Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:39 PM GMT

PDB ID	:	1BU6
Title	:	CRYSTAL STRUCTURES OF ESCHERICHIA COLI GLYCEROL KINASE AND THE MUTANT A65T IN AN INACTIVE TETRAMER: CONFORMATIONAL CHANGES AND IMPLICATIONS FOR ALLOSTERIC REGULATION
Authors	:	Feese, M.D.; Faber, H.R.; Bystrom, C.E.; Pettigrew, D.W.; Remington, S.J.
Deposited on	:	1998-08-30
Resolution	:	2.37 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 (1)) were used in the production of this report:

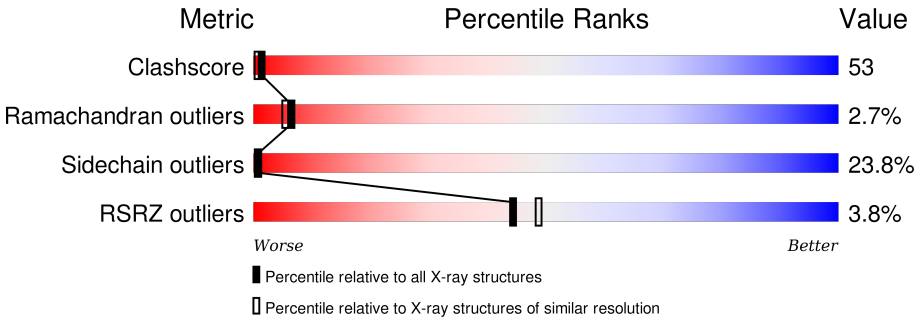
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.37 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	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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.

Mol	Chain	Length	Quality of chain
1	O	501	5% 26% 45% 22% 7%
1	X	501	4% 28% 45% 19% 7%
1	Y	501	2% 29% 44% 23%
1	Z	501	4% 26% 48% 21% 5%

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
2	SO4	O	502	-	-	X	-
2	SO4	X	502	-	-	-	X
2	SO4	Y	502	-	-	-	X
3	GOL	O	504	-	-	-	X
3	GOL	X	503	-	-	-	X
3	GOL	Y	503	-	-	-	X
3	GOL	Z	504	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15815 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.

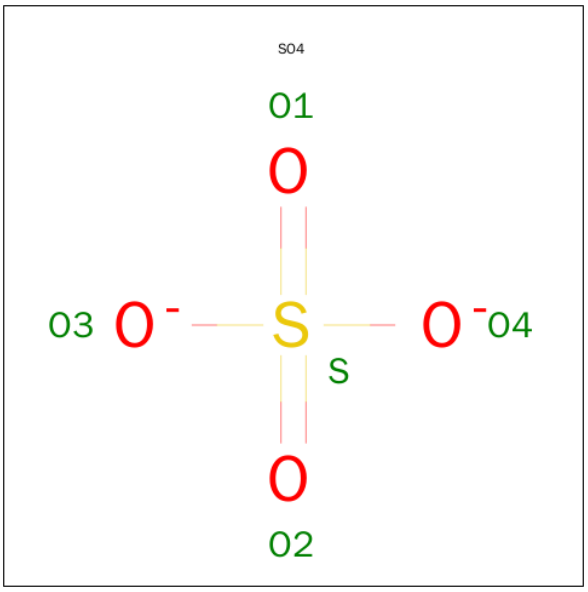
- Molecule 1 is a protein called PROTEIN (GLYCEROL KINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	497	Total	C	N	O	S	0	0	0
			3891	2452	680	740	19			
1	Y	499	Total	C	N	O	S	0	0	0
			3921	2471	686	745	19			
1	Z	498	Total	C	N	O	S	0	0	0
			3913	2465	686	743	19			
1	X	498	Total	C	N	O	S	0	0	0
			3896	2456	681	740	19			

There are 4 discrepancies between the modelled and reference sequences:

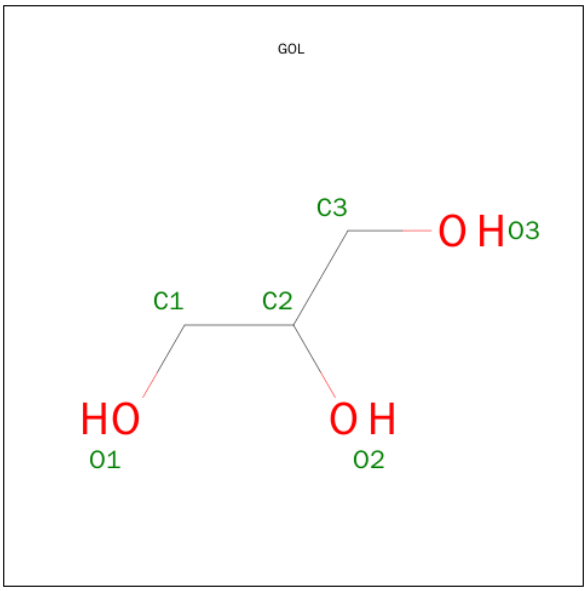
Chain	Residue	Modelled	Actual	Comment	Reference
O	65	THR	ALA	ENGINEERED	UNP P0A6F3
Y	65	THR	ALA	ENGINEERED	UNP P0A6F3
Z	65	THR	ALA	ENGINEERED	UNP P0A6F3
X	65	THR	ALA	ENGINEERED	UNP P0A6F3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	O	1	Total O S 5 4 1	0	0
2	Z	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	Y	1	Total O S 5 4 1	0	0
2	Z	1	Total O S 5 4 1	0	0
2	X	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total C O 6 3 3	0	0
3	Y	1	Total C O 6 3 3	0	0
3	Z	1	Total C O 6 3 3	0	0
3	X	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

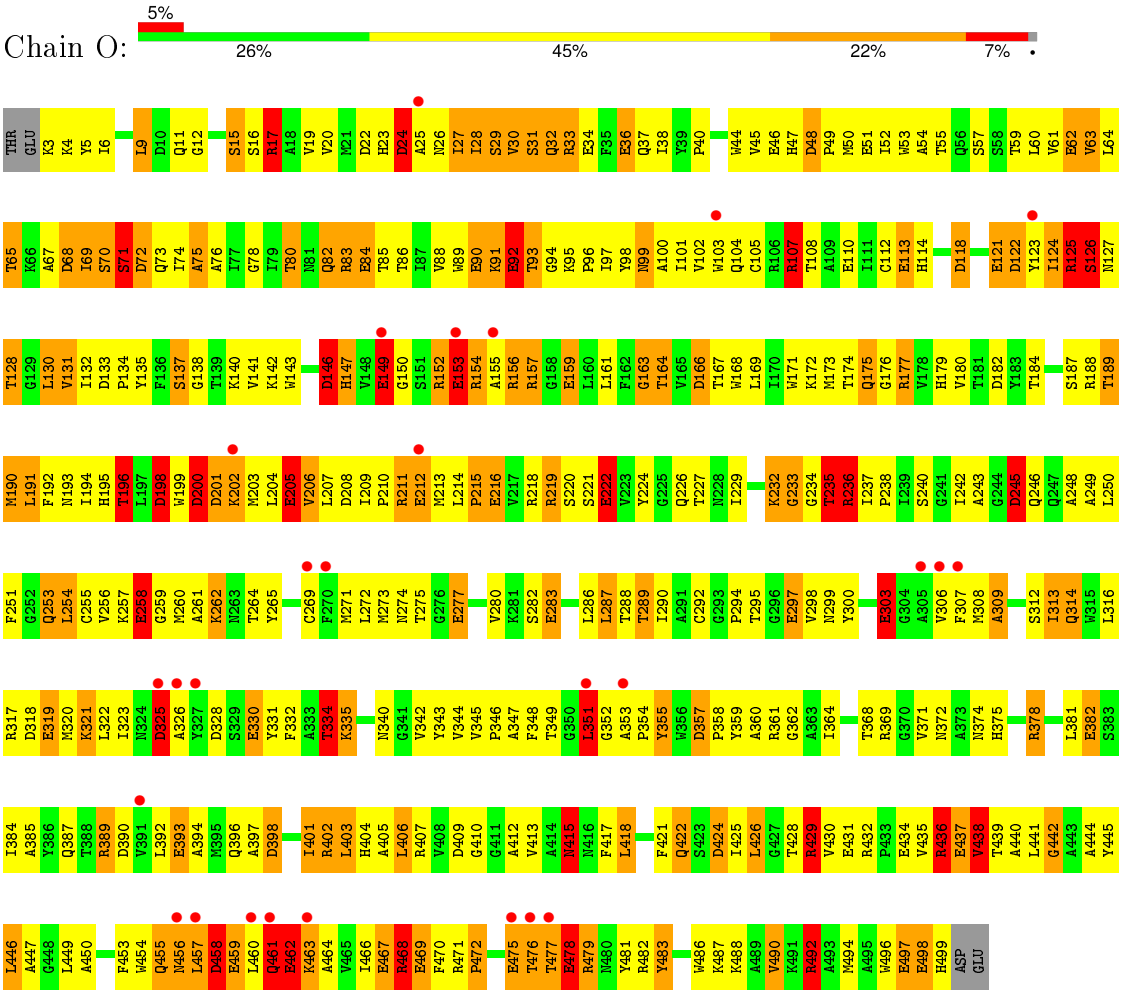
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	29	Total O 29 29	0	0
4	X	42	Total O 42 42	0	0
4	Y	38	Total O 38 38	0	0
4	Z	31	Total O 31 31	0	0

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.

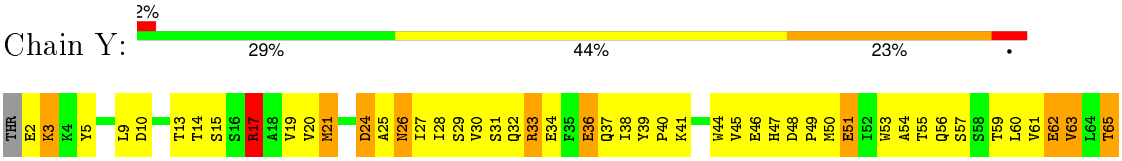
- Molecule 1: PROTEIN (GLYCEROL KINASE)

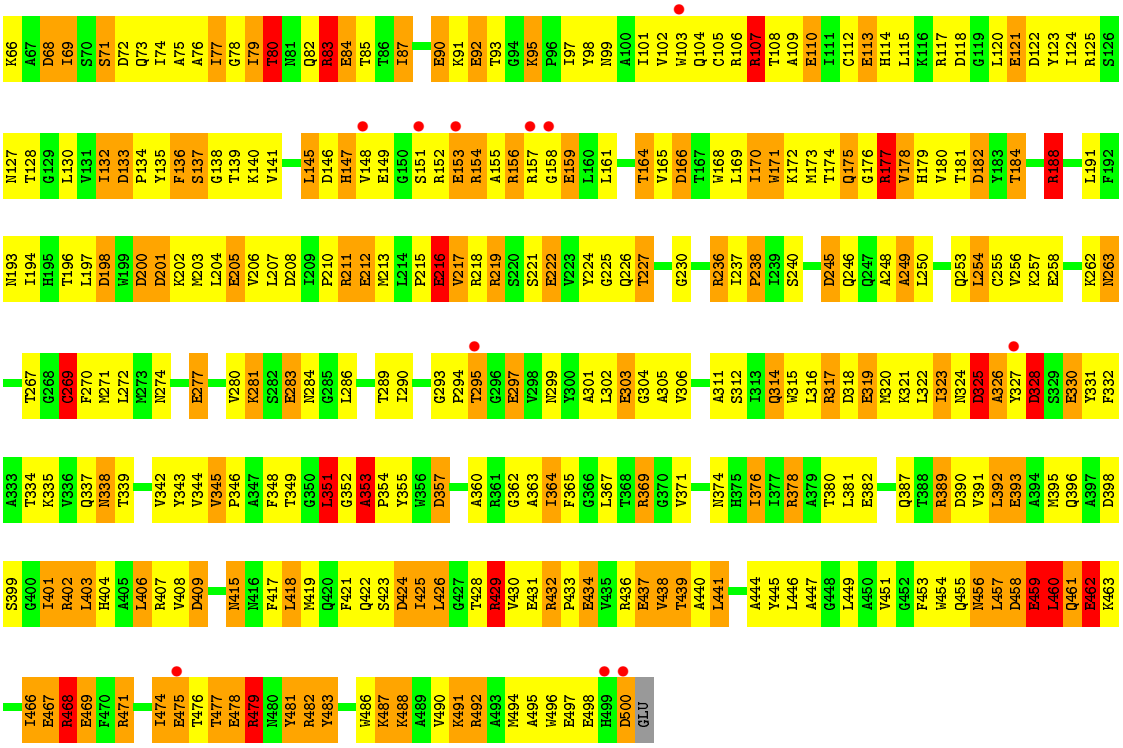
Chain O:



- Molecule 1: PROTEIN (GLYCEROL KINASE)

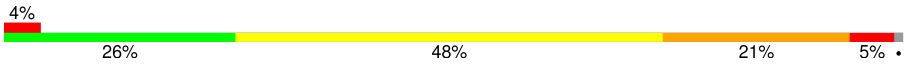
Chain Y:

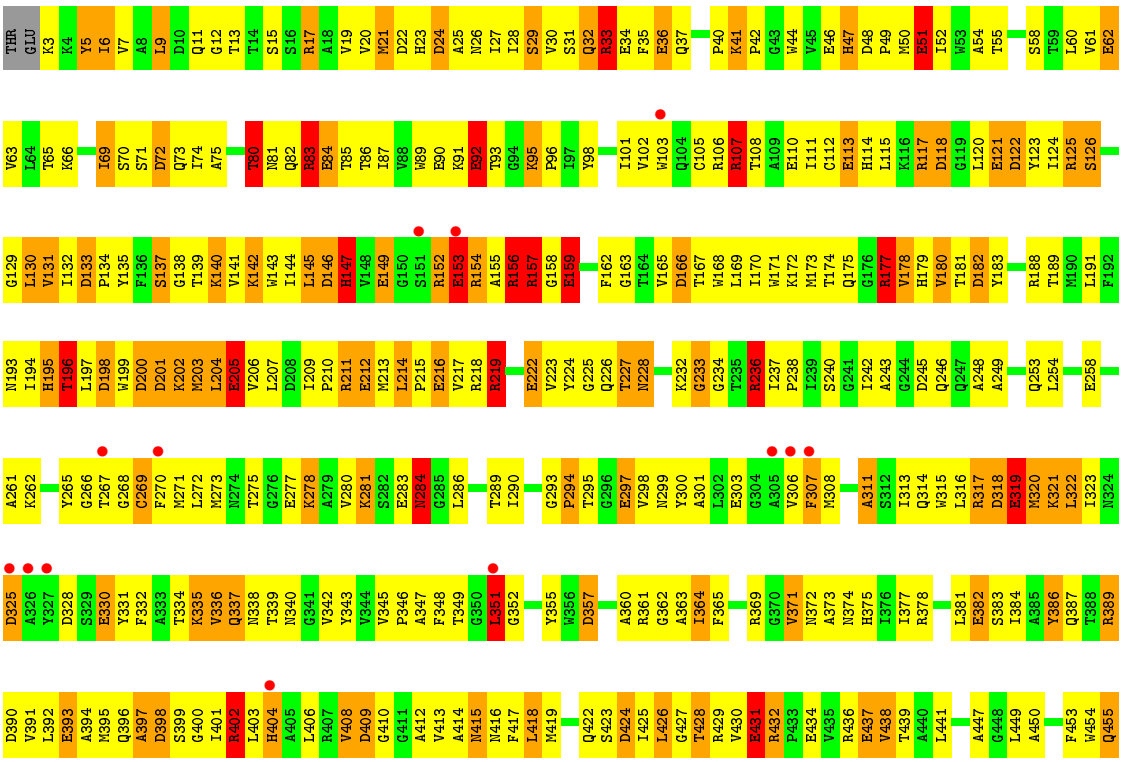


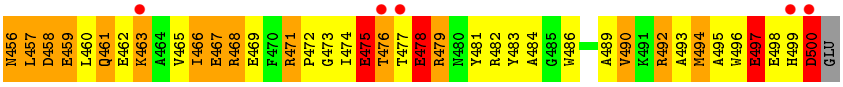


- Molecule 1: PROTEIN (GLYCEROL KINASE)

Chain Z:

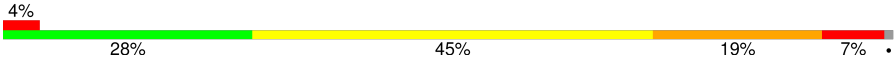


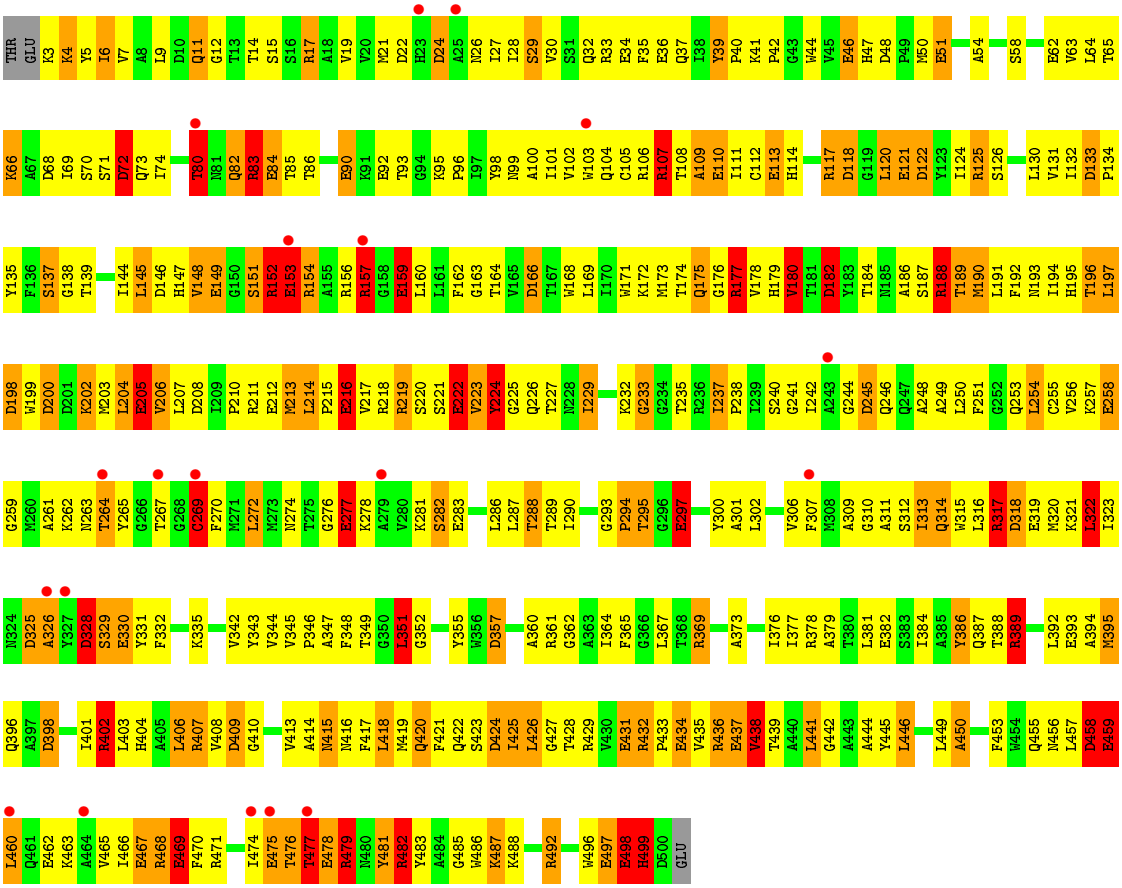




• Molecule 1: PROTEIN (GLYCEROL KINASE)

Chain X:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.90Å 119.00Å 109.30Å 90.00° 103.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.37 37.01 – 2.37	Depositor EDS
% Data completeness (in resolution range)	74.0 (20.00-2.37) 72.3 (37.01-2.37)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.49 (at 2.37Å)	Xtriage
Refinement program	TNT V. 5-F-6	Depositor
R, R_{free}	0.167 , (Not available) 0.157 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 128.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	3 of 69682 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15815	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.80 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.8628e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	O	1.34	35/3970 (0.9%)	1.71	83/5387 (1.5%)
1	X	1.37	39/3975 (1.0%)	1.76	96/5393 (1.8%)
1	Y	1.34	40/4001 (1.0%)	1.75	102/5427 (1.9%)
1	Z	1.32	36/3992 (0.9%)	1.71	69/5413 (1.3%)
All	All	1.34	150/15938 (0.9%)	1.74	350/21620 (1.6%)

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	X	2	0
1	Z	1	0
All	All	3	0

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	475	GLU	CD-OE2	16.71	1.44	1.25
1	Y	475	GLU	CD-OE2	12.24	1.39	1.25
1	Z	36	GLU	CD-OE2	10.65	1.37	1.25
1	Y	84	GLU	CD-OE1	10.23	1.36	1.25
1	Y	434	GLU	CD-OE2	10.15	1.36	1.25
1	O	475	GLU	CD-OE1	9.90	1.36	1.25
1	Z	149	GLU	CD-OE1	9.86	1.36	1.25
1	X	277	GLU	CD-OE2	9.64	1.36	1.25
1	Z	34	GLU	CD-OE1	9.49	1.36	1.25
1	Z	475	GLU	CD-OE2	9.44	1.36	1.25
1	O	92	GLU	CD-OE1	9.33	1.35	1.25
1	Y	216	GLU	CD-OE1	9.14	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	121	GLU	CD-OE1	9.11	1.35	1.25
1	Y	92	GLU	CD-OE1	9.08	1.35	1.25
1	X	153	GLU	CD-OE2	8.99	1.35	1.25
1	O	36	GLU	CD-OE2	8.98	1.35	1.25
1	O	434	GLU	CD-OE2	8.93	1.35	1.25
1	O	277	GLU	CD-OE2	8.86	1.35	1.25
1	X	258	GLU	CD-OE2	8.85	1.35	1.25
1	Z	110	GLU	CD-OE2	8.72	1.35	1.25
1	X	205	GLU	CD-OE2	8.67	1.35	1.25
1	X	437	GLU	CD-OE2	8.64	1.35	1.25
1	X	434	GLU	CD-OE1	8.58	1.35	1.25
1	O	462	GLU	CD-OE1	8.57	1.35	1.25
1	Z	92	GLU	CD-OE2	8.57	1.35	1.25
1	X	431	GLU	CD-OE1	8.54	1.35	1.25
1	Y	462	GLU	CD-OE1	8.53	1.35	1.25
1	Z	462	GLU	CD-OE2	8.51	1.35	1.25
1	Y	153	GLU	CD-OE1	8.49	1.34	1.25
1	O	34	GLU	CD-OE1	8.47	1.34	1.25
1	Z	437	GLU	CD-OE2	8.47	1.34	1.25
1	X	283	GLU	CD-OE1	8.47	1.34	1.25
1	Z	51	GLU	CD-OE1	8.38	1.34	1.25
1	Y	459	GLU	CD-OE2	8.36	1.34	1.25
1	O	153	GLU	CD-OE2	8.33	1.34	1.25
1	O	497	GLU	CD-OE2	8.33	1.34	1.25
1	X	149	GLU	CD-OE1	8.30	1.34	1.25
1	Y	382	GLU	CD-OE2	8.29	1.34	1.25
1	Y	437	GLU	CD-OE2	8.16	1.34	1.25
1	X	478	GLU	CD-OE1	8.12	1.34	1.25
1	O	62	GLU	CD-OE2	8.09	1.34	1.25
1	Y	36	GLU	CD-OE2	8.05	1.34	1.25
1	X	92	GLU	CD-OE2	8.02	1.34	1.25
1	Y	34	GLU	CD-OE1	7.97	1.34	1.25
1	Y	469	GLU	CD-OE2	7.93	1.34	1.25
1	O	459	GLU	CD-OE1	7.93	1.34	1.25
1	X	36	GLU	CD-OE2	7.91	1.34	1.25
1	X	34	GLU	CD-OE1	7.89	1.34	1.25
1	Z	153	GLU	CD-OE1	7.87	1.34	1.25
1	Y	110	GLU	CD-OE1	7.87	1.34	1.25
1	X	459	GLU	CD-OE2	7.84	1.34	1.25
1	Z	283	GLU	CD-OE1	7.81	1.34	1.25
1	X	330	GLU	CD-OE1	7.80	1.34	1.25
1	Z	205	GLU	CD-OE2	7.79	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	283	GLU	CD-OE1	7.76	1.34	1.25
1	O	149	GLU	CD-OE1	7.75	1.34	1.25
1	Y	258	GLU	CD-OE1	7.70	1.34	1.25
1	O	216	GLU	CD-OE2	7.65	1.34	1.25
1	X	462	GLU	CD-OE2	7.65	1.34	1.25
1	O	437	GLU	CD-OE1	7.64	1.34	1.25
1	X	110	GLU	CD-OE1	7.61	1.34	1.25
1	X	51	GLU	CD-OE1	7.58	1.33	1.25
1	O	212	GLU	CD-OE2	7.57	1.33	1.25
1	Z	459	GLU	CD-OE1	7.53	1.33	1.25
1	Y	498	GLU	CD-OE1	7.52	1.33	1.25
1	Y	205	GLU	CD-OE2	7.46	1.33	1.25
1	X	297	GLU	CD-OE1	7.46	1.33	1.25
1	O	498	GLU	CD-OE1	7.39	1.33	1.25
1	Y	330	GLU	CD-OE2	7.38	1.33	1.25
1	O	205	GLU	CD-OE1	7.32	1.33	1.25
1	X	62	GLU	CD-OE2	7.31	1.33	1.25
1	Z	382	GLU	CD-OE2	7.29	1.33	1.25
1	Z	258	GLU	CD-OE1	7.28	1.33	1.25
1	Z	277	GLU	CD-OE1	7.26	1.33	1.25
1	O	467	GLU	CD-OE2	7.25	1.33	1.25
1	X	469	GLU	CD-OE1	7.17	1.33	1.25
1	Z	330	GLU	CD-OE1	7.16	1.33	1.25
1	Z	497	GLU	CD-OE2	7.12	1.33	1.25
1	X	117	ARG	NE-CZ	7.11	1.42	1.33
1	Y	149	GLU	CD-OE1	7.10	1.33	1.25
1	Y	467	GLU	CD-OE2	7.10	1.33	1.25
1	O	469	GLU	CD-OE2	7.09	1.33	1.25
1	O	330	GLU	CD-OE1	7.08	1.33	1.25
1	X	216	GLU	CD-OE2	7.08	1.33	1.25
1	X	319	GLU	CD-OE2	7.07	1.33	1.25
1	Z	159	GLU	CD-OE1	7.04	1.33	1.25
1	Y	84	GLU	CD-OE2	-6.96	1.18	1.25
1	X	121	GLU	CD-OE1	6.94	1.33	1.25
1	Y	431	GLU	CD-OE2	6.87	1.33	1.25
1	Z	393	GLU	CD-OE1	6.83	1.33	1.25
1	X	498	GLU	CD-OE1	6.81	1.33	1.25
1	O	110	GLU	CD-OE1	6.74	1.33	1.25
1	X	222	GLU	CD-OE2	6.73	1.33	1.25
1	O	283	GLU	CD-OE1	6.67	1.32	1.25
1	O	478	GLU	CD-OE2	6.63	1.32	1.25
1	O	382	GLU	CD-OE2	6.62	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	478	GLU	CD-OE2	6.62	1.32	1.25
1	X	159	GLU	CD-OE2	6.62	1.32	1.25
1	Y	269	CYS	CB-SG	-6.57	1.71	1.82
1	O	258	GLU	CD-OE1	6.56	1.32	1.25
1	Z	222	GLU	CD-OE2	6.49	1.32	1.25
1	Z	431	GLU	CD-OE1	6.42	1.32	1.25
1	Z	62	GLU	CD-OE2	6.38	1.32	1.25
1	O	393	GLU	CD-OE2	6.36	1.32	1.25
1	Y	497	GLU	CD-OE1	6.33	1.32	1.25
1	Z	498	GLU	CD-OE1	6.31	1.32	1.25
1	Y	393	GLU	CD-OE1	6.31	1.32	1.25
1	Y	62	GLU	CD-OE1	6.28	1.32	1.25
1	X	212	GLU	CD-OE2	6.27	1.32	1.25
1	Y	478	GLU	CD-OE2	6.26	1.32	1.25
1	Z	121	GLU	CD-OE2	6.25	1.32	1.25
1	Y	212	GLU	CD-OE2	6.23	1.32	1.25
1	Y	297	GLU	CD-OE2	6.21	1.32	1.25
1	Y	121	GLU	CD-OE1	6.19	1.32	1.25
1	Z	212	GLU	CD-OE1	6.18	1.32	1.25
1	Y	113	GLU	CD-OE2	6.17	1.32	1.25
1	O	222	GLU	CD-OE1	6.17	1.32	1.25
1	Y	46	GLU	CD-OE1	-6.16	1.18	1.25
1	X	393	GLU	CD-OE1	6.14	1.32	1.25
1	O	90	GLU	CD-OE2	6.08	1.32	1.25
1	X	467	GLU	CD-OE2	6.08	1.32	1.25
1	Y	277	GLU	CD-OE1	6.06	1.32	1.25
1	X	497	GLU	CD-OE2	6.03	1.32	1.25
1	O	84	GLU	CD-OE1	6.01	1.32	1.25
1	Z	467	GLU	CD-OE2	6.00	1.32	1.25
1	Y	222	GLU	CD-OE2	5.99	1.32	1.25
1	O	159	GLU	CD-OE1	5.98	1.32	1.25
1	Z	216	GLU	CD-OE2	5.98	1.32	1.25
1	Z	269	CYS	CB-SG	-5.94	1.72	1.81
1	Y	159	GLU	CD-OE1	5.91	1.32	1.25
1	Z	84	GLU	CD-OE1	5.90	1.32	1.25
1	O	431	GLU	CD-OE1	5.79	1.32	1.25
1	X	113	GLU	CD-OE2	5.76	1.31	1.25
1	Z	113	GLU	CD-OE2	5.72	1.31	1.25
1	Z	297	GLU	CD-OE1	5.56	1.31	1.25
1	O	319	GLU	CD-OE2	5.46	1.31	1.25
1	Y	482	ARG	NE-CZ	5.46	1.40	1.33
1	Y	402	ARG	NE-CZ	5.44	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	157	ARG	NE-CZ	5.39	1.40	1.33
1	X	84	GLU	CD-OE1	5.39	1.31	1.25
1	Z	46	GLU	CD-OE2	5.35	1.31	1.25
1	X	269	CYS	CB-SG	-5.31	1.73	1.81
1	X	84	GLU	N-CA	5.29	1.56	1.46
1	O	113	GLU	CD-OE1	5.28	1.31	1.25
1	Z	90	GLU	CD-OE2	5.24	1.31	1.25
1	X	46	GLU	CD-OE2	5.16	1.31	1.25
1	Y	90	GLU	CD-OE1	5.15	1.31	1.25
1	Z	434	GLU	CD-OE1	5.05	1.31	1.25
1	X	117	ARG	CD-NE	5.05	1.55	1.46
1	Y	319	GLU	CD-OE2	5.04	1.31	1.25

All (350) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	107	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	Z	479	ARG	NE-CZ-NH1	12.15	126.38	120.30
1	O	200	ASP	CB-CG-OD2	-11.71	107.76	118.30
1	X	479	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	Y	407	ARG	NE-CZ-NH2	-10.35	115.13	120.30
1	Z	107	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	X	152	ARG	NE-CZ-NH1	10.17	125.39	120.30
1	Z	200	ASP	CB-CG-OD2	-9.93	109.36	118.30
1	Z	361	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	Y	483	TYR	CB-CG-CD1	9.70	126.82	121.00
1	Y	107	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	O	133	ASP	CB-CG-OD1	-9.67	109.59	118.30
1	O	107	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	Y	318	ASP	CB-CG-OD2	-9.52	109.73	118.30
1	Y	402	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	O	135	TYR	CB-CG-CD1	9.38	126.63	121.00
1	Y	458	ASP	CB-CG-OD2	-9.33	109.90	118.30
1	Y	208	ASP	CB-CG-OD2	9.33	126.69	118.30
1	Y	492	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	X	39	TYR	CB-CG-CD1	9.28	126.57	121.00
1	Y	351	LEU	C-N-CA	-9.22	102.94	122.30
1	Z	361	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	O	325	ASP	CB-CG-OD2	-9.21	110.02	118.30
1	O	492	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	Y	353	ALA	N-CA-CB	9.15	122.91	110.10
1	X	146	ASP	CB-CG-OD2	-9.13	110.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	118	ASP	CB-CG-OD1	8.94	126.35	118.30
1	Y	68	ASP	CB-CG-OD1	-8.91	110.28	118.30
1	Y	481	TYR	CB-CG-CD1	-8.83	115.70	121.00
1	Y	198	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	Y	208	ASP	CB-CG-OD1	-8.79	110.39	118.30
1	X	224	TYR	CB-CG-CD1	-8.77	115.74	121.00
1	X	482	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	Z	245	ASP	CB-CG-OD2	-8.60	110.56	118.30
1	O	429	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	X	288	THR	CA-CB-CG2	-8.53	100.46	112.40
1	Z	458	ASP	CB-CG-OD1	-8.48	110.67	118.30
1	O	83	ARG	C-N-CA	-8.42	100.64	121.70
1	X	118	ASP	CB-CG-OD2	-8.37	110.76	118.30
1	X	39	TYR	CB-CG-CD2	-8.37	115.98	121.00
1	Z	33	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	Y	318	ASP	CB-CG-OD1	8.34	125.81	118.30
1	X	83	ARG	C-N-CA	-8.29	100.98	121.70
1	Y	245	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	Z	156	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	O	128	THR	CA-CB-CG2	-8.06	101.11	112.40
1	Y	325	ASP	CB-CG-OD2	-8.04	111.06	118.30
1	X	317	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	Y	17	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	X	133	ASP	CB-CG-OD1	-7.97	111.12	118.30
1	X	351	LEU	C-N-CA	-7.97	105.56	122.30
1	Y	479	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	X	245	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	X	152	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	X	458	ASP	CB-CG-OD1	-7.87	111.22	118.30
1	Y	407	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	X	200	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	X	154	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	X	219	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	X	182	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	O	458	ASP	CB-CG-OD1	-7.72	111.35	118.30
1	X	386	TYR	CB-CG-CD1	-7.70	116.38	121.00
1	O	490	VAL	CA-CB-CG1	-7.69	99.36	110.90
1	Z	83	ARG	C-N-CA	-7.68	102.51	121.70
1	Y	83	ARG	C-N-CA	-7.63	102.63	121.70
1	X	166	ASP	CB-CG-OD1	-7.63	111.44	118.30
1	Z	122	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	O	200	ASP	CB-CG-OD1	7.61	125.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	122	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	Y	211	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	Z	409	ASP	CB-CG-OD1	7.51	125.06	118.30
1	Y	10	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	X	83	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	X	133	ASP	CB-CG-OD2	7.34	124.91	118.30
1	Y	107	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	O	152	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	X	146	ASP	CB-CG-OD1	7.30	124.87	118.30
1	X	166	ASP	CB-CG-OD2	7.30	124.87	118.30
1	Y	328	ASP	CB-CG-OD1	7.29	124.86	118.30
1	O	146	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	O	402	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	Y	245	ASP	CB-CG-OD1	7.25	124.83	118.30
1	X	188	ARG	CG-CD-NE	7.24	127.00	111.80
1	Y	24	ASP	CB-CG-OD1	-7.23	111.79	118.30
1	Y	369	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	X	188	ARG	CD-NE-CZ	7.19	133.66	123.60
1	O	156	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	Y	481	TYR	N-CA-CB	-7.14	97.75	110.60
1	Y	146	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	O	378	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	Y	345	VAL	CA-CB-CG2	-7.04	100.34	110.90
1	X	137	SER	N-CA-CB	7.03	121.05	110.50
1	X	389	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	X	24	ASP	CB-CG-OD1	-7.03	111.98	118.30
1	X	318	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	Y	147	HIS	CA-CB-CG	-6.99	101.72	113.60
1	Z	317	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	Z	201	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	Z	409	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	Y	475	GLU	N-CA-CB	-6.94	98.10	110.60
1	O	357	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	Z	133	ASP	CB-CG-OD1	6.92	124.53	118.30
1	X	180	VAL	CA-CB-CG1	6.91	121.26	110.90
1	Y	468	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	Z	24	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	O	24	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	O	107	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	O	126	SER	N-CA-CB	6.81	120.71	110.50
1	O	479	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	Y	188	ARG	NE-CZ-NH1	6.79	123.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	80	THR	CA-CB-CG2	-6.79	102.90	112.40
1	Z	424	ASP	CB-CG-OD1	6.77	124.39	118.30
1	X	409	ASP	CB-CG-OD1	6.77	124.39	118.30
1	Y	106	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	Z	118	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	X	177	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	O	147	HIS	CA-CB-CG	-6.71	102.20	113.60
1	O	236	ARG	NE-CZ-NH1	-6.67	116.96	120.30
1	Y	211	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	X	188	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	O	436	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	X	68	ASP	CB-CG-OD1	-6.64	112.33	118.30
1	O	118	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	O	182	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	X	109	ALA	N-CA-CB	-6.62	100.83	110.10
1	Z	500	ASP	CB-CG-OD1	6.61	124.25	118.30
1	X	208	ASP	CB-CG-OD2	6.60	124.24	118.30
1	Y	106	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	Y	249	ALA	CB-CA-C	6.59	119.99	110.10
1	O	454	TRP	N-CA-CB	6.58	122.45	110.60
1	O	72	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	Z	269	CYS	CB-CA-C	-6.57	97.25	110.40
1	Y	432	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	O	15	SER	N-CA-CB	-6.57	100.65	110.50
1	Y	483	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	Y	328	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	Z	339	THR	CA-CB-CG2	-6.51	103.28	112.40
1	O	289	THR	N-CA-CB	6.51	122.67	110.30
1	X	328	ASP	CB-CG-OD1	6.50	124.15	118.30
1	Y	5	TYR	CB-CG-CD1	-6.49	117.10	121.00
1	Z	177	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	O	440	ALA	N-CA-CB	6.48	119.17	110.10
1	Y	479	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	O	436	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	O	468	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	X	432	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	X	24	ASP	CB-CG-OD2	6.44	124.10	118.30
1	X	148	VAL	CB-CA-C	-6.44	99.17	111.40
1	X	122	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	O	198	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	X	402	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	O	325	ASP	CB-CG-OD1	6.38	124.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	424	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	X	80	THR	N-CA-CB	6.35	122.37	110.30
1	O	68	ASP	CB-CG-OD1	-6.33	112.61	118.30
1	Z	414	ALA	CB-CA-C	6.33	119.59	110.10
1	O	83	ARG	O-C-N	-6.32	112.59	122.70
1	X	14	THR	N-CA-CB	-6.31	98.31	110.30
1	Z	351	LEU	C-N-CA	-6.29	109.09	122.30
1	Y	409	ASP	CB-CG-OD1	6.29	123.96	118.30
1	Y	154	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	Z	325	ASP	CB-CG-OD2	-6.28	112.64	118.30
1	Y	72	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	Z	236	ARG	N-CA-CB	-6.27	99.31	110.60
1	O	458	ASP	CB-CG-OD2	6.25	123.93	118.30
1	O	398	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	Y	409	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	O	318	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	X	318	ASP	CB-CG-OD1	6.23	123.90	118.30
1	X	402	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	X	481	TYR	CB-CG-CD1	-6.21	117.27	121.00
1	O	198	ASP	CB-CG-OD2	6.21	123.89	118.30
1	Y	357	ASP	CB-CG-OD1	6.21	123.89	118.30
1	X	325	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	X	147	HIS	CB-CA-C	6.19	122.78	110.40
1	Y	458	ASP	CB-CG-OD1	6.17	123.85	118.30
1	Z	500	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	O	83	ARG	CA-C-N	6.15	130.72	117.20
1	O	90	GLU	N-CA-CB	6.14	121.66	110.60
1	Y	166	ASP	CB-CG-OD2	6.13	123.82	118.30
1	Y	156	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	Z	219	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	Y	200	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	O	30	VAL	CB-CA-C	-6.09	99.83	111.40
1	Y	219	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	Y	404	HIS	CB-CA-C	6.08	122.56	110.40
1	Z	245	ASP	CB-CG-OD1	6.08	123.77	118.30
1	Z	424	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	X	117	ARG	CD-NE-CZ	6.06	132.09	123.60
1	Z	147	HIS	CA-CB-CG	-6.04	103.33	113.60
1	Y	83	ARG	N-CA-C	6.03	127.27	111.00
1	X	458	ASP	CB-CG-OD2	6.01	123.71	118.30
1	Z	147	HIS	CB-CA-C	6.01	122.42	110.40
1	X	264	THR	CA-CB-CG2	-5.99	104.02	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	429	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	X	409	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	Z	83	ARG	N-CA-C	5.97	127.12	111.00
1	O	48	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	X	499	HIS	N-CA-CB	5.96	121.32	110.60
1	Y	314	GLN	CB-CA-C	5.95	122.30	110.40
1	Y	118	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	Y	133	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	X	198	ASP	CB-CG-OD1	5.91	123.62	118.30
1	Y	122	ASP	CB-CG-OD1	5.91	123.62	118.30
1	Z	130	LEU	CA-CB-CG	-5.91	101.71	115.30
1	X	224	TYR	CB-CG-CD2	5.91	124.54	121.00
1	X	245	ASP	CB-CG-OD1	5.90	123.61	118.30
1	X	404	HIS	N-CA-CB	5.90	121.22	110.60
1	Z	402	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	O	125	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	X	177	ARG	N-CA-CB	5.87	121.17	110.60
1	Z	72	ASP	CB-CG-OD1	-5.86	113.02	118.30
1	X	68	ASP	CB-CG-OD2	5.86	123.57	118.30
1	Y	357	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	Y	353	ALA	CB-CA-C	-5.85	101.33	110.10
1	O	70	SER	N-CA-CB	5.85	119.27	110.50
1	X	198	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	Y	402	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	X	398	ASP	CB-CG-OD2	5.81	123.53	118.30
1	O	48	ASP	CB-CG-OD2	5.79	123.51	118.30
1	Z	414	ALA	N-CA-CB	5.75	118.15	110.10
1	O	235	THR	CA-CB-CG2	-5.74	104.36	112.40
1	Z	284	ASN	N-CA-C	5.74	126.51	111.00
1	Y	14	THR	OG1-CB-CG2	5.74	123.20	110.00
1	Z	5	TYR	CB-CA-C	-5.74	98.92	110.40
1	Z	17	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	O	118	ASP	CB-CA-C	5.72	121.84	110.40
1	X	5	TYR	CB-CA-C	-5.71	98.98	110.40
1	O	83	ARG	N-CA-C	5.70	126.39	111.00
1	Z	201	ASP	CB-CG-OD1	5.70	123.43	118.30
1	O	409	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	Z	146	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	X	172	LYS	N-CA-CB	5.69	120.83	110.60
1	O	75	ALA	N-CA-CB	5.68	118.06	110.10
1	O	424	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	Y	177	ARG	NE-CZ-NH1	5.67	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	263	ASN	N-CA-CB	5.67	120.80	110.60
1	O	415	ASN	CB-CA-C	-5.66	99.08	110.40
1	Z	133	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	O	93	THR	N-CA-CB	-5.63	99.60	110.30
1	Y	236	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	Y	269	CYS	CB-CA-C	-5.62	99.15	110.40
1	Z	389	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	X	208	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	O	483	TYR	CB-CG-CD1	5.61	124.36	121.00
1	X	84	GLU	N-CA-CB	5.60	120.69	110.60
1	Y	482	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	X	83	ARG	N-CA-C	5.59	126.08	111.00
1	Y	378	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	X	11	GLN	CB-CA-C	5.58	121.57	110.40
1	O	122	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	Z	471	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	X	189	THR	CA-CB-CG2	-5.56	104.62	112.40
1	Z	311	ALA	CB-CA-C	5.56	118.44	110.10
1	Z	357	ASP	CB-CG-OD1	5.55	123.29	118.30
1	Z	118	ASP	CB-CG-OD1	5.54	123.29	118.30
1	X	159	GLU	N-CA-C	5.54	125.95	111.00
1	O	325	ASP	CB-CA-C	5.53	121.47	110.40
1	Z	5	TYR	CA-C-N	-5.53	105.03	117.20
1	Y	181	THR	CA-CB-CG2	-5.51	104.68	112.40
1	O	314	GLN	CB-CA-C	-5.51	99.38	110.40
1	Y	10	ASP	CB-CG-OD2	5.51	123.26	118.30
1	O	166	ASP	CB-CG-OD2	5.51	123.25	118.30
1	O	292	CYS	CB-CA-C	-5.49	99.42	110.40
1	Y	389	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	Z	47	HIS	CA-CB-CG	5.47	122.91	113.60
1	O	483	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	X	388	THR	N-CA-CB	-5.47	99.92	110.30
1	X	438	VAL	CA-CB-CG1	-5.46	102.71	110.90
1	Y	457	LEU	CA-CB-CG	-5.46	102.75	115.30
1	X	357	ASP	CB-CG-OD1	5.46	123.21	118.30
1	Y	166	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	O	122	ASP	N-CA-CB	5.45	120.41	110.60
1	Z	408	VAL	CB-CA-C	-5.45	101.05	111.40
1	X	398	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	X	407	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	Y	17	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	Y	325	ASP	CB-CG-OD1	5.42	123.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	163	GLY	C-N-CA	5.42	135.25	121.70
1	Z	195	HIS	CA-CB-CG	-5.41	104.41	113.60
1	X	357	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	O	166	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	X	269	CYS	CA-CB-SG	-5.40	104.29	114.00
1	X	424	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	X	479	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	Y	24	ASP	CB-CG-OD2	5.37	123.14	118.30
1	O	245	ASP	CB-CG-OD1	5.37	123.13	118.30
1	Z	386	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	Y	80	THR	N-CA-CB	5.36	120.47	110.30
1	O	357	ASP	CB-CG-OD1	5.35	123.11	118.30
1	Z	198	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	X	90	GLU	CB-CG-CD	-5.34	99.78	114.20
1	Y	326	ALA	N-CA-CB	5.33	117.56	110.10
1	X	432	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	O	300	TYR	CA-CB-CG	-5.32	103.29	113.40
1	Z	389	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	X	475	GLU	N-CA-CB	-5.30	101.05	110.60
1	Y	14	THR	CA-CB-CG2	5.30	119.82	112.40
1	Z	211	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	Z	177	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	Y	171	TRP	N-CA-CB	-5.28	101.10	110.60
1	X	281	LYS	CB-CA-C	5.27	120.93	110.40
1	Y	201	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	O	334	THR	CA-CB-CG2	-5.26	105.04	112.40
1	X	33	ARG	N-CA-CB	5.26	120.06	110.60
1	X	83	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	Y	39	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	Z	492	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	X	394	ALA	CA-C-N	-5.24	105.67	117.20
1	Y	354	PRO	CB-CA-C	-5.24	98.90	112.00
1	Z	432	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	X	72	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	Y	441	LEU	CB-CA-C	-5.23	100.26	110.20
1	O	303	GLU	CG-CD-OE1	-5.23	107.84	118.30
1	Z	196	THR	N-CA-CB	-5.22	100.38	110.30
1	O	17	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	Y	154	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	Y	72	ASP	CB-CG-OD2	5.20	122.98	118.30
1	O	196	THR	N-CA-CB	-5.20	100.43	110.30
1	O	468	ARG	NE-CZ-NH1	5.20	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	42	PRO	N-CA-CB	5.19	109.53	103.30
1	Y	184	THR	CA-CB-CG2	-5.18	105.14	112.40
1	O	153	GLU	CA-CB-CG	-5.18	102.00	113.40
1	O	351	LEU	C-N-CA	-5.18	111.43	122.30
1	O	355	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	Z	33	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	Z	404	HIS	CB-CA-C	5.16	120.72	110.40
1	X	328	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	O	438	VAL	CA-CB-CG2	-5.15	103.18	110.90
1	Z	319	GLU	CG-CD-OE1	-5.14	108.02	118.30
1	X	369	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	X	86	THR	N-CA-CB	-5.12	100.57	110.30
1	Z	203	MET	CA-CB-CG	-5.12	104.60	113.30
1	X	219	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	Y	323	ILE	N-CA-C	-5.11	97.19	111.00
1	Y	468	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	Y	389	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	Y	117	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	O	83	ARG	N-CA-CB	5.10	119.78	110.60
1	Y	460	LEU	CA-CB-CG	-5.08	103.61	115.30
1	Y	429	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	Z	157	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	X	188	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	O	133	ASP	CB-CG-OD2	5.05	122.85	118.30
1	Y	326	ALA	CB-CA-C	5.05	117.67	110.10
1	X	481	TYR	CA-CB-CG	-5.05	103.81	113.40
1	O	75	ALA	CB-CA-C	-5.04	102.54	110.10
1	Y	76	ALA	CB-CA-C	-5.03	102.56	110.10
1	Y	487	LYS	CB-CA-C	5.01	120.42	110.40
1	Y	77	ILE	CB-CA-C	-5.00	101.59	111.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	Z	149	GLU	CA
1	X	147	HIS	CA
1	X	404	HIS	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

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	O	3891	0	3804	450	0
1	X	3896	0	3811	414	0
1	Y	3921	0	3839	406	0
1	Z	3913	0	3841	448	0
2	O	10	0	0	2	0
2	X	5	0	0	0	0
2	Y	5	0	0	0	0
2	Z	10	0	0	2	0
3	O	6	0	8	1	0
3	X	6	0	8	1	0
3	Y	6	0	8	3	0
3	Z	6	0	8	7	0
4	O	29	0	0	3	0
4	X	42	0	0	7	0
4	Y	38	0	0	4	0
4	Z	31	0	0	2	0
All	All	15815	0	15327	1658	0

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 53.

All (1658) 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:Y:33:ARG:HH22	1:Z:58:SER:HB2	1.15	1.11
1:O:287:LEU:HD12	1:O:303:GLU:HG2	1.31	1.11
1:Y:456:ASN:ND2	1:Y:458:ASP:H	1.51	1.08
1:Z:468:ARG:HG3	1:Z:468:ARG:HH11	1.19	1.07
1:Z:154:ARG:HB3	1:Z:159:GLU:HG3	1.32	1.05
1:O:17:ARG:HG3	1:O:32:GLN:HG3	1.38	1.05
1:Z:92:GLU:HG2	1:Z:93:THR:HG23	1.40	1.04
1:Z:320:MET:HE1	1:X:373:ALA:HA	1.40	1.04
1:Z:112:CYS:HB3	1:Z:132:ILE:HG22	1.35	1.04
1:O:189:THR:HB	1:O:191:LEU:HD12	1.37	1.03
1:O:128:THR:HG21	1:O:130:LEU:HD22	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:125:ARG:HB2	1:Z:125:ARG:HH11	1.20	1.02
1:O:203:MET:HA	1:O:206:VAL:HG23	1.41	1.00
1:O:330:GLU:HG3	1:O:415:ASN:HD21	1.23	1.00
1:Y:9:LEU:HB2	1:Y:79:ILE:HD12	1.42	1.00
1:Z:460:LEU:HA	1:Z:463:LYS:HD2	1.44	0.99
1:Z:83:ARG:HH11	1:Z:83:ARG:HB2	1.24	0.99
1:Y:272:LEU:HG	1:Y:303:GLU:HB2	1.42	0.98
1:Z:424:ASP:HB3	1:Z:474:ILE:HD12	1.42	0.98
1:Y:85:THR:HG23	1:Y:102:VAL:HA	1.40	0.98
1:Y:219:ARG:HH22	1:Y:295:THR:HG23	1.25	0.98
1:X:17:ARG:HG3	1:X:32:GLN:HG2	1.40	0.98
1:O:261:ALA:HB2	1:O:273:MET:HB2	1.46	0.98
1:O:460:LEU:HD12	1:O:463:LYS:HE3	1.44	0.96
1:Z:415:ASN:HD21	1:Z:417:PHE:HB3	1.29	0.95
1:X:237:ILE:HG22	1:X:238:PRO:HD2	1.48	0.95
1:Y:33:ARG:NH2	1:Z:58:SER:HB2	1.84	0.92
1:Z:145:LEU:HB3	1:Z:152:ARG:NH1	1.84	0.92
1:X:475:GLU:HB3	1:X:478:GLU:HG2	1.49	0.92
1:X:396:GLN:HE21	1:X:403:LEU:H	1.15	0.92
1:Y:415:ASN:HD21	1:Y:417:PHE:HB3	1.34	0.92
1:X:111:ILE:H	1:X:111:ILE:HD12	1.32	0.92
1:Y:219:ARG:NH2	1:Y:295:THR:HG23	1.84	0.91
1:X:108:THR:HA	1:X:111:ILE:HD13	1.50	0.91
1:Y:421:PHE:CZ	1:Y:425:ILE:HD13	2.06	0.91
1:Z:261:ALA:HB2	1:Z:273:MET:HB2	1.54	0.90
1:X:124:ILE:HG12	1:X:203:MET:HE1	1.51	0.90
1:Z:174:THR:HG21	1:Z:178:VAL:HG13	1.53	0.90
1:Z:154:ARG:CB	1:Z:159:GLU:HG3	2.02	0.90
1:O:127:ASN:HD22	1:O:193:ASN:ND2	1.70	0.89
1:Z:112:CYS:HB3	1:Z:132:ILE:CG2	2.01	0.88
1:O:460:LEU:HA	1:O:463:LYS:HE2	1.55	0.88
1:O:161:LEU:HD22	1:O:179:HIS:CE1	2.07	0.88
1:X:154:ARG:HB3	1:X:159:GLU:HG2	1.54	0.88
1:Y:196:THR:HG22	1:Y:198:ASP:N	1.88	0.88
1:Y:271:MET:HE2	1:Y:391:VAL:HG23	1.53	0.87
1:Y:468:ARG:HG3	1:Y:468:ARG:HH11	1.40	0.87
1:O:85:THR:HG23	1:O:102:VAL:HA	1.55	0.87
1:Z:351:LEU:HD22	1:Z:360:ALA:CB	2.03	0.87
1:Z:84:GLU:OE2	1:Z:188:ARG:HD2	1.74	0.86
1:Z:156:ARG:HG3	1:Z:156:ARG:HH11	1.38	0.86
1:Y:424:ASP:HB3	1:Y:474:ILE:HG21	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:146:ASP:HB2	1:Z:147:HIS:CE1	2.10	0.86
1:O:127:ASN:HD22	1:O:193:ASN:HD21	1.24	0.86
1:Y:65:THR:HG21	1:Z:54:ALA:HA	1.56	0.85
1:Y:475:GLU:HG2	1:Y:477:THR:HB	1.57	0.85
1:Y:344:VAL:HG22	1:Y:364:ILE:HD12	1.57	0.85
1:Z:17:ARG:CG	1:Z:32:GLN:HG2	2.05	0.85
1:Y:180:VAL:HG23	1:Y:216:GLU:HG2	1.59	0.85
1:O:128:THR:HG22	1:O:130:LEU:HD13	1.58	0.85
1:Z:152:ARG:O	1:Z:156:ARG:HG2	1.76	0.85
1:Y:65:THR:CG2	1:Z:54:ALA:HA	2.07	0.84
1:O:105:CYS:SG	1:O:107:ARG:HD2	2.17	0.84
1:O:330:GLU:HG3	1:O:415:ASN:ND2	1.92	0.83
1:Y:456:ASN:HD21	1:Y:458:ASP:H	1.24	0.83
1:Y:323:ILE:HG22	1:Y:332:PHE:CD2	2.13	0.83
1:Z:125:ARG:CB	1:Z:125:ARG:HH11	1.92	0.83
1:O:457:LEU:HA	1:O:460:LEU:HD23	1.61	0.83
1:X:154:ARG:HA	1:X:157:ARG:HH11	1.41	0.83
1:O:193:ASN:HB3	1:O:196:THR:CG2	2.09	0.82
1:Y:475:GLU:HG2	1:Y:478:GLU:H	1.43	0.82
1:Y:344:VAL:HG22	1:Y:364:ILE:CD1	2.09	0.82
1:Z:6:ILE:CG2	1:Z:21:MET:HB3	2.09	0.82
1:O:155:ALA:HB1	1:O:210:PRO:HG2	1.61	0.82
1:Y:396:GLN:HE22	1:Y:402:ARG:HD3	1.43	0.82
1:Y:475:GLU:CG	1:Y:477:THR:HB	2.09	0.82
1:O:54:ALA:HA	1:X:65:THR:HG21	1.61	0.82
1:X:406:LEU:HD13	1:X:408:VAL:HG12	1.61	0.82
1:Z:320:MET:HE1	1:X:376:ILE:HD12	1.60	0.82
1:Y:328:ASP:HB3	1:Y:332:PHE:CE2	2.15	0.81
1:X:237:ILE:CG2	1:X:238:PRO:HD2	2.10	0.81
1:Z:315:TRP:CD1	1:Z:319:GLU:HG2	2.16	0.81
1:Z:23:HIS:HA	1:Z:453:PHE:CE2	2.16	0.81
1:Z:387:GLN:O	1:Z:390:ASP:HB2	1.78	0.81
1:Z:17:ARG:HG2	1:Z:32:GLN:HG2	1.63	0.81
1:Y:328:ASP:HB3	1:Y:332:PHE:HE2	1.43	0.81
1:X:154:ARG:NE	1:X:159:GLU:HG2	1.96	0.81
1:Z:347:ALA:HB2	1:Z:351:LEU:HD13	1.63	0.81
1:Y:256:VAL:HG11	1:Y:294:PRO:CA	2.11	0.80
1:O:359:TYR:CE1	1:O:499:HIS:HB3	2.16	0.80
1:X:111:ILE:CG2	1:X:139:THR:HG22	2.12	0.80
1:X:154:ARG:HB3	1:X:159:GLU:CG	2.11	0.80
1:O:154:ARG:HB3	1:O:159:GLU:HB2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:112:CYS:HB3	1:X:132:ILE:HG22	1.62	0.80
1:Y:147:HIS:HB3	4:Y:539:HOH:O	1.81	0.79
1:O:387:GLN:O	1:O:390:ASP:HB2	1.83	0.79
1:Y:422:GLN:O	1:Y:426:LEU:HD22	1.82	0.79
1:O:460:LEU:HD22	1:O:460:LEU:H	1.48	0.79
1:Z:320:MET:CE	1:X:376:ILE:HD12	2.11	0.79
1:Z:415:ASN:ND2	1:Z:417:PHE:HB3	1.96	0.79
1:O:180:VAL:CG2	1:O:218:ARG:HG3	2.13	0.79
1:Z:83:ARG:HH11	1:Z:83:ARG:CB	1.96	0.79
1:Y:161:LEU:HD22	1:Y:179:HIS:CE1	2.18	0.79
1:Y:80:THR:CG2	1:Y:245:ASP:HA	2.12	0.78
1:X:256:VAL:HG11	1:X:294:PRO:HB3	1.63	0.78
1:Z:83:ARG:NH1	1:Z:83:ARG:HB2	1.98	0.78
1:Y:323:ILE:HG22	1:Y:332:PHE:CE2	2.19	0.78
1:X:83:ARG:HD2	1:X:244:GLY:HA3	1.65	0.78
1:Z:203:MET:HA	1:Z:206:VAL:HG12	1.65	0.78
1:X:314:GLN:HG3	1:X:317:ARG:NH2	1.99	0.78
1:Y:54:ALA:HA	1:Z:65:THR:CG2	2.14	0.78
1:Z:28:ILE:HG22	1:Z:29:SER:HB3	1.65	0.78
1:Z:458:ASP:HA	1:Z:461:GLN:HG3	1.64	0.77
1:Z:21:MET:HA	1:Z:26:ASN:O	1.83	0.77
1:X:29:SER:HB3	1:X:63:VAL:CG2	2.13	0.77
1:Z:115:LEU:HA	1:Z:120:LEU:HD12	1.66	0.77
1:O:17:ARG:HG3	1:O:32:GLN:CG	2.15	0.77
1:Y:155:ALA:HB1	1:Y:213:MET:CE	2.15	0.77
1:Y:196:THR:HG22	1:Y:198:ASP:H	1.49	0.77
1:Y:155:ALA:HB1	1:Y:213:MET:HE2	1.66	0.77
1:Y:295:THR:HG22	1:Y:297:GLU:CD	2.06	0.76
1:Z:174:THR:HG21	1:Z:178:VAL:CG1	2.15	0.76
1:X:80:THR:HG21	1:X:245:ASP:HA	1.65	0.76
1:O:437:GLU:O	1:O:441:LEU:HD23	1.85	0.76
1:X:459:GLU:C	1:X:460:LEU:HD13	2.05	0.76
1:O:237:ILE:HG23	1:O:238:PRO:HD2	1.66	0.76
1:X:482:ARG:CB	1:X:482:ARG:HH11	1.97	0.76
1:O:128:THR:HG21	1:O:130:LEU:CD2	2.14	0.76
1:X:159:GLU:O	1:X:160:LEU:HD23	1.85	0.76
1:X:240:SER:HB2	1:X:450:ALA:HB3	1.66	0.76
1:Y:406:LEU:HD13	1:Y:408:VAL:CG1	2.16	0.76
1:Y:179:HIS:ND1	1:Y:215:PRO:HA	2.00	0.76
1:O:173:MET:HB3	1:O:227:THR:HG21	1.68	0.76
1:X:330:GLU:HG3	1:X:415:ASN:HD21	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:403:LEU:HD23	1:O:405:ALA:O	1.86	0.76
1:Y:271:MET:CE	1:Y:391:VAL:HG23	2.15	0.76
1:O:173:MET:HB3	1:O:227:THR:CG2	2.16	0.76
1:Y:483:TYR:CE2	1:Y:487:LYS:HE2	2.21	0.76
1:O:250:LEU:CD1	1:O:255:CYS:HB2	2.16	0.75
1:O:173:MET:O	1:O:227:THR:HG22	1.86	0.75
1:Z:362:GLY:HA3	1:X:367:LEU:HB2	1.67	0.75
1:Y:48:ASP:HB3	1:Y:51:GLU:HB2	1.68	0.75
1:Z:173:MET:O	1:Z:227:THR:HG23	1.85	0.75
1:O:460:LEU:HA	1:O:463:LYS:CE	2.16	0.75
1:Z:170:ILE:CD1	1:Z:242:ILE:HD11	2.17	0.75
1:O:313:ILE:HD11	1:O:381:LEU:HD23	1.69	0.75
1:Y:121:GLU:O	1:Y:125:ARG:HB2	1.85	0.75
1:O:154:ARG:HA	1:O:159:GLU:HG3	1.68	0.74
1:Y:54:ALA:HA	1:Z:65:THR:HG21	1.69	0.74
1:O:421:PHE:O	1:O:424:ASP:HB2	1.86	0.74
1:O:460:LEU:CD1	1:O:463:LYS:HE3	2.15	0.74
1:X:108:THR:CA	1:X:111:ILE:HD13	2.16	0.74
1:O:193:ASN:HB3	1:O:196:THR:HG22	1.68	0.74
1:O:201:ASP:O	1:O:205:GLU:HB3	1.87	0.74
1:Z:6:ILE:HG22	1:Z:21:MET:HB3	1.68	0.74
1:O:203:MET:HA	1:O:206:VAL:CG2	2.17	0.74
1:O:54:ALA:HA	1:X:65:THR:CG2	2.18	0.74
1:X:422:GLN:HE21	1:X:426:LEU:HD22	1.52	0.74
1:Z:105:CYS:SG	1:Z:107:ARG:HD2	2.28	0.74
1:O:130:LEU:HD23	1:O:190:MET:HG3	1.68	0.74
1:Y:256:VAL:HG11	1:Y:294:PRO:HA	1.70	0.74
1:Y:83:ARG:NH1	1:Y:246:GLN:HG2	2.02	0.74
1:Z:203:MET:HA	1:Z:206:VAL:CG1	2.17	0.74
1:Z:193:ASN:HB3	1:Z:196:THR:HG22	1.70	0.73
1:O:80:THR:HG21	1:O:245:ASP:HA	1.69	0.73
1:O:65:THR:CG2	1:X:54:ALA:HA	2.18	0.73
1:Z:424:ASP:O	1:Z:479:ARG:NH1	2.20	0.73
1:X:124:ILE:HG12	1:X:203:MET:CE	2.16	0.73
1:Y:468:ARG:NH1	1:Y:468:ARG:HG3	2.01	0.73
1:Z:378:ARG:O	1:Z:382:GLU:HG3	1.88	0.73
1:Z:147:HIS:N	1:Z:147:HIS:ND1	2.36	0.73
1:X:486:TRP:CD1	1:X:487:LYS:HD2	2.24	0.73
1:O:460:LEU:O	1:O:463:LYS:HG2	1.89	0.73
1:X:478:GLU:O	1:X:481:TYR:HB3	1.88	0.73
1:Y:19:VAL:HG11	1:Y:27:ILE:HD12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:21:MET:HA	1:X:26:ASN:O	1.88	0.73
1:Z:86:THR:OG1	1:Z:137:SER:HB3	1.88	0.73
1:Y:90:GLU:HB2	1:Y:93:THR:OG1	1.89	0.73
1:O:455:GLN:HB3	1:O:459:GLU:OE2	1.89	0.72
1:Y:55:THR:O	1:Y:59:THR:HG23	1.88	0.72
1:X:189:THR:OG1	1:X:191:LEU:HB2	1.89	0.72
1:X:410:GLY:O	1:X:413:VAL:HG22	1.88	0.72
1:X:154:ARG:HA	1:X:157:ARG:NH1	2.05	0.72
1:Z:332:PHE:HA	1:Z:335:LYS:HD3	1.71	0.72
1:O:317:ARG:HB2	1:O:323:ILE:HD11	1.70	0.72
1:X:328:ASP:O	1:X:331:TYR:HB3	1.88	0.72
1:Y:180:VAL:CG2	1:Y:218:ARG:HG3	2.20	0.72
1:X:483:TYR:O	1:X:486:TRP:HB3	1.89	0.72
1:O:203:MET:CA	1:O:206:VAL:HG23	2.19	0.72
1:Z:402:ARG:HG3	1:Z:402:ARG:HH11	1.54	0.72
1:Z:458:ASP:HA	1:Z:461:GLN:CG	2.19	0.72
1:X:3:LYS:N	1:X:4:LYS:HZ3	1.87	0.72
1:X:111:ILE:HG21	1:X:139:THR:HG22	1.71	0.72
1:O:128:THR:CG2	1:O:130:LEU:HD22	2.19	0.71
1:X:418:LEU:HD13	1:X:419:MET:CE	2.19	0.71
1:Z:84:GLU:HB2	1:Z:103:TRP:HB3	1.71	0.71
1:X:17:ARG:HD3	1:X:17:ARG:N	2.05	0.71
1:O:156:ARG:CG	1:O:210:PRO:HG3	2.20	0.71
1:Y:434:GLU:HG3	1:Y:467:GLU:HB2	1.72	0.71
1:Y:112:CYS:HA	1:Y:115:LEU:HD23	1.70	0.71
1:Z:143:TRP:O	1:Z:147:HIS:ND1	2.23	0.71
1:X:267:THR:HG23	1:X:311:ALA:HB2	1.71	0.71
1:O:17:ARG:HD3	1:O:17:ARG:N	2.05	0.71
1:Y:80:THR:HG22	1:Y:245:ASP:HA	1.71	0.71
1:X:295:THR:HG23	1:X:297:GLU:OE2	1.91	0.71
1:Y:458:ASP:HA	1:Y:461:GLN:HE21	1.55	0.71
1:X:482:ARG:CA	1:X:482:ARG:HH11	2.03	0.71
1:X:434:GLU:HG3	1:X:467:GLU:HB2	1.71	0.71
1:X:202:LYS:O	1:X:206:VAL:HG23	1.89	0.71
1:O:357:ASP:OD2	1:O:360:ALA:HB2	1.90	0.71
1:Z:154:ARG:CA	1:Z:159:GLU:HG3	2.20	0.71
1:O:80:THR:CG2	1:O:245:ASP:HA	2.21	0.71
1:Z:157:ARG:HB3	1:Z:157:ARG:HH11	1.54	0.71
1:Z:340:ASN:HD22	1:Z:371:VAL:HG23	1.56	0.71
1:Y:271:MET:HE2	1:Y:391:VAL:CG2	2.20	0.71
1:O:250:LEU:HD11	1:O:255:CYS:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:255:CYS:HB3	1:O:260:MET:HB3	1.73	0.71
1:O:179:HIS:CD2	1:O:215:PRO:HB3	2.26	0.71
1:O:65:THR:HG23	1:X:54:ALA:HA	1.73	0.71
1:Z:12:GLY:HA3	1:Z:17:ARG:NH1	2.06	0.71
1:Z:17:ARG:HG3	1:Z:32:GLN:HG2	1.73	0.71
1:O:124:ILE:HD13	1:O:203:MET:CE	2.20	0.71
1:X:120:LEU:O	1:X:124:ILE:HG13	1.90	0.71
1:O:254:LEU:O	1:O:256:VAL:HG22	1.91	0.70
1:Y:483:TYR:CD2	1:Y:487:LYS:HE2	2.27	0.70
1:Y:50:MET:HA	1:Y:50:MET:HE3	1.72	0.70
1:Y:156:ARG:O	1:Y:212:GLU:HG2	1.91	0.70
1:Z:483:TYR:O	1:Z:486:TRP:HB3	1.91	0.70
1:O:258:GLU:HB2	1:O:275:THR:C	2.12	0.70
1:Y:469:GLU:HB3	1:Y:471:ARG:NH2	2.06	0.70
1:O:458:ASP:O	1:O:461:GLN:HG3	1.91	0.70
1:Z:429:ARG:HG2	1:Z:471:ARG:HG2	1.74	0.70
1:Y:21:MET:HA	1:Y:26:ASN:O	1.91	0.70
1:Z:19:VAL:CG1	1:Z:27:ILE:HG23	2.22	0.70
1:X:435:VAL:HG11	1:X:441:LEU:HD11	1.73	0.70
1:Z:322:LEU:N	1:Z:322:LEU:HD23	2.07	0.70
1:O:224:TYR:CE2	1:O:242:ILE:HG13	2.26	0.70
1:X:322:LEU:H	1:X:322:LEU:HD23	1.56	0.70
1:O:84:GLU:OE2	1:O:188:ARG:HD2	1.92	0.70
1:Y:78:GLY:C	1:Y:79:ILE:HD13	2.12	0.70
1:Z:146:ASP:HB2	1:Z:147:HIS:ND1	2.06	0.70
1:X:90:GLU:HB2	1:X:93:THR:OG1	1.92	0.70
1:Z:460:LEU:HA	1:Z:463:LYS:CD	2.22	0.70
1:X:3:LYS:HD3	1:X:72:ASP:O	1.92	0.70
1:O:251:PHE:CE2	1:O:446:LEU:HD13	2.27	0.70
1:X:322:LEU:N	1:X:322:LEU:HD23	2.06	0.69
1:X:210:PRO:O	1:X:213:MET:HG3	1.92	0.69
1:Y:475:GLU:HB3	1:Y:478:GLU:HB2	1.73	0.69
1:Y:478:GLU:O	1:Y:481:TYR:HB3	1.92	0.69
1:X:80:THR:CG2	1:X:245:ASP:HA	2.22	0.69
1:Z:267:THR:HG23	1:Z:311:ALA:HB2	1.73	0.69
1:X:346:PRO:HA	1:X:348:PHE:CE1	2.27	0.69
1:Y:90:GLU:HG3	1:Y:95:LYS:O	1.92	0.69
1:O:265:TYR:HB3	1:O:412:ALA:HB3	1.74	0.69
1:O:483:TYR:O	1:O:486:TRP:HB3	1.91	0.69
1:Z:313:ILE:HD11	1:Z:381:LEU:HD23	1.73	0.69
1:Y:90:GLU:OE2	1:Y:93:THR:HG21	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:196:THR:CG2	1:O:198:ASP:H	2.06	0.69
1:X:313:ILE:HD12	1:X:313:ILE:H	1.57	0.69
1:Z:80:THR:HG21	1:Z:248:ALA:CB	2.23	0.69
1:Z:92:GLU:CG	1:Z:93:THR:HG23	2.20	0.69
1:Z:147:HIS:N	1:Z:147:HIS:HD1	1.91	0.69
1:O:85:THR:HG23	1:O:102:VAL:CA	2.22	0.69
1:O:83:ARG:NE	3:O:504:GOL:O2	2.26	0.69
1:X:64:LEU:CD2	1:X:69:ILE:HB	2.22	0.69
1:X:64:LEU:HD23	1:X:69:ILE:HB	1.75	0.69
1:X:250:LEU:HD12	1:X:255:CYS:HB2	1.75	0.68
1:O:128:THR:HG21	1:O:130:LEU:HB2	1.75	0.68
1:Z:6:ILE:HD13	1:Z:7:VAL:N	2.08	0.68
1:O:234:GLY:N	2:O:502:SO4:O2	2.26	0.68
1:Z:403:LEU:H	1:Z:403:LEU:HD12	1.59	0.68
1:Y:85:THR:CG2	1:Y:102:VAL:HA	2.22	0.68
1:X:415:ASN:HD21	1:X:417:PHE:HB3	1.58	0.68
1:Y:399:SER:HB2	1:Y:401:ILE:HD12	1.74	0.68
1:Z:468:ARG:HG3	1:Z:468:ARG:NH1	1.96	0.68
1:Z:328:ASP:O	1:Z:331:TYR:HB3	1.93	0.68
1:O:202:LYS:HD3	1:O:206:VAL:HG22	1.75	0.68
1:Z:429:ARG:CG	1:Z:471:ARG:HG2	2.24	0.68
1:Y:415:ASN:ND2	1:Y:417:PHE:HB3	2.08	0.68
1:O:415:ASN:HD21	1:O:417:PHE:HB3	1.59	0.67
1:X:227:THR:N	1:X:237:ILE:O	2.25	0.67
1:X:351:LEU:HD22	1:X:360:ALA:HB3	1.75	0.67
1:O:188:ARG:HH22	1:O:303:GLU:CD	1.97	0.67
1:O:127:ASN:ND2	1:O:193:ASN:HD21	1.90	0.67
1:X:426:LEU:HB3	1:X:428:THR:HB	1.76	0.67
1:X:287:LEU:O	1:X:302:LEU:HD23	1.94	0.67
1:X:347:ALA:HA	4:X:523:HOH:O	1.94	0.67
1:X:415:ASN:ND2	1:X:417:PHE:HB3	2.09	0.67
1:Z:147:HIS:HB3	4:Z:535:HOH:O	1.93	0.67
1:X:460:LEU:N	1:X:460:LEU:HD13	2.09	0.67
1:Z:278:LYS:HE3	1:Z:280:VAL:CG2	2.25	0.67
1:Y:418:LEU:HD13	1:Y:419:MET:CE	2.25	0.67
1:O:155:ALA:CB	1:O:210:PRO:HG2	2.24	0.67
1:Z:237:ILE:HG23	1:Z:238:PRO:HD2	1.75	0.67
1:Z:347:ALA:HB2	1:Z:351:LEU:CD1	2.25	0.67
1:X:186:ALA:O	1:X:189:THR:HG23	1.94	0.67
1:O:410:GLY:O	1:O:413:VAL:HG22	1.93	0.67
1:O:23:HIS:HA	1:O:453:PHE:CE2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:460:LEU:O	1:Z:463:LYS:HB2	1.95	0.66
1:Z:325:ASP:O	1:Z:328:ASP:HB2	1.95	0.66
1:O:216:GLU:OE2	1:O:218:ARG:HD3	1.95	0.66
1:X:29:SER:HB3	1:X:63:VAL:HG23	1.76	0.66
1:Z:313:ILE:HD11	1:Z:381:LEU:CD2	2.25	0.66
1:Z:253:GLN:NE2	1:Z:409:ASP:OD2	2.27	0.66
1:O:152:ARG:NH2	1:O:208:ASP:HB3	2.08	0.66
1:Z:44:TRP:HA	1:Z:105:CYS:SG	2.36	0.66
1:X:418:LEU:HD13	1:X:419:MET:HE2	1.77	0.66
1:Z:496:TRP:CZ3	1:X:488:LYS:HD2	2.31	0.66
1:O:86:THR:OG1	1:O:137:SER:HB3	1.96	0.66
1:Z:83:ARG:NH1	3:Z:504:GOL:O2	2.28	0.66
1:O:150:GLY:O	1:O:153:GLU:HB2	1.95	0.66
1:O:141:VAL:HG11	1:O:209:ILE:HG12	1.76	0.66
1:Y:201:ASP:OD1	1:Y:211:ARG:NH1	2.29	0.66
1:Z:12:GLY:HA3	1:Z:17:ARG:HH12	1.61	0.66
1:X:179:HIS:CD2	1:X:215:PRO:HB3	2.30	0.66
1:Z:269:CYS:HB2	1:Z:306:VAL:HB	1.77	0.66
1:Z:40:PRO:HG2	1:Z:44:TRP:HB3	1.77	0.66
1:Y:33:ARG:HH22	1:Z:58:SER:CB	2.00	0.66
1:Z:203:MET:CA	1:Z:206:VAL:HG12	2.25	0.66
1:Z:203:MET:O	1:Z:206:VAL:HG12	1.96	0.66
1:X:108:THR:HB	1:X:139:THR:HB	1.78	0.66
1:Y:83:ARG:HD3	1:Y:245:ASP:OD1	1.96	0.66
1:X:478:GLU:O	1:X:482:ARG:HG2	1.96	0.66
1:Y:19:VAL:CG1	1:Y:27:ILE:HD12	2.25	0.66
1:Y:90:GLU:OE2	1:Y:95:LYS:HD2	1.96	0.66
1:X:438:VAL:HA	1:X:441:LEU:HD13	1.78	0.66
1:X:148:VAL:HB	1:X:151:SER:OG	1.96	0.66
1:Z:166:ASP:N	1:Z:166:ASP:OD1	2.27	0.65
1:Z:466:ILE:N	1:Z:466:ILE:HD13	2.10	0.65
1:O:128:THR:CG2	1:O:130:LEU:HB2	2.27	0.65
1:Y:174:THR:O	1:Y:176:GLY:N	2.29	0.65
1:O:468:ARG:HD2	1:O:470:PHE:CE1	2.31	0.65
1:Y:227:THR:N	1:Y:237:ILE:O	2.29	0.65
1:O:15:SER:O	1:O:17:ARG:NH1	2.30	0.65
1:O:193:ASN:HB3	1:O:196:THR:HG21	1.78	0.65
1:Y:196:THR:CG2	1:Y:198:ASP:HB3	2.26	0.65
1:X:219:ARG:NH2	1:X:295:THR:O	2.29	0.65
1:X:214:LEU:N	1:X:214:LEU:HD23	2.11	0.65
1:X:178:VAL:CG1	1:X:180:VAL:HB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:40:PRO:HG2	1:O:44:TRP:HB2	1.77	0.65
1:Z:157:ARG:HG3	1:Z:157:ARG:O	1.96	0.65
1:Z:315:TRP:HD1	1:Z:319:GLU:HG2	1.57	0.65
1:Z:22:ASP:OD1	1:Z:24:ASP:N	2.28	0.65
1:Y:40:PRO:HD2	1:Y:44:TRP:HB2	1.77	0.65
1:O:123:TYR:O	1:O:126:SER:N	2.30	0.65
1:X:406:LEU:CD1	1:X:408:VAL:HG12	2.26	0.65
1:O:236:ARG:NH2	2:O:502:SO4:O2	2.30	0.65
1:Z:201:ASP:OD2	1:Z:211:ARG:NH1	2.30	0.65
1:O:211:ARG:HA	1:O:214:LEU:HD13	1.78	0.65
1:X:22:ASP:OD1	1:X:24:ASP:N	2.29	0.65
1:O:421:PHE:O	1:O:425:ILE:HG22	1.96	0.65
1:X:193:ASN:HB3	1:X:196:THR:CG2	2.27	0.65
1:Z:240:SER:HB2	1:Z:450:ALA:CB	2.27	0.65
1:X:169:LEU:O	1:X:173:MET:HG3	1.97	0.65
1:O:156:ARG:HG2	1:O:210:PRO:HG3	1.78	0.65
1:Y:87:ILE:HD12	1:Y:168:TRP:CG	2.32	0.65
1:Z:226:GLN:NE2	1:Z:236:ARG:HG2	2.12	0.65
1:Z:40:PRO:HG2	1:Z:44:TRP:CB	2.25	0.65
1:O:202:LYS:HE2	1:O:205:GLU:HG2	1.78	0.64
1:Z:212:GLU:OE1	1:Z:212:GLU:N	2.30	0.64
1:O:261:ALA:HB2	1:O:273:MET:CB	2.26	0.64
1:O:378:ARG:O	1:O:382:GLU:HG3	1.96	0.64
1:Y:226:GLN:HG2	1:Y:238:PRO:HA	1.79	0.64
1:O:362:GLY:C	1:Y:367:LEU:HB2	2.17	0.64
1:O:62:GLU:HB3	1:X:58:SER:OG	1.98	0.64
1:O:127:ASN:ND2	1:O:193:ASN:ND2	2.43	0.64
1:Y:466:ILE:O	1:Y:466:ILE:HD13	1.97	0.64
1:Y:280:VAL:CG1	1:Y:302:LEU:HD21	2.28	0.64
1:O:240:SER:HB2	1:O:450:ALA:CB	2.27	0.64
1:Z:49:PRO:HB3	1:Z:87:ILE:HD13	1.80	0.64
1:O:283:GLU:HB2	1:O:398:ASP:OD1	1.97	0.64
1:Y:418:LEU:HD13	1:Y:419:MET:HE2	1.80	0.64
1:O:237:ILE:CG2	1:O:238:PRO:HD2	2.28	0.64
1:Y:428:THR:HG22	1:Y:429:ARG:O	1.98	0.64
1:Z:253:GLN:HG2	1:Z:438:VAL:HG21	1.80	0.64
1:O:211:ARG:HG2	1:O:211:ARG:O	1.98	0.64
1:X:105:CYS:SG	1:X:107:ARG:HB3	2.36	0.64
1:X:180:VAL:CG2	1:X:218:ARG:HG3	2.27	0.64
1:Z:497:GLU:HG2	4:Z:529:HOH:O	1.98	0.64
1:Z:365:PHE:CZ	1:Z:492:ARG:HB3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:320:MET:HE1	1:X:373:ALA:CA	2.21	0.64
1:X:240:SER:HB2	1:X:450:ALA:CB	2.28	0.64
1:O:442:GLY:O	1:O:445:TYR:HB2	1.97	0.64
1:X:133:ASP:OD2	1:X:135:TYR:HB2	1.98	0.64
1:O:458:ASP:HA	1:O:461:GLN:CG	2.28	0.64
1:X:154:ARG:HB3	1:X:159:GLU:CB	2.28	0.64
1:X:154:ARG:O	1:X:159:GLU:HB2	1.98	0.64
1:Z:62:GLU:O	1:Z:66:LYS:HB2	1.98	0.64
1:O:124:ILE:HD13	1:O:203:MET:HE3	1.78	0.63
1:Z:403:LEU:N	1:Z:403:LEU:HD12	2.13	0.63
1:Y:68:ASP:C	1:Y:69:ILE:HD13	2.19	0.63
1:O:59:THR:O	1:O:63:VAL:HG22	1.98	0.63
1:Y:376:ILE:N	1:Y:376:ILE:HD13	2.13	0.63
1:Z:486:TRP:O	1:Z:490:VAL:HG23	1.99	0.63
1:X:381:LEU:HD23	1:X:381:LEU:N	2.11	0.63
1:Y:105:CYS:SG	1:Y:107:ARG:HD2	2.39	0.63
1:O:458:ASP:HA	1:O:461:GLN:HG3	1.81	0.63
1:Y:19:VAL:HG12	1:Y:27:ILE:HG23	1.81	0.63
1:O:456:ASN:O	1:O:459:GLU:HG3	1.98	0.63
1:Z:226:GLN:HA	1:Z:237:ILE:O	1.98	0.63
1:Z:351:LEU:HD22	1:Z:360:ALA:HB2	1.81	0.63
1:O:174:THR:HA	1:O:177:ARG:NH2	2.13	0.63
1:O:428:THR:HG22	1:O:429:ARG:O	1.99	0.63
1:Z:141:VAL:HG12	1:Z:145:LEU:HD22	1.80	0.63
1:Z:152:ARG:O	1:Z:155:ALA:HB3	1.99	0.63
1:O:396:GLN:NE2	1:O:403:LEU:H	1.95	0.63
1:O:462:GLU:H	1:O:462:GLU:CD	2.03	0.62
1:Y:415:ASN:ND2	1:Y:418:LEU:H	1.97	0.62
1:X:313:ILE:HD12	1:X:313:ILE:N	2.13	0.62
1:O:362:GLY:CA	1:Y:367:LEU:HB2	2.28	0.62
1:X:345:VAL:O	1:X:362:GLY:HA2	1.99	0.62
1:O:85:THR:HA	1:O:101:ILE:O	1.99	0.62
1:X:108:THR:OG1	1:X:134:PRO:HB3	1.99	0.62
1:X:154:ARG:CZ	1:X:159:GLU:HG2	2.28	0.62
1:X:471:ARG:HG3	1:X:471:ARG:NH1	2.12	0.62
1:X:111:ILE:N	1:X:111:ILE:HD12	2.12	0.62
1:X:216:GLU:OE2	1:X:218:ARG:NH1	2.32	0.62
1:Y:65:THR:HG22	1:Y:66:LYS:N	2.15	0.62
1:Y:325:ASP:O	1:Y:328:ASP:HB2	1.99	0.62
1:Z:125:ARG:HB2	1:Z:125:ARG:NH1	2.05	0.62
1:Y:9:LEU:HB2	1:Y:79:ILE:CD1	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:83:ARG:NH1	3:Z:504:GOL:O1	2.27	0.62
1:Y:387:GLN:O	1:Y:390:ASP:HB2	1.99	0.62
1:Y:193:ASN:HB2	1:Y:200:ASP:OD2	2.00	0.62
1:Y:93:THR:OG1	1:Y:95:LYS:N	2.29	0.62
1:X:152:ARG:HH11	1:X:152:ARG:HG2	1.65	0.62
1:Z:169:LEU:O	1:Z:173:MET:HG3	1.99	0.62
1:Y:112:CYS:HB3	1:Y:132:ILE:HG22	1.81	0.62
1:O:496:TRP:CZ3	1:Y:488:LYS:HD2	2.34	0.62
1:O:313:ILE:HD11	1:O:381:LEU:CD2	2.29	0.62
1:Y:295:THR:HG22	1:Y:297:GLU:OE1	2.00	0.62
1:Y:50:MET:CE	1:Y:50:MET:HA	2.30	0.62
1:Y:281:LYS:NZ	1:Y:283:GLU:OE2	2.29	0.62
1:O:260:MET:O	1:O:273:MET:HA	2.00	0.61
1:Z:23:HIS:HA	1:Z:453:PHE:CZ	2.35	0.61
1:Z:415:ASN:ND2	1:Z:418:LEU:H	1.98	0.61
1:X:256:VAL:HG11	1:X:294:PRO:CB	2.30	0.61
1:Y:432:ARG:O	1:Y:467:GLU:N	2.34	0.61
1:Z:275:THR:O	1:Z:278:LYS:HG2	2.01	0.61
1:O:71:SER:HA	1:O:74:ILE:HD12	1.81	0.61
1:O:295:THR:OG1	1:O:297:GLU:HG2	2.00	0.61
1:X:180:VAL:HG21	1:X:218:ARG:HG3	1.80	0.61
1:Z:203:MET:SD	1:Z:206:VAL:HG11	2.40	0.61
1:O:313:ILE:N	1:O:313:ILE:HD13	2.16	0.61
1:O:415:ASN:ND2	1:O:418:LEU:H	1.98	0.61
1:Y:280:VAL:HG12	1:Y:302:LEU:HD21	1.82	0.61
1:Y:170:ILE:HG22	1:Y:171:TRP:N	2.14	0.61
1:Z:191:LEU:HD11	1:Z:209:ILE:HD13	1.81	0.61
1:O:65:THR:HG23	1:X:54:ALA:CB	2.31	0.61
1:X:84:GLU:HG2	1:X:103:TRP:HB3	1.83	0.61
1:X:389:ARG:HG2	1:X:483:TYR:CE1	2.36	0.61
1:Y:476:THR:O	1:Y:479:ARG:N	2.32	0.61
1:Y:325:ASP:HB2	1:Y:328:ASP:OD1	2.00	0.61
1:Z:476:THR:HA	1:Z:479:ARG:HG2	1.82	0.61
1:Y:128:THR:OG1	1:Y:130:LEU:HB2	2.01	0.61
1:Y:180:VAL:HG21	1:Y:218:ARG:HG3	1.81	0.61
1:O:432:ARG:NE	1:O:467:GLU:OE1	2.34	0.61
1:X:486:TRP:HD1	1:X:487:LYS:HD2	1.63	0.61
1:Y:115:LEU:N	1:Y:115:LEU:HD22	2.15	0.61
1:Z:233:GLY:HA2	2:Z:502:SO4:O2	2.01	0.61
1:Y:17:ARG:HG3	1:Y:32:GLN:HG3	1.81	0.61
1:X:194:ILE:HG22	1:X:290:ILE:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:429:ARG:HA	1:X:470:PHE:O	2.00	0.60
1:X:12:GLY:HA3	1:X:17:ARG:HH12	1.65	0.60
1:O:415:ASN:ND2	1:O:417:PHE:HB3	2.16	0.60
1:O:396:GLN:HE21	1:O:403:LEU:H	1.49	0.60
1:X:152:ARG:CG	1:X:152:ARG:HH11	2.14	0.60
1:Z:336:VAL:HG13	1:Z:338:ASN:O	2.01	0.60
1:O:328:ASP:O	1:O:331:TYR:HB3	2.00	0.60
1:X:111:ILE:HG22	1:X:139:THR:HG22	1.83	0.60
1:X:194:ILE:HG22	1:X:290:ILE:HD12	1.82	0.60
1:X:258:GLU:HA	1:X:274:ASN:O	2.02	0.60
1:Y:351:LEU:HD22	1:Y:360:ALA:CB	2.31	0.60
1:X:386:TYR:HE1	1:X:425:ILE:CD1	2.14	0.60
1:O:214:LEU:HD12	1:O:214:LEU:N	2.16	0.60
1:Z:194:ILE:HD12	1:Z:300:TYR:CE2	2.37	0.60
1:Z:203:MET:C	1:Z:206:VAL:HG12	2.21	0.60
1:Z:138:GLY:N	1:Z:189:THR:O	2.33	0.60
1:O:458:ASP:N	1:O:458:ASP:OD1	2.29	0.60
1:Y:48:ASP:OD1	1:Y:49:PRO:HD2	2.01	0.60
1:Z:456:ASN:HD22	1:Z:458:ASP:N	1.99	0.60
1:O:362:GLY:HA3	1:Y:367:LEU:HB2	1.83	0.60
1:O:475:GLU:O	1:O:477:THR:N	2.35	0.60
1:Y:458:ASP:HA	1:Y:461:GLN:NE2	2.16	0.60
1:O:422:GLN:HA	1:O:425:ILE:CG2	2.32	0.60
1:X:293:GLY:O	1:X:295:THR:N	2.34	0.60
1:Y:316:LEU:HA	1:Y:320:MET:HB2	1.84	0.60
1:Z:457:LEU:O	1:Z:461:GLN:HG2	2.02	0.60
1:Y:61:VAL:HG21	1:Z:61:VAL:HG21	1.84	0.59
1:O:202:LYS:HD3	1:O:202:LYS:C	2.23	0.59
1:O:458:ASP:HA	1:O:461:GLN:CD	2.23	0.59
1:X:111:ILE:H	1:X:111:ILE:CD1	2.08	0.59
1:X:227:THR:O	1:X:237:ILE:N	2.31	0.59
1:X:80:THR:HG21	1:X:248:ALA:HB3	1.84	0.59
1:X:471:ARG:HH11	1:X:471:ARG:HG3	1.66	0.59
1:O:200:ASP:OD1	1:O:202:LYS:HB3	2.02	0.59
1:O:179:HIS:NE2	1:O:215:PRO:HB3	2.18	0.59
1:O:497:GLU:HG3	1:O:498:GLU:N	2.17	0.59
1:Z:237:ILE:CG2	1:Z:238:PRO:HD2	2.31	0.59
1:X:122:ASP:O	1:X:126:SER:HB2	2.02	0.59
1:Z:403:LEU:CD1	1:Z:403:LEU:H	2.15	0.59
1:X:258:GLU:HB3	1:X:276:GLY:N	2.17	0.59
1:Z:413:VAL:HG23	1:Z:436:ARG:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:85:THR:HG23	1:Y:102:VAL:CA	2.25	0.59
1:O:85:THR:CG2	1:O:102:VAL:HA	2.28	0.59
1:Y:328:ASP:O	1:Y:331:TYR:HB3	2.01	0.59
1:O:156:ARG:HG3	1:O:210:PRO:HG3	1.83	0.59
1:O:84:GLU:HB2	1:O:103:TRP:HB3	1.83	0.59
1:X:396:GLN:HG2	1:X:401:ILE:O	2.01	0.59
1:Z:402:ARG:HG3	1:Z:402:ARG:NH1	2.15	0.59
1:O:331:TYR:O	1:O:335:LYS:HG2	2.02	0.59
1:X:184:THR:O	1:X:187:SER:HB3	2.03	0.59
1:O:153:GLU:OE2	1:O:153:GLU:HA	1.90	0.59
1:Y:19:VAL:CG1	1:Y:27:ILE:HG23	2.32	0.59
1:X:351:LEU:HD22	1:X:360:ALA:CB	2.32	0.59
1:O:85:THR:HG23	1:O:101:ILE:C	2.23	0.59
1:Y:406:LEU:HD13	1:Y:408:VAL:HG12	1.85	0.59
1:X:178:VAL:HG12	1:X:180:VAL:HB	1.85	0.59
1:O:227:THR:N	1:O:237:ILE:O	2.34	0.59
1:X:407:ARG:CZ	1:X:466:ILE:HD11	2.32	0.59
1:O:271:MET:CE	1:O:392:LEU:HD12	2.32	0.59
1:Z:131:VAL:HG13	1:Z:132:ILE:N	2.16	0.58
1:Z:460:LEU:CA	1:Z:463:LYS:HD2	2.28	0.58
1:Z:49:PRO:O	1:Z:52:ILE:HB	2.03	0.58
1:X:180:VAL:HG23	1:X:216:GLU:HG2	1.84	0.58
1:Y:500:ASP:OD1	1:Y:500:ASP:N	2.36	0.58
1:O:134:PRO:O	1:O:140:LYS:NZ	2.34	0.58
1:O:124:ILE:HD13	1:O:203:MET:HE1	1.85	0.58
1:Z:424:ASP:OD1	1:Z:473:GLY:N	2.29	0.58
1:Y:256:VAL:HG11	1:Y:294:PRO:CB	2.34	0.58
1:X:415:ASN:HD22	1:X:415:ASN:C	2.06	0.58
1:X:438:VAL:HA	1:X:441:LEU:CD1	2.33	0.58
1:X:313:ILE:CD1	1:X:313:ILE:H	2.16	0.58
1:O:204:LEU:HD22	1:O:209:ILE:O	2.03	0.58
1:X:193:ASN:HB3	1:X:196:THR:HG21	1.85	0.58
1:Z:36:GLU:HG3	1:Z:37:GLN:N	2.19	0.58
1:O:316:LEU:HA	1:O:320:MET:HB2	1.86	0.58
1:Z:219:ARG:HG3	1:Z:222:GLU:OE1	2.03	0.58
1:Y:475:GLU:OE1	1:Y:478:GLU:HB2	2.03	0.58
1:Y:20:VAL:O	1:Y:28:ILE:N	2.29	0.58
1:X:286:LEU:HD13	1:X:395:MET:CE	2.34	0.58
1:Z:386:TYR:HB3	1:Z:486:TRP:CE2	2.38	0.58
1:X:130:LEU:HD12	1:X:190:MET:CB	2.33	0.58
1:X:47:HIS:CD2	1:X:82:GLN:HE22	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:157:ARG:CB	1:Z:157:ARG:HH11	2.17	0.58
1:O:196:THR:HG21	4:O:514:HOH:O	2.03	0.58
1:O:210:PRO:O	1:O:213:MET:HG2	2.03	0.58
1:Y:80:THR:HG21	1:Y:245:ASP:HA	1.84	0.58
1:O:328:ASP:HB3	1:O:332:PHE:CE2	2.39	0.58
1:Z:499:HIS:CD2	1:Z:500:ASP:H	2.21	0.58
1:Z:156:ARG:O	1:Z:212:GLU:HG2	2.04	0.58
1:Y:217:VAL:C	1:Y:218:ARG:HG2	2.24	0.58
1:X:456:ASN:O	1:X:459:GLU:HB2	2.02	0.58
1:Z:330:GLU:O	1:Z:334:THR:HG23	2.04	0.58
1:X:157:ARG:HH12	1:X:159:GLU:CD	2.07	0.58
1:Z:401:ILE:HG22	1:Z:402:ARG:N	2.19	0.58
1:Y:226:GLN:HA	1:Y:237:ILE:O	2.04	0.58
1:Z:343:TYR:O	1:Z:364:ILE:HA	2.04	0.58
1:Z:106:ARG:HD2	1:Z:349:THR:O	2.03	0.58
1:Y:123:TYR:CD2	1:Y:203:MET:HE3	2.38	0.57
1:O:29:SER:OG	1:O:63:VAL:HG12	2.03	0.57
1:Z:265:TYR:HB3	1:Z:412:ALA:HB3	1.86	0.57
1:X:309:ALA:O	1:X:312:SER:HB2	2.03	0.57
1:X:84:GLU:OE1	1:X:188:ARG:NH1	2.37	0.57
1:O:5:TYR:CE2	1:O:69:ILE:HG12	2.38	0.57
1:Y:33:ARG:HH21	1:Z:33:ARG:HH21	1.52	0.57
1:Z:278:LYS:HE3	1:Z:280:VAL:HG23	1.85	0.57
1:Y:491:LYS:HA	1:Y:494:MET:CE	2.34	0.57
1:X:352:GLY:N	4:X:524:HOH:O	2.36	0.57
1:O:261:ALA:HA	1:O:272:LEU:O	2.05	0.57
1:X:310:GLY:HA2	1:X:313:ILE:HD13	1.86	0.57
1:Y:456:ASN:ND2	1:Y:458:ASP:N	2.37	0.57
1:Z:115:LEU:HA	1:Z:120:LEU:CD1	2.32	0.57
1:Y:424:ASP:CB	1:Y:474:ILE:HG21	2.29	0.57
1:Y:54:ALA:HA	1:Z:65:THR:HG23	1.85	0.57
1:O:251:PHE:HE2	1:O:445:TYR:HB3	1.70	0.57
1:Y:491:LYS:HA	1:Y:494:MET:HE2	1.87	0.57
1:Y:325:ASP:O	1:Y:328:ASP:N	2.29	0.57
1:O:174:THR:C	1:O:175:GLN:HG2	2.24	0.57
1:X:423:SER:O	1:X:427:GLY:N	2.37	0.57
1:Y:77:ILE:HG22	1:Y:78:GLY:N	2.20	0.57
1:X:478:GLU:HG3	1:X:479:ARG:N	2.19	0.57
1:O:424:ASP:HA	1:O:472:PRO:HA	1.86	0.57
1:O:325:ASP:O	1:O:328:ASP:N	2.35	0.57
1:Z:30:VAL:HG12	1:Z:31:SER:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:161:LEU:HD22	1:O:179:HIS:HE1	1.64	0.57
1:Y:345:VAL:N	1:Y:363:ALA:O	2.33	0.57
1:X:457:LEU:O	1:X:460:LEU:N	2.31	0.57
1:Y:38:ILE:O	1:Y:45:VAL:HA	2.03	0.57
1:X:422:GLN:NE2	1:X:426:LEU:HD22	2.19	0.57
1:X:106:ARG:HD2	1:X:349:THR:O	2.04	0.56
1:Z:422:GLN:HE21	1:Z:426:LEU:HD22	1.70	0.56
1:O:70:SER:OG	1:O:73:GLN:NE2	2.39	0.56
1:X:342:VAL:HG12	1:X:343:TYR:N	2.20	0.56
1:O:30:VAL:HG12	1:O:31:SER:N	2.19	0.56
1:Z:156:ARG:HD3	1:Z:210:PRO:HG3	1.86	0.56
1:Z:347:ALA:CB	1:Z:351:LEU:HD13	2.33	0.56
1:X:200:ASP:O	1:X:204:LEU:HD13	2.05	0.56
1:Z:122:ASP:O	1:Z:126:SER:HB2	2.04	0.56
1:X:482:ARG:HB3	1:X:482:ARG:HH11	1.70	0.56
1:X:249:ALA:HB2	1:X:439:THR:OG1	2.05	0.56
1:X:250:LEU:CD1	1:X:255:CYS:HB2	2.36	0.56
1:O:496:TRP:CE3	1:Y:488:LYS:HD2	2.40	0.56
1:O:128:THR:HB	1:O:130:LEU:H	1.70	0.56
1:X:401:ILE:HG22	1:X:403:LEU:HD12	1.87	0.56
1:X:157:ARG:HB2	1:X:157:ARG:CZ	2.35	0.56
1:O:143:TRP:O	1:O:147:HIS:ND1	2.31	0.56
1:Y:120:LEU:O	1:Y:124:ILE:HG13	2.05	0.56
1:Y:60:LEU:O	1:Y:63:VAL:HG23	2.06	0.56
1:Z:157:ARG:HH11	1:Z:157:ARG:CG	2.19	0.56
1:X:251:PHE:CE2	1:X:446:LEU:HD11	2.40	0.56
1:X:294:PRO:HD2	1:X:297:GLU:OE2	2.05	0.56
1:Z:62:GLU:HA	1:Z:65:THR:HG22	1.87	0.56
1:X:386:TYR:HE1	1:X:425:ILE:HD13	1.71	0.56
1:X:47:HIS:HD2	1:X:82:GLN:HE22	1.54	0.56
1:Z:293:GLY:O	1:Z:295:THR:N	2.38	0.56
1:Y:2:GLU:O	1:Y:73:GLN:HA	2.06	0.56
1:Y:13:THR:HG22	1:Y:13:THR:O	2.06	0.56
1:Z:467:GLU:OE1	1:Z:468:ARG:HB2	2.06	0.56
1:O:137:SER:OG	1:O:189:THR:HA	2.04	0.56
1:X:437:GLU:C	1:X:441:LEU:HD12	2.26	0.56
1:Z:253:GLN:CG	1:Z:438:VAL:HG21	2.35	0.56
1:O:430:VAL:O	1:O:469:GLU:HA	2.05	0.56
1:Y:202:LYS:O	1:Y:206:VAL:N	2.29	0.56
1:Y:9:LEU:HD13	1:Y:77:ILE:CG2	2.36	0.56
1:Z:295:THR:HB	1:Z:297:GLU:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:196:THR:HG23	1:O:198:ASP:N	2.21	0.56
1:Y:474:ILE:HG12	1:Y:475:GLU:N	2.21	0.56
1:O:204:LEU:CD2	1:O:209:ILE:HG22	2.36	0.56
1:Z:191:LEU:O	1:Z:199:TRP:HE3	1.89	0.56
1:Y:240:SER:O	1:Y:447:ALA:HA	2.05	0.56
1:Z:125:ARG:CG	1:Z:125:ARG:HH11	2.19	0.56
1:Z:156:ARG:C	1:Z:158:GLY:H	2.08	0.56
1:O:317:ARG:HB2	1:O:323:ILE:CD1	2.35	0.56
1:O:40:PRO:HG2	1:O:44:TRP:CB	2.35	0.56
1:O:189:THR:CB	1:O:191:LEU:HD12	2.23	0.56
1:X:456:ASN:HD22	1:X:458:ASP:HB2	1.71	0.56
1:Y:483:TYR:O	1:Y:486:TRP:HB3	2.06	0.56
1:O:394:ALA:O	1:O:397:ALA:HB3	2.05	0.56
1:Z:108:THR:HB	1:Z:139:THR:HB	1.89	0.56
1:O:65:THR:HG21	1:X:54:ALA:HA	1.88	0.55
1:Z:320:MET:O	1:Z:322:LEU:HD23	2.05	0.55
1:O:124:ILE:HG23	1:O:203:MET:CE	2.36	0.55
1:O:422:GLN:HA	1:O:425:ILE:HG22	1.88	0.55
1:Z:394:ALA:O	1:Z:397:ALA:HB3	2.06	0.55
1:Y:269:CYS:HB2	1:Y:306:VAL:HB	1.89	0.55
1:O:104:GLN:HB3	1:O:349:THR:HG21	1.87	0.55
1:Y:346:PRO:HG3	4:Y:512:HOH:O	2.06	0.55
1:O:15:SER:OG	1:O:17:ARG:NH1	2.39	0.55
1:Y:78:GLY:O	1:Y:79:ILE:HD13	2.06	0.55
1:Z:48:ASP:O	1:Z:52:ILE:HG13	2.07	0.55
1:Z:351:LEU:HD22	1:Z:360:ALA:HB1	1.88	0.55
1:Y:28:ILE:HD13	1:Y:28:ILE:N	2.20	0.55
1:X:351:LEU:HB2	1:X:357:ASP:HB3	1.88	0.55
1:O:23:HIS:HA	1:O:453:PHE:HE2	1.71	0.55
1:Y:123:TYR:HD2	1:Y:203:MET:HE3	1.71	0.55
1:Y:346:PRO:HA	1:Y:348:PHE:CE1	2.41	0.55
1:O:22:ASP:OD1	1:O:24:ASP:N	2.39	0.55
1:O:401:ILE:HG13	1:O:402:ARG:N	2.22	0.55
1:Z:318:ASP:O	1:Z:321:LYS:HE2	2.07	0.55
1:X:482:ARG:HA	1:X:482:ARG:HH11	1.70	0.55
1:X:251:PHE:CD2	1:X:446:LEU:HD11	2.42	0.55
1:O:422:GLN:O	1:O:426:LEU:HD22	2.07	0.55
1:Y:108:THR:HB	1:Y:139:THR:HB	1.88	0.55
1:X:378:ARG:O	1:X:382:GLU:HG3	2.06	0.55
1:O:164:THR:O	1:O:167:THR:HB	2.07	0.55
1:O:202:LYS:O	1:O:205:GLU:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:86:THR:HG23	1:Z:162:PHE:HE1	1.71	0.55
1:X:477:THR:O	1:X:481:TYR:HB2	2.06	0.55
1:O:269:CYS:HB2	1:O:306:VAL:HB	1.88	0.55
1:O:32:GLN:O	1:O:33:ARG:HD3	2.07	0.55
1:O:124:ILE:HG21	1:O:190:MET:SD	2.47	0.55
1:Z:210:PRO:O	1:Z:213:MET:HG2	2.07	0.55
1:Y:102:VAL:HG12	1:Y:103:TRP:N	2.21	0.55
1:O:331:TYR:CZ	1:O:335:LYS:HE3	2.42	0.55
1:X:174:THR:O	1:X:175:GLN:HG2	2.07	0.55
1:Z:170:ILE:HD11	1:Z:242:ILE:HD11	1.88	0.55
1:Y:82:GLN:HG3	1:Y:82:GLN:O	2.07	0.55
1:X:15:SER:O	1:X:17:ARG:NH1	2.39	0.55
1:Y:389:ARG:HH12	1:Y:479:ARG:HG3	1.72	0.55
1:X:254:LEU:O	1:X:256:VAL:N	2.40	0.55
1:X:83:ARG:NH1	3:X:503:GOL:O1	2.39	0.55
1:O:70:SER:H	1:O:73:GLN:HE22	1.55	0.55
1:O:460:LEU:CA	1:O:463:LYS:HE2	2.34	0.54
1:X:316:LEU:HA	1:X:320:MET:HB2	1.88	0.54
1:X:196:THR:HG22	1:X:198:ASP:H	1.72	0.54
1:X:312:SER:O	1:X:315:TRP:HB3	2.07	0.54
1:Z:316:LEU:HA	1:Z:320:MET:HB2	1.88	0.54
1:O:460:LEU:O	1:O:463:LYS:HE2	2.06	0.54
1:O:64:LEU:CD2	1:O:74:ILE:HD11	2.37	0.54
1:Y:222:GLU:O	1:Y:240:SER:HA	2.07	0.54
1:Z:363:ALA:HA	1:X:364:ILE:O	2.08	0.54
1:X:110:GLU:O	1:X:113:GLU:N	2.40	0.54
1:X:475:GLU:HG2	1:X:477:THR:OG1	2.07	0.54
1:X:159:GLU:HB3	1:X:160:LEU:HG	1.88	0.54
1:X:320:MET:O	1:X:322:LEU:HD23	2.07	0.54
1:Y:312:SER:O	1:Y:315:TRP:HB3	2.07	0.54
1:Y:191:LEU:CD2	1:Y:207:LEU:HD12	2.37	0.54
1:Z:130:LEU:N	1:Z:130:LEU:HD23	2.16	0.54
1:Z:152:ARG:C	1:Z:156:ARG:HG2	2.28	0.54
1:X:84:GLU:HG2	1:X:103:TRP:CB	2.37	0.54
1:X:317:ARG:HB2	1:X:323:ILE:HG13	1.89	0.54
1:X:386:TYR:HB3	1:X:486:TRP:CE2	2.42	0.54
1:X:3:LYS:N	1:X:4:LYS:NZ	2.54	0.54
1:X:497:GLU:HG3	1:X:498:GLU:N	2.22	0.54
1:O:196:THR:HG22	1:O:198:ASP:H	1.72	0.54
1:Z:106:ARG:NH1	1:Z:307:PHE:HE2	2.04	0.54
1:Z:317:ARG:O	1:Z:321:LYS:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:188:ARG:HH22	1:Z:303:GLU:CD	2.11	0.54
1:Z:473:GLY:C	1:Z:474:ILE:HG13	2.28	0.54
1:Z:399:SER:HB2	1:Z:401:ILE:HD12	1.90	0.54
1:X:202:LYS:O	1:X:205:GLU:HB3	2.08	0.54
1:X:213:MET:C	1:X:214:LEU:HD23	2.28	0.54
1:Z:133:ASP:CG	1:Z:134:PRO:HD2	2.28	0.54
1:Z:240:SER:O	1:Z:447:ALA:HA	2.08	0.54
1:O:332:PHE:HA	1:O:374:ASN:HD21	1.73	0.54
1:Y:392:LEU:O	1:Y:392:LEU:HG	2.08	0.54
1:O:31:SER:HB3	1:O:62:GLU:OE2	2.07	0.54
1:Z:171:TRP:CE3	1:Z:172:LYS:HD2	2.43	0.54
1:Z:200:ASP:HB3	1:Z:203:MET:HB2	1.90	0.54
1:X:180:VAL:HG22	1:X:218:ARG:CG	2.38	0.54
1:X:44:TRP:CE2	1:X:107:ARG:HB2	2.43	0.54
1:Z:194:ILE:HD12	1:Z:300:TYR:HE2	1.72	0.54
1:Y:468:ARG:CG	1:Y:468:ARG:HH11	2.15	0.53
1:Z:289:THR:O	1:Z:301:ALA:N	2.40	0.53
1:O:322:LEU:CD2	1:Y:322:LEU:HD21	2.37	0.53
1:X:445:TYR:N	1:X:445:TYR:CD1	2.75	0.53
1:O:130:LEU:O	1:O:131:VAL:HG23	2.08	0.53
1:O:402:ARG:HH21	1:O:404:HIS:CD2	2.26	0.53
1:Z:423:SER:O	1:Z:427:GLY:N	2.35	0.53
1:O:92:GLU:HB3	1:O:93:THR:HG23	1.89	0.53
1:O:457:LEU:O	1:O:460:LEU:HB2	2.08	0.53
1:Y:180:VAL:HG22	1:Y:218:ARG:HG3	1.90	0.53
1:Z:362:GLY:CA	1:X:367:LEU:HB2	2.36	0.53
1:Z:40:PRO:HG2	1:Z:44:TRP:HE3	1.72	0.53
1:Y:429:ARG:HG2	1:Y:469:GLU:CD	2.28	0.53
1:Y:174:THR:HG21	1:Y:178:VAL:HG13	1.90	0.53
1:O:406:LEU:HD22	1:O:407:ARG:N	2.23	0.53
1:X:37:GLN:OE1	1:X:47:HIS:HE1	1.91	0.53
1:Z:422:GLN:NE2	1:Z:426:LEU:HD22	2.23	0.53
1:X:70:SER:O	1:X:73:GLN:OE1	2.26	0.53
1:Y:40:PRO:HG2	1:Y:44:TRP:HE3	1.73	0.53
1:X:85:THR:HG23	1:X:102:VAL:HA	1.91	0.53
1:Z:92:GLU:HG2	1:Z:93:THR:N	2.23	0.53
1:Y:406:LEU:HD13	1:Y:408:VAL:HG13	1.90	0.53
1:Y:115:LEU:HD22	1:Y:115:LEU:H	1.72	0.53
1:O:70:SER:H	1:O:73:GLN:NE2	2.06	0.53
1:X:166:ASP:N	1:X:166:ASP:OD1	2.41	0.53
1:O:128:THR:O	1:O:128:THR:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:234:GLY:H	1:O:236:ARG:NH2	2.06	0.53
1:X:144:ILE:O	1:X:148:VAL:HG23	2.08	0.53
1:Y:127:ASN:HD22	1:Y:193:ASN:HD21	1.56	0.53
1:Z:352:GLY:O	1:Z:355:TYR:N	2.37	0.53
1:X:253:GLN:O	1:X:254:LEU:HB2	2.09	0.53
1:Z:401:ILE:HG22	1:Z:402:ARG:H	1.72	0.53
1:X:469:GLU:HG2	1:X:471:ARG:CZ	2.38	0.53
1:Y:169:LEU:O	1:Y:173:MET:HG3	2.09	0.53
1:Y:182:ASP:OD2	1:Y:184:THR:HG23	2.09	0.53
1:Z:183:TYR:CE1	1:Z:217:VAL:HG12	2.43	0.53
1:X:9:LEU:N	1:X:9:LEU:HD12	2.24	0.53
1:Y:456:ASN:O	1:Y:459:GLU:HB2	2.08	0.53
1:O:65:THR:HG23	1:X:54:ALA:CA	2.38	0.53
1:Y:330:GLU:O	1:Y:334:THR:HG23	2.09	0.53
1:O:152:ARG:O	1:O:156:ARG:HG3	2.08	0.53
1:O:152:ARG:HH21	1:O:208:ASP:HB3	1.71	0.53
1:Z:173:MET:HB3	1:Z:227:THR:HG21	1.90	0.53
1:Z:19:VAL:HG12	1:Z:20:VAL:N	2.23	0.53
1:O:51:GLU:O	1:O:55:THR:HG23	2.09	0.53
1:Y:272:LEU:CG	1:Y:303:GLU:HB2	2.28	0.53
1:X:90:GLU:HB2	1:X:93:THR:HG1	1.74	0.53
1:O:156:ARG:HA	1:O:212:GLU:OE1	2.09	0.53
1:X:216:GLU:OE2	1:X:218:ARG:HD3	2.08	0.53
1:Z:5:TYR:CE2	1:Z:69:ILE:HD13	2.43	0.53
1:Z:162:PHE:CD1	1:Z:163:GLY:N	2.77	0.53
1:Y:44:TRP:CD1	1:Y:44:TRP:N	2.75	0.53
1:O:142:LYS:O	1:O:146:ASP:OD1	2.26	0.53
1:X:19:VAL:HG11	1:X:27:ILE:CD1	2.39	0.53
1:X:476:THR:O	1:X:479:ARG:N	2.42	0.52
1:Y:415:ASN:HD22	1:Y:418:LEU:H	1.55	0.52
1:X:65:THR:CG2	1:X:66:LYS:N	2.72	0.52
1:Z:389:ARG:O	1:Z:393:GLU:HG2	2.09	0.52
1:Y:456:ASN:ND2	1:Y:458:ASP:OD1	2.42	0.52
1:Z:83:ARG:HH12	3:Z:504:GOL:C1	2.23	0.52
1:Y:297:GLU:OE1	1:Y:297:GLU:N	2.33	0.52
1:X:191:LEU:HD22	1:X:204:LEU:HD12	1.91	0.52
1:X:44:TRP:CD1	1:X:44:TRP:N	2.75	0.52
1:Z:499:HIS:CG	1:Z:500:ASP:N	2.77	0.52
1:Y:9:LEU:HD13	1:Y:77:ILE:HG21	1.91	0.52
1:Z:83:ARG:NH1	3:Z:504:GOL:C2	2.72	0.52
1:Z:123:TYR:CE2	1:Z:202:LYS:HG2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:20:VAL:O	1:Y:27:ILE:HA	2.10	0.52
1:Z:311:ALA:HA	1:Z:314:GLN:HG2	1.92	0.52
1:O:253:GLN:NE2	1:O:407:ARG:HG3	2.24	0.52
1:O:62:GLU:HA	1:O:65:THR:HG22	1.90	0.52
1:Z:135:TYR:OH	3:Z:504:GOL:O1	2.24	0.52
1:O:101:ILE:CG2	1:O:140:LYS:HG2	2.40	0.52
1:Y:49:PRO:HB3	1:Y:87:ILE:HD13	1.90	0.52
1:O:44:TRP:CD1	1:O:44:TRP:N	2.75	0.52
1:O:82:GLN:NE2	1:O:85:THR:OG1	2.42	0.52
1:X:174:THR:C	1:X:175:GLN:HG2	2.30	0.52
1:Y:98:TYR:CD2	1:Y:99:ASN:N	2.78	0.52
1:X:106:ARG:NH1	1:X:307:PHE:CE2	2.78	0.52
1:Z:174:THR:CG2	1:Z:178:VAL:HG13	2.32	0.52
1:X:80:THR:HG22	1:X:245:ASP:N	2.24	0.52
1:Z:115:LEU:N	1:Z:115:LEU:HD12	2.25	0.52
1:Z:461:GLN:C	1:Z:463:LYS:H	2.12	0.52
1:X:154:ARG:NH1	1:X:160:LEU:HD21	2.24	0.52
1:Z:41:LYS:O	1:Z:44:TRP:HB2	2.10	0.52
1:Y:430:VAL:O	1:Y:469:GLU:HA	2.09	0.52
1:O:204:LEU:HD23	1:O:209:ILE:HB	1.92	0.52
1:Z:129:GLY:C	1:Z:130:LEU:HD23	2.30	0.52
1:X:19:VAL:HG11	1:X:27:ILE:HD12	1.92	0.52
1:Y:137:SER:O	1:Y:141:VAL:HG23	2.09	0.52
1:Z:357:ASP:OD2	1:Z:360:ALA:HB2	2.10	0.52
1:X:125:ARG:N	4:X:534:HOH:O	2.43	0.52
1:O:123:TYR:CZ	1:O:202:LYS:HG3	2.45	0.51
1:Y:103:TRP:CE3	1:Y:104:GLN:HG3	2.45	0.51
1:O:196:THR:HG23	1:O:198:ASP:H	1.75	0.51
1:Y:396:GLN:NE2	1:Y:402:ARG:HA	2.25	0.51
1:O:317:ARG:O	1:O:321:LYS:HA	2.10	0.51
1:O:317:ARG:HA	1:O:323:ILE:CG1	2.40	0.51
1:X:180:VAL:CG2	1:X:216:GLU:HG2	2.39	0.51
1:Y:455:GLN:H	1:Y:459:GLU:CD	2.12	0.51
1:Z:386:TYR:HB3	1:Z:486:TRP:CD2	2.44	0.51
1:O:209:ILE:O	1:O:209:ILE:HG22	2.10	0.51
1:X:196:THR:HG23	1:X:196:THR:O	2.10	0.51
1:Z:436:ARG:HD2	1:Z:436:ARG:N	2.25	0.51
1:Y:59:THR:O	1:Y:63:VAL:HG22	2.10	0.51
1:Y:61:VAL:O	1:Y:65:THR:HB	2.10	0.51
1:Z:147:HIS:H	1:Z:147:HIS:HD1	1.56	0.51
1:Z:156:ARG:HG3	1:Z:156:ARG:NH1	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:161:LEU:HD13	1:Y:179:HIS:CD2	2.45	0.51
1:O:226:GLN:HA	1:O:237:ILE:O	2.11	0.51
1:Z:37:GLN:OE1	1:Z:47:HIS:HE1	1.93	0.51
1:X:98:TYR:CD2	1:X:99:ASN:N	2.78	0.51
1:O:221:SER:O	1:O:222:GLU:HB2	2.10	0.51
1:X:259:GLY:N	1:X:274:ASN:O	2.41	0.51
1:X:85:THR:HA	1:X:101:ILE:O	2.10	0.51
1:X:241:GLY:C	1:X:242:ILE:HG13	2.31	0.51
1:Z:415:ASN:O	1:Z:419:MET:HG2	2.10	0.51
1:O:154:ARG:CA	1:O:159:GLU:HG3	2.40	0.51
1:Y:428:THR:CG2	1:Y:429:ARG:N	2.74	0.51
1:Y:351:LEU:HD22	1:Y:360:ALA:HB1	1.92	0.51
1:X:35:PHE:HE2	1:X:47:HIS:CD2	2.29	0.51
1:X:48:ASP:O	1:X:51:GLU:N	2.43	0.51
1:Z:179:HIS:ND1	1:Z:215:PRO:HA	2.26	0.51
1:O:280:VAL:O	1:O:288:THR:HG21	2.11	0.51
1:Y:455:GLN:N	1:Y:459:GLU:OE1	2.41	0.51
1:O:85:THR:HG23	1:O:101:ILE:O	2.11	0.51
1:O:157:ARG:HB2	1:O:159:GLU:HG3	1.93	0.51
1:Z:40:PRO:CG	1:Z:44:TRP:HB3	2.40	0.51
1:O:224:TYR:CZ	1:O:242:ILE:HG13	2.46	0.51
1:X:153:GLU:O	1:X:156:ARG:N	2.42	0.51
1:Z:298:VAL:O	1:Z:299:ASN:OD1	2.28	0.51
1:Z:120:LEU:O	1:Z:124:ILE:HD12	2.10	0.51
1:Z:49:PRO:HG2	1:Z:96:PRO:CG	2.40	0.51
1:Y:193:ASN:HB3	1:Y:196:THR:HB	1.92	0.51
1:Y:191:LEU:HD21	1:Y:207:LEU:CD1	2.41	0.51
1:Y:441:LEU:HD13	1:Y:445:TYR:OH	2.11	0.51
1:Z:180:VAL:HG21	1:Z:218:ARG:HG3	1.91	0.51
1:Y:219:ARG:HH22	1:Y:295:THR:CG2	2.09	0.51
1:Y:486:TRP:O	1:Y:490:VAL:N	2.37	0.51
1:O:166:ASP:OD1	1:O:166:ASP:N	2.44	0.51
1:Z:428:THR:HG23	1:Z:429:ARG:O	2.11	0.51
1:X:7:VAL:CG2	1:X:74:ILE:HG23	2.40	0.51
1:Y:98:TYR:HD2	1:Y:99:ASN:O	1.94	0.51
1:Y:456:ASN:HD21	1:Y:458:ASP:CB	2.23	0.50
1:Z:83:ARG:HH11	1:Z:83:ARG:CG	2.24	0.50
1:Y:80:THR:HG22	1:Y:245:ASP:CA	2.37	0.50
1:O:384:ILE:HG22	1:O:385:ALA:N	2.24	0.50
1:O:114:HIS:ND1	1:O:114:HIS:N	2.56	0.50
1:Z:115:LEU:N	1:Z:115:LEU:CD1	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:121:GLU:HA	1:O:132:ILE:HD11	1.93	0.50
1:Y:295:THR:N	1:Y:297:GLU:OE1	2.38	0.50
1:O:250:LEU:HD11	1:O:255:CYS:CB	2.40	0.50
1:Z:415:ASN:HB3	1:Z:418:LEU:HB2	1.93	0.50
1:Y:179:HIS:CE1	1:Y:215:PRO:HA	2.46	0.50
1:X:251:PHE:HE1	1:X:293:GLY:O	1.95	0.50
1:X:7:VAL:HA	1:X:19:VAL:O	2.12	0.50
1:Y:141:VAL:HG12	1:Y:145:LEU:HD22	1.92	0.50
1:O:57:SER:O	1:O:60:LEU:HB3	2.12	0.50
1:O:16:SER:C	1:O:17:ARG:HD3	2.32	0.50
1:Z:48:ASP:HB3	1:Z:51:GLU:HB2	1.94	0.50
1:Z:51:GLU:O	1:Z:55:THR:HG23	2.11	0.50
1:Z:348:PHE:CE2	1:X:367:LEU:HB3	2.46	0.50
1:Y:441:LEU:HD13	1:Y:445:TYR:CZ	2.46	0.50
1:O:68:ASP:HB2	1:X:50:MET:CE	2.41	0.50
1:Z:206:VAL:HG13	1:Z:207:LEU:N	2.26	0.50
1:O:98:TYR:CE2	1:O:101:ILE:HD11	2.47	0.50
1:Z:180:VAL:HG22	1:Z:181:THR:H	1.77	0.50
1:Y:369:ARG:HB2	4:Y:525:HOH:O	2.11	0.50
1:Y:456:ASN:HD21	1:Y:458:ASP:N	2.00	0.50
1:Z:89:TRP:CE3	1:Z:89:TRP:N	2.80	0.50
1:O:458:ASP:C	1:O:461:GLN:HG3	2.32	0.50
1:Y:345:VAL:O	1:Y:362:GLY:HA2	2.12	0.50
1:Z:80:THR:CG2	1:Z:248:ALA:HB2	2.41	0.50
1:X:342:VAL:HG13	1:X:365:PHE:O	2.11	0.50
1:O:108:THR:OG1	1:O:134:PRO:HB3	2.12	0.50
1:X:326:ALA:O	1:X:329:SER:OG	2.28	0.50
1:X:232:LYS:O	1:X:233:GLY:O	2.30	0.50
1:O:415:ASN:HD22	1:O:415:ASN:C	2.15	0.50
1:X:225:GLY:O	1:X:238:PRO:HA	2.11	0.50
1:Z:225:GLY:O	1:Z:238:PRO:HA	2.12	0.50
1:Z:142:LYS:O	1:Z:145:LEU:HB2	2.12	0.50
1:Y:127:ASN:HD22	1:Y:193:ASN:ND2	2.10	0.50
1:O:345:VAL:O	1:O:362:GLY:HA2	2.12	0.50
1:Y:355:TYR:OH	1:Y:390:ASP:OD2	2.29	0.50
1:O:332:PHE:O	1:O:374:ASN:ND2	2.39	0.50
1:Y:202:LYS:HG3	1:Y:206:VAL:HG23	1.93	0.50
1:O:368:THR:O	1:O:371:VAL:HB	2.12	0.50
1:O:12:GLY:HA3	1:O:17:ARG:HH12	1.77	0.50
1:Y:317:ARG:NH1	1:Y:326:ALA:HB2	2.26	0.50
1:Z:294:PRO:HD2	1:Z:297:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:128:THR:HG21	1:O:130:LEU:CB	2.41	0.49
1:X:330:GLU:HG3	1:X:415:ASN:ND2	2.24	0.49
1:X:320:MET:HB3	1:X:322:LEU:HG	1.94	0.49
1:O:4:LYS:N	1:O:73:GLN:O	2.45	0.49
1:O:149:GLU:H	1:O:149:GLU:CD	2.16	0.49
1:O:250:LEU:HD12	1:O:255:CYS:HB2	1.92	0.49
1:O:85:THR:HG22	1:O:100:ALA:HB1	1.94	0.49
1:X:295:THR:OG1	1:X:295:THR:O	2.29	0.49
1:Z:19:VAL:HG13	1:Z:27:ILE:HG23	1.94	0.49
1:O:234:GLY:N	1:O:236:ARG:HH21	2.10	0.49
1:O:187:SER:HB3	1:O:289:THR:HG22	1.92	0.49
1:Z:140:LYS:O	1:Z:144:ILE:HG13	2.12	0.49
1:Z:415:ASN:HD22	1:Z:417:PHE:N	2.10	0.49
1:O:85:THR:HG23	1:O:102:VAL:N	2.27	0.49
1:Z:320:MET:HE3	1:X:373:ALA:HB2	1.95	0.49
1:Y:330:GLU:HG3	1:Y:415:ASN:ND2	2.27	0.49
1:O:154:ARG:HB3	1:O:159:GLU:CB	2.41	0.49
1:Y:93:THR:OG1	1:Y:95:LYS:HB3	2.12	0.49
1:Y:226:GLN:HB3	1:Y:236:ARG:HB3	1.94	0.49
1:Y:84:GLU:OE2	1:Y:188:ARG:NH1	2.45	0.49
1:Z:174:THR:O	1:Z:177:ARG:N	2.29	0.49
1:X:351:LEU:HB3	1:X:355:TYR:HB2	1.95	0.49
1:O:444:ALA:O	1:O:447:ALA:N	2.45	0.49
1:O:28:ILE:N	1:O:28:ILE:CD1	2.76	0.49
1:O:48:ASP:OD1	1:O:49:PRO:HD2	2.12	0.49
1:O:308:MET:HE3	1:O:349:THR:HG23	1.95	0.49
1:Z:455:GLN:N	1:Z:459:GLU:OE2	2.27	0.49
1:O:153:GLU:O	1:O:156:ARG:N	2.45	0.49
1:Y:269:CYS:CB	1:Y:306:VAL:HB	2.42	0.49
1:Z:246:GLN:O	1:Z:249:ALA:HB3	2.12	0.49
1:Y:284:ASN:OD1	1:Y:398:ASP:OD1	2.30	0.49
1:Y:338:ASN:CB	1:Y:482:ARG:HH22	2.25	0.49
1:Z:392:LEU:C	1:Z:392:LEU:HD23	2.33	0.49
1:Z:432:ARG:HD2	1:Z:467:GLU:OE1	2.11	0.49
1:X:435:VAL:HG12	1:X:435:VAL:O	2.13	0.49
1:X:162:PHE:CG	1:X:163:GLY:N	2.79	0.49
1:O:130:LEU:HD22	1:O:190:MET:HA	1.94	0.49
1:Z:475:GLU:HG3	1:Z:478:GLU:OE1	2.12	0.49
1:O:155:ALA:CB	1:O:213:MET:HE1	2.43	0.49
1:Z:401:ILE:CG2	1:Z:402:ARG:H	2.26	0.49
1:O:251:PHE:CE2	1:O:446:LEU:CD1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:489:ALA:O	1:Z:492:ARG:N	2.46	0.49
1:X:258:GLU:HB3	1:X:276:GLY:CA	2.42	0.49
1:X:286:LEU:HD13	1:X:395:MET:HE3	1.94	0.49
1:Y:80:THR:HG23	1:Y:248:ALA:HB2	1.95	0.49
1:X:3:LYS:HA	1:X:73:GLN:O	2.13	0.49
1:X:126:SER:O	1:X:195:HIS:HE1	1.95	0.49
1:X:343:TYR:OH	1:X:485:GLY:HA3	2.12	0.49
1:X:164:THR:OG1	1:X:166:ASP:OD1	2.30	0.49
1:Y:342:VAL:HG12	1:Y:343:TYR:N	2.27	0.49
1:Y:33:ARG:NH2	1:Z:33:ARG:HH21	2.11	0.49
1:Y:85:THR:HG23	1:Y:101:ILE:O	2.12	0.49
1:X:482:ARG:H	1:X:482:ARG:HG2	1.41	0.49
1:X:396:GLN:NE2	1:X:403:LEU:H	1.95	0.49
1:X:263:ASN:HB2	1:X:406:LEU:HD11	1.95	0.49
1:Z:331:TYR:CE2	1:Z:335:LYS:NZ	2.79	0.49
1:X:465:VAL:HG12	1:X:466:ILE:N	2.28	0.49
1:X:196:THR:HG22	1:X:197:LEU:N	2.28	0.49
1:X:331:TYR:O	1:X:335:LYS:HG3	2.13	0.48
1:X:320:MET:CE	1:X:320:MET:HA	2.37	0.48
1:X:64:LEU:HD22	1:X:69:ILE:HB	1.94	0.48
1:O:332:PHE:HA	1:O:374:ASN:ND2	2.27	0.48
1:Z:194:ILE:HG13	1:Z:195:HIS:CE1	2.48	0.48
1:O:320:MET:HB3	1:O:322:LEU:HG	1.94	0.48
1:Y:154:ARG:HB3	1:Y:159:GLU:HB2	1.95	0.48
1:O:202:LYS:O	1:O:206:VAL:HG22	2.13	0.48
1:Z:284:ASN:OD1	1:Z:398:ASP:OD1	2.31	0.48
1:O:372:ASN:O	1:O:375:HIS:HB2	2.13	0.48
1:Y:221:SER:OG	1:Y:446:LEU:O	2.27	0.48
1:Y:303:GLU:HG3	1:Y:304:GLY:N	2.27	0.48
1:O:155:ALA:HB1	1:O:213:MET:CE	2.43	0.48
1:O:180:VAL:HG21	1:O:218:ARG:HG3	1.95	0.48
1:O:422:GLN:CA	1:O:425:ILE:HG22	2.43	0.48
1:Z:223:VAL:HG22	1:Z:240:SER:HB3	1.95	0.48
1:X:6:ILE:HG21	1:X:444:ALA:HB1	1.94	0.48
1:O:478:GLU:O	1:O:481:TYR:N	2.47	0.48
1:X:106:ARG:O	1:X:108:THR:N	2.46	0.48
1:O:245:ASP:O	1:O:249:ALA:N	2.45	0.48
1:Z:346:PRO:HG3	1:Z:383:SER:HB2	1.94	0.48
1:O:422:GLN:NE2	1:O:426:LEU:HD22	2.27	0.48
1:X:180:VAL:HG22	1:X:218:ARG:HG2	1.95	0.48
1:Z:289:THR:O	1:Z:300:TYR:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:142:LYS:CD	1:O:207:LEU:HD22	2.43	0.48
1:O:147:HIS:HB3	4:O:533:HOH:O	2.12	0.48
1:O:322:LEU:HD21	1:Y:322:LEU:HD21	1.95	0.48
1:O:309:ALA:O	1:O:312:SER:HB2	2.13	0.48
1:Z:203:MET:HA	1:Z:206:VAL:HG11	1.94	0.48
1:Z:95:LYS:HE3	1:Z:96:PRO:O	2.13	0.48
1:Z:40:PRO:HG2	1:Z:44:TRP:CE3	2.49	0.48
1:Z:382:GLU:OE2	1:Z:482:ARG:NH2	2.47	0.48
1:X:409:ASP:HB2	1:X:438:VAL:HG21	1.95	0.48
1:Y:69:ILE:HD13	1:Y:69:ILE:N	2.27	0.48
1:X:130:LEU:HD12	1:X:190:MET:HA	1.94	0.48
1:X:130:LEU:CD1	1:X:190:MET:HB2	2.44	0.48
1:O:456:ASN:HD22	1:O:458:ASP:N	2.11	0.48
1:O:468:ARG:HD2	1:O:470:PHE:CZ	2.49	0.48
1:X:217:VAL:HG12	1:X:218:ARG:N	2.28	0.48
1:O:61:VAL:O	1:O:65:THR:HB	2.13	0.48
1:Z:474:ILE:HG23	1:Z:478:GLU:HB2	1.94	0.48
1:O:250:LEU:HD13	1:O:262:LYS:HG2	1.96	0.48
1:O:459:GLU:O	1:O:462:GLU:OE1	2.32	0.48
1:X:457:LEU:HD23	1:X:457:LEU:HA	1.63	0.48
1:O:138:GLY:O	1:O:141:VAL:HB	2.13	0.48
1:O:340:ASN:HB2	1:O:375:HIS:CD2	2.49	0.48
1:Y:338:ASN:HB3	1:Y:482:ARG:NH2	2.28	0.48
1:Y:451:VAL:O	1:Y:451:VAL:HG23	2.14	0.48
1:O:47:HIS:O	1:O:99:ASN:HB3	2.14	0.48
1:Z:48:ASP:OD1	1:Z:49:PRO:HD2	2.14	0.48
1:Z:44:TRP:N	1:Z:44:TRP:CD1	2.78	0.48
1:Y:19:VAL:HG11	1:Y:27:ILE:CD1	2.42	0.48
1:O:346:PRO:HA	1:O:348:PHE:CE1	2.49	0.48
1:Y:254:LEU:HA	1:Y:254:LEU:HD12	1.73	0.48
1:O:128:THR:HG21	1:O:130:LEU:CG	2.43	0.48
1:O:24:ASP:O	1:O:25:ALA:HB3	2.14	0.48
1:X:346:PRO:HA	1:X:348:PHE:HE1	1.77	0.48
1:Y:281:LYS:HD2	1:Y:281:LYS:O	2.13	0.48
1:Y:170:ILE:CG2	1:Y:171:TRP:N	2.73	0.48
1:Z:89:TRP:HB2	1:Z:95:LYS:O	2.13	0.47
1:Y:210:PRO:HB2	1:Y:213:MET:HE2	1.94	0.47
1:Y:33:ARG:NE	1:Z:33:ARG:CZ	2.77	0.47
1:O:131:VAL:CG1	1:O:132:ILE:N	2.77	0.47
1:O:130:LEU:CD2	1:O:190:MET:HG3	2.41	0.47
1:O:28:ILE:HG22	1:O:29:SER:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:89:TRP:HA	1:O:96:PRO:HA	1.96	0.47
1:O:342:VAL:HG12	1:O:343:TYR:N	2.29	0.47
1:O:258:GLU:HA	1:O:274:ASN:O	2.14	0.47
1:O:351:LEU:HB3	1:O:355:TYR:HB2	1.97	0.47
1:X:153:GLU:O	1:X:156:ARG:HB2	2.14	0.47
1:Z:381:LEU:O	1:Z:384:ILE:HB	2.14	0.47
1:Z:365:PHE:CE1	1:Z:492:ARG:HB3	2.49	0.47
1:X:229:ILE:N	4:X:525:HOH:O	2.36	0.47
1:Z:481:TYR:O	1:Z:484:ALA:HB3	2.13	0.47
1:Y:204:LEU:HD23	1:Y:204:LEU:N	2.29	0.47
1:Z:124:ILE:HG13	1:Z:203:MET:CE	2.44	0.47
1:O:259:GLY:N	1:O:274:ASN:O	2.40	0.47
1:O:461:GLN:H	1:O:461:GLN:HG2	1.32	0.47
1:Z:6:ILE:HG23	1:Z:21:MET:HB3	1.94	0.47
1:O:352:GLY:O	1:O:355:TYR:N	2.40	0.47
1:O:64:LEU:HD22	1:O:74:ILE:HD11	1.96	0.47
1:X:289:THR:O	1:X:301:ALA:N	2.41	0.47
1:X:264:THR:HG22	1:X:265:TYR:N	2.28	0.47
1:X:103:TRP:CZ3	1:X:104:GLN:HG3	2.49	0.47
1:Y:83:ARG:NH1	3:Y:503:GOL:C2	2.78	0.47
1:Z:346:PRO:HA	1:Z:348:PHE:CE1	2.50	0.47
1:O:447:ALA:O	1:O:450:ALA:HB3	2.15	0.47
1:X:114:HIS:CD2	1:X:114:HIS:N	2.81	0.47
1:Z:154:ARG:HA	1:Z:157:ARG:HG2	1.95	0.47
1:Y:102:VAL:CG1	1:Y:103:TRP:N	2.77	0.47
1:X:386:TYR:CE1	1:X:425:ILE:HD13	2.48	0.47
1:Y:339:THR:HG22	1:Y:378:ARG:HG2	1.97	0.47
1:Y:101:ILE:HG22	1:Y:140:LYS:HD3	1.96	0.47
1:O:460:LEU:HD22	1:O:460:LEU:N	2.22	0.47
1:O:461:GLN:O	1:O:463:LYS:N	2.48	0.47
1:O:456:ASN:ND2	1:O:458:ASP:HB2	2.30	0.47
1:X:474:ILE:HG23	1:X:478:GLU:HG3	1.96	0.47
1:O:80:THR:HG23	1:O:248:ALA:HB2	1.96	0.47
1:Z:6:ILE:HD13	1:Z:6:ILE:C	2.34	0.47
1:O:242:ILE:HG22	1:O:243:ALA:N	2.30	0.47
1:O:174:THR:CA	1:O:177:ARG:NH2	2.78	0.47
1:Z:499:HIS:CG	1:Z:500:ASP:H	2.32	0.47
1:O:142:LYS:HD3	1:O:207:LEU:HD22	1.97	0.47
1:Y:3:LYS:HZ3	1:Y:3:LYS:CB	2.26	0.47
1:O:125:ARG:HG3	1:O:125:ARG:O	2.13	0.47
1:Y:3:LYS:HZ3	1:Y:75:ALA:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:249:ALA:HB2	1:Y:439:THR:OG1	2.15	0.47
1:X:254:LEU:HA	1:X:254:LEU:HD12	1.73	0.47
1:Z:342:VAL:CG2	1:Z:371:VAL:HG21	2.45	0.47
1:Y:24:ASP:O	1:Y:25:ALA:HB3	2.14	0.47
1:Z:293:GLY:C	1:Z:295:THR:H	2.18	0.47
1:X:74:ILE:N	1:X:74:ILE:HD13	2.29	0.47
1:Z:114:HIS:ND1	1:Z:114:HIS:N	2.59	0.47
1:O:31:SER:CB	1:O:62:GLU:HG3	2.44	0.47
1:Z:28:ILE:HD12	1:Z:28:ILE:N	2.30	0.47
1:X:302:LEU:HD23	1:X:302:LEU:HA	1.77	0.47
1:X:46:GLU:HA	1:X:100:ALA:O	2.14	0.47
1:O:492:ARG:HH11	1:O:492:ARG:HG2	1.78	0.47
1:O:492:ARG:HD3	1:Y:496:TRP:HZ3	1.80	0.47
1:Z:115:LEU:CA	1:Z:120:LEU:HD12	2.42	0.47
1:O:415:ASN:HD22	1:O:417:PHE:N	2.13	0.47
1:Y:130:LEU:HD13	1:Y:136:PHE:CD2	2.50	0.47
1:X:478:GLU:HA	1:X:481:TYR:CB	2.44	0.47
1:Y:415:ASN:ND2	1:Y:417:PHE:H	2.13	0.47
1:Z:234:GLY:H	1:Z:236:ARG:NH2	2.13	0.47
1:Z:396:GLN:HG2	1:Z:401:ILE:O	2.14	0.47
1:X:6:ILE:HD12	1:X:453:PHE:CD2	2.50	0.47
1:Z:392:LEU:O	1:Z:395:MET:HB3	2.15	0.47
1:Y:114:HIS:N	1:Y:114:HIS:CD2	2.81	0.47
1:Z:408:VAL:HG22	1:Z:431:GLU:O	2.14	0.47
1:O:54:ALA:HB2	1:X:65:THR:HG23	1.96	0.46
1:Y:280:VAL:HG13	1:Y:281:LYS:N	2.30	0.46
1:Y:376:ILE:HD12	1:Y:376:ILE:HA	1.69	0.46
1:X:241:GLY:O	1:X:242:ILE:HG13	2.15	0.46
1:Z:13:THR:OG1	2:Z:503:SO4:O1	2.29	0.46
1:Y:389:ARG:O	1:Y:393:GLU:HG3	2.15	0.46
1:Z:227:THR:N	1:Z:237:ILE:O	2.43	0.46
1:O:317:ARG:HA	1:O:323:ILE:HG12	1.97	0.46
1:Z:80:THR:CG2	1:Z:248:ALA:CB	2.93	0.46
1:Z:214:LEU:HB3	1:Z:215:PRO:HD2	1.98	0.46
1:Y:270:PHE:HE1	4:Y:527:HOH:O	1.98	0.46
1:O:54:ALA:CB	1:X:65:THR:HG23	2.46	0.46
1:X:180:VAL:CG2	1:X:218:ARG:CG	2.92	0.46
1:Y:41:LYS:HD3	1:Y:44:TRP:CZ2	2.50	0.46
1:X:286:LEU:CD1	1:X:395:MET:CE	2.94	0.46
1:Y:202:LYS:O	1:Y:205:GLU:N	2.49	0.46
1:Z:5:TYR:CE2	1:Z:69:ILE:CD1	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:98:TYR:CG	1:Y:99:ASN:N	2.83	0.46
1:Z:373:ALA:O	1:Z:377:ILE:N	2.44	0.46
1:Z:12:GLY:O	1:Z:35:PHE:HZ	1.98	0.46
1:Y:112:CYS:SG	1:Y:139:THR:HG21	2.55	0.46
1:X:346:PRO:CA	1:X:348:PHE:CE1	2.97	0.46
1:X:196:THR:CG2	1:X:198:ASP:N	2.78	0.46
1:Y:438:VAL:O	1:Y:441:LEU:HB2	2.16	0.46
1:Z:85:THR:HG23	1:Z:102:VAL:HA	1.97	0.46
1:Z:157:ARG:NH1	1:Z:157:ARG:CG	2.78	0.46
1:Z:456:ASN:ND2	1:Z:459:GLU:N	2.63	0.46
1:Y:415:ASN:HD22	1:Y:417:PHE:N	2.14	0.46
1:X:263:ASN:CB	1:X:406:LEU:HD11	2.45	0.46
1:Y:179:HIS:CE1	1:Y:215:PRO:CA	2.98	0.46
1:X:459:GLU:HB3	1:X:460:LEU:HD13	1.97	0.46
1:X:204:LEU:N	1:X:204:LEU:CD1	2.79	0.46
1:O:351:LEU:HD22	1:O:360:ALA:CB	2.46	0.46
1:O:214:LEU:CD1	1:O:214:LEU:N	2.79	0.46
1:Z:179:HIS:CE1	1:Z:215:PRO:HA	2.50	0.46
1:Z:494:MET:O	1:Z:495:ALA:HB3	2.16	0.46
1:X:456:ASN:ND2	1:X:458:ASP:HB2	2.31	0.46
1:Y:429:ARG:HG2	1:Y:469:GLU:OE2	2.15	0.46
1:X:348:PHE:CD1	1:X:348:PHE:N	2.83	0.46
1:O:234:GLY:H	1:O:236:ARG:HH21	1.63	0.46
1:X:179:HIS:NE2	1:X:215:PRO:HB3	2.31	0.46
1:X:196:THR:CG2	1:X:198:ASP:H	2.29	0.46
1:O:340:ASN:HD22	1:O:371:VAL:HG23	1.81	0.46
1:O:298:VAL:CG1	1:O:299:ASN:N	2.79	0.46
1:Z:143:TRP:CE3	1:Z:144:ILE:HA	2.51	0.46
1:Z:146:ASP:HB2	1:Z:147:HIS:HD1	1.77	0.46
1:Y:256:VAL:HG12	1:Y:294:PRO:HG3	1.98	0.46
1:Z:332:PHE:O	1:Z:335:LYS:HB2	2.16	0.46
1:Y:136:PHE:O	1:Y:140:LYS:HG3	2.16	0.46
1:X:389:ARG:HG2	1:X:483:TYR:CZ	2.50	0.46
1:Z:19:VAL:HG13	1:Z:27:ILE:CG2	2.46	0.46
1:Y:36:GLU:HG3	1:Y:37:GLN:N	2.30	0.46
1:X:270:PHE:N	1:X:270:PHE:CD1	2.84	0.46
1:Z:9:LEU:HD12	1:Z:9:LEU:HA	1.61	0.46
1:Z:124:ILE:HG13	1:Z:203:MET:HE2	1.98	0.46
1:O:91:LYS:HB2	1:O:161:LEU:HG	1.96	0.46
1:X:154:ARG:CB	1:X:159:GLU:CB	2.93	0.46
1:X:263:ASN:O	1:X:408:VAL:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:161:LEU:HD22	1:Y:179:HIS:NE2	2.29	0.46
1:Y:54:ALA:CA	1:Z:65:THR:HG23	2.46	0.46
1:O:389:ARG:HB2	1:O:426:LEU:HD13	1.98	0.46
1:O:471:ARG:HA	1:O:472:PRO:HD3	1.84	0.46
1:X:24:ASP:N	1:X:24:ASP:OD1	2.48	0.46
1:O:26:ASN:O	1:O:28:ILE:HD13	2.14	0.46
1:O:407:ARG:HD3	1:O:407:ARG:HA	1.53	0.46
1:Y:71:SER:HA	1:Y:74:ILE:HD12	1.98	0.46
1:Z:115:LEU:HG	1:Z:120:LEU:HD13	1.98	0.46
1:Z:456:ASN:HD22	1:Z:459:GLU:H	1.63	0.46
1:X:154:ARG:NH2	1:X:159:GLU:CG	2.79	0.46
1:Z:23:HIS:CA	1:Z:453:PHE:CZ	2.99	0.46
1:X:438:VAL:N	1:X:441:LEU:HD12	2.31	0.46
1:Z:308:MET:HE3	1:Z:311:ALA:HB3	1.98	0.46
1:O:496:TRP:CZ3	1:Y:488:LYS:HG2	2.51	0.46
1:Z:410:GLY:O	1:Z:413:VAL:HG22	2.16	0.46
1:X:41:LYS:HB2	1:X:42:PRO:CD	2.46	0.46
1:Z:157:ARG:NH1	1:Z:157:ARG:HG2	2.30	0.45
1:Z:118:ASP:HB2	1:Z:120:LEU:CD1	2.45	0.45
1:Z:83:ARG:HH12	3:Z:504:GOL:C2	2.29	0.45
1:Y:486:TRP:CE2	1:Y:490:VAL:CG2	2.99	0.45
1:O:332:PHE:CA	1:O:374:ASN:ND2	2.79	0.45
1:O:406:LEU:HA	1:O:406:LEU:HD23	1.61	0.45
1:X:130:LEU:HD12	1:X:190:MET:CA	2.47	0.45
1:O:233:GLY:C	1:O:235:THR:H	2.17	0.45
1:Z:271:MET:C	1:Z:272:LEU:HD12	2.37	0.45
1:O:460:LEU:CD2	1:O:460:LEU:H	2.25	0.45
1:Z:101:ILE:HG23	1:Z:107:ARG:NH1	2.31	0.45
1:X:4:LYS:H	1:X:4:LYS:HG2	1.51	0.45
1:Y:280:VAL:HG11	1:Y:302:LEU:HD21	1.97	0.45
1:Z:54:ALA:O	1:Z:58:SER:OG	2.29	0.45
1:X:478:GLU:HB2	4:X:545:HOH:O	2.16	0.45
1:X:251:PHE:CE2	1:X:446:LEU:CD1	2.98	0.45
1:Y:20:VAL:O	1:Y:28:ILE:HG12	2.15	0.45
1:Y:433:PRO:O	1:Y:467:GLU:HB3	2.16	0.45
1:Z:371:VAL:HG12	1:Z:371:VAL:O	2.14	0.45
1:X:277:GLU:O	1:X:300:TYR:HD2	1.99	0.45
1:Z:120:LEU:C	1:Z:124:ILE:HD12	2.37	0.45
1:Z:162:PHE:CG	1:Z:163:GLY:N	2.81	0.45
1:Z:272:LEU:HG	1:Z:303:GLU:HB2	1.97	0.45
1:Z:474:ILE:O	1:Z:479:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:27:ILE:HG22	1:O:28:ILE:N	2.30	0.45
1:O:27:ILE:HD13	1:O:27:ILE:N	2.31	0.45
1:Y:165:VAL:O	1:Y:169:LEU:HG	2.16	0.45
1:Z:456:ASN:HD22	1:Z:458:ASP:H	1.65	0.45
1:Z:50:MET:HE1	1:Z:168:TRP:HH2	1.81	0.45
1:Y:474:ILE:HG21	1:Y:474:ILE:HD12	1.72	0.45
1:Y:364:ILE:HG22	1:Y:365:PHE:N	2.31	0.45
1:O:468:ARG:HD3	1:O:469:GLU:N	2.31	0.45
1:Z:191:LEU:HD23	1:Z:191:LEU:HA	1.54	0.45
1:Z:436:ARG:N	1:Z:436:ARG:CD	2.79	0.45
1:O:406:LEU:CD2	1:O:407:ARG:N	2.79	0.45
1:Y:145:LEU:HD12	1:Y:145:LEU:HA	1.58	0.45
1:X:39:TYR:HA	1:X:40:PRO:HD2	1.63	0.45
1:Y:110:GLU:O	1:Y:113:GLU:HB2	2.17	0.45
1:O:457:LEU:HA	1:O:457:LEU:HD22	1.73	0.45
1:X:154:ARG:NH2	1:X:159:GLU:HG3	2.31	0.45
1:Y:344:VAL:HG22	1:Y:364:ILE:HD13	1.94	0.45
1:Y:331:TYR:CE1	1:Y:335:LYS:HD3	2.52	0.45
1:Z:28:ILE:CD1	1:Z:28:ILE:N	2.79	0.45
1:X:428:THR:CG2	1:X:429:ARG:N	2.79	0.45
1:Z:401:ILE:CG2	1:Z:402:ARG:N	2.79	0.45
1:X:130:LEU:HD12	1:X:190:MET:CG	2.47	0.45
1:O:402:ARG:NH2	1:O:404:HIS:HA	2.31	0.45
1:X:261:ALA:HA	1:X:272:LEU:O	2.17	0.45
1:O:457:LEU:O	1:O:460:LEU:N	2.50	0.45
1:X:154:ARG:HE	1:X:159:GLU:HG2	1.77	0.45
1:X:83:ARG:HB2	1:X:83:ARG:HH11	1.82	0.45
1:O:44:TRP:HD1	1:O:44:TRP:N	2.14	0.45
1:O:240:SER:HB2	1:O:450:ALA:HB3	1.96	0.45
1:O:271:MET:HE3	1:O:406:LEU:HD11	1.99	0.45
1:X:342:VAL:CG1	1:X:343:TYR:N	2.79	0.45
1:X:269:CYS:HB3	1:X:306:VAL:HB	1.98	0.45
1:O:219:ARG:CG	1:O:220:SER:N	2.80	0.45
1:O:246:GLN:OE1	1:O:246:GLN:HA	2.16	0.45
1:Y:103:TRP:CZ3	1:Y:104:GLN:HG2	2.51	0.45
1:Y:381:LEU:HD12	1:Y:417:PHE:CD2	2.52	0.45
1:O:80:THR:HG21	1:O:248:ALA:CB	2.46	0.45
1:Y:83:ARG:CZ	1:Y:246:GLN:HG2	2.46	0.45
1:O:27:ILE:CD1	1:O:27:ILE:N	2.80	0.45
1:Y:415:ASN:HD22	1:Y:417:PHE:H	1.64	0.45
1:Z:15:SER:OG	1:Z:17:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:335:LYS:HB3	1:Z:374:ASN:ND2	2.32	0.45
1:Z:240:SER:HB2	1:Z:450:ALA:HB3	1.98	0.45
1:O:353:ALA:CB	1:O:354:PRO:HA	2.40	0.45
1:Z:473:GLY:O	1:Z:474:ILE:HG13	2.17	0.45
1:Z:475:GLU:HG3	1:Z:475:GLU:H	1.64	0.45
1:Z:390:ASP:O	1:Z:393:GLU:HB2	2.17	0.45
1:O:347:ALA:HB2	1:O:351:LEU:HD13	1.99	0.45
1:O:357:ASP:HA	1:O:358:PRO:HD2	1.83	0.45
1:O:93:THR:OG1	1:O:94:GLY:N	2.50	0.45
1:Y:403:LEU:N	1:Y:403:LEU:HD13	2.32	0.45
1:Z:124:ILE:HD13	1:Z:132:ILE:CG1	2.48	0.44
1:Y:293:GLY:N	1:Y:297:GLU:O	2.28	0.44
1:Y:19:VAL:CG1	1:Y:27:ILE:CG2	2.95	0.44
1:X:418:LEU:HD23	1:X:418:LEU:HA	1.67	0.44
1:O:410:GLY:O	1:O:413:VAL:HG13	2.18	0.44
1:Y:69:ILE:HA	1:Y:69:ILE:HD12	1.79	0.44
1:Y:357:ASP:OD2	1:Y:494:MET:HB3	2.17	0.44
1:Y:202:LYS:O	1:Y:206:VAL:HB	2.17	0.44
1:Z:5:TYR:O	1:Z:75:ALA:N	2.45	0.44
1:O:36:GLU:HG3	1:O:37:GLN:N	2.31	0.44
1:O:422:GLN:NE2	1:O:426:LEU:CD2	2.80	0.44
1:Z:323:ILE:HG22	1:Z:332:PHE:CE2	2.51	0.44
1:O:83:ARG:HE	1:O:83:ARG:HB2	1.66	0.44
1:X:351:LEU:HD13	1:X:351:LEU:HA	1.41	0.44
1:X:6:ILE:CG2	1:X:7:VAL:N	2.79	0.44
1:X:192:PHE:HB2	1:X:199:TRP:CZ3	2.52	0.44
1:Y:274:ASN:HD21	1:Y:299:ASN:HD22	1.63	0.44
1:Y:475:GLU:CD	1:Y:477:THR:HB	2.37	0.44
1:Y:328:ASP:O	1:Y:331:TYR:N	2.51	0.44
1:X:297:GLU:HG3	1:X:297:GLU:H	1.24	0.44
1:Y:156:ARG:C	1:Y:158:GLY:H	2.19	0.44
1:X:344:VAL:HG23	1:X:379:ALA:CB	2.48	0.44
1:O:50:MET:O	1:O:53:TRP:HB3	2.17	0.44
1:Z:286:LEU:N	1:Z:286:LEU:HD23	2.32	0.44
1:Z:351:LEU:N	1:Z:357:ASP:O	2.51	0.44
1:O:359:TYR:CZ	1:O:499:HIS:HB3	2.52	0.44
1:Y:486:TRP:CD1	1:Y:487:LYS:HG3	2.52	0.44
1:X:483:TYR:O	1:X:487:LYS:HG2	2.18	0.44
1:Z:403:LEU:CD1	1:Z:403:LEU:N	2.78	0.44
1:Z:438:VAL:HA	1:Z:441:LEU:HD12	2.00	0.44
1:O:362:GLY:O	1:Y:367:LEU:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:78:GLY:HA2	1:O:447:ALA:HB2	1.99	0.44
1:Y:338:ASN:CB	1:Y:482:ARG:NH2	2.81	0.44
1:Z:266:GLY:N	1:Z:268:GLY:O	2.50	0.44
1:O:122:ASP:O	1:O:126:SER:OG	2.27	0.44
1:Z:348:PHE:N	1:Z:348:PHE:CD1	2.78	0.44
1:Z:40:PRO:CG	1:Z:44:TRP:HE3	2.30	0.44
1:X:322:LEU:N	1:X:322:LEU:CD2	2.80	0.44
1:Y:3:LYS:HB3	1:Y:3:LYS:HZ3	1.83	0.44
1:Z:430:VAL:O	1:Z:469:GLU:HA	2.17	0.44
1:O:457:LEU:O	1:O:461:GLN:HG2	2.17	0.44
1:Y:344:VAL:C	1:Y:345:VAL:HG23	2.37	0.44
1:O:213:MET:HB3	1:O:213:MET:HE3	1.71	0.44
1:O:251:PHE:CZ	1:O:446:LEU:CD1	3.01	0.44
1:Y:44:TRP:N	1:Y:44:TRP:HD1	2.14	0.44
1:Z:81:ASN:N	1:Z:81:ASN:ND2	2.66	0.44
1:X:109:ALA:HA	1:X:134:PRO:HG3	2.00	0.44
1:Y:196:THR:O	1:Y:197:LEU:HB2	2.18	0.44
1:Y:83:ARG:HH11	3:Y:503:GOL:C2	2.31	0.44
1:X:317:ARG:NE	1:X:326:ALA:HB2	2.33	0.44
1:O:282:SER:OG	1:O:398:ASP:OD2	2.28	0.44
1:X:469:GLU:HG2	1:X:471:ARG:NH2	2.33	0.44
1:X:125:ARG:HB2	4:X:534:HOH:O	2.18	0.44
1:Y:109:ALA:HA	1:Y:134:PRO:HG3	2.00	0.44
1:O:163:GLY:HA2	4:O:529:HOH:O	2.17	0.44
1:O:466:ILE:O	1:O:466:ILE:HG22	2.17	0.44
1:O:330:GLU:O	1:O:334:THR:OG1	2.28	0.44
1:Z:171:TRP:HE3	1:Z:172:LYS:HD2	1.82	0.44
1:O:23:HIS:HE1	1:O:453:PHE:O	2.00	0.44
1:X:471:ARG:CG	1:X:471:ARG:HH11	2.31	0.44
1:Z:106:ARG:NH1	1:Z:307:PHE:CE2	2.85	0.44
1:X:182:ASP:OD2	1:X:220:SER:OG	2.25	0.44
1:X:436:ARG:HE	1:X:436:ARG:HB2	1.41	0.44
1:Z:188:ARG:HA	1:Z:188:ARG:HD3	1.61	0.44
1:Y:196:THR:HG23	1:Y:198:ASP:HB3	1.98	0.44
1:X:314:GLN:HG3	1:X:317:ARG:HH21	1.79	0.44
1:Y:486:TRP:HD1	1:Y:487:LYS:HG3	1.83	0.44
1:Z:170:ILE:HD13	1:Z:242:ILE:HD11	1.97	0.44
1:Z:193:ASN:OD1	1:Z:196:THR:HB	2.18	0.44
1:Y:225:GLY:O	1:Y:238:PRO:HA	2.18	0.44
1:Y:439:THR:HG22	1:Y:440:ALA:N	2.32	0.44
1:O:53:TRP:HA	1:O:53:TRP:HE3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:84:GLU:HB2	1:Y:103:TRP:HB3	1.99	0.43
1:Y:396:GLN:OE1	1:Y:402:ARG:HB2	2.18	0.43
1:O:441:LEU:N	1:O:441:LEU:CD2	2.80	0.43
1:X:426:LEU:HA	1:X:426:LEU:HD12	1.85	0.43
1:X:156:ARG:HH11	1:X:156:ARG:HD2	1.59	0.43
1:Z:37:GLN:NE2	1:Z:47:HIS:CE1	2.86	0.43
1:Y:338:ASN:HD22	1:Y:338:ASN:N	2.16	0.43
1:Z:337:GLN:HG2	1:Z:337:GLN:H	1.34	0.43
1:Y:54:ALA:CB	1:Z:65:THR:HG23	2.48	0.43
1:X:286:LEU:CD1	1:X:395:MET:HE2	2.48	0.43
1:Y:184:THR:HG23	1:Y:184:THR:H	1.44	0.43
1:O:232:LYS:O	1:O:233:GLY:O	2.36	0.43
1:O:75:ALA:O	1:O:76:ALA:HB2	2.18	0.43
1:O:317:ARG:HA	1:O:323:ILE:HG13	2.00	0.43
1:Y:280:VAL:HG12	1:Y:280:VAL:O	2.15	0.43
1:O:3:LYS:HA	1:O:73:GLN:C	2.38	0.43
1:Y:441:LEU:O	1:Y:444:ALA:HB3	2.18	0.43
1:Y:454:TRP:CD1	1:Y:460:LEU:HD21	2.53	0.43
1:X:103:TRP:CE3	1:X:104:GLN:HG3	2.53	0.43
1:Y:344:VAL:HG13	1:Y:364:ILE:HD13	1.99	0.43
1:X:487:LYS:HB3	1:X:487:LYS:HE3	1.69	0.43
1:Z:80:THR:HG22	1:Z:243:ALA:O	2.19	0.43
1:Z:24:ASP:O	1:Z:25:ALA:HB3	2.18	0.43
1:X:152:ARG:NH1	1:X:152:ARG:HG2	2.33	0.43
1:Z:37:GLN:HE22	1:Z:47:HIS:CE1	2.37	0.43
1:Y:57:SER:O	1:Y:60:LEU:HB3	2.17	0.43
1:Y:271:MET:O	1:Y:303:GLU:HA	2.18	0.43
1:Z:474:ILE:HG23	1:Z:478:GLU:CB	2.48	0.43
1:X:17:ARG:HG3	1:X:32:GLN:CG	2.29	0.43
1:Z:17:ARG:HG3	1:Z:32:GLN:HA	2.00	0.43
1:O:446:LEU:HA	1:O:446:LEU:HD12	1.58	0.43
1:O:475:GLU:C	1:O:477:THR:H	2.20	0.43
1:Z:182:ASP:HA	1:Z:218:ARG:O	2.18	0.43
1:O:68:ASP:HB2	1:X:50:MET:HE2	2.00	0.43
1:O:128:THR:CG2	1:O:130:LEU:CB	2.97	0.43
1:O:128:THR:CG2	1:O:130:LEU:HD13	2.39	0.43
1:O:255:CYS:HB3	1:O:260:MET:CB	2.45	0.43
1:X:460:LEU:H	1:X:460:LEU:HD22	1.83	0.43
1:X:377:ILE:HD13	1:X:377:ILE:HG21	1.56	0.43
1:Z:154:ARG:HB3	1:Z:159:GLU:CG	2.24	0.43
1:Z:456:ASN:HD22	1:Z:456:ASN:C	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:456:ASN:ND2	1:Z:459:GLU:H	2.16	0.43
1:O:458:ASP:CA	1:O:461:GLN:HG3	2.47	0.43
1:X:65:THR:HG23	1:X:66:LYS:N	2.31	0.43
1:O:436:ARG:C	1:O:438:VAL:H	2.22	0.43
1:Z:372:ASN:H	1:Z:375:HIS:CE1	2.36	0.43
1:Z:95:LYS:HA	1:Z:96:PRO:HD3	1.66	0.43
1:Y:104:GLN:HB3	1:Y:349:THR:HG21	2.00	0.43
1:X:474:ILE:HG23	1:X:478:GLU:CG	2.48	0.43
1:Y:421:PHE:CE2	1:Y:425:ILE:HD13	2.53	0.43
1:O:193:ASN:C	1:O:195:HIS:H	2.21	0.43
1:O:101:ILE:HG22	1:O:140:LYS:HG2	2.01	0.43
1:Y:335:LYS:HE3	1:Y:374:ASN:HD21	1.84	0.43
1:Y:93:THR:CB	1:Y:95:LYS:HB3	2.48	0.43
1:Z:402:ARG:HD2	1:Z:404:HIS:CE1	2.54	0.43
1:X:6:ILE:CD1	1:X:453:PHE:CD2	3.01	0.43
1:Y:250:LEU:CD1	1:Y:255:CYS:HB2	2.49	0.43
1:O:344:VAL:HG22	1:O:364:ILE:HG12	2.01	0.43
1:Y:462:GLU:HA	1:Y:462:GLU:OE1	2.16	0.43
1:X:402:ARG:HB2	1:X:402:ARG:HE	1.43	0.43
1:Y:456:ASN:HD21	1:Y:458:ASP:CG	2.22	0.43
1:O:124:ILE:H	1:O:124:ILE:HG12	1.24	0.43
1:Z:152:ARG:O	1:Z:156:ARG:N	2.35	0.43
1:X:482:ARG:HA	1:X:482:ARG:NH1	2.33	0.43
1:O:80:THR:HG21	1:O:248:ALA:HB3	2.01	0.43
1:Y:396:GLN:CD	1:Y:402:ARG:HA	2.39	0.43
1:X:422:GLN:O	1:X:426:LEU:HD22	2.19	0.43
1:Y:95:LYS:HG2	1:Y:95:LYS:O	2.19	0.43
1:Y:164:THR:HB	1:Y:166:ASP:OD1	2.19	0.43
1:O:168:TRP:O	1:O:172:LYS:HG2	2.19	0.43
1:Z:115:LEU:CD1	1:Z:115:LEU:H	2.32	0.43
1:X:90:GLU:HA	1:X:160:LEU:CD2	2.49	0.43
1:Y:90:GLU:HB2	1:Y:93:THR:HG1	1.82	0.43
1:X:191:LEU:HD21	1:X:207:LEU:CD1	2.49	0.43
1:X:432:ARG:HA	1:X:433:PRO:HD2	1.87	0.43
1:Y:253:GLN:O	1:Y:254:LEU:HB2	2.18	0.43
1:X:282:SER:HA	1:X:398:ASP:OD2	2.18	0.43
1:O:192:PHE:HB2	1:O:199:TRP:CZ3	2.54	0.43
1:Y:30:VAL:O	1:Y:66:LYS:NZ	2.31	0.42
1:Z:168:TRP:CZ3	1:Z:172:LYS:HD3	2.54	0.42
1:Y:293:GLY:HA3	1:Y:297:GLU:CD	2.40	0.42
1:Y:256:VAL:CG1	1:Y:294:PRO:CG	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:88:VAL:HA	1:O:161:LEU:O	2.18	0.42
1:Z:66:LYS:HB3	1:Z:66:LYS:HE3	1.80	0.42
1:X:6:ILE:CD1	1:X:453:PHE:CG	3.02	0.42
1:X:421:PHE:O	1:X:424:ASP:HB2	2.19	0.42
1:Y:194:ILE:HG22	1:Y:290:ILE:HD11	1.99	0.42
1:Z:124:ILE:CG1	1:Z:203:MET:HE1	2.49	0.42
1:O:202:LYS:HD3	1:O:206:VAL:CG2	2.47	0.42
1:Z:137:SER:OG	1:Z:189:THR:HA	2.19	0.42
1:O:80:THR:CG2	1:O:248:ALA:CB	2.97	0.42
1:O:382:GLU:HB3	1:O:421:PHE:CE2	2.54	0.42
1:Y:115:LEU:HA	1:Y:115:LEU:HD13	1.62	0.42
1:Y:15:SER:OG	1:Y:17:ARG:NH1	2.52	0.42
1:Y:351:LEU:CD2	1:Y:360:ALA:CB	2.97	0.42
1:X:154:ARG:C	1:X:159:GLU:HB2	2.40	0.42
1:O:422:GLN:HE21	1:O:426:LEU:HD22	1.83	0.42
1:Y:28:ILE:HG23	1:Y:28:ILE:HD12	1.80	0.42
1:O:264:THR:CG2	1:O:265:TYR:N	2.81	0.42
1:Y:237:ILE:HG23	1:Y:238:PRO:HD2	2.01	0.42
1:O:211:ARG:CA	1:O:214:LEU:HD13	2.48	0.42
1:Y:488:LYS:HB3	1:Y:488:LYS:HE3	1.82	0.42
1:X:190:MET:N	4:X:518:HOH:O	2.51	0.42
1:O:67:ALA:CB	1:O:69:ILE:HD12	2.49	0.42
1:Y:494:MET:O	1:Y:495:ALA:HB3	2.19	0.42
1:O:142:LYS:HD3	1:O:207:LEU:CD2	2.49	0.42
1:Y:409:ASP:CB	1:Y:438:VAL:HG21	2.49	0.42
1:O:184:THR:HG23	1:O:184:THR:H	1.47	0.42
1:Y:130:LEU:HD23	1:Y:130:LEU:N	2.33	0.42
1:X:104:GLN:HB3	1:X:349:THR:HG21	2.01	0.42
1:Y:180:VAL:HG22	1:Y:216:GLU:O	2.20	0.42
1:X:432:ARG:NH2	1:X:468:ARG:HD3	2.35	0.42
1:Z:496:TRP:CZ3	1:X:488:LYS:CD	3.01	0.42
1:O:335:LYS:HB2	1:O:374:ASN:ND2	2.33	0.42
1:Y:491:LYS:HA	1:Y:494:MET:HG3	2.01	0.42
1:Z:183:TYR:CD2	1:Z:298:VAL:CG2	3.03	0.42
1:X:264:THR:O	1:X:269:CYS:HA	2.20	0.42
1:Z:206:VAL:CG1	1:Z:207:LEU:N	2.83	0.42
1:Z:458:ASP:CA	1:Z:461:GLN:HG3	2.44	0.42
1:Z:103:TRP:HB2	1:Z:135:TYR:CE1	2.54	0.42
1:O:82:GLN:HA	1:O:245:ASP:OD2	2.20	0.42
1:X:460:LEU:HD22	1:X:460:LEU:N	2.35	0.42
1:O:396:GLN:HE21	1:O:403:LEU:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:180:VAL:HG11	1:X:224:TYR:HB3	2.02	0.42
1:Z:219:ARG:O	1:Z:224:TYR:OH	2.28	0.42
1:O:19:VAL:HG12	1:O:20:VAL:N	2.34	0.42
1:O:307:PHE:HD2	1:O:349:THR:O	2.02	0.42
1:O:130:LEU:HD12	1:O:130:LEU:HA	1.60	0.42
1:Z:135:TYR:O	1:Z:140:LYS:NZ	2.49	0.42
1:Y:47:HIS:CE1	1:Y:102:VAL:HG21	2.55	0.42
1:Z:453:PHE:CE2	1:Z:454:TRP:CZ2	3.08	0.42
1:X:254:LEU:HD11	1:X:457:LEU:HD22	1.99	0.42
1:O:425:ILE:O	1:O:425:ILE:HG13	2.18	0.42
1:O:471:ARG:CB	1:O:472:PRO:HD2	2.48	0.42
1:O:207:LEU:HD23	1:O:207:LEU:HA	1.91	0.42
1:Z:391:VAL:CG2	1:Z:392:LEU:N	2.76	0.42
1:O:33:ARG:HH12	1:O:62:GLU:CD	2.23	0.42
1:Z:457:LEU:HA	1:Z:457:LEU:HD23	1.47	0.42
1:O:108:THR:HG22	1:O:143:TRP:HB2	2.01	0.42
1:O:359:TYR:O	1:O:497:GLU:N	2.40	0.42
1:O:435:VAL:HG23	1:O:437:GLU:OE1	2.19	0.42
1:X:47:HIS:O	1:X:99:ASN:HB3	2.20	0.42
1:Y:191:LEU:HD21	1:Y:207:LEU:HD13	2.01	0.42
1:Y:145:LEU:HD12	1:Y:151:SER:OG	2.19	0.42
1:Y:33:ARG:NH2	1:Z:33:ARG:NH2	2.68	0.42
1:Z:156:ARG:HG2	1:Z:156:ARG:H	1.66	0.42
1:O:80:THR:HG22	1:O:245:ASP:N	2.34	0.42
1:X:446:LEU:HD12	1:X:446:LEU:HA	1.84	0.42
1:Y:486:TRP:CE2	1:Y:490:VAL:HG21	2.55	0.42
1:X:386:TYR:HE1	1:X:425:ILE:HD11	1.84	0.42
1:X:431:GLU:O	1:X:433:PRO:HD3	2.19	0.42
1:X:320:MET:CA	1:X:320:MET:CE	2.97	0.42
1:Z:492:ARG:NH1	1:X:492:ARG:O	2.53	0.42
1:X:381:LEU:O	1:X:384:ILE:HB	2.20	0.42
1:X:171:TRP:CE2	1:X:176:GLY:HA2	2.54	0.42
1:O:308:MET:HE3	1:Y:369:ARG:HG3	2.02	0.42
1:Z:153:GLU:H	1:Z:153:GLU:CD	2.21	0.42
1:O:245:ASP:O	1:O:248:ALA:HB3	2.19	0.42
1:X:191:LEU:CD2	1:X:207:LEU:HD12	2.50	0.42
1:X:433:PRO:O	1:X:467:GLU:HB3	2.20	0.42
1:O:38:ILE:HB	1:O:46:GLU:O	2.20	0.42
1:X:152:ARG:CG	1:X:152:ARG:NH1	2.79	0.42
1:Y:133:ASP:OD1	1:Y:135:TYR:HB2	2.20	0.42
1:Z:456:ASN:ND2	1:Z:459:GLU:HG3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:137:SER:HA	1:Z:140:LYS:HD2	2.02	0.42
1:X:249:ALA:O	1:X:253:GLN:N	2.53	0.42
1:X:409:ASP:CB	1:X:438:VAL:HG21	2.49	0.42
1:Y:174:THR:C	1:Y:176:GLY:H	2.22	0.42
1:Z:179:HIS:CE1	1:Z:215:PRO:CA	3.03	0.42
1:Z:270:PHE:CD1	1:Z:270:PHE:N	2.87	0.42
1:Y:9:LEU:HD23	1:Y:56:GLN:CG	2.50	0.41
1:Z:142:LYS:HG3	1:Z:146:ASP:OD2	2.20	0.41
1:O:259:GLY:HA2	1:O:273:MET:HE1	2.02	0.41
1:O:25:ALA:HB3	1:O:463:LYS:CD	2.50	0.41
1:X:83:ARG:NH1	1:X:246:GLN:HG2	2.35	0.41
1:Y:87:ILE:HD13	1:Y:87:ILE:HG21	1.86	0.41
1:X:420:GLN:OE1	1:X:471:ARG:O	2.37	0.41
1:X:130:LEU:HD12	1:X:190:MET:HG3	2.02	0.41
1:O:289:THR:HB	1:O:290:ILE:H	1.48	0.41
1:O:9:LEU:HA	1:O:9:LEU:HD12	1.60	0.41
1:O:103:TRP:CZ3	1:O:104:GLN:HG3	2.56	0.41
1:Z:103:TRP:CD2	3:Z:504:GOL:H11	2.55	0.41
1:Z:351:LEU:HB3	1:Z:355:TYR:HB2	2.02	0.41
1:Y:475:GLU:CB	1:Y:478:GLU:HB2	2.48	0.41
1:X:323:ILE:HD12	1:X:326:ALA:HA	2.01	0.41
1:Y:263:ASN:O	1:Y:408:VAL:HA	2.19	0.41
1:X:415:ASN:HD22	1:X:416:ASN:N	2.19	0.41
1:Y:108:THR:HG21	1:Y:139:THR:C	2.41	0.41
1:O:360:ALA:O	1:O:361:ARG:HD3	2.19	0.41
1:O:325:ASP:O	1:O:328:ASP:HB2	2.20	0.41
1:Z:426:LEU:HA	1:Z:426:LEU:HD12	1.77	0.41
1:O:340:ASN:HB2	1:O:375:HIS:NE2	2.35	0.41
1:Y:342:VAL:HG21	1:Y:371:VAL:HG11	2.01	0.41
1:O:353:ALA:HB1	1:O:354:PRO:HA	2.01	0.41
1:Z:71:SER:O	1:Z:74:ILE:HD12	2.21	0.41
1:Y:33:ARG:HB2	1:Y:59:THR:CG2	2.50	0.41
1:Z:124:ILE:HD13	1:Z:132:ILE:HG12	2.01	0.41
1:Y:323:ILE:HD12	1:Y:326:ALA:HA	2.02	0.41
1:Z:315:TRP:O	1:Z:319:GLU:HB2	2.19	0.41
1:X:248:ALA:O	1:X:442:GLY:HA3	2.20	0.41
1:Y:433:PRO:HA	1:Y:466:ILE:HA	2.01	0.41
1:Y:50:MET:O	1:Y:53:TRP:HB3	2.20	0.41
1:Y:429:ARG:NH1	1:Y:469:GLU:OE2	2.54	0.41
1:Y:226:GLN:HG2	1:Y:238:PRO:CA	2.47	0.41
1:X:217:VAL:CG1	1:X:218:ARG:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:38:ILE:O	1:O:40:PRO:HD3	2.19	0.41
1:Z:397:ALA:HB3	1:Z:398:ASP:H	1.58	0.41
1:O:353:ALA:HA	1:O:354:PRO:HA	1.67	0.41
1:O:128:THR:CB	1:O:130:LEU:HB2	2.51	0.41
1:Y:294:PRO:HD2	1:Y:297:GLU:OE2	2.21	0.41
1:Y:95:LYS:HE2	1:Y:95:LYS:HB3	1.81	0.41
1:X:156:ARG:HG3	1:X:210:PRO:HG3	2.02	0.41
1:X:179:HIS:CE1	1:X:215:PRO:HA	2.56	0.41
1:Z:191:LEU:HD22	1:Z:204:LEU:HD13	2.03	0.41
1:Y:316:LEU:HD11	1:Y:380:THR:HG21	2.02	0.41
1:X:344:VAL:HG23	1:X:379:ALA:HB3	2.02	0.41
1:Z:81:ASN:HB2	1:Z:165:VAL:CG1	2.50	0.41
1:Y:286:LEU:HD13	1:Y:395:MET:HE2	2.01	0.41
1:Y:352:GLY:O	1:Y:353:ALA:HB2	2.20	0.41
1:O:381:LEU:HD12	1:O:417:PHE:CD2	2.56	0.41
1:Y:294:PRO:O	1:Y:457:LEU:HD12	2.20	0.41
1:Y:469:GLU:O	1:Y:471:ARG:NH1	2.54	0.41
1:X:179:HIS:CE1	1:X:215:PRO:CA	3.04	0.41
1:O:345:VAL:HA	1:O:346:PRO:HD3	1.50	0.41
1:O:53:TRP:HA	1:O:53:TRP:CE3	2.55	0.41
1:Y:267:THR:HG23	1:Y:311:ALA:HB2	2.02	0.41
1:Y:289:THR:HG23	1:Y:301:ALA:HB3	2.02	0.41
1:Y:97:ILE:HD12	1:Y:148:VAL:HG21	2.01	0.41
1:X:108:THR:CB	1:X:139:THR:HB	2.47	0.41
1:X:433:PRO:HA	1:X:465:VAL:O	2.20	0.41
1:Z:113:GLU:O	1:Z:117:ARG:HG2	2.20	0.41
1:Y:33:ARG:HH21	1:Z:33:ARG:NH2	2.16	0.41
1:O:128:THR:HB	1:O:130:LEU:HB2	2.03	0.41
1:O:205:GLU:CG	1:O:206:VAL:N	2.82	0.41
1:Z:86:THR:HG23	1:Z:162:PHE:CE1	2.52	0.41
1:Y:256:VAL:CG1	1:Y:294:PRO:CD	2.99	0.41
1:X:90:GLU:HA	1:X:160:LEU:HD23	2.03	0.41
1:Z:80:THR:HG21	1:Z:248:ALA:HB3	2.02	0.41
1:X:64:LEU:HD22	1:X:69:ILE:CG2	2.50	0.41
1:Z:153:GLU:HB2	1:Z:154:ARG:H	1.31	0.41
1:Z:461:GLN:HE21	1:Z:461:GLN:HB3	1.35	0.41
1:Y:317:ARG:NH1	1:Y:326:ALA:CB	2.83	0.41
1:Y:331:TYR:O	1:Y:335:LYS:HG3	2.20	0.41
1:O:153:GLU:OE1	1:O:153:GLU:N	2.53	0.41
1:X:249:ALA:O	1:X:253:GLN:HB2	2.20	0.41
1:Z:396:GLN:HA	1:Z:399:SER:HG	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:438:VAL:CA	1:X:441:LEU:CD1	2.99	0.41
1:O:486:TRP:O	1:O:490:VAL:HG23	2.21	0.41
1:O:64:LEU:HD21	1:O:74:ILE:HD11	2.02	0.41
1:Y:305:ALA:O	1:Y:353:ALA:HB3	2.21	0.41
1:Z:345:VAL:HG11	1:Z:493:ALA:HB3	2.03	0.41
1:Y:33:ARG:HH12	1:Y:62:GLU:CD	2.24	0.41
1:Y:33:ARG:HE	1:Z:33:ARG:NH2	2.19	0.41
1:Z:205:GLU:CG	1:Z:206:VAL:N	2.81	0.41
1:Z:131:VAL:HG12	1:Z:131:VAL:O	2.18	0.41
1:Z:125:ARG:CG	1:Z:125:ARG:NH1	2.78	0.41
1:Z:49:PRO:HB2	1:Z:168:TRP:CZ2	2.55	0.41
1:Z:87:ILE:O	1:Z:163:GLY:N	2.54	0.41
1:Y:188:ARG:HA	1:Y:188:ARG:HD2	1.63	0.41
1:Y:476:THR:HG22	1:Y:477:THR:N	2.35	0.41
1:O:155:ALA:CB	1:O:213:MET:CE	2.99	0.41
1:Z:396:GLN:O	1:Z:400:GLY:N	2.44	0.41
1:X:438:VAL:N	1:X:441:LEU:CD1	2.84	0.41
1:X:435:VAL:CG1	1:X:441:LEU:HD11	2.47	0.41
1:Z:496:TRP:CH2	1:X:488:LYS:HD2	2.56	0.41
1:Z:492:ARG:HD2	1:X:496:TRP:HZ3	1.86	0.41
1:Y:68:ASP:O	1:Y:69:ILE:HD13	2.20	0.41
1:X:174:THR:HB	1:X:177:ARG:NH1	2.36	0.41
1:O:340:ASN:ND2	1:O:371:VAL:HG23	2.36	0.41
1:Y:338:ASN:HB3	1:Y:482:ARG:HH22	1.84	0.41
1:X:288:THR:HG22	1:X:289:THR:N	2.31	0.41
1:Z:117:ARG:H	1:Z:117:ARG:HG2	1.63	0.41
1:Z:60:LEU:C	1:Z:60:LEU:HD12	2.39	0.41
1:Y:230:GLY:HA3	1:Z:228:ASN:O	2.21	0.41
1:Y:33:ARG:NE	1:Z:33:ARG:NH2	2.69	0.41
1:Y:62:GLU:HB2	1:Z:58:SER:HB3	2.02	0.41
1:O:369:ARG:NH1	1:Y:104:GLN:OE1	2.54	0.41
1:Y:424:ASP:CB	1:Y:474:ILE:CG2	2.99	0.41
1:X:222:GLU:O	1:X:240:SER:HA	2.21	0.41
1:X:169:LEU:HD23	1:X:169:LEU:HA	1.90	0.41
1:O:271:MET:CE	1:O:392:LEU:CD1	2.98	0.41
1:O:340:ASN:HD22	1:O:371:VAL:CG2	2.34	0.41
1:O:171:TRP:CE2	1:O:176:GLY:HA2	2.56	0.41
1:Y:172:LYS:HA	1:Y:172:LYS:HD2	1.93	0.41
1:X:29:SER:CB	1:X:63:VAL:HG23	2.48	0.40
1:Y:483:TYR:CE2	1:Y:487:LYS:CE	2.98	0.40
1:X:328:ASP:HB3	1:X:332:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:254:LEU:HA	1:O:254:LEU:HD12	1.80	0.40
1:X:414:ALA:HB2	1:X:436:ARG:NH1	2.36	0.40
1:Y:175:GLN:CA	1:Y:175:GLN:NE2	2.82	0.40
1:O:62:GLU:HA	1:O:65:THR:CG2	2.50	0.40
1:Z:111:ILE:O	1:Z:115:LEU:HD13	2.21	0.40
1:Y:457:LEU:HD23	1:Y:457:LEU:HA	1.66	0.40
1:O:193:ASN:OD1	1:O:195:HIS:HB2	2.20	0.40
1:Y:83:ARG:NH1	3:Y:503:GOL:H2	2.37	0.40
1:X:95:LYS:HA	1:X:96:PRO:HD3	1.90	0.40
1:X:223:VAL:HG12	1:X:223:VAL:O	2.21	0.40
1:Y:30:VAL:HG12	1:Y:31:SER:N	2.36	0.40
1:Z:154:ARG:HB3	1:Z:154:ARG:HE	1.42	0.40
1:Z:475:GLU:O	1:Z:478:GLU:N	2.50	0.40
1:X:478:GLU:HA	1:X:481:TYR:HB2	2.02	0.40
1:Y:486:TRP:CZ2	1:Y:490:VAL:CG2	3.04	0.40
1:Z:253:GLN:O	1:Z:254:LEU:HB2	2.21	0.40
1:X:384:ILE:O	1:X:387:GLN:HB2	2.21	0.40
1:X:194:ILE:HG22	1:X:290:ILE:HD11	2.03	0.40
1:X:499:HIS:CD2	1:X:499:HIS:H	2.39	0.40
1:Z:316:LEU:HD23	1:Z:316:LEU:HA	1.79	0.40
1:X:478:GLU:HA	1:X:481:TYR:HB3	2.03	0.40
1:Y:418:LEU:CD1	1:Y:419:MET:CE	2.98	0.40
1:O:112:CYS:SG	1:O:134:PRO:HD3	2.62	0.40
1:Z:98:TYR:OH	1:Z:107:ARG:NH2	2.55	0.40
1:X:407:ARG:NH1	1:X:466:ILE:HD11	2.37	0.40
1:Y:21:MET:HG2	1:Y:25:ALA:C	2.41	0.40
1:Z:314:GLN:NE2	1:X:369:ARG:HH22	2.19	0.40
1:X:347:ALA:O	1:X:361:ARG:HA	2.21	0.40
1:O:44:TRP:C	1:O:45:VAL:HG23	2.41	0.40
1:Z:413:VAL:HG23	1:Z:436:ARG:CG	2.50	0.40
1:Z:427:GLY:C	1:Z:472:PRO:HG3	2.42	0.40
1:O:48:ASP:HA	1:O:49:PRO:HD3	1.91	0.40
1:O:488:LYS:HD3	1:Y:496:TRP:CZ3	2.55	0.40
1:O:192:PHE:HB2	1:O:199:TRP:CE3	2.56	0.40
1:X:145:LEU:HA	1:X:145:LEU:HD12	1.61	0.40
1:O:286:LEU:N	1:O:286:LEU:HD23	2.37	0.40
1:Z:124:ILE:CG1	1:Z:203:MET:CE	2.98	0.40
1:Z:456:ASN:O	1:Z:459:GLU:HB2	2.22	0.40
1:Y:271:MET:HE2	1:Y:271:MET:HB3	1.84	0.40
1:X:482:ARG:CA	1:X:482:ARG:NH1	2.79	0.40
1:O:80:THR:HG22	1:O:245:ASP:HA	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:346:PRO:CG	1:Z:383:SER:HB2	2.51	0.40
1:O:204:LEU:CD2	1:O:209:ILE:CG2	2.99	0.40
1:Z:166:ASP:CG	1:Z:167:THR:H	2.23	0.40
1:Z:183:TYR:HB3	1:Z:290:ILE:HD13	2.03	0.40
1:Z:81:ASN:N	1:Z:81:ASN:HD22	2.19	0.40
1:Z:337:GLN:HE21	1:Z:337:GLN:HB3	1.40	0.40
1:Z:281:LYS:NZ	1:Z:281:LYS:HB3	2.36	0.40

There are no symmetry-related clashes.

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	O	495/501 (99%)	420 (85%)	58 (12%)	17 (3%)	5 3
1	X	496/501 (99%)	436 (88%)	42 (8%)	18 (4%)	4 3
1	Y	497/501 (99%)	442 (89%)	46 (9%)	9 (2%)	11 12
1	Z	496/501 (99%)	448 (90%)	39 (8%)	9 (2%)	11 12
All	All	1984/2004 (99%)	1746 (88%)	185 (9%)	53 (3%)	6 5

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	149	GLU
1	O	232	LYS
1	O	233	GLY
1	O	461	GLN
1	Y	175	GLN
1	Z	149	GLU
1	Z	476	THR
1	X	107	ARG

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Mol	Chain	Res	Type
1	X	159	GLU
1	X	233	GLY
1	X	322	LEU
1	X	438	VAL
1	O	326	ALA
1	O	462	GLU
1	O	464	ALA
1	O	476	THR
1	Y	325	ASP
1	Y	453	PHE
1	Z	153	GLU
1	Z	284	ASN
1	X	149	GLU
1	X	326	ALA
1	X	450	ALA
1	X	477	THR
1	O	71	SER
1	Y	138	GLY
1	Z	232	LYS
1	Z	233	GLY
1	Z	294	PRO
1	X	153	GLU
1	X	223	VAL
1	O	92	GLU
1	O	99	ASN
1	O	309	ALA
1	Y	92	GLU
1	X	294	PRO
1	X	458	ASP
1	X	463	LYS
1	X	476	THR
1	O	222	GLU
1	Y	177	ARG
1	Y	353	ALA
1	Y	477	THR
1	Z	397	ALA
1	Z	398	ASP
1	O	294	PRO
1	Y	438	VAL
1	X	157	ARG
1	X	138	GLY
1	X	206	VAL

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Mol	Chain	Res	Type
1	O	442	GLY
1	O	472	PRO
1	O	194	ILE

5.3.2 Protein sidechains

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	O	404/413 (98%)	299 (74%)	105 (26%)	0 0
1	X	404/413 (98%)	309 (76%)	95 (24%)	1 1
1	Y	408/413 (99%)	322 (79%)	86 (21%)	1 1
1	Z	408/413 (99%)	308 (76%)	100 (24%)	1 1
All	All	1624/1652 (98%)	1238 (76%)	386 (24%)	1 1

All (386) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	6	ILE
1	O	9	LEU
1	O	11	GLN
1	O	17	ARG
1	O	24	ASP
1	O	27	ILE
1	O	28	ILE
1	O	29	SER
1	O	31	SER
1	O	32	GLN
1	O	33	ARG
1	O	52	ILE
1	O	63	VAL
1	O	65	THR
1	O	69	ILE
1	O	71	SER
1	O	72	ASP
1	O	80	THR

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Mol	Chain	Res	Type
1	O	82	GLN
1	O	90	GLU
1	O	91	LYS
1	O	92	GLU
1	O	95	LYS
1	O	97	ILE
1	O	107	ARG
1	O	113	GLU
1	O	118	ASP
1	O	124	ILE
1	O	125	ARG
1	O	126	SER
1	O	130	LEU
1	O	131	VAL
1	O	137	SER
1	O	146	ASP
1	O	149	GLU
1	O	153	GLU
1	O	154	ARG
1	O	164	THR
1	O	169	LEU
1	O	175	GLN
1	O	177	ARG
1	O	189	THR
1	O	190	MET
1	O	191	LEU
1	O	196	THR
1	O	198	ASP
1	O	200	ASP
1	O	201	ASP
1	O	202	LYS
1	O	205	GLU
1	O	206	VAL
1	O	211	ARG
1	O	215	PRO
1	O	219	ARG
1	O	229	ILE
1	O	235	THR
1	O	236	ARG
1	O	245	ASP
1	O	253	GLN
1	O	254	LEU

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Mol	Chain	Res	Type
1	O	257	LYS
1	O	258	GLU
1	O	262	LYS
1	O	277	GLU
1	O	287	LEU
1	O	297	GLU
1	O	303	GLU
1	O	313	ILE
1	O	314	GLN
1	O	319	GLU
1	O	321	LYS
1	O	325	ASP
1	O	334	THR
1	O	335	LYS
1	O	351	LEU
1	O	389	ARG
1	O	393	GLU
1	O	401	ILE
1	O	403	LEU
1	O	406	LEU
1	O	415	ASN
1	O	418	LEU
1	O	422	GLN
1	O	426	LEU
1	O	429	ARG
1	O	436	ARG
1	O	438	VAL
1	O	439	THR
1	O	446	LEU
1	O	449	LEU
1	O	455	GLN
1	O	456	ASN
1	O	457	LEU
1	O	458	ASP
1	O	461	GLN
1	O	463	LYS
1	O	468	ARG
1	O	476	THR
1	O	477	THR
1	O	478	GLU
1	O	479	ARG
1	O	482	ARG

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Mol	Chain	Res	Type
1	O	487	LYS
1	O	492	ARG
1	O	494	MET
1	Y	3	LYS
1	Y	17	ARG
1	Y	21	MET
1	Y	26	ASN
1	Y	29	SER
1	Y	33	ARG
1	Y	51	GLU
1	Y	63	VAL
1	Y	65	THR
1	Y	69	ILE
1	Y	71	SER
1	Y	79	ILE
1	Y	80	THR
1	Y	83	ARG
1	Y	87	ILE
1	Y	91	LYS
1	Y	95	LYS
1	Y	107	ARG
1	Y	132	ILE
1	Y	136	PHE
1	Y	137	SER
1	Y	145	LEU
1	Y	152	ARG
1	Y	153	GLU
1	Y	157	ARG
1	Y	164	THR
1	Y	170	ILE
1	Y	177	ARG
1	Y	178	VAL
1	Y	182	ASP
1	Y	188	ARG
1	Y	216	GLU
1	Y	217	VAL
1	Y	224	TYR
1	Y	227	THR
1	Y	238	PRO
1	Y	254	LEU
1	Y	257	LYS
1	Y	262	LYS

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Mol	Chain	Res	Type
1	Y	269	CYS
1	Y	277	GLU
1	Y	281	LYS
1	Y	295	THR
1	Y	303	GLU
1	Y	314	GLN
1	Y	317	ARG
1	Y	319	GLU
1	Y	321	LYS
1	Y	324	ASN
1	Y	325	ASP
1	Y	327	TYR
1	Y	328	ASP
1	Y	337	GLN
1	Y	338	ASN
1	Y	351	LEU
1	Y	364	ILE
1	Y	376	ILE
1	Y	392	LEU
1	Y	401	ILE
1	Y	403	LEU
1	Y	406	LEU
1	Y	415	ASN
1	Y	418	LEU
1	Y	423	SER
1	Y	425	ILE
1	Y	426	LEU
1	Y	429	ARG
1	Y	436	ARG
1	Y	437	GLU
1	Y	439	THR
1	Y	449	LEU
1	Y	456	ASN
1	Y	459	GLU
1	Y	460	LEU
1	Y	461	GLN
1	Y	462	GLU
1	Y	463	LYS
1	Y	466	ILE
1	Y	468	ARG
1	Y	471	ARG
1	Y	474	ILE

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Mol	Chain	Res	Type
1	Y	479	ARG
1	Y	488	LYS
1	Y	491	LYS
1	Y	492	ARG
1	Y	500	ASP
1	Z	3	LYS
1	Z	6	ILE
1	Z	9	LEU
1	Z	11	GLN
1	Z	21	MET
1	Z	29	SER
1	Z	32	GLN
1	Z	33	ARG
1	Z	41	LYS
1	Z	51	GLU
1	Z	63	VAL
1	Z	69	ILE
1	Z	70	SER
1	Z	72	ASP
1	Z	73	GLN
1	Z	80	THR
1	Z	82	GLN
1	Z	83	ARG
1	Z	91	LYS
1	Z	92	GLU
1	Z	95	LYS
1	Z	107	ARG
1	Z	117	ARG
1	Z	121	GLU
1	Z	125	ARG
1	Z	126	SER
1	Z	131	VAL
1	Z	137	SER
1	Z	140	LYS
1	Z	142	LYS
1	Z	145	LEU
1	Z	147	HIS
1	Z	152	ARG
1	Z	154	ARG
1	Z	156	ARG
1	Z	157	ARG
1	Z	159	GLU

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Mol	Chain	Res	Type
1	Z	166	ASP
1	Z	175	GLN
1	Z	177	ARG
1	Z	178	VAL
1	Z	180	VAL
1	Z	182	ASP
1	Z	196	THR
1	Z	197	LEU
1	Z	198	ASP
1	Z	202	LYS
1	Z	204	LEU
1	Z	205	GLU
1	Z	214	LEU
1	Z	216	GLU
1	Z	219	ARG
1	Z	227	THR
1	Z	228	ASN
1	Z	236	ARG
1	Z	262	LYS
1	Z	278	LYS
1	Z	281	LYS
1	Z	284	ASN
1	Z	307	PHE
1	Z	318	ASP
1	Z	319	GLU
1	Z	320	MET
1	Z	321	LYS
1	Z	322	LEU
1	Z	335	LYS
1	Z	336	VAL
1	Z	337	GLN
1	Z	351	LEU
1	Z	364	ILE
1	Z	369	ARG
1	Z	371	VAL
1	Z	402	ARG
1	Z	406	LEU
1	Z	415	ASN
1	Z	416	ASN
1	Z	418	LEU
1	Z	425	ILE
1	Z	426	LEU

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Mol	Chain	Res	Type
1	Z	428	THR
1	Z	431	GLU
1	Z	437	GLU
1	Z	438	VAL
1	Z	439	THR
1	Z	449	LEU
1	Z	455	GLN
1	Z	456	ASN
1	Z	457	LEU
1	Z	461	GLN
1	Z	463	LYS
1	Z	465	VAL
1	Z	466	ILE
1	Z	468	ARG
1	Z	475	GLU
1	Z	477	THR
1	Z	478	GLU
1	Z	490	VAL
1	Z	494	MET
1	Z	497	GLU
1	Z	500	ASP
1	X	4	LYS
1	X	6	ILE
1	X	11	GLN
1	X	17	ARG
1	X	28	ILE
1	X	29	SER
1	X	30	VAL
1	X	66	LYS
1	X	71	SER
1	X	72	ASP
1	X	80	THR
1	X	82	GLN
1	X	83	ARG
1	X	107	ARG
1	X	117	ARG
1	X	118	ASP
1	X	120	LEU
1	X	121	GLU
1	X	125	ARG
1	X	131	VAL
1	X	137	SER

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Mol	Chain	Res	Type
1	X	145	LEU
1	X	151	SER
1	X	152	ARG
1	X	157	ARG
1	X	159	GLU
1	X	168	TRP
1	X	175	GLN
1	X	177	ARG
1	X	180	VAL
1	X	182	ASP
1	X	188	ARG
1	X	190	MET
1	X	196	THR
1	X	197	LEU
1	X	202	LYS
1	X	204	LEU
1	X	205	GLU
1	X	211	ARG
1	X	213	MET
1	X	214	LEU
1	X	216	GLU
1	X	221	SER
1	X	222	GLU
1	X	224	TYR
1	X	226	GLN
1	X	229	ILE
1	X	235	THR
1	X	237	ILE
1	X	254	LEU
1	X	257	LYS
1	X	262	LYS
1	X	269	CYS
1	X	272	LEU
1	X	277	GLU
1	X	278	LYS
1	X	282	SER
1	X	295	THR
1	X	297	GLU
1	X	313	ILE
1	X	314	GLN
1	X	317	ARG
1	X	318	ASP

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Mol	Chain	Res	Type
1	X	321	LYS
1	X	322	LEU
1	X	325	ASP
1	X	328	ASP
1	X	329	SER
1	X	351	LEU
1	X	389	ARG
1	X	392	LEU
1	X	395	MET
1	X	402	ARG
1	X	406	LEU
1	X	415	ASN
1	X	418	LEU
1	X	420	GLN
1	X	425	ILE
1	X	426	LEU
1	X	436	ARG
1	X	441	LEU
1	X	446	LEU
1	X	449	LEU
1	X	455	GLN
1	X	459	GLU
1	X	460	LEU
1	X	468	ARG
1	X	469	GLU
1	X	477	THR
1	X	479	ARG
1	X	482	ARG
1	X	487	LYS
1	X	492	ARG
1	X	498	GLU
1	X	499	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	11	GLN
1	O	23	HIS
1	O	47	HIS
1	O	73	GLN
1	O	81	ASN
1	O	82	GLN

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Mol	Chain	Res	Type
1	O	127	ASN
1	O	179	HIS
1	O	185	ASN
1	O	253	GLN
1	O	299	ASN
1	O	324	ASN
1	O	374	ASN
1	O	396	GLN
1	O	415	ASN
1	O	422	GLN
1	O	455	GLN
1	O	456	ASN
1	Y	47	HIS
1	Y	114	HIS
1	Y	127	ASN
1	Y	175	GLN
1	Y	179	HIS
1	Y	195	HIS
1	Y	299	ASN
1	Y	314	GLN
1	Y	338	ASN
1	Y	374	ASN
1	Y	396	GLN
1	Y	415	ASN
1	Y	456	ASN
1	Y	461	GLN
1	Z	23	HIS
1	Z	47	HIS
1	Z	73	GLN
1	Z	81	ASN
1	Z	127	ASN
1	Z	185	ASN
1	Z	226	GLN
1	Z	228	ASN
1	Z	314	GLN
1	Z	337	GLN
1	Z	340	ASN
1	Z	374	ASN
1	Z	415	ASN
1	Z	420	GLN
1	Z	455	GLN
1	Z	456	ASN

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Mol	Chain	Res	Type
1	Z	461	GLN
1	Z	499	HIS
1	X	23	HIS
1	X	47	HIS
1	X	81	ASN
1	X	114	HIS
1	X	127	ASN
1	X	147	HIS
1	X	185	ASN
1	X	195	HIS
1	X	226	GLN
1	X	299	ASN
1	X	337	GLN
1	X	396	GLN
1	X	415	ASN
1	X	420	GLN
1	X	422	GLN
1	X	499	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	SO4	O	502	-	4,4,4	2.31	1 (25%)	6,6,6	0.44	0
2	SO4	O	503	-	4,4,4	4.07	2 (50%)	6,6,6	0.62	0
3	GOL	O	504	-	5,5,5	0.85	0	5,5,5	0.80	0
2	SO4	X	502	-	4,4,4	2.77	3 (75%)	6,6,6	0.25	0
3	GOL	X	503	-	5,5,5	0.29	0	5,5,5	0.71	0
2	SO4	Y	502	-	4,4,4	3.43	1 (25%)	6,6,6	0.44	0
3	GOL	Y	503	-	5,5,5	0.30	0	5,5,5	0.31	0
2	SO4	Z	502	-	4,4,4	1.47	1 (25%)	6,6,6	0.24	0
2	SO4	Z	503	-	4,4,4	3.01	3 (75%)	6,6,6	0.48	0
3	GOL	Z	504	-	5,5,5	0.20	0	5,5,5	0.85	0

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
2	SO4	O	502	-	-	0/0/0/0	0/0/0/0
2	SO4	O	503	-	-	0/0/0/0	0/0/0/0
3	GOL	O	504	-	-	0/4/4/4	0/0/0/0
2	SO4	X	502	-	-	0/0/0/0	0/0/0/0
3	GOL	X	503	-	-	0/4/4/4	0/0/0/0
2	SO4	Y	502	-	-	0/0/0/0	0/0/0/0
3	GOL	Y	503	-	-	0/4/4/4	0/0/0/0
2	SO4	Z	502	-	-	0/0/0/0	0/0/0/0
2	SO4	Z	503	-	-	0/0/0/0	0/0/0/0
3	GOL	Z	504	-	-	0/4/4/4	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	502	SO4	O1-S	-4.33	1.32	1.47
2	X	502	SO4	O2-S	2.30	1.55	1.47
2	X	502	SO4	O3-S	2.36	1.55	1.47
2	Z	503	SO4	O1-S	2.72	1.56	1.47
2	Z	502	SO4	O2-S	2.78	1.56	1.47
2	Z	503	SO4	O2-S	3.35	1.58	1.47
2	Z	503	SO4	O4-S	3.98	1.61	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	502	SO4	O1-S	4.42	1.62	1.47
2	O	503	SO4	O4-S	4.74	1.64	1.47
2	Y	502	SO4	O3-S	6.37	1.70	1.47
2	O	503	SO4	O3-S	6.57	1.71	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	502	SO4	2	0
3	O	504	GOL	1	0
3	X	503	GOL	1	0
3	Y	503	GOL	3	0
2	Z	502	SO4	1	0
2	Z	503	SO4	1	0
3	Z	504	GOL	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	O	497/501 (99%)	0.17	27 (5%)	29	34	10, 36, 67, 75	0
1	X	498/501 (99%)	0.04	19 (3%)	44	49	13, 34, 67, 75	0
1	Y	499/501 (99%)	-0.02	11 (2%)	65	68	13, 34, 65, 75	0
1	Z	498/501 (99%)	-0.04	18 (3%)	46	51	12, 33, 62, 75	0
All	All	1992/2004 (99%)	0.04	75 (3%)	44	49	10, 34, 65, 75	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	158	GLY	5.8
1	Y	499	HIS	5.1
1	Y	327	TYR	5.0
1	O	460	LEU	4.9
1	X	460	LEU	4.6
1	O	463	LYS	4.3
1	O	326	ALA	4.2
1	O	456	ASN	4.2
1	Y	475	GLU	4.1
1	O	306	VAL	3.9
1	Z	476	THR	3.7
1	Z	500	ASP	3.3
1	O	457	LEU	3.2
1	Y	157	ARG	3.1
1	O	476	THR	3.1
1	Y	148	VAL	3.0
1	Y	500	ASP	3.0
1	O	103	TRP	3.0
1	O	305	ALA	3.0
1	X	327	TYR	3.0
1	O	269	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	Z	306	VAL	3.0
1	X	157	ARG	2.9
1	O	270	PHE	2.8
1	Y	153	GLU	2.8
1	Z	477	THR	2.8
1	O	327	TYR	2.7
1	O	153	GLU	2.7
1	O	307	PHE	2.7
1	O	123	TYR	2.7
1	X	153	GLU	2.6
1	X	264	THR	2.6
1	Z	404	HIS	2.6
1	X	243	ALA	2.6
1	X	326	ALA	2.6
1	Z	327	TYR	2.6
1	O	353	ALA	2.6
1	Z	499	HIS	2.6
1	O	391	VAL	2.6
1	O	25	ALA	2.5
1	Z	307	PHE	2.5
1	X	474	ILE	2.5
1	X	267	THR	2.4
1	X	477	THR	2.4
1	Y	103	TRP	2.4
1	Z	325	ASP	2.4
1	O	477	THR	2.4
1	Z	463	LYS	2.4
1	X	307	PHE	2.3
1	Z	305	ALA	2.3
1	O	202	LYS	2.3
1	X	475	GLU	2.3
1	Z	267	THR	2.3
1	Z	103	TRP	2.3
1	X	103	TRP	2.3
1	Z	326	ALA	2.2
1	X	464	ALA	2.2
1	Y	151	SER	2.2
1	O	212	GLU	2.2
1	Z	151	SER	2.2
1	X	23	HIS	2.2
1	X	25	ALA	2.2
1	X	279	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	Z	153	GLU	2.2
1	O	351	LEU	2.2
1	O	149	GLU	2.1
1	Z	351	LEU	2.1
1	X	80	THR	2.1
1	O	155	ALA	2.1
1	O	461	GLN	2.1
1	Z	270	PHE	2.0
1	O	325	ASP	2.0
1	O	475	GLU	2.0
1	Y	295	THR	2.0
1	X	269	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	X	502	5/5	0.97	0.33	3.05	30,75,75,75	0
3	GOL	Y	503	6/6	0.99	0.27	2.64	11,18,30,63	0
2	SO4	Y	502	5/5	0.95	0.27	2.59	36,67,75,75	0
3	GOL	X	503	6/6	0.97	0.30	2.46	5,20,29,35	0
3	GOL	O	504	6/6	0.94	0.31	2.13	12,23,29,40	0
3	GOL	Z	504	6/6	0.98	0.26	1.99	5,16,20,54	0
2	SO4	Z	503	5/5	0.96	0.26	1.93	51,60,75,75	0
2	SO4	O	503	5/5	0.93	0.24	1.59	37,48,75,75	0
2	SO4	O	502	5/5	0.99	0.11	-0.45	11,36,68,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	Z	502	5/5	0.99	0.10	-0.77	27,48,75,75	0

6.5 Other polymers

There are no such residues in this entry.