Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:21 PM GMT

PDB ID	:	1A49
Title	:	BIS MG-ATP-K-OXALATE COMPLEX OF PYRUVATE KINASE
Authors	:	Larsen, T.M.; Benning, M.M.; Rayment, I.; Reed, G.H.
Deposited on	:	1998-02-12
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

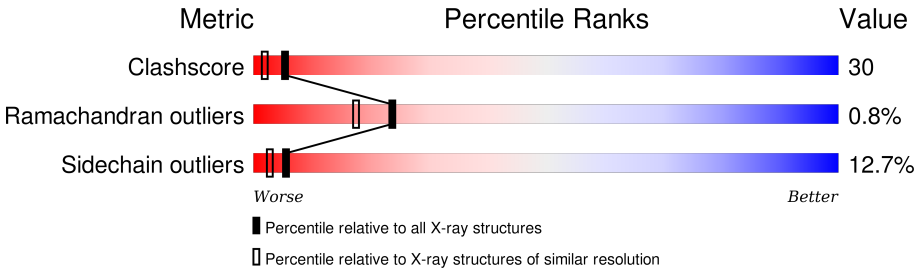
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	530	40% 40% 16%
1	B	530	49% 38% 10%
1	C	530	38% 44% 14%
1	D	530	45% 42% 9%
1	E	530	47% 37% 12%
1	F	530	44% 41% 11%
1	G	530	43% 43% 12%

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Mol	Chain	Length	Quality of chain
1	H	530	54% 36% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	533	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34001 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PYRUVATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	B	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	C	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	D	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	E	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	F	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	G	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	H	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		
2	H	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		

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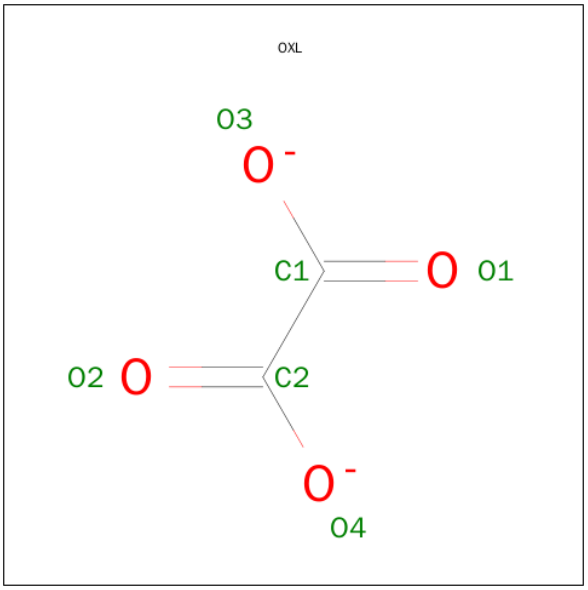
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).

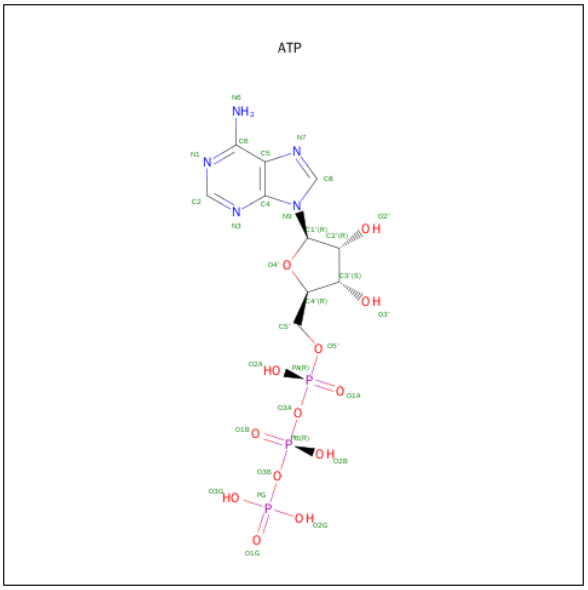


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 2 4	0	0
3	B	1	Total C O 6 2 4	0	0
3	C	1	Total C O 6 2 4	0	0
3	D	1	Total C O 6 2 4	0	0
3	E	1	Total C O 6 2 4	0	0
3	F	1	Total C O 6 2 4	0	0
3	G	1	Total C O 6 2 4	0	0
3	H	1	Total C O 6 2 4	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0
4	E	2	Total Mg 2 2	0	0
4	H	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	2	Total Mg 2 2	0	0
4	A	2	Total Mg 2 2	0	0
4	F	2	Total Mg 2 2	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 31 10 5 13 3	0	0
5	C	1	Total C N O P 31 10 5 13 3	0	0
5	D	1	Total C N O P 31 10 5 13 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	195	Total	O	0	0
			195	195		
6	B	270	Total	O	0	0
			270	270		
6	C	178	Total	O	0	0
			178	178		
6	D	272	Total	O	0	0
			272	272		
6	E	279	Total	O	0	0
			279	279		
6	F	197	Total	O	0	0
			197	197		
6	G	228	Total	O	0	0
			228	228		
6	H	302	Total	O	0	0
			302	302		

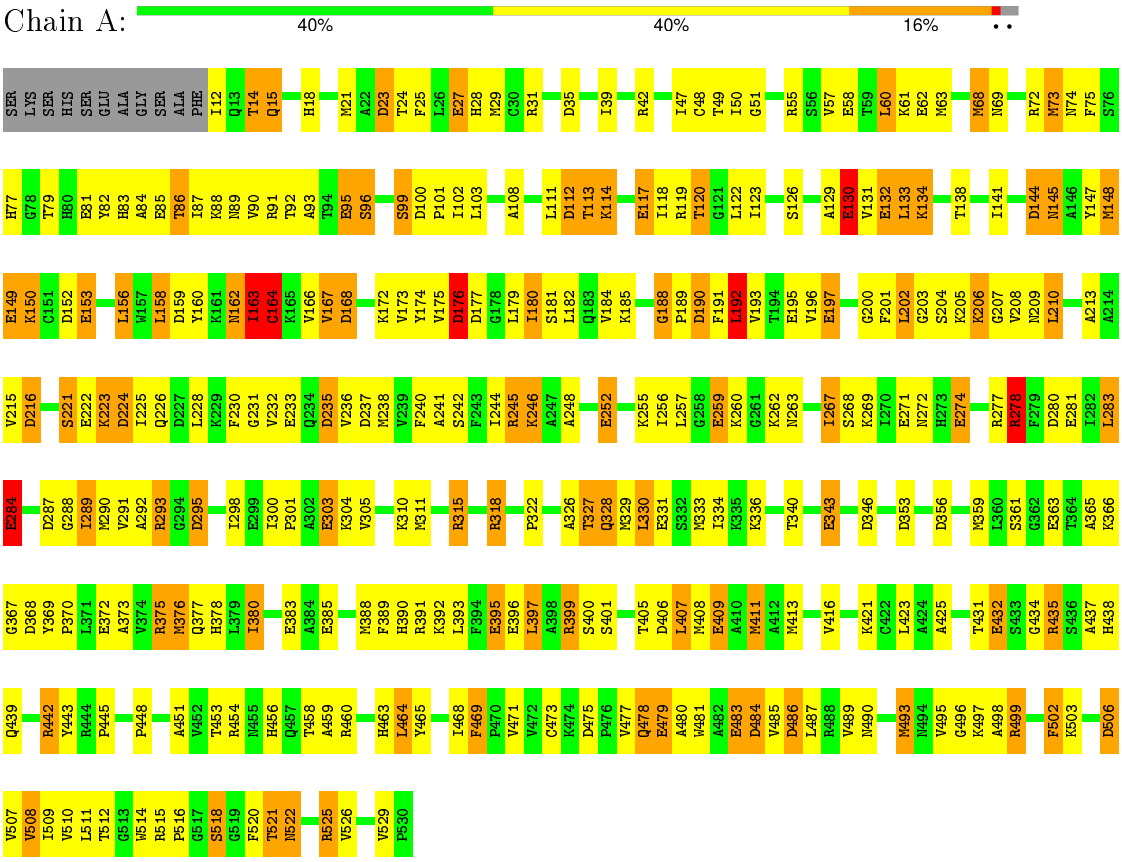
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

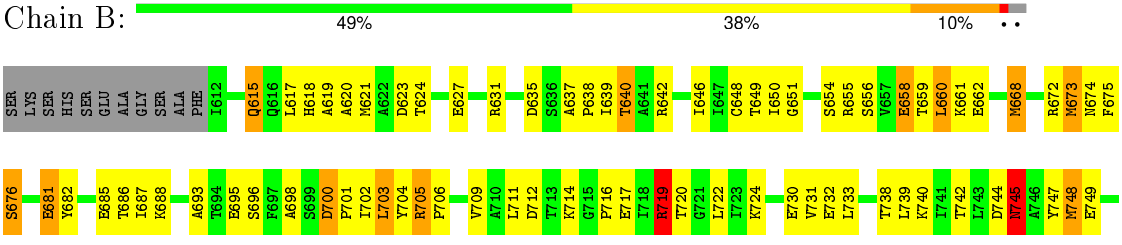
- Molecule 1: PYRUVATE KINASE

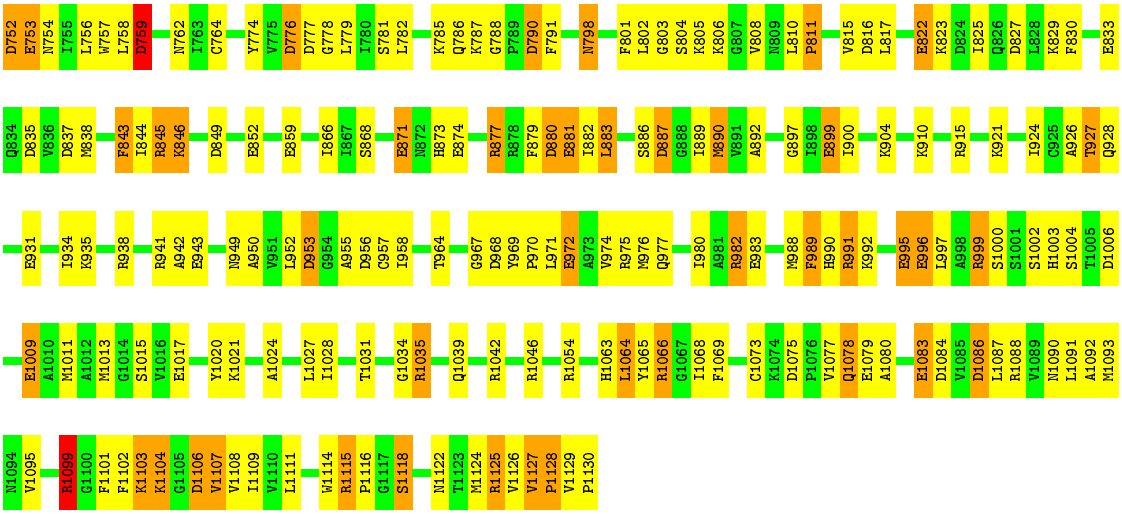
Chain A:



- Molecule 1: PYRUVATE KINASE

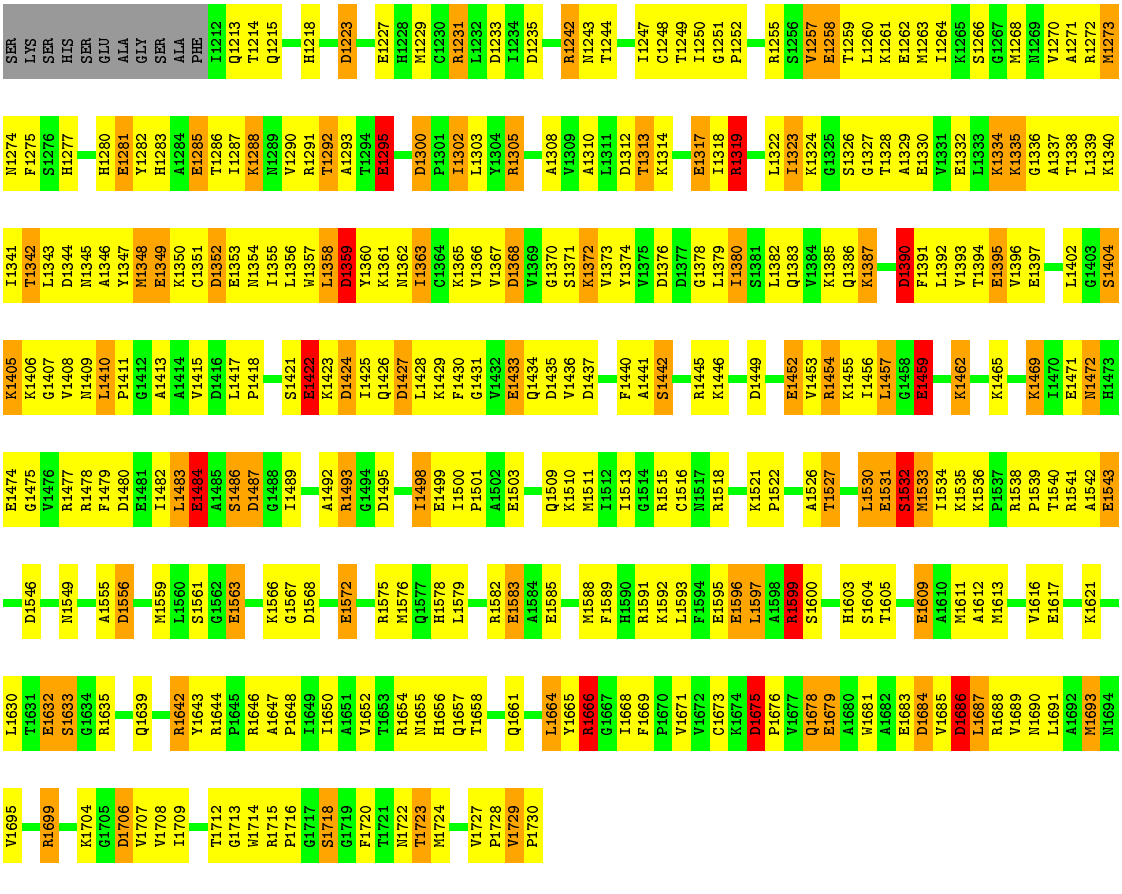
Chain B:





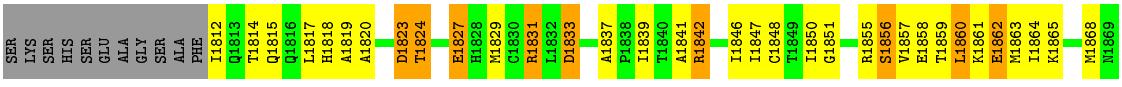
• Molecule 1: PYRUVATE KINASE

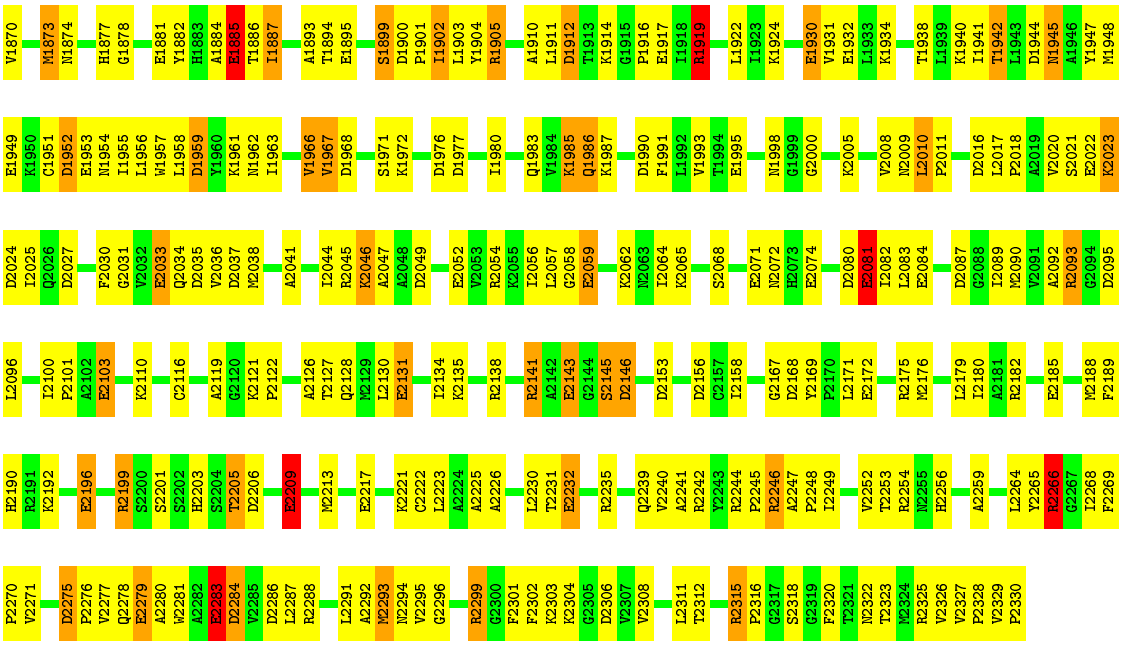
Chain C:



• Molecule 1: PYRUVATE KINASE

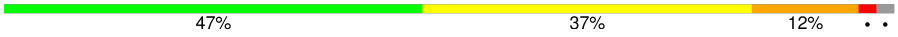
Chain D:

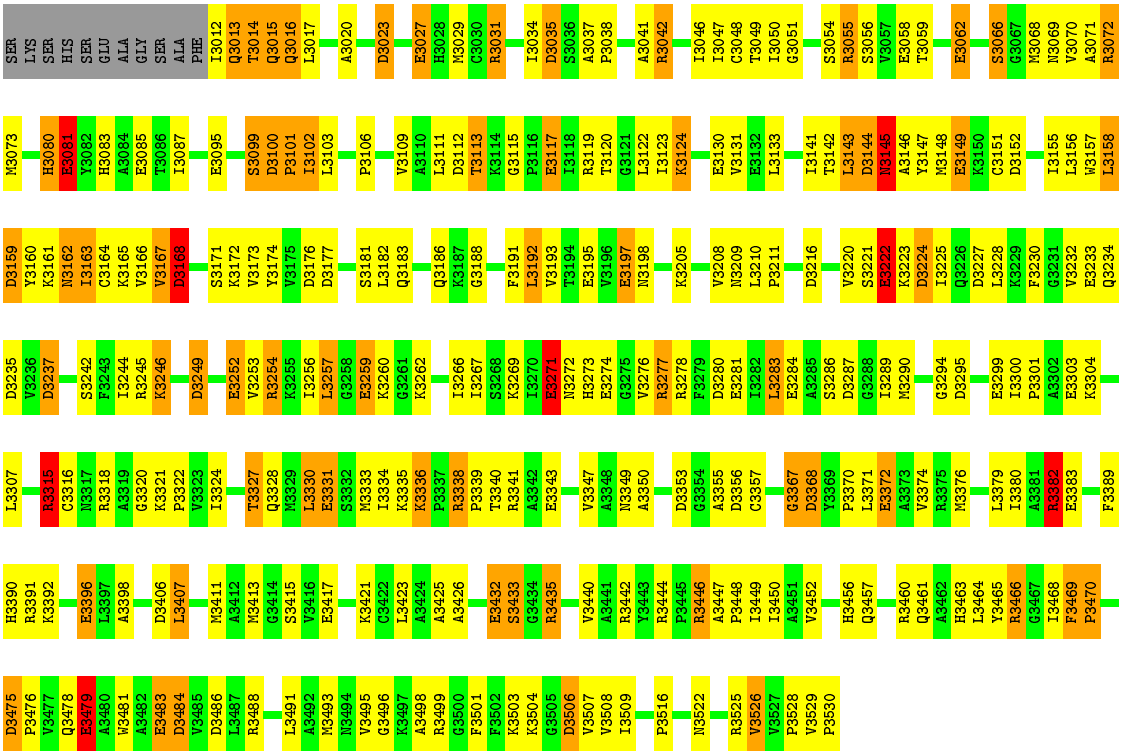




• Molecule 1: PYRUVATE KINASE

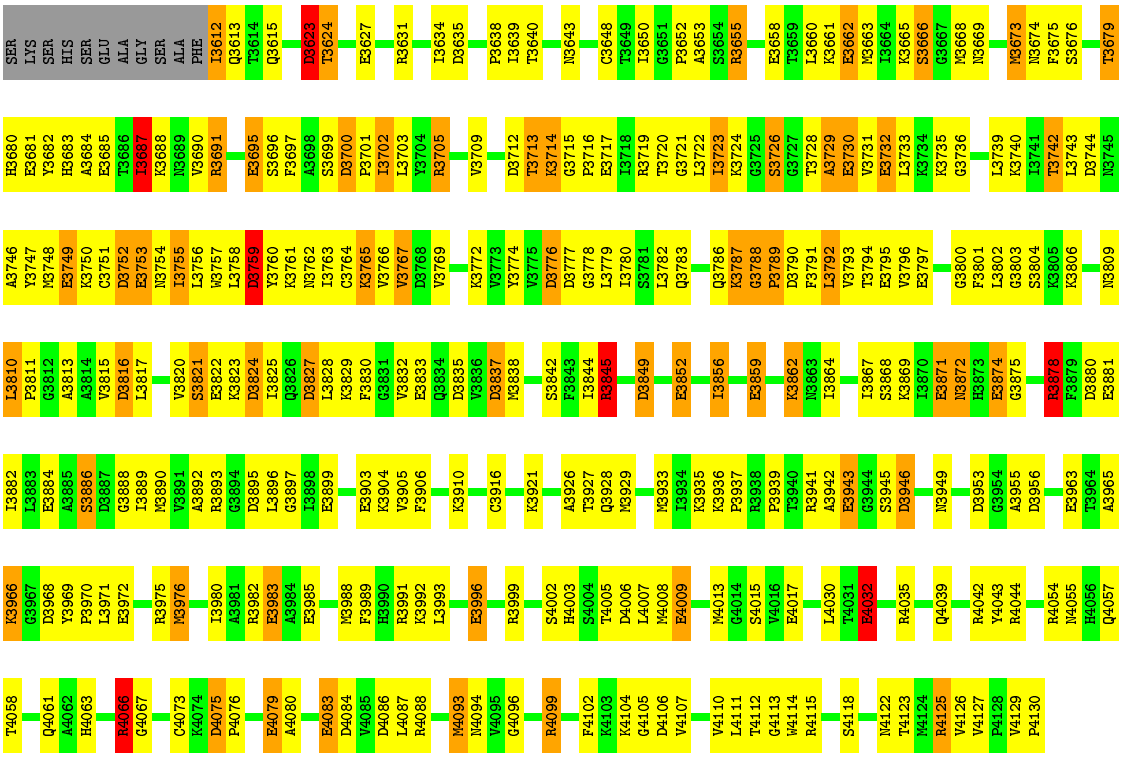
Chain E:





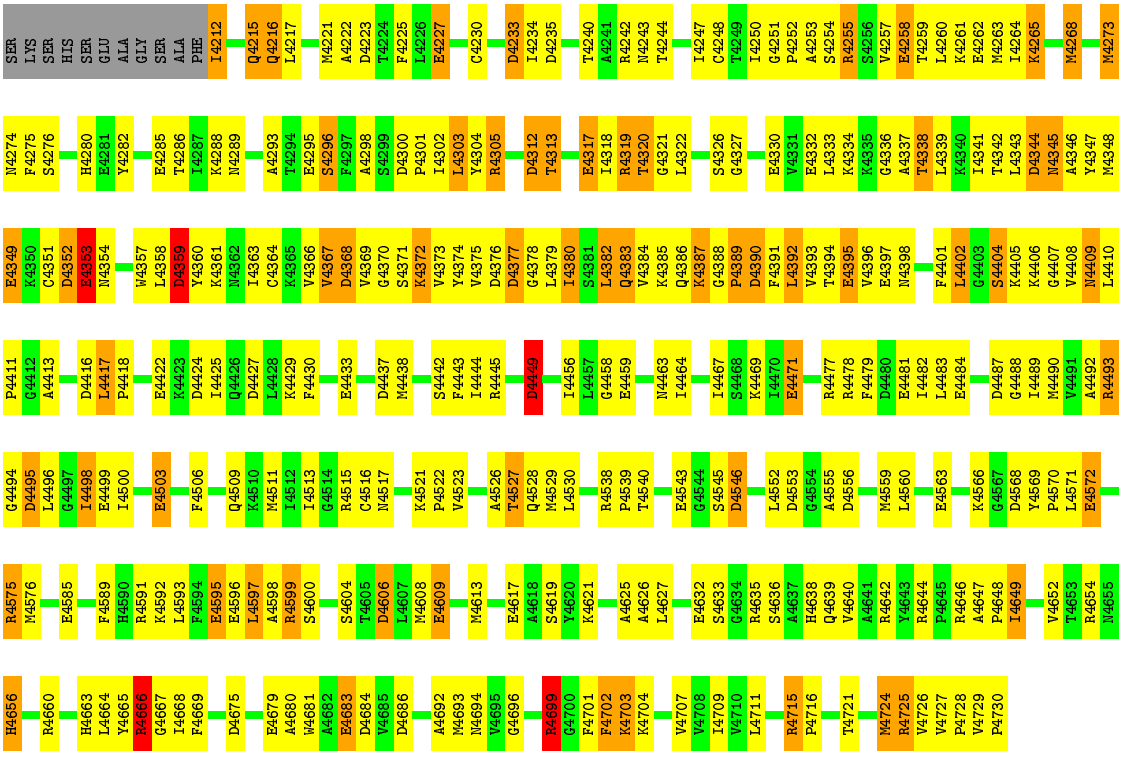
• Molecule 1: PYRUVATE KINASE

Chain F:



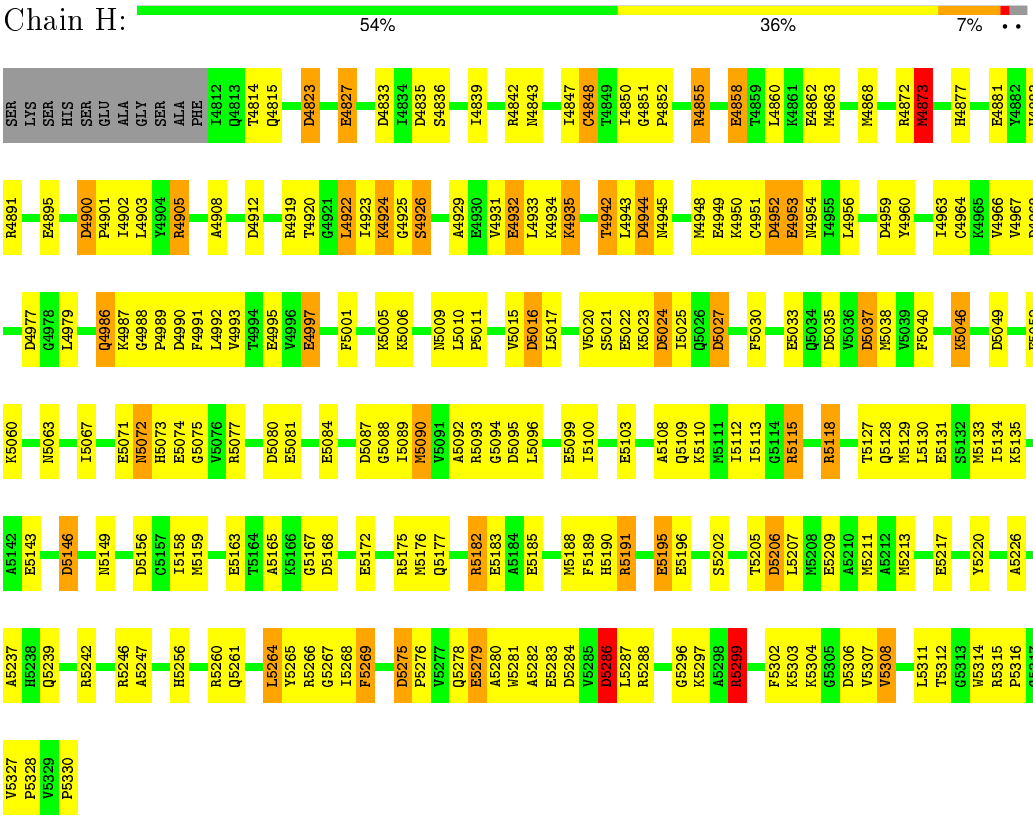
• Molecule 1: PYRUVATE KINASE

Chain G:



• Molecule 1: PYRUVATE KINASE

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.30Å 216.50Å 258.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	87.0 (30.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT V. 5-D	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	34001	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, MG, K, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.36	35/4041 (0.9%)	1.29	48/5452 (0.9%)
1	B	1.38	29/4041 (0.7%)	1.31	58/5452 (1.1%)
1	C	1.30	36/4041 (0.9%)	1.34	63/5452 (1.2%)
1	D	1.38	35/4041 (0.9%)	1.30	57/5452 (1.0%)
1	E	1.37	32/4041 (0.8%)	1.32	52/5452 (1.0%)
1	F	1.31	31/4041 (0.8%)	1.32	64/5452 (1.2%)
1	G	1.34	30/4041 (0.7%)	1.30	50/5452 (0.9%)
1	H	1.36	27/4041 (0.7%)	1.31	63/5452 (1.2%)
All	All	1.35	255/32328 (0.8%)	1.31	455/43616 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	H	1	0
All	All	1	2

All (255) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4595	GLU	CD-OE1	11.92	1.38	1.25
1	B	681	GLU	CD-OE2	11.16	1.38	1.25
1	B	627	GLU	CD-OE2	10.56	1.37	1.25
1	A	27	GLU	CD-OE2	10.12	1.36	1.25
1	F	3797	GLU	CD-OE1	10.11	1.36	1.25
1	F	3903	GLU	CD-OE1	9.81	1.36	1.25
1	B	874	GLU	CD-OE1	9.72	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	GLU	CD-OE1	9.34	1.35	1.25
1	H	5195	GLU	CD-OE1	9.21	1.35	1.25
1	H	5279	GLU	CD-OE2	9.19	1.35	1.25
1	E	3081	GLU	CD-OE2	9.02	1.35	1.25
1	H	5099	GLU	CD-OE2	8.86	1.35	1.25
1	C	1317	GLU	CD-OE2	8.71	1.35	1.25
1	E	3396	GLU	CD-OE1	8.58	1.35	1.25
1	B	899	GLU	CD-OE2	8.52	1.35	1.25
1	A	222	GLU	CD-OE2	8.50	1.35	1.25
1	E	3331	GLU	CD-OE2	8.42	1.34	1.25
1	D	2283	GLU	CD-OE1	8.32	1.34	1.25
1	C	1353	GLU	CD-OE2	8.30	1.34	1.25
1	E	3149	GLU	CD-OE2	8.26	1.34	1.25
1	B	871	GLU	CD-OE2	8.14	1.34	1.25
1	F	4079	GLU	CD-OE2	8.13	1.34	1.25
1	E	3271	GLU	CD-OE2	8.10	1.34	1.25
1	B	881	GLU	CD-OE2	-8.05	1.16	1.25
1	A	432	GLU	CD-OE2	8.04	1.34	1.25
1	D	1917	GLU	CD-OE2	8.03	1.34	1.25
1	C	1503	GLU	CD-OE1	7.97	1.34	1.25
1	H	4997	GLU	CD-OE2	7.96	1.34	1.25
1	B	833	GLU	CD-OE2	7.91	1.34	1.25
1	G	4258	GLU	CD-OE1	7.82	1.34	1.25
1	A	331	GLU	CD-OE2	7.79	1.34	1.25
1	A	483	GLU	CD-OE1	7.76	1.34	1.25
1	B	983	GLU	CD-OE1	-7.75	1.17	1.25
1	C	1459	GLU	CD-OE1	7.72	1.34	1.25
1	D	2103	GLU	CD-OE1	7.70	1.34	1.25
1	E	3222	GLU	CD-OE2	7.67	1.34	1.25
1	D	2143	GLU	CD-OE2	7.61	1.34	1.25
1	C	1595	GLU	CD-OE1	7.56	1.33	1.25
1	G	4433	GLU	CD-OE2	7.49	1.33	1.25
1	D	2033	GLU	CD-OE2	7.47	1.33	1.25
1	H	5131	GLU	CD-OE1	7.47	1.33	1.25
1	D	2279	GLU	CD-OE2	7.44	1.33	1.25
1	D	2196	GLU	CD-OE1	7.42	1.33	1.25
1	G	4227	GLU	CD-OE2	7.39	1.33	1.25
1	F	3795	GLU	CD-OE1	7.38	1.33	1.25
1	G	4481	GLU	CD-OE1	7.36	1.33	1.25
1	D	1827	GLU	CD-OE2	7.28	1.33	1.25
1	G	4349	GLU	CD-OE2	7.28	1.33	1.25
1	B	822	GLU	CD-OE2	7.24	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	3479	GLU	CD-OE2	7.23	1.33	1.25
1	F	3859	GLU	CD-OE1	7.21	1.33	1.25
1	G	4679	GLU	CD-OE2	7.19	1.33	1.25
1	G	4683	GLU	CD-OE1	7.18	1.33	1.25
1	C	1471	GLU	CD-OE2	7.17	1.33	1.25
1	D	1995	GLU	CD-OE1	7.16	1.33	1.25
1	G	4422	GLU	CD-OE1	7.14	1.33	1.25
1	C	1395	GLU	CD-OE1	7.12	1.33	1.25
1	D	1895	GLU	CD-OE1	7.11	1.33	1.25
1	C	1679	GLU	CD-OE2	7.09	1.33	1.25
1	C	1531	GLU	CD-OE2	7.09	1.33	1.25
1	E	3372	GLU	CD-OE1	7.08	1.33	1.25
1	B	943	GLU	CD-OE2	7.07	1.33	1.25
1	A	259	GLU	CD-OE1	7.07	1.33	1.25
1	F	3985	GLU	CD-OE1	7.05	1.33	1.25
1	A	85	GLU	CD-OE2	7.05	1.33	1.25
1	D	2022	GLU	CD-OE2	7.04	1.33	1.25
1	E	3259	GLU	CD-OE1	7.03	1.33	1.25
1	F	3871	GLU	CD-OE2	7.01	1.33	1.25
1	A	153	GLU	CD-OE2	6.99	1.33	1.25
1	E	3027	GLU	CD-OE2	6.96	1.33	1.25
1	E	3085	GLU	CD-OE1	6.94	1.33	1.25
1	G	4596	GLU	CD-OE1	6.91	1.33	1.25
1	C	1422	GLU	CD-OE1	6.91	1.33	1.25
1	B	749	GLU	CD-OE2	6.90	1.33	1.25
1	E	3062	GLU	CD-OE2	6.89	1.33	1.25
1	E	3483	GLU	CD-OE2	6.89	1.33	1.25
1	F	3972	GLU	CD-OE1	6.87	1.33	1.25
1	B	931	GLU	CD-OE2	6.87	1.33	1.25
1	H	4949	GLU	CD-OE2	6.86	1.33	1.25
1	C	1452	GLU	CD-OE2	6.85	1.33	1.25
1	D	1858	GLU	CD-OE2	6.84	1.33	1.25
1	A	197	GLU	CD-OE2	6.82	1.33	1.25
1	D	2185	GLU	CD-OE2	-6.79	1.18	1.25
1	H	5283	GLU	CD-OE2	6.78	1.33	1.25
1	A	81	GLU	CD-OE2	6.74	1.33	1.25
1	C	1258	GLU	CD-OE2	6.74	1.33	1.25
1	E	3195	GLU	CD-OE2	6.73	1.33	1.25
1	E	3299	GLU	CD-OE2	6.70	1.33	1.25
1	B	695	GLU	CD-OE1	6.70	1.33	1.25
1	B	1079	GLU	CD-OE2	6.70	1.33	1.25
1	G	4632	GLU	CD-OE1	-6.69	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	395	GLU	CD-OE1	6.68	1.32	1.25
1	B	658	GLU	CD-OE2	6.67	1.32	1.25
1	G	4353	GLU	CD-OE2	6.66	1.32	1.25
1	F	3749	GLU	CD-OE2	6.63	1.32	1.25
1	B	995	GLU	CD-OE2	6.61	1.32	1.25
1	F	3833	GLU	CD-OE2	6.60	1.32	1.25
1	A	274	GLU	CD-OE1	6.60	1.32	1.25
1	F	3695	GLU	CD-OE1	6.58	1.32	1.25
1	C	1572	GLU	CD-OE1	6.55	1.32	1.25
1	D	1953	GLU	CD-OE2	6.55	1.32	1.25
1	A	95	GLU	CD-OE1	6.51	1.32	1.25
1	E	3338	ARG	NE-CZ	6.48	1.41	1.33
1	D	2033	GLU	CD-OE1	-6.48	1.18	1.25
1	F	3658	GLU	CD-OE2	6.47	1.32	1.25
1	E	3417	GLU	CD-OE1	6.46	1.32	1.25
1	E	3130	GLU	CD-OE2	6.42	1.32	1.25
1	C	1499	GLU	CD-OE2	6.42	1.32	1.25
1	G	4285	GLU	CD-OE1	6.38	1.32	1.25
1	F	3996	GLU	CD-OE1	6.37	1.32	1.25
1	A	233	GLU	CD-OE2	6.36	1.32	1.25
1	A	363	GLU	CD-OE1	6.33	1.32	1.25
1	G	4617	GLU	CD-OE2	6.33	1.32	1.25
1	C	1632	GLU	CD-OE2	6.31	1.32	1.25
1	D	1949	GLU	CD-OE2	6.30	1.32	1.25
1	E	3058	GLU	CD-OE1	6.30	1.32	1.25
1	E	3095	GLU	CD-OE1	6.30	1.32	1.25
1	G	4503	GLU	CD-OE1	6.29	1.32	1.25
1	A	252	GLU	CD-OE2	6.28	1.32	1.25
1	E	3233	GLU	CD-OE2	6.25	1.32	1.25
1	F	3963	GLU	CD-OE1	6.25	1.32	1.25
1	B	852	GLU	CD-OE2	6.24	1.32	1.25
1	G	4609	GLU	CD-OE2	6.22	1.32	1.25
1	C	1262	GLU	CD-OE2	6.22	1.32	1.25
1	F	4083	GLU	CD-OE1	6.18	1.32	1.25
1	G	4317	GLU	CD-OE2	6.18	1.32	1.25
1	D	1930	GLU	CD-OE2	6.17	1.32	1.25
1	E	3284	GLU	CD-OE2	6.17	1.32	1.25
1	G	4262	GLU	CD-OE2	6.17	1.32	1.25
1	A	27	GLU	CB-CG	6.16	1.63	1.52
1	B	972	GLU	CD-OE1	6.15	1.32	1.25
1	H	5185	GLU	CD-OE2	-6.15	1.18	1.25
1	D	2052	GLU	CD-OE1	6.15	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4563	GLU	CD-OE1	6.12	1.32	1.25
1	C	1349	GLU	CD-OE2	6.10	1.32	1.25
1	C	1330	GLU	CD-OE2	6.09	1.32	1.25
1	C	1599	ARG	NE-CZ	6.08	1.41	1.33
1	G	4572	GLU	CD-OE1	6.08	1.32	1.25
1	A	479	GLU	CD-OE2	6.06	1.32	1.25
1	C	1227	GLU	CD-OE1	6.06	1.32	1.25
1	G	4459	GLU	CD-OE2	6.05	1.32	1.25
1	H	4953	GLU	CD-OE2	6.04	1.32	1.25
1	F	3753	GLU	CD-OE2	6.03	1.32	1.25
1	F	4017	GLU	CD-OE1	6.02	1.32	1.25
1	G	4484	GLU	CD-OE1	6.01	1.32	1.25
1	B	753	GLU	CD-OE2	6.00	1.32	1.25
1	H	5172	GLU	CD-OE1	5.99	1.32	1.25
1	B	662	GLU	CD-OE2	5.99	1.32	1.25
1	D	2266	ARG	NE-CZ	-5.97	1.25	1.33
1	A	409	GLU	CD-OE2	5.97	1.32	1.25
1	H	5196	GLU	CD-OE1	5.96	1.32	1.25
1	H	5232	GLU	CD-OE1	5.95	1.32	1.25
1	C	1617	GLU	CD-OE1	5.95	1.32	1.25
1	F	3681	GLU	CD-OE2	5.95	1.32	1.25
1	A	132	GLU	CD-OE1	5.94	1.32	1.25
1	H	4995	GLU	CD-OE1	5.94	1.32	1.25
1	B	996	GLU	CD-OE1	5.92	1.32	1.25
1	E	3252	GLU	CD-OE1	5.91	1.32	1.25
1	H	5059	GLU	CD-OE2	5.90	1.32	1.25
1	B	1017	GLU	CD-OE1	5.88	1.32	1.25
1	E	3117	GLU	CD-OE2	5.87	1.32	1.25
1	E	3174	TYR	CB-CG	-5.84	1.42	1.51
1	E	3281	GLU	CD-OE1	5.83	1.32	1.25
1	A	58	GLU	CD-OE2	5.81	1.32	1.25
1	E	3367	GLY	N-CA	5.81	1.54	1.46
1	E	3432	GLU	CD-OE2	5.81	1.32	1.25
1	H	5163	GLU	CD-OE1	5.80	1.32	1.25
1	A	149	GLU	CD-OE1	5.76	1.31	1.25
1	C	1484	GLU	CD-OE2	5.75	1.31	1.25
1	C	1666	ARG	CD-NE	-5.75	1.36	1.46
1	A	303	GLU	CD-OE1	5.74	1.31	1.25
1	D	1932	GLU	CD-OE1	5.74	1.31	1.25
1	F	3943	GLU	CD-OE1	-5.74	1.19	1.25
1	F	3685	GLU	CD-OE1	5.73	1.31	1.25
1	G	4252	PRO	CA-C	-5.73	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	3383	GLU	CD-OE2	5.72	1.31	1.25
1	G	4543	GLU	CD-OE2	5.72	1.31	1.25
1	H	4881	GLU	CD-OE2	5.69	1.31	1.25
1	H	4858	GLU	CD-OE2	5.68	1.31	1.25
1	D	2081	GLU	CD-OE1	5.67	1.31	1.25
1	A	442	ARG	CA-CB	-5.66	1.41	1.53
1	A	385	GLU	CD-OE1	5.63	1.31	1.25
1	A	62	GLU	CD-OE1	5.61	1.31	1.25
1	A	284	GLU	CD-OE1	5.60	1.31	1.25
1	G	4632	GLU	CD-OE2	5.60	1.31	1.25
1	F	3852	GLU	CD-OE2	5.59	1.31	1.25
1	F	4032	GLU	CD-OE1	5.59	1.31	1.25
1	D	1932	GLU	CD-OE2	-5.59	1.19	1.25
1	C	1683	GLU	CD-OE1	5.57	1.31	1.25
1	D	2172	GLU	CD-OE2	5.57	1.31	1.25
1	B	1083	GLU	CD-OE2	5.55	1.31	1.25
1	H	4862	GLU	CD-OE2	5.55	1.31	1.25
1	B	730	GLU	CD-OE2	5.54	1.31	1.25
1	B	803	GLY	CA-C	5.54	1.60	1.51
1	D	2074	GLU	CD-OE1	5.54	1.31	1.25
1	B	1009	GLU	CD-OE2	5.53	1.31	1.25
1	E	3303	GLU	CD-OE2	-5.53	1.19	1.25
1	D	2084	GLU	CD-OE2	5.52	1.31	1.25
1	F	3730	GLU	CD-OE2	5.51	1.31	1.25
1	D	1885	GLU	CD-OE1	5.47	1.31	1.25
1	C	1596	GLU	CD-OE1	5.47	1.31	1.25
1	H	5103	GLU	CD-OE1	5.46	1.31	1.25
1	F	3662	GLU	CD-OE2	5.45	1.31	1.25
1	G	4585	GLU	CD-OE2	-5.45	1.19	1.25
1	A	331	GLU	CD-OE1	-5.43	1.19	1.25
1	A	343	GLU	CD-OE1	-5.42	1.19	1.25
1	D	2138	ARG	CZ-NH1	5.41	1.40	1.33
1	C	1285	GLU	CD-OE1	5.39	1.31	1.25
1	C	1397	GLU	CD-OE1	5.39	1.31	1.25
1	H	5074	GLU	CD-OE1	5.39	1.31	1.25
1	C	1543	GLU	CD-OE2	5.38	1.31	1.25
1	A	383	GLU	CD-OE1	5.34	1.31	1.25
1	F	3732	GLU	CD-OE1	5.33	1.31	1.25
1	F	3874	GLU	CD-OE1	5.32	1.31	1.25
1	B	1092	ALA	C-N	-5.32	1.21	1.34
1	H	4895	GLU	CD-OE1	5.32	1.31	1.25
1	D	2232	GLU	CD-OE1	5.31	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	305	VAL	C-O	5.31	1.33	1.23
1	B	685	GLU	CD-OE1	5.30	1.31	1.25
1	G	4398	ASN	CA-CB	5.29	1.67	1.53
1	A	130	GLU	CD-OE2	5.28	1.31	1.25
1	D	1881	GLU	CD-OE2	5.27	1.31	1.25
1	H	5217	GLU	CD-OE2	5.27	1.31	1.25
1	G	4585	GLU	CD-OE1	5.26	1.31	1.25
1	G	4609	GLU	CD-OE1	-5.26	1.19	1.25
1	D	2138	ARG	NE-CZ	5.25	1.39	1.33
1	D	2209	GLU	CD-OE1	5.25	1.31	1.25
1	C	1295	GLU	CD-OE1	-5.24	1.19	1.25
1	E	3197	GLU	CD-OE2	5.24	1.31	1.25
1	H	5185	GLU	CD-OE1	5.24	1.31	1.25
1	A	281	GLU	CD-OE2	5.24	1.31	1.25
1	D	2059	GLU	CD-OE1	5.23	1.31	1.25
1	C	1583	GLU	CD-OE2	-5.22	1.20	1.25
1	D	2217	GLU	CD-OE1	5.21	1.31	1.25
1	H	5022	GLU	CD-OE2	5.21	1.31	1.25
1	F	3822	GLU	CD-OE2	5.21	1.31	1.25
1	H	4827	GLU	CD-OE1	5.20	1.31	1.25
1	H	5084	GLU	CD-OE1	-5.19	1.20	1.25
1	F	3983	GLU	CD-OE1	-5.19	1.20	1.25
1	G	4295	GLU	CD-OE2	5.19	1.31	1.25
1	A	195	GLU	CD-OE2	5.17	1.31	1.25
1	D	1862	GLU	CD-OE2	5.17	1.31	1.25
1	C	1609	GLU	CD-OE1	-5.15	1.20	1.25
1	C	1295	GLU	CD-OE2	5.14	1.31	1.25
1	H	5084	GLU	CD-OE2	5.14	1.31	1.25
1	F	4009	GLU	CD-OE1	5.13	1.31	1.25
1	F	3963	GLU	CD-OE2	-5.12	1.20	1.25
1	F	3943	GLU	CD-OE2	5.12	1.31	1.25
1	E	3470	PRO	N-CA	-5.10	1.38	1.47
1	C	1281	GLU	CD-OE2	5.08	1.31	1.25
1	C	1332	GLU	CD-OE1	5.06	1.31	1.25
1	C	1402	LEU	N-CA	-5.05	1.36	1.46
1	C	1563	GLU	CD-OE1	5.04	1.31	1.25
1	D	2131	GLU	CD-OE1	5.04	1.31	1.25
1	B	955	ALA	C-O	-5.00	1.13	1.23

All (455) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1919	ARG	NE-CZ-NH1	13.83	127.21	120.30
1	C	1666	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	F	4066	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	B	1127	VAL	C-N-CD	-11.65	94.97	120.60
1	D	1919	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	C	1666	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	B	776	ASP	CB-CG-OD1	-10.22	109.10	118.30
1	G	4352	ASP	CB-CG-OD1	10.14	127.43	118.30
1	G	4352	ASP	CB-CG-OD2	-10.11	109.20	118.30
1	H	4952	ASP	CB-CG-OD2	-9.91	109.38	118.30
1	B	668	MET	CG-SD-CE	-9.61	84.82	100.20
1	E	3152	ASP	CB-CG-OD1	9.37	126.74	118.30
1	F	3788	GLY	C-N-CD	-9.29	100.15	120.60
1	B	956	ASP	CB-CG-OD2	-9.26	109.97	118.30
1	D	2138	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	E	3152	ASP	CB-CG-OD2	-9.16	110.06	118.30
1	B	880	ASP	CB-CG-OD2	9.02	126.42	118.30
1	E	3119	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	G	4449	ASP	CB-CG-OD1	8.89	126.31	118.30
1	H	4835	ASP	CB-CG-OD1	-8.86	110.32	118.30
1	G	4376	ASP	CB-CG-OD1	-8.69	110.48	118.30
1	D	2095	ASP	CB-CG-OD1	-8.66	110.51	118.30
1	E	3224	ASP	CB-CG-OD1	-8.62	110.54	118.30
1	D	2266	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	G	4684	ASP	CB-CG-OD1	-8.45	110.69	118.30
1	B	776	ASP	CB-CG-OD2	8.43	125.89	118.30
1	E	3356	ASP	CB-CG-OD1	-8.39	110.75	118.30
1	H	5024	ASP	CB-CG-OD2	-8.37	110.77	118.30
1	D	1976	ASP	CB-CG-OD2	8.35	125.81	118.30
1	C	1493	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	D	2095	ASP	CB-CG-OD2	8.22	125.69	118.30
1	H	5284	ASP	CB-CG-OD1	-8.21	110.92	118.30
1	A	506	ASP	CB-CG-OD2	8.19	125.67	118.30
1	A	188	GLY	C-N-CD	-8.06	102.87	120.60
1	B	837	ASP	CB-CG-OD1	-8.03	111.07	118.30
1	H	4952	ASP	CB-CG-OD1	8.00	125.50	118.30
1	B	880	ASP	CB-CG-OD1	-7.98	111.12	118.30
1	H	5275	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	D	1952	ASP	CB-CG-OD1	7.92	125.43	118.30
1	H	5027	ASP	CB-CG-OD1	-7.78	111.30	118.30
1	H	5024	ASP	CB-CG-OD1	7.76	125.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	5138	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	E	3315	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	C	1437	ASP	CB-CG-OD1	-7.71	111.36	118.30
1	F	3712	ASP	CB-CG-OD1	-7.70	111.37	118.30
1	H	5037	ASP	CB-CG-OD1	-7.64	111.43	118.30
1	C	1454	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	F	3623	ASP	CB-CG-OD2	7.60	125.14	118.30
1	A	177	ASP	CB-CG-OD1	-7.59	111.47	118.30
1	B	956	ASP	CB-CG-OD1	7.58	125.12	118.30
1	H	4872	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	G	4449	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	H	5288	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	G	4546	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	C	1427	ASP	CB-CG-OD1	-7.54	111.52	118.30
1	H	5087	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	E	3210	LEU	C-N-CD	-7.52	104.05	120.60
1	E	3176	ASP	CB-CG-OD1	-7.48	111.57	118.30
1	D	1976	ASP	CB-CG-OD1	-7.46	111.58	118.30
1	F	3956	ASP	CB-CG-OD1	-7.45	111.60	118.30
1	F	3631	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	G	4684	ASP	CB-CG-OD2	7.43	124.99	118.30
1	H	5299	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	D	1905	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	C	1675	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	H	4835	ASP	CB-CG-OD2	7.35	124.91	118.30
1	F	3878	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	F	4099	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	B	1099	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	D	2080	ASP	CB-CG-OD1	-7.32	111.71	118.30
1	H	5288	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	499	ARG	NE-CZ-NH2	7.31	123.96	120.30
1	E	3119	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	C	1480	ASP	CB-CG-OD1	-7.30	111.73	118.30
1	D	2299	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	F	3705	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	E	3499	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	F	3776	ASP	CB-CG-OD1	-7.26	111.76	118.30
1	C	1305	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	H	5175	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	C	1699	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	G	4699	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	E	3072	ARG	NE-CZ-NH2	-7.19	116.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	3338	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	C	1568	ASP	CB-CG-OD1	-7.19	111.83	118.30
1	G	4424	ASP	CB-CG-OD2	7.17	124.76	118.30
1	D	2035	ASP	CB-CG-OD1	-7.13	111.88	118.30
1	A	406	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	B	705	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	A	475	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	B	849	ASP	CB-CG-OD1	7.08	124.67	118.30
1	B	1075	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	E	3066	SER	CB-CA-C	7.02	123.44	110.10
1	H	5220	TYR	CB-CG-CD2	-7.02	116.79	121.00
1	E	3216	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	B	759	ASP	CB-CA-C	-6.97	96.46	110.40
1	G	4575	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	D	2275	ASP	CB-CG-OD1	-6.94	112.06	118.30
1	E	3224	ASP	CB-CG-OD2	6.93	124.54	118.30
1	D	2306	ASP	CB-CG-OD1	6.93	124.53	118.30
1	G	4223	ASP	CB-CG-OD1	6.92	124.53	118.30
1	C	1675	ASP	CB-CG-OD1	6.90	124.51	118.30
1	E	3042	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	H	5090	MET	CG-SD-CE	-6.88	89.19	100.20
1	D	1919	ARG	CD-NE-CZ	6.88	133.23	123.60
1	C	1493	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	506	ASP	CB-CG-OD1	-6.87	112.12	118.30
1	F	4006	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	A	35	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	A	112	ASP	CB-CG-OD1	-6.83	112.16	118.30
1	C	1319	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	E	3249	ASP	CB-CG-OD1	6.81	124.43	118.30
1	H	5168	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	C	1686	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	G	4675	ASP	CB-CG-OD1	-6.76	112.22	118.30
1	E	3356	ASP	CB-CG-OD2	6.76	124.38	118.30
1	A	399	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	144	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	F	4075	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	E	3042	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	G	4556	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	H	5206	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	B	759	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	F	3712	ASP	CB-CG-OD2	6.68	124.31	118.30
1	C	1480	ASP	CB-CG-OD2	6.67	124.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	2206	ASP	CB-CG-OD2	6.67	124.30	118.30
1	H	4912	ASP	CB-CG-OD1	-6.66	112.30	118.30
1	C	1231	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	B	790	ASP	CB-CG-OD1	-6.63	112.33	118.30
1	H	5284	ASP	CB-CG-OD2	6.61	124.25	118.30
1	F	4106	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	F	3956	ASP	CB-CG-OD2	6.60	124.24	118.30
1	F	3946	ASP	CB-CG-OD1	-6.60	112.36	118.30
1	B	700	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	D	1831	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	406	ASP	CB-CG-OD1	6.58	124.22	118.30
1	E	3035	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	C	1424	ASP	CB-CG-OD1	-6.55	112.40	118.30
1	D	2087	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	A	235	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	B	953	ASP	CB-CG-OD2	6.53	124.18	118.30
1	H	4990	ASP	CB-CG-OD1	-6.51	112.44	118.30
1	G	4725	ARG	NE-CZ-NH2	6.51	123.55	120.30
1	B	877	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	F	4084	ASP	CB-CG-OD2	6.50	124.15	118.30
1	D	2156	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	C	1231	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	G	4223	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	C	1235	ASP	CB-CG-OD1	-6.49	112.46	118.30
1	F	3845	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	E	3254	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	F	3946	ASP	CB-CG-OD2	6.44	124.10	118.30
1	C	1242	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	G	4568	ASP	CB-CG-OD2	6.44	124.09	118.30
1	B	1006	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	G	4235	ASP	CB-CG-OD1	-6.43	112.51	118.30
1	E	3159	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	C	1556	ASP	CB-CG-OD2	6.42	124.08	118.30
1	F	3968	ASP	CB-CG-OD1	-6.42	112.53	118.30
1	B	623	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	E	3176	ASP	CB-CG-OD2	6.38	124.05	118.30
1	B	1086	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	G	4568	ASP	CB-CG-OD1	-6.37	112.56	118.30
1	H	5191	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	953	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	C	1556	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	F	4106	ASP	CB-CG-OD2	6.36	124.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	318	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	H	5115	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	C	1495	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	G	4344	ASP	CB-CG-OD1	-6.34	112.60	118.30
1	F	4125	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	F	3824	ASP	CB-CG-OD2	6.33	123.99	118.30
1	E	3237	ASP	CB-CG-OD1	-6.32	112.62	118.30
1	H	5037	ASP	CB-CG-OD2	6.31	123.98	118.30
1	F	3623	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	E	3112	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	F	4086	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	A	235	ASP	CB-CG-OD2	6.29	123.96	118.30
1	C	1435	ASP	CB-CG-OD2	-6.28	112.64	118.30
1	F	3953	ASP	CB-CG-OD1	-6.26	112.66	118.30
1	B	719	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	C	1568	ASP	CB-CG-OD2	6.25	123.92	118.30
1	D	1952	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	D	2016	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	G	4368	ASP	CB-CG-OD1	6.23	123.91	118.30
1	C	1223	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	2168	ASP	CB-CG-OD1	6.23	123.91	118.30
1	B	1106	ASP	CB-CG-OD2	6.23	123.91	118.30
1	E	3177	ASP	CB-CG-OD2	6.22	123.90	118.30
1	E	3237	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	112	ASP	CB-CG-OD2	6.22	123.90	118.30
1	F	3759	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	A	100	ASP	CB-CG-OD1	-6.18	112.73	118.30
1	C	1684	ASP	CB-CG-OD1	-6.17	112.74	118.30
1	A	176	ASP	CB-CG-OD2	6.17	123.86	118.30
1	C	1233	ASP	CB-CG-OD1	-6.17	112.75	118.30
1	F	4084	ASP	CB-CG-OD1	-6.16	112.75	118.30
1	E	3112	ASP	CB-CG-OD2	6.16	123.84	118.30
1	F	3790	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	B	890	MET	CG-SD-CE	6.14	110.02	100.20
1	G	4305	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	H	4873	MET	CG-SD-CE	6.13	110.00	100.20
1	F	3895	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	C	1300	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	D	2080	ASP	CB-CG-OD2	6.12	123.80	118.30
1	G	4312	ASP	CB-CG-OD1	-6.11	112.80	118.30
1	H	5220	TYR	CB-CG-CD1	6.11	124.67	121.00
1	A	315	ARG	NE-CZ-NH1	6.11	123.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	4944	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	G	4686	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	G	4493	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	35	ASP	CB-CG-OD2	6.08	123.77	118.30
1	C	1242	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	2035	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	2275	ASP	CB-CG-OD2	6.05	123.75	118.30
1	G	4606	ASP	CB-CG-OD1	6.05	123.75	118.30
1	G	4675	ASP	CB-CG-OD2	6.05	123.74	118.30
1	G	4666	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	1020	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	E	3406	ASP	CB-CG-OD1	-6.04	112.86	118.30
1	F	3880	ASP	CB-CG-OD2	6.04	123.73	118.30
1	G	4376	ASP	CB-CG-OD2	6.03	123.73	118.30
1	C	1359	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	A	23	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	E	3023	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	C	1454	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	D	2235	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	D	2027	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	G	4319	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	G	4416	ASP	CB-CG-OD1	5.95	123.65	118.30
1	G	4416	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	D	2146	ASP	CB-CG-OD1	-5.94	112.96	118.30
1	B	623	ASP	CB-CG-OD1	5.93	123.64	118.30
1	E	3216	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	190	ASP	CB-CG-OD1	5.93	123.64	118.30
1	C	1487	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	E	3277	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	H	5138	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	D	2093	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	H	5266	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	B	1035	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	F	3827	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	H	4823	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	B	816	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	A	293	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	712	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	B	1106	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	D	2138	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	D	1833	ASP	CB-CG-OD1	-5.88	113.00	118.30
1	F	3849	ASP	CB-CG-OD2	-5.88	113.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	968	ASP	CB-CG-OD1	-5.87	113.01	118.30
1	D	2306	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	F	3968	ASP	CB-CG-OD2	5.87	123.58	118.30
1	F	3635	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	E	3475	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	152	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	F	3635	ASP	CB-CG-OD2	5.85	123.57	118.30
1	H	4959	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	177	ASP	CB-CG-OD2	5.84	123.55	118.30
1	H	4959	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	B	991	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	D	1842	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	E	3484	ASP	CB-CG-OD2	5.83	123.54	118.30
1	B	837	ASP	CB-CG-OD2	5.82	123.54	118.30
1	C	1729	VAL	C-N-CD	-5.82	107.79	120.60
1	F	4115	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	D	2284	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	A	216	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	C	1684	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	295	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	B	759	ASP	N-CA-CB	-5.77	100.22	110.60
1	H	4990	ASP	CB-CG-OD2	5.77	123.49	118.30
1	H	5206	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	152	ASP	CB-CG-OD1	5.76	123.48	118.30
1	F	3700	ASP	CB-CG-OD1	-5.76	113.11	118.30
1	F	3816	ASP	CB-CG-OD2	5.75	123.48	118.30
1	C	1437	ASP	CB-CG-OD2	5.75	123.47	118.30
1	C	1495	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	486	ASP	CB-CG-OD1	-5.74	113.13	118.30
1	E	3235	ASP	CB-CG-OD2	5.74	123.46	118.30
1	F	3880	ASP	CB-CG-OD1	-5.73	113.14	118.30
1	H	5016	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	A	163	ILE	O-C-N	5.73	131.87	122.70
1	F	3744	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	G	4606	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	E	3486	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	C	1300	ASP	CB-CG-OD1	5.71	123.44	118.30
1	H	5027	ASP	CB-CG-OD2	5.71	123.44	118.30
1	H	5095	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	H	5175	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	H	4823	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	635	ASP	CB-CG-OD2	5.69	123.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	3816	ASP	N-CA-CB	5.69	120.84	110.60
1	D	1833	ASP	CB-CG-OD2	5.69	123.42	118.30
1	E	3249	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	C	1646	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	G	4390	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	486	ASP	CB-CG-OD2	5.67	123.41	118.30
1	C	1319	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	B	700	ASP	CB-CG-OD2	5.66	123.40	118.30
1	C	1427	ASP	CB-CG-OD2	5.66	123.39	118.30
1	C	1435	ASP	CB-CG-OD1	5.65	123.39	118.30
1	C	1686	ASP	CB-CG-OD2	5.65	123.39	118.30
1	G	4233	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	1235	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	777	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	A	484	ASP	CB-CG-OD1	-5.64	113.23	118.30
1	H	5095	ASP	CB-CG-OD2	5.64	123.37	118.30
1	B	1084	ASP	CB-CG-OD1	-5.63	113.23	118.30
1	F	3895	ASP	CB-CG-OD2	5.63	123.37	118.30
1	D	2024	ASP	CB-CG-OD1	-5.63	113.23	118.30
1	D	1823	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	G	4424	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	B	835	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	H	5054	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	1359	ASP	CB-CG-OD1	5.62	123.36	118.30
1	G	4553	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	A	287	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	B	752	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	B	849	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	C	1706	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	D	2146	ASP	CB-CG-OD2	5.60	123.34	118.30
1	D	1912	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	F	3790	ASP	CB-CG-OD1	5.59	123.33	118.30
1	H	5080	ASP	CB-CG-OD2	5.57	123.31	118.30
1	D	2315	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	190	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	192	LEU	N-CA-CB	5.55	121.50	110.40
1	F	4035	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	224	ASP	CB-CG-OD2	5.53	123.27	118.30
1	G	4390	ASP	CB-CG-OD1	5.53	123.27	118.30
1	H	5118	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	712	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	1599	ARG	NE-CZ-NH1	5.49	123.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	4842	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	D	2037	ASP	CB-CG-OD1	-5.48	113.36	118.30
1	F	4086	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	368	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	E	3277	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	E	3475	ASP	CB-CG-OD1	5.46	123.22	118.30
1	G	4487	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	B	790	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	635	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	C	1223	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	G	4487	ASP	CB-CG-OD1	5.42	123.18	118.30
1	C	1644	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	G	4599	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	346	ASP	CB-CG-OD2	5.41	123.16	118.30
1	C	1591	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	1706	ASP	CB-CG-OD2	5.39	123.15	118.30
1	D	2049	ASP	CB-CG-OD1	5.39	123.15	118.30
1	E	3444	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	F	4006	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	176	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	C	1646	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	H	5146	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	1990	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	E	3072	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	1990	ASP	CB-CG-OD1	5.37	123.13	118.30
1	F	3953	ASP	CB-CG-OD2	5.37	123.13	118.30
1	E	3177	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	H	5286	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	E	3144	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	A	159	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	B	1006	ASP	CB-CG-OD1	5.35	123.12	118.30
1	G	4377	ASP	CB-CG-OD2	5.35	123.12	118.30
1	E	3382	ARG	N-CA-CB	5.35	120.23	110.60
1	H	5275	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	835	ASP	CB-CG-OD2	5.34	123.11	118.30
1	E	3486	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	1075	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	1233	ASP	CB-CG-OD2	5.34	123.10	118.30
1	F	4066	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	G	4686	ASP	CB-CG-OD2	5.33	123.10	118.30
1	E	3484	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	E	3023	ASP	CB-CG-OD1	5.32	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1086	ASP	CB-CG-OD1	5.32	123.08	118.30
1	A	368	ASP	CB-CG-OD1	5.31	123.08	118.30
1	G	4312	ASP	CB-CG-OD2	5.31	123.08	118.30
1	F	3691	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	F	3752	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	144	ASP	CB-CG-OD2	5.30	123.07	118.30
1	E	3035	ASP	CB-CG-OD1	5.29	123.06	118.30
1	F	4075	ASP	CB-CG-OD2	5.29	123.06	118.30
1	G	4233	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	C	1433	GLU	OE1-CD-OE2	5.26	129.62	123.30
1	D	2168	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	B	964	THR	CA-CB-CG2	-5.26	105.04	112.40
1	D	2087	ASP	CB-CG-OD1	5.26	123.03	118.30
1	H	5306	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	C	1352	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	E	3100	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	1424	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	2153	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	H	5168	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	484	ASP	CB-CG-OD2	5.23	123.01	118.30
1	F	3816	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	F	3700	ASP	CB-CG-OD2	5.23	123.00	118.30
1	G	4495	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	B	968	ASP	CB-CG-OD2	5.22	123.00	118.30
1	H	5205	THR	CA-CB-OG1	5.22	119.97	109.00
1	D	1912	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	2206	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	G	4724	MET	CG-SD-CE	5.21	108.54	100.20
1	H	4912	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	915	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	H	5054	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	H	5205	THR	CA-CB-CG2	5.19	119.67	112.40
1	D	1977	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	1487	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	2199	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	H	4977	ASP	CB-CG-OD2	5.19	122.97	118.30
1	F	4042	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	295	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	887	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	F	3835	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	1115	ARG	CB-CA-C	5.16	120.72	110.40
1	C	1449	ASP	CB-CG-OD2	-5.16	113.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	845	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	278	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	H	5087	ASP	CB-CG-OD1	5.16	122.94	118.30
1	D	2286	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	C	1352	ASP	CB-CG-OD1	5.14	122.92	118.30
1	D	2016	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	3776	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	100	ASP	CB-CG-OD2	5.13	122.92	118.30
1	E	3168	ASP	N-CA-CB	5.13	119.83	110.60
1	D	2156	ASP	CB-CG-OD1	5.12	122.91	118.30
1	H	4977	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	H	4900	ASP	CB-CG-OD1	5.11	122.90	118.30
1	H	5016	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	1546	ASP	CB-CG-OD2	5.10	122.89	118.30
1	F	3991	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	525	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	744	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	D	2024	ASP	CB-CG-OD2	5.09	122.88	118.30
1	G	4359	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	A	356	ASP	CB-CG-OD1	5.09	122.88	118.30
1	H	5156	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	1344	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	C	1390	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	D	1842	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	F	3837	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	F	3752	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	H	5035	ASP	CB-CG-OD2	5.06	122.85	118.30
1	E	3168	ASP	CA-CB-CG	5.05	124.51	113.40
1	F	3759	ASP	CB-CA-C	-5.05	100.30	110.40
1	F	3744	ASP	CB-CG-OD2	5.04	122.84	118.30
1	G	4575	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	999	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	F	3687	ILE	CB-CA-C	-5.03	101.54	111.60
1	F	3777	ASP	CB-CG-OD2	5.02	122.82	118.30
1	G	4427	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	E	3368	ASP	CB-CG-OD2	5.00	122.80	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	5205	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	759	ASP	Mainchain
1	C	1599	ARG	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3978	0	4055	326	2
1	B	3978	0	4056	216	1
1	C	3978	0	4055	321	3
1	D	3978	0	4055	251	5
1	E	3978	0	4056	221	14
1	F	3978	0	4055	240	2
1	G	3978	0	4055	276	2
1	H	3978	0	4055	187	18
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	6	0	0	2	0
3	B	6	0	0	0	0
3	C	6	0	0	1	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	1	0
3	G	6	0	0	1	0
3	H	6	0	0	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	2	0	0	0	0
4	H	1	0	0	0	0
5	A	31	0	12	3	0
5	C	31	0	12	3	0
5	D	31	0	12	1	0
5	E	31	0	12	0	0
5	F	31	0	12	0	0
5	G	31	0	12	1	0
6	A	195	0	0	11	0
6	B	270	0	0	17	0
6	C	178	0	0	11	0
6	D	272	0	0	21	0
6	E	279	0	0	15	0
6	F	197	0	0	9	0
6	G	228	0	0	7	0
6	H	302	0	0	12	3
All	All	34001	0	32514	1940	25

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (1940) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ARG:NH2	6:A:6596:HOH:O	1.57	1.36
1:C:1248:CYS:HB2	1:C:1268:MET:HE3	1.25	1.19
1:E:3142:THR:HG22	1:E:3144:ASP:H	1.05	1.10
1:H:5130:LEU:HD13	1:H:5133:MET:HE3	1.20	1.09
1:G:4665:TYR:HB2	1:G:4668:ILE:HD12	1.36	1.07
1:C:1678:GLN:HB2	1:C:1684:ASP:HB2	1.31	1.06
1:F:3624:THR:HG22	1:F:3627:GLU:H	1.21	1.05
1:A:122:LEU:HD23	1:A:204:SER:HB3	1.41	1.02
1:G:4367:VAL:HG22	1:G:4371:SER:HB3	1.42	1.01
1:E:3493:MET:HE1	1:E:3529:VAL:HA	1.45	0.99
1:E:3048:CYS:HB2	1:E:3068:MET:HE3	1.45	0.99
1:B:928:GLN:NE2	1:D:2141:ARG:H	1.63	0.96
1:B:648:CYS:HB2	1:B:668:MET:HE3	1.44	0.96
1:G:4680:ALA:HB3	1:G:4683:GLU:HG3	1.48	0.96
1:H:4850:ILE:HD11	1:H:4868:MET:HE1	1.46	0.96
1:D:2044:ILE:HG22	1:D:2082:ILE:HD12	1.47	0.96
1:F:3941:ARG:H	1:H:5128:GLN:HE21	1.13	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:LEU:HD23	1:B:1099:ARG:NH2	1.82	0.95
1:C:1257:VAL:HG21	1:C:1292:THR:HG22	1.48	0.94
1:E:3376:MET:HA	1:E:3376:MET:HE3	1.47	0.93
1:A:431:THR:HG21	1:A:434:GLY:HA2	1.49	0.93
1:A:191:PHE:HE2	1:A:193:VAL:HG23	1.32	0.93
1:A:160:TYR:HD2	1:A:163:ILE:HB	1.30	0.92
1:E:3160:TYR:HD2	1:E:3163:ILE:HB	1.34	0.92
1:E:3493:MET:HE3	1:E:3529:VAL:HG13	1.52	0.92
1:B:815:VAL:HB	1:B:817:LEU:HD12	1.51	0.92
1:G:4593:LEU:HD21	1:G:4644:ARG:HG3	1.53	0.91
1:F:3743:LEU:HD11	1:F:3761:LYS:HA	1.51	0.91
1:G:4479:PHE:CZ	1:G:4483:LEU:HD22	2.06	0.90
1:C:1479:PHE:HE1	1:C:1489:ILE:HD12	1.35	0.90
1:C:1322:LEU:HD12	1:C:1349:GLU:HG2	1.53	0.90
1:G:4389:PRO:HD2	1:G:4391:PHE:CE2	2.08	0.89
1:C:1248:CYS:HB2	1:C:1268:MET:CE	2.02	0.89
1:H:5020:VAL:HG13	1:H:5024:ASP:HB2	1.55	0.89
1:A:328:GLN:NE2	1:C:1541:ARG:H	1.71	0.89
1:A:514:TRP:H	1:A:522:ASN:HD21	1.17	0.88
1:G:4408:VAL:HG12	1:G:4410:LEU:HD11	1.56	0.88
1:A:141:ILE:HG21	1:A:158:LEU:HD22	1.56	0.88
1:E:3142:THR:HG22	1:E:3144:ASP:N	1.88	0.87
1:C:1693:MET:CE	1:C:1729:VAL:HG22	2.04	0.87
1:H:5015:VAL:HG11	1:H:5017:LEU:HD12	1.57	0.87
1:C:1319:ARG:H	1:C:1359:ASP:HB2	1.39	0.86
1:G:4408:VAL:HG12	1:G:4410:LEU:CD1	2.06	0.86
1:E:3050:ILE:HD11	1:E:3068:MET:HE3	1.55	0.86
1:F:3928:GLN:NE2	1:H:5141:ARG:H	1.74	0.86
1:D:1850:ILE:HD11	1:D:1868:MET:CE	2.05	0.86
1:G:4276:SER:HB3	1:G:4319:ARG:HE	1.41	0.85
1:E:3191:PHE:HE1	1:E:3193:VAL:HG23	1.39	0.85
1:A:126:SER:HB3	1:A:129:ALA:HB2	1.57	0.85
1:B:648:CYS:HB2	1:B:668:MET:CE	2.06	0.85
1:A:120:THR:HG22	1:A:205:LYS:N	1.90	0.85
1:A:118:ILE:CG2	1:A:208:VAL:HB	2.06	0.85
1:D:1850:ILE:HB	1:D:1873:MET:HE3	1.57	0.85
1:H:5327:VAL:HG13	1:H:5328:PRO:HD2	1.58	0.85
1:H:5133:MET:HE1	1:H:5139:PRO:HG3	1.57	0.84
1:D:1850:ILE:HD11	1:D:1868:MET:HE1	1.57	0.84
1:F:3941:ARG:H	1:H:5128:GLN:NE2	1.73	0.84
1:C:1477:ARG:NH2	1:C:1478:ARG:HH11	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:976:MET:HE2	1:B:980:ILE:HD11	1.58	0.84
1:A:103:LEU:HD11	1:A:498:ALA:HB1	1.59	0.83
1:H:4850:ILE:HD11	1:H:4868:MET:CE	2.07	0.83
1:A:225:ILE:HG23	1:A:256:ILE:CG2	2.08	0.83
1:D:1902:ILE:HG13	1:D:2295:VAL:HG22	1.61	0.83
1:D:1824:THR:HG22	1:D:1827:GLU:HB2	1.60	0.83
1:H:4942:THR:HG23	1:H:4944:ASP:H	1.39	0.83
1:D:2176:MET:HA	1:D:2176:MET:HE3	1.59	0.83
1:D:2201:SER:HA	1:D:2203:HIS:CE1	2.13	0.83
1:H:4848:CYS:HB2	1:H:4868:MET:HE3	1.61	0.83
1:D:1824:THR:HG23	1:D:1827:GLU:H	1.43	0.83
1:F:3726:SER:CB	1:F:3729:ALA:HB2	2.08	0.82
1:A:160:TYR:O	1:A:163:ILE:HG22	1.79	0.82
1:D:1899:SER:O	1:D:1901:PRO:HD3	1.80	0.82
1:A:431:THR:CG2	1:A:434:GLY:HA2	2.08	0.82
1:E:3493:MET:CE	1:E:3529:VAL:HG13	2.10	0.82
1:E:3186:GLN:HB3	1:E:3193:VAL:HB	1.60	0.82
1:H:4873:MET:HG3	1:H:4887:ILE:HD11	1.61	0.82
1:H:5130:LEU:HD13	1:H:5133:MET:CE	2.09	0.82
1:F:3624:THR:CG2	1:F:3627:GLU:H	1.92	0.82
1:B:720:THR:HG22	1:B:758:LEU:CD2	2.10	0.81
1:A:328:GLN:HE21	1:C:1541:ARG:H	1.25	0.81
1:E:3050:ILE:HD11	1:E:3068:MET:CE	2.10	0.81
1:D:1824:THR:HG22	1:D:1827:GLU:CB	2.10	0.81
1:D:2176:MET:CE	1:D:2179:LEU:HB2	2.10	0.81
1:C:1442:SER:HA	1:C:1469:LYS:HD3	1.63	0.81
1:H:4848:CYS:HB2	1:H:4868:MET:CE	2.10	0.81
1:B:1109:ILE:CD1	1:B:1126:VAL:HG22	2.10	0.81
1:E:3160:TYR:O	1:E:3163:ILE:HG22	1.80	0.81
1:G:4367:VAL:HG22	1:G:4371:SER:CB	2.11	0.81
1:F:3949:ASN:HD21	1:H:5110:LYS:NZ	1.79	0.81
1:A:118:ILE:HG22	1:A:208:VAL:HB	1.63	0.80
1:F:3776:ASP:HB3	1:F:3779:LEU:HB3	1.64	0.80
1:A:277:ARG:NH2	1:A:278:ARG:NH1	2.30	0.80
1:G:4305:ARG:HD3	1:G:4699:ARG:NH1	1.96	0.80
1:C:1678:GLN:HB2	1:C:1684:ASP:CB	2.11	0.80
1:G:4333:LEU:HG	1:G:4402:LEU:HD23	1.62	0.80
1:E:3106:PRO:HG2	1:E:3470:PRO:HB2	1.63	0.80
1:H:5133:MET:HE2	1:H:5139:PRO:HB3	1.62	0.80
1:G:4322:LEU:HD23	1:G:4404:SER:CB	2.12	0.80
1:F:3803:GLY:HA3	1:F:3806:LYS:HE2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASN:HB3	1:A:463:HIS:ND1	1.98	0.79
1:E:3162:ASN:HD21	1:E:3165:LYS:HD3	1.47	0.79
1:D:1905:ARG:NH1	1:D:2299:ARG:HH21	1.79	0.79
1:F:3726:SER:HB3	1:F:3729:ALA:HB2	1.62	0.79
1:F:3648:CYS:HB2	1:F:3668:MET:CE	2.13	0.79
1:E:3341:ARG:H	1:G:4528:GLN:HE21	1.30	0.79
1:A:120:THR:HG22	1:A:205:LYS:H	1.44	0.79
1:E:3158:LEU:HD11	1:E:3208:VAL:HG21	1.64	0.79
1:C:1409:ASN:O	1:C:1411:PRO:HD3	1.83	0.79
1:E:3493:MET:CE	1:E:3530:PRO:HD2	2.12	0.79
1:B:928:GLN:HE21	1:D:2141:ARG:H	1.27	0.79
1:A:327:THR:HG22	1:A:328:GLN:HG3	1.63	0.79
1:A:391:ARG:O	1:A:395:GLU:HG3	1.83	0.79
1:C:1343:LEU:CD2	1:C:1361:LYS:HA	2.12	0.79
1:D:2304:LYS:HG3	1:D:2330:PRO:C	2.02	0.78
1:G:4680:ALA:HB3	1:G:4683:GLU:CG	2.14	0.78
1:D:1945:ASN:HD21	1:D:1961:LYS:NZ	1.80	0.78
1:A:191:PHE:CE2	1:A:193:VAL:HG23	2.17	0.78
1:C:1693:MET:HE2	1:C:1729:VAL:HG22	1.66	0.78
1:H:5311:LEU:HB3	1:H:5321:THR:CG2	2.13	0.78
1:G:4313:THR:CG2	1:G:4442:SER:H	1.97	0.78
1:B:1104:LYS:HB3	1:B:1130:PRO:C	2.04	0.78
1:G:4313:THR:HG22	1:G:4442:SER:H	1.47	0.78
1:C:1259:THR:O	1:C:1263:MET:HG3	1.83	0.78
1:B:897:GLY:HA3	1:D:2141:ARG:HE	1.49	0.77
1:C:1534:ILE:HG23	1:C:1567:GLY:HA2	1.67	0.77
1:G:4339:LEU:HD11	1:G:4354:ASN:CA	2.15	0.77
1:C:1479:PHE:CE1	1:C:1489:ILE:HD12	2.19	0.77
1:H:4905:ARG:NH2	1:H:5299:ARG:HD3	1.99	0.77
1:D:1848:CYS:HB2	1:D:1868:MET:CE	2.13	0.77
1:D:1824:THR:CG2	1:D:1827:GLU:H	1.96	0.77
1:E:3509:ILE:CD1	1:E:3526:VAL:HG23	2.14	0.77
1:H:4926:SER:HB3	1:H:4929:ALA:H	1.48	0.77
1:G:4216:GLN:HE22	1:G:4233:ASP:H	1.33	0.77
1:B:759:ASP:HB3	6:B:6599:HOH:O	1.85	0.77
1:C:1257:VAL:HG21	1:C:1292:THR:CG2	2.15	0.77
1:A:288:GLY:O	1:A:289:ILE:HD13	1.84	0.77
1:B:989:PHE:CE2	1:B:992:LYS:HD2	2.20	0.76
1:C:1347:TYR:CD2	1:C:1355:ILE:HG21	2.19	0.76
1:H:4952:ASP:HB2	1:H:4953:GLU:OE1	1.85	0.76
1:G:4369:VAL:HA	1:G:4384:VAL:HG12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1477:ARG:HH22	1:C:1478:ARG:HH11	1.34	0.76
1:D:2284:ASP:O	1:D:2288:ARG:HG3	1.86	0.76
1:C:1376:ASP:OD2	1:C:1406:LYS:HE2	1.84	0.76
1:C:1477:ARG:HH22	1:C:1478:ARG:NH1	1.82	0.76
1:F:3724:LYS:HG3	6:F:7473:HOH:O	1.85	0.76
1:A:47:ILE:HG22	1:A:359:MET:HG3	1.66	0.76
1:D:2038:MET:CE	1:D:2264:LEU:HD11	2.16	0.76
1:H:5133:MET:HE1	1:H:5139:PRO:CG	2.15	0.76
1:A:47:ILE:CG2	1:A:359:MET:HG3	2.16	0.76
1:C:1286:THR:O	1:C:1290:VAL:HG23	1.86	0.76
1:E:3341:ARG:H	1:G:4528:GLN:NE2	1.83	0.75
1:G:4257:VAL:O	1:G:4261:LYS:HG3	1.86	0.75
1:C:1472:ASN:ND2	1:C:1475:GLY:H	1.82	0.75
1:D:2141:ARG:HG2	1:D:2141:ARG:HH11	1.50	0.75
1:A:131:VAL:CG1	1:A:202:LEU:HD23	2.15	0.75
1:E:3481:TRP:CG	1:E:3516:PRO:HD3	2.21	0.75
1:C:1493:ARG:HD3	1:C:1526:ALA:O	1.86	0.75
1:C:1723:THR:HG23	1:D:2325:ARG:HG3	1.68	0.75
1:F:3752:ASP:OD1	1:F:3755:ILE:HD13	1.87	0.75
1:A:50:ILE:HB	1:A:73:MET:CE	2.15	0.75
1:E:3113:THR:HG22	1:E:3242:SER:H	1.52	0.75
1:G:4715:ARG:HB3	1:G:4716:PRO:HD2	1.67	0.75
1:F:3845:ARG:HG2	1:F:3874:GLU:HB3	1.66	0.75
1:E:3479:GLU:HG3	6:E:6695:HOH:O	1.85	0.75
1:D:2201:SER:HA	1:D:2203:HIS:HE1	1.51	0.75
1:D:1958:LEU:CD2	1:D:2008:VAL:HG21	2.16	0.75
1:G:4360:TYR:HE2	1:G:4366:VAL:HG21	1.52	0.75
1:E:3068:MET:HE1	1:E:3071:ALA:HB2	1.68	0.75
1:B:815:VAL:HG22	6:B:6919:HOH:O	1.86	0.75
1:E:3246:LYS:HD2	1:E:3249:ASP:OD1	1.87	0.75
1:G:4438:MET:HA	1:G:4464:ILE:HG23	1.68	0.75
1:E:3191:PHE:C	1:E:3192:LEU:HD22	2.07	0.75
1:G:4250:ILE:HB	1:G:4273:MET:CE	2.17	0.75
1:B:651:GLY:O	1:B:655:ARG:HG3	1.86	0.75
1:C:1404:SER:O	1:C:1406:LYS:HD3	1.86	0.74
1:G:4250:ILE:HD11	1:G:4268:MET:CE	2.18	0.74
1:C:1428:LEU:HD13	1:C:1456:ILE:HB	1.69	0.74
1:A:113:THR:CG2	1:A:242:SER:H	2.00	0.74
1:C:1678:GLN:HA	1:C:1678:GLN:NE2	2.02	0.74
1:F:3949:ASN:HD21	1:H:5110:LYS:HZ1	1.32	0.74
1:G:4371:SER:H	1:G:4384:VAL:HB	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1406:LYS:HE3	5:C:1735:ATP:O3'	1.87	0.74
1:D:2295:VAL:HG12	1:D:2299:ARG:HD2	1.68	0.74
1:E:3160:TYR:CD2	1:E:3163:ILE:HB	2.21	0.74
1:G:4248:CYS:HB2	1:G:4268:MET:CE	2.18	0.74
1:G:4250:ILE:HB	1:G:4273:MET:HE3	1.68	0.74
1:C:1368:ASP:HB3	6:C:7539:HOH:O	1.88	0.74
1:A:515:ARG:HD2	6:A:6021:HOH:O	1.86	0.74
6:B:6064:HOH:O	1:D:1824:THR:HG21	1.86	0.74
1:C:1728:PRO:O	1:C:1730:PRO:HD3	1.88	0.74
1:B:815:VAL:HB	1:B:817:LEU:CD1	2.17	0.73
1:C:1693:MET:HE3	1:C:1729:VAL:HG22	1.70	0.73
1:G:4305:ARG:HH22	1:G:4663:HIS:HE1	1.36	0.73
1:B:1087:LEU:HD23	1:B:1088:ARG:N	2.03	0.73
1:D:1986:GLN:HB3	1:D:1993:VAL:HB	1.70	0.73
1:F:3732:GLU:HB2	1:F:3801:PHE:CD1	2.22	0.73
1:G:4498:ILE:N	1:G:4498:ILE:HD13	2.02	0.73
1:B:823:LYS:HE3	1:B:827:ASP:OD2	1.88	0.73
1:C:1671:VAL:HG12	1:C:1691:LEU:HD21	1.70	0.73
1:G:4348:MET:HA	1:G:4357:TRP:CD2	2.24	0.73
1:C:1343:LEU:HD13	1:C:1390:ASP:O	1.89	0.73
1:F:3750:LYS:O	1:F:3755:ILE:HD11	1.88	0.73
1:H:5209:GLU:O	1:H:5213:MET:HG3	1.88	0.73
1:H:5020:VAL:HG11	1:H:5025:ILE:HG12	1.70	0.73
1:D:2038:MET:HE2	1:D:2264:LEU:HD11	1.71	0.73
1:B:991:ARG:O	1:B:995:GLU:HG3	1.88	0.73
1:C:1422:GLU:O	1:C:1425:ILE:HB	1.88	0.73
1:F:3723:ILE:HA	1:F:3751:CYS:O	1.89	0.73
1:E:3316:CYS:HB3	1:E:3321:LYS:O	1.89	0.73
1:C:1665:TYR:HB2	1:C:1668:ILE:HD12	1.70	0.73
1:A:399:ARG:NH2	1:C:1223:ASP:HB2	2.04	0.73
1:C:1291:ARG:O	1:C:1295:GLU:HG2	1.89	0.73
1:G:4680:ALA:CB	1:G:4683:GLU:HG3	2.18	0.73
1:G:4681:TRP:CD2	1:G:4716:PRO:HD3	2.24	0.73
1:A:14:THR:HG23	1:A:15:GLN:HB2	1.69	0.73
1:B:976:MET:HE3	1:B:980:ILE:HG13	1.70	0.72
1:F:3892:ALA:HB1	3:F:4133:OXL:C2	2.19	0.72
1:B:938:ARG:HH22	1:D:1998:ASN:HD21	1.37	0.72
1:E:3493:MET:HE2	1:E:3530:PRO:HD2	1.71	0.72
1:B:1091:LEU:O	1:B:1095:VAL:HG23	1.89	0.72
1:D:2176:MET:HE3	1:D:2179:LEU:HB2	1.69	0.72
1:C:1313:THR:HG22	1:C:1442:SER:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ALA:O	1:A:96:SER:HB3	1.89	0.72
1:F:3763:ILE:O	1:F:3767:VAL:HG13	1.90	0.72
1:D:2265:TYR:HB2	1:D:2268:ILE:HD12	1.70	0.72
1:F:3739:LEU:HD21	1:F:3756:LEU:HB2	1.71	0.72
1:A:102:ILE:HG22	1:A:103:LEU:CD1	2.20	0.72
1:F:3740:LYS:HE2	1:F:3791:PHE:CD2	2.24	0.72
1:C:1257:VAL:CG2	1:C:1292:THR:HG22	2.19	0.72
1:A:167:VAL:HG21	1:A:184:VAL:HG21	1.72	0.72
1:A:503:LYS:O	1:A:506:ASP:HB2	1.89	0.71
1:H:5108:ALA:O	1:H:5112:ILE:HG13	1.88	0.71
1:A:181:SER:C	1:A:182:LEU:HD23	2.10	0.71
1:B:703:LEU:CD2	1:B:1099:ARG:NH2	2.54	0.71
1:G:4647:ALA:HB1	1:G:4648:PRO:HD2	1.72	0.71
1:F:4008:MET:HG3	1:F:4039:GLN:HG2	1.71	0.71
1:A:484:ASP:O	1:A:487:LEU:HB3	1.91	0.71
1:A:421:LYS:HE2	1:B:1013:MET:SD	2.30	0.71
1:A:511:LEU:HD22	1:A:521:THR:HG23	1.71	0.71
1:A:18:HIS:O	1:A:21:MET:HB2	1.91	0.71
1:D:1839:ILE:O	1:D:2182:ARG:HD2	1.90	0.71
1:A:55:ARG:HD2	1:A:82:TYR:CZ	2.26	0.71
1:G:4322:LEU:CD2	1:G:4327:GLY:HA2	2.20	0.71
1:G:4704:LYS:HG2	1:G:4730:PRO:C	2.10	0.71
1:E:3172:LYS:HE2	1:E:3197:GLU:OE1	1.91	0.71
1:E:3099:SER:O	1:E:3101:PRO:HD3	1.91	0.70
1:A:481:TRP:O	1:A:485:VAL:HG23	1.90	0.70
1:E:3300:ILE:HB	1:E:3301:PRO:HD2	1.73	0.70
1:G:4243:ASN:HB3	1:G:4667:GLY:HA2	1.71	0.70
1:A:225:ILE:HG23	1:A:256:ILE:HG21	1.74	0.70
1:C:1323:ILE:HG22	1:C:1324:LYS:HG3	1.73	0.70
1:H:5311:LEU:HB3	1:H:5321:THR:HG21	1.74	0.70
1:A:231:GLY:O	1:A:236:VAL:HG13	1.92	0.70
1:D:1910:ALA:HB2	1:D:2038:MET:HG3	1.73	0.70
1:E:3276:VAL:HG11	1:G:4234:ILE:HD13	1.73	0.70
1:D:2176:MET:HE2	1:D:2180:ILE:HG13	1.74	0.70
1:G:4322:LEU:HD23	1:G:4404:SER:HB3	1.71	0.70
1:F:3723:ILE:HD11	1:F:3803:GLY:O	1.91	0.70
1:D:1814:THR:HG22	1:D:1815:GLN:HG3	1.72	0.70
1:A:145:ASN:O	1:A:148:MET:HB2	1.92	0.70
1:F:3650:ILE:HD11	1:F:3668:MET:CE	2.22	0.70
1:G:4509:GLN:O	1:G:4513:ILE:HG13	1.92	0.70
1:H:4963:ILE:O	1:H:4967:VAL:HG22	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3432:GLU:HA	1:E:3432:GLU:OE1	1.91	0.70
1:G:4339:LEU:HD11	1:G:4354:ASN:HA	1.72	0.69
1:C:1387:LYS:HB3	1:C:1392:LEU:HD12	1.74	0.69
1:B:705:ARG:NE	1:B:1099:ARG:HH12	1.90	0.69
1:A:192:LEU:N	1:A:192:LEU:HD22	2.07	0.69
1:F:3928:GLN:HE21	1:H:5141:ARG:H	1.39	0.69
1:E:3027:GLU:O	1:E:3031:ARG:HG3	1.92	0.69
1:A:126:SER:HB3	1:A:129:ALA:CB	2.22	0.69
1:C:1343:LEU:HD21	1:C:1361:LYS:HA	1.74	0.69
1:F:3740:LYS:HE2	1:F:3791:PHE:CG	2.27	0.69
1:E:3142:THR:CG2	1:E:3144:ASP:H	1.97	0.69
1:F:3648:CYS:HB2	1:F:3668:MET:HE2	1.73	0.69
1:A:51:GLY:O	1:A:55:ARG:HG3	1.91	0.69
1:C:1609:GLU:O	1:C:1613:MET:HG3	1.93	0.69
1:A:413:MET:SD	1:B:1021:LYS:HD3	2.32	0.69
1:C:1250:ILE:HB	1:C:1273:MET:HE1	1.75	0.69
1:C:1678:GLN:CB	1:C:1684:ASP:HB2	2.18	0.69
1:D:1902:ILE:HG22	1:D:1903:LEU:CD2	2.23	0.69
1:H:4873:MET:CG	1:H:4887:ILE:HD11	2.22	0.69
1:A:160:TYR:CD2	1:A:163:ILE:HB	2.20	0.69
1:H:4942:THR:CG2	1:H:4944:ASP:H	2.06	0.69
1:F:3650:ILE:HD11	1:F:3668:MET:HE2	1.75	0.69
1:D:1814:THR:HG23	1:D:1837:ALA:O	1.91	0.69
1:E:3253:VAL:HG12	1:E:3257:LEU:CD2	2.23	0.69
1:E:3245:ARG:HB3	1:E:3274:GLU:HG2	1.75	0.69
1:D:1851:GLY:O	1:D:1855:ARG:HG3	1.93	0.69
1:A:225:ILE:HG23	1:A:256:ILE:HG23	1.73	0.68
1:H:5191:ARG:O	1:H:5195:GLU:HG3	1.93	0.68
1:E:3371:LEU:HB2	6:E:6194:HOH:O	1.93	0.68
1:B:705:ARG:CZ	1:B:1099:ARG:HH12	2.05	0.68
1:A:172:LYS:HE3	1:A:197:GLU:OE1	1.92	0.68
1:H:4964:CYS:HB2	6:H:6481:HOH:O	1.93	0.68
1:F:3652:PRO:HD2	1:F:3965:ALA:O	1.93	0.68
1:G:4469:LYS:HD2	1:G:4490:MET:SD	2.33	0.68
1:G:4250:ILE:HD11	1:G:4268:MET:HE1	1.76	0.68
1:E:3051:GLY:O	1:E:3055:ARG:HG3	1.94	0.68
1:H:4815:GLN:HG3	1:H:4839:ILE:HG23	1.74	0.68
1:H:4847:ILE:HG21	1:H:5159:MET:CE	2.24	0.68
1:H:5133:MET:CE	1:H:5139:PRO:HB3	2.23	0.68
1:C:1326:SER:HB3	1:C:1329:ALA:CB	2.24	0.68
1:G:4332:GLU:HA	1:G:4401:PHE:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1270:VAL:HG22	1:C:1308:ALA:HB3	1.75	0.68
1:C:1500:ILE:HB	1:C:1501:PRO:HD2	1.75	0.68
1:A:55:ARG:HD2	1:A:82:TYR:OH	1.93	0.68
1:B:703:LEU:CD2	1:B:1099:ARG:HH21	2.07	0.68
1:G:4305:ARG:NH2	1:G:4663:HIS:HE1	1.91	0.68
1:C:1423:LYS:O	1:C:1426:GLN:HB3	1.93	0.68
1:H:5130:LEU:CD1	1:H:5133:MET:HE3	2.12	0.68
1:E:3252:GLU:O	1:E:3256:ILE:HG12	1.92	0.68
1:H:4945:ASN:HB3	1:H:4948:MET:HE2	1.76	0.67
1:H:4843:ASN:HB3	1:H:5267:GLY:CA	2.22	0.67
1:F:3733:LEU:HD11	1:F:3802:LEU:HD22	1.76	0.67
1:D:2281:TRP:CG	1:D:2316:PRO:HD3	2.29	0.67
1:B:703:LEU:HD23	1:B:1099:ARG:HH21	1.58	0.67
1:E:3481:TRP:CD1	1:E:3516:PRO:HD3	2.29	0.67
1:G:4255:ARG:HD2	1:G:4282:TYR:OH	1.95	0.67
1:D:2044:ILE:CG2	1:D:2082:ILE:HD12	2.24	0.67
1:D:1855:ARG:NH2	1:D:1885:GLU:HG2	2.09	0.67
1:D:2171:LEU:O	1:D:2175:ARG:HG3	1.95	0.67
1:F:3828:LEU:O	1:F:3832:VAL:HG23	1.94	0.67
1:A:122:LEU:HD23	1:A:204:SER:CB	2.22	0.67
1:C:1322:LEU:HB2	1:C:1349:GLU:HA	1.76	0.67
1:A:328:GLN:HE22	1:C:1540:THR:HA	1.60	0.67
1:D:2291:LEU:O	1:D:2295:VAL:HG23	1.93	0.67
1:C:1251:GLY:O	1:C:1255:ARG:HG3	1.94	0.67
1:H:4850:ILE:N	1:H:4850:ILE:HD13	2.10	0.67
1:D:1958:LEU:HD21	1:D:2008:VAL:HG21	1.75	0.67
1:B:1109:ILE:HD12	1:B:1126:VAL:HG22	1.75	0.67
1:F:4093:MET:CE	1:F:4129:VAL:HG22	2.25	0.67
1:G:4322:LEU:HD22	1:G:4326:SER:O	1.95	0.67
1:A:69:ASN:HB3	1:A:463:HIS:CE1	2.30	0.67
1:E:3254:ARG:NH2	1:E:3287:ASP:OD2	2.28	0.67
1:B:618:HIS:CE1	1:B:631:ARG:HD3	2.30	0.67
1:C:1370:GLY:O	1:C:1383:GLN:NE2	2.28	0.66
1:C:1305:ARG:NE	1:C:1699:ARG:NH2	2.43	0.66
1:F:4113:GLY:HA2	1:F:4122:ASN:OD1	1.95	0.66
1:C:1248:CYS:CB	1:C:1268:MET:HE3	2.15	0.66
1:A:191:PHE:HE2	1:A:193:VAL:CG2	2.08	0.66
1:F:3722:LEU:O	1:F:3751:CYS:N	2.25	0.66
1:D:2030:PHE:CE1	1:D:2034:GLN:HG3	2.30	0.66
1:D:2239:GLN:O	1:D:2242:ARG:HG2	1.95	0.66
1:B:1078:GLN:HA	1:B:1078:GLN:NE2	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1362:ASN:ND2	1:C:1365:LYS:HD2	2.10	0.66
1:E:3392:LYS:O	1:E:3396:GLU:HG3	1.96	0.66
1:B:928:GLN:NE2	1:D:2141:ARG:N	2.41	0.66
1:G:4243:ASN:HB3	1:G:4667:GLY:CA	2.25	0.66
1:H:4968:ASP:OD1	6:H:7656:HOH:O	2.11	0.66
1:C:1339:LEU:HD12	1:C:1340:LYS:H	1.61	0.66
1:E:3192:LEU:N	1:E:3192:LEU:HD22	2.11	0.66
1:A:167:VAL:CG2	1:A:184:VAL:HG21	2.25	0.66
1:G:4681:TRP:CG	1:G:4716:PRO:HD3	2.31	0.66
1:A:15:GLN:HG3	1:A:39:ILE:HG23	1.77	0.66
1:C:1250:ILE:HB	1:C:1273:MET:CE	2.26	0.66
1:G:4479:PHE:HZ	1:G:4483:LEU:HD22	1.60	0.66
1:C:1421:SER:O	1:C:1424:ASP:HB2	1.96	0.66
1:A:144:ASP:HB3	1:A:147:TYR:HD1	1.61	0.66
1:E:3145:ASN:O	1:E:3148:MET:HB2	1.96	0.66
1:H:4920:THR:HB	1:H:4956:LEU:HD11	1.77	0.66
1:B:873:HIS:O	1:B:877:ARG:HG3	1.96	0.66
1:H:5311:LEU:HD22	1:H:5321:THR:HG23	1.77	0.66
1:D:1919:ARG:H	1:D:1959:ASP:HB2	1.61	0.66
1:F:3687:ILE:HD13	1:F:3709:VAL:HG11	1.77	0.66
1:E:3372:GLU:OE1	1:E:3372:GLU:N	2.29	0.66
1:C:1250:ILE:HD11	1:C:1268:MET:CE	2.27	0.65
1:B:938:ARG:HH22	1:D:1998:ASN:ND2	1.94	0.65
1:G:4555:ALA:O	1:G:4666:ARG:NH1	2.30	0.65
1:C:1327:GLY:HA2	1:C:1404:SER:CB	2.26	0.65
1:G:4388:GLY:HA3	1:G:4391:PHE:CE2	2.32	0.65
1:B:928:GLN:NE2	1:D:2141:ARG:HH11	1.94	0.65
1:H:5015:VAL:HG11	1:H:5017:LEU:CD1	2.26	0.65
1:A:99:SER:O	1:A:101:PRO:HD3	1.95	0.65
1:F:4075:ASP:HB3	1:F:4076:PRO:HD2	1.79	0.65
1:E:3167:VAL:HG22	1:E:3171:SER:CB	2.26	0.65
1:F:3612:ILE:N	6:F:7480:HOH:O	2.29	0.65
1:D:2280:ALA:HB3	1:D:2283:GLU:HG3	1.78	0.65
1:F:3731:VAL:O	1:F:3802:LEU:N	2.29	0.65
1:C:1456:ILE:HD13	1:C:1456:ILE:N	2.10	0.65
1:A:340:THR:OG1	1:A:343:GLU:HG3	1.97	0.65
1:D:2033:GLU:HG3	6:D:6683:HOH:O	1.95	0.65
1:E:3330:LEU:HD12	1:E:3343:GLU:HB3	1.77	0.65
1:A:131:VAL:HG12	1:A:202:LEU:HD23	1.76	0.65
1:C:1255:ARG:HD2	1:C:1282:TYR:CZ	2.31	0.65
1:F:3669:ASN:HB3	1:F:4063:HIS:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:O	1:A:191:PHE:HB2	1.96	0.65
1:C:1343:LEU:HD23	1:C:1361:LYS:HA	1.77	0.65
1:A:486:ASP:O	1:A:490:ASN:ND2	2.29	0.65
1:H:5023:LYS:NZ	1:H:5027:ASP:OD2	2.28	0.65
1:F:3802:LEU:HD12	1:F:3803:GLY:N	2.12	0.65
1:C:1647:ALA:HB1	1:C:1648:PRO:HD2	1.79	0.65
1:A:23:ASP:HB2	6:A:7647:HOH:O	1.97	0.65
1:E:3160:TYR:HD2	1:E:3163:ILE:CB	2.06	0.65
1:G:4409:ASN:C	1:G:4410:LEU:HD12	2.17	0.65
1:C:1511:MET:O	1:C:1515:ARG:HG3	1.97	0.65
1:D:2188:MET:HE2	1:D:2266:ARG:HH21	1.62	0.65
1:D:1848:CYS:HB2	1:D:1868:MET:HE2	1.77	0.64
1:G:4345:ASN:O	1:G:4348:MET:HG3	1.97	0.64
1:E:3012:ILE:HG22	1:E:3013:GLN:N	2.12	0.64
1:E:3457:GLN:O	1:E:3461:GLN:HG3	1.96	0.64
1:E:3188:GLY:HA3	1:E:3191:PHE:CE2	2.32	0.64
1:F:3726:SER:HB2	1:F:3729:ALA:HB2	1.78	0.64
1:G:4360:TYR:CE2	1:G:4366:VAL:HG21	2.32	0.64
1:A:454:ARG:NH2	1:A:484:ASP:OD2	2.30	0.64
1:H:4979:LEU:HD12	1:H:4979:LEU:O	1.96	0.64
1:F:3928:GLN:HE22	1:H:5140:THR:HA	1.62	0.64
1:C:1431:GLY:O	1:C:1436:VAL:HG22	1.97	0.64
1:A:280:ASP:OD1	1:A:315:ARG:NH1	2.30	0.64
1:G:4221:MET:HE1	1:H:5202:SER:HB2	1.79	0.64
1:A:48:CYS:SG	1:A:68:MET:HE2	2.37	0.64
1:F:3624:THR:HG22	1:F:3627:GLU:N	2.04	0.64
1:E:3493:MET:HE1	1:E:3530:PRO:HD2	1.78	0.64
1:B:1027:LEU:HD23	1:B:1109:ILE:HB	1.80	0.64
1:C:1345:ASN:O	1:C:1348:MET:HB3	1.98	0.64
1:A:478:GLN:HB2	1:A:484:ASP:HB2	1.80	0.64
1:G:4302:ILE:HD12	1:G:4694:ASN:CB	2.28	0.64
1:F:3766:VAL:HG13	1:F:3813:ALA:HB1	1.78	0.64
1:F:3743:LEU:CD1	1:F:3761:LYS:HA	2.24	0.64
1:F:3732:GLU:HB2	1:F:3801:PHE:CE1	2.33	0.64
1:G:4341:ILE:HB	1:G:4392:LEU:HB2	1.78	0.64
1:A:221:SER:HB2	1:A:224:ASP:H	1.62	0.64
1:B:1054:ARG:HD2	6:B:7433:HOH:O	1.98	0.64
1:C:1363:ILE:O	1:C:1367:VAL:HG12	1.96	0.64
1:B:740:LYS:HE2	1:B:742:THR:HG22	1.78	0.64
1:G:4493:ARG:HD3	1:G:4526:ALA:O	1.98	0.64
1:F:3715:GLY:O	1:F:3717:GLU:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASN:HB2	6:A:6418:HOH:O	1.98	0.64
1:B:639:ILE:O	1:B:982:ARG:HD2	1.98	0.64
1:G:4379:LEU:HD12	1:G:4379:LEU:O	1.97	0.64
1:F:3752:ASP:CG	1:F:3754:ASN:H	2.00	0.63
1:E:3253:VAL:HG12	1:E:3257:LEU:HD23	1.80	0.63
1:G:4251:GLY:O	1:G:4255:ARG:HG3	1.98	0.63
1:B:971:LEU:O	1:B:975:ARG:HD2	1.98	0.63
1:D:2245:PRO:HD2	6:D:6587:HOH:O	1.98	0.63
1:F:3856:ILE:N	1:F:3856:ILE:HD13	2.12	0.63
1:F:3648:CYS:HB2	1:F:3668:MET:HE3	1.80	0.63
1:H:4923:ILE:O	1:H:4925:GLY:N	2.32	0.63
1:C:1661:GLN:O	1:C:1664:LEU:HB2	1.98	0.63
1:C:1531:GLU:N	1:C:1543:GLU:OE2	2.31	0.63
1:G:4409:ASN:C	1:G:4411:PRO:HD3	2.19	0.63
1:D:1905:ARG:CZ	1:D:2299:ARG:HH21	2.10	0.63
1:H:5109:GLN:O	1:H:5113:ILE:HG13	1.98	0.63
1:A:223:LYS:O	1:A:226:GLN:HB2	1.98	0.63
1:E:3041:ALA:HB2	1:E:3501:PHE:CE1	2.33	0.63
1:B:1103:LYS:HG3	1:B:1106:ASP:OD2	1.99	0.63
1:D:2141:ARG:HG2	1:D:2141:ARG:NH1	2.10	0.63
1:G:4243:ASN:CB	1:G:4667:GLY:HA2	2.28	0.63
1:B:871:GLU:HG2	1:B:892:ALA:HB3	1.79	0.63
1:F:3787:LYS:HB3	1:F:3792:LEU:HD12	1.81	0.63
1:C:1250:ILE:HD11	1:C:1268:MET:HE3	1.80	0.63
1:G:4322:LEU:O	1:G:4351:CYS:HB2	1.99	0.63
1:C:1715:ARG:HB3	1:C:1716:PRO:HD2	1.80	0.63
1:H:5275:ASP:OD2	1:H:5287:LEU:HD21	1.97	0.63
1:A:49:THR:HG22	1:A:365:ALA:HB2	1.80	0.63
1:A:113:THR:HG22	1:A:242:SER:CB	2.29	0.63
1:G:4591:ARG:NH1	1:G:4592:LYS:HD2	2.14	0.63
1:F:3941:ARG:NH2	1:H:5094:GLY:O	2.30	0.63
1:G:4410:LEU:O	1:G:4413:ALA:HB3	1.99	0.63
1:H:5311:LEU:HB3	1:H:5321:THR:HG23	1.81	0.63
1:A:181:SER:O	1:A:182:LEU:HD23	1.99	0.63
1:C:1382:LEU:HD21	1:C:1396:VAL:HG22	1.81	0.63
1:D:1850:ILE:HD11	1:D:1868:MET:HE3	1.81	0.62
1:E:3448:PRO:HB3	1:E:3469:PHE:CE1	2.34	0.62
1:A:188:GLY:HA3	1:A:191:PHE:CE1	2.34	0.62
1:A:160:TYR:HD2	1:A:163:ILE:CB	2.07	0.62
1:B:1091:LEU:O	1:B:1091:LEU:HD12	2.00	0.62
1:D:1855:ARG:HD2	1:D:1882:TYR:OH	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1685:VAL:O	1:C:1689:VAL:HG23	2.00	0.62
1:F:4104:LYS:HG3	1:F:4130:PRO:C	2.19	0.62
1:B:731:VAL:CG1	1:B:753:GLU:HB3	2.29	0.62
1:A:84:ALA:HB2	1:A:230:PHE:HZ	1.64	0.62
1:E:3113:THR:HG21	6:E:6225:HOH:O	1.99	0.62
1:D:1941:ILE:HA	1:D:1956:LEU:O	1.99	0.62
1:C:1273:MET:HE2	1:C:1286:THR:HG22	1.82	0.62
1:G:4257:VAL:HG23	1:G:4289:ASN:HB3	1.81	0.62
1:A:113:THR:HG22	1:A:242:SER:HB2	1.80	0.62
1:C:1326:SER:HB3	1:C:1329:ALA:HB3	1.82	0.62
1:C:1360:TYR:HE2	1:C:1366:VAL:HG11	1.62	0.62
1:B:740:LYS:HE2	1:B:742:THR:CG2	2.28	0.62
1:H:5092:ALA:HB1	3:H:5333:OXL:C2	2.29	0.62
1:A:134:LYS:O	1:A:196:VAL:HB	1.99	0.62
1:E:3068:MET:HE1	1:E:3071:ALA:CB	2.29	0.62
1:F:3723:ILE:HD13	1:F:3723:ILE:N	2.14	0.62
1:A:113:THR:HG21	1:A:242:SER:H	1.63	0.62
1:A:399:ARG:HD2	6:C:6758:HOH:O	1.99	0.62
1:B:999:ARG:HH12	1:D:1823:ASP:CB	2.11	0.62
1:G:4293:ALA:O	1:G:4296:SER:HB3	1.99	0.62
1:H:4905:ARG:HH22	1:H:5299:ARG:HD3	1.62	0.62
1:D:2281:TRP:CD1	1:D:2316:PRO:HD3	2.34	0.62
1:B:999:ARG:HH12	1:D:1823:ASP:HB2	1.65	0.62
1:F:3966:LYS:HG2	1:F:3966:LYS:O	1.99	0.62
1:E:3376:MET:CE	1:E:3376:MET:HA	2.27	0.62
1:D:1848:CYS:HB2	1:D:1868:MET:HE3	1.79	0.62
1:F:3752:ASP:OD1	1:F:3755:ILE:N	2.31	0.62
1:E:3014:THR:HG23	1:E:3015:GLN:HB2	1.82	0.62
1:C:1453:VAL:HG12	1:C:1457:LEU:HD22	1.82	0.62
1:D:1945:ASN:ND2	1:D:1961:LYS:NZ	2.48	0.62
1:E:3481:TRP:HB2	1:E:3516:PRO:HG3	1.80	0.62
1:G:4273:MET:HE3	1:G:4286:THR:HG21	1.80	0.62
1:E:3083:HIS:O	1:E:3087:ILE:HG13	2.00	0.62
1:C:1339:LEU:HD12	1:C:1340:LYS:N	2.15	0.62
1:E:3172:LYS:HE3	1:E:3183:GLN:HB2	1.81	0.61
1:C:1255:ARG:HD2	1:C:1282:TYR:OH	1.99	0.61
1:H:5275:ASP:HB3	1:H:5276:PRO:HD2	1.82	0.61
1:H:5281:TRP:CD1	1:H:5316:PRO:HD3	2.35	0.61
1:A:48:CYS:HB2	1:A:68:MET:HE2	1.81	0.61
1:F:3999:ARG:HH12	1:H:4823:ASP:HB2	1.65	0.61
1:B:866:ILE:O	1:B:887:ASP:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:GLN:O	1:A:442:ARG:HG2	2.01	0.61
1:B:1003:HIS:HB2	6:B:7042:HOH:O	1.99	0.61
1:C:1362:ASN:ND2	1:C:1365:LYS:HB2	2.16	0.61
1:G:4302:ILE:HD12	1:G:4694:ASN:HB2	1.82	0.61
1:G:4370:GLY:N	1:G:4384:VAL:O	2.28	0.61
1:F:3928:GLN:NE2	1:H:5140:THR:HB	2.15	0.61
1:F:3999:ARG:NH1	1:H:4823:ASP:HB2	2.15	0.61
1:G:4305:ARG:HD3	1:G:4699:ARG:CZ	2.31	0.61
1:C:1272:ARG:NE	1:C:1312:ASP:OD2	2.31	0.61
1:C:1317:GLU:OE1	1:C:1319:ARG:NH1	2.33	0.61
1:A:29:MET:CE	1:C:1510:LYS:HB3	2.31	0.61
1:A:237:ASP:OD1	1:A:460:ARG:NH1	2.31	0.61
1:G:4471:GLU:HA	1:G:4496:LEU:HB2	1.82	0.61
1:B:873:HIS:CE1	1:B:900:ILE:HG22	2.36	0.61
1:C:1280:HIS:NE2	1:C:1427:ASP:OD1	2.30	0.61
1:D:2090:MET:HE2	1:D:2092:ALA:HB2	1.81	0.61
1:C:1382:LEU:CD2	1:C:1396:VAL:HG22	2.31	0.61
1:A:510:VAL:HG12	1:A:512:THR:HG23	1.83	0.61
1:A:246:LYS:HG3	1:A:248:ALA:HB3	1.83	0.61
1:C:1532:SER:HB2	1:C:1543:GLU:OE1	2.01	0.61
1:G:4387:LYS:HG3	1:G:4392:LEU:HD11	1.82	0.61
1:C:1385:LYS:HB2	1:C:1393:VAL:O	2.01	0.61
1:E:3465:TYR:HB2	1:E:3468:ILE:HD12	1.83	0.61
1:H:5067:ILE:HD12	1:H:5088:GLY:HA3	1.83	0.60
1:D:1952:ASP:OD1	1:D:1954:ASN:N	2.33	0.60
1:D:2064:ILE:HD11	6:D:7414:HOH:O	2.01	0.60
1:B:1127:VAL:HG12	1:B:1128:PRO:N	2.16	0.60
1:C:1378:GLY:HA3	1:C:1498:ILE:HG13	1.81	0.60
1:B:714:LYS:NZ	1:B:717:GLU:OE2	2.35	0.60
1:A:456:HIS:CD2	1:A:456:HIS:H	2.18	0.60
1:D:1902:ILE:C	1:D:1903:LEU:HD23	2.22	0.60
1:G:4498:ILE:HD13	1:G:4498:ILE:H	1.67	0.60
1:B:731:VAL:HG11	1:B:753:GLU:HB3	1.82	0.60
1:D:1902:ILE:HG22	1:D:1903:LEU:HD21	1.82	0.60
1:G:4333:LEU:N	1:G:4333:LEU:HD23	2.15	0.60
1:F:3720:THR:HG22	1:F:3721:GLY:O	2.02	0.60
1:A:221:SER:HB2	1:A:224:ASP:CG	2.22	0.60
1:B:941:ARG:H	1:D:2128:GLN:NE2	1.99	0.60
1:B:617:LEU:O	1:B:621:MET:HG2	2.01	0.60
1:C:1493:ARG:NH1	1:C:1527:THR:O	2.35	0.60
1:D:2241:ALA:O	1:D:2244:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3367:GLY:HA3	6:E:7134:HOH:O	2.00	0.60
1:G:4725:ARG:HD3	1:H:5314:TRP:CE3	2.37	0.60
1:A:310:LYS:NZ	1:A:353:ASP:OD1	2.35	0.60
1:H:4945:ASN:HB3	1:H:4948:MET:CE	2.32	0.60
1:C:1362:ASN:HD22	1:C:1365:LYS:HD2	1.67	0.60
1:D:1914:LYS:NZ	1:D:2023:LYS:HD3	2.17	0.60
1:B:722:LEU:HA	1:B:804:SER:HB3	1.84	0.60
1:A:141:ILE:CG2	1:A:158:LEU:HD22	2.30	0.60
1:A:292:ALA:HB1	3:A:533:OXL:C2	2.32	0.60
1:H:4923:ILE:HD12	1:H:4931:VAL:HG23	1.83	0.60
1:G:4348:MET:HG2	1:G:4357:TRP:CZ2	2.37	0.60
1:E:3411:MET:SD	1:F:4126:VAL:HG23	2.41	0.60
1:D:1873:MET:HE2	1:D:1886:THR:HG22	1.82	0.60
1:A:172:LYS:HE3	1:A:197:GLU:CD	2.22	0.60
1:G:4344:ASP:OD2	1:G:4346:ALA:HB3	2.00	0.60
1:A:300:ILE:HB	1:A:301:PRO:HD2	1.84	0.60
1:D:2044:ILE:HG22	1:D:2082:ILE:CD1	2.27	0.59
1:E:3376:MET:HE2	1:E:3380:ILE:HG13	1.83	0.59
1:G:4385:LYS:HB2	1:G:4393:VAL:O	2.02	0.59
1:G:4322:LEU:HA	1:G:4404:SER:HB3	1.84	0.59
1:G:4248:CYS:HB2	1:G:4268:MET:HE2	1.84	0.59
1:H:5130:LEU:HD23	1:H:5143:GLU:HB3	1.84	0.59
1:C:1472:ASN:HD21	1:C:1475:GLY:H	1.45	0.59
1:A:48:CYS:HB2	1:A:68:MET:CE	2.33	0.59
1:G:4704:LYS:HE2	1:G:4730:PRO:O	2.02	0.59
1:C:1459:GLU:O	1:C:1462:LYS:HG2	2.03	0.59
1:C:1714:TRP:HD1	1:C:1715:ARG:HE	1.49	0.59
1:A:113:THR:CG2	1:A:242:SER:HB2	2.32	0.59
1:B:1031:THR:HG21	1:B:1034:GLY:HA2	1.84	0.59
1:G:4388:GLY:HA3	1:G:4391:PHE:CZ	2.37	0.59
1:H:4847:ILE:HG21	1:H:5159:MET:HE2	1.84	0.59
1:A:49:THR:OG1	1:A:72:ARG:HD3	2.02	0.59
1:E:3426:ALA:HA	1:E:3447:ALA:HB1	1.84	0.59
1:G:4633:SER:OG	1:G:4635:ARG:HG3	2.02	0.59
1:E:3237:ASP:OD1	1:E:3460:ARG:HD2	2.03	0.59
1:A:130:GLU:HA	1:A:202:LEU:O	2.02	0.59
1:B:934:ILE:HG23	1:B:967:GLY:HA2	1.85	0.59
1:D:2141:ARG:HD3	6:D:6362:HOH:O	2.02	0.59
1:D:2252:VAL:HG21	1:D:2292:ALA:HB2	1.83	0.59
1:E:3113:THR:CG2	1:E:3242:SER:H	2.14	0.59
1:B:720:THR:HA	1:B:758:LEU:HD23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1714:TRP:CE3	1:D:2325:ARG:HD3	2.38	0.59
1:C:1305:ARG:HE	1:C:1699:ARG:NH2	2.01	0.59
1:C:1366:VAL:HG22	1:C:1413:ALA:HB1	1.84	0.59
1:C:1599:ARG:NH1	1:D:1823:ASP:HB3	2.17	0.59
1:C:1509:GLN:HG2	1:C:1513:ILE:HD12	1.84	0.59
1:B:1114:TRP:CD1	1:B:1115:ARG:HG3	2.38	0.59
1:B:1099:ARG:HB3	1:B:1101:PHE:CE1	2.37	0.59
1:E:3315:ARG:NH1	1:G:4230:CYS:O	2.29	0.59
1:A:506:ASP:O	1:A:529:VAL:HG23	2.03	0.58
1:E:3269:LYS:HE2	1:E:3271:GLU:OE2	2.03	0.58
1:C:1313:THR:CG2	1:C:1442:SER:H	2.16	0.58
1:C:1442:SER:CA	1:C:1469:LYS:HD3	2.32	0.58
1:G:4322:LEU:C	1:G:4351:CYS:HB2	2.23	0.58
1:A:147:TYR:HA	1:A:150:LYS:HB2	1.86	0.58
1:F:4075:ASP:CB	1:F:4087:LEU:HD21	2.33	0.58
1:D:1817:LEU:O	1:D:1820:ALA:HB3	2.03	0.58
1:B:844:ILE:HG13	1:B:868:SER:HB3	1.84	0.58
1:C:1727:VAL:HG13	1:C:1728:PRO:HD2	1.85	0.58
1:H:5015:VAL:HG12	1:H:5017:LEU:H	1.69	0.58
1:D:2278:GLN:HB2	1:D:2284:ASP:HB2	1.85	0.58
1:C:1360:TYR:HE2	1:C:1366:VAL:CG1	2.15	0.58
1:A:238:MET:CE	1:A:464:LEU:HD22	2.33	0.58
1:D:1910:ALA:CB	1:D:2038:MET:HG3	2.34	0.58
1:A:144:ASP:HB3	1:A:147:TYR:CD1	2.38	0.58
1:H:5281:TRP:CG	1:H:5316:PRO:HD3	2.38	0.58
1:A:451:ALA:HB2	1:A:468:ILE:HG23	1.85	0.58
1:B:1125:ARG:HD2	6:B:7774:HOH:O	2.03	0.58
1:G:4322:LEU:HD23	1:G:4404:SER:HB2	1.85	0.58
1:A:173:VAL:HG13	1:A:210:LEU:HD11	1.85	0.58
1:E:3440:VAL:HG12	1:E:3449:ILE:CD1	2.33	0.58
1:H:5096:LEU:O	1:H:5100:ILE:HG12	2.04	0.58
1:F:4032:GLU:OE1	1:F:4054:ARG:N	2.30	0.58
1:E:3142:THR:HG22	1:E:3143:LEU:N	2.18	0.58
1:F:3731:VAL:HG12	1:F:3802:LEU:HB3	1.85	0.58
1:F:3859:GLU:O	1:F:3862:LYS:HG3	2.04	0.58
1:E:3475:ASP:HB3	1:E:3476:PRO:HD2	1.86	0.58
1:H:4873:MET:HE3	1:H:4887:ILE:HD13	1.86	0.57
1:C:1313:THR:HG21	6:C:6158:HOH:O	2.03	0.57
1:A:439:GLN:HA	1:A:439:GLN:OE1	2.04	0.57
1:E:3407:LEU:HG	1:F:4126:VAL:HG11	1.86	0.57
1:C:1484:GLU:HG3	6:C:6559:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2145:SER:HB2	6:D:6669:HOH:O	2.04	0.57
1:G:4342:THR:HG21	1:G:4347:TYR:CD2	2.39	0.57
1:D:1887:ILE:N	1:D:1887:ILE:HD13	2.19	0.57
1:G:4391:PHE:HE1	1:G:4393:VAL:HG23	1.68	0.57
1:H:5314:TRP:CD1	1:H:5315:ARG:HG3	2.39	0.57
1:H:4851:GLY:O	1:H:4855:ARG:HG2	2.04	0.57
1:F:3660:LEU:HD13	1:F:3690:VAL:HA	1.86	0.57
1:C:1492:ALA:HB1	3:C:1733:OXL:C2	2.34	0.57
1:G:4389:PRO:HD2	1:G:4391:PHE:HE2	1.65	0.57
1:C:1376:ASP:N	1:C:1407:GLY:O	2.34	0.57
1:G:4593:LEU:HG	1:G:4597:LEU:HD22	1.85	0.57
1:F:3650:ILE:CG1	1:F:3673:MET:HE1	2.34	0.57
1:B:1103:LYS:N	1:B:1106:ASP:OD2	2.30	0.57
1:E:3080:HIS:HE1	1:E:3227:ASP:OD1	1.86	0.57
1:B:745:ASN:ND2	1:B:757:TRP:HE1	2.01	0.57
1:G:4409:ASN:O	1:G:4410:LEU:HD12	2.05	0.57
1:B:976:MET:HE3	1:B:980:ILE:CG1	2.35	0.57
1:A:503:LYS:NZ	6:A:7773:HOH:O	2.36	0.57
1:H:4843:ASN:HB3	1:H:5267:GLY:N	2.19	0.57
1:F:3838:MET:HA	1:F:3864:ILE:HG23	1.85	0.57
1:D:2190:HIS:HD2	6:D:6458:HOH:O	1.88	0.57
1:B:928:GLN:HE22	1:D:2141:ARG:HH11	1.52	0.57
1:C:1322:LEU:CD1	1:C:1349:GLU:HG2	2.30	0.57
1:G:4321:GLY:HA3	1:G:4357:TRP:HE3	1.69	0.57
1:A:241:ALA:O	1:A:244:ILE:HG12	2.03	0.57
1:E:3355:ALA:O	1:E:3466:ARG:NH1	2.38	0.57
1:A:122:LEU:HB2	1:A:149:GLU:HA	1.85	0.57
1:G:4384:VAL:HA	1:G:4394:THR:HG22	1.85	0.57
1:G:4322:LEU:HD21	1:G:4327:GLY:HA2	1.84	0.57
1:G:4250:ILE:CG1	1:G:4273:MET:HE1	2.35	0.57
1:H:4920:THR:O	1:H:5005:LYS:HA	2.04	0.57
1:A:77:HIS:CD2	5:A:535:ATP:H2'	2.39	0.57
1:D:1877:HIS:CE1	5:D:2335:ATP:H2'	2.40	0.57
1:A:330:LEU:HD22	1:A:377:GLN:HG3	1.86	0.57
1:F:3623:ASP:N	1:F:3623:ASP:OD1	2.36	0.57
1:G:4369:VAL:HA	1:G:4384:VAL:CG1	2.35	0.57
1:G:4250:ILE:HD11	1:G:4268:MET:HE3	1.85	0.57
1:B:774:TYR:CE2	1:B:811:PRO:HG3	2.40	0.57
1:A:372:GLU:HA	1:A:375:ARG:HD2	1.87	0.57
1:C:1633:SER:OG	1:C:1635:ARG:HG3	2.04	0.57
1:F:3726:SER:HB3	1:F:3729:ALA:CB	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3802:LEU:HD12	1:F:3803:GLY:H	1.70	0.56
1:E:3167:VAL:HG22	1:E:3171:SER:HB2	1.86	0.56
1:E:3259:GLU:O	1:E:3262:LYS:HG2	2.05	0.56
1:D:2045:ARG:C	1:D:2046:LYS:HG3	2.25	0.56
1:A:163:ILE:HG23	1:A:163:ILE:O	2.06	0.56
1:D:2295:VAL:CG1	1:D:2299:ARG:HD2	2.35	0.56
1:F:3748:MET:HG3	1:F:3757:TRP:CE2	2.39	0.56
1:C:1366:VAL:CG2	1:C:1413:ALA:HB1	2.35	0.56
1:C:1373:VAL:N	1:C:1382:LEU:O	2.33	0.56
1:C:1242:ARG:HB2	1:C:1578:HIS:CE1	2.40	0.56
1:G:4625:ALA:HB1	1:G:4702:PHE:HB3	1.87	0.56
1:C:1343:LEU:HD23	1:C:1361:LYS:CD	2.35	0.56
1:A:86:THR:HG22	1:A:87:ILE:N	2.19	0.56
1:B:624:THR:HB	1:D:2196:GLU:CD	2.25	0.56
1:B:706:PRO:O	1:B:1063:HIS:HE1	1.88	0.56
1:E:3382:ARG:HH11	1:E:3382:ARG:CG	2.19	0.56
1:D:2008:VAL:HG12	1:D:2010:LEU:CD2	2.36	0.56
1:D:1842:ARG:NH1	1:D:1846:ILE:HG13	2.19	0.56
1:C:1611:MET:SD	1:D:2326:VAL:HG23	2.46	0.56
1:B:739:LEU:HD12	1:B:754:ASN:C	2.26	0.56
1:E:3390:HIS:HD2	6:E:6377:HOH:O	1.87	0.56
1:F:3872:ASN:HD22	1:F:3875:GLY:H	1.54	0.56
1:A:407:LEU:HD21	1:B:1107:VAL:HG21	1.87	0.56
1:H:5020:VAL:HG12	1:H:5021:SER:O	2.05	0.56
1:G:4276:SER:HB3	1:G:4319:ARG:NE	2.16	0.56
1:G:4729:VAL:HG12	1:G:4730:PRO:HD2	1.88	0.56
1:F:3787:LYS:HB3	1:F:3792:LEU:CD1	2.36	0.56
1:C:1261:LYS:HG3	1:C:1293:ALA:HB1	1.87	0.56
1:A:133:LEU:N	1:A:133:LEU:HD13	2.20	0.56
1:G:4665:TYR:CB	1:G:4668:ILE:HD12	2.22	0.56
1:B:823:LYS:NZ	6:B:6941:HOH:O	2.38	0.56
1:D:2135:LYS:O	1:D:2169:TYR:HE2	1.89	0.56
1:D:1819:ALA:HA	1:D:1831:ARG:HD2	1.87	0.56
1:F:3638:PRO:HG3	1:F:3983:GLU:CD	2.26	0.56
1:F:3928:GLN:HE21	1:H:5140:THR:HB	1.69	0.56
1:A:50:ILE:HD11	1:A:68:MET:HE1	1.88	0.56
1:A:511:LEU:HB3	1:A:521:THR:CG2	2.36	0.56
1:C:1318:ILE:CG2	1:C:1408:VAL:HB	2.36	0.56
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.41	0.56
1:E:3163:ILE:HG12	1:E:3163:ILE:O	2.04	0.55
1:D:1958:LEU:HD22	1:D:2008:VAL:HG21	1.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1363:ILE:HA	1:C:1366:VAL:HG12	1.88	0.55
1:A:48:CYS:CB	1:A:68:MET:HE2	2.36	0.55
1:G:4320:THR:O	1:G:4405:LYS:HA	2.05	0.55
1:D:1815:GLN:CG	1:D:1839:ILE:HG23	2.36	0.55
1:B:1054:ARG:HG2	1:B:1073:CYS:HB3	1.89	0.55
1:C:1374:TYR:O	1:C:1408:VAL:HA	2.05	0.55
1:C:1452:GLU:O	1:C:1455:LYS:HB3	2.06	0.55
1:D:1954:ASN:O	1:D:1955:ILE:HG13	2.06	0.55
1:A:411:MET:HE1	1:A:522:ASN:O	2.07	0.55
1:G:4333:LEU:C	1:G:4334:LYS:HG2	2.26	0.55
1:C:1360:TYR:HD2	1:C:1363:ILE:HB	1.71	0.55
1:B:804:SER:O	1:B:806:LYS:HD3	2.06	0.55
1:G:4275:PHE:HE2	1:G:4280:HIS:CD2	2.24	0.55
1:C:1345:ASN:O	1:C:1347:TYR:N	2.39	0.55
1:A:123:ILE:HD11	1:A:202:LEU:CD2	2.37	0.55
1:E:3343:GLU:O	1:E:3347:VAL:HG23	2.07	0.55
1:A:108:ALA:HB2	1:A:460:ARG:HB3	1.89	0.55
1:B:934:ILE:HG22	1:B:935:LYS:HD3	1.88	0.55
1:C:1675:ASP:HB3	1:C:1676:PRO:HD2	1.87	0.55
1:G:4444:ILE:HD12	1:G:4449:ASP:HB2	1.88	0.55
1:G:4640:VAL:CG1	1:G:4649:ILE:HD13	2.37	0.55
1:F:3679:THR:OG1	1:F:3680:HIS:N	2.38	0.55
1:B:928:GLN:NE2	1:D:2141:ARG:HG2	2.21	0.55
1:E:3160:TYR:CE2	1:E:3162:ASN:HB3	2.42	0.55
1:B:716:PRO:HG2	1:B:843:PHE:CD2	2.41	0.55
1:A:14:THR:HG23	1:A:15:GLN:N	2.22	0.55
1:B:731:VAL:O	1:B:801:PHE:HA	2.07	0.55
1:A:416:VAL:HG22	1:A:445:PRO:HG3	1.89	0.55
1:E:3333:MET:HA	1:E:3336:LYS:O	2.07	0.55
1:E:3339:PRO:HG3	1:E:3376:MET:HG2	1.89	0.55
1:A:209:ASN:C	1:A:210:LEU:HD13	2.27	0.55
1:B:1114:TRP:C	1:B:1115:ARG:HG3	2.26	0.55
1:F:3643:ASN:HB3	1:F:4067:GLY:HA2	1.89	0.55
1:A:328:GLN:NE2	1:C:1540:THR:HB	2.22	0.55
1:A:131:VAL:HG11	1:A:202:LEU:HD23	1.89	0.55
1:C:1681:TRP:CH2	1:C:1716:PRO:HA	2.42	0.55
1:F:3825:ILE:O	1:F:3829:LYS:HG2	2.06	0.55
1:D:1934:LYS:HG3	6:D:7630:HOH:O	2.07	0.55
1:F:3971:LEU:O	1:F:3975:ARG:HG3	2.07	0.55
1:E:3048:CYS:HB2	1:E:3068:MET:CE	2.28	0.55
1:C:1244:THR:N	1:C:1585:GLU:OE2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1532:SER:OG	1:C:1540:THR:HG23	2.07	0.55
1:F:3890:MET:HE1	1:F:3892:ALA:HB2	1.88	0.55
1:G:4729:VAL:CG1	1:G:4730:PRO:HD2	2.36	0.55
1:G:4217:LEU:O	1:G:4221:MET:HG2	2.06	0.55
1:H:4848:CYS:HB2	1:H:4868:MET:HE2	1.89	0.54
1:F:3757:TRP:C	1:F:3758:LEU:HD23	2.27	0.54
1:H:4960:TYR:OH	1:H:5016:ASP:HB2	2.07	0.54
1:H:4847:ILE:HG21	1:H:5159:MET:HE3	1.89	0.54
1:B:1080:ALA:HB3	1:B:1083:GLU:CD	2.27	0.54
1:A:333:MET:CE	1:A:373:ALA:HA	2.37	0.54
1:A:295:ASP:O	1:A:298:ILE:HG22	2.06	0.54
1:C:1650:ILE:HD13	1:C:1650:ILE:N	2.23	0.54
1:B:654:SER:O	1:B:660:LEU:HD13	2.07	0.54
1:H:5239:GLN:OE1	1:H:5242:ARG:HD3	2.08	0.54
1:D:2116:CYS:HB3	1:D:2121:LYS:O	2.07	0.54
1:E:3122:LEU:HB2	1:E:3149:GLU:HA	1.89	0.54
1:B:1115:ARG:HB3	1:B:1116:PRO:CD	2.37	0.54
1:E:3324:ILE:HG12	1:E:3357:CYS:HB2	1.89	0.54
1:C:1533:MET:HA	1:C:1536:LYS:O	2.07	0.54
1:A:514:TRP:H	1:A:522:ASN:ND2	1.96	0.54
1:B:656:SER:O	1:B:660:LEU:HB2	2.07	0.54
1:B:687:ILE:HD13	1:B:709:VAL:HG11	1.89	0.54
1:B:720:THR:HG22	1:B:758:LEU:HD23	1.89	0.54
1:C:1431:GLY:HA2	1:C:1434:GLN:HB2	1.90	0.54
1:A:29:MET:HE2	1:C:1510:LYS:HB3	1.89	0.54
1:A:133:LEU:N	1:A:200:GLY:O	2.38	0.54
1:A:333:MET:HG2	1:A:336:LYS:O	2.08	0.54
1:D:2083:LEU:O	1:D:2121:LYS:NZ	2.39	0.54
1:D:2054:ARG:NH2	1:D:2062:LYS:O	2.39	0.54
1:D:2275:ASP:HB2	1:D:2287:LEU:HD21	1.89	0.54
1:F:4066:ARG:HG3	1:F:4067:GLY:N	2.22	0.54
1:E:3222:GLU:HG2	1:E:3223:LYS:N	2.22	0.54
1:A:252:GLU:O	1:A:255:LYS:N	2.40	0.54
1:G:4437:ASP:OD1	1:G:4660:ARG:HD2	2.08	0.54
1:F:3928:GLN:NE2	1:H:5141:ARG:N	2.51	0.54
1:A:221:SER:CB	1:A:224:ASP:H	2.20	0.54
1:A:453:THR:CG2	1:A:459:ALA:HB2	2.37	0.54
1:C:1421:SER:HB2	1:C:1424:ASP:H	1.72	0.54
1:F:3788:GLY:N	1:F:3791:PHE:O	2.28	0.54
1:C:1341:ILE:HB	1:C:1392:LEU:HB2	1.90	0.54
1:E:3382:ARG:NH1	6:E:6645:HOH:O	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3160:TYR:HB3	1:E:3163:ILE:CG2	2.37	0.54
1:D:2093:ARG:HD3	1:D:2126:ALA:O	2.07	0.54
1:G:4477:ARG:NH2	1:G:4478:ARG:NH1	2.55	0.54
1:E:3123:ILE:HD13	1:E:3151:CYS:HB2	1.88	0.54
1:G:4339:LEU:CD1	1:G:4354:ASN:HA	2.37	0.54
1:B:1104:LYS:HA	1:B:1129:VAL:HG12	1.89	0.54
1:A:123:ILE:HD11	1:A:202:LEU:HG	1.90	0.54
1:B:619:ALA:HA	1:B:631:ARG:HD2	1.90	0.54
1:C:1287:ILE:O	1:C:1290:VAL:HB	2.08	0.53
1:G:4391:PHE:CE1	1:G:4393:VAL:HG23	2.43	0.53
1:E:3301:PRO:HG2	1:E:3304:LYS:HD2	1.89	0.53
1:H:4900:ASP:OD2	1:H:4903:LEU:HG	2.08	0.53
1:G:4300:ASP:OD2	1:G:4303:LEU:HB2	2.07	0.53
1:H:4952:ASP:OD1	1:H:4954:ASN:N	2.32	0.53
1:C:1671:VAL:CG1	1:C:1691:LEU:HD21	2.37	0.53
1:A:409:GLU:O	1:A:413:MET:HG3	2.07	0.53
1:F:3824:ASP:O	1:F:3827:ASP:HB2	2.08	0.53
1:H:5073:HIS:O	1:H:5077:ARG:HG3	2.08	0.53
1:G:4669:PHE:CZ	1:G:4699:ARG:HD2	2.43	0.53
1:B:1087:LEU:C	1:B:1087:LEU:HD23	2.29	0.53
1:C:1430:PHE:O	1:C:1434:GLN:HG2	2.09	0.53
1:B:740:LYS:HE3	1:B:791:PHE:HB2	1.90	0.53
1:B:745:ASN:HD22	1:B:745:ASN:N	2.07	0.53
1:B:825:ILE:HG22	1:B:829:LYS:NZ	2.23	0.53
1:C:1213:GLN:OE1	1:C:1213:GLN:HA	2.08	0.53
1:A:203:GLY:HA3	1:A:206:LYS:HE2	1.91	0.53
1:H:4883:HIS:O	1:H:4887:ILE:HG12	2.09	0.53
1:A:268:SER:HB2	1:A:289:ILE:CD1	2.39	0.53
1:C:1345:ASN:C	1:C:1347:TYR:H	2.12	0.53
1:C:1255:ARG:NH2	1:C:1282:TYR:O	2.40	0.53
1:H:5275:ASP:HB3	1:H:5276:PRO:CD	2.38	0.53
1:A:310:LYS:NZ	1:C:1549:ASN:HD21	2.05	0.53
1:A:141:ILE:HA	1:A:156:LEU:O	2.08	0.53
1:F:3650:ILE:HG13	1:F:3673:MET:HE1	1.89	0.53
1:C:1715:ARG:HB3	1:C:1716:PRO:CD	2.37	0.53
1:A:172:LYS:HE3	1:A:197:GLU:OE2	2.08	0.53
1:B:748:MET:HB2	1:B:757:TRP:CE2	2.44	0.53
1:C:1335:LYS:HG3	1:C:1336:GLY:N	2.24	0.53
1:C:1526:ALA:HB1	1:C:1559:MET:CE	2.39	0.53
1:E:3068:MET:CE	1:E:3071:ALA:HB2	2.37	0.53
1:C:1706:ASP:O	1:C:1728:PRO:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1421:SER:N	1:C:1424:ASP:HB2	2.23	0.53
1:H:5040:PHE:CE2	1:H:5159:MET:HE1	2.43	0.53
1:C:1255:ARG:HH22	1:C:1285:GLU:HB3	1.72	0.53
1:F:3787:LYS:HA	1:F:3792:LEU:HD12	1.90	0.53
1:C:1378:GLY:CA	1:C:1498:ILE:HG13	2.39	0.53
1:H:5242:ARG:NH2	6:H:7298:HOH:O	2.31	0.53
1:D:2320:PHE:CE2	1:D:2322:ASN:HB3	2.44	0.53
1:E:3017:LEU:O	1:E:3020:ALA:HB3	2.07	0.53
1:H:5133:MET:HE1	1:H:5176:MET:HG2	1.91	0.53
1:B:703:LEU:CG	1:B:1099:ARG:HH21	2.21	0.53
1:H:5015:VAL:CG1	1:H:5017:LEU:HG	2.39	0.53
1:C:1347:TYR:HE2	1:C:1355:ILE:CD1	2.21	0.53
1:H:4931:VAL:HG11	1:H:4953:GLU:OE1	2.08	0.53
1:C:1383:GLN:HG2	1:C:1385:LYS:HE2	1.91	0.53
1:C:1650:ILE:CD1	1:C:1669:PHE:HB2	2.38	0.53
1:E:3506:ASP:O	1:E:3528:PRO:HA	2.09	0.53
1:C:1593:LEU:CD1	1:C:1597:LEU:HD22	2.39	0.53
1:A:162:ASN:O	1:A:164:CYS:N	2.42	0.53
1:B:654:SER:HA	1:B:659:THR:HG21	1.91	0.53
1:E:3115:GLY:O	1:E:3117:GLU:N	2.41	0.53
1:E:3495:VAL:O	1:E:3498:ALA:HB3	2.09	0.53
1:E:3068:MET:HE2	1:E:3071:ALA:HA	1.91	0.53
1:G:4257:VAL:CG2	1:G:4289:ASN:HB3	2.39	0.53
1:F:3752:ASP:OD2	1:F:3754:ASN:HB2	2.09	0.53
1:A:487:LEU:C	1:A:487:LEU:HD23	2.29	0.53
1:D:2281:TRP:CH2	1:D:2316:PRO:HA	2.44	0.53
1:F:3717:GLU:OE2	1:F:3719:ARG:NH2	2.40	0.53
1:B:941:ARG:H	1:D:2128:GLN:HE21	1.57	0.53
1:A:141:ILE:N	1:A:192:LEU:O	2.33	0.53
1:G:4319:ARG:O	1:G:4359:ASP:HB2	2.09	0.53
1:H:5327:VAL:CG1	1:H:5328:PRO:HD2	2.36	0.53
1:A:290:MET:HE2	1:A:292:ALA:HB2	1.91	0.53
1:G:4591:ARG:O	1:G:4595:GLU:HG3	2.09	0.53
1:D:2083:LEU:HD21	1:D:2119:ALA:CB	2.39	0.53
1:B:648:CYS:CB	1:B:668:MET:HE3	2.30	0.52
1:G:4321:GLY:N	1:G:4357:TRP:O	2.42	0.52
1:E:3168:ASP:O	1:E:3171:SER:HB2	2.09	0.52
1:E:3054:SER:HA	1:E:3059:THR:HG21	1.92	0.52
1:H:5038:MET:CE	1:H:5264:LEU:HD22	2.39	0.52
1:A:322:PRO:HG3	1:A:465:TYR:CE2	2.43	0.52
1:F:3634:ILE:HG23	6:F:6961:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3260:LYS:O	1:E:3260:LYS:HG3	2.08	0.52
1:D:2269:PHE:CD1	1:D:2269:PHE:N	2.76	0.52
1:C:1477:ARG:NH2	1:C:1478:ARG:NH1	2.46	0.52
1:D:2122:PRO:HG3	1:D:2265:TYR:CE2	2.44	0.52
1:F:3758:LEU:HD23	1:F:3758:LEU:N	2.24	0.52
1:A:454:ARG:HG2	1:A:473:CYS:HB3	1.91	0.52
1:E:3433:SER:OG	1:E:3435:ARG:HB3	2.10	0.52
1:E:3440:VAL:HG12	1:E:3449:ILE:HD11	1.91	0.52
1:C:1539:PRO:HD2	6:C:7859:HOH:O	2.08	0.52
1:F:3665:LYS:HE2	1:F:3697:PHE:HE2	1.75	0.52
1:A:191:PHE:CD2	1:A:192:LEU:N	2.78	0.52
1:E:3160:TYR:HB3	1:E:3163:ILE:HG22	1.90	0.52
1:A:328:GLN:NE2	1:C:1541:ARG:N	2.49	0.52
1:F:3742:THR:N	1:F:3756:LEU:O	2.35	0.52
1:A:173:VAL:N	1:A:182:LEU:O	2.30	0.52
1:G:4255:ARG:NE	1:G:4282:TYR:CZ	2.78	0.52
1:G:4443:PHE:O	1:G:4445:ARG:HG3	2.09	0.52
1:E:3335:LYS:HE3	6:E:6947:HOH:O	2.08	0.52
1:A:27:GLU:O	1:A:31:ARG:HG3	2.09	0.52
1:H:5046:LYS:O	1:H:5049:ASP:HB2	2.09	0.52
1:G:4408:VAL:CG1	1:G:4410:LEU:HD11	2.33	0.52
1:F:3731:VAL:O	1:F:3801:PHE:HA	2.09	0.52
1:F:3893:ARG:HA	1:F:3896:LEU:HB3	1.91	0.52
1:D:1847:ILE:HG12	1:D:1870:VAL:HB	1.90	0.52
1:E:3328:GLN:HE22	1:G:4540:THR:HA	1.74	0.52
1:C:1372:LYS:HA	1:C:1382:LEU:O	2.10	0.52
1:A:456:HIS:CD2	1:A:456:HIS:N	2.78	0.52
1:H:4873:MET:HE3	1:H:4886:THR:HG22	1.92	0.52
1:C:1343:LEU:HD23	1:C:1361:LYS:HD2	1.91	0.52
1:G:4363:ILE:HG23	1:G:4364:CYS:N	2.25	0.52
1:H:5226:ALA:HA	1:H:5247:ALA:HB1	1.92	0.52
1:A:89:ASN:N	1:A:89:ASN:HD22	2.08	0.52
1:E:3209:ASN:O	1:E:3211:PRO:HD3	2.10	0.52
1:A:525:ARG:HB2	1:A:525:ARG:HH11	1.75	0.52
1:B:650:ILE:HD11	1:B:668:MET:CE	2.40	0.52
1:A:50:ILE:HD13	1:A:50:ILE:N	2.25	0.52
1:D:1824:THR:HG22	1:D:1827:GLU:HB3	1.90	0.52
1:C:1687:LEU:O	1:C:1690:ASN:HB2	2.09	0.52
1:C:1681:TRP:CZ2	1:C:1716:PRO:HA	2.45	0.52
1:C:1352:ASP:OD1	1:C:1354:ASN:N	2.29	0.52
1:B:1024:ALA:HA	1:B:1107:VAL:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1860:LEU:HB3	1:D:1893:ALA:CB	2.40	0.52
1:B:838:MET:SD	1:B:1064:LEU:HD21	2.50	0.52
1:A:181:SER:O	1:A:197:GLU:HB2	2.09	0.51
1:H:5314:TRP:O	1:H:5315:ARG:HG2	2.10	0.51
1:G:4344:ASP:O	1:G:4346:ALA:N	2.43	0.51
1:B:739:LEU:HD12	1:B:754:ASN:O	2.10	0.51
1:E:3073:MET:CE	1:E:3109:VAL:HG13	2.40	0.51
1:G:4336:GLY:HA2	1:G:4395:GLU:CD	2.31	0.51
1:G:4248:CYS:HB2	1:G:4268:MET:HE3	1.92	0.51
1:H:4851:GLY:HA3	1:H:5165:ALA:O	2.10	0.51
1:F:3717:GLU:CD	1:F:3719:ARG:HE	2.13	0.51
1:E:3042:ARG:CZ	1:E:3046:ILE:HD12	2.40	0.51
1:B:924:ILE:HG12	1:B:957:CYS:HB2	1.91	0.51
1:D:1911:LEU:HD23	1:D:1911:LEU:C	2.31	0.51
1:D:2047:ALA:HB2	1:D:2081:GLU:HG3	1.91	0.51
1:G:4276:SER:OG	1:G:4317:GLU:OE2	2.29	0.51
1:B:720:THR:O	1:B:805:LYS:HA	2.11	0.51
1:B:999:ARG:NH1	1:D:1823:ASP:HB2	2.25	0.51
1:F:3675:PHE:CZ	1:F:3683:HIS:CD2	2.99	0.51
1:C:1522:PRO:HA	1:C:1556:ASP:OD2	2.10	0.51
1:B:658:GLU:HG2	6:B:7821:HOH:O	2.11	0.51
1:G:4571:LEU:O	1:G:4575:ARG:HG3	2.10	0.51
1:A:283:LEU:HD22	1:A:283:LEU:O	2.11	0.51
1:B:1028:ILE:HG13	1:B:1108:VAL:HG11	1.93	0.51
1:D:1945:ASN:HD21	1:D:1961:LYS:HZ3	1.55	0.51
1:A:293:ARG:HD3	1:A:326:ALA:O	2.09	0.51
1:F:3889:ILE:HG22	1:F:3890:MET:N	2.26	0.51
1:A:210:LEU:HB3	1:A:213:ALA:CB	2.41	0.51
1:F:3674:ASN:OD1	1:F:3676:SER:HB2	2.11	0.51
1:F:3774:TYR:HB3	1:F:3778:GLY:HA2	1.92	0.51
1:B:969:TYR:HB3	1:B:972:GLU:HB2	1.92	0.51
1:G:4503:GLU:N	1:G:4503:GLU:OE1	2.39	0.51
1:E:3456:HIS:H	1:E:3456:HIS:CD2	2.28	0.51
1:C:1639:GLN:OE1	1:C:1642:ARG:HD3	2.10	0.51
1:E:3162:ASN:ND2	1:E:3165:LYS:HD3	2.20	0.51
1:E:3191:PHE:CE1	1:E:3193:VAL:HG23	2.32	0.51
1:G:4305:ARG:NH2	1:G:4663:HIS:CE1	2.77	0.51
1:E:3341:ARG:N	1:G:4528:GLN:NE2	2.56	0.51
1:E:3509:ILE:HD12	1:E:3526:VAL:HG23	1.90	0.51
1:F:3717:GLU:OE2	1:F:3719:ARG:NE	2.43	0.51
1:F:3764:CYS:SG	1:F:3792:LEU:HD13	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ALA:HB1	1:A:468:ILE:HD13	1.92	0.51
1:G:4305:ARG:HH22	1:G:4663:HIS:CE1	2.22	0.51
1:E:3221:SER:O	1:E:3224:ASP:HB2	2.09	0.51
1:B:1065:TYR:HB2	1:B:1068:ILE:HD12	1.93	0.51
1:B:703:LEU:HG	1:B:1099:ARG:HH21	1.75	0.51
1:C:1686:ASP:O	1:C:1690:ASN:ND2	2.44	0.51
1:C:1427:ASP:O	1:C:1430:PHE:HB3	2.11	0.51
1:D:1952:ASP:OD1	1:D:1955:ILE:N	2.40	0.51
1:D:1940:LYS:HB3	1:D:1955:ILE:HG12	1.93	0.51
1:A:245:ARG:HG2	1:A:274:GLU:HB3	1.93	0.51
1:B:949:ASN:HD21	1:D:2110:LYS:HZ1	1.59	0.51
1:A:411:MET:HG2	1:A:521:THR:O	2.11	0.51
1:E:3456:HIS:CD2	1:E:3456:HIS:N	2.79	0.51
1:F:4057:GLN:O	1:F:4061:GLN:HG3	2.11	0.51
1:E:3230:PHE:CE1	1:E:3234:GLN:HG3	2.46	0.51
1:G:4494:GLY:CA	1:G:4527:THR:HG21	2.41	0.51
1:A:122:LEU:HD12	1:A:149:GLU:HG2	1.92	0.51
1:C:1347:TYR:O	1:C:1350:LYS:N	2.31	0.51
1:A:399:ARG:NH2	1:C:1223:ASP:OD2	2.44	0.51
1:E:3392:LYS:NZ	1:G:4225:PHE:HB2	2.26	0.51
1:A:318:ARG:HD2	6:A:6148:HOH:O	2.11	0.51
1:A:451:ALA:HB2	1:A:468:ILE:CG2	2.41	0.51
1:D:2192:LYS:HE3	1:D:2196:GLU:OE2	2.11	0.51
1:A:75:PHE:CE1	1:A:111:LEU:HG	2.45	0.51
1:G:4319:ARG:HH11	1:G:4407:GLY:CA	2.24	0.50
1:G:4250:ILE:HB	1:G:4273:MET:HE1	1.93	0.50
1:C:1652:VAL:CG1	1:C:1691:LEU:HD23	2.41	0.50
1:A:303:GLU:OE2	1:C:1579:LEU:HG	2.11	0.50
1:F:4096:GLY:HA3	1:F:4102:PHE:CZ	2.46	0.50
1:H:4967:VAL:O	1:H:4987:LYS:NZ	2.36	0.50
1:F:4093:MET:HE1	1:F:4129:VAL:HG22	1.92	0.50
1:E:3469:PHE:N	1:E:3469:PHE:CD1	2.79	0.50
1:A:120:THR:HG22	1:A:205:LYS:CA	2.41	0.50
1:F:3722:LEU:HB2	1:F:3749:GLU:HA	1.93	0.50
1:D:1959:ASP:HB3	6:D:7872:HOH:O	2.12	0.50
1:F:3829:LYS:HE2	1:F:3856:ILE:HG23	1.93	0.50
1:F:3688:LYS:HE3	6:F:7669:HOH:O	2.10	0.50
1:B:926:ALA:O	1:B:927:THR:HB	2.12	0.50
1:A:118:ILE:HG21	1:A:208:VAL:HB	1.91	0.50
1:D:1905:ARG:NH1	1:D:2299:ARG:NH2	2.55	0.50
1:A:326:ALA:HB1	1:A:359:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1357:TRP:CE3	1:C:1358:LEU:N	2.79	0.50
1:C:1360:TYR:CE2	1:C:1366:VAL:HG11	2.44	0.50
1:F:3976:MET:O	1:F:3980:ILE:HG13	2.11	0.50
1:G:4492:ALA:HB1	3:G:4733:OXL:C2	2.41	0.50
1:A:83:HIS:O	1:A:87:ILE:HG13	2.12	0.50
1:F:3893:ARG:HH22	1:F:3946:ASP:CG	2.14	0.50
1:B:941:ARG:HG2	1:D:2128:GLN:NE2	2.27	0.50
1:F:3869:LYS:HE2	1:F:3871:GLU:OE2	2.10	0.50
1:F:3615:GLN:NE2	6:F:7151:HOH:O	2.44	0.50
1:H:4986:GLN:HG2	1:H:4993:VAL:CG2	2.42	0.50
1:E:3068:MET:HE2	1:E:3070:VAL:O	2.12	0.50
1:F:3722:LEU:HD12	1:F:3749:GLU:OE1	2.12	0.50
1:G:4377:ASP:HA	1:G:4498:ILE:HD11	1.94	0.50
1:C:1326:SER:HB3	1:C:1329:ALA:HB2	1.91	0.50
1:C:1255:ARG:NH2	1:C:1285:GLU:HB3	2.26	0.50
1:F:4075:ASP:HB2	1:F:4087:LEU:HD21	1.92	0.50
1:F:3612:ILE:O	1:F:3612:ILE:HG22	2.10	0.50
1:A:315:ARG:HD3	1:A:318:ARG:HH12	1.77	0.50
1:F:3810:LEU:HB3	1:F:3813:ALA:HB3	1.92	0.50
1:A:57:VAL:HG22	1:A:89:ASN:CB	2.42	0.50
1:A:111:LEU:HD23	1:A:111:LEU:C	2.31	0.50
1:E:3228:LEU:O	1:E:3232:VAL:HG23	2.10	0.50
1:D:1873:MET:CE	1:D:1886:THR:HG22	2.42	0.50
1:D:1945:ASN:HD21	1:D:1961:LYS:HZ1	1.57	0.50
1:B:788:GLY:HA3	1:B:791:PHE:CE1	2.46	0.50
1:A:333:MET:HE2	1:A:373:ALA:HA	1.93	0.50
1:G:4652:VAL:HG21	1:G:4692:ALA:HB2	1.93	0.50
1:F:3655:ARG:HD2	1:F:3682:TYR:CZ	2.47	0.50
1:H:4974:TYR:CE2	1:H:5011:PRO:HG3	2.47	0.50
1:D:1967:VAL:HG12	1:D:1987:LYS:HE3	1.94	0.50
1:F:4003:HIS:HB2	6:F:7655:HOH:O	2.11	0.50
1:F:3662:GLU:O	1:F:3666:SER:OG	2.29	0.50
1:D:1966:VAL:O	1:D:1966:VAL:HG23	2.12	0.50
1:H:5020:VAL:HG13	1:H:5024:ASP:CB	2.34	0.50
1:A:145:ASN:C	1:A:147:TYR:H	2.15	0.50
1:D:2190:HIS:NE2	1:D:2246:ARG:HG3	2.26	0.50
1:C:1270:VAL:HG13	1:C:1308:ALA:HB3	1.94	0.50
1:A:102:ILE:HG22	1:A:103:LEU:HD12	1.94	0.50
1:F:3890:MET:HE3	1:F:3926:ALA:CB	2.42	0.50
1:B:1078:GLN:HA	1:B:1078:GLN:HE21	1.77	0.50
1:G:4379:LEU:HG	1:G:4380:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1114:TRP:HE1	1:B:1115:ARG:HE	1.59	0.50
1:C:1675:ASP:CB	1:C:1676:PRO:HD2	2.40	0.50
1:H:4974:TYR:HB2	1:H:5009:ASN:HB2	1.93	0.50
1:F:4009:GLU:OE2	1:F:4043:TYR:OH	2.28	0.50
1:G:4467:ILE:HD12	1:G:4488:GLY:HA3	1.94	0.50
1:E:3522:ASN:O	1:F:4125:ARG:HG2	2.12	0.50
1:C:1572:GLU:OE1	1:C:1572:GLU:N	2.42	0.50
1:D:2203:HIS:N	1:D:2203:HIS:ND1	2.60	0.49
1:F:3675:PHE:CE1	1:F:3683:HIS:CD2	3.00	0.49
1:G:4222:ALA:CB	1:G:4227:GLU:HG2	2.42	0.49
1:G:4506:PHE:HB2	6:G:7616:HOH:O	2.12	0.49
1:G:4711:LEU:HB3	1:G:4721:THR:OG1	2.12	0.49
1:A:393:LEU:HG	1:A:397:LEU:HD22	1.93	0.49
1:G:4352:ASP:OD1	1:G:4354:ASN:N	2.37	0.49
1:D:2293:MET:HG2	1:D:2330:PRO:HD2	1.94	0.49
1:G:4703:LYS:O	1:G:4729:VAL:HB	2.13	0.49
1:E:3181:SER:O	1:E:3197:GLU:HB2	2.13	0.49
1:G:4302:ILE:HD12	1:G:4694:ASN:HB3	1.93	0.49
1:B:827:ASP:O	1:B:830:PHE:HB3	2.12	0.49
1:H:5314:TRP:HD1	1:H:5315:ARG:HG3	1.77	0.49
1:C:1287:ILE:HG22	1:C:1291:ARG:HD2	1.94	0.49
1:D:2046:LYS:HB3	1:D:2081:GLU:OE2	2.13	0.49
1:D:1902:ILE:CG1	1:D:2295:VAL:HG22	2.38	0.49
1:G:4334:LYS:O	1:G:4337:ALA:HB3	2.12	0.49
1:B:618:HIS:ND1	1:B:631:ARG:HD3	2.26	0.49
1:G:4696:GLY:HA3	1:G:4702:PHE:CZ	2.46	0.49
1:F:3815:VAL:O	1:F:3817:LEU:N	2.45	0.49
1:D:2103:GLU:OE1	1:D:2103:GLU:N	2.35	0.49
1:B:700:ASP:O	1:B:703:LEU:N	2.45	0.49
1:C:1348:MET:HA	1:C:1357:TRP:CG	2.48	0.49
1:F:3721:GLY:CA	1:F:3757:TRP:HE3	2.25	0.49
1:C:1323:ILE:CG2	1:C:1324:LYS:HG3	2.41	0.49
1:D:1940:LYS:HE3	1:D:1991:PHE:CB	2.43	0.49
1:A:432:GLU:O	1:A:458:THR:HG21	2.11	0.49
1:B:762:ASN:ND2	6:B:6065:HOH:O	2.46	0.49
1:C:1247:ILE:HB	1:C:1559:MET:HG3	1.92	0.49
1:H:5130:LEU:HD22	1:H:5133:MET:HE2	1.94	0.49
1:E:3162:ASN:OD1	1:E:3165:LYS:HE2	2.13	0.49
1:A:514:TRP:N	1:A:522:ASN:HD21	1.99	0.49
1:A:120:THR:CG2	1:A:206:LYS:H	2.26	0.49
1:A:87:ILE:HG22	1:A:91:ARG:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2225:ALA:HB1	1:D:2302:PHE:HB3	1.95	0.49
1:C:1260:LEU:O	1:C:1264:ILE:HG13	2.12	0.49
1:C:1268:MET:HE2	1:C:1270:VAL:O	2.13	0.49
1:H:4873:MET:CG	1:H:4887:ILE:CD1	2.90	0.49
1:H:4923:ILE:HA	1:H:4951:CYS:O	2.12	0.49
1:A:113:THR:HG21	1:A:242:SER:N	2.26	0.49
1:E:3252:GLU:HG2	6:E:7122:HOH:O	2.12	0.49
1:B:1031:THR:CG2	1:B:1034:GLY:HA2	2.42	0.49
1:A:238:MET:HE1	1:A:464:LEU:HD22	1.94	0.49
1:H:4833:ASP:HB3	1:H:4836:SER:HB2	1.95	0.49
1:F:3786:GLN:O	1:F:3793:VAL:N	2.29	0.49
1:D:1861:LYS:O	1:D:1865:LYS:HG3	2.11	0.49
1:C:1417:LEU:HB3	1:C:1418:PRO:HD2	1.93	0.49
1:F:3899:GLU:HB3	6:F:7614:HOH:O	2.11	0.49
1:H:5093:ARG:NH2	1:H:5129:MET:HG2	2.28	0.49
1:G:4212:ILE:HD13	1:G:4233:ASP:OD2	2.12	0.49
1:A:113:THR:HG22	1:A:242:SER:H	1.77	0.49
1:D:1940:LYS:HE3	1:D:1991:PHE:CG	2.48	0.49
1:F:3680:HIS:NE2	1:F:3827:ASP:OD1	2.30	0.49
1:B:1091:LEU:C	1:B:1091:LEU:HD12	2.33	0.49
1:D:1855:ARG:HH22	1:D:1885:GLU:HG2	1.78	0.49
1:D:1884:ALA:HB2	1:D:2030:PHE:HZ	1.78	0.49
1:E:3328:GLN:HE21	1:G:4540:THR:HB	1.77	0.49
1:G:4396:VAL:O	1:G:4396:VAL:HG12	2.11	0.49
1:A:123:ILE:HD11	1:A:202:LEU:HD21	1.95	0.49
1:G:4320:THR:HG22	1:G:4406:LYS:H	1.77	0.49
1:D:1814:THR:CG2	1:D:1815:GLN:N	2.76	0.49
1:E:3168:ASP:HB3	6:E:6720:HOH:O	2.13	0.49
1:G:4445:ARG:O	1:G:4478:ARG:HD3	2.13	0.49
1:A:328:GLN:HE21	1:C:1541:ARG:N	2.02	0.48
1:A:511:LEU:CD2	1:A:521:THR:HG23	2.42	0.48
1:D:1958:LEU:HD13	1:D:1963:ILE:HD12	1.94	0.48
1:G:4358:LEU:HD21	1:G:4363:ILE:HD12	1.95	0.48
1:D:2083:LEU:HD21	1:D:2119:ALA:HB2	1.95	0.48
1:H:5063:ASN:HB2	6:H:7909:HOH:O	2.12	0.48
1:F:3691:ARG:O	1:F:3695:GLU:HG2	2.12	0.48
1:E:3157:TRP:CH2	1:E:3159:ASP:HB3	2.48	0.48
1:C:1305:ARG:HG3	1:C:1699:ARG:HH21	1.77	0.48
1:C:1657:GLN:O	1:C:1661:GLN:HG3	2.14	0.48
1:A:29:MET:HE3	1:C:1510:LYS:HB3	1.94	0.48
1:A:24:THR:HB	1:C:1596:GLU:CD	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ILE:HD13	1:A:526:VAL:HG22	1.93	0.48
1:E:3289:ILE:HG22	1:E:3290:MET:N	2.27	0.48
1:A:388:MET:HB2	1:A:390:HIS:CE1	2.48	0.48
1:A:118:ILE:HG12	1:A:160:TYR:HB2	1.94	0.48
1:C:1479:PHE:CZ	1:C:1483:LEU:HG	2.48	0.48
1:D:2176:MET:HE3	1:D:2176:MET:CA	2.38	0.48
1:A:79:THR:H	1:A:82:TYR:HB3	1.78	0.48
1:C:1351:CYS:O	1:C:1352:ASP:HB3	2.13	0.48
1:E:3145:ASN:N	1:E:3145:ASN:HD22	2.11	0.48
1:A:57:VAL:HG22	1:A:89:ASN:HA	1.94	0.48
1:D:2230:LEU:HD22	1:D:2312:THR:HG22	1.95	0.48
1:H:5072:ASN:ND2	1:H:5075:GLY:H	2.10	0.48
1:D:1942:THR:HG22	1:D:1944:ASP:H	1.78	0.48
1:G:4319:ARG:H	1:G:4359:ASP:HB2	1.78	0.48
1:F:3650:ILE:HD11	1:F:3668:MET:HE1	1.93	0.48
1:G:4313:THR:HG21	6:G:6263:HOH:O	2.12	0.48
1:A:73:MET:HE2	1:A:86:THR:HG21	1.94	0.48
1:C:1243:ASN:H	1:C:1585:GLU:CD	2.14	0.48
1:A:240:PHE:HB3	1:A:269:LYS:HD2	1.95	0.48
1:G:4709:ILE:HG23	1:G:4724:MET:SD	2.53	0.48
1:G:4646:ARG:HB3	6:G:6227:HOH:O	2.12	0.48
1:B:747:TYR:CD1	1:B:747:TYR:N	2.81	0.48
1:A:495:VAL:CG1	1:A:499:ARG:HG3	2.44	0.48
1:F:3941:ARG:N	1:H:5128:GLN:NE2	2.52	0.48
1:D:2008:VAL:HG12	1:D:2010:LEU:HD21	1.95	0.48
1:D:1855:ARG:NH2	1:D:1885:GLU:HB3	2.29	0.48
1:H:4815:GLN:OE1	1:H:5246:ARG:HD3	2.14	0.48
1:A:329:MET:O	1:A:343:GLU:HB3	2.14	0.48
1:A:73:MET:CE	1:A:86:THR:HG21	2.44	0.48
1:C:1652:VAL:HG13	1:C:1691:LEU:HD23	1.94	0.48
1:G:4275:PHE:HB2	1:G:4312:ASP:O	2.14	0.48
1:F:3955:ALA:O	1:F:4066:ARG:NH1	2.40	0.48
1:C:1588:MET:SD	1:C:1666:ARG:NH2	2.87	0.48
1:C:1707:VAL:HG12	1:C:1708:VAL:N	2.28	0.48
1:C:1273:MET:HE3	1:C:1286:THR:HG21	1.95	0.48
1:G:4383:GLN:O	1:G:4394:THR:HG22	2.14	0.48
1:E:3173:VAL:HB	1:E:3182:LEU:HB2	1.94	0.48
1:E:3457:GLN:HB2	1:E:3460:ARG:NH1	2.29	0.48
1:A:240:PHE:CD1	1:A:240:PHE:N	2.81	0.48
1:H:5282:ALA:O	1:H:5286:ASP:HB2	2.14	0.48
1:E:3160:TYR:CD2	1:E:3163:ILE:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4873:MET:CE	1:H:4887:ILE:HD13	2.43	0.48
1:B:1015:SER:HB3	1:B:1109:ILE:HG21	1.96	0.48
1:A:113:THR:HG23	1:A:114:LYS:N	2.29	0.48
1:A:49:THR:HB	1:A:361:SER:HA	1.95	0.48
1:A:57:VAL:HG22	1:A:89:ASN:CA	2.42	0.48
1:D:2011:PRO:HB3	6:D:7715:HOH:O	2.14	0.48
1:G:4288:LYS:HE2	6:G:7504:HOH:O	2.13	0.48
1:G:4339:LEU:HD11	1:G:4354:ASN:C	2.34	0.48
1:D:2046:LYS:N	1:D:2082:ILE:HD11	2.28	0.48
1:A:290:MET:HE3	1:A:326:ALA:CB	2.44	0.48
1:E:3172:LYS:HA	1:E:3172:LYS:HD2	1.40	0.48
1:A:425:ALA:HB1	1:A:502:PHE:HB3	1.96	0.48
1:A:334:ILE:HG23	1:A:367:GLY:HA2	1.96	0.48
1:H:4988:GLY:HA3	1:H:4991:PHE:CE2	2.49	0.48
1:C:1247:ILE:HG23	1:C:1270:VAL:HB	1.96	0.48
1:C:1287:ILE:HG21	1:C:1291:ARG:NH1	2.28	0.48
1:B:720:THR:HG22	1:B:758:LEU:HD21	1.90	0.48
1:C:1356:LEU:HD12	1:C:1357:TRP:N	2.29	0.48
1:H:4847:ILE:CG2	1:H:5159:MET:HE2	2.43	0.48
1:F:3988:MET:SD	1:F:4066:ARG:NH2	2.87	0.48
1:D:2296:GLY:HA3	1:D:2302:PHE:CZ	2.49	0.48
1:H:5135:LYS:HB2	6:H:6489:HOH:O	2.13	0.48
1:C:1530:LEU:O	1:C:1563:GLU:HG2	2.14	0.48
1:D:1850:ILE:HG13	1:D:1873:MET:HE1	1.96	0.47
1:D:1899:SER:OG	1:D:1900:ASP:N	2.46	0.47
1:G:4715:ARG:CB	1:G:4716:PRO:HD2	2.35	0.47
1:A:489:VAL:O	1:A:493:MET:HG2	2.14	0.47
1:F:3655:ARG:HD2	1:F:3682:TYR:OH	2.14	0.47
1:F:3910:LYS:NZ	1:H:5149:ASN:HD21	2.12	0.47
1:B:724:LYS:HE2	1:B:752:ASP:HB3	1.96	0.47
1:E:3350:ALA:O	1:E:3353:ASP:HB2	2.13	0.47
1:A:469:PHE:CD1	1:A:469:PHE:N	2.82	0.47
1:C:1258:GLU:O	1:C:1258:GLU:HG2	2.13	0.47
1:B:758:LEU:HD22	1:B:808:VAL:HG21	1.96	0.47
1:C:1347:TYR:HD2	1:C:1355:ILE:HG21	1.77	0.47
1:C:1342:THR:O	1:C:1357:TRP:HA	2.14	0.47
1:D:2009:ASN:C	1:D:2010:LEU:HD22	2.34	0.47
1:F:3893:ARG:HD3	1:F:3926:ALA:O	2.14	0.47
1:G:4704:LYS:HA	1:G:4729:VAL:O	2.13	0.47
1:D:2188:MET:SD	1:D:2266:ARG:NH2	2.87	0.47
1:B:617:LEU:O	1:B:620:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2134:ILE:HG23	1:D:2167:GLY:HA2	1.97	0.47
1:C:1300:ASP:OD1	1:C:1303:LEU:HD12	2.14	0.47
1:G:4264:ILE:HG22	1:G:4265:LYS:N	2.28	0.47
1:C:1630:LEU:HD22	1:C:1712:THR:HG22	1.95	0.47
1:A:289:ILE:CG2	1:A:290:MET:N	2.77	0.47
1:B:1028:ILE:HG13	1:B:1108:VAL:CG1	2.44	0.47
1:B:950:ALA:O	1:B:953:ASP:HB2	2.13	0.47
1:D:1833:ASP:HA	6:D:7034:HOH:O	2.12	0.47
1:F:3699:SER:O	1:F:3701:PRO:HD3	2.14	0.47
1:F:3663:MET:CE	1:F:3668:MET:HE3	2.44	0.47
1:A:292:ALA:HB1	3:A:533:OXL:C1	2.44	0.47
1:F:3755:ILE:HG12	1:F:3755:ILE:O	2.13	0.47
1:C:1428:LEU:CD1	1:C:1456:ILE:HB	2.43	0.47
1:E:3023:ASP:HA	1:E:3391:ARG:NH2	2.29	0.47
1:B:745:ASN:HD22	1:B:757:TRP:HE1	1.63	0.47
1:D:2190:HIS:CD2	1:D:2246:ARG:HG3	2.49	0.47
1:G:4640:VAL:HG12	1:G:4649:ILE:HD13	1.97	0.47
1:B:972:GLU:OE1	1:B:972:GLU:N	2.43	0.47
1:G:4598:ALA:CB	1:G:4613:MET:HE1	2.44	0.47
1:G:4336:GLY:N	1:G:4396:VAL:O	2.47	0.47
1:B:640:THR:O	1:B:982:ARG:HD3	2.15	0.47
1:B:1114:TRP:HE1	1:B:1115:ARG:NE	2.13	0.47
1:A:238:MET:HE2	1:A:464:LEU:CD2	2.44	0.47
1:B:988:MET:SD	1:B:1066:ARG:NH2	2.87	0.47
1:A:60:LEU:O	1:A:63:MET:N	2.47	0.47
1:E:3331:GLU:HA	1:E:3331:GLU:OE1	2.13	0.47
1:B:1118:SER:HB2	6:B:6107:HOH:O	2.15	0.47
1:C:1441:ALA:O	1:C:1469:LYS:HG3	2.15	0.47
1:B:1129:VAL:HA	1:B:1130:PRO:HD2	1.69	0.47
1:A:182:LEU:HD23	1:A:182:LEU:N	2.26	0.47
1:C:1318:ILE:HG22	1:C:1408:VAL:HB	1.96	0.47
1:D:2256:HIS:N	1:D:2256:HIS:CD2	2.82	0.47
1:C:1275:PHE:N	1:C:1275:PHE:CD1	2.81	0.47
1:G:4370:GLY:HA2	1:G:4383:GLN:NE2	2.29	0.47
1:A:522:ASN:N	1:A:522:ASN:HD22	2.12	0.47
1:E:3141:ILE:O	1:E:3191:PHE:HB2	2.15	0.47
1:H:4877:HIS:O	1:H:4883:HIS:NE2	2.45	0.47
1:H:4887:ILE:O	1:H:4891:ARG:HG3	2.14	0.47
1:F:3663:MET:HE3	1:F:3668:MET:HE3	1.95	0.47
1:H:4923:ILE:C	1:H:4925:GLY:H	2.18	0.47
1:C:1252:PRO:HG3	5:C:1735:ATP:C2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1376:ASP:CG	1:C:1406:LYS:HE2	2.35	0.47
1:C:1326:SER:CB	1:C:1329:ALA:HB2	2.44	0.47
1:C:1360:TYR:HD2	1:C:1363:ILE:CB	2.28	0.47
1:F:3872:ASN:ND2	1:F:3875:GLY:H	2.10	0.47
1:C:1650:ILE:HD12	1:C:1669:PHE:HB2	1.97	0.47
1:A:57:VAL:HG23	1:A:89:ASN:CG	2.35	0.47
1:B:776:ASP:O	1:B:779:LEU:HG	2.14	0.47
1:D:2311:LEU:HA	1:D:2323:THR:O	2.15	0.47
1:F:4080:ALA:O	1:F:4083:GLU:HB2	2.15	0.47
1:F:3929:MET:O	1:F:3943:GLU:HG2	2.15	0.47
1:B:859:GLU:HG3	6:B:7831:HOH:O	2.14	0.47
1:F:3783:GLN:O	1:F:3794:THR:HA	2.15	0.47
1:D:2072:ASN:HB2	6:D:6557:HOH:O	2.14	0.47
1:B:904:LYS:NZ	6:B:7033:HOH:O	2.47	0.47
1:A:392:LYS:HE2	1:A:396:GLU:OE2	2.14	0.47
1:D:1902:ILE:O	1:D:1903:LEU:HD23	2.15	0.47
1:C:1343:LEU:N	1:C:1343:LEU:HD12	2.30	0.47
1:C:1727:VAL:CG1	1:C:1728:PRO:HD2	2.45	0.47
1:C:1704:LYS:HD2	1:C:1730:PRO:O	2.14	0.47
1:C:1688:ARG:O	1:C:1691:LEU:HB3	2.14	0.47
1:F:3721:GLY:CA	1:F:3757:TRP:CE3	2.98	0.47
1:E:3245:ARG:CB	1:E:3274:GLU:HG2	2.45	0.47
1:D:2315:ARG:HB3	1:D:2316:PRO:HD2	1.97	0.47
1:F:4093:MET:HE2	1:F:4129:VAL:HG22	1.96	0.47
1:C:1526:ALA:HB1	1:C:1559:MET:HE1	1.97	0.47
1:A:141:ILE:HG23	1:A:156:LEU:O	2.15	0.47
1:G:4483:LEU:HD13	1:G:4489:ILE:HG13	1.96	0.47
1:D:2252:VAL:HG22	1:D:2271:VAL:HB	1.96	0.47
1:F:3713:THR:HG22	1:F:3842:SER:H	1.80	0.47
1:D:2205:THR:HG23	1:D:2205:THR:O	2.15	0.47
1:B:719:ARG:HH11	1:B:719:ARG:CG	2.27	0.47
1:H:4922:LEU:HB3	1:H:4926:SER:O	2.15	0.47
1:B:655:ARG:HD2	1:B:682:TYR:OH	2.14	0.47
1:F:3889:ILE:CG2	1:F:3890:MET:N	2.78	0.47
1:B:740:LYS:HE3	1:B:791:PHE:CB	2.44	0.47
1:C:1555:ALA:O	1:C:1666:ARG:NH1	2.39	0.47
1:B:719:ARG:HH11	1:B:719:ARG:HG3	1.79	0.47
1:E:3049:THR:HA	1:E:3072:ARG:O	2.14	0.47
1:E:3507:VAL:CG1	1:E:3508:VAL:N	2.78	0.47
1:H:5094:GLY:HA3	6:H:6869:HOH:O	2.13	0.46
1:F:3733:LEU:HD12	1:F:3780:ILE:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4363:ILE:CG2	1:G:4364:CYS:N	2.78	0.46
1:H:4843:ASN:HB3	1:H:5267:GLY:HA2	1.96	0.46
1:B:738:THR:CG2	1:B:739:LEU:N	2.78	0.46
1:F:3661:LYS:O	1:F:3665:LYS:HG3	2.14	0.46
1:H:5115:ARG:NH2	6:H:6821:HOH:O	2.48	0.46
1:E:3023:ASP:HB3	1:F:3999:ARG:NH2	2.30	0.46
1:G:4275:PHE:HZ	1:G:4430:PHE:CE2	2.34	0.46
1:F:3688:LYS:HG2	6:F:7669:HOH:O	2.15	0.46
1:G:4639:GLN:NE2	1:G:4639:GLN:HA	2.27	0.46
1:B:910:LYS:HB3	1:D:1829:MET:HG2	1.97	0.46
1:E:3318:ARG:HD2	6:E:6699:HOH:O	2.14	0.46
1:G:4516:CYS:HB3	1:G:4521:LYS:O	2.15	0.46
1:G:4638:HIS:HD2	6:G:7226:HOH:O	1.99	0.46
1:F:3933:MET:HA	1:F:3936:LYS:O	2.15	0.46
1:C:1250:ILE:HG12	1:C:1271:ALA:HB1	1.98	0.46
1:G:4322:LEU:HD22	1:G:4326:SER:C	2.35	0.46
1:A:50:ILE:HB	1:A:73:MET:HE2	1.96	0.46
1:F:3756:LEU:HD12	1:F:3757:TRP:N	2.30	0.46
1:A:407:LEU:HA	1:A:407:LEU:HD12	1.51	0.46
1:D:1894:THR:HG22	1:D:1904:TYR:HE1	1.79	0.46
1:G:4276:SER:CB	1:G:4319:ARG:HH21	2.28	0.46
1:H:4952:ASP:OD1	1:H:4954:ASN:HB2	2.15	0.46
1:A:409:GLU:HB3	1:B:1021:LYS:HE2	1.97	0.46
1:E:3069:ASN:HB3	1:E:3463:HIS:CD2	2.50	0.46
1:H:4908:ALA:HB2	1:H:5260:ARG:HB3	1.98	0.46
1:G:4253:ALA:HB2	1:G:4566:LYS:HA	1.97	0.46
1:B:928:GLN:NE2	1:D:2141:ARG:NH1	2.62	0.46
1:E:3328:GLN:NE2	1:G:4540:THR:HA	2.31	0.46
1:H:5134:ILE:HG23	1:H:5167:GLY:HA2	1.96	0.46
1:B:889:ILE:HG22	1:B:890:MET:N	2.31	0.46
1:F:3904:LYS:HD3	1:H:5183:GLU:CD	2.36	0.46
1:F:4030:LEU:HG	1:F:4112:THR:HG22	1.97	0.46
1:E:3142:THR:HG21	1:E:3144:ASP:HB3	1.98	0.46
1:B:976:MET:CE	1:B:980:ILE:HD11	2.38	0.46
1:E:3273:HIS:CE1	1:E:3300:ILE:HG22	2.51	0.46
1:A:318:ARG:HD3	6:A:6437:HOH:O	2.16	0.46
1:A:77:HIS:NE2	5:A:535:ATP:H2'	2.31	0.46
1:D:2192:LYS:HB2	6:D:7588:HOH:O	2.14	0.46
1:A:507:VAL:CG1	1:A:508:VAL:N	2.79	0.46
1:A:435:ARG:HA	1:A:438:HIS:CD2	2.50	0.46
1:C:1249:THR:OG1	1:C:1561:SER:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1260:LEU:HD13	1:C:1290:VAL:HA	1.97	0.46
1:G:4368:ASP:O	1:G:4371:SER:HB2	2.15	0.46
1:B:845:ARG:O	1:B:846:LYS:HB3	2.14	0.46
1:G:4348:MET:HA	1:G:4357:TRP:CE3	2.49	0.46
1:C:1609:GLU:HB3	1:D:2221:LYS:HE2	1.98	0.46
1:B:871:GLU:O	1:B:899:GLU:HG3	2.16	0.46
1:F:4075:ASP:HB3	1:F:4076:PRO:CD	2.45	0.46
1:D:2089:ILE:CG2	1:D:2090:MET:N	2.79	0.46
1:B:881:GLU:HG3	1:B:882:ILE:N	2.31	0.46
1:F:3992:LYS:O	1:F:3996:GLU:HG3	2.15	0.46
1:E:3370:PRO:O	1:E:3374:VAL:HG23	2.16	0.46
1:E:3491:LEU:HA	1:E:3491:LEU:HD12	1.72	0.46
1:H:5265:TYR:N	1:H:5265:TYR:CD1	2.84	0.46
1:H:4935:LYS:HE3	1:H:4997:GLU:O	2.16	0.46
1:E:3493:MET:HE1	1:E:3530:PRO:CD	2.45	0.46
1:A:188:GLY:HA3	1:A:191:PHE:CD1	2.50	0.46
1:F:3743:LEU:HD13	1:F:3743:LEU:HA	1.82	0.46
1:A:120:THR:O	1:A:205:LYS:HA	2.16	0.46
1:A:51:GLY:C	1:A:55:ARG:HG3	2.35	0.46
1:B:1114:TRP:NE1	1:B:1115:ARG:NE	2.64	0.46
1:G:4274:ASN:ND2	5:G:4735:ATP:O3G	2.40	0.46
1:G:4598:ALA:HB1	1:G:4613:MET:HE1	1.97	0.46
1:D:2232:GLU:HB3	6:D:7100:HOH:O	2.14	0.46
1:H:5230:LEU:HG	1:H:5312:THR:HG22	1.98	0.46
1:G:4656:HIS:N	1:G:4656:HIS:ND1	2.62	0.46
1:A:495:VAL:HG12	1:A:499:ARG:HG3	1.97	0.46
1:A:174:TYR:HA	1:A:180:ILE:O	2.16	0.46
1:B:673:MET:N	1:B:673:MET:SD	2.88	0.46
1:A:12:ILE:HG22	1:A:12:ILE:O	2.14	0.46
1:G:4522:PRO:HG3	1:G:4665:TYR:CE2	2.51	0.46
1:A:102:ILE:C	1:A:103:LEU:HD12	2.37	0.46
1:H:4873:MET:CE	1:H:4886:THR:HG22	2.46	0.46
1:C:1327:GLY:HA2	1:C:1404:SER:HB2	1.95	0.46
1:F:3789:PRO:HD2	1:F:3791:PHE:CE1	2.51	0.46
1:E:3172:LYS:HE2	1:E:3197:GLU:CD	2.36	0.46
1:E:3012:ILE:CG2	1:E:3013:GLN:N	2.79	0.46
1:A:77:HIS:CE1	5:A:535:ATP:H3'	2.51	0.46
1:F:4110:VAL:HG21	1:F:4127:VAL:HG21	1.98	0.46
1:C:1305:ARG:NE	1:C:1699:ARG:HH21	2.14	0.45
1:E:3425:ALA:O	1:E:3426:ALA:HB2	2.16	0.45
1:B:1114:TRP:CD1	1:B:1115:ARG:CD	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4054:ARG:HG2	1:F:4073:CYS:HB3	1.97	0.45
1:H:5030:PHE:O	1:H:5033:GLU:HB2	2.15	0.45
1:F:3820:VAL:HG21	1:F:3852:GLU:HB3	1.98	0.45
1:B:642:ARG:CZ	1:B:646:ILE:HD12	2.46	0.45
1:C:1655:ASN:HB3	1:C:1658:THR:HB	1.98	0.45
1:F:3724:LYS:C	1:F:3726:SER:H	2.20	0.45
1:C:1347:TYR:CE2	1:C:1355:ILE:CD1	2.98	0.45
1:A:132:GLU:HA	1:A:201:PHE:HA	1.98	0.45
1:F:4105:GLY:N	1:F:4129:VAL:O	2.39	0.45
1:E:3475:ASP:HB3	1:E:3476:PRO:CD	2.45	0.45
1:A:42:ARG:HB2	1:A:378:HIS:CE1	2.51	0.45
1:H:4966:VAL:HB	6:H:7523:HOH:O	2.14	0.45
1:B:958:ILE:HG13	1:B:977:GLN:NE2	2.30	0.45
1:H:5182:ARG:NH1	6:H:7313:HOH:O	2.47	0.45
1:C:1287:ILE:CG2	1:C:1291:ARG:NH1	2.80	0.45
1:D:2009:ASN:O	1:D:2010:LEU:HD22	2.15	0.45
1:E:3283:LEU:HD22	1:E:3321:LYS:HD2	1.99	0.45
1:G:4647:ALA:CB	1:G:4648:PRO:HD2	2.38	0.45
1:D:2281:TRP:CD2	1:D:2316:PRO:HD3	2.50	0.45
1:B:774:TYR:HB3	1:B:778:GLY:HA2	1.99	0.45
1:B:674:ASN:OD1	1:B:676:SER:HB2	2.16	0.45
1:A:514:TRP:CE3	1:B:1125:ARG:HD3	2.52	0.45
1:H:4953:GLU:CD	1:H:4953:GLU:H	2.11	0.45
1:G:4318:ILE:HG23	1:G:4360:TYR:HB2	1.98	0.45
1:C:1687:LEU:HG	1:C:1688:ARG:N	2.29	0.45
1:E:3316:CYS:O	1:E:3320:GLY:N	2.50	0.45
1:F:3766:VAL:CG1	1:F:3813:ALA:HB1	2.45	0.45
1:G:4493:ARG:NH2	1:G:4546:ASP:OD1	2.50	0.45
1:E:3440:VAL:CG1	1:E:3449:ILE:HD13	2.46	0.45
1:E:3503:LYS:O	1:E:3506:ASP:HB2	2.16	0.45
1:D:2301:PHE:CD1	1:D:2301:PHE:N	2.84	0.45
1:F:3752:ASP:C	1:F:3754:ASN:H	2.19	0.45
1:G:4358:LEU:CD2	1:G:4363:ILE:HD12	2.47	0.45
1:D:1914:LYS:HZ2	1:D:2023:LYS:HD3	1.80	0.45
1:B:1080:ALA:HB3	1:B:1083:GLU:CG	2.47	0.45
1:H:5296:GLY:HA3	1:H:5302:PHE:CZ	2.52	0.45
1:G:4511:MET:O	1:G:4515:ARG:HG3	2.16	0.45
1:D:2231:THR:O	1:D:2253:THR:HB	2.16	0.45
1:C:1532:SER:O	1:C:1534:ILE:N	2.49	0.45
1:A:511:LEU:HB3	1:A:521:THR:HG21	1.98	0.45
1:F:3928:GLN:HE22	1:H:5140:THR:CA	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3890:MET:HE1	1:F:3892:ALA:CB	2.47	0.45
1:G:4666:ARG:HG3	1:G:4667:GLY:N	2.30	0.45
1:C:1305:ARG:HE	1:C:1699:ARG:CZ	2.30	0.45
1:A:408:MET:SD	1:A:520:PHE:HD2	2.40	0.45
1:A:123:ILE:HD11	1:A:202:LEU:CG	2.47	0.45
1:G:4364:CYS:O	1:G:4387:LYS:HE3	2.17	0.45
1:C:1318:ILE:HG12	1:C:1360:TYR:HB2	1.98	0.45
1:E:3440:VAL:HG12	1:E:3449:ILE:HD13	1.97	0.45
1:G:4608:MET:SD	1:G:4721:THR:HG22	2.56	0.45
1:D:2222:CYS:O	1:D:2223:LEU:HB2	2.16	0.45
1:A:267:ILE:N	1:A:267:ILE:CD1	2.80	0.45
1:B:928:GLN:HB2	1:D:2141:ARG:HB2	1.98	0.45
1:F:3928:GLN:NE2	1:H:5140:THR:CB	2.79	0.45
1:G:4248:CYS:SG	1:G:4268:MET:HB2	2.56	0.45
1:A:14:THR:CG2	1:A:15:GLN:HB2	2.43	0.45
1:F:3748:MET:HG3	1:F:3757:TRP:CZ2	2.51	0.45
1:G:4729:VAL:HA	1:G:4730:PRO:HD3	1.70	0.45
1:H:5089:ILE:CG2	1:H:5090:MET:N	2.79	0.45
1:A:480:ALA:HB3	1:A:483:GLU:HB2	1.99	0.45
1:E:3103:LEU:HD12	1:E:3103:LEU:HA	1.58	0.45
1:F:3928:GLN:NE2	1:H:5140:THR:CA	2.80	0.45
1:A:103:LEU:N	1:A:103:LEU:CD1	2.80	0.45
1:D:1910:ALA:HB2	1:D:2038:MET:CG	2.42	0.45
1:G:4621:LYS:HD2	1:G:4621:LYS:O	2.17	0.45
1:A:180:ILE:CG2	1:A:182:LEU:HD21	2.47	0.45
1:A:330:LEU:CD2	1:A:377:GLN:HG3	2.46	0.45
1:G:4477:ARG:HD3	6:G:7521:HOH:O	2.17	0.45
1:C:1335:LYS:CG	1:C:1336:GLY:N	2.80	0.45
1:C:1302:ILE:HA	1:C:1695:VAL:HG22	1.98	0.45
1:D:1916:PRO:HG3	1:D:2045:ARG:NH2	2.32	0.45
1:G:4410:LEU:N	1:G:4411:PRO:HD3	2.31	0.45
1:A:310:LYS:HZ1	1:C:1549:ASN:HD21	1.63	0.45
1:B:844:ILE:HG13	1:B:868:SER:CB	2.47	0.45
1:B:825:ILE:CG2	1:B:829:LYS:NZ	2.80	0.45
1:G:4636:SER:O	1:G:4639:GLN:HB2	2.17	0.45
1:F:3684:ALA:HB2	1:F:3830:PHE:HZ	1.82	0.45
1:B:675:PHE:CD1	1:B:711:LEU:HG	2.52	0.45
1:F:4111:LEU:HD23	1:F:4123:THR:O	2.17	0.45
1:C:1632:GLU:OE1	1:C:1654:ARG:HB2	2.17	0.45
1:D:2065:LYS:HA	1:D:2065:LYS:HD3	1.75	0.45
1:F:3648:CYS:CB	1:F:3668:MET:HE3	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:992:LYS:O	1:B:996:GLU:HG3	2.17	0.44
1:A:167:VAL:CG2	1:A:168:ASP:N	2.80	0.44
1:A:180:ILE:HG22	1:A:182:LEU:HD21	1.99	0.44
1:A:209:ASN:O	1:A:210:LEU:HD13	2.17	0.44
1:C:1664:LEU:HD12	1:C:1664:LEU:HA	1.78	0.44
1:F:3705:ARG:NE	1:F:4099:ARG:NH2	2.65	0.44
1:H:5279:GLU:HG3	1:H:5280:ALA:N	2.32	0.44
1:C:1274:ASN:O	1:C:1283:HIS:NE2	2.50	0.44
1:B:843:PHE:CE2	1:B:845:ARG:HD3	2.51	0.44
1:D:2291:LEU:O	1:D:2291:LEU:HD12	2.17	0.44
1:E:3015:GLN:OE1	1:E:3446:ARG:HD3	2.17	0.44
1:G:4471:GLU:OE1	1:G:4495:ASP:HB2	2.17	0.44
1:G:4471:GLU:O	1:G:4499:GLU:HG3	2.17	0.44
1:A:300:ILE:HB	1:A:301:PRO:CD	2.46	0.44
1:B:660:LEU:HB3	1:B:693:ALA:CB	2.47	0.44
1:C:1707:VAL:CG1	1:C:1708:VAL:N	2.80	0.44
1:D:2327:VAL:HG12	1:D:2328:PRO:O	2.18	0.44
1:D:1948:MET:HA	1:D:1957:TRP:CG	2.52	0.44
1:C:1429:LYS:HB3	6:C:7061:HOH:O	2.17	0.44
1:E:3277:ARG:NE	6:E:7207:HOH:O	2.49	0.44
1:H:5133:MET:CE	1:H:5139:PRO:CB	2.95	0.44
1:C:1319:ARG:NE	1:C:1405:LYS:O	2.43	0.44
1:B:1127:VAL:CG1	1:B:1128:PRO:N	2.79	0.44
1:A:202:LEU:O	1:A:202:LEU:HG	2.17	0.44
1:F:3720:THR:CG2	1:F:3721:GLY:N	2.80	0.44
1:C:1314:LYS:HE3	1:C:1427:ASP:OD2	2.17	0.44
1:F:3764:CYS:HB2	6:F:7678:HOH:O	2.17	0.44
1:F:3910:LYS:HZ1	1:H:5149:ASN:HD21	1.65	0.44
1:A:520:PHE:N	1:A:520:PHE:CD1	2.86	0.44
1:D:1968:ASP:O	1:D:1971:SER:HB2	2.17	0.44
1:F:3886:SER:O	1:F:3921:LYS:HE2	2.17	0.44
1:E:3244:ILE:HD13	1:E:3244:ILE:HA	1.77	0.44
1:A:522:ASN:H	1:A:522:ASN:HD22	1.64	0.44
1:E:3415:SER:HB3	1:E:3509:ILE:HG21	1.98	0.44
1:A:131:VAL:O	1:A:201:PHE:HA	2.17	0.44
1:H:4979:LEU:HD21	6:H:7671:HOH:O	2.17	0.44
1:F:3719:ARG:H	1:F:3759:ASP:HB2	1.82	0.44
1:G:4516:CYS:CB	1:G:4523:VAL:HB	2.47	0.44
1:H:5089:ILE:HG22	1:H:5090:MET:N	2.31	0.44
1:G:4242:ARG:HD2	1:G:4244:THR:O	2.18	0.44
1:E:3452:VAL:HG11	1:E:3488:ARG:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1947:TYR:N	1:D:1947:TYR:CD1	2.86	0.44
1:C:1379:LEU:HG	1:C:1380:ILE:HG12	2.00	0.44
1:A:328:GLN:NE2	1:C:1540:THR:CA	2.80	0.44
1:F:4008:MET:CG	1:F:4039:GLN:HG2	2.43	0.44
1:B:1009:GLU:O	1:B:1013:MET:HG3	2.17	0.44
1:A:148:MET:HB3	1:A:148:MET:HE3	1.76	0.44
1:E:3450:ILE:HD11	1:E:3501:PHE:HD2	1.83	0.44
1:F:3774:TYR:CE2	1:F:3811:PRO:HG2	2.52	0.44
1:F:3774:TYR:HE2	1:F:3811:PRO:HG2	1.81	0.44
1:D:2031:GLY:O	1:D:2036:VAL:HG13	2.17	0.44
1:A:369:TYR:N	1:A:370:PRO:CD	2.81	0.44
1:E:3068:MET:CE	1:E:3071:ALA:HA	2.47	0.44
1:D:2288:ARG:O	1:D:2291:LEU:HB3	2.18	0.44
1:G:4333:LEU:CG	1:G:4402:LEU:HD23	2.38	0.44
1:F:3650:ILE:CD1	1:F:3668:MET:HE1	2.47	0.44
1:F:3893:ARG:NH2	1:F:3946:ASP:OD1	2.50	0.44
1:D:2089:ILE:HG22	1:D:2090:MET:N	2.33	0.44
1:G:4444:ILE:HD13	1:G:4444:ILE:HA	1.77	0.44
1:A:259:GLU:O	1:A:262:LYS:HG2	2.18	0.44
1:H:5328:PRO:O	1:H:5330:PRO:HD3	2.18	0.44
1:C:1472:ASN:HD22	1:C:1472:ASN:C	2.21	0.44
1:A:409:GLU:OE1	1:A:443:TYR:OH	2.36	0.44
1:F:4122:ASN:N	1:F:4122:ASN:OD1	2.42	0.44
1:H:5049:ASP:O	1:H:5052:GLU:HB2	2.17	0.44
1:B:949:ASN:HD21	1:D:2110:LYS:NZ	2.16	0.44
1:H:4919:ARG:HA	1:H:5006:LYS:O	2.18	0.44
1:B:615:GLN:O	1:B:615:GLN:HG2	2.17	0.44
1:D:1850:ILE:HB	1:D:1873:MET:CE	2.39	0.44
1:C:1621:LYS:NZ	1:D:2201:SER:O	2.51	0.44
1:A:114:LYS:HG2	1:A:117:GLU:OE2	2.17	0.44
1:A:515:ARG:HB3	1:A:516:PRO:HD2	1.99	0.44
1:A:75:PHE:CD1	1:A:75:PHE:N	2.84	0.44
1:E:3349:ASN:HB3	6:E:6204:HOH:O	2.18	0.44
1:B:990:HIS:HD2	6:B:6334:HOH:O	2.00	0.44
1:D:2017:LEU:HB3	1:D:2018:PRO:HD2	1.98	0.44
1:G:4373:VAL:O	1:G:4382:LEU:HB2	2.17	0.44
1:H:4933:LEU:HA	1:H:4933:LEU:HD23	1.71	0.44
1:G:4338:THR:HG23	1:G:4339:LEU:N	2.32	0.44
1:D:2044:ILE:HG13	1:D:2068:SER:HB3	2.00	0.44
1:C:1532:SER:C	1:C:1534:ILE:H	2.20	0.44
1:B:1124:MET:HG2	1:B:1125:ARG:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LYS:HA	1:A:182:LEU:O	2.18	0.44
1:H:4960:TYR:CD2	1:H:4963:ILE:HB	2.53	0.44
1:B:1078:GLN:NE2	1:B:1078:GLN:CA	2.79	0.44
1:G:4379:LEU:C	1:G:4379:LEU:HD12	2.37	0.44
1:A:246:LYS:HG3	6:A:7641:HOH:O	2.18	0.44
1:F:3821:SER:O	1:F:3824:ASP:HB2	2.18	0.44
1:B:825:ILE:HG22	1:B:829:LYS:HZ2	1.81	0.44
1:G:4529:MET:O	1:G:4530:LEU:HD23	2.18	0.44
1:C:1603:HIS:CG	1:C:1604:SER:N	2.86	0.44
1:D:1874:ASN:HA	1:D:1912:ASP:HB3	2.00	0.44
1:D:2056:ILE:HD13	1:D:2056:ILE:N	2.32	0.44
1:B:650:ILE:HD11	1:B:668:MET:HE1	2.00	0.43
1:E:3163:ILE:O	1:E:3163:ILE:HG23	2.17	0.43
1:G:4222:ALA:HB1	1:G:4227:GLU:HG2	2.00	0.43
1:F:3716:PRO:HB3	1:F:3817:LEU:HB3	2.00	0.43
1:B:990:HIS:HE1	6:B:6944:HOH:O	2.01	0.43
1:C:1310:ALA:HB1	1:C:1440:PHE:CZ	2.53	0.43
1:B:650:ILE:HD11	1:B:668:MET:HE2	2.00	0.43
1:C:1534:ILE:HG23	1:C:1567:GLY:CA	2.41	0.43
1:E:3304:LYS:O	1:E:3307:LEU:HB2	2.18	0.43
1:B:873:HIS:HE1	1:B:899:GLU:O	2.01	0.43
1:E:3012:ILE:HD12	1:E:3035:ASP:HB3	1.98	0.43
1:G:4274:ASN:HA	1:G:4312:ASP:HB3	2.00	0.43
1:A:57:VAL:HG22	1:A:89:ASN:HB3	2.00	0.43
1:H:4860:LEU:O	1:H:4863:MET:HB2	2.18	0.43
1:B:970:PRO:O	1:B:974:VAL:HG23	2.17	0.43
1:F:3897:GLY:HA2	1:F:3905:VAL:CG2	2.49	0.43
1:D:1980:ILE:HD11	1:D:2000:GLY:HA3	1.98	0.43
1:G:4522:PRO:HD3	1:G:4665:TYR:CE2	2.53	0.43
1:H:4850:ILE:HD11	1:H:4868:MET:HE3	1.96	0.43
1:D:2046:LYS:HB2	6:D:7884:HOH:O	2.18	0.43
1:A:160:TYR:CD2	1:A:163:ILE:N	2.85	0.43
1:G:4313:THR:HG22	1:G:4442:SER:N	2.26	0.43
1:C:1382:LEU:HD23	1:C:1396:VAL:HA	1.99	0.43
1:A:301:PRO:HG2	1:A:304:LYS:HD2	2.00	0.43
1:D:1856:SER:O	1:D:1860:LEU:HB2	2.18	0.43
1:D:2057:LEU:HB2	6:D:7550:HOH:O	2.18	0.43
1:C:1445:ARG:HB3	1:C:1474:GLU:OE1	2.18	0.43
1:C:1347:TYR:CE2	1:C:1355:ILE:HD13	2.53	0.43
1:A:91:ARG:O	1:A:95:GLU:HG2	2.17	0.43
1:C:1428:LEU:HD12	1:C:1456:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1077:VAL:HG12	1:B:1078:GLN:O	2.18	0.43
1:A:456:HIS:H	1:A:456:HIS:HD2	1.65	0.43
1:E:3334:ILE:HA	6:E:7134:HOH:O	2.16	0.43
1:C:1588:MET:HE3	6:C:7860:HOH:O	2.18	0.43
1:B:990:HIS:CD2	1:B:990:HIS:H	2.35	0.43
1:B:997:LEU:O	1:B:1000:SER:OG	2.29	0.43
1:H:4932:GLU:HG3	1:H:5001:PHE:CZ	2.54	0.43
1:C:1343:LEU:HD23	1:C:1361:LYS:HD3	2.01	0.43
1:G:4621:LYS:HE2	1:H:5209:GLU:HB3	2.00	0.43
1:E:3272:ASN:OD1	1:E:3274:GLU:N	2.52	0.43
1:A:49:THR:O	1:A:365:ALA:HB2	2.18	0.43
1:F:3906:PHE:O	1:F:3910:LYS:HG3	2.18	0.43
1:B:779:LEU:HD23	1:B:779:LEU:HA	1.78	0.43
1:F:3942:ALA:HB2	1:H:5146:ASP:OD2	2.19	0.43
1:B:688:LYS:HE3	6:B:7688:HOH:O	2.17	0.43
1:D:1983:GLN:HG2	1:D:1985:LYS:HE2	2.01	0.43
1:E:3120:THR:O	1:E:3205:LYS:HA	2.18	0.43
1:G:4339:LEU:HA	1:G:4339:LEU:HD12	1.32	0.43
1:B:700:ASP:O	1:B:702:ILE:N	2.51	0.43
1:C:1322:LEU:HA	1:C:1322:LEU:HD23	1.65	0.43
1:G:4300:ASP:HA	1:G:4301:PRO:HD3	1.81	0.43
1:F:3676:SER:HA	1:F:3714:LYS:HG3	2.01	0.43
1:G:4619:SER:N	1:G:4709:ILE:HD11	2.34	0.43
1:F:3820:VAL:HB	1:F:3852:GLU:OE1	2.18	0.43
1:D:2100:ILE:HB	1:D:2101:PRO:HD2	2.01	0.43
1:H:5130:LEU:HD22	1:H:5133:MET:CE	2.49	0.43
1:D:2252:VAL:CG2	1:D:2292:ALA:HB2	2.48	0.43
1:G:4681:TRP:NE1	1:G:4715:ARG:HA	2.33	0.43
1:B:651:GLY:C	1:B:655:ARG:HG3	2.39	0.43
1:C:1368:ASP:O	1:C:1371:SER:HB2	2.19	0.43
1:A:493:MET:HE1	1:A:529:VAL:HG22	1.99	0.43
1:A:454:ARG:HH22	1:A:484:ASP:CG	2.18	0.43
1:E:3257:LEU:HA	1:E:3257:LEU:HD13	1.86	0.43
1:D:1855:ARG:NH2	1:D:1885:GLU:CG	2.79	0.43
1:E:3461:GLN:O	1:E:3464:LEU:HB2	2.19	0.43
1:H:5242:ARG:NE	6:H:7298:HOH:O	2.50	0.43
1:G:4660:ARG:HD2	1:G:4660:ARG:HH11	1.66	0.43
1:A:283:LEU:HD22	1:A:283:LEU:C	2.38	0.43
1:A:245:ARG:HD3	1:A:272:ASN:HD21	1.84	0.43
1:C:1612:ALA:O	1:C:1616:VAL:HG23	2.19	0.43
1:C:1718:SER:C	1:C:1720:PHE:H	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5307:VAL:CG1	1:H:5308:VAL:N	2.82	0.43
1:A:192:LEU:N	1:A:192:LEU:CD2	2.79	0.43
1:G:4498:ILE:N	1:G:4498:ILE:CD1	2.80	0.43
1:A:228:LEU:O	1:A:232:VAL:HG23	2.19	0.43
1:C:1366:VAL:O	1:C:1366:VAL:HG22	2.18	0.43
1:C:1457:LEU:HD12	1:C:1457:LEU:HA	1.53	0.43
1:C:1654:ARG:HG2	1:C:1673:CYS:O	2.19	0.43
1:A:119:ARG:HD3	1:A:207:GLY:HA2	2.00	0.43
1:H:5015:VAL:CG1	1:H:5017:LEU:H	2.31	0.43
1:C:1263:MET:HA	1:C:1266:SER:HB2	2.00	0.43
1:D:2275:ASP:HA	1:D:2276:PRO:HD3	1.88	0.43
1:C:1539:PRO:HG3	1:C:1576:MET:HG2	2.00	0.43
1:D:1859:THR:O	1:D:1862:GLU:N	2.51	0.43
1:C:1410:LEU:HD12	1:C:1410:LEU:HA	1.79	0.43
1:G:4298:ALA:HA	1:G:4304:TYR:CD1	2.54	0.43
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.89	0.43
1:C:1322:LEU:HD12	1:C:1349:GLU:CG	2.37	0.43
1:D:1902:ILE:HG22	1:D:1903:LEU:HD23	2.00	0.43
1:C:1387:LYS:HB3	1:C:1392:LEU:CD1	2.46	0.43
1:C:1339:LEU:HD12	1:C:1354:ASN:O	2.19	0.43
1:F:3817:LEU:HA	1:F:3817:LEU:HD23	1.59	0.43
1:B:698:ALA:HA	1:B:704:TYR:CD1	2.54	0.43
1:D:1878:GLY:HA2	6:D:6138:HOH:O	2.18	0.43
1:E:3016:GLN:NE2	6:E:6187:HOH:O	2.52	0.43
1:B:764:CYS:O	1:B:787:LYS:NZ	2.39	0.43
1:H:5304:LYS:HB2	1:H:5330:PRO:O	2.19	0.42
1:D:2304:LYS:HG3	1:D:2330:PRO:O	2.17	0.42
1:A:291:VAL:HG12	1:A:293:ARG:HG3	2.00	0.42
1:F:3739:LEU:HD21	1:F:3756:LEU:CB	2.43	0.42
1:A:144:ASP:O	1:A:147:TYR:N	2.51	0.42
1:C:1305:ARG:HE	1:C:1699:ARG:HH21	1.65	0.42
1:D:2020:VAL:CG1	1:D:2025:ILE:HD11	2.48	0.42
1:D:2021:SER:O	1:D:2025:ILE:HG12	2.19	0.42
1:A:74:ASN:HA	1:A:112:ASP:HB3	2.01	0.42
1:E:3100:ASP:C	1:E:3102:ILE:H	2.22	0.42
1:D:2265:TYR:HB2	1:D:2268:ILE:CD1	2.44	0.42
1:A:238:MET:CE	1:A:464:LEU:CD2	2.97	0.42
1:G:4640:VAL:HG12	1:G:4649:ILE:CD1	2.48	0.42
1:C:1720:PHE:CZ	1:C:1722:ASN:HB3	2.54	0.42
1:B:880:ASP:HB2	6:B:7833:HOH:O	2.19	0.42
1:G:4260:LEU:HA	1:G:4263:MET:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:MET:O	1:A:380:ILE:HG13	2.18	0.42
1:G:4372:LYS:NZ	1:G:4397:GLU:OE1	2.50	0.42
1:E:3266:ILE:O	1:E:3266:ILE:HG22	2.19	0.42
1:E:3144:ASP:O	1:E:3146:ALA:N	2.52	0.42
1:A:158:LEU:HA	1:A:158:LEU:HD12	1.47	0.42
1:E:3191:PHE:HE1	1:E:3193:VAL:CG2	2.22	0.42
1:E:3186:GLN:CB	1:E:3193:VAL:HB	2.39	0.42
1:G:4322:LEU:HB2	1:G:4349:GLU:HA	2.01	0.42
1:G:4313:THR:HG21	1:G:4442:SER:H	1.81	0.42
1:C:1305:ARG:NH1	6:C:7519:HOH:O	2.52	0.42
1:G:4217:LEU:HD23	1:G:4217:LEU:HA	1.86	0.42
1:F:3867:ILE:HA	1:F:3888:GLY:O	2.19	0.42
1:G:4569:TYR:HB3	1:G:4572:GLU:HB2	2.01	0.42
1:H:5256:HIS:CD2	1:H:5256:HIS:H	2.37	0.42
1:G:4560:LEU:HA	1:G:4560:LEU:HD23	1.70	0.42
1:E:3144:ASP:HB3	1:E:3147:TYR:HD2	1.85	0.42
1:E:3162:ASN:HD22	1:E:3162:ASN:HA	1.59	0.42
1:A:425:ALA:O	1:A:448:PRO:HD2	2.19	0.42
1:A:57:VAL:O	1:A:61:LYS:HG3	2.19	0.42
1:H:5158:ILE:HD12	1:H:5177:GLN:HG2	2.02	0.42
1:F:3881:GLU:HG3	1:F:3882:ILE:N	2.34	0.42
1:A:25:PHE:O	1:A:28:HIS:HB3	2.20	0.42
1:H:5188:MET:CE	1:H:5190:HIS:NE2	2.83	0.42
1:B:637:ALA:HA	1:B:638:PRO:HD3	1.83	0.42
1:F:3735:LYS:HA	1:F:3796:VAL:HG12	2.01	0.42
1:F:3726:SER:HB3	1:F:3729:ALA:N	2.34	0.42
1:H:4843:ASN:CB	1:H:5267:GLY:HA2	2.48	0.42
1:E:3198:ASN:HD21	1:G:4538:ARG:HH22	1.67	0.42
1:A:328:GLN:HE21	1:C:1540:THR:HB	1.84	0.42
1:G:4337:ALA:O	1:G:4395:GLU:HA	2.19	0.42
1:D:1958:LEU:CD1	1:D:1963:ILE:HD12	2.50	0.42
1:G:4387:LYS:HA	1:G:4392:LEU:CD1	2.50	0.42
1:C:1687:LEU:HA	1:C:1690:ASN:HD22	1.85	0.42
1:D:1863:MET:HG3	1:D:2171:LEU:CD2	2.49	0.42
1:G:4374:TYR:HB3	1:G:4378:GLY:HA2	2.02	0.42
1:D:2071:GLU:HB3	1:D:2092:ALA:HB3	2.01	0.42
1:B:935:LYS:HD2	1:B:935:LYS:HA	1.70	0.42
1:D:1818:HIS:CD2	1:D:1831:ARG:HD3	2.54	0.42
1:G:4300:ASP:OD1	1:G:4301:PRO:HD2	2.20	0.42
1:F:3675:PHE:CE2	1:F:3683:HIS:HD2	2.37	0.42
1:D:2096:LEU:O	1:D:2100:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:VAL:HG21	1:B:843:PHE:HE2	1.85	0.42
1:F:3743:LEU:HD12	1:F:3761:LYS:HG2	2.01	0.42
1:C:1406:LYS:HD2	1:C:1406:LYS:HA	1.40	0.42
1:H:4945:ASN:CB	1:H:4948:MET:HE2	2.47	0.42
1:C:1305:ARG:CG	1:C:1699:ARG:HH21	2.33	0.42
1:E:3457:GLN:HB2	1:E:3460:ARG:HH12	1.84	0.42
1:A:439:GLN:OE1	1:A:442:ARG:HD3	2.18	0.42
1:G:4303:LEU:HA	1:G:4303:LEU:HD22	1.78	0.42
1:H:5261:GLN:O	1:H:5264:LEU:HB2	2.20	0.42
1:C:1417:LEU:HA	1:C:1418:PRO:HD3	1.78	0.42
1:E:3111:LEU:C	1:E:3111:LEU:HD23	2.40	0.42
1:C:1250:ILE:HD11	1:C:1268:MET:HE1	2.02	0.42
1:H:4873:MET:HG3	1:H:4887:ILE:CD1	2.38	0.42
1:A:210:LEU:HB3	1:A:213:ALA:HB3	2.02	0.42
1:E:3300:ILE:HB	1:E:3301:PRO:CD	2.46	0.42
1:G:4251:GLY:C	1:G:4255:ARG:HG3	2.39	0.42
1:C:1363:ILE:HA	1:C:1366:VAL:CG1	2.48	0.42
1:E:3271:GLU:OE1	1:E:3295:ASP:HB2	2.20	0.42
1:C:1575:ARG:O	1:C:1578:HIS:HB3	2.20	0.42
1:E:3103:LEU:O	1:E:3103:LEU:HG	2.20	0.42
1:D:1841:ALA:CB	1:D:2248:PRO:HG3	2.50	0.42
1:E:3062:GLU:HA	1:E:3062:GLU:OE1	2.19	0.42
1:G:4701:PHE:HA	1:G:4701:PHE:HD1	1.63	0.42
1:A:328:GLN:HE22	1:C:1540:THR:CA	2.30	0.42
1:G:4341:ILE:N	1:G:4392:LEU:O	2.46	0.42
1:E:3496:GLY:O	1:E:3501:PHE:N	2.46	0.42
1:A:375:ARG:O	1:A:378:HIS:HB3	2.20	0.42
1:D:1857:VAL:O	1:D:1861:LYS:HG3	2.19	0.42
1:G:4259:THR:O	1:G:4263:MET:HG2	2.19	0.42
1:B:733:LEU:HD11	1:B:802:LEU:HD22	2.02	0.42
1:H:5269:PHE:N	1:H:5269:PHE:CD1	2.88	0.42
1:B:846:LYS:N	1:B:846:LYS:HD2	2.35	0.42
1:G:4273:MET:HE2	1:G:4286:THR:HG22	2.01	0.42
1:E:3145:ASN:HD21	1:E:3161:LYS:NZ	2.17	0.42
1:A:224:ASP:O	1:A:228:LEU:HG	2.20	0.42
1:G:4417:LEU:HD12	1:G:4417:LEU:HA	1.71	0.42
1:D:1922:LEU:O	1:D:1951:CYS:HB2	2.19	0.42
1:F:3639:ILE:O	1:F:3982:ARG:HD2	2.20	0.42
1:G:4539:PRO:HG3	1:G:4576:MET:HG2	2.01	0.42
1:G:4339:LEU:N	1:G:4394:THR:O	2.40	0.41
1:F:3928:GLN:NE2	1:H:5140:THR:HA	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ILE:H	1:A:225:ILE:HG13	1.64	0.41
1:D:1900:ASP:OD2	1:D:1903:LEU:HG	2.20	0.41
1:H:4942:THR:CG2	1:H:4944:ASP:N	2.79	0.41
1:D:2293:MET:CG	1:D:2330:PRO:HD2	2.50	0.41
1:D:1894:THR:HG22	1:D:1904:TYR:CE1	2.55	0.41
1:C:1713:GLY:HA2	1:C:1722:ASN:OD1	2.20	0.41
1:F:3993:LEU:HD21	1:F:4044:ARG:HG3	2.02	0.41
1:E:3280:ASP:HB2	6:E:6959:HOH:O	2.20	0.41
1:D:2041:ALA:O	1:D:2044:ILE:HG12	2.20	0.41
1:A:277:ARG:NH2	1:A:278:ARG:CZ	2.83	0.41
1:F:3733:LEU:N	1:F:3800:GLY:O	2.48	0.41
1:G:4320:THR:HG23	1:G:4321:GLY:N	2.35	0.41
1:A:478:GLN:HB2	1:A:484:ASP:CB	2.50	0.41
1:E:3225:ILE:HD12	1:E:3256:ILE:HD12	2.02	0.41
1:C:1647:ALA:HB1	1:C:1648:PRO:CD	2.49	0.41
1:E:3411:MET:SD	1:F:4126:VAL:CG2	3.08	0.41
1:A:244:ILE:HD13	1:A:244:ILE:HA	1.86	0.41
1:G:4247:ILE:HB	1:G:4559:MET:HG3	2.02	0.41
1:C:1288:LYS:HD3	6:C:7421:HOH:O	2.19	0.41
1:A:284:GLU:HA	6:A:6607:HOH:O	2.20	0.41
1:H:4943:LEU:HD23	1:H:4943:LEU:HA	1.85	0.41
1:E:3165:LYS:HG3	1:E:3165:LYS:O	2.20	0.41
1:B:1111:LEU:HD21	1:B:1124:MET:HB2	2.01	0.41
1:E:3192:LEU:N	1:E:3192:LEU:CD2	2.80	0.41
1:A:68:MET:HE2	1:A:68:MET:HB2	1.89	0.41
1:E:3274:GLU:O	1:E:3278:ARG:HG3	2.20	0.41
1:B:866:ILE:HG21	1:B:866:ILE:HD13	1.77	0.41
1:D:2130:LEU:HD23	1:D:2143:GLU:HB3	2.01	0.41
1:H:5081:GLU:HG2	6:H:6315:HOH:O	2.21	0.41
1:G:4726:VAL:HG23	1:H:5211:MET:SD	2.60	0.41
1:F:3746:ALA:HB3	1:F:3747:TYR:CD1	2.55	0.41
1:D:2158:ILE:H	1:D:2158:ILE:HG12	1.71	0.41
1:G:4410:LEU:N	1:G:4411:PRO:CD	2.82	0.41
1:A:90:VAL:HG12	1:A:91:ARG:N	2.34	0.41
1:D:1851:GLY:O	1:D:1855:ARG:N	2.54	0.41
1:D:2030:PHE:CE1	1:D:2034:GLN:CG	3.03	0.41
1:C:1360:TYR:CD2	1:C:1363:ILE:HB	2.52	0.41
1:H:4900:ASP:O	1:H:4902:ILE:N	2.54	0.41
1:C:1465:LYS:HA	1:C:1487:ASP:OD2	2.20	0.41
1:B:879:PHE:CZ	1:B:883:LEU:HG	2.55	0.41
1:C:1218:HIS:O	1:C:1231:ARG:NH1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1516:CYS:HB3	1:C:1521:LYS:O	2.20	0.41
1:F:3849:ASP:N	1:F:3849:ASP:OD1	2.52	0.41
1:E:3220:VAL:O	1:E:3220:VAL:HG12	2.18	0.41
1:E:3047:ILE:HG12	1:E:3070:VAL:HB	2.01	0.41
1:D:1873:MET:CE	1:D:1886:THR:CG2	2.99	0.41
1:C:1609:GLU:HG2	1:C:1643:TYR:OH	2.19	0.41
1:C:1338:THR:HG22	1:C:1339:LEU:N	2.35	0.41
1:G:4215:GLN:HB3	1:G:4217:LEU:HG	2.01	0.41
1:F:3760:TYR:HE2	1:F:3766:VAL:HG21	1.85	0.41
1:C:1599:ARG:HG3	6:D:6052:HOH:O	2.20	0.41
1:A:246:LYS:CG	1:A:248:ALA:HB3	2.50	0.41
1:G:4639:GLN:O	1:G:4642:ARG:HG2	2.19	0.41
6:B:6588:HOH:O	1:D:2131:GLU:HB3	2.20	0.41
1:E:3423:LEU:HD12	1:F:4005:THR:HG21	2.01	0.41
1:A:176:ASP:HB3	1:A:179:LEU:CB	2.51	0.41
1:C:1287:ILE:O	1:C:1290:VAL:N	2.53	0.41
1:G:4669:PHE:HZ	1:G:4699:ARG:HD2	1.85	0.41
1:C:1428:LEU:HA	1:C:1428:LEU:HD23	1.82	0.41
1:A:210:LEU:CB	1:A:213:ALA:HB3	2.50	0.41
1:E:3172:LYS:HA	1:E:3182:LEU:O	2.20	0.41
1:A:401:SER:HB2	1:B:1021:LYS:HZ3	1.86	0.41
1:E:3272:ASN:OD1	1:E:3274:GLU:HB3	2.20	0.41
1:B:617:LEU:HD23	1:B:617:LEU:HA	1.89	0.41
1:G:4478:ARG:O	1:G:4482:ILE:HG13	2.21	0.41
1:F:3936:LYS:HA	1:F:3937:PRO:HD3	1.90	0.41
1:B:889:ILE:CG2	1:B:890:MET:N	2.83	0.41
1:F:3746:ALA:HB3	1:F:3747:TYR:CE1	2.54	0.41
1:D:2226:ALA:HA	1:D:2247:ALA:HB1	2.03	0.41
1:F:3700:ASP:OD2	1:F:3703:LEU:HD13	2.21	0.41
1:D:2271:VAL:HG11	1:D:2291:LEU:HG	2.03	0.41
1:B:1087:LEU:CD2	1:B:1088:ARG:N	2.79	0.41
1:C:1391:PHE:O	1:C:1392:LEU:HD13	2.21	0.41
1:C:1500:ILE:HB	1:C:1501:PRO:CD	2.49	0.41
1:B:731:VAL:HG12	1:B:732:GLU:N	2.35	0.41
1:B:693:ALA:O	1:B:696:SER:OG	2.29	0.41
1:B:1011:MET:HE1	1:B:1122:ASN:O	2.21	0.41
1:G:4429:LYS:HE2	1:G:4456:ILE:O	2.21	0.41
1:D:1864:ILE:HD13	1:D:1864:ILE:HG21	1.79	0.41
1:G:4319:ARG:H	1:G:4359:ASP:CB	2.33	0.41
1:C:1409:ASN:ND2	6:C:6568:HOH:O	2.51	0.41
1:A:454:ARG:CG	1:A:473:CYS:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1814:THR:HG22	1:D:1815:GLN:N	2.35	0.41
1:F:3653:ALA:HB2	1:F:3966:LYS:HA	2.03	0.41
1:H:5067:ILE:HD12	1:H:5088:GLY:CA	2.51	0.41
1:C:1708:VAL:CG1	1:C:1709:ILE:N	2.81	0.41
1:B:781:SER:HB3	1:B:798:ASN:HB2	2.03	0.41
1:A:518:SER:HB2	6:A:7722:HOH:O	2.21	0.41
1:C:1605:THR:HG22	6:D:6122:HOH:O	2.20	0.41
1:G:4727:VAL:HA	1:G:4728:PRO:HD3	1.92	0.41
1:D:2294:ASN:HD22	1:D:2294:ASN:HA	1.71	0.41
1:F:4007:LEU:HA	1:F:4007:LEU:HD23	1.64	0.41
1:C:1526:ALA:HB1	1:C:1559:MET:HE2	2.02	0.41
1:E:3143:LEU:HA	1:E:3143:LEU:HD12	1.65	0.41
1:A:191:PHE:CG	1:A:192:LEU:N	2.82	0.41
1:A:511:LEU:HD22	1:A:521:THR:CG2	2.44	0.41
1:A:47:ILE:HG22	1:A:359:MET:CG	2.42	0.41
1:C:1345:ASN:C	1:C:1347:TYR:N	2.74	0.41
1:G:4273:MET:CE	1:G:4286:THR:CG2	2.99	0.41
1:C:1421:SER:O	1:C:1425:ILE:HG13	2.21	0.41
1:A:173:VAL:HG13	1:A:210:LEU:CD1	2.49	0.41
1:G:4626:ALA:HA	1:G:4647:ALA:HB1	2.03	0.41
1:H:4945:ASN:O	1:H:4948:MET:HB2	2.21	0.41
1:B:1054:ARG:HH11	1:B:1054:ARG:HD2	1.64	0.41
1:A:133:LEU:CD1	1:A:133:LEU:N	2.84	0.41
1:E:3289:ILE:CG2	1:E:3290:MET:N	2.84	0.41
1:A:60:LEU:HA	1:A:60:LEU:HD12	1.43	0.41
1:F:4030:LEU:HD23	1:F:4030:LEU:N	2.35	0.41
1:A:176:ASP:O	1:A:179:LEU:HB2	2.21	0.41
1:C:1334:LYS:HB3	1:C:1334:LYS:HE3	1.82	0.41
1:G:4463:ASN:HA	1:G:4463:ASN:HD22	1.62	0.41
1:H:5237:ALA:HB1	1:H:5268:ILE:HD13	2.02	0.41
1:F:3702:ILE:CD1	1:F:4094:ASN:HB2	2.50	0.41
1:F:3844:ILE:HG13	1:F:3868:SER:HB3	2.03	0.41
1:B:790:ASP:OD1	1:B:790:ASP:O	2.38	0.41
1:E:3037:ALA:HA	1:E:3038:PRO:HD3	1.91	0.41
1:B:976:MET:CE	1:B:980:ILE:CG1	2.99	0.41
1:D:2329:VAL:HA	1:D:2330:PRO:HD3	1.90	0.41
1:A:73:MET:CE	1:A:86:THR:CG2	2.99	0.41
1:G:4374:TYR:HA	1:G:4380:ILE:O	2.20	0.41
1:G:4625:ALA:CB	1:G:4702:PHE:HB3	2.51	0.41
1:D:1819:ALA:HB2	1:D:1831:ARG:HB2	2.03	0.41
1:F:3837:ASP:HB3	1:F:4061:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1579:LEU:HD12	1:C:1579:LEU:HA	1.81	0.41
1:H:4986:GLN:HG2	1:H:4993:VAL:HB	2.02	0.41
1:F:4030:LEU:HD13	1:F:4088:ARG:HB2	2.03	0.41
1:F:4099:ARG:HA	1:F:4099:ARG:HD3	1.84	0.41
1:C:1720:PHE:CE2	1:C:1722:ASN:HB3	2.56	0.41
1:F:3878:ARG:O	1:F:3881:GLU:HG2	2.20	0.41
1:F:3735:LYS:HG2	1:F:3736:GLY:N	2.35	0.41
1:G:4726:VAL:CG2	1:H:5211:MET:SD	3.09	0.41
1:D:2209:GLU:O	1:D:2213:MET:HG3	2.21	0.41
1:C:1535:LYS:HD3	1:C:1535:LYS:HA	1.91	0.41
1:E:3142:THR:CG2	1:E:3143:LEU:N	2.84	0.40
1:H:5020:VAL:CG1	1:H:5025:ILE:CG1	2.99	0.40
1:G:4402:LEU:HA	1:G:4402:LEU:HD22	1.77	0.40
1:G:4273:MET:HE3	1:G:4286:THR:CG2	2.49	0.40
1:F:3788:GLY:HA3	1:F:3791:PHE:CZ	2.57	0.40
1:H:4847:ILE:CG2	1:H:5159:MET:CE	2.97	0.40
1:E:3145:ASN:ND2	1:E:3161:LYS:NZ	2.69	0.40
1:D:2192:LYS:CG	6:D:7588:HOH:O	2.69	0.40
1:C:1611:MET:HE3	1:C:1724:MET:HB2	2.03	0.40
1:G:4275:PHE:CE2	1:G:4280:HIS:CD2	3.06	0.40
1:B:942:ALA:HB1	1:D:2146:ASP:HB2	2.03	0.40
1:B:825:ILE:O	1:B:829:LYS:HG3	2.21	0.40
1:E:3335:LYS:HE2	1:E:3368:ASP:OD2	2.20	0.40
1:F:3842:SER:HA	1:F:3869:LYS:HD3	2.03	0.40
1:B:673:MET:CE	1:B:686:THR:HG22	2.51	0.40
1:E:3398:ALA:CB	1:E:3413:MET:CE	2.99	0.40
1:E:3421:LYS:HD3	1:F:4013:MET:SD	2.61	0.40
1:C:1656:HIS:N	1:C:1656:HIS:CD2	2.88	0.40
1:C:1371:SER:O	1:C:1383:GLN:HA	2.22	0.40
1:A:57:VAL:CG2	1:A:89:ASN:CB	3.00	0.40
1:H:5037:ASP:OD1	1:H:5260:ARG:HD2	2.20	0.40
1:E:3294:GLY:HA3	1:E:3327:THR:HG21	2.04	0.40
1:C:1215:GLN:HA	6:C:6142:HOH:O	2.21	0.40
1:D:2240:VAL:HG12	1:D:2249:ILE:CD1	2.51	0.40
6:A:7332:HOH:O	1:C:1542:ALA:HB3	2.20	0.40
1:G:4654:ARG:HH11	1:G:4654:ARG:HD2	1.77	0.40
1:E:3340:THR:HB	1:G:4528:GLN:HE21	1.86	0.40
1:A:47:ILE:CB	1:A:359:MET:HG3	2.51	0.40
1:C:1456:ILE:N	1:C:1456:ILE:CD1	2.79	0.40
1:C:1272:ARG:HE	1:C:1312:ASP:CG	2.22	0.40
1:G:4608:MET:HG3	1:G:4639:GLN:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1429:LYS:O	1:C:1433:GLU:HG2	2.21	0.40
1:F:4055:ASN:O	1:F:4058:THR:HB	2.21	0.40
1:D:2254:ARG:HD2	6:D:7101:HOH:O	2.20	0.40
1:E:3478:GLN:HB2	1:E:3484:ASP:HB2	2.02	0.40
1:G:4570:PRO:HD2	6:G:6548:HOH:O	2.19	0.40
1:A:216:ASP:OD1	1:A:216:ASP:O	2.39	0.40
1:A:235:ASP:O	1:A:235:ASP:OD1	2.39	0.40
1:G:4353:GLU:HG2	1:G:4353:GLU:H	1.44	0.40
1:C:1250:ILE:CG2	1:C:1286:THR:CG2	3.00	0.40
1:C:1273:MET:CE	1:C:1286:THR:CG2	2.99	0.40
1:D:1850:ILE:CG1	1:D:1873:MET:HE1	2.51	0.40
1:C:1357:TRP:CD2	1:C:1358:LEU:N	2.90	0.40
1:C:1277:HIS:NE2	5:C:1735:ATP:H3'	2.36	0.40
1:H:5275:ASP:CB	1:H:5276:PRO:CD	2.99	0.40
1:A:451:ALA:CB	1:A:468:ILE:CG2	2.99	0.40
1:F:3809:ASN:C	1:F:3811:PRO:HD3	2.42	0.40
1:D:2311:LEU:HD23	1:D:2323:THR:O	2.20	0.40
1:C:1482:ILE:O	1:C:1486:SER:OG	2.38	0.40
1:C:1273:MET:CE	1:C:1286:THR:HG22	2.49	0.40
1:F:3650:ILE:HD12	1:F:3650:ILE:HG23	1.82	0.40
1:B:1128:PRO:O	1:B:1130:PRO:HD3	2.22	0.40
1:G:4363:ILE:O	1:G:4366:VAL:HB	2.21	0.40
1:F:3721:GLY:N	1:F:3757:TRP:HE3	2.19	0.40
1:A:454:ARG:CZ	1:A:477:VAL:HG22	2.51	0.40
1:E:3287:ASP:O	1:E:3322:PRO:HD2	2.21	0.40
1:H:4852:PRO:HD2	1:H:5165:ALA:O	2.21	0.40
1:D:2246:ARG:HD3	6:D:6077:HOH:O	2.22	0.40
1:D:2093:ARG:NH2	1:D:2146:ASP:OD1	2.55	0.40
1:F:3939:PRO:HG3	1:F:3976:MET:HG2	2.03	0.40
1:F:3916:CYS:HB3	1:F:3921:LYS:O	2.22	0.40
1:G:4417:LEU:HA	1:G:4418:PRO:HD3	1.89	0.40
1:F:3702:ILE:HD12	1:F:4094:ASN:HB3	2.03	0.40
1:F:3969:TYR:N	1:F:3970:PRO:CD	2.83	0.40
1:G:4606:ASP:O	1:G:4609:GLU:HB2	2.22	0.40
1:D:2259:ALA:HB1	1:D:2270:PRO:HB2	2.02	0.40
1:B:649:THR:OG1	1:B:672:ARG:NH1	2.50	0.40
1:E:3525:ARG:HD3	1:F:4114:TRP:CE3	2.57	0.40

All (25) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3149:GLU:OE1	1:H:4934:LYS:CE[3_655]	0.65	1.55
1:E:3149:GLU:CD	1:H:4934:LYS:NZ[3_655]	1.12	1.08
1:E:3081:GLU:OE1	1:H:4924:LYS:NZ[3_655]	1.15	1.05
1:E:3149:GLU:CD	1:H:4934:LYS:CE[3_655]	1.22	0.98
1:D:1924:LYS:NZ	1:H:4858:GLU:OE1[1_455]	1.29	0.91
1:E:3149:GLU:OE1	1:H:4934:LYS:CD[3_655]	1.43	0.77
1:E:3124:LYS:O	6:H:6943:HOH:O[3_655]	1.55	0.65
1:E:3149:GLU:OE2	1:H:4934:LYS:NZ[3_655]	1.58	0.62
1:D:1948:MET:CE	1:F:3765:LYS:NZ[4_465]	1.65	0.55
1:E:3149:GLU:OE1	1:H:4934:LYS:NZ[3_655]	1.68	0.52
1:E:3124:LYS:C	6:H:6943:HOH:O[3_655]	1.72	0.48
1:D:1924:LYS:CE	1:H:4858:GLU:OE1[1_455]	1.74	0.46
1:D:1945:ASN:OD1	1:F:3816:ASP:OD2[4_465]	1.83	0.37
1:E:3149:GLU:OE2	1:H:4934:LYS:CE[3_655]	1.88	0.32
1:E:3081:GLU:OE1	1:H:4924:LYS:CE[3_655]	1.92	0.28
1:C:1387:LYS:O	1:H:4987:LYS:CB[3_645]	1.97	0.23
1:C:1386:GLN:CB	1:H:4989:PRO:CD[3_645]	2.00	0.20
1:D:1924:LYS:NZ	1:H:4858:GLU:CD[1_455]	2.01	0.19
1:E:3149:GLU:CG	1:H:4934:LYS:NZ[3_655]	2.03	0.17
1:A:277:ARG:NH1	1:G:4425:ILE:CD1[4_465]	2.08	0.12
1:E:3081:GLU:CD	1:H:4924:LYS:NZ[3_655]	2.10	0.10
1:A:277:ARG:CZ	1:G:4425:ILE:CD1[4_465]	2.11	0.09
1:B:801:PHE:CE2	6:H:7250:HOH:O[1_455]	2.11	0.09
1:E:3081:GLU:CD	1:H:4924:LYS:CE[3_655]	2.14	0.06
1:C:1385:LYS:O	1:H:4989:PRO:CG[3_645]	2.14	0.06

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	517/530 (98%)	480 (93%)	33 (6%)	4 (1%)	24 17
1	B	517/530 (98%)	492 (95%)	20 (4%)	5 (1%)	19 13
1	C	517/530 (98%)	471 (91%)	41 (8%)	5 (1%)	19 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	517/530 (98%)	493 (95%)	21 (4%)	3 (1%)	30	24
1	E	517/530 (98%)	488 (94%)	24 (5%)	5 (1%)	19	13
1	F	517/530 (98%)	490 (95%)	23 (4%)	4 (1%)	24	17
1	G	517/530 (98%)	488 (94%)	25 (5%)	4 (1%)	24	17
1	H	517/530 (98%)	490 (95%)	24 (5%)	3 (1%)	30	24
All	All	4136/4240 (98%)	3892 (94%)	211 (5%)	33 (1%)	24	17

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	PRO
1	C	1533	MET
1	E	3506	ASP
1	F	3729	ALA
1	F	3789	PRO
1	H	4924	LYS
1	A	221	SER
1	C	1346	ALA
1	D	2058	GLY
1	F	3730	GLU
1	G	4345	ASN
1	G	4389	PRO
1	A	164	CYS
1	B	745	ASN
1	D	2277	VAL
1	E	3013	GLN
1	C	1337	ALA
1	E	3145	ASN
1	B	1002	SER
1	C	1527	THR
1	C	1532	SER
1	D	2127	THR
1	E	3327	THR
1	G	4458	GLY
1	A	327	THR
1	B	927	THR
1	B	1128	PRO
1	F	3927	THR
1	G	4527	THR
1	H	4901	PRO

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Mol	Chain	Res	Type
1	H	5127	THR
1	B	701	PRO
1	E	3163	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	426/434 (98%)	349 (82%)	77 (18%)	2 1
1	B	426/434 (98%)	379 (89%)	47 (11%)	8 4
1	C	426/434 (98%)	358 (84%)	68 (16%)	3 1
1	D	426/434 (98%)	384 (90%)	42 (10%)	10 6
1	E	426/434 (98%)	372 (87%)	54 (13%)	5 3
1	F	426/434 (98%)	373 (88%)	53 (12%)	6 3
1	G	426/434 (98%)	368 (86%)	58 (14%)	5 2
1	H	426/434 (98%)	391 (92%)	35 (8%)	14 10
All	All	3408/3472 (98%)	2974 (87%)	434 (13%)	5 3

All (434) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	15	GLN
1	A	60	LEU
1	A	68	MET
1	A	73	MET
1	A	86	THR
1	A	88	LYS
1	A	92	THR
1	A	96	SER
1	A	99	SER
1	A	113	THR
1	A	114	LYS

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Mol	Chain	Res	Type
1	A	120	THR
1	A	130	GLU
1	A	133	LEU
1	A	134	LYS
1	A	138	THR
1	A	145	ASN
1	A	148	MET
1	A	150	LYS
1	A	153	GLU
1	A	156	LEU
1	A	158	LEU
1	A	162	ASN
1	A	163	ILE
1	A	164	CYS
1	A	166	VAL
1	A	167	VAL
1	A	168	ASP
1	A	175	VAL
1	A	176	ASP
1	A	180	ILE
1	A	185	LYS
1	A	190	ASP
1	A	192	LEU
1	A	202	LEU
1	A	206	LYS
1	A	210	LEU
1	A	215	VAL
1	A	223	LYS
1	A	245	ARG
1	A	246	LYS
1	A	257	LEU
1	A	260	LYS
1	A	267	ILE
1	A	271	GLU
1	A	278	ARG
1	A	283	LEU
1	A	284	GLU
1	A	289	ILE
1	A	311	MET
1	A	328	GLN
1	A	330	LEU
1	A	366	LYS

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Mol	Chain	Res	Type
1	A	375	ARG
1	A	376	MET
1	A	380	ILE
1	A	389	PHE
1	A	397	LEU
1	A	400	SER
1	A	405	THR
1	A	407	LEU
1	A	411	MET
1	A	423	LEU
1	A	435	ARG
1	A	464	LEU
1	A	469	PHE
1	A	471	VAL
1	A	478	GLN
1	A	479	GLU
1	A	493	MET
1	A	497	LYS
1	A	502	PHE
1	A	508	VAL
1	A	518	SER
1	A	521	THR
1	A	522	ASN
1	B	615	GLN
1	B	640	THR
1	B	660	LEU
1	B	661	LYS
1	B	673	MET
1	B	676	SER
1	B	681	GLU
1	B	703	LEU
1	B	719	ARG
1	B	745	ASN
1	B	748	MET
1	B	756	LEU
1	B	759	ASP
1	B	782	LEU
1	B	785	LYS
1	B	786	GLN
1	B	798	ASN
1	B	810	LEU
1	B	811	PRO

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Mol	Chain	Res	Type
1	B	822	GLU
1	B	843	PHE
1	B	846	LYS
1	B	883	LEU
1	B	886	SER
1	B	921	LYS
1	B	952	LEU
1	B	982	ARG
1	B	989	PHE
1	B	1004	SER
1	B	1035	ARG
1	B	1039	GLN
1	B	1042	ARG
1	B	1046	ARG
1	B	1064	LEU
1	B	1066	ARG
1	B	1069	PHE
1	B	1078	GLN
1	B	1086	ASP
1	B	1090	ASN
1	B	1093	MET
1	B	1099	ARG
1	B	1102	PHE
1	B	1103	LYS
1	B	1104	LYS
1	B	1107	VAL
1	B	1118	SER
1	B	1125	ARG
1	C	1214	THR
1	C	1229	MET
1	C	1257	VAL
1	C	1273	MET
1	C	1281	GLU
1	C	1288	LYS
1	C	1292	THR
1	C	1295	GLU
1	C	1302	ILE
1	C	1313	THR
1	C	1319	ARG
1	C	1323	ILE
1	C	1328	THR
1	C	1334	LYS

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Mol	Chain	Res	Type
1	C	1335	LYS
1	C	1342	THR
1	C	1348	MET
1	C	1358	LEU
1	C	1359	ASP
1	C	1363	ILE
1	C	1368	ASP
1	C	1372	LYS
1	C	1380	ILE
1	C	1387	LYS
1	C	1390	ASP
1	C	1394	THR
1	C	1395	GLU
1	C	1404	SER
1	C	1405	LYS
1	C	1410	LEU
1	C	1415	VAL
1	C	1422	GLU
1	C	1442	SER
1	C	1446	LYS
1	C	1454	ARG
1	C	1457	LEU
1	C	1459	GLU
1	C	1462	LYS
1	C	1469	LYS
1	C	1472	ASN
1	C	1483	LEU
1	C	1484	GLU
1	C	1486	SER
1	C	1498	ILE
1	C	1518	ARG
1	C	1530	LEU
1	C	1532	SER
1	C	1538	ARG
1	C	1566	LYS
1	C	1582	ARG
1	C	1583	GLU
1	C	1589	PHE
1	C	1592	LYS
1	C	1597	LEU
1	C	1599	ARG
1	C	1600	SER

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Mol	Chain	Res	Type
1	C	1633	SER
1	C	1642	ARG
1	C	1664	LEU
1	C	1666	ARG
1	C	1675	ASP
1	C	1678	GLN
1	C	1679	GLU
1	C	1686	ASP
1	C	1687	LEU
1	C	1693	MET
1	C	1718	SER
1	C	1723	THR
1	D	1812	ILE
1	D	1824	THR
1	D	1856	SER
1	D	1860	LEU
1	D	1873	MET
1	D	1885	GLU
1	D	1887	ILE
1	D	1899	SER
1	D	1902	ILE
1	D	1919	ARG
1	D	1930	GLU
1	D	1931	VAL
1	D	1938	THR
1	D	1942	THR
1	D	1945	ASN
1	D	1959	ASP
1	D	1962	ASN
1	D	1966	VAL
1	D	1967	VAL
1	D	1972	LYS
1	D	1985	LYS
1	D	1986	GLN
1	D	2005	LYS
1	D	2010	LEU
1	D	2023	LYS
1	D	2046	LYS
1	D	2059	GLU
1	D	2081	GLU
1	D	2141	ARG
1	D	2145	SER

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Mol	Chain	Res	Type
1	D	2189	PHE
1	D	2199	ARG
1	D	2205	THR
1	D	2209	GLU
1	D	2246	ARG
1	D	2266	ARG
1	D	2279	GLU
1	D	2283	GLU
1	D	2293	MET
1	D	2303	LYS
1	D	2308	VAL
1	D	2318	SER
1	E	3014	THR
1	E	3015	GLN
1	E	3016	GLN
1	E	3029	MET
1	E	3031	ARG
1	E	3034	ILE
1	E	3055	ARG
1	E	3056	SER
1	E	3066	SER
1	E	3080	HIS
1	E	3081	GLU
1	E	3099	SER
1	E	3101	PRO
1	E	3102	ILE
1	E	3113	THR
1	E	3124	LYS
1	E	3131	VAL
1	E	3133	LEU
1	E	3143	LEU
1	E	3145	ASN
1	E	3155	ILE
1	E	3156	LEU
1	E	3158	LEU
1	E	3162	ASN
1	E	3164	CYS
1	E	3166	VAL
1	E	3167	VAL
1	E	3168	ASP
1	E	3192	LEU
1	E	3222	GLU

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Mol	Chain	Res	Type
1	E	3246	LYS
1	E	3257	LEU
1	E	3267	ILE
1	E	3271	GLU
1	E	3283	LEU
1	E	3286	SER
1	E	3315	ARG
1	E	3330	LEU
1	E	3336	LYS
1	E	3338	ARG
1	E	3379	LEU
1	E	3382	ARG
1	E	3389	PHE
1	E	3407	LEU
1	E	3433	SER
1	E	3435	ARG
1	E	3442	ARG
1	E	3446	ARG
1	E	3466	ARG
1	E	3469	PHE
1	E	3479	GLU
1	E	3483	GLU
1	E	3504	LYS
1	E	3526	VAL
1	F	3612	ILE
1	F	3613	GLN
1	F	3623	ASP
1	F	3624	THR
1	F	3640	THR
1	F	3655	ARG
1	F	3666	SER
1	F	3673	MET
1	F	3679	THR
1	F	3687	ILE
1	F	3696	SER
1	F	3702	ILE
1	F	3713	THR
1	F	3714	LYS
1	F	3723	ILE
1	F	3726	SER
1	F	3728	THR
1	F	3742	THR

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Mol	Chain	Res	Type
1	F	3753	GLU
1	F	3755	ILE
1	F	3759	ASP
1	F	3762	ASN
1	F	3765	LYS
1	F	3767	VAL
1	F	3769	VAL
1	F	3772	LYS
1	F	3782	LEU
1	F	3787	LYS
1	F	3792	LEU
1	F	3804	SER
1	F	3810	LEU
1	F	3821	SER
1	F	3823	LYS
1	F	3845	ARG
1	F	3856	ILE
1	F	3862	LYS
1	F	3872	ASN
1	F	3878	ARG
1	F	3884	GLU
1	F	3886	SER
1	F	3935	LYS
1	F	3945	SER
1	F	3966	LYS
1	F	3976	MET
1	F	3989	PHE
1	F	4002	SER
1	F	4015	SER
1	F	4032	GLU
1	F	4066	ARG
1	F	4079	GLU
1	F	4093	MET
1	F	4107	VAL
1	F	4118	SER
1	G	4212	ILE
1	G	4215	GLN
1	G	4216	GLN
1	G	4240	THR
1	G	4254	SER
1	G	4255	ARG
1	G	4258	GLU

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Mol	Chain	Res	Type
1	G	4265	LYS
1	G	4268	MET
1	G	4273	MET
1	G	4296	SER
1	G	4303	LEU
1	G	4313	THR
1	G	4320	THR
1	G	4330	GLU
1	G	4338	THR
1	G	4343	LEU
1	G	4353	GLU
1	G	4359	ASP
1	G	4361	LYS
1	G	4367	VAL
1	G	4372	LYS
1	G	4375	VAL
1	G	4380	ILE
1	G	4382	LEU
1	G	4383	GLN
1	G	4386	GLN
1	G	4387	LYS
1	G	4390	ASP
1	G	4392	LEU
1	G	4395	GLU
1	G	4402	LEU
1	G	4404	SER
1	G	4409	ASN
1	G	4417	LEU
1	G	4449	ASP
1	G	4471	GLU
1	G	4498	ILE
1	G	4500	ILE
1	G	4517	ASN
1	G	4545	SER
1	G	4552	LEU
1	G	4589	PHE
1	G	4597	LEU
1	G	4599	ARG
1	G	4600	SER
1	G	4604	SER
1	G	4627	LEU
1	G	4649	ILE

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Mol	Chain	Res	Type
1	G	4656	HIS
1	G	4664	LEU
1	G	4666	ARG
1	G	4693	MET
1	G	4699	ARG
1	G	4702	PHE
1	G	4703	LYS
1	G	4707	VAL
1	G	4715	ARG
1	H	4814	THR
1	H	4827	GLU
1	H	4848	CYS
1	H	4855	ARG
1	H	4873	MET
1	H	4905	ARG
1	H	4922	LEU
1	H	4926	SER
1	H	4932	GLU
1	H	4935	LYS
1	H	4942	THR
1	H	4950	LYS
1	H	4972	LYS
1	H	4986	GLN
1	H	4992	LEU
1	H	5010	LEU
1	H	5046	LYS
1	H	5060	LYS
1	H	5071	GLU
1	H	5072	ASN
1	H	5118	ARG
1	H	5182	ARG
1	H	5189	PHE
1	H	5206	ASP
1	H	5207	LEU
1	H	5264	LEU
1	H	5269	PHE
1	H	5278	GLN
1	H	5286	ASP
1	H	5297	LYS
1	H	5299	ARG
1	H	5303	LYS
1	H	5308	VAL

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Mol	Chain	Res	Type
1	H	5318	SER
1	H	5321	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	89	ASN
1	A	145	ASN
1	A	162	ASN
1	A	198	ASN
1	A	209	ASN
1	A	263	ASN
1	A	273	HIS
1	A	328	GLN
1	A	349	ASN
1	A	377	GLN
1	A	438	HIS
1	A	456	HIS
1	A	522	ASN
1	B	643	ASN
1	B	689	ASN
1	B	745	ASN
1	B	762	ASN
1	B	783	GLN
1	B	798	ASN
1	B	826	GLN
1	B	863	ASN
1	B	928	GLN
1	B	949	ASN
1	B	977	GLN
1	B	990	HIS
1	B	1056	HIS
1	B	1063	HIS
1	B	1078	GLN
1	C	1218	HIS
1	C	1243	ASN
1	C	1345	ASN
1	C	1362	ASN
1	C	1409	ASN
1	C	1426	GLN
1	C	1463	ASN

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Mol	Chain	Res	Type
1	C	1472	ASN
1	C	1528	GLN
1	C	1549	ASN
1	C	1577	GLN
1	C	1590	HIS
1	C	1656	HIS
1	C	1678	GLN
1	C	1690	ASN
1	D	1818	HIS
1	D	1843	ASN
1	D	1889	ASN
1	D	1945	ASN
1	D	1986	GLN
1	D	1998	ASN
1	D	2073	HIS
1	D	2128	GLN
1	D	2149	ASN
1	D	2177	GLN
1	D	2190	HIS
1	D	2238	HIS
1	D	2256	HIS
1	D	2257	GLN
1	D	2263	HIS
1	D	2294	ASN
1	E	3043	ASN
1	E	3080	HIS
1	E	3089	ASN
1	E	3145	ASN
1	E	3162	ASN
1	E	3198	ASN
1	E	3263	ASN
1	E	3328	GLN
1	E	3349	ASN
1	E	3377	GLN
1	E	3390	HIS
1	E	3463	HIS
1	F	3613	GLN
1	F	3615	GLN
1	F	3618	HIS
1	F	3683	HIS
1	F	3689	ASN
1	F	3786	GLN

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Mol	Chain	Res	Type
1	F	3798	ASN
1	F	3809	ASN
1	F	3863	ASN
1	F	3872	ASN
1	F	3873	HIS
1	F	3928	GLN
1	F	3949	ASN
1	F	4063	HIS
1	G	4215	GLN
1	G	4216	GLN
1	G	4243	ASN
1	G	4289	ASN
1	G	4345	ASN
1	G	4383	GLN
1	G	4409	ASN
1	G	4463	ASN
1	G	4528	GLN
1	G	4549	ASN
1	G	4577	GLN
1	G	4638	HIS
1	H	4843	ASN
1	H	4889	ASN
1	H	4986	GLN
1	H	5063	ASN
1	H	5072	ASN
1	H	5128	GLN
1	H	5149	ASN
1	H	5177	GLN
1	H	5256	HIS
1	H	5261	GLN
1	H	5263	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 22 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OXL	A	533	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	A	535	2,4	24,33,33	1.49	5 (20%)	31,52,52	1.49	4 (12%)
3	OXL	B	1133	4	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	C	1733	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	C	1735	2,4	24,33,33	1.63	4 (16%)	31,52,52	1.17	4 (12%)
3	OXL	D	2333	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	D	2335	2,4	24,33,33	1.55	5 (20%)	31,52,52	1.29	6 (19%)
3	OXL	E	3533	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	E	3535	2,4	24,33,33	1.65	4 (16%)	31,52,52	1.18	2 (6%)
3	OXL	F	4133	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	F	4135	2,4	24,33,33	1.62	4 (16%)	31,52,52	1.05	1 (3%)
3	OXL	G	4733	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	G	4735	2,4	24,33,33	1.65	4 (16%)	31,52,52	1.25	3 (9%)
3	OXL	H	5333	4	0,5,5	0.00	-	0,6,6	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	A	533	4	-	0/0/4/4	0/0/0/0
5	ATP	A	535	2,4	-	0/18/38/38	0/3/3/3
3	OXL	B	1133	4	-	0/0/4/4	0/0/0/0
3	OXL	C	1733	4	-	0/0/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	C	1735	2,4	-	0/18/38/38	0/3/3/3
3	OXL	D	2333	4	-	0/0/4/4	0/0/0/0
5	ATP	D	2335	2,4	-	0/18/38/38	0/3/3/3
3	OXL	E	3533	4	-	0/0/4/4	0/0/0/0
5	ATP	E	3535	2,4	-	0/18/38/38	0/3/3/3
3	OXL	F	4133	4	-	0/0/4/4	0/0/0/0
5	ATP	F	4135	2,4	-	0/18/38/38	0/3/3/3
3	OXL	G	4733	4	-	0/0/4/4	0/0/0/0
5	ATP	G	4735	2,4	-	0/18/38/38	0/3/3/3
3	OXL	H	5333	4	-	0/0/4/4	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3535	ATP	PG-O3G	-5.19	1.36	1.54
5	D	2335	ATP	PG-O3G	-4.40	1.38	1.54
5	G	4735	ATP	PG-O3G	-4.32	1.39	1.54
5	C	1735	ATP	PG-O3G	-3.99	1.40	1.54
5	C	1735	ATP	O4'-C1'	-3.94	1.36	1.41
5	G	4735	ATP	O4'-C1'	-3.91	1.36	1.41
5	A	535	ATP	PG-O3G	-3.77	1.41	1.54
5	F	4135	ATP	PG-O3G	-3.37	1.42	1.54
5	E	3535	ATP	PG-O2G	-2.88	1.44	1.54
5	D	2335	ATP	PA-O2A	-2.31	1.45	1.54
5	D	2335	ATP	PG-O2G	-2.24	1.46	1.54
5	G	4735	ATP	PA-O2A	-2.23	1.45	1.54
5	A	535	ATP	PG-O2G	-2.22	1.46	1.54
5	C	1735	ATP	PG-O2G	-2.15	1.47	1.54
5	G	4735	ATP	PG-O1G	-2.12	1.44	1.51
5	A	535	ATP	PB-O2B	-2.03	1.46	1.54
5	F	4135	ATP	C6-N6	2.08	1.41	1.34
5	D	2335	ATP	PA-O5'	2.15	1.68	1.59
5	D	2335	ATP	C4-N3	2.16	1.38	1.35
5	E	3535	ATP	PA-O5'	2.18	1.69	1.59
5	A	535	ATP	C4-N3	2.21	1.38	1.35
5	E	3535	ATP	C2-N1	2.27	1.38	1.33
5	C	1735	ATP	C2-N1	3.13	1.39	1.33
5	F	4135	ATP	PA-O5'	3.47	1.74	1.59
5	A	535	ATP	C2-N1	3.86	1.41	1.33
5	F	4135	ATP	C2-N1	3.94	1.41	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	3535	ATP	C2'-C1'-N9	-2.93	109.81	114.29
5	A	535	ATP	O3A-PA-O5'	-2.92	95.19	102.94
5	G	4735	ATP	C1'-N9-C4	-2.78	122.75	126.94
5	D	2335	ATP	O3A-PA-O5'	-2.63	95.96	102.94
5	C	1735	ATP	C2'-C1'-N9	-2.57	110.37	114.29
5	G	4735	ATP	C2'-C1'-N9	-2.49	110.48	114.29
5	C	1735	ATP	O2G-PG-O1G	-2.31	103.14	110.58
5	A	535	ATP	C1'-N9-C4	-2.14	123.72	126.94
5	D	2335	ATP	O3G-PG-O1G	-2.13	103.72	110.58
5	A	535	ATP	O2G-PG-O1G	-2.06	103.96	110.58
5	D	2335	ATP	O2B-PB-O3B	-2.06	95.76	105.09
5	C	1735	ATP	C2'-C3'-C4'	-2.05	98.39	102.61
5	E	3535	ATP	C1'-N9-C4	-2.00	123.92	126.94
5	F	4135	ATP	N6-C6-N1	2.06	123.63	119.20
5	D	2335	ATP	C4-C5-N7	2.07	111.38	109.48
5	D	2335	ATP	O4'-C1'-N9	2.07	112.44	108.10
5	C	1735	ATP	O2B-PB-O3A	2.28	115.43	105.09
5	D	2335	ATP	O3G-PG-O3B	2.31	115.58	105.09
5	G	4735	ATP	O3A-PA-O5'	4.00	113.55	102.94
5	A	535	ATP	O2B-PB-O3B	4.90	127.32	105.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	533	OXL	2	0
5	A	535	ATP	3	0
3	C	1733	OXL	1	0
5	C	1735	ATP	3	0
5	D	2335	ATP	1	0
3	F	4133	OXL	1	0
3	G	4733	OXL	1	0
5	G	4735	ATP	1	0
3	H	5333	OXL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.