



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:04 AM GMT

PDB ID : 2VPY
Title : POLYSULFIDE REDUCTASE WITH BOUND QUINONE INHIBITOR,
PENTACHLOROPHENOL (PCP)
Authors : Jormakka, M.; Yokoyama, K.; Yano, T.; Tamakoshi, M.; Akimoto, S.; Shimamura, T.; Curmi, P.; Iwata, S.
Deposited on : 2008-03-09
Resolution : 2.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

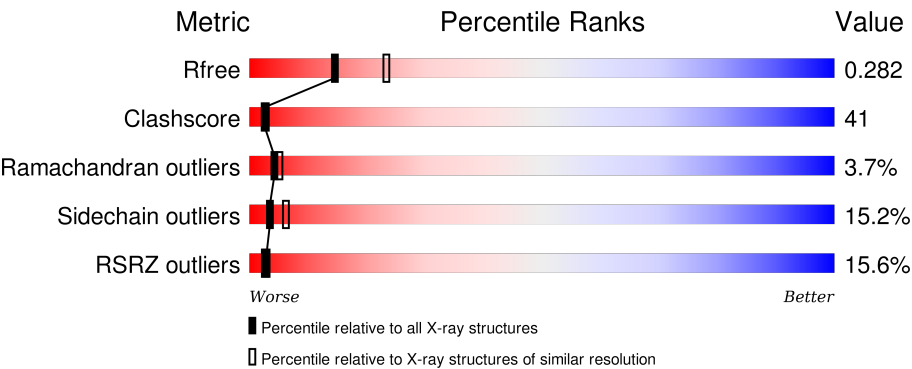
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R _{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	A	765	<div><div>16%</div><div><div></div><div>43%</div><div>38%</div><div>13%</div><div>• •</div></div></div>
1	E	765	<div><div>14%</div><div><div></div><div>42%</div><div>38%</div><div>13%</div><div>• •</div></div></div>
2	B	195	<div><div>8%</div><div><div></div><div>51%</div><div>38%</div><div>8%</div><div>• •</div></div></div>
2	F	195	<div><div>9%</div><div><div></div><div>56%</div><div>33%</div><div>9%</div><div>• •</div></div></div>
3	C	253	<div><div>15%</div><div><div></div><div>63%</div><div>28%</div><div>7%</div><div>• •</div></div></div>

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Mol	Chain	Length	Quality of chain
3	G	253	

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
4	SF4	B	1196	-	-	X	-
4	SF4	F	1194	-	-	X	-
4	SF4	F	1195	-	-	X	-
7	PCI	C	1252	-	-	X	-
7	PCI	G	1251	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20217 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 THIOSULFATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			
1	E	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			

- Molecule 2 is a protein called NRFC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	194	Total	C	N	O	S	0	0	1
			1475	930	256	269	20			
2	F	194	Total	C	N	O	S	0	0	1
			1475	930	256	269	20			

- Molecule 3 is a protein called HYPOTHETICAL MEMBRANE SPANNING PROTEIN.

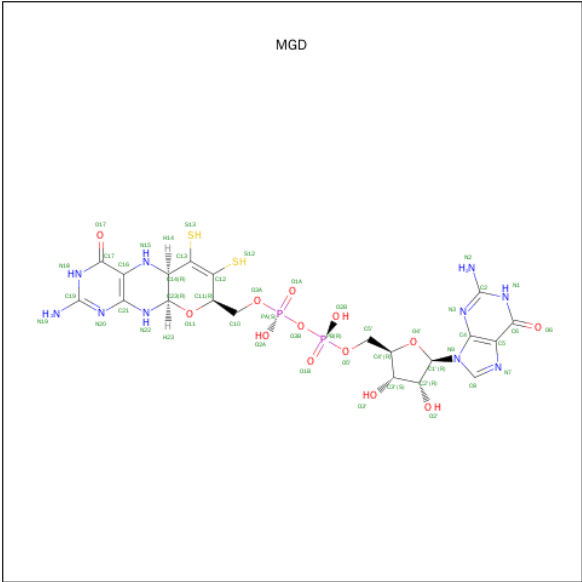
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			
3	G	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

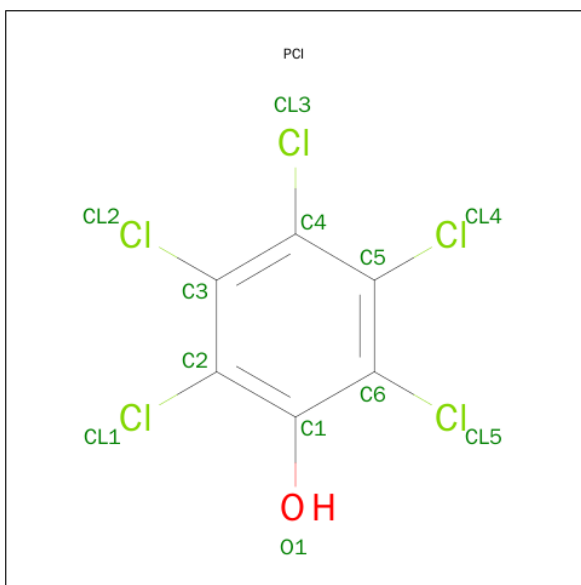


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 6 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		
6	E	1	Total	Mo	0	0
			1	1		

- Molecule 7 is PENTACHLOROPHENOL (three-letter code: PCI) (formula: C₆HCl₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	Cl	O	0	0
			12	6	5	1		
7	G	1	Total	C	Cl	O	0	0
			12	6	5	1		

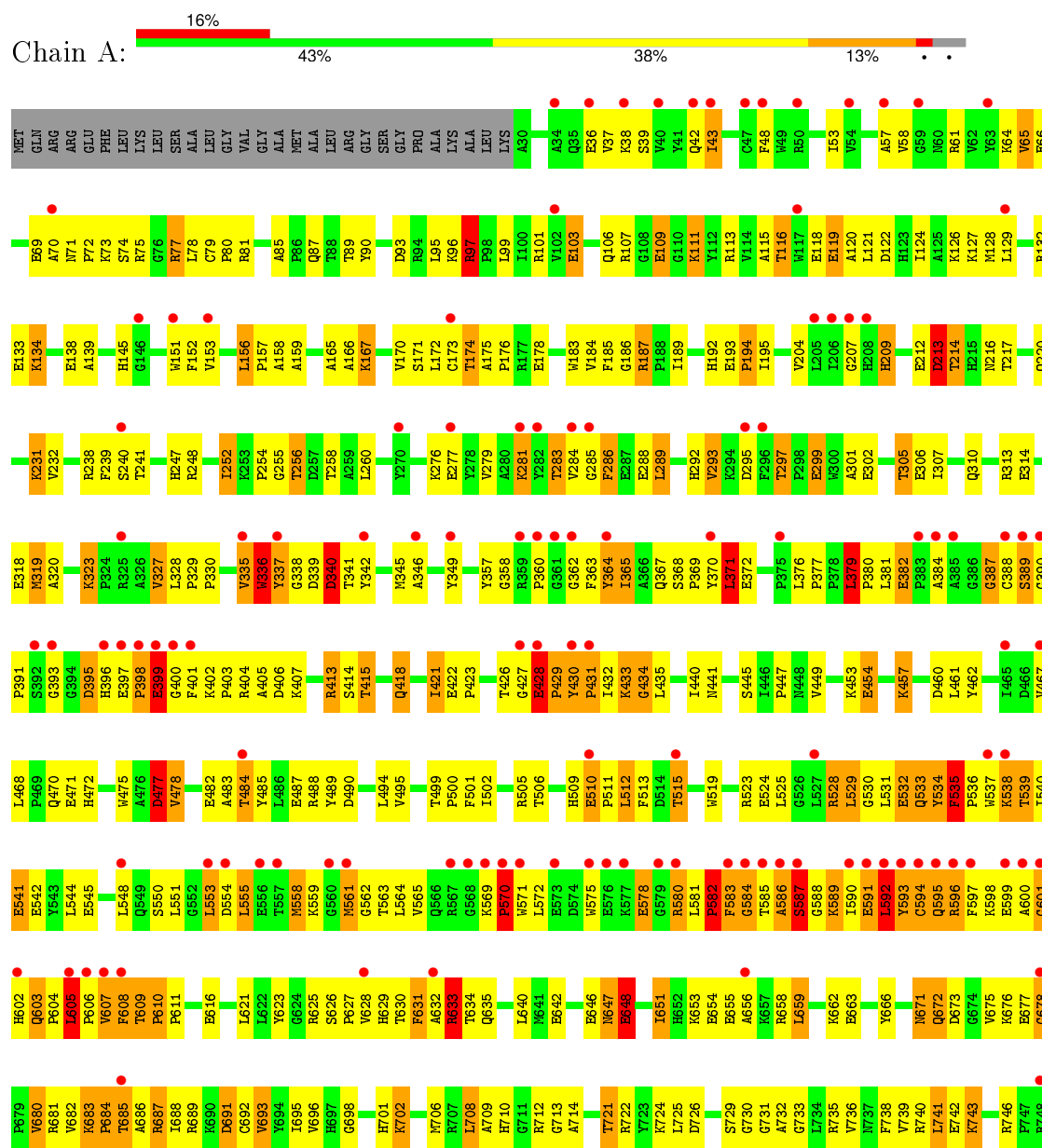
- Molecule 8 is water.

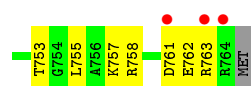
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	387	Total	O	0	0
			387	387		
8	B	150	Total	O	0	0
			150	150		
8	C	90	Total	O	0	0
			90	90		
8	E	452	Total	O	0	0
			452	452		
8	F	129	Total	O	0	0
			129	129		
8	G	77	Total	O	0	0
			77	77		

3 Residue-property plots

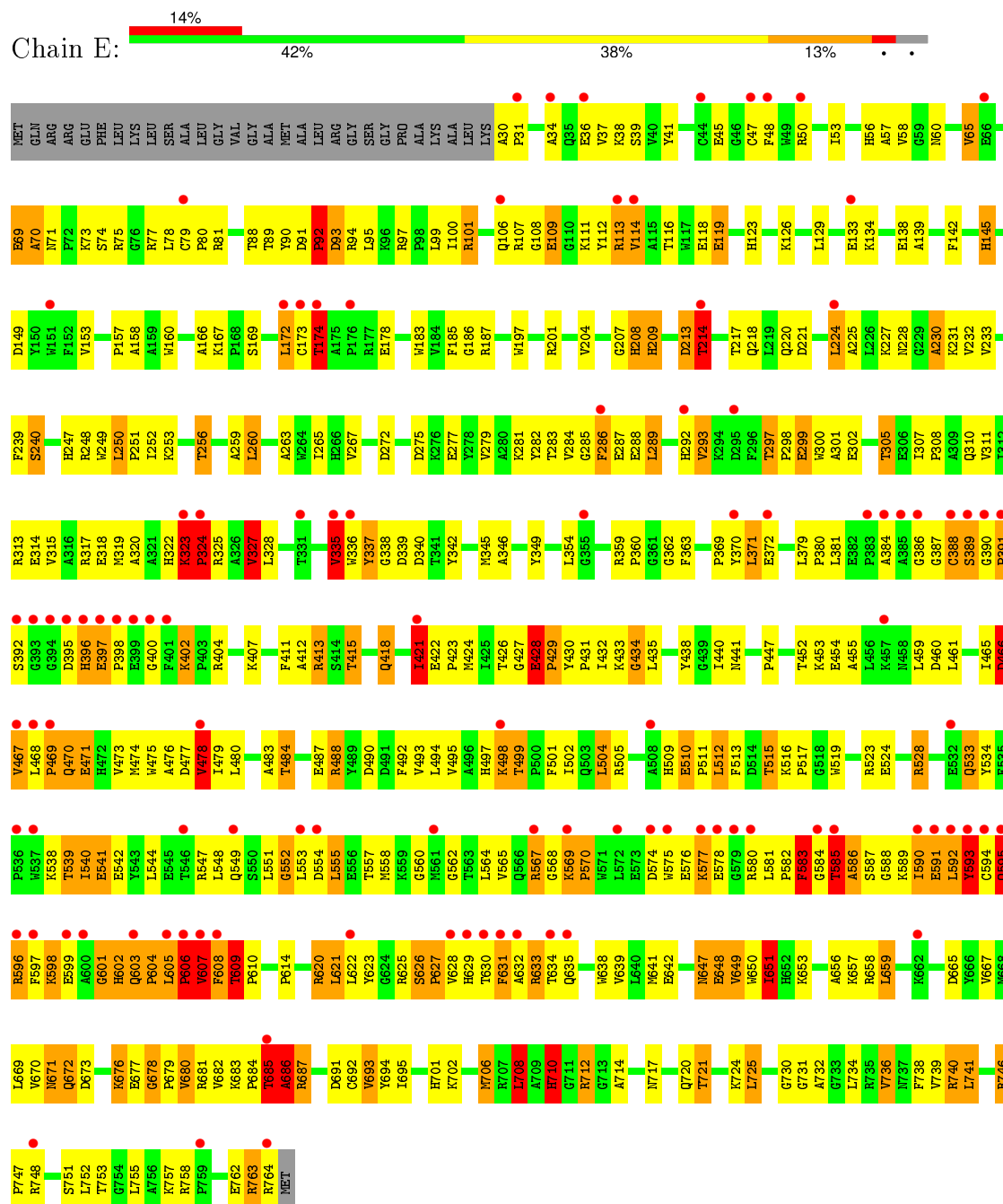
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: THIOSULFATE REDUCTASE

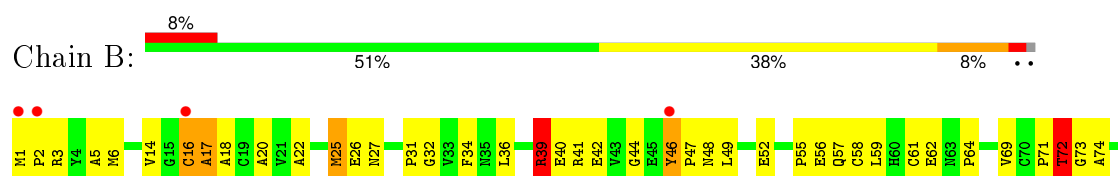


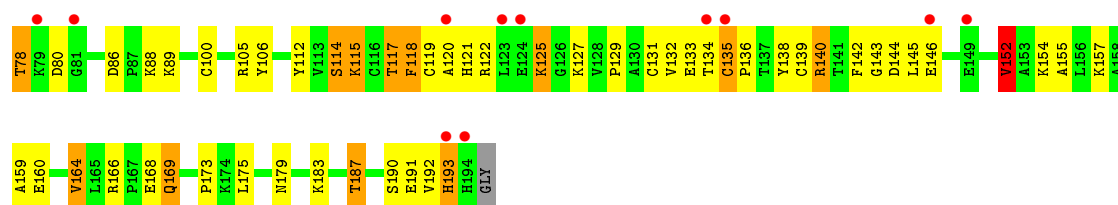


● Molecule 1: THIOSULFATE REDUCTASE

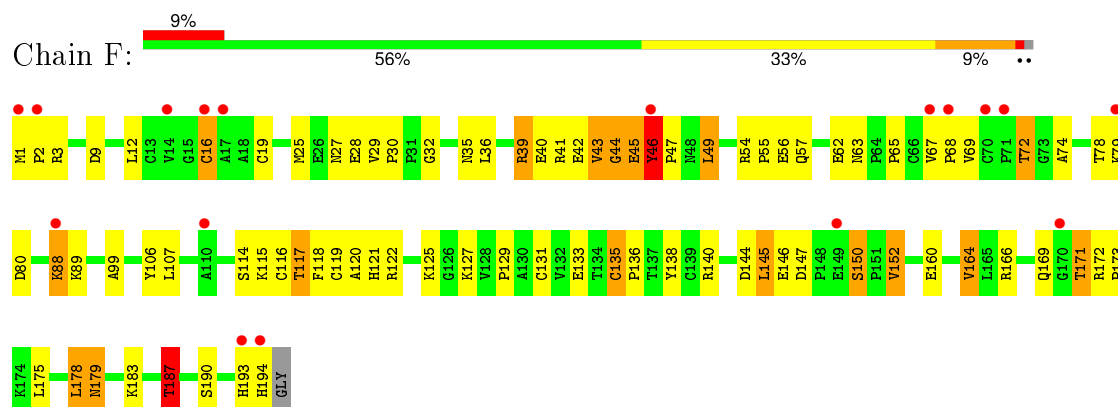


- Molecule 2: NRFC PROTEIN

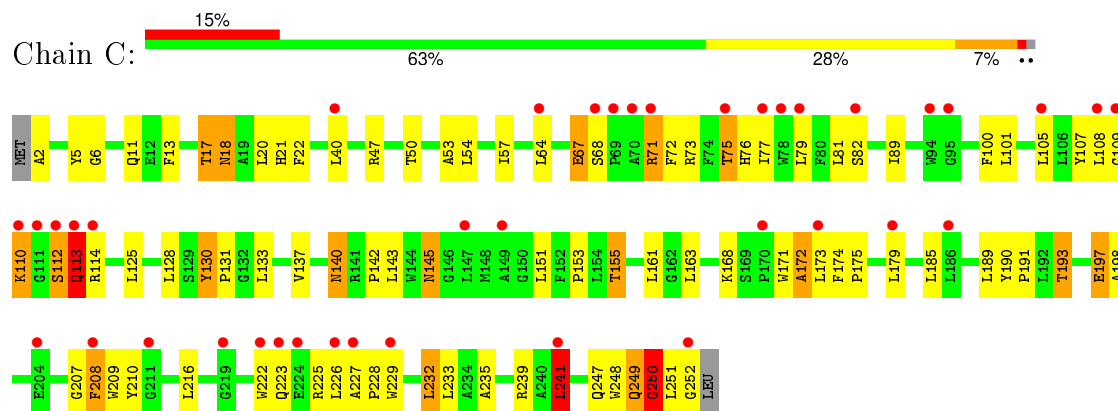




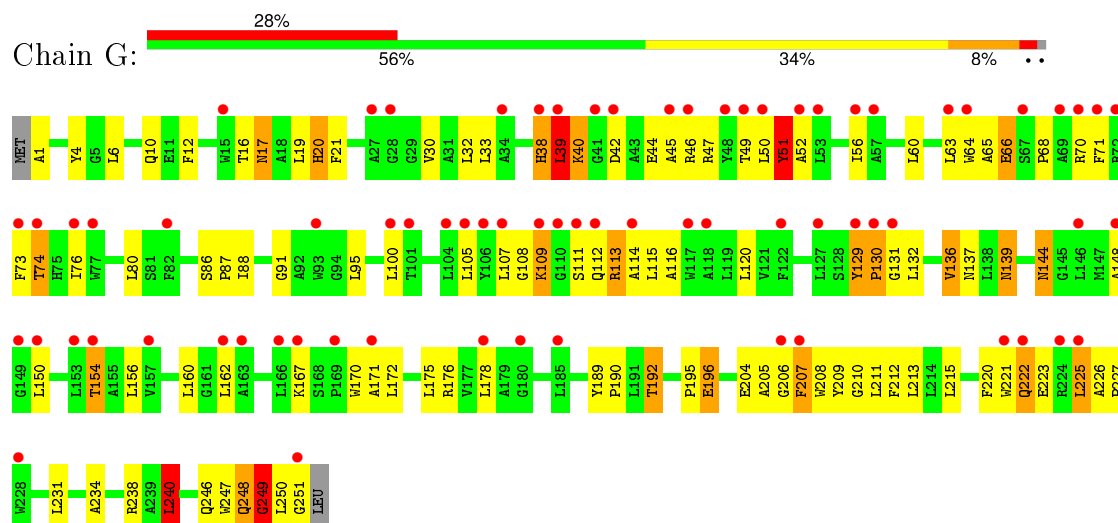
• Molecule 2: NRFC PROTEIN



• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN



• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.12Å 165.19Å 243.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.58 – 2.50 39.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.58-2.50) 98.7 (39.58-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.283 , 0.289 0.277 , 0.282	Depositor DCC
R_{free} test set	3224 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 160975 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	20217	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SF4, PCI, MO, MGD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.83	9/6079 (0.1%)	1.08	28/8267 (0.3%)
1	E	0.93	21/6079 (0.3%)	1.29	74/8267 (0.9%)
2	B	0.83	3/1512 (0.2%)	1.20	9/2058 (0.4%)
2	F	0.86	2/1512 (0.1%)	1.21	14/2058 (0.7%)
3	C	0.81	3/2016 (0.1%)	0.89	8/2764 (0.3%)
3	G	0.71	1/2016 (0.0%)	1.09	17/2764 (0.6%)
All	All	0.85	39/19214 (0.2%)	1.15	150/26178 (0.6%)

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	E	0	2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	592	LEU	CG-CD1	15.29	2.08	1.51
2	F	135	CYS	CB-SG	14.39	2.06	1.82
1	E	323	LYS	C-O	12.36	1.46	1.23
3	C	114	ARG	NE-CZ	11.87	1.48	1.33
1	E	240	SER	CA-CB	-11.46	1.35	1.52
1	A	648	GLU	CB-CG	10.09	1.71	1.52
2	F	16	CYS	CB-SG	9.01	1.97	1.82
1	A	399	GLU	CD-OE2	-8.72	1.16	1.25
2	B	135	CYS	CB-SG	8.71	1.97	1.82
3	C	114	ARG	CZ-NH1	8.56	1.44	1.33
1	E	324	PRO	CG-CD	8.30	1.78	1.50
1	E	324	PRO	CA-C	8.07	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	173	CYS	CB-SG	7.43	1.94	1.82
2	B	16	CYS	CB-SG	7.33	1.94	1.82
1	E	388	CYS	CA-CB	-6.46	1.39	1.53
1	A	336	TRP	CB-CG	-6.34	1.38	1.50
3	G	109	LYS	C-N	6.32	1.44	1.33
1	E	387	GLY	C-N	6.26	1.48	1.34
1	E	648	GLU	CB-CG	6.11	1.63	1.52
1	A	337	TYR	CB-CG	6.06	1.60	1.51
2	B	100	CYS	CB-SG	6.01	1.92	1.82
1	E	324	PRO	N-CA	5.91	1.57	1.47
1	E	387	GLY	C-O	-5.90	1.14	1.23
1	E	595	GLN	CA-CB	-5.89	1.41	1.53
1	A	97	ARG	NE-CZ	5.87	1.40	1.33
1	E	231	LYS	CA-CB	-5.84	1.41	1.53
1	E	324	PRO	N-CD	5.74	1.55	1.47
1	E	594	CYS	C-O	-5.65	1.12	1.23
1	A	364	TYR	C-O	-5.65	1.12	1.23
1	A	601	GLY	CA-C	-5.56	1.43	1.51
1	E	323	LYS	C-N	5.50	1.44	1.34
1	E	230	ALA	C-O	-5.47	1.12	1.23
1	E	324	PRO	CB-CG	-5.38	1.23	1.50
1	A	535	PHE	CB-CG	-5.19	1.42	1.51
1	E	421	ILE	CA-CB	-5.19	1.43	1.54
1	E	478	VAL	CA-CB	5.16	1.65	1.54
1	E	231	LYS	CB-CG	-5.12	1.38	1.52
1	A	173	CYS	CB-SG	5.11	1.91	1.82
3	C	114	ARG	CD-NE	5.06	1.55	1.46

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	323	LYS	C-N-CD	-24.04	67.71	120.60
1	E	324	PRO	CA-N-CD	-15.99	89.11	111.50
1	E	323	LYS	O-C-N	-13.09	96.24	121.10
3	G	249	GLY	N-CA-C	11.65	142.23	113.10
2	F	171	THR	N-CA-C	10.52	139.41	111.00
1	E	387	GLY	CA-C-O	10.32	139.17	120.60
1	A	583	PHE	C-N-CA	10.21	143.74	122.30
1	E	324	PRO	N-CA-C	-9.81	86.59	112.10
1	E	240	SER	N-CA-CB	-9.70	95.95	110.50
2	F	44	GLY	N-CA-C	9.65	137.24	113.10
2	B	46	TYR	N-CA-C	9.62	136.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	172	LEU	CA-CB-CG	-9.21	94.11	115.30
1	E	585	THR	CA-CB-CG2	-8.88	99.97	112.40
1	A	691	ASP	CB-CA-C	-8.79	92.82	110.40
1	A	592	LEU	N-CA-C	8.48	133.89	111.00
1	A	401	PHE	N-CA-C	8.45	133.81	111.00
1	E	680	VAL	CB-CA-C	-8.27	95.69	111.40
3	G	207	PHE	CB-CA-C	-8.24	93.92	110.40
1	E	185	PHE	N-CA-C	-8.15	88.98	111.00
1	E	387	GLY	C-N-CA	-8.14	101.35	121.70
1	E	388	CYS	N-CA-C	7.95	132.46	111.00
2	B	169	GLN	N-CA-C	-7.91	89.64	111.00
1	E	725	LEU	CA-CB-CG	7.86	133.37	115.30
2	B	46	TYR	CB-CA-C	-7.84	94.72	110.40
1	E	686	ALA	N-CA-C	7.83	132.14	111.00
1	E	583	PHE	N-CA-C	7.79	132.04	111.00
1	E	595	GLN	N-CA-CB	-7.75	96.66	110.60
1	E	593	TYR	CB-CA-C	-7.70	95.00	110.40
2	F	39	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	E	387	GLY	CA-C-N	-7.63	100.41	117.20
1	E	659	LEU	N-CA-C	-7.54	90.64	111.00
1	E	582	PRO	N-CA-C	7.53	131.68	112.10
1	E	593	TYR	N-CA-CB	7.50	124.09	110.60
1	E	327	VAL	CB-CA-C	-7.47	97.20	111.40
1	E	585	THR	CB-CA-C	7.35	131.45	111.60
1	A	327	VAL	CB-CA-C	-7.29	97.55	111.40
3	G	114	ALA	N-CA-C	-7.24	91.46	111.00
1	E	323	LYS	CB-CA-C	7.23	124.86	110.40
1	E	731	GLY	N-CA-C	7.20	131.09	113.10
3	G	240	LEU	CA-CB-CG	7.16	131.78	115.30
1	E	390	GLY	N-CA-C	-7.06	95.46	113.10
1	E	467	VAL	N-CA-C	6.86	129.53	111.00
1	E	685	THR	C-N-CA	6.83	138.78	121.70
3	G	225	LEU	N-CA-C	-6.79	92.68	111.00
1	A	648	GLU	N-CA-CB	-6.76	98.44	110.60
3	C	113	GLN	N-CA-C	6.74	129.19	111.00
3	G	131	GLY	N-CA-C	-6.69	96.37	113.10
1	E	708	LEU	CA-CB-CG	6.63	130.56	115.30
1	A	185	PHE	C-N-CA	-6.63	108.38	122.30
2	F	54	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	E	603	GLN	N-CA-C	6.61	128.84	111.00
2	F	152	VAL	CB-CA-C	-6.60	98.86	111.40
1	A	340	ASP	N-CA-C	6.58	128.76	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	16	CYS	N-CA-C	-6.57	93.27	111.00
2	B	72	THR	N-CA-C	-6.54	93.34	111.00
1	E	594	CYS	O-C-N	-6.52	112.26	122.70
1	E	594	CYS	N-CA-C	6.47	128.47	111.00
1	A	741	LEU	CA-CB-CG	6.39	130.00	115.30
1	E	594	CYS	N-CA-CB	-6.38	99.12	110.60
3	C	250	GLY	N-CA-C	6.34	128.95	113.10
1	E	710	HIS	C-N-CA	-6.33	109.00	122.30
1	E	92	PRO	N-CA-C	-6.29	95.75	112.10
1	A	477	ASP	N-CA-C	-6.27	94.08	111.00
1	A	582	PRO	N-CA-C	6.25	128.34	112.10
2	F	145	LEU	CA-CB-CG	6.22	129.60	115.30
1	E	593	TYR	CB-CG-CD1	-6.21	117.28	121.00
1	E	593	TYR	N-CA-C	-6.17	94.34	111.00
1	A	213	ASP	N-CA-C	-6.16	94.37	111.00
2	F	39	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	E	428	GLU	N-CA-C	6.11	127.49	111.00
2	B	152	VAL	CB-CA-C	-6.05	99.89	111.40
1	E	214	THR	N-CA-CB	-6.00	98.90	110.30
2	F	43	VAL	N-CA-C	-5.97	94.89	111.00
1	E	590	ILE	CB-CA-C	-5.96	99.69	111.60
1	A	364	TYR	N-CA-C	5.95	127.07	111.00
3	G	4	TYR	N-CA-C	-5.95	94.94	111.00
2	F	46	TYR	N-CA-C	5.93	127.02	111.00
1	E	213	ASP	N-CA-C	-5.92	95.01	111.00
1	E	388	CYS	CA-CB-SG	5.92	124.65	114.00
1	A	659	LEU	N-CA-C	-5.91	95.04	111.00
3	G	248	GLN	N-CA-CB	-5.91	99.96	110.60
1	A	97	ARG	NE-CZ-NH1	-5.91	117.34	120.30
1	E	606	PRO	N-CA-C	-5.87	96.83	112.10
1	E	324	PRO	N-CD-CG	-5.86	94.41	103.20
1	E	712	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	379	LEU	CA-CB-CG	5.81	128.67	115.30
1	E	400	GLY	N-CA-C	-5.78	98.64	113.10
1	A	433	LYS	N-CA-C	-5.76	95.44	111.00
3	C	226	LEU	CA-CB-CG	5.75	128.52	115.30
1	A	109	GLU	N-CA-C	-5.74	95.50	111.00
2	F	16	CYS	C-N-CA	-5.73	107.38	121.70
1	E	651	ILE	CB-CA-C	-5.71	100.18	111.60
1	E	593	TYR	CB-CG-CD2	5.70	124.42	121.00
3	C	114	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	E	741	LEU	CA-CB-CG	5.67	128.33	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	169	GLN	C-N-CA	-5.66	110.41	122.30
2	B	72	THR	N-CA-CB	-5.66	99.54	110.30
3	G	109	LYS	CA-C-N	-5.66	104.88	116.20
1	E	337	TYR	N-CA-C	5.65	126.25	111.00
1	E	34	ALA	C-N-CA	5.65	135.81	121.70
3	C	114	ARG	N-CA-C	-5.60	95.87	111.00
3	G	130	PRO	N-CA-C	-5.60	97.55	112.10
1	E	173	CYS	CA-CB-SG	5.59	124.07	114.00
1	E	207	GLY	N-CA-C	-5.59	99.14	113.10
3	C	6	GLY	N-CA-C	-5.56	99.21	113.10
3	C	241	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	319	MET	CA-CB-CG	5.52	122.69	113.30
1	E	710	HIS	N-CA-C	5.52	125.91	111.00
1	A	570	PRO	O-C-N	-5.49	113.92	122.70
1	A	706	MET	N-CA-C	-5.48	96.19	111.00
1	E	379	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	401	PHE	CA-C-O	-5.45	108.66	120.10
1	E	335	VAL	CB-CA-C	5.43	121.72	111.40
1	A	364	TYR	C-N-CA	5.41	135.22	121.70
1	E	335	VAL	N-CA-CB	-5.40	99.62	111.50
1	E	706	MET	N-CA-C	-5.38	96.48	111.00
1	E	710	HIS	CA-C-N	5.35	126.90	116.20
1	A	583	PHE	CB-CA-C	-5.33	99.73	110.40
1	A	365	ILE	N-CA-CB	5.32	123.03	110.80
3	G	6	LEU	CA-CB-CG	5.30	127.48	115.30
1	E	583	PHE	N-CA-CB	-5.29	101.08	110.60
3	G	109	LYS	O-C-N	5.28	132.18	123.20
3	G	207	PHE	CB-CG-CD1	-5.27	117.11	120.80
3	G	213	LEU	CA-CB-CG	5.26	127.41	115.30
1	E	687	ARG	CB-CG-CD	-5.25	97.94	111.60
1	E	323	LYS	C-N-CA	5.24	144.02	122.00
2	B	16	CYS	N-CA-C	-5.23	96.87	111.00
2	B	39	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	E	601	GLY	N-CA-C	5.23	126.17	113.10
1	E	174	THR	N-CA-CB	-5.23	100.37	110.30
1	E	665	ASP	N-CA-C	5.23	125.11	111.00
1	E	260	LEU	CA-CB-CG	5.19	127.24	115.30
1	E	692	CYS	CB-CA-C	-5.18	100.04	110.40
1	E	686	ALA	N-CA-CB	-5.17	102.86	110.10
1	E	185	PHE	C-N-CA	-5.16	111.47	122.30
1	E	736	VAL	N-CA-CB	-5.15	100.16	111.50
1	E	363	PHE	CB-CG-CD2	-5.14	117.20	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	231	LYS	N-CA-CB	-5.13	101.37	110.60
2	F	54	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	534	TYR	N-CA-C	-5.08	97.28	111.00
1	E	586	ALA	N-CA-CB	-5.08	103.00	110.10
2	F	187	THR	N-CA-CB	-5.07	100.66	110.30
1	A	376	LEU	CA-CB-CG	5.06	126.95	115.30
1	E	213	ASP	CB-CG-OD1	5.05	122.85	118.30
3	G	51	TYR	N-CA-C	-5.05	97.37	111.00
3	C	5	TYR	N-CA-C	-5.04	97.39	111.00
3	G	39	LEU	CA-CB-CG	5.03	126.88	115.30
3	G	248	GLN	CA-C-N	-5.03	106.15	116.20
2	F	16	CYS	CA-C-N	5.01	128.22	117.20
1	A	371	LEU	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	323	LYS	Mainchain,Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5896	0	5813	579	3
1	E	5896	0	5814	528	3
2	B	1475	0	1453	135	0
2	F	1475	0	1454	104	0
3	C	1948	0	2001	116	0
3	G	1948	0	2004	129	0
4	A	8	0	0	0	0
4	B	32	0	0	4	0
4	E	8	0	0	1	0
4	F	32	0	0	6	0
5	A	94	0	44	7	0
5	E	94	0	44	12	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1	0	0	0	0
7	C	12	0	0	11	0
7	G	12	0	1	10	0
8	A	387	0	0	77	0
8	B	150	0	0	38	0
8	C	90	0	0	7	0
8	E	452	0	0	114	0
8	F	129	0	0	22	0
8	G	77	0	0	23	0
All	All	20217	0	18628	1551	3

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 41.

All (1551) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:HIS:CE1	1:A:606:PRO:HG3	1.48	1.45
1:E:324:PRO:CG	1:E:324:PRO:CD	1.78	1.45
1:E:592:LEU:HA	1:E:603:GLN:NE2	1.24	1.44
2:F:135:CYS:SG	2:F:135:CYS:CB	2.06	1.43
1:E:605:LEU:CD2	1:E:605:LEU:H	1.28	1.39
1:A:186:GLY:HA3	1:A:583:PHE:C	1.45	1.35
1:A:591:GLU:OE2	1:A:604:PRO:HG3	1.24	1.34
1:A:184:VAL:CG2	1:A:592:LEU:HD23	1.59	1.32
1:A:582:PRO:HB2	8:A:2097:HOH:O	1.26	1.28
1:E:591:GLU:OE1	1:E:604:PRO:HB3	1.24	1.26
2:B:46:TYR:HB2	8:B:2032:HOH:O	1.33	1.26
1:A:604:PRO:O	1:A:606:PRO:HD2	1.37	1.23
1:E:477:ASP:O	1:E:478:VAL:HG23	1.32	1.22
1:E:605:LEU:HD23	1:E:605:LEU:N	1.42	1.22
2:B:41:ARG:HH11	2:B:187:THR:CG2	1.53	1.21
1:E:388:CYS:HB2	1:E:593:TYR:OH	1.36	1.20
1:A:601:GLY:HA2	8:A:2284:HOH:O	1.05	1.20
3:G:207:PHE:CE2	3:G:211:LEU:HD13	1.75	1.20
1:E:602:HIS:CE1	1:E:606:PRO:HG3	1.76	1.19
3:C:171:TRP:CE3	3:C:171:TRP:O	1.97	1.17
1:E:36:GLU:O	1:E:58:VAL:HG22	1.01	1.17
1:E:562:GLY:O	8:E:2316:HOH:O	1.59	1.16
1:A:337:TYR:O	1:A:340:ASP:OD2	1.59	1.16
1:A:395:ASP:O	1:A:399:GLU:HB2	1.43	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HH21	1:A:763:ARG:NH2	1.43	1.16
1:E:592:LEU:CA	1:E:603:GLN:HE21	1.56	1.15
1:A:42:GLN:O	1:A:53:ILE:HG13	1.45	1.15
1:E:477:ASP:O	1:E:478:VAL:CG2	1.95	1.15
1:A:583:PHE:CE2	1:A:588:GLY:N	2.16	1.14
1:E:36:GLU:O	1:E:58:VAL:CG2	1.96	1.14
2:F:57:GLN:NE2	2:F:140:ARG:HH22	1.44	1.14
1:A:584:GLY:HA2	8:A:2277:HOH:O	0.96	1.13
1:A:395:ASP:HA	1:A:399:GLU:CG	1.78	1.13
1:A:69:GLU:O	8:A:2034:HOH:O	1.65	1.12
1:A:284:VAL:O	1:A:590:ILE:HG22	1.47	1.12
1:E:116:THR:HG22	1:E:119:GLU:HB3	1.24	1.12
2:B:134:THR:HG23	2:B:134:THR:O	1.47	1.12
3:G:1:ALA:HB1	8:G:2001:HOH:O	1.51	1.11
1:E:607:VAL:O	1:E:607:VAL:HG12	1.46	1.10
1:E:607:VAL:O	1:E:607:VAL:CG1	1.97	1.09
1:A:428:GLU:HB3	1:A:429:PRO:HD2	1.34	1.09
1:A:397:GLU:HB3	1:A:398:PRO:HD3	1.15	1.09
1:E:323:LYS:HD3	1:E:354:LEU:CA	1.82	1.09
1:A:184:VAL:HG23	1:A:592:LEU:CD2	1.82	1.09
1:A:601:GLY:CA	8:A:2284:HOH:O	1.68	1.09
1:A:43:ILE:HG13	1:A:505:ARG:HB3	1.21	1.09
1:A:604:PRO:O	1:A:606:PRO:CD	2.01	1.09
1:E:591:GLU:OE1	1:E:604:PRO:CB	2.00	1.09
1:A:77:ARG:NH1	2:B:138:TYR:HE2	1.50	1.09
2:B:134:THR:O	2:B:134:THR:CG2	1.97	1.08
1:E:97:ARG:HG3	8:E:2194:HOH:O	1.52	1.08
1:A:288:GLU:HB3	1:A:591:GLU:HG3	1.37	1.07
1:E:605:LEU:N	1:E:605:LEU:CD2	1.92	1.07
1:A:632:ALA:O	1:A:635:GLN:HG2	1.56	1.06
1:A:467:VAL:HB	8:A:2230:HOH:O	1.55	1.06
1:E:602:HIS:CD2	1:E:604:PRO:HD2	1.89	1.06
1:A:97:ARG:NH2	1:A:763:ARG:HH22	1.52	1.06
2:F:57:GLN:HE22	2:F:140:ARG:NH2	1.52	1.06
1:E:602:HIS:NE2	1:E:604:PRO:HD2	1.72	1.05
1:E:591:GLU:CD	1:E:604:PRO:HB3	1.75	1.05
1:E:339:ASP:HB2	1:E:607:VAL:HG11	1.39	1.04
1:A:591:GLU:OE2	1:A:604:PRO:CG	2.05	1.04
1:E:592:LEU:CA	1:E:603:GLN:NE2	2.17	1.04
1:E:763:ARG:HG2	8:E:2442:HOH:O	1.56	1.04
1:A:186:GLY:HA3	1:A:583:PHE:O	1.58	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:TYR:CD1	8:B:2032:HOH:O	2.09	1.04
1:A:602:HIS:CE1	1:A:606:PRO:CG	2.41	1.03
1:E:95:LEU:HD12	1:E:466:ASP:O	1.57	1.03
1:E:626:SER:HB2	8:E:2349:HOH:O	1.56	1.03
2:B:41:ARG:HD2	2:B:187:THR:HG21	1.38	1.02
1:E:511:PRO:HB3	1:E:515:THR:HG22	1.41	1.02
1:A:279:VAL:HG13	1:A:283:THR:HG21	1.38	1.02
3:C:22:PHE:O	3:C:239:ARG:NH1	1.91	1.02
1:A:395:ASP:CA	1:A:399:GLU:HG3	1.87	1.02
1:A:592:LEU:O	1:A:593:TYR:HB2	1.56	1.02
1:A:165:ALA:O	1:A:415:THR:HG21	1.57	1.02
1:E:429:PRO:HD2	8:E:2259:HOH:O	1.57	1.02
1:E:413:ARG:HD3	8:E:2251:HOH:O	1.59	1.01
1:A:685:THR:HB	2:B:42:GLU:OE2	1.60	1.01
3:G:207:PHE:HE2	3:G:211:LEU:HD13	1.11	1.01
3:C:17:THR:CG2	3:C:67:GLU:HG3	1.90	1.01
1:E:602:HIS:HE1	1:E:606:PRO:CG	1.73	1.01
2:B:41:ARG:HD2	2:B:187:THR:CG2	1.89	1.01
3:G:38:HIS:HD2	3:G:45:ALA:HB1	1.24	1.00
1:E:592:LEU:HD23	1:E:603:GLN:HE22	1.24	1.00
1:E:116:THR:CG2	1:E:119:GLU:H	1.75	1.00
1:E:47:CYS:HB2	8:E:2451:HOH:O	1.60	1.00
1:A:569:LYS:O	8:A:2272:HOH:O	1.79	1.00
1:A:172:LEU:HD13	1:A:445:SER:O	1.61	1.00
1:E:598:LYS:HD2	8:E:2332:HOH:O	1.61	1.00
1:E:602:HIS:HE1	1:E:606:PRO:HG3	0.84	1.00
1:A:395:ASP:HA	1:A:399:GLU:HG3	1.00	1.00
1:E:224:LEU:HD12	8:E:2134:HOH:O	1.61	0.99
1:E:230:ALA:O	8:E:2140:HOH:O	1.77	0.99
1:E:323:LYS:HD3	1:E:354:LEU:HA	1.02	0.99
1:A:603:GLN:HB3	1:A:604:PRO:HD3	1.39	0.98
2:F:57:GLN:NE2	2:F:140:ARG:NH2	2.11	0.98
1:E:608:PHE:O	8:E:2337:HOH:O	1.80	0.98
2:B:41:ARG:HH11	2:B:187:THR:HG22	1.25	0.98
1:A:763:ARG:HG2	8:A:2379:HOH:O	1.62	0.98
1:A:632:ALA:O	1:A:635:GLN:CG	2.11	0.97
1:E:653:LYS:HD2	1:E:686:ALA:HB2	1.44	0.97
3:C:130:TYR:OH	7:C:1252:PCI:O1	1.80	0.97
1:E:342:TYR:CD1	1:E:607:VAL:HB	1.98	0.97
1:A:42:GLN:O	1:A:53:ILE:CG1	2.11	0.97
1:A:583:PHE:HE2	1:A:588:GLY:N	1.58	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:TYR:CE2	8:B:2031:HOH:O	2.17	0.97
1:A:170:VAL:O	1:A:175:ALA:HB2	1.62	0.97
2:B:192:VAL:HG21	8:B:2020:HOH:O	1.66	0.96
3:C:171:TRP:CD2	3:C:171:TRP:O	2.19	0.96
3:G:221:TRP:HE3	3:G:225:LEU:HD22	1.27	0.96
1:A:651:ILE:HD11	1:A:682:VAL:HG13	1.45	0.96
3:C:155:THR:HG22	3:C:239:ARG:HE	1.30	0.95
1:A:186:GLY:CA	1:A:583:PHE:C	2.34	0.95
2:B:160:GLU:H	2:B:179:ASN:HD21	1.14	0.95
1:E:764:ARG:N	8:E:2446:HOH:O	1.99	0.95
1:A:585:THR:O	1:A:586:ALA:HB3	1.67	0.94
3:G:111:SER:HB3	8:G:2034:HOH:O	1.65	0.94
1:A:116:THR:HG22	1:A:119:GLU:H	1.25	0.94
1:E:590:ILE:HG13	8:E:2182:HOH:O	1.67	0.94
3:G:206:GLY:O	3:G:209:TYR:N	2.00	0.94
2:F:41:ARG:HD2	2:F:187:THR:CG2	1.98	0.94
1:A:360:PRO:HD3	1:A:571:TRP:CE3	2.02	0.94
1:E:428:GLU:O	1:E:430:TYR:N	2.01	0.93
1:E:112:TYR:OH	1:E:474:MET:O	1.86	0.93
1:A:97:ARG:HH21	1:A:763:ARG:HH22	0.98	0.93
1:A:531:LEU:O	1:A:534:TYR:O	1.86	0.93
2:F:46:TYR:HB3	8:F:2035:HOH:O	1.67	0.93
1:E:349:TYR:OH	1:E:591:GLU:HA	1.69	0.92
1:A:599:GLU:O	8:A:2283:HOH:O	1.87	0.92
1:A:580:ARG:HH11	1:A:580:ARG:CB	1.83	0.92
2:F:41:ARG:HD2	2:F:187:THR:HG23	1.48	0.92
1:E:551:LEU:O	1:E:553:LEU:N	2.01	0.92
1:A:591:GLU:HB3	1:A:603:GLN:NE2	1.83	0.92
1:A:680:VAL:HG11	8:A:2313:HOH:O	1.69	0.92
2:B:46:TYR:CB	8:B:2032:HOH:O	2.00	0.92
1:E:533:GLN:HE21	1:E:533:GLN:H	1.16	0.92
1:A:434:GLY:HA2	1:A:461:LEU:O	1.70	0.91
1:E:397:GLU:HB3	1:E:398:PRO:HD3	1.52	0.91
1:A:335:VAL:CG1	1:A:732:ALA:O	2.19	0.91
1:A:608:PHE:CD1	1:A:608:PHE:O	2.23	0.91
1:A:729:SER:O	1:A:731:GLY:N	2.04	0.91
1:A:349:TYR:OH	1:A:591:GLU:O	1.89	0.91
2:B:72:THR:HG22	2:B:74:ALA:H	1.33	0.91
3:C:207:GLY:O	3:C:210:TYR:N	2.03	0.91
1:A:591:GLU:CD	1:A:604:PRO:HG3	1.91	0.90
1:A:763:ARG:HB2	8:A:2381:HOH:O	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:604:PRO:O	1:E:606:PRO:HD3	1.71	0.90
1:E:92:PRO:O	1:E:94:ARG:N	2.04	0.90
3:G:221:TRP:CE3	3:G:225:LEU:HD22	2.07	0.90
1:A:116:THR:CG2	1:A:119:GLU:H	1.83	0.90
1:A:186:GLY:HA3	1:A:584:GLY:N	1.87	0.90
1:E:116:THR:HG23	1:E:119:GLU:H	1.36	0.90
2:F:41:ARG:HH11	2:F:187:THR:CG2	1.85	0.90
1:E:297:THR:HG22	1:E:300:TRP:H	1.37	0.90
3:G:38:HIS:CD2	3:G:45:ALA:HB1	2.06	0.89
1:A:397:GLU:HB3	1:A:398:PRO:CD	2.03	0.89
1:E:635:GLN:O	1:E:641:MET:CG	2.20	0.89
1:E:635:GLN:O	1:E:641:MET:HG3	1.73	0.89
1:E:569:LYS:HD2	8:E:2322:HOH:O	1.70	0.89
1:E:95:LEU:CD1	1:E:466:ASP:O	2.20	0.88
2:B:146:GLU:HG2	8:B:2110:HOH:O	1.73	0.88
1:A:314:GLU:O	1:A:318:GLU:HG3	1.72	0.88
3:G:154:THR:HG22	3:G:238:ARG:HE	1.36	0.88
2:F:160:GLU:H	2:F:179:ASN:HD21	1.19	0.88
1:A:607:VAL:HG12	1:A:607:VAL:O	1.73	0.88
3:C:17:THR:HG21	3:C:67:GLU:HG3	1.55	0.88
1:E:209:HIS:HE1	1:E:625:ARG:H	1.21	0.88
1:A:397:GLU:CB	1:A:398:PRO:HD3	2.04	0.88
1:A:184:VAL:HG23	1:A:592:LEU:HD23	0.89	0.87
1:E:606:PRO:O	1:E:608:PHE:N	2.06	0.87
3:C:140:ASN:HD22	3:C:140:ASN:H	1.22	0.87
1:E:493:VAL:HG13	8:E:2014:HOH:O	1.74	0.87
1:A:276:LYS:HA	8:A:2152:HOH:O	1.74	0.87
2:B:16:CYS:O	2:B:16:CYS:SG	2.32	0.87
1:A:629:HIS:ND1	1:A:634:THR:HG23	1.88	0.87
2:F:2:PRO:HD2	2:F:80:ASP:OD2	1.75	0.87
3:C:128:LEU:HB3	8:C:2063:HOH:O	1.73	0.87
2:B:159:ALA:O	2:F:183:LYS:HE2	1.74	0.86
1:E:324:PRO:HD3	8:E:2170:HOH:O	1.73	0.86
3:C:108:LEU:O	3:C:110:LYS:HG2	1.74	0.86
2:B:41:ARG:NH1	2:B:187:THR:CG2	2.38	0.86
3:C:172:ALA:HA	3:C:175:PRO:HG2	1.56	0.86
2:F:65:PRO:HD2	4:F:1196:SF4:S4	2.15	0.86
1:E:605:LEU:N	1:E:605:LEU:HD22	1.90	0.86
3:C:168:LYS:HE2	8:C:2065:HOH:O	1.74	0.86
1:A:42:GLN:NE2	1:A:505:ARG:HD3	1.90	0.85
3:G:139:ASN:HD22	3:G:139:ASN:H	1.24	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:VAL:HG23	1:A:587:SER:HB3	1.58	0.85
1:A:335:VAL:O	1:A:733:GLY:HA2	1.75	0.85
1:E:614:PRO:HG2	8:E:2343:HOH:O	1.75	0.85
3:G:206:GLY:O	3:G:210:GLY:N	2.08	0.85
1:A:335:VAL:HG11	1:A:732:ALA:O	1.74	0.85
1:E:590:ILE:CG1	8:E:2182:HOH:O	2.23	0.85
1:E:323:LYS:CD	1:E:354:LEU:HA	1.98	0.85
1:E:301:ALA:O	1:E:305:THR:HB	1.77	0.85
1:A:604:PRO:C	1:A:606:PRO:CD	2.46	0.85
1:E:608:PHE:CD1	1:E:608:PHE:O	2.30	0.84
2:B:25:MET:CE	2:B:25:MET:HA	2.07	0.84
2:F:47:PRO:HD2	8:F:2035:HOH:O	1.75	0.84
1:A:519:TRP:CE2	1:A:540:ILE:HG12	2.12	0.84
1:A:400:GLY:HA3	8:A:2196:HOH:O	1.77	0.84
1:A:97:ARG:NH2	1:A:763:ARG:NH2	2.16	0.84
1:A:601:GLY:N	8:A:2284:HOH:O	1.94	0.84
1:A:653:LYS:HG3	1:A:684:PRO:O	1.78	0.84
3:G:196:GLU:HG2	8:G:2056:HOH:O	1.76	0.84
1:E:116:THR:CG2	1:E:119:GLU:HB3	2.08	0.84
2:B:117:THR:HG21	8:B:2095:HOH:O	1.78	0.84
1:A:42:GLN:NE2	1:A:485:TYR:O	2.11	0.83
1:E:498:LYS:HE2	8:E:2297:HOH:O	1.78	0.83
1:A:184:VAL:CG2	1:A:592:LEU:CD2	2.50	0.83
2:B:46:TYR:HD1	8:B:2032:HOH:O	1.50	0.83
1:A:207:GLY:O	5:A:1766:MGD:O5'	1.96	0.83
1:E:305:THR:HG22	1:E:307:ILE:H	1.43	0.83
1:E:388:CYS:SG	1:E:413:ARG:NE	2.51	0.83
2:F:57:GLN:HE22	2:F:140:ARG:HH22	1.11	0.83
2:F:146:GLU:HG2	8:F:2004:HOH:O	1.77	0.83
1:E:510:GLU:HG3	8:E:2301:HOH:O	1.77	0.83
1:A:602:HIS:ND1	1:A:606:PRO:HG3	1.93	0.83
1:E:562:GLY:C	8:E:2316:HOH:O	2.06	0.83
1:A:256:THR:HG21	1:A:305:THR:HA	1.61	0.83
1:A:607:VAL:HG13	1:A:609:THR:OG1	1.79	0.82
2:F:72:THR:HG22	2:F:74:ALA:H	1.44	0.82
3:C:53:ALA:O	3:C:57:ILE:HG13	1.78	0.82
1:A:591:GLU:HB3	1:A:603:GLN:HE22	1.43	0.82
1:A:183:TRP:CH2	1:A:596:ARG:HD3	2.13	0.82
1:E:116:THR:HG22	1:E:119:GLU:CB	2.09	0.82
1:A:93:ASP:OD1	1:A:758:ARG:NH2	2.11	0.82
1:A:186:GLY:CA	1:A:583:PHE:O	2.28	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:TYR:HE2	8:B:2031:HOH:O	1.57	0.82
1:E:428:GLU:O	1:E:429:PRO:C	2.13	0.82
1:E:494:LEU:HD22	1:E:502:ILE:HG12	1.62	0.81
1:E:305:THR:CG2	1:E:307:ILE:H	1.93	0.81
1:A:591:GLU:O	1:A:592:LEU:HD12	1.80	0.81
1:E:283:THR:HG22	8:E:2181:HOH:O	1.78	0.81
1:A:183:TRP:HH2	1:A:596:ARG:HD3	1.46	0.81
1:E:81:ARG:HG2	1:E:628:VAL:O	1.80	0.81
1:A:429:PRO:O	1:A:430:TYR:CD2	2.33	0.81
1:A:77:ARG:NH1	2:B:138:TYR:CE2	2.35	0.81
1:A:740:ARG:NH1	8:A:2361:HOH:O	2.12	0.81
1:E:648:GLU:HG2	1:E:681:ARG:HH12	1.44	0.80
1:E:629:HIS:ND1	1:E:634:THR:HG23	1.97	0.80
1:A:629:HIS:HA	1:A:634:THR:HG21	1.63	0.80
1:A:604:PRO:C	1:A:606:PRO:HD3	2.01	0.80
1:A:48:PHE:CE1	1:A:145:HIS:CE1	2.70	0.80
1:A:580:ARG:HH11	1:A:580:ARG:HB3	1.44	0.80
1:E:109:GLU:HG3	8:E:2066:HOH:O	1.80	0.80
3:C:140:ASN:ND2	3:C:140:ASN:H	1.80	0.80
1:E:89:THR:OG1	1:E:484:THR:HG21	1.82	0.80
1:E:608:PHE:CD1	1:E:608:PHE:C	2.55	0.80
1:A:413:ARG:CD	1:A:413:ARG:H	1.95	0.80
1:E:308:PRO:HB2	8:E:2198:HOH:O	1.82	0.80
1:A:602:HIS:HE1	1:A:606:PRO:HG3	1.03	0.80
1:A:686:ALA:HB3	8:A:2332:HOH:O	1.81	0.80
1:A:116:THR:HG22	1:A:119:GLU:HB3	1.62	0.80
1:E:256:THR:HG21	1:E:305:THR:HA	1.62	0.79
3:C:64:LEU:HD22	7:C:1252:PCI:C4	2.12	0.79
2:B:41:ARG:NH1	2:B:187:THR:HG22	1.97	0.79
3:C:155:THR:CG2	3:C:239:ARG:HE	1.95	0.79
1:E:488:ARG:HD3	1:E:490:ASP:OD2	1.82	0.79
8:B:2146:HOH:O	3:C:251:LEU:HD11	1.81	0.79
1:E:95:LEU:HD21	8:E:2278:HOH:O	1.82	0.79
1:E:342:TYR:HD1	1:E:607:VAL:HB	1.42	0.79
3:C:155:THR:HG21	3:C:239:ARG:HG2	1.65	0.79
1:A:70:ALA:O	8:A:2037:HOH:O	1.98	0.79
1:A:585:THR:O	1:A:586:ALA:CB	2.30	0.79
1:A:390:GLY:H	1:A:595:GLN:HE22	1.31	0.79
1:A:75:ARG:HD2	1:A:220:GLN:HE22	1.45	0.78
1:A:583:PHE:HE2	1:A:588:GLY:H	1.25	0.78
1:E:469:PRO:O	1:E:706:MET:HG3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:LEU:H	1:A:605:LEU:CD2	1.97	0.78
1:A:279:VAL:HG13	1:A:283:THR:CG2	2.10	0.78
3:C:207:GLY:O	3:C:209:TRP:N	2.16	0.78
1:A:183:TRP:HE1	1:A:413:ARG:HH22	1.32	0.78
1:A:605:LEU:HD23	1:A:605:LEU:H	1.48	0.78
3:G:111:SER:O	3:G:115:LEU:HD12	1.84	0.77
1:E:438:TYR:HD2	8:E:2094:HOH:O	1.66	0.77
1:A:138:GLU:OE2	1:A:402:LYS:HB2	1.84	0.77
1:A:633:ARG:HD2	5:A:1765:MGD:O2B	1.83	0.77
1:A:651:ILE:HD11	1:A:682:VAL:CG1	2.14	0.77
2:B:57:GLN:HE22	2:B:140:ARG:HH22	1.29	0.77
1:E:539:THR:HG23	1:E:542:GLU:H	1.49	0.77
2:B:160:GLU:H	2:B:179:ASN:ND2	1.81	0.77
1:E:109:GLU:CG	8:E:2066:HOH:O	2.31	0.77
1:E:277:GLU:O	1:E:281:LYS:HG2	1.84	0.77
2:F:1:MET:HA	8:F:2001:HOH:O	1.85	0.77
1:E:685:THR:HG22	2:F:42:GLU:CD	2.04	0.77
1:A:320:ALA:O	1:A:323:LYS:HG2	1.85	0.77
1:E:311:VAL:HB	8:E:2198:HOH:O	1.84	0.77
3:C:173:LEU:HG	3:C:173:LEU:O	1.84	0.77
1:E:592:LEU:CD2	1:E:603:GLN:HE22	1.98	0.76
1:A:153:VAL:HG11	1:A:167:LYS:HE2	1.67	0.76
1:E:453:LYS:HG2	1:E:475:TRP:CH2	2.20	0.76
1:A:42:GLN:HE22	1:A:505:ARG:HD3	1.49	0.76
1:A:393:GLY:HA3	1:A:407:LYS:HE3	1.66	0.76
1:E:95:LEU:HD11	8:E:2278:HOH:O	1.84	0.76
2:B:41:ARG:HH11	2:B:187:THR:HG23	1.49	0.76
1:A:75:ARG:HH11	1:A:220:GLN:NE2	1.83	0.76
1:E:604:PRO:O	1:E:606:PRO:CD	2.33	0.76
3:C:155:THR:HG21	3:C:239:ARG:CG	2.16	0.76
1:A:677:GLU:O	1:A:678:GLY:O	2.03	0.76
1:E:297:THR:HG23	1:E:299:GLU:H	1.49	0.76
1:A:393:GLY:HA3	1:A:407:LYS:CE	2.16	0.76
1:A:457:LYS:HA	8:A:2224:HOH:O	1.85	0.76
1:A:672:GLN:NE2	1:A:738:PHE:H	1.84	0.76
1:E:592:LEU:HD23	1:E:603:GLN:NE2	2.00	0.75
1:A:209:HIS:HE1	1:A:625:ARG:H	1.34	0.75
3:C:235:ALA:O	3:C:239:ARG:HG3	1.86	0.75
1:E:421:ILE:O	1:E:421:ILE:HG23	1.84	0.75
3:G:234:ALA:O	3:G:238:ARG:HG3	1.84	0.75
1:A:231:LYS:HA	1:A:247:HIS:CD2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:CYS:HA	1:A:593:TYR:OH	1.85	0.75
1:E:397:GLU:HB3	1:E:398:PRO:CD	2.16	0.75
3:G:21:PHE:O	3:G:238:ARG:NH1	2.20	0.75
1:E:75:ARG:HH11	1:E:220:GLN:HE21	1.34	0.75
1:E:421:ILE:O	1:E:421:ILE:CG2	2.34	0.75
1:A:395:ASP:O	1:A:399:GLU:CB	2.28	0.75
3:C:64:LEU:HD22	7:C:1252:PCI:C3	2.16	0.75
1:E:239:PHE:HB3	1:E:687:ARG:HB3	1.68	0.75
1:A:647:ASN:C	1:A:648:GLU:HG3	2.07	0.75
1:A:342:TYR:CD1	1:A:607:VAL:HB	2.22	0.74
2:F:117:THR:HG23	2:F:120:ALA:H	1.52	0.74
1:E:473:VAL:HG11	8:E:2278:HOH:O	1.87	0.74
2:F:67:VAL:HB	2:F:68:PRO:HD3	1.67	0.74
1:A:232:VAL:H	1:A:247:HIS:HD2	1.32	0.74
1:E:339:ASP:CB	1:E:607:VAL:HG11	2.18	0.74
1:A:170:VAL:O	1:A:175:ALA:CB	2.36	0.74
1:E:431:PRO:HD2	8:E:2262:HOH:O	1.88	0.74
1:E:69:GLU:O	1:E:70:ALA:HB3	1.88	0.74
1:A:721:THR:HG22	1:A:722:ARG:HG3	1.69	0.74
3:G:222:GLN:OE1	3:G:222:GLN:HA	1.88	0.74
1:E:75:ARG:HH11	1:E:220:GLN:NE2	1.84	0.74
3:C:241:LEU:C	3:C:241:LEU:HD12	2.08	0.74
1:E:297:THR:CG2	1:E:299:GLU:H	2.00	0.73
2:B:16:CYS:O	2:B:18:ALA:N	2.19	0.73
3:G:206:GLY:O	3:G:207:PHE:C	2.26	0.73
1:E:717:ASN:HD22	5:E:1765:MGD:H192	1.36	0.73
2:F:41:ARG:HH11	2:F:187:THR:HG23	1.52	0.73
1:E:397:GLU:CB	1:E:398:PRO:HD3	2.18	0.73
3:G:107:LEU:O	3:G:109:LYS:N	2.20	0.73
1:E:38:LYS:HG3	8:E:2021:HOH:O	1.88	0.73
1:A:377:PRO:HG2	1:A:533:GLN:HG3	1.71	0.73
1:A:285:GLY:O	1:A:590:ILE:HG23	1.88	0.73
1:A:428:GLU:HB3	1:A:429:PRO:CD	2.15	0.73
1:E:113:ARG:NH1	1:E:114:VAL:HG13	2.02	0.73
1:E:605:LEU:HD23	1:E:605:LEU:H	0.57	0.73
1:E:511:PRO:HB3	1:E:515:THR:CG2	2.18	0.73
2:F:72:THR:HG23	2:F:89:LYS:HB3	1.71	0.73
1:E:100:ILE:HG12	1:E:478:VAL:HG22	1.69	0.73
1:A:390:GLY:N	1:A:595:GLN:HE22	1.87	0.73
3:G:139:ASN:ND2	3:G:139:ASN:H	1.87	0.73
1:A:427:GLY:O	1:A:428:GLU:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ILE:HD13	1:A:656:ALA:HB2	1.68	0.72
1:A:629:HIS:CA	1:A:634:THR:HG21	2.19	0.72
2:B:25:MET:HE2	2:B:25:MET:HA	1.71	0.72
3:G:63:LEU:HD13	7:G:1251:PCI:CL5	2.26	0.72
1:A:595:GLN:CG	1:A:595:GLN:O	2.37	0.72
3:C:171:TRP:O	3:C:172:ALA:HB2	1.89	0.72
1:A:519:TRP:NE1	1:A:540:ILE:HG12	2.03	0.72
1:E:88:THR:HG23	1:E:468:LEU:HD21	1.70	0.72
1:E:539:THR:HG22	1:E:542:GLU:CB	2.20	0.72
1:A:510:GLU:HG3	8:A:2024:HOH:O	1.90	0.72
1:A:625:ARG:HH22	5:A:1765:MGD:H15	1.38	0.72
1:E:100:ILE:HG23	1:E:478:VAL:HG22	1.70	0.72
3:G:206:GLY:HA2	3:G:209:TYR:HB3	1.70	0.72
1:A:595:GLN:HG3	1:A:595:GLN:O	1.89	0.72
2:B:190:SER:HB3	3:C:252:GLY:N	2.03	0.72
1:A:467:VAL:HG13	8:A:2050:HOH:O	1.90	0.72
1:E:91:ASP:O	1:E:92:PRO:O	2.08	0.72
1:E:635:GLN:H	1:E:635:GLN:NE2	1.88	0.72
1:A:393:GLY:HA3	1:A:407:LYS:NZ	2.04	0.72
1:A:346:ALA:HB2	1:A:605:LEU:CD1	2.19	0.71
3:G:76:ILE:O	3:G:80:LEU:HG	1.90	0.71
1:A:184:VAL:HG22	1:A:592:LEU:HD23	1.71	0.71
1:E:116:THR:HG21	8:E:2072:HOH:O	1.90	0.71
1:A:653:LYS:HD2	1:A:686:ALA:H	1.53	0.71
1:A:422:GLU:HB3	1:A:423:PRO:HD3	1.72	0.71
1:E:297:THR:CG2	1:E:299:GLU:HG2	2.21	0.71
3:C:108:LEU:O	3:C:110:LYS:CG	2.39	0.71
1:A:209:HIS:O	1:A:213:ASP:HB3	1.89	0.71
3:C:101:LEU:O	3:C:105:LEU:HD12	1.90	0.71
1:A:428:GLU:O	1:A:429:PRO:C	2.26	0.71
1:A:301:ALA:O	1:A:305:THR:HB	1.91	0.71
2:F:40:GLU:HB2	8:F:2021:HOH:O	1.91	0.71
1:A:605:LEU:HD23	1:A:605:LEU:N	2.06	0.71
3:C:21:HIS:HE1	3:C:64:LEU:HD11	1.56	0.71
1:E:232:VAL:H	1:E:247:HIS:CD2	2.09	0.71
1:E:478:VAL:HG23	8:E:2283:HOH:O	1.90	0.70
2:B:41:ARG:HD2	2:B:187:THR:HG23	1.73	0.70
1:E:209:HIS:HE1	1:E:625:ARG:N	1.89	0.70
1:E:183:TRP:HH2	1:E:596:ARG:HD3	1.55	0.70
1:A:284:VAL:O	1:A:590:ILE:CG2	2.35	0.70
2:B:47:PRO:O	2:B:48:ASN:OD1	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:HIS:ND1	3:C:64:LEU:HG	2.05	0.70
1:E:648:GLU:HG2	1:E:681:ARG:NH1	2.06	0.70
1:E:232:VAL:H	1:E:247:HIS:HD2	1.40	0.70
3:C:197:GLU:HG2	8:C:2074:HOH:O	1.89	0.70
1:A:166:ALA:HB2	1:A:415:THR:HG23	1.72	0.70
1:A:729:SER:OG	1:A:729:SER:O	2.01	0.70
1:A:382:GLU:HA	8:A:2188:HOH:O	1.90	0.70
1:E:673:ASP:OD2	1:E:721:THR:CG2	2.40	0.70
1:E:465:ILE:O	1:E:466:ASP:HB3	1.90	0.70
2:F:55:PRO:HG2	4:F:1194:SF4:S2	2.30	0.70
8:A:2015:HOH:O	2:B:25:MET:HE1	1.91	0.70
1:E:671:ASN:C	1:E:671:ASN:HD22	1.95	0.70
1:A:611:PRO:HB3	8:A:2139:HOH:O	1.90	0.70
1:A:592:LEU:O	1:A:593:TYR:CB	2.37	0.70
1:E:762:GLU:HB2	8:E:2445:HOH:O	1.90	0.70
2:B:47:PRO:HD3	8:B:2034:HOH:O	1.92	0.69
1:A:367:GLN:HG3	8:A:2271:HOH:O	1.92	0.69
1:A:561:MET:O	1:A:563:THR:N	2.24	0.69
1:A:89:THR:OG1	1:A:484:THR:HG21	1.92	0.69
2:F:57:GLN:HE21	2:F:140:ARG:HH22	1.40	0.69
1:E:69:GLU:O	1:E:70:ALA:CB	2.40	0.69
1:E:139:ALA:O	1:E:433:LYS:O	2.10	0.69
2:F:169:GLN:NE2	8:F:2107:HOH:O	2.25	0.69
1:E:591:GLU:OE2	1:E:604:PRO:HG3	1.92	0.69
1:A:632:ALA:O	1:A:635:GLN:HG3	1.92	0.69
1:A:152:PHE:O	1:A:157:PRO:HD3	1.91	0.69
1:E:259:ALA:HB3	8:E:2196:HOH:O	1.92	0.69
1:E:734:LEU:HD22	8:E:2419:HOH:O	1.91	0.69
1:E:577:LYS:HE2	8:E:2323:HOH:O	1.92	0.69
1:E:118:GLU:HG3	8:E:2307:HOH:O	1.93	0.69
1:E:746:ARG:HG3	1:E:746:ARG:HH11	1.58	0.69
1:A:342:TYR:HD1	1:A:607:VAL:HB	1.56	0.69
3:G:63:LEU:HD22	7:G:1251:PCI:C6	2.23	0.69
2:F:3:ARG:HG2	8:F:2003:HOH:O	1.92	0.69
1:A:186:GLY:H	1:A:583:PHE:HA	1.58	0.69
1:E:183:TRP:CH2	1:E:596:ARG:HD3	2.28	0.69
1:A:604:PRO:C	1:A:606:PRO:HD2	2.10	0.69
1:E:589:LYS:HG2	1:E:592:LEU:HD12	1.75	0.69
1:E:438:TYR:CD2	8:E:2094:HOH:O	2.44	0.69
1:A:673:ASP:OD2	1:A:721:THR:HG21	1.92	0.69
3:G:12:PHE:CZ	3:G:246:GLN:HG2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:591:GLU:HG3	1:E:591:GLU:O	1.92	0.69
1:A:395:ASP:C	1:A:399:GLU:HB2	2.13	0.69
1:E:97:ARG:NH2	1:E:763:ARG:HD2	2.07	0.69
1:A:79:CYS:HB2	1:A:80:PRO:HD2	1.75	0.69
2:F:117:THR:HG21	8:F:2077:HOH:O	1.91	0.69
2:F:3:ARG:HD2	2:F:62:GLU:OE2	1.92	0.69
1:A:36:GLU:O	1:A:58:VAL:HG22	1.93	0.69
3:G:51:TYR:N	8:G:2015:HOH:O	2.26	0.68
1:A:396:HIS:HB3	1:A:403:PRO:HB3	1.74	0.68
2:B:46:TYR:CE2	8:B:2033:HOH:O	2.46	0.68
1:A:483:ALA:HA	1:A:515:THR:CG2	2.23	0.68
1:A:642:GLU:HG2	2:B:34:PHE:HZ	1.59	0.68
1:A:286:PHE:HA	1:A:590:ILE:HG21	1.75	0.68
1:E:602:HIS:CD2	1:E:604:PRO:CD	2.71	0.68
1:A:116:THR:HG22	1:A:119:GLU:N	2.06	0.68
1:A:174:THR:HG23	1:A:178:GLU:HG2	1.76	0.68
1:E:71:ASN:HD22	1:E:74:SER:H	1.40	0.68
1:A:429:PRO:O	1:A:430:TYR:CG	2.46	0.68
3:G:115:LEU:HD13	8:G:2032:HOH:O	1.93	0.68
3:C:21:HIS:CE1	3:C:64:LEU:HD21	2.29	0.68
2:B:6:MET:HE3	8:B:2045:HOH:O	1.94	0.68
1:E:651:ILE:HD11	1:E:682:VAL:CG1	2.24	0.68
1:A:606:PRO:O	1:A:608:PHE:N	2.26	0.68
1:E:339:ASP:HB2	1:E:607:VAL:CG1	2.22	0.68
1:E:708:LEU:HA	8:E:2408:HOH:O	1.93	0.68
1:A:232:VAL:H	1:A:247:HIS:CD2	2.11	0.68
1:E:424:MET:HG2	1:E:459:LEU:HD21	1.76	0.68
1:E:153:VAL:HG11	1:E:167:LYS:HE2	1.76	0.68
3:G:206:GLY:HA2	3:G:209:TYR:CB	2.24	0.68
1:E:673:ASP:OD2	1:E:721:THR:HG21	1.93	0.68
3:C:145:ASN:HD22	3:C:145:ASN:C	1.95	0.68
1:A:349:TYR:CE2	1:A:590:ILE:O	2.47	0.68
1:E:100:ILE:HG23	1:E:478:VAL:CG2	2.23	0.67
1:A:73:LYS:NZ	1:A:192:HIS:HD2	1.91	0.67
1:E:589:LYS:HB3	1:E:592:LEU:HB2	1.75	0.67
1:E:305:THR:HG23	1:E:307:ILE:HG12	1.76	0.67
1:E:434:GLY:HA2	1:E:461:LEU:O	1.93	0.67
3:G:129:TYR:CD2	3:G:130:PRO:HD3	2.29	0.67
2:B:72:THR:HG21	2:B:89:LYS:O	1.94	0.67
1:A:602:HIS:ND1	1:A:606:PRO:CG	2.54	0.67
2:F:72:THR:HG21	2:F:89:LYS:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:GLU:HB3	1:A:580:ARG:HD3	1.76	0.67
3:G:225:LEU:HB3	8:G:2068:HOH:O	1.93	0.67
2:F:47:PRO:CD	8:F:2035:HOH:O	2.37	0.67
2:F:160:GLU:H	2:F:179:ASN:ND2	1.93	0.67
1:E:346:ALA:N	1:E:605:LEU:HD12	2.10	0.67
1:A:488:ARG:NH2	5:A:1765:MGD:O6	2.28	0.67
1:A:305:THR:HG22	1:A:307:ILE:H	1.60	0.67
2:F:43:VAL:HG23	8:F:2121:HOH:O	1.95	0.67
1:E:465:ILE:O	1:E:466:ASP:CB	2.43	0.66
1:A:400:GLY:CA	8:A:2196:HOH:O	2.37	0.66
1:E:575:TRP:O	1:E:578:GLU:HB2	1.94	0.66
1:A:293:VAL:O	1:A:293:VAL:HG13	1.94	0.66
1:E:253:LYS:O	1:E:256:THR:HB	1.94	0.66
1:A:338:GLY:O	1:A:726:ASP:HA	1.95	0.66
2:B:17:ALA:HB1	2:B:20:ALA:HB3	1.77	0.66
1:A:413:ARG:HD2	1:A:413:ARG:H	1.59	0.66
1:A:608:PHE:C	1:A:608:PHE:CD1	2.64	0.66
1:A:75:ARG:HH11	1:A:220:GLN:HE21	1.43	0.66
1:A:330:PRO:HD2	8:A:2168:HOH:O	1.94	0.66
1:A:336:TRP:HD1	1:A:336:TRP:H	1.43	0.66
1:A:183:TRP:CB	1:A:592:LEU:HD22	2.25	0.66
1:E:589:LYS:NZ	8:E:2326:HOH:O	2.27	0.66
2:B:46:TYR:O	8:B:2029:HOH:O	2.14	0.66
1:E:75:ARG:HD2	1:E:220:GLN:HE22	1.61	0.66
3:G:207:PHE:HE2	3:G:211:LEU:CD1	2.00	0.66
1:E:311:VAL:CB	8:E:2198:HOH:O	2.42	0.66
1:E:488:ARG:HB2	1:E:517:PRO:HB3	1.76	0.66
1:E:642:GLU:OE2	2:F:32:GLY:N	2.24	0.66
1:A:195:ILE:HA	1:A:362:GLY:O	1.95	0.66
1:A:37:VAL:HG12	1:A:38:LYS:N	2.10	0.66
2:B:121:HIS:O	2:B:125:LYS:HE2	1.96	0.66
1:A:349:TYR:HE1	1:A:605:LEU:HD21	1.61	0.66
1:E:30:ALA:HB3	8:E:2002:HOH:O	1.94	0.66
1:A:484:THR:HG22	1:A:487:GLU:HG3	1.78	0.66
1:A:339:ASP:HB3	1:A:607:VAL:HG11	1.77	0.66
1:E:551:LEU:O	1:E:553:LEU:HB2	1.96	0.66
1:A:519:TRP:CE2	1:A:540:ILE:CG1	2.78	0.66
1:E:686:ALA:HB1	8:E:2386:HOH:O	1.95	0.66
1:A:305:THR:O	1:A:306:GLU:HB2	1.95	0.66
1:A:511:PRO:HB3	1:A:515:THR:HG22	1.76	0.66
1:E:97:ARG:HH21	1:E:763:ARG:NH1	1.92	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:470:GLN:HG2	1:E:706:MET:SD	2.36	0.65
1:A:642:GLU:OE2	2:B:31:PRO:O	2.14	0.65
1:A:71:ASN:HD22	1:A:74:SER:H	1.41	0.65
3:C:222:TRP:CG	3:C:223:GLN:N	2.59	0.65
1:A:134:LYS:HE2	8:A:2079:HOH:O	1.95	0.65
1:E:632:ALA:O	1:E:635:GLN:NE2	2.29	0.65
3:G:63:LEU:CD1	7:G:1251:PCI:CL5	2.81	0.65
1:E:639:VAL:HG11	2:F:25:MET:HE3	1.77	0.65
1:E:391:PRO:O	1:E:413:ARG:HG2	1.96	0.65
1:E:490:ASP:O	8:E:2290:HOH:O	2.14	0.65
1:E:720:GLN:HB3	8:E:2419:HOH:O	1.96	0.65
1:A:603:GLN:HB3	1:A:604:PRO:CD	2.23	0.65
1:E:589:LYS:HG2	1:E:592:LEU:CD1	2.27	0.65
1:A:95:LEU:HD11	1:A:468:LEU:O	1.95	0.65
2:F:78:THR:HG21	8:F:2059:HOH:O	1.96	0.65
1:E:174:THR:HG23	1:E:178:GLU:HG2	1.78	0.65
2:F:117:THR:HG22	2:F:119:CYS:H	1.60	0.65
2:B:44:GLY:O	2:B:49:LEU:HD13	1.97	0.65
1:A:139:ALA:O	1:A:433:LYS:O	2.14	0.65
1:A:672:GLN:HE22	1:A:738:PHE:H	1.42	0.65
2:B:78:THR:HG21	8:B:2068:HOH:O	1.97	0.65
2:F:88:LYS:O	3:G:74:THR:HG22	1.96	0.65
2:F:45:GLU:HB2	8:F:2028:HOH:O	1.96	0.64
1:A:238:ARG:HG3	1:A:688:ILE:HD12	1.78	0.64
2:B:25:MET:HA	2:B:25:MET:HE3	1.78	0.64
1:A:153:VAL:CG1	1:A:167:LYS:HE2	2.28	0.64
1:A:495:VAL:HG13	8:A:2020:HOH:O	1.96	0.64
1:E:622:LEU:HD22	5:E:1766:MGD:H8	1.78	0.64
1:A:755:LEU:O	1:A:758:ARG:HD3	1.97	0.64
3:G:63:LEU:HD22	7:G:1251:PCI:C5	2.27	0.64
3:G:150:LEU:O	3:G:154:THR:HB	1.98	0.64
1:A:152:PHE:O	1:A:157:PRO:CD	2.46	0.64
1:A:127:LYS:HE2	8:A:2228:HOH:O	1.98	0.64
1:A:580:ARG:CB	1:A:580:ARG:NH1	2.58	0.64
2:F:78:THR:HG22	2:F:80:ASP:H	1.61	0.64
1:A:387:GLY:O	1:A:593:TYR:CE1	2.51	0.64
1:A:166:ALA:HB2	1:A:415:THR:CG2	2.26	0.64
1:E:539:THR:CG2	1:E:542:GLU:H	2.10	0.64
1:E:585:THR:OG1	1:E:589:LYS:HE3	1.97	0.64
1:A:580:ARG:HH11	1:A:580:ARG:HB2	1.63	0.64
1:A:647:ASN:H	1:A:647:ASN:HD22	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:206:GLY:O	3:G:209:TYR:CA	2.45	0.64
2:B:134:THR:O	2:B:134:THR:HG22	1.92	0.64
2:B:44:GLY:O	2:B:49:LEU:CD1	2.45	0.64
1:A:183:TRP:HB2	1:A:592:LEU:HD22	1.80	0.64
1:A:604:PRO:O	1:A:606:PRO:HD3	1.92	0.64
1:E:588:GLY:HA3	8:E:2178:HOH:O	1.97	0.64
1:E:267:VAL:HG22	8:E:2200:HOH:O	1.97	0.64
1:A:391:PRO:O	1:A:413:ARG:HB3	1.98	0.63
1:A:95:LEU:HD12	1:A:467:VAL:C	2.18	0.63
1:A:231:LYS:HA	1:A:247:HIS:NE2	2.12	0.63
1:A:642:GLU:HG2	2:B:34:PHE:CZ	2.32	0.63
1:A:239:PHE:HB3	1:A:687:ARG:HB3	1.81	0.63
1:A:687:ARG:NH2	2:B:40:GLU:OE2	2.31	0.63
1:E:597:PHE:HB3	8:E:2327:HOH:O	1.97	0.63
1:E:284:VAL:HG12	1:E:592:LEU:CD1	2.28	0.63
8:E:2386:HOH:O	2:F:49:LEU:HD11	1.99	0.63
1:E:553:LEU:HD21	1:E:557:THR:HG21	1.81	0.63
1:A:581:LEU:HD11	8:A:2274:HOH:O	1.98	0.63
1:A:99:LEU:O	1:A:478:VAL:HA	1.99	0.63
3:C:47:ARG:NH1	3:C:107:TYR:O	2.31	0.63
2:B:117:THR:HG22	2:B:119:CYS:N	2.13	0.63
1:E:282:TYR:O	1:E:587:SER:HB3	1.98	0.63
2:B:47:PRO:CD	8:B:2034:HOH:O	2.46	0.63
1:A:581:LEU:CD1	8:A:2274:HOH:O	2.46	0.63
1:A:635:GLN:O	1:A:709:ALA:HB2	1.98	0.63
1:A:388:CYS:HA	1:A:593:TYR:CE1	2.33	0.63
1:E:318:GLU:O	1:E:322:HIS:HD2	1.82	0.63
1:A:349:TYR:CE1	1:A:605:LEU:HD21	2.34	0.62
1:E:633:ARG:HD2	5:E:1765:MGD:O2B	1.98	0.62
3:G:221:TRP:HZ3	3:G:225:LEU:HD13	1.63	0.62
2:F:193:HIS:HB2	8:F:2129:HOH:O	1.98	0.62
1:A:314:GLU:HG2	8:A:2165:HOH:O	1.98	0.62
1:E:670:VAL:HG22	1:E:676:LYS:HG3	1.80	0.62
1:A:335:VAL:HG13	1:A:732:ALA:O	1.97	0.62
1:E:708:LEU:O	1:E:712:ARG:HD2	2.00	0.62
1:A:293:VAL:CG1	1:A:293:VAL:O	2.46	0.62
1:A:539:THR:CG2	1:A:541:GLU:HG2	2.30	0.62
2:F:41:ARG:HD2	2:F:187:THR:HG21	1.78	0.62
1:E:310:GLN:NE2	1:E:314:GLU:OE2	2.32	0.62
1:E:477:ASP:C	1:E:478:VAL:HG23	2.13	0.62
1:E:511:PRO:CB	1:E:515:THR:HG22	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:672:GLN:NE2	1:E:738:PHE:H	1.97	0.62
2:B:117:THR:HB	8:B:2010:HOH:O	1.99	0.62
1:E:740:ARG:NH1	8:E:2428:HOH:O	2.32	0.62
1:A:428:GLU:O	1:A:430:TYR:N	2.33	0.62
2:F:41:ARG:HH11	2:F:187:THR:HG22	1.65	0.62
1:E:297:THR:HG23	1:E:299:GLU:HG2	1.82	0.62
1:E:418:GLN:H	1:E:418:GLN:NE2	1.97	0.62
1:A:346:ALA:HB2	1:A:605:LEU:HD13	1.80	0.62
3:G:105:LEU:HG	8:G:2032:HOH:O	1.98	0.61
2:B:192:VAL:HG12	2:B:193:HIS:N	2.15	0.61
1:E:297:THR:HG21	8:E:2087:HOH:O	2.00	0.61
1:E:608:PHE:C	8:E:2337:HOH:O	2.30	0.61
1:E:649:VAL:HG13	1:E:695:ILE:CG2	2.30	0.61
1:A:685:THR:HB	2:B:42:GLU:CD	2.20	0.61
1:E:569:LYS:CD	8:E:2322:HOH:O	2.38	0.61
1:E:495:VAL:CG2	8:E:2299:HOH:O	2.48	0.61
1:A:603:GLN:CB	1:A:604:PRO:HD3	2.24	0.61
3:G:105:LEU:HB3	8:G:2011:HOH:O	2.00	0.61
2:B:2:PRO:HB3	2:B:144:ASP:CG	2.20	0.61
1:A:413:ARG:NE	1:A:413:ARG:H	1.97	0.61
1:A:292:HIS:NE2	1:A:604:PRO:HB2	2.16	0.61
1:A:653:LYS:CG	1:A:684:PRO:O	2.48	0.61
1:E:669:LEU:CD2	1:E:741:LEU:HD22	2.30	0.61
1:A:428:GLU:CB	1:A:429:PRO:HD2	2.23	0.61
1:A:335:VAL:HG13	1:A:732:ALA:C	2.20	0.61
1:E:90:TYR:OH	1:E:509:HIS:HE1	1.83	0.61
1:A:360:PRO:HD3	1:A:571:TRP:CZ3	2.35	0.61
1:E:116:THR:HG22	1:E:119:GLU:H	1.56	0.61
3:C:241:LEU:C	3:C:241:LEU:CD1	2.68	0.61
1:E:539:THR:HG22	1:E:542:GLU:HB2	1.83	0.61
2:B:72:THR:HG23	2:B:89:LYS:HB3	1.83	0.61
1:A:121:LEU:HD13	1:A:524:GLU:HB3	1.83	0.61
1:E:606:PRO:CD	1:E:607:VAL:H	2.12	0.60
1:A:428:GLU:O	1:A:430:TYR:O	2.19	0.60
1:E:607:VAL:O	1:E:607:VAL:HG13	1.97	0.60
1:A:53:ILE:HD12	1:A:65:VAL:HG22	1.83	0.60
1:A:630:THR:H	1:A:634:THR:HG21	1.66	0.60
2:F:194:HIS:N	8:F:2128:HOH:O	2.33	0.60
1:A:594:CYS:O	1:A:598:LYS:HG3	2.01	0.60
1:E:647:ASN:HD21	1:E:714:ALA:H	1.48	0.60
3:C:171:TRP:O	3:C:172:ALA:CB	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:GLN:HG3	1:A:701:HIS:NE2	2.16	0.60
2:F:43:VAL:CG2	8:F:2121:HOH:O	2.50	0.60
1:E:479:ILE:O	1:E:480:LEU:HD23	2.02	0.60
3:C:130:TYR:CD2	3:C:131:PRO:HD3	2.36	0.60
2:B:27:ASN:HD21	2:B:121:HIS:CE1	2.20	0.60
1:E:108:GLY:HA3	8:E:2064:HOH:O	2.01	0.60
1:A:631:PHE:O	1:A:698:GLY:HA3	2.01	0.60
1:A:345:MET:HG2	1:A:592:LEU:HD21	1.84	0.60
3:G:38:HIS:CE1	8:G:2011:HOH:O	2.54	0.60
1:E:539:THR:HG22	1:E:542:GLU:HB3	1.83	0.60
1:A:109:GLU:OE2	1:A:111:LYS:HE2	2.01	0.60
1:A:345:MET:HE3	1:A:592:LEU:HD11	1.84	0.60
3:G:208:TRP:CE3	3:G:208:TRP:HA	2.37	0.60
1:A:120:ALA:HB3	8:A:2068:HOH:O	2.01	0.60
1:A:427:GLY:O	1:A:430:TYR:O	2.19	0.59
1:A:204:VAL:HB	1:A:328:LEU:HG	1.84	0.59
1:A:319:MET:CE	1:A:328:LEU:HD11	2.31	0.59
1:A:646:GLU:O	1:A:648:GLU:OE2	2.20	0.59
1:A:382:GLU:HB3	8:A:2189:HOH:O	2.02	0.59
1:A:558:MET:HE2	1:A:558:MET:HA	1.83	0.59
2:B:88:LYS:O	3:C:75:THR:HG22	2.01	0.59
2:F:164:VAL:HG22	2:F:173:PRO:HB2	1.84	0.59
3:C:155:THR:CG2	3:C:239:ARG:NE	2.65	0.59
2:B:117:THR:CG2	2:B:120:ALA:H	2.15	0.59
1:A:256:THR:CG2	1:A:305:THR:HA	2.30	0.59
2:B:3:ARG:HG2	8:B:2001:HOH:O	2.02	0.59
1:A:607:VAL:O	1:A:607:VAL:CG1	2.46	0.59
1:A:42:GLN:O	1:A:53:ILE:HG12	2.02	0.59
1:E:81:ARG:NH1	1:E:630:THR:OG1	2.32	0.59
1:A:534:TYR:O	1:A:535:PHE:HB2	2.02	0.59
2:B:57:GLN:HE22	2:B:140:ARG:NH2	1.98	0.59
1:E:642:GLU:HG3	8:E:2436:HOH:O	2.02	0.59
2:B:142:PHE:C	2:B:152:VAL:HG22	2.22	0.59
1:E:591:GLU:O	1:E:603:GLN:NE2	2.36	0.59
1:E:209:HIS:CE1	1:E:625:ARG:H	2.12	0.59
1:E:418:GLN:H	1:E:418:GLN:HE21	1.49	0.59
1:A:710:HIS:O	8:A:2346:HOH:O	2.17	0.59
1:E:81:ARG:HE	1:E:214:THR:HG22	1.67	0.59
1:A:252:ILE:CD1	1:A:256:THR:HG22	2.32	0.59
2:B:166:ARG:HH22	3:C:249:GLN:NE2	2.00	0.59
3:C:197:GLU:CD	3:C:197:GLU:H	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:189:TYR:O	3:G:192:THR:HB	2.03	0.59
1:A:708:LEU:HD22	1:A:755:LEU:HB3	1.84	0.58
2:B:166:ARG:NH2	3:C:249:GLN:NE2	2.50	0.58
8:B:2028:HOH:O	3:C:2:ALA:HB1	2.02	0.58
1:A:540:ILE:O	1:A:544:LEU:HG	2.03	0.58
1:A:583:PHE:CE2	1:A:587:SER:C	2.76	0.58
1:E:391:PRO:HG3	1:E:411:PHE:CZ	2.38	0.58
2:B:57:GLN:O	2:B:58:CYS:C	2.41	0.58
1:A:558:MET:CE	1:A:561:MET:SD	2.91	0.58
1:E:679:PRO:HG2	1:E:747:PRO:HB3	1.85	0.58
1:A:633:ARG:CD	5:A:1765:MGD:O2B	2.51	0.58
3:C:207:GLY:O	3:C:208:PHE:C	2.39	0.58
1:A:107:ARG:HG2	1:A:475:TRP:O	2.02	0.58
1:E:671:ASN:ND2	1:E:673:ASP:H	2.01	0.58
2:F:166:ARG:HH22	3:G:248:GLN:HE21	1.51	0.58
1:A:364:TYR:HB2	1:A:570:PRO:HB3	1.84	0.58
3:G:196:GLU:CD	3:G:196:GLU:H	2.04	0.58
1:E:647:ASN:H	1:E:647:ASN:HD22	1.49	0.58
2:B:36:LEU:HD11	8:B:2104:HOH:O	2.03	0.58
1:A:39:SER:HB2	8:A:2005:HOH:O	2.03	0.58
1:E:79:CYS:HB2	1:E:80:PRO:HD2	1.86	0.58
1:E:483:ALA:N	1:E:516:LYS:O	2.25	0.58
1:E:345:MET:HB2	1:E:605:LEU:HD13	1.85	0.58
1:A:37:VAL:HG13	1:A:57:ALA:O	2.04	0.58
1:A:471:GLU:HG2	1:A:471:GLU:O	2.04	0.58
1:A:426:THR:HG23	8:A:2052:HOH:O	2.03	0.58
1:A:583:PHE:HE2	1:A:588:GLY:CA	2.16	0.57
1:E:386:GLY:O	1:E:388:CYS:SG	2.48	0.57
3:C:171:TRP:CG	3:C:171:TRP:O	2.57	0.57
1:E:474:MET:HE2	8:E:2069:HOH:O	2.03	0.57
3:C:128:LEU:HD22	8:C:2063:HOH:O	2.04	0.57
2:B:57:GLN:NE2	2:B:140:ARG:HH22	1.99	0.57
1:A:483:ALA:HA	1:A:515:THR:HG21	1.86	0.57
1:E:204:VAL:HB	1:E:328:LEU:HG	1.86	0.57
1:E:549:GLN:HG3	8:E:2313:HOH:O	2.04	0.57
1:E:279:VAL:O	1:E:283:THR:HB	2.03	0.57
3:C:239:ARG:NH2	8:C:2084:HOH:O	2.35	0.57
3:G:115:LEU:HB3	8:G:2032:HOH:O	2.04	0.57
3:G:39:LEU:HD13	3:G:116:ALA:HB3	1.86	0.57
1:E:77:ARG:NE	8:E:2046:HOH:O	2.37	0.57
1:E:129:LEU:O	1:E:133:GLU:HG2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:THR:CG2	1:E:119:GLU:N	2.57	0.57
1:E:686:ALA:CB	8:E:2386:HOH:O	2.52	0.57
3:C:140:ASN:HD22	3:C:140:ASN:N	1.99	0.57
1:E:687:ARG:NH2	2:F:40:GLU:OE2	2.37	0.57
3:G:154:THR:HG21	3:G:238:ARG:HG2	1.87	0.57
1:A:609:THR:O	1:A:610:PRO:C	2.43	0.57
1:E:590:ILE:HB	8:E:2182:HOH:O	2.04	0.57
1:A:357:TYR:HA	1:A:363:PHE:HB2	1.86	0.57
3:G:220:PHE:HD1	8:G:2064:HOH:O	1.87	0.57
1:A:75:ARG:NH1	1:A:220:GLN:NE2	2.51	0.57
3:C:17:THR:CG2	3:C:67:GLU:CG	2.75	0.57
3:C:89:ILE:HD12	7:C:1252:PCI:C6	2.34	0.57
1:E:311:VAL:CG2	8:E:2198:HOH:O	2.52	0.57
3:G:30:VAL:HG12	3:G:52:ALA:HB2	1.87	0.57
1:E:604:PRO:C	1:E:606:PRO:HD3	2.25	0.57
3:G:156:LEU:HD12	3:G:178:LEU:HD13	1.87	0.57
1:E:724:LYS:HG2	8:E:2424:HOH:O	2.04	0.57
3:C:112:SER:O	3:C:113:GLN:HG2	2.05	0.57
1:E:592:LEU:HA	1:E:603:GLN:HE22	1.55	0.57
1:E:590:ILE:O	1:E:592:LEU:HG	2.05	0.57
3:G:206:GLY:C	3:G:209:TYR:H	2.07	0.57
1:A:380:PRO:HD3	1:A:534:TYR:OH	2.04	0.57
1:E:591:GLU:OE1	1:E:604:PRO:CA	2.53	0.56
1:E:320:ALA:O	1:E:323:LYS:HB2	2.05	0.56
1:A:519:TRP:CZ2	1:A:540:ILE:HG13	2.40	0.56
1:E:342:TYR:HD1	1:E:607:VAL:CB	2.14	0.56
1:A:319:MET:HE1	1:A:328:LEU:HD11	1.85	0.56
1:A:122:ASP:OD1	1:A:528:ARG:NH1	2.37	0.56
1:A:602:HIS:CD2	1:A:604:PRO:HD2	2.41	0.56
2:B:57:GLN:NE2	8:B:2045:HOH:O	2.38	0.56
1:A:678:GLY:HA3	8:A:2330:HOH:O	2.05	0.56
1:E:651:ILE:HD13	1:E:656:ALA:HB2	1.86	0.56
1:A:81:ARG:HE	1:A:214:THR:HG22	1.69	0.56
1:A:388:CYS:HA	1:A:593:TYR:CZ	2.40	0.56
1:A:384:ALA:N	8:A:2190:HOH:O	2.30	0.56
3:G:226:ALA:HB3	3:G:227:PRO:HD3	1.87	0.56
1:E:186:GLY:HA3	1:E:584:GLY:N	2.21	0.56
3:G:49:THR:HG21	8:G:2011:HOH:O	2.04	0.56
1:E:539:THR:HG23	1:E:541:GLU:HG2	1.88	0.56
1:A:367:GLN:O	1:A:500:PRO:HG3	2.05	0.56
2:F:44:GLY:O	2:F:45:GLU:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:396:HIS:CE1	1:E:404:ARG:H	2.24	0.56
1:A:658:ARG:C	1:A:659:LEU:O	2.37	0.56
2:B:114:SER:O	2:B:115:LYS:HB3	2.06	0.56
1:A:335:VAL:HG13	1:A:733:GLY:HA2	1.88	0.56
3:C:207:GLY:HA2	3:C:210:TYR:HB3	1.88	0.56
1:A:346:ALA:HB2	1:A:605:LEU:HD12	1.88	0.56
1:E:470:GLN:NE2	8:E:2279:HOH:O	2.39	0.56
1:E:109:GLU:HG2	8:E:2066:HOH:O	2.01	0.55
1:A:630:THR:N	1:A:634:THR:HG21	2.22	0.55
1:E:286:PHE:CB	8:E:2182:HOH:O	2.54	0.55
2:B:121:HIS:O	2:B:125:LYS:CE	2.53	0.55
1:A:186:GLY:C	1:A:583:PHE:O	2.44	0.55
1:A:580:ARG:NH1	1:A:580:ARG:HB2	2.21	0.55
1:A:151:TRP:O	1:A:156:LEU:HB2	2.06	0.55
1:A:193:GLU:HG2	8:A:2120:HOH:O	2.07	0.55
1:A:286:PHE:CA	1:A:590:ILE:HG21	2.36	0.55
1:A:607:VAL:HG13	1:A:609:THR:CB	2.36	0.55
1:A:295:ASP:HB2	8:A:2160:HOH:O	2.06	0.55
3:C:67:GLU:O	3:C:67:GLU:HG2	2.07	0.55
3:C:130:TYR:CZ	7:C:1252:PCI:O1	2.60	0.55
2:F:72:THR:HG22	2:F:74:ALA:N	2.17	0.55
1:E:93:ASP:OD1	1:E:758:ARG:NH2	2.40	0.55
1:A:187:ARG:NH2	1:A:367:GLN:NE2	2.55	0.55
1:A:53:ILE:HD12	1:A:65:VAL:CG2	2.37	0.55
1:A:428:GLU:OE2	1:A:428:GLU:HA	2.01	0.55
1:E:81:ARG:HD2	1:E:630:THR:OG1	2.07	0.55
1:A:483:ALA:CA	1:A:515:THR:HG23	2.37	0.55
1:E:607:VAL:HG23	8:E:2148:HOH:O	2.07	0.55
1:A:582:PRO:C	8:A:2097:HOH:O	2.44	0.55
2:F:41:ARG:CD	2:F:187:THR:HG23	2.31	0.55
1:E:208:HIS:HE1	1:E:218:GLN:NE2	2.04	0.55
2:F:39:ARG:HD2	2:F:56:GLU:OE2	2.06	0.55
1:E:519:TRP:CE2	1:E:540:ILE:CG1	2.90	0.55
1:E:346:ALA:H	1:E:605:LEU:HD12	1.71	0.55
3:G:207:PHE:O	3:G:211:LEU:N	2.40	0.55
1:A:42:GLN:CD	1:A:505:ARG:HB2	2.27	0.55
1:E:551:LEU:O	1:E:552:GLY:C	2.46	0.55
1:A:422:GLU:HB2	8:A:2206:HOH:O	2.06	0.55
1:E:396:HIS:HB3	1:E:407:LYS:HE3	1.89	0.55
1:A:467:VAL:CG2	8:A:2230:HOH:O	2.55	0.54
1:E:209:HIS:CG	5:E:1766:MGD:H5'1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:154:THR:HG22	3:G:238:ARG:NE	2.15	0.54
1:A:80:PRO:HD3	2:B:18:ALA:HB2	1.89	0.54
1:E:568:GLY:O	1:E:570:PRO:HD3	2.07	0.54
1:E:635:GLN:N	1:E:635:GLN:NE2	2.53	0.54
3:G:63:LEU:CD2	7:G:1251:PCI:C1	2.85	0.54
1:A:558:MET:HE2	1:A:561:MET:SD	2.48	0.54
1:E:553:LEU:CD2	1:E:557:THR:HG21	2.37	0.54
1:E:345:MET:CB	1:E:605:LEU:HD13	2.37	0.54
1:E:99:LEU:O	1:E:478:VAL:HA	2.08	0.54
1:E:598:LYS:HB3	1:E:599:GLU:OE1	2.08	0.54
1:A:358:GLY:O	1:A:571:TRP:HA	2.07	0.54
1:E:88:THR:HG21	1:E:467:VAL:HG11	1.88	0.54
1:E:281:LYS:HG3	1:E:282:TYR:CE1	2.43	0.54
1:E:658:ARG:C	1:E:659:LEU:O	2.35	0.54
1:A:421:ILE:HG22	1:A:421:ILE:O	2.06	0.54
1:E:359:ARG:HD3	8:E:2101:HOH:O	2.07	0.54
1:A:345:MET:CE	1:A:592:LEU:HD11	2.38	0.54
1:A:519:TRP:CD1	1:A:540:ILE:HG21	2.42	0.54
2:B:140:ARG:NH2	8:B:2045:HOH:O	2.40	0.54
1:E:388:CYS:HB2	1:E:593:TYR:HH	1.63	0.54
2:B:22:ALA:HB2	2:B:134:THR:HG21	1.90	0.54
1:E:81:ARG:HE	1:E:214:THR:CG2	2.20	0.54
1:A:231:LYS:HB2	1:A:247:HIS:CD2	2.43	0.54
1:A:336:TRP:O	1:A:735:ARG:HB2	2.07	0.54
2:B:2:PRO:HB3	2:B:144:ASP:HB2	1.90	0.54
3:G:70:ARG:HG2	3:G:71:PHE:H	1.72	0.54
2:B:192:VAL:HG12	2:B:193:HIS:H	1.72	0.54
1:E:315:VAL:HG12	1:E:319:MET:HE3	1.90	0.54
1:E:586:ALA:HB3	8:E:2326:HOH:O	2.07	0.54
1:A:81:ARG:HH21	1:A:214:THR:HG22	1.72	0.54
3:G:66:GLU:HG2	3:G:66:GLU:O	2.08	0.54
1:A:152:PHE:O	1:A:157:PRO:CG	2.56	0.54
1:E:391:PRO:HG2	1:E:392:SER:H	1.72	0.54
1:E:81:ARG:NE	1:E:214:THR:HG22	2.22	0.54
1:A:320:ALA:O	1:A:323:LYS:CG	2.55	0.54
2:B:72:THR:CG2	2:B:74:ALA:H	2.14	0.53
2:F:67:VAL:CB	2:F:68:PRO:HD3	2.38	0.53
1:A:36:GLU:HG2	1:A:36:GLU:O	2.08	0.53
1:A:415:THR:HG22	8:A:2204:HOH:O	2.09	0.53
2:F:2:PRO:HB3	2:F:144:ASP:CG	2.28	0.53
1:E:284:VAL:HG12	1:E:592:LEU:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:221:TRP:HD1	8:G:2033:HOH:O	1.91	0.53
2:B:117:THR:HG22	2:B:119:CYS:H	1.74	0.53
1:A:583:PHE:CZ	1:A:587:SER:HA	2.44	0.53
1:A:536:PRO:HG2	1:A:537:TRP:H	1.74	0.53
3:G:76:ILE:HG12	3:G:80:LEU:HD11	1.91	0.53
1:E:186:GLY:H	1:E:583:PHE:HA	1.73	0.53
1:E:397:GLU:CG	1:E:398:PRO:HD3	2.39	0.53
3:C:207:GLY:C	3:C:209:TRP:N	2.61	0.53
1:E:635:GLN:O	1:E:641:MET:HG2	2.04	0.53
1:A:525:LEU:O	1:A:529:LEU:HG	2.08	0.53
1:E:422:GLU:H	1:E:423:PRO:HD2	1.73	0.53
1:A:535:PHE:N	1:A:536:PRO:CD	2.71	0.53
1:A:388:CYS:O	1:A:391:PRO:HD3	2.09	0.53
3:G:144:ASN:OD1	3:G:192:THR:CG2	2.57	0.53
1:A:689:ARG:NH2	1:A:691:ASP:OD2	2.37	0.53
1:A:591:GLU:CB	1:A:603:GLN:HE22	2.18	0.53
1:E:622:LEU:HD22	8:E:2426:HOH:O	2.08	0.53
1:E:467:VAL:HG12	1:E:468:LEU:HG	1.90	0.53
2:B:2:PRO:HD2	2:B:80:ASP:OD2	2.08	0.53
1:E:37:VAL:HA	1:E:57:ALA:O	2.09	0.53
1:E:342:TYR:CE1	1:E:607:VAL:HB	2.41	0.53
1:A:647:ASN:HD21	1:A:714:ALA:H	1.57	0.53
1:A:457:LYS:HD3	8:A:2223:HOH:O	2.09	0.53
1:A:558:MET:HE1	1:A:561:MET:SD	2.49	0.53
1:A:134:LYS:CE	8:A:2079:HOH:O	2.54	0.53
3:G:46:ARG:HG3	8:G:2014:HOH:O	2.07	0.53
1:E:336:TRP:O	1:E:340:ASP:OD1	2.27	0.53
1:A:427:GLY:C	1:A:428:GLU:O	2.48	0.52
1:A:81:ARG:HE	1:A:214:THR:CG2	2.23	0.52
1:E:519:TRP:CE2	1:E:540:ILE:HG13	2.44	0.52
1:A:413:ARG:N	1:A:413:ARG:HD2	2.23	0.52
1:E:100:ILE:HG12	1:E:478:VAL:HG13	1.91	0.52
1:A:79:CYS:CB	1:A:80:PRO:HD2	2.39	0.52
1:A:708:LEU:N	1:A:708:LEU:HD23	2.24	0.52
1:E:69:GLU:HA	8:E:2039:HOH:O	2.08	0.52
2:B:2:PRO:HB3	2:B:144:ASP:CB	2.39	0.52
1:E:755:LEU:O	1:E:758:ARG:HD3	2.09	0.52
3:C:145:ASN:ND2	3:C:145:ASN:C	2.61	0.52
1:E:45:GLU:HG3	8:E:2011:HOH:O	2.09	0.52
1:A:671:ASN:HD21	1:A:675:VAL:H	1.58	0.52
1:E:209:HIS:CD2	5:E:1766:MGD:H5'1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:2168:HOH:O	2:F:46:TYR:HB2	2.09	0.52
2:B:183:LYS:HE3	8:B:2143:HOH:O	2.09	0.52
2:B:32:GLY:N	8:B:2011:HOH:O	2.40	0.52
1:A:183:TRP:HB3	1:A:592:LEU:HD22	1.90	0.52
1:A:96:LYS:HB3	1:A:513:PHE:HB3	1.92	0.52
8:B:2075:HOH:O	3:C:82:SER:HB3	2.09	0.52
1:A:113:ARG:NH2	8:A:2066:HOH:O	2.42	0.52
1:E:454:GLU:HG2	8:E:2274:HOH:O	2.09	0.52
1:A:572:LEU:HD22	8:A:2274:HOH:O	2.09	0.52
1:E:627:PRO:HB2	2:F:16:CYS:HA	1.91	0.52
1:A:364:TYR:HB2	1:A:570:PRO:CB	2.40	0.52
3:G:225:LEU:CB	8:G:2068:HOH:O	2.56	0.52
1:A:379:LEU:O	1:A:380:PRO:C	2.48	0.52
1:E:635:GLN:HE21	1:E:635:GLN:H	1.57	0.52
3:C:140:ASN:O	3:C:142:PRO:HD3	2.09	0.52
1:E:345:MET:HB3	1:E:605:LEU:CD1	2.40	0.52
3:G:207:PHE:CD2	3:G:207:PHE:C	2.82	0.52
1:E:621:LEU:HD22	1:E:622:LEU:O	2.09	0.52
3:G:63:LEU:CD2	7:G:1251:PCI:C6	2.88	0.52
1:A:519:TRP:CG	1:A:540:ILE:HG21	2.44	0.52
2:F:166:ARG:HH22	3:G:248:GLN:NE2	2.07	0.52
2:F:115:LYS:HG3	2:F:116:CYS:O	2.10	0.52
3:G:240:LEU:C	3:G:240:LEU:HD12	2.30	0.52
3:G:38:HIS:CE1	3:G:105:LEU:HD22	2.44	0.52
2:B:122:ARG:HB3	2:B:127:LYS:HB2	1.90	0.52
1:A:284:VAL:CG2	1:A:587:SER:HB3	2.35	0.52
3:G:206:GLY:CA	3:G:209:TYR:CB	2.88	0.52
1:A:239:PHE:O	1:A:687:ARG:HD2	2.10	0.52
2:B:139:CYS:SG	4:B:1194:SF4:S3	3.08	0.52
1:E:41:TYR:HE1	1:E:560:GLY:O	1.93	0.52
1:A:454:GLU:HG2	8:A:2102:HOH:O	2.10	0.51
3:C:140:ASN:ND2	3:C:140:ASN:N	2.55	0.51
1:A:627:PRO:HB2	2:B:16:CYS:HA	1.93	0.51
2:B:27:ASN:HD21	2:B:121:HIS:HE1	1.57	0.51
1:E:519:TRP:NE1	1:E:540:ILE:HG12	2.25	0.51
2:B:117:THR:CG2	2:B:117:THR:O	2.58	0.51
1:E:684:PRO:O	1:E:685:THR:C	2.48	0.51
1:A:73:LYS:NZ	1:A:192:HIS:CD2	2.75	0.51
3:G:172:LEU:O	3:G:176:ARG:HG3	2.11	0.51
1:A:345:MET:HE1	1:A:605:LEU:HD22	1.92	0.51
1:E:100:ILE:HG12	1:E:478:VAL:CG2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:512:LEU:O	1:E:515:THR:HB	2.11	0.51
1:A:523:ARG:HG3	1:A:535:PHE:HB3	1.92	0.51
1:E:632:ALA:C	1:E:635:GLN:NE2	2.63	0.51
2:B:117:THR:HG23	2:B:117:THR:O	2.11	0.51
1:E:591:GLU:CD	1:E:604:PRO:CB	2.61	0.51
1:E:606:PRO:CG	1:E:607:VAL:N	2.73	0.51
1:E:91:ASP:C	1:E:92:PRO:O	2.49	0.51
1:A:71:ASN:HD21	1:A:73:LYS:HB2	1.75	0.51
1:E:606:PRO:HG2	1:E:607:VAL:N	2.26	0.51
3:G:139:ASN:N	3:G:139:ASN:HD22	2.02	0.51
1:A:519:TRP:CZ2	1:A:540:ILE:CG1	2.94	0.51
1:A:48:PHE:HE1	1:A:145:HIS:CE1	2.28	0.51
1:A:422:GLU:HB3	1:A:423:PRO:CD	2.40	0.51
1:A:583:PHE:CE2	1:A:588:GLY:CA	2.91	0.51
3:C:17:THR:HG22	3:C:18:ASN:N	2.26	0.51
1:E:225:ALA:O	1:E:230:ALA:HB3	2.11	0.51
1:A:232:VAL:N	1:A:247:HIS:HD2	2.04	0.51
1:A:195:ILE:HG12	1:A:329:PRO:HB3	1.93	0.51
1:A:214:THR:HG23	1:A:214:THR:O	2.11	0.51
1:A:231:LYS:CA	1:A:247:HIS:CD2	2.93	0.51
1:A:396:HIS:CB	1:A:403:PRO:HB3	2.40	0.51
1:A:336:TRP:CD1	1:A:336:TRP:N	2.69	0.51
2:B:160:GLU:N	2:B:179:ASN:HD21	1.97	0.51
1:E:651:ILE:HD11	1:E:682:VAL:HG13	1.92	0.51
3:G:40:LYS:O	3:G:40:LYS:HG3	2.11	0.51
3:C:68:SER:O	3:C:71:ARG:HB3	2.11	0.51
1:A:585:THR:HG22	1:A:585:THR:O	2.10	0.51
3:C:174:PHE:H	3:C:175:PRO:HD2	1.76	0.51
1:A:390:GLY:H	1:A:595:GLN:NE2	2.05	0.51
2:B:86:ASP:OD1	2:B:88:LYS:HB2	2.11	0.51
3:G:189:TYR:HB3	3:G:190:PRO:HD3	1.93	0.51
2:B:155:ALA:HB1	8:B:2113:HOH:O	2.11	0.51
1:E:201:ARG:HD3	8:E:2124:HOH:O	2.10	0.50
2:F:190:SER:O	2:F:194:HIS:N	2.43	0.50
1:A:183:TRP:HB3	1:A:592:LEU:O	2.11	0.50
2:B:46:TYR:CD2	8:B:2033:HOH:O	2.64	0.50
1:A:673:ASP:OD2	1:A:721:THR:CG2	2.58	0.50
1:A:483:ALA:HA	1:A:515:THR:HG23	1.90	0.50
1:A:554:ASP:N	1:A:554:ASP:OD2	2.45	0.50
1:E:701:HIS:O	1:E:710:HIS:O	2.28	0.50
1:E:371:LEU:HD13	1:E:547:ARG:CZ	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:HD2	1:A:220:GLN:NE2	2.20	0.50
1:A:345:MET:HE1	1:A:605:LEU:CD2	2.40	0.50
1:A:605:LEU:N	1:A:606:PRO:CD	2.73	0.50
8:A:2041:HOH:O	2:B:133:GLU:HG3	2.12	0.50
1:E:153:VAL:CG1	1:E:167:LYS:HE2	2.42	0.50
1:A:654:GLU:HG3	8:A:2319:HOH:O	2.11	0.50
3:G:132:LEU:O	3:G:136:VAL:HB	2.12	0.50
3:C:151:LEU:O	3:C:155:THR:HB	2.12	0.50
3:C:50:THR:O	3:C:54:LEU:HG	2.11	0.50
1:E:36:GLU:HB3	8:E:2005:HOH:O	2.11	0.50
1:E:630:THR:HG23	8:E:2451:HOH:O	2.11	0.50
1:E:519:TRP:CE2	1:E:540:ILE:HG12	2.46	0.50
1:A:285:GLY:C	1:A:590:ILE:HG23	2.32	0.50
1:E:345:MET:CB	1:E:605:LEU:CD1	2.90	0.50
1:A:428:GLU:CB	1:A:429:PRO:CD	2.87	0.50
1:A:93:ASP:CG	1:A:758:ARG:HH22	2.14	0.50
1:A:187:ARG:HH22	1:A:367:GLN:NE2	2.10	0.50
1:A:599:GLU:HB2	8:A:2280:HOH:O	2.12	0.50
1:E:256:THR:CG2	1:E:305:THR:HA	2.36	0.50
1:E:311:VAL:HG23	8:E:2198:HOH:O	2.10	0.50
1:E:671:ASN:ND2	1:E:671:ASN:C	2.64	0.50
1:A:548:LEU:HD13	1:A:558:MET:HB2	1.94	0.50
2:F:78:THR:CG2	2:F:79:LYS:N	2.76	0.49
1:A:231:LYS:HB2	1:A:247:HIS:CG	2.47	0.49
3:G:63:LEU:HD21	7:G:1251:PCI:C1	2.42	0.49
2:B:47:PRO:CG	8:B:2034:HOH:O	2.60	0.49
2:B:36:LEU:CD1	8:B:2104:HOH:O	2.60	0.49
1:A:289:LEU:HD12	1:A:590:ILE:HD11	1.94	0.49
1:A:592:LEU:O	1:A:592:LEU:HD13	2.12	0.49
1:A:118:GLU:CD	1:A:118:GLU:H	2.15	0.49
1:E:160:TRP:O	1:E:160:TRP:CG	2.65	0.49
1:E:97:ARG:HH22	1:E:763:ARG:HD2	1.76	0.49
1:E:252:ILE:HG12	1:E:256:THR:HG22	1.94	0.49
1:E:93:ASP:O	1:E:469:PRO:HD3	2.12	0.49
1:E:685:THR:HG22	2:F:42:GLU:OE2	2.12	0.49
1:E:142:PHE:CG	1:E:157:PRO:HG3	2.47	0.49
1:E:286:PHE:C	1:E:288:GLU:H	2.14	0.49
1:E:623:TYR:HA	1:E:695:ILE:O	2.12	0.49
1:A:305:THR:HG23	1:A:307:ILE:HD12	1.94	0.49
2:F:35:ASN:HD22	2:F:106:TYR:HE2	1.60	0.49
1:E:265:ILE:HD11	1:E:349:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:651:ILE:HD11	1:E:682:VAL:HG12	1.94	0.49
3:G:227:PRO:O	3:G:231:LEU:HB2	2.12	0.49
1:E:497:HIS:O	1:E:498:LYS:C	2.50	0.49
2:F:35:ASN:ND2	2:F:106:TYR:HE2	2.11	0.49
1:E:380:PRO:HD3	1:E:534:TYR:OH	2.12	0.49
3:C:21:HIS:CE1	3:C:64:LEU:CG	2.96	0.49
1:A:276:LYS:CA	8:A:2152:HOH:O	2.47	0.49
1:E:620:ARG:HB3	8:E:2392:HOH:O	2.12	0.49
1:E:305:THR:HG23	1:E:307:ILE:H	1.75	0.49
8:B:2081:HOH:O	3:C:251:LEU:HD11	2.12	0.49
2:F:172:ARG:N	2:F:173:PRO:HD3	2.28	0.49
3:G:70:ARG:HG2	3:G:71:PHE:N	2.27	0.49
1:A:449:VAL:O	1:A:453:LYS:HG3	2.12	0.49
3:C:248:TRP:CE2	3:C:250:GLY:HA3	2.48	0.49
1:E:116:THR:HG23	1:E:119:GLU:N	2.16	0.49
3:G:63:LEU:HD22	7:G:1251:PCI:C1	2.43	0.49
1:E:724:LYS:CG	8:E:2424:HOH:O	2.61	0.49
1:A:404:ARG:HG3	1:A:406:ASP:OD2	2.13	0.49
1:A:429:PRO:C	1:A:430:TYR:CD2	2.85	0.49
3:G:17:ASN:O	3:G:21:PHE:HD1	1.95	0.49
1:A:393:GLY:HA3	1:A:407:LYS:HZ1	1.78	0.49
1:A:345:MET:CE	1:A:605:LEU:HD22	2.43	0.48
2:F:16:CYS:O	2:F:16:CYS:SG	2.71	0.48
1:E:112:TYR:CZ	1:E:474:MET:O	2.65	0.48
1:E:247:HIS:CE1	8:E:2149:HOH:O	2.66	0.48
2:F:88:LYS:O	3:G:74:THR:CG2	2.60	0.48
1:E:601:GLY:HA2	8:E:2334:HOH:O	2.13	0.48
1:E:335:VAL:HG13	1:E:732:ALA:O	2.13	0.48
1:A:103:GLU:HA	1:A:103:GLU:OE1	2.13	0.48
1:A:209:HIS:CE1	1:A:625:ARG:H	2.23	0.48
1:A:635:GLN:C	1:A:709:ALA:HB2	2.33	0.48
1:A:310:GLN:HG3	8:A:2164:HOH:O	2.13	0.48
3:C:21:HIS:CE1	3:C:64:LEU:CD2	2.97	0.48
1:A:43:ILE:HB	1:A:505:ARG:HH21	1.79	0.48
1:A:37:VAL:CG1	1:A:38:LYS:N	2.75	0.48
1:E:495:VAL:HG21	8:E:2299:HOH:O	2.12	0.48
2:B:55:PRO:HB2	8:B:2104:HOH:O	2.12	0.48
3:G:70:ARG:CG	3:G:71:PHE:N	2.76	0.48
1:E:336:TRP:O	1:E:338:GLY:N	2.47	0.48
1:E:197:TRP:CG	1:E:221:ASP:HB3	2.49	0.48
1:E:119:GLU:HG2	8:E:2075:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:46:TYR:C	2:F:46:TYR:CD1	2.85	0.48
1:E:149:ASP:CB	8:E:2094:HOH:O	2.61	0.48
3:C:77:ILE:HG12	3:C:81:LEU:HD11	1.95	0.48
1:E:166:ALA:HB2	1:E:415:THR:CG2	2.42	0.48
1:A:342:TYR:CD2	1:A:605:LEU:HA	2.49	0.48
1:E:591:GLU:OE2	1:E:604:PRO:HB3	2.12	0.48
3:C:172:ALA:CA	3:C:175:PRO:HG2	2.35	0.48
3:G:222:GLN:C	8:G:2068:HOH:O	2.51	0.48
1:A:116:THR:HG23	1:A:118:GLU:N	2.29	0.48
1:E:397:GLU:HB3	8:E:2242:HOH:O	2.13	0.48
1:A:75:ARG:NH1	1:A:220:GLN:HE21	2.07	0.48
1:E:469:PRO:O	1:E:706:MET:CG	2.59	0.48
3:G:144:ASN:C	3:G:144:ASN:HD22	2.16	0.48
1:E:214:THR:HG21	1:E:627:PRO:O	2.12	0.48
1:E:553:LEU:HD21	1:E:557:THR:CG2	2.43	0.48
3:C:108:LEU:HB3	3:C:110:LYS:HG3	1.96	0.48
3:G:139:ASN:ND2	8:G:2041:HOH:O	2.46	0.48
1:A:305:THR:CG2	1:A:307:ILE:HB	2.43	0.48
1:A:512:LEU:O	1:A:515:THR:HB	2.13	0.48
1:A:195:ILE:N	1:A:195:ILE:HD12	2.27	0.48
3:G:52:ALA:O	3:G:56:ILE:HG13	2.14	0.48
3:G:100:LEU:HB3	8:G:2031:HOH:O	2.14	0.48
1:A:101:ARG:HB2	1:A:477:ASP:HA	1.96	0.48
1:A:132:ARG:CD	8:A:2077:HOH:O	2.60	0.48
1:A:284:VAL:HG12	1:A:285:GLY:N	2.28	0.48
1:E:591:GLU:O	1:E:591:GLU:CG	2.60	0.48
1:A:483:ALA:CA	1:A:515:THR:CG2	2.90	0.48
1:A:124:ILE:HD11	1:A:478:VAL:HG11	1.96	0.48
1:A:623:TYR:HA	1:A:695:ILE:O	2.13	0.48
3:G:206:GLY:CA	3:G:209:TYR:HB3	2.43	0.48
3:C:64:LEU:HD21	7:C:1252:PCI:C1	2.44	0.48
1:E:632:ALA:C	1:E:635:GLN:HE22	2.17	0.48
1:A:519:TRP:CG	1:A:540:ILE:CG2	2.96	0.48
1:A:256:THR:O	1:A:256:THR:HG23	2.14	0.48
1:E:315:VAL:HG12	1:E:319:MET:CE	2.44	0.48
1:E:97:ARG:HH21	1:E:763:ARG:CZ	2.27	0.48
1:A:683:LYS:HA	1:A:684:PRO:HD2	1.66	0.48
1:A:107:ARG:HB2	8:A:2224:HOH:O	2.13	0.48
1:A:369:PRO:HG2	1:A:494:LEU:HB3	1.96	0.48
1:E:677:GLU:O	1:E:678:GLY:O	2.31	0.48
1:A:299:GLU:OE2	1:A:313:ARG:NH2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:397:GLU:CB	1:E:398:PRO:CD	2.85	0.47
1:E:313:ARG:HD3	1:E:317:ARG:NH2	2.30	0.47
1:E:75:ARG:NH1	1:E:220:GLN:HE21	2.07	0.47
1:A:81:ARG:HH21	1:A:214:THR:CG2	2.27	0.47
1:E:519:TRP:CZ2	1:E:540:ILE:HG13	2.49	0.47
1:E:412:ALA:HB1	1:E:413:ARG:NH1	2.29	0.47
1:E:424:MET:CE	1:E:455:ALA:HB1	2.44	0.47
1:E:647:ASN:HD22	1:E:647:ASN:N	2.07	0.47
1:A:64:LYS:CE	2:B:26:GLU:HB2	2.43	0.47
1:E:302:GLU:HG2	1:E:302:GLU:O	2.14	0.47
2:B:46:TYR:HE2	8:B:2033:HOH:O	1.93	0.47
2:B:41:ARG:NH1	2:B:187:THR:HG23	2.19	0.47
1:A:519:TRP:CD2	1:A:540:ILE:HG23	2.48	0.47
1:E:433:LYS:HB3	1:E:460:ASP:HB2	1.96	0.47
2:B:78:THR:HG22	2:B:80:ASP:H	1.80	0.47
1:A:533:GLN:HG2	1:A:534:TYR:N	2.28	0.47
1:A:575:TRP:O	1:A:580:ARG:HG2	2.15	0.47
1:E:606:PRO:CG	1:E:607:VAL:H	2.27	0.47
1:A:69:GLU:C	8:A:2034:HOH:O	2.35	0.47
1:E:466:ASP:HA	5:E:1765:MGD:N2	2.29	0.47
1:E:239:PHE:CB	1:E:687:ARG:HB3	2.41	0.47
2:F:63:ASN:HB2	8:F:2110:HOH:O	2.13	0.47
2:B:191:GLU:HG3	8:B:2144:HOH:O	2.14	0.47
1:A:85:ALA:HA	8:A:2044:HOH:O	2.13	0.47
3:C:64:LEU:CD2	7:C:1252:PCI:C4	2.89	0.47
1:A:534:TYR:O	1:A:535:PHE:CB	2.63	0.47
1:A:595:GLN:HA	1:A:598:LYS:HD2	1.97	0.47
1:E:574:ASP:HA	1:E:577:LYS:HD3	1.95	0.47
1:A:64:LYS:HE2	2:B:26:GLU:HB2	1.95	0.47
2:F:29:VAL:HA	2:F:30:PRO:HD3	1.68	0.47
1:A:285:GLY:C	1:A:590:ILE:CG2	2.83	0.47
1:E:346:ALA:N	1:E:605:LEU:CD1	2.76	0.47
1:E:275:ASP:N	1:E:323:LYS:HE3	2.29	0.47
1:A:647:ASN:C	1:A:648:GLU:CG	2.81	0.47
1:E:683:LYS:HE2	1:E:685:THR:HB	1.95	0.47
1:A:548:LEU:O	1:A:553:LEU:O	2.33	0.47
1:A:647:ASN:HD22	1:A:647:ASN:N	2.07	0.47
1:E:672:GLN:H	1:E:672:GLN:NE2	2.13	0.47
1:A:555:LEU:O	1:A:559:LYS:HG3	2.14	0.47
1:A:591:GLU:O	1:A:592:LEU:CD1	2.58	0.47
1:E:428:GLU:O	1:E:430:TYR:CA	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:GLN:CD	8:B:2045:HOH:O	2.54	0.47
1:A:295:ASP:O	1:A:297:THR:HG22	2.15	0.47
1:A:671:ASN:ND2	1:A:675:VAL:H	2.12	0.47
1:E:48:PHE:CZ	1:E:145:HIS:CE1	3.03	0.47
1:A:391:PRO:O	1:A:413:ARG:CB	2.63	0.47
1:E:453:LYS:HG2	1:E:475:TRP:CZ2	2.50	0.47
3:G:247:TRP:CE2	3:G:249:GLY:HA3	2.50	0.47
1:E:287:GLU:N	1:E:287:GLU:OE1	2.48	0.47
1:E:606:PRO:CD	1:E:607:VAL:N	2.78	0.46
3:G:208:TRP:HE3	3:G:208:TRP:HA	1.80	0.46
1:A:337:TYR:O	1:A:340:ASP:CG	2.45	0.46
1:A:193:GLU:CG	8:A:2120:HOH:O	2.62	0.46
1:E:609:THR:HG23	8:E:2338:HOH:O	2.15	0.46
2:B:5:ALA:HB3	2:B:145:LEU:HD13	1.97	0.46
1:A:286:PHE:HA	1:A:590:ILE:CG2	2.43	0.46
1:E:591:GLU:OE2	1:E:604:PRO:CG	2.62	0.46
1:A:42:GLN:OE1	1:A:506:THR:N	2.48	0.46
2:F:57:GLN:HE22	2:F:140:ARG:HH21	1.55	0.46
1:E:81:ARG:HB2	4:E:1764:SF4:S3	2.54	0.46
3:C:155:THR:CG2	3:C:239:ARG:CG	2.89	0.46
8:B:2078:HOH:O	7:C:1252:PCI:CL3	2.58	0.46
1:A:305:THR:CG2	1:A:307:ILE:H	2.25	0.46
3:C:57:ILE:HG21	3:C:100:PHE:HB2	1.97	0.46
1:E:651:ILE:HD12	1:E:684:PRO:HA	1.97	0.46
3:G:63:LEU:HD11	7:G:1251:PCI:CL5	2.51	0.46
3:C:229:TRP:O	3:C:233:LEU:HG	2.14	0.46
1:A:686:ALA:CB	8:A:2332:HOH:O	2.50	0.46
1:A:194:PRO:O	1:A:363:PHE:HA	2.15	0.46
3:G:46:ARG:CG	8:G:2014:HOH:O	2.64	0.46
2:B:168:GLU:C	2:B:169:GLN:O	2.50	0.46
1:A:488:ARG:HD3	1:A:490:ASP:OD2	2.15	0.46
1:E:308:PRO:CB	8:E:2198:HOH:O	2.51	0.46
2:F:117:THR:HG22	2:F:119:CYS:N	2.27	0.46
3:G:205:ALA:HB1	3:G:240:LEU:CD2	2.45	0.46
1:A:592:LEU:HD13	1:A:592:LEU:C	2.35	0.46
1:E:100:ILE:CG2	1:E:478:VAL:HG22	2.44	0.46
3:C:171:TRP:HE3	3:C:171:TRP:O	1.81	0.46
3:C:21:HIS:CE1	3:C:64:LEU:HD11	2.43	0.46
1:A:175:ALA:HB3	1:A:176:PRO:HD3	1.97	0.46
1:E:297:THR:HG21	1:E:299:GLU:HG2	1.96	0.46
1:E:169:SER:O	1:E:174:THR:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:669:LEU:HD23	1:E:741:LEU:HD22	1.96	0.46
3:G:160:LEU:HB3	3:G:175:LEU:HB2	1.96	0.46
1:A:530:GLY:HA2	1:A:532:GLU:OE2	2.15	0.46
2:B:129:PRO:HB3	4:B:1195:SF4:S3	2.56	0.46
2:B:64:PRO:HB3	4:B:1196:SF4:S3	2.56	0.46
3:C:185:LEU:O	3:C:189:LEU:HG	2.15	0.46
1:A:183:TRP:HE1	1:A:413:ARG:NH2	2.08	0.46
1:A:596:ARG:NH1	1:A:600:ALA:CB	2.78	0.46
1:A:209:HIS:HD2	5:A:1766:MGD:O2A	1.98	0.46
1:A:490:ASP:OD2	1:A:505:ARG:NH1	2.48	0.46
1:E:620:ARG:CG	1:E:620:ARG:O	2.63	0.46
1:E:421:ILE:HD11	1:E:452:THR:HG23	1.98	0.46
3:C:222:TRP:CD1	3:C:223:GLN:N	2.83	0.46
2:F:147:ASP:O	2:F:150:SER:HB2	2.15	0.46
3:G:91:GLY:O	3:G:95:LEU:HD12	2.15	0.46
3:C:190:TYR:HB3	3:C:191:PRO:HD3	1.98	0.46
1:A:341:THR:OG1	1:A:729:SER:HB3	2.15	0.46
1:A:335:VAL:HG13	1:A:733:GLY:CA	2.45	0.46
1:A:124:ILE:O	1:A:128:MET:HG3	2.16	0.46
2:F:166:ARG:HD2	8:F:2105:HOH:O	2.16	0.46
1:E:327:VAL:HG13	1:E:362:GLY:HA2	1.97	0.46
1:E:639:VAL:HG21	2:F:25:MET:HE3	1.97	0.46
1:E:48:PHE:CE1	1:E:145:HIS:CE1	3.04	0.46
1:A:676:LYS:NZ	1:A:742:GLU:OE1	2.48	0.46
1:A:605:LEU:N	1:A:605:LEU:CD2	2.67	0.46
3:G:206:GLY:HA2	3:G:209:TYR:HB2	1.97	0.46
1:E:717:ASN:ND2	5:E:1765:MGD:H192	2.08	0.46
2:F:55:PRO:CG	4:F:1194:SF4:S2	3.02	0.46
1:E:299:GLU:OE2	1:E:313:ARG:NH2	2.27	0.46
1:E:708:LEU:HD22	8:E:2408:HOH:O	2.15	0.46
1:E:248:ARG:NH1	1:E:318:GLU:OE2	2.49	0.46
3:G:16:THR:HG21	3:G:66:GLU:HB2	1.98	0.46
1:E:39:SER:OG	1:E:56:HIS:ND1	2.39	0.46
1:A:430:TYR:HB2	1:A:431:PRO:HD3	1.98	0.45
1:E:97:ARG:NH2	1:E:763:ARG:NH1	2.61	0.45
3:C:21:HIS:C	3:C:21:HIS:CD2	2.90	0.45
1:A:116:THR:HG22	1:A:119:GLU:CB	2.41	0.45
1:E:468:LEU:HB3	1:E:469:PRO:HD2	1.97	0.45
2:F:117:THR:HG23	2:F:117:THR:O	2.15	0.45
1:A:548:LEU:C	1:A:553:LEU:O	2.55	0.45
1:E:647:ASN:H	1:E:647:ASN:ND2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:TYR:CE1	2:B:114:SER:HB3	2.50	0.45
2:B:118:PHE:HD1	2:B:118:PHE:HA	1.66	0.45
1:E:412:ALA:HB1	1:E:413:ARG:HH12	1.81	0.45
1:E:95:LEU:CD1	8:E:2278:HOH:O	2.56	0.45
1:A:682:VAL:HG12	1:A:684:PRO:HD3	1.99	0.45
2:B:88:LYS:O	3:C:75:THR:CG2	2.64	0.45
1:A:279:VAL:HA	1:A:283:THR:HB	1.99	0.45
1:E:397:GLU:CB	8:E:2242:HOH:O	2.64	0.45
1:E:256:THR:HG23	8:E:2196:HOH:O	2.16	0.45
1:A:122:ASP:HB2	8:A:2070:HOH:O	2.15	0.45
2:B:61:CYS:HB2	4:B:1196:SF4:S3	2.57	0.45
1:E:88:THR:CG2	1:E:467:VAL:HG11	2.47	0.45
1:A:284:VAL:HB	1:A:589:LYS:HA	1.99	0.45
1:A:43:ILE:HB	1:A:505:ARG:NH2	2.31	0.45
1:A:405:ALA:HB2	1:A:430:TYR:CZ	2.52	0.45
2:F:16:CYS:O	4:F:1194:SF4:S3	2.75	0.45
8:E:2134:HOH:O	2:F:138:TYR:CE1	2.70	0.45
1:E:263:ALA:HB2	1:E:301:ALA:HB2	1.98	0.45
1:E:484:THR:HB	1:E:487:GLU:OE1	2.16	0.45
1:E:149:ASP:HA	8:E:2094:HOH:O	2.16	0.45
1:E:447:PRO:HB3	8:E:2419:HOH:O	2.16	0.45
2:F:44:GLY:HA3	8:F:2025:HOH:O	2.16	0.45
1:A:255:GLY:HA2	1:A:337:TYR:CE1	2.51	0.45
1:A:77:ARG:NH2	8:A:2041:HOH:O	2.39	0.45
1:E:113:ARG:HB3	8:E:2044:HOH:O	2.17	0.45
1:E:622:LEU:HB2	1:E:693:VAL:O	2.17	0.45
1:A:170:VAL:HG12	1:A:171:SER:N	2.31	0.45
2:B:112:TYR:HB3	3:C:73:ARG:NH2	2.31	0.45
1:A:702:LYS:HG3	8:A:2234:HOH:O	2.16	0.45
2:F:125:LYS:HE2	8:F:2078:HOH:O	2.17	0.45
1:A:583:PHE:CZ	1:A:587:SER:CA	2.99	0.45
1:E:116:THR:HG22	1:E:119:GLU:N	2.27	0.45
3:C:64:LEU:HD21	7:C:1252:PCI:C6	2.46	0.45
1:E:112:TYR:OH	1:E:476:ALA:O	2.35	0.45
1:E:533:GLN:HE21	1:E:533:GLN:N	1.98	0.45
1:E:638:TRP:O	1:E:642:GLU:HB2	2.17	0.45
1:A:586:ALA:O	1:A:587:SER:CB	2.64	0.45
1:E:100:ILE:CG1	1:E:478:VAL:HG22	2.44	0.45
1:A:116:THR:HG23	1:A:118:GLU:H	1.81	0.45
1:A:422:GLU:N	1:A:423:PRO:HD2	2.31	0.45
1:E:576:GLU:C	1:E:578:GLU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:730:GLY:HA3	8:E:2252:HOH:O	2.16	0.45
3:G:44:GLU:OE1	3:G:47:ARG:NH1	2.49	0.45
1:A:499:THR:HB	1:A:565:VAL:CG1	2.47	0.45
1:A:288:GLU:HB3	1:A:591:GLU:CG	2.28	0.45
3:G:206:GLY:CA	3:G:209:TYR:HB2	2.47	0.45
1:A:159:ALA:HA	1:A:380:PRO:HD2	1.99	0.45
3:G:195:PRO:HD2	3:G:196:GLU:OE2	2.17	0.45
1:E:239:PHE:O	1:E:687:ARG:HD2	2.17	0.45
1:A:156:LEU:HB3	1:A:157:PRO:HD3	1.99	0.45
1:A:483:ALA:HB2	1:A:515:THR:CG2	2.47	0.45
1:A:212:GLU:OE1	1:A:240:SER:HB2	2.17	0.45
1:A:72:PRO:HG2	1:A:501:PHE:CD2	2.52	0.45
3:G:148:ALA:HA	8:G:2047:HOH:O	2.17	0.45
1:A:115:ALA:HB1	1:A:119:GLU:HG2	1.99	0.44
1:A:252:ILE:HG13	1:A:307:ILE:HD11	1.98	0.44
2:F:117:THR:HB	8:F:2012:HOH:O	2.15	0.44
1:A:81:ARG:NE	1:A:214:THR:HG22	2.32	0.44
2:F:35:ASN:ND2	2:F:106:TYR:CE2	2.84	0.44
1:E:166:ALA:HB2	1:E:415:THR:HG21	1.99	0.44
1:A:628:VAL:HG13	1:A:640:LEU:HD22	1.99	0.44
1:A:655:GLU:CD	1:A:658:ARG:HH22	2.20	0.44
1:E:53:ILE:HD12	1:E:65:VAL:HG22	1.99	0.44
1:A:753:THR:CG2	1:A:757:LYS:HE2	2.47	0.44
1:A:569:LYS:HA	1:A:570:PRO:HD3	1.73	0.44
3:G:39:LEU:HD13	3:G:116:ALA:CB	2.47	0.44
1:A:81:ARG:NH2	1:A:214:THR:HG22	2.31	0.44
8:F:2029:HOH:O	3:G:250:LEU:HD12	2.16	0.44
3:C:228:PRO:O	3:C:232:LEU:HD12	2.18	0.44
1:E:492:PHE:HZ	1:E:548:LEU:HG	1.82	0.44
1:A:349:TYR:HH	1:A:591:GLU:C	2.05	0.44
1:A:207:GLY:O	5:A:1766:MGD:PB	2.75	0.44
1:A:42:GLN:OE1	1:A:506:THR:O	2.35	0.44
2:B:190:SER:CB	3:C:252:GLY:N	2.77	0.44
3:C:143:LEU:CD2	3:C:198:ALA:HB1	2.47	0.44
1:A:184:VAL:HG22	1:A:592:LEU:CG	2.47	0.44
1:E:734:LEU:CD2	8:E:2419:HOH:O	2.59	0.44
2:F:190:SER:N	3:G:251:GLY:N	2.65	0.44
3:G:205:ALA:HB1	3:G:240:LEU:HD22	1.98	0.44
1:E:504:LEU:HD22	1:E:505:ARG:N	2.33	0.44
1:A:647:ASN:H	1:A:647:ASN:ND2	2.12	0.44
1:E:250:LEU:HD13	1:E:307:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:LEU:CG	3:C:173:LEU:O	2.62	0.44
1:A:680:VAL:HG22	1:A:714:ALA:HB2	1.99	0.44
2:B:72:THR:CG2	2:B:73:GLY:N	2.80	0.44
2:B:25:MET:CE	2:B:25:MET:CA	2.87	0.44
1:E:539:THR:CG2	1:E:541:GLU:HG2	2.47	0.44
1:E:204:VAL:HG21	1:E:319:MET:CE	2.47	0.44
1:E:423:PRO:HB2	1:E:432:ILE:HG13	1.99	0.44
1:E:201:ARG:CD	8:E:2124:HOH:O	2.65	0.44
2:F:107:LEU:HD21	3:G:68:PRO:HG2	2.00	0.44
3:G:206:GLY:O	3:G:209:TYR:CB	2.66	0.44
1:E:553:LEU:CD2	1:E:557:THR:CG2	2.95	0.44
1:E:297:THR:HG22	1:E:299:GLU:H	1.81	0.44
1:E:142:PHE:CD1	1:E:157:PRO:HB3	2.53	0.44
1:E:342:TYR:CD1	1:E:607:VAL:CB	2.86	0.44
3:C:145:ASN:OD1	3:C:193:THR:CG2	2.65	0.44
1:E:524:GLU:OE1	1:E:528:ARG:NH2	2.51	0.44
2:B:52:GLU:OE2	2:B:187:THR:HB	2.18	0.43
1:A:65:VAL:HG13	1:A:78:LEU:HD21	2.00	0.43
3:G:112:GLN:N	8:G:2034:HOH:O	2.50	0.43
1:E:204:VAL:HG21	1:E:319:MET:HE1	2.00	0.43
1:A:254:PRO:HG2	1:A:692:CYS:SG	2.57	0.43
1:E:227:LYS:HE2	2:F:12:LEU:HD11	1.99	0.43
3:G:222:GLN:CA	3:G:222:GLN:OE1	2.62	0.43
1:E:499:THR:HA	1:E:567:ARG:O	2.19	0.43
1:E:708:LEU:HD22	1:E:755:LEU:HB3	2.00	0.43
3:G:60:LEU:HD23	3:G:63:LEU:HD12	1.98	0.43
1:E:575:TRP:HB3	1:E:580:ARG:O	2.18	0.43
1:E:79:CYS:CB	1:E:80:PRO:HD2	2.48	0.43
3:G:42:ASP:OD1	3:G:44:GLU:HG3	2.18	0.43
2:F:9:ASP:HA	2:F:178:LEU:HB2	1.99	0.43
1:E:158:ALA:HB1	1:E:381:LEU:O	2.17	0.43
1:A:666:TYR:CZ	1:A:681:ARG:HG3	2.53	0.43
3:G:33:LEU:HD23	3:G:33:LEU:HA	1.71	0.43
1:A:186:GLY:N	1:A:583:PHE:HA	2.27	0.43
3:C:153:PRO:HB3	8:C:2063:HOH:O	2.17	0.43
2:B:166:ARG:HG2	8:B:2146:HOH:O	2.19	0.43
3:C:133:LEU:O	3:C:137:VAL:HG22	2.18	0.43
1:A:587:SER:O	1:A:589:LYS:HE2	2.18	0.43
3:G:207:PHE:HB3	3:G:208:TRP:H	1.42	0.43
1:A:761:ASP:C	1:A:763:ARG:H	2.21	0.43
1:E:630:THR:HA	5:E:1766:MGD:C17	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ALA:CB	1:A:415:THR:CG2	2.95	0.43
1:A:482:GLU:HG2	1:A:483:ALA:H	1.84	0.43
1:A:73:LYS:HZ3	1:A:192:HIS:CD2	2.36	0.43
1:A:689:ARG:NE	1:A:691:ASP:OD2	2.50	0.43
1:A:113:ARG:NE	8:A:2066:HOH:O	2.52	0.43
1:E:548:LEU:CD1	1:E:555:LEU:HA	2.48	0.43
1:A:184:VAL:HG22	1:A:592:LEU:CB	2.48	0.43
1:A:651:ILE:HG23	1:A:693:VAL:HG23	2.00	0.43
2:B:132:VAL:HA	2:B:140:ARG:HG3	2.01	0.43
1:E:247:HIS:N	1:E:247:HIS:CD2	2.85	0.43
1:A:96:LYS:HB3	1:A:513:PHE:CB	2.48	0.43
2:F:129:PRO:HB3	4:F:1195:SF4:S2	2.59	0.43
1:A:388:CYS:HA	1:A:593:TYR:HE1	1.80	0.43
3:C:64:LEU:CD2	7:C:1252:PCI:C5	2.96	0.43
1:E:488:ARG:HG3	8:E:2288:HOH:O	2.18	0.43
1:A:371:LEU:HD23	1:A:551:LEU:CD1	2.49	0.43
3:C:172:ALA:HA	3:C:175:PRO:CG	2.37	0.43
1:E:630:THR:HA	5:E:1766:MGD:N18	2.34	0.43
1:A:743:LYS:HG3	8:A:2365:HOH:O	2.18	0.43
1:A:42:GLN:NE2	1:A:505:ARG:CD	2.74	0.43
1:A:488:ARG:CD	1:A:490:ASP:OD2	2.67	0.43
3:C:208:PHE:CD2	3:C:208:PHE:C	2.90	0.43
1:A:721:THR:OG1	8:A:2354:HOH:O	2.21	0.43
1:E:746:ARG:CG	1:E:746:ARG:HH11	2.30	0.43
1:A:319:MET:CE	1:A:328:LEU:CD1	2.97	0.43
1:E:583:PHE:CD2	1:E:583:PHE:N	2.81	0.43
3:G:65:ALA:O	3:G:70:ARG:NH1	2.52	0.43
1:A:158:ALA:HB1	1:A:381:LEU:O	2.18	0.43
3:C:125:LEU:HD23	3:C:125:LEU:HA	1.95	0.43
1:E:285:GLY:HA3	1:E:592:LEU:HD11	2.01	0.43
1:E:426:THR:C	1:E:428:GLU:N	2.72	0.43
2:F:79:LYS:HD2	2:F:79:LYS:HA	1.81	0.43
3:C:222:TRP:CD1	3:C:222:TRP:C	2.91	0.43
1:A:418:GLN:HG3	1:A:418:GLN:H	1.49	0.43
1:A:596:ARG:CZ	1:A:600:ALA:HB1	2.49	0.43
1:E:627:PRO:CB	2:F:16:CYS:HA	2.49	0.43
3:C:155:THR:CG2	3:C:239:ARG:CD	2.97	0.43
1:A:489:TYR:CD1	1:A:540:ILE:HD13	2.54	0.43
1:A:193:GLU:HB2	1:A:195:ILE:CD1	2.48	0.43
1:E:370:TYR:OH	1:E:372:GLU:HG3	2.18	0.43
1:E:123:HIS:CE1	8:E:2080:HOH:O	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:VAL:HG13	1:E:293:VAL:O	2.18	0.43
1:A:506:THR:CG2	8:A:2248:HOH:O	2.66	0.42
1:A:523:ARG:HG2	1:A:523:ARG:HH11	1.83	0.42
3:C:207:GLY:HA2	3:C:210:TYR:CB	2.49	0.42
2:B:159:ALA:O	2:F:183:LYS:CE	2.59	0.42
2:B:164:VAL:HG22	2:B:173:PRO:HB2	2.00	0.42
1:A:635:GLN:HG2	1:A:635:GLN:H	1.38	0.42
3:C:21:HIS:ND1	3:C:64:LEU:CG	2.80	0.42
2:B:192:VAL:CG1	2:B:193:HIS:H	2.32	0.42
1:E:540:ILE:O	1:E:544:LEU:HG	2.19	0.42
2:F:99:ALA:HB2	3:G:137:ASN:ND2	2.34	0.42
1:E:614:PRO:HB3	1:E:738:PHE:CD2	2.54	0.42
2:F:164:VAL:CG2	2:F:173:PRO:HB2	2.49	0.42
3:G:86:SER:O	3:G:87:PRO:C	2.55	0.42
1:E:289:LEU:HD12	1:E:590:ILE:HG21	2.00	0.42
1:E:591:GLU:O	1:E:603:GLN:HG2	2.18	0.42
2:B:41:ARG:CD	2:B:187:THR:HG23	2.46	0.42
3:C:130:TYR:CE1	7:C:1252:PCI:O1	2.72	0.42
1:E:30:ALA:N	1:E:31:PRO:CD	2.82	0.42
1:A:371:LEU:HD23	1:A:371:LEU:HA	1.94	0.42
1:E:384:ALA:HB1	8:E:2240:HOH:O	2.20	0.42
2:B:71:PRO:HB2	3:C:79:LEU:CD1	2.49	0.42
1:A:90:TYR:OH	1:A:509:HIS:HE1	2.01	0.42
1:A:349:TYR:OH	1:A:592:LEU:HG	2.19	0.42
1:A:589:LYS:O	1:A:592:LEU:CA	2.67	0.42
1:E:595:GLN:O	1:E:595:GLN:HG3	2.19	0.42
1:A:65:VAL:CG1	1:A:78:LEU:HD21	2.49	0.42
1:E:622:LEU:O	1:E:623:TYR:HB3	2.19	0.42
2:B:117:THR:HG23	2:B:120:ALA:H	1.84	0.42
8:B:2081:HOH:O	3:C:251:LEU:CD1	2.66	0.42
1:A:483:ALA:CB	1:A:515:THR:CG2	2.97	0.42
1:A:555:LEU:HA	1:A:555:LEU:HD23	1.83	0.42
1:E:492:PHE:CZ	1:E:548:LEU:HG	2.55	0.42
1:E:325:ARG:NH1	8:E:2214:HOH:O	2.34	0.42
1:A:129:LEU:O	1:A:133:GLU:HG2	2.20	0.42
1:A:581:LEU:HD23	1:A:583:PHE:HE1	1.85	0.42
1:E:590:ILE:HG22	1:E:591:GLU:N	2.34	0.42
3:C:174:PHE:N	3:C:175:PRO:HD2	2.35	0.42
1:E:630:THR:H	1:E:634:THR:HG21	1.84	0.42
3:C:17:THR:HG21	8:C:2014:HOH:O	2.18	0.42
3:G:154:THR:CG2	3:G:238:ARG:CG	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:ARG:HD2	8:E:2014:HOH:O	2.18	0.42
1:E:371:LEU:HD12	1:E:494:LEU:HD21	2.02	0.42
1:A:231:LYS:HB3	1:A:231:LYS:HE3	1.64	0.42
1:A:73:LYS:HZ1	1:A:192:HIS:HD2	1.63	0.42
1:A:433:LYS:HD3	1:A:460:ASP:OD2	2.20	0.42
1:A:541:GLU:O	1:A:545:GLU:HG2	2.19	0.42
1:E:622:LEU:HD23	1:E:622:LEU:HA	1.92	0.42
3:G:20:HIS:CE1	3:G:63:LEU:HD21	2.55	0.42
2:F:27:ASN:HD21	2:F:121:HIS:HE1	1.68	0.42
1:A:447:PRO:HD3	8:A:2216:HOH:O	2.19	0.42
2:B:57:GLN:O	2:B:59:LEU:HD23	2.20	0.42
2:F:117:THR:CG2	2:F:119:CYS:N	2.82	0.42
1:E:53:ILE:HD12	1:E:65:VAL:CG2	2.49	0.42
1:E:501:PHE:HB3	1:E:565:VAL:HG13	2.01	0.42
1:A:66:GLU:HG3	8:A:2040:HOH:O	2.20	0.42
1:E:391:PRO:HD2	1:E:595:GLN:OE1	2.20	0.42
1:A:561:MET:O	1:A:563:THR:O	2.38	0.42
3:C:143:LEU:HD23	3:C:198:ALA:HB1	2.02	0.42
3:C:161:LEU:CD1	3:C:179:LEU:HD12	2.50	0.42
1:E:138:GLU:CD	1:E:402:LYS:HB2	2.40	0.42
1:E:523:ARG:HG2	1:E:523:ARG:HH11	1.85	0.42
1:A:589:LYS:H	1:A:589:LYS:HG2	1.60	0.42
1:E:592:LEU:HA	1:E:603:GLN:HE21	0.64	0.42
1:E:625:ARG:HH22	5:E:1765:MGD:H15	1.67	0.42
1:A:138:GLU:CD	1:A:402:LYS:HB2	2.40	0.42
1:A:457:LYS:HD2	8:A:2224:HOH:O	2.20	0.42
2:B:3:ARG:HD2	2:B:62:GLU:OE2	2.19	0.42
1:E:186:GLY:HA3	1:E:583:PHE:C	2.41	0.42
1:E:288:GLU:HG3	8:E:2186:HOH:O	2.20	0.41
1:E:391:PRO:HD3	1:E:595:GLN:CD	2.40	0.41
1:E:369:PRO:HG2	1:E:494:LEU:HB3	2.02	0.41
2:B:166:ARG:HH22	3:C:249:GLN:HE21	1.66	0.41
3:G:240:LEU:CD1	3:G:240:LEU:C	2.88	0.41
1:E:335:VAL:CG1	1:E:335:VAL:O	2.68	0.41
1:A:494:LEU:HD22	1:A:502:ILE:HG12	2.01	0.41
2:B:169:GLN:NE2	8:B:2129:HOH:O	2.37	0.41
1:E:53:ILE:HG22	1:E:78:LEU:HD11	2.02	0.41
2:F:27:ASN:O	2:F:28:GLU:C	2.58	0.41
2:F:135:CYS:HA	2:F:136:PRO:HD3	1.75	0.41
1:A:430:TYR:HB2	1:A:431:PRO:CD	2.50	0.41
1:A:629:HIS:ND1	1:A:634:THR:CG2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:LEU:O	3:C:109:GLY:C	2.59	0.41
1:E:494:LEU:HD23	1:E:502:ILE:HG23	2.02	0.41
1:E:648:GLU:CG	1:E:681:ARG:NH1	2.80	0.41
3:C:193:THR:HG23	3:C:193:THR:O	2.20	0.41
1:E:670:VAL:HB	1:E:740:ARG:HG3	2.01	0.41
1:A:712:ARG:NH2	8:A:2348:HOH:O	2.52	0.41
1:E:106:GLN:NE2	8:E:2062:HOH:O	2.53	0.41
1:E:95:LEU:CD2	8:E:2278:HOH:O	2.52	0.41
1:E:201:ARG:NH2	1:E:228:ASN:O	2.43	0.41
1:A:501:PHE:HA	1:A:564:LEU:O	2.20	0.41
3:G:73:PHE:HA	8:G:2022:HOH:O	2.21	0.41
3:G:19:LEU:O	3:G:19:LEU:HD23	2.20	0.41
1:E:604:PRO:O	1:E:606:PRO:HD2	2.18	0.41
3:G:208:TRP:O	3:G:212:PHE:CD2	2.73	0.41
3:G:63:LEU:HD22	7:G:1251:PCI:C4	2.51	0.41
2:F:166:ARG:NH2	3:G:248:GLN:HG3	2.35	0.41
1:A:122:ASP:CB	8:A:2070:HOH:O	2.68	0.41
1:A:113:ARG:CZ	8:A:2066:HOH:O	2.69	0.41
3:C:227:ALA:HB3	3:C:228:PRO:HD3	2.03	0.41
1:A:626:SER:HB2	1:A:696:VAL:HG11	2.02	0.41
2:B:157:LYS:HD3	8:F:2039:HOH:O	2.20	0.41
1:A:241:THR:HG21	2:B:14:VAL:HB	2.02	0.41
1:A:277:GLU:HB3	1:A:281:LYS:NZ	2.35	0.41
2:F:122:ARG:HG2	2:F:127:LYS:HE3	2.03	0.41
1:E:345:MET:HB3	1:E:605:LEU:HD11	2.02	0.41
1:E:649:VAL:HG13	1:E:695:ILE:HG23	2.01	0.41
2:B:192:VAL:CG1	2:B:193:HIS:N	2.81	0.41
3:G:223:GLU:N	8:G:2068:HOH:O	2.52	0.41
1:E:497:HIS:HB3	1:E:499:THR:O	2.20	0.41
1:E:71:ASN:HD21	1:E:73:LYS:HB2	1.86	0.41
1:E:424:MET:HE2	1:E:455:ALA:HB1	2.01	0.41
1:E:314:GLU:HG3	8:E:2202:HOH:O	2.19	0.41
1:E:107:ARG:O	1:E:108:GLY:C	2.56	0.41
1:E:422:GLU:N	1:E:423:PRO:CD	2.83	0.41
2:B:135:CYS:HA	2:B:136:PRO:HD3	1.88	0.41
1:E:753:THR:HG22	1:E:757:LYS:HE3	2.01	0.41
1:A:462:TYR:OH	1:A:472:HIS:O	2.31	0.41
2:F:19:CYS:HB2	2:F:131:CYS:HB2	2.02	0.41
1:E:606:PRO:HG2	1:E:607:VAL:H	1.85	0.41
2:F:78:THR:HG23	2:F:79:LYS:N	2.35	0.41
1:A:722:ARG:NE	8:A:2356:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:ARG:NH2	3:G:248:GLN:NE2	2.68	0.41
1:E:292:HIS:HD2	8:E:2085:HOH:O	2.02	0.41
1:E:101:ARG:HB2	1:E:477:ASP:HA	2.03	0.41
1:A:395:ASP:CA	1:A:399:GLU:CG	2.68	0.41
1:E:297:THR:HG22	1:E:300:TRP:N	2.17	0.41
1:A:449:VAL:CG1	1:A:453:LYS:HE3	2.51	0.41
1:A:248:ARG:HB3	8:A:2136:HOH:O	2.20	0.41
1:A:538:LYS:HE2	1:A:538:LYS:N	2.35	0.41
1:E:283:THR:HG23	1:E:590:ILE:HG13	2.03	0.41
1:A:423:PRO:HB2	1:A:432:ILE:HD12	2.02	0.41
2:F:36:LEU:HD22	4:F:1195:SF4:S4	2.61	0.41
1:A:370:TYR:CD2	1:A:551:LEU:HD21	2.56	0.41
1:E:60:ASN:ND2	8:E:2022:HOH:O	2.52	0.41
1:E:346:ALA:HB2	1:E:605:LEU:HD12	2.02	0.41
1:E:470:GLN:O	1:E:471:GLU:C	2.59	0.41
3:G:32:LEU:HD12	3:G:120:LEU:HD12	2.03	0.41
3:G:170:TRP:CE3	3:G:171:ALA:N	2.89	0.41
1:E:249:TRP:CZ2	1:E:251:PRO:HB3	2.55	0.41
1:E:630:THR:O	1:E:631:PHE:O	2.38	0.41
1:A:523:ARG:HG2	1:A:523:ARG:NH1	2.35	0.41
3:G:150:LEU:HA	3:G:150:LEU:HD23	1.87	0.41
2:F:72:THR:HG21	2:F:89:LYS:C	2.40	0.41
1:A:422:GLU:N	1:A:423:PRO:CD	2.84	0.41
1:E:435:LEU:HB3	1:E:459:LEU:CD1	2.51	0.41
1:A:435:LEU:O	1:A:462:TYR:HA	2.21	0.41
1:E:621:LEU:HD22	1:E:622:LEU:N	2.36	0.40
3:C:76:HIS:O	3:C:79:LEU:HB2	2.21	0.40
1:A:588:GLY:HA3	8:A:2156:HOH:O	2.21	0.40
1:E:427:GLY:O	1:E:428:GLU:O	2.39	0.40
1:E:620:ARG:HA	1:E:738:PHE:HD2	1.86	0.40
1:A:389:SER:CA	1:A:595:GLN:HE22	2.35	0.40
1:E:422:GLU:N	1:E:423:PRO:HD2	2.35	0.40
1:E:197:TRP:CB	1:E:221:ASP:HB3	2.51	0.40
2:B:39:ARG:HD2	2:B:56:GLU:OE2	2.22	0.40
1:E:323:LYS:HD3	1:E:354:LEU:C	2.39	0.40
1:A:647:ASN:ND2	1:A:713:GLY:HA3	2.35	0.40
1:A:232:VAL:N	1:A:247:HIS:CD2	2.84	0.40
1:A:548:LEU:HD23	1:A:548:LEU:HA	1.79	0.40
1:A:558:MET:CE	1:A:558:MET:HA	2.46	0.40
1:E:233:VAL:HG13	1:E:248:ARG:HB2	2.03	0.40
3:C:71:ARG:HG2	3:C:72:PHE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:47:ARG:O	3:G:50:LEU:O	2.39	0.40
2:B:117:THR:HG22	2:B:119:CYS:CA	2.51	0.40
2:B:143:GLY:N	2:B:152:VAL:CG2	2.84	0.40
1:E:422:GLU:HG3	8:E:2107:HOH:O	2.20	0.40
3:C:13:PHE:CZ	3:C:247:GLN:HG2	2.56	0.40
1:A:258:THR:HB	1:A:608:PHE:HA	2.03	0.40
5:E:1766:MGD:H8	8:E:2426:HOH:O	2.21	0.40
1:E:625:ARG:HD2	5:E:1766:MGD:C17	2.52	0.40
1:E:650:TRP:HB2	1:E:694:TYR:HB3	2.03	0.40
1:E:650:TRP:O	1:E:693:VAL:HG22	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:OE2	1:E:133:GLU:C[2_674]	1.63	0.57
1:A:399:GLU:OE2	1:E:134:LYS:N[2_674]	1.75	0.45
1:A:399:GLU:OE2	1:E:133:GLU:O[2_674]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	733/765 (96%)	653 (89%)	46 (6%)	34 (5%)	3	3
1	E	733/765 (96%)	635 (87%)	63 (9%)	35 (5%)	3	3
2	B	192/195 (98%)	177 (92%)	12 (6%)	3 (2%)	12	21
2	F	192/195 (98%)	179 (93%)	9 (5%)	4 (2%)	9	14
3	C	249/253 (98%)	232 (93%)	12 (5%)	5 (2%)	9	15
3	G	249/253 (98%)	221 (89%)	21 (8%)	7 (3%)	6	9
All	All	2348/2426 (97%)	2097 (89%)	163 (7%)	88 (4%)	4	5

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	TRP
1	A	340	ASP
1	A	428	GLU
1	A	429	PRO
1	A	431	PRO
1	A	535	PHE
1	A	562	GLY
1	A	570	PRO
1	A	586	ALA
1	A	587	SER
1	A	593	TYR
1	A	605	LEU
1	A	678	GLY
1	A	687	ARG
1	A	730	GLY
2	B	17	ALA
3	C	208	PHE
3	C	250	GLY
1	E	92	PRO
1	E	93	ASP
1	E	109	GLU
1	E	324	PRO
1	E	396	HIS
1	E	397	GLU
1	E	428	GLU
1	E	552	GLY
1	E	567	ARG
1	E	583	PHE
1	E	593	TYR
1	E	607	VAL
1	E	631	PHE
1	E	678	GLY
1	E	686	ALA
2	F	46	TYR
3	G	108	GLY
3	G	113	ARG
3	G	222	GLN
1	A	365	ILE
1	A	399	GLU
1	A	430	TYR
1	A	434	GLY
1	A	582	PRO

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Mol	Chain	Res	Type
1	A	592	LEU
1	A	607	VAL
1	A	631	PHE
1	A	633	ARG
2	B	193	HIS
3	C	112	SER
3	C	172	ALA
1	E	337	TYR
1	E	391	PRO
1	E	606	PRO
1	E	685	THR
2	F	179	ASN
3	G	39	LEU
3	G	51	TYR
3	G	249	GLY
1	A	216	ASN
1	A	389	SER
1	A	398	PRO
1	E	389	SER
1	E	429	PRO
1	E	466	ASP
1	E	469	PRO
1	E	471	GLU
1	E	513	PHE
1	E	570	PRO
1	E	627	PRO
2	F	45	GLU
2	F	178	LEU
1	A	478	VAL
2	B	115	LYS
1	E	478	VAL
1	E	763	ARG
3	G	38	HIS
1	A	387	GLY
3	C	113	GLN
1	E	70	ALA
1	E	710	HIS
1	A	610	PRO
1	A	684	PRO
1	E	610	PRO
1	A	584	GLY
1	A	609	THR

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Mol	Chain	Res	Type
1	E	434	GLY
1	A	194	PRO
1	E	604	PRO
1	E	609	THR

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	A	610/632 (96%)	499 (82%)	111 (18%)	2	3
1	E	610/632 (96%)	506 (83%)	104 (17%)	2	4
2	B	162/163 (99%)	144 (89%)	18 (11%)	8	14
2	F	162/163 (99%)	147 (91%)	15 (9%)	11	21
3	C	185/187 (99%)	164 (89%)	21 (11%)	7	13
3	G	185/187 (99%)	163 (88%)	22 (12%)	6	12
All	All	1914/1964 (98%)	1623 (85%)	291 (15%)	3	6

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ILE
1	A	61	ARG
1	A	65	VAL
1	A	77	ARG
1	A	87	GLN
1	A	97	ARG
1	A	103	GLU
1	A	106	GLN
1	A	111	LYS
1	A	116	THR
1	A	119	GLU
1	A	126	LYS
1	A	134	LYS
1	A	156	LEU

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Mol	Chain	Res	Type
1	A	167	LYS
1	A	174	THR
1	A	187	ARG
1	A	189	ILE
1	A	209	HIS
1	A	213	ASP
1	A	214	THR
1	A	217	THR
1	A	231	LYS
1	A	252	ILE
1	A	256	THR
1	A	260	LEU
1	A	281	LYS
1	A	283	THR
1	A	286	PHE
1	A	289	LEU
1	A	293	VAL
1	A	297	THR
1	A	299	GLU
1	A	302	GLU
1	A	305	THR
1	A	323	LYS
1	A	327	VAL
1	A	335	VAL
1	A	368	SER
1	A	371	LEU
1	A	372	GLU
1	A	379	LEU
1	A	382	GLU
1	A	395	ASP
1	A	413	ARG
1	A	414	SER
1	A	415	THR
1	A	418	GLN
1	A	421	ILE
1	A	428	GLU
1	A	440	ILE
1	A	441	ASN
1	A	454	GLU
1	A	457	LYS
1	A	470	GLN
1	A	477	ASP

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Mol	Chain	Res	Type
1	A	484	THR
1	A	510	GLU
1	A	512	LEU
1	A	515	THR
1	A	528	ARG
1	A	529	LEU
1	A	532	GLU
1	A	533	GLN
1	A	538	LYS
1	A	539	THR
1	A	541	GLU
1	A	542	GLU
1	A	550	SER
1	A	553	LEU
1	A	555	LEU
1	A	558	MET
1	A	561	MET
1	A	578	GLU
1	A	580	ARG
1	A	587	SER
1	A	589	LYS
1	A	591	GLU
1	A	592	LEU
1	A	594	CYS
1	A	595	GLN
1	A	596	ARG
1	A	597	PHE
1	A	603	GLN
1	A	605	LEU
1	A	608	PHE
1	A	616	GLU
1	A	621	LEU
1	A	633	ARG
1	A	647	ASN
1	A	648	GLU
1	A	651	ILE
1	A	662	LYS
1	A	663	GLU
1	A	671	ASN
1	A	672	GLN
1	A	680	VAL
1	A	683	LYS

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Mol	Chain	Res	Type
1	A	685	THR
1	A	693	VAL
1	A	702	LYS
1	A	708	LEU
1	A	721	THR
1	A	724	LYS
1	A	725	LEU
1	A	736	VAL
1	A	739	VAL
1	A	741	LEU
1	A	743	LYS
1	A	746	ARG
1	A	762	GLU
2	B	1	MET
2	B	25	MET
2	B	39	ARG
2	B	69	VAL
2	B	72	THR
2	B	78	THR
2	B	105	ARG
2	B	114	SER
2	B	117	THR
2	B	118	PHE
2	B	125	LYS
2	B	131	CYS
2	B	140	ARG
2	B	152	VAL
2	B	154	LYS
2	B	164	VAL
2	B	175	LEU
2	B	187	THR
3	C	11	GLN
3	C	17	THR
3	C	18	ASN
3	C	20	LEU
3	C	40	LEU
3	C	67	GLU
3	C	71	ARG
3	C	75	THR
3	C	110	LYS
3	C	130	TYR
3	C	140	ASN

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Mol	Chain	Res	Type
3	C	145	ASN
3	C	155	THR
3	C	163	LEU
3	C	193	THR
3	C	197	GLU
3	C	216	LEU
3	C	225	ARG
3	C	232	LEU
3	C	241	LEU
3	C	249	GLN
1	E	65	VAL
1	E	69	GLU
1	E	101	ARG
1	E	111	LYS
1	E	113	ARG
1	E	114	VAL
1	E	119	GLU
1	E	126	LYS
1	E	145	HIS
1	E	172	LEU
1	E	174	THR
1	E	187	ARG
1	E	208	HIS
1	E	209	HIS
1	E	213	ASP
1	E	214	THR
1	E	217	THR
1	E	224	LEU
1	E	240	SER
1	E	250	LEU
1	E	256	THR
1	E	260	LEU
1	E	272	ASP
1	E	286	PHE
1	E	289	LEU
1	E	293	VAL
1	E	297	THR
1	E	298	PRO
1	E	299	GLU
1	E	305	THR
1	E	327	VAL
1	E	335	VAL

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Mol	Chain	Res	Type
1	E	360	PRO
1	E	371	LEU
1	E	389	SER
1	E	395	ASP
1	E	402	LYS
1	E	413	ARG
1	E	415	THR
1	E	418	GLN
1	E	421	ILE
1	E	428	GLU
1	E	440	ILE
1	E	441	ASN
1	E	466	ASP
1	E	470	GLN
1	E	484	THR
1	E	488	ARG
1	E	498	LYS
1	E	499	THR
1	E	504	LEU
1	E	510	GLU
1	E	512	LEU
1	E	515	THR
1	E	528	ARG
1	E	533	GLN
1	E	538	LYS
1	E	539	THR
1	E	540	ILE
1	E	541	GLU
1	E	554	ASP
1	E	555	LEU
1	E	558	MET
1	E	564	LEU
1	E	569	LYS
1	E	577	LYS
1	E	581	LEU
1	E	585	THR
1	E	591	GLU
1	E	595	GLN
1	E	596	ARG
1	E	598	LYS
1	E	602	HIS
1	E	605	LEU

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Mol	Chain	Res	Type
1	E	607	VAL
1	E	608	PHE
1	E	609	THR
1	E	620	ARG
1	E	621	LEU
1	E	626	SER
1	E	633	ARG
1	E	647	ASN
1	E	649	VAL
1	E	651	ILE
1	E	657	LYS
1	E	667	VAL
1	E	671	ASN
1	E	672	GLN
1	E	676	LYS
1	E	680	VAL
1	E	685	THR
1	E	691	ASP
1	E	693	VAL
1	E	702	LYS
1	E	708	LEU
1	E	721	THR
1	E	725	LEU
1	E	736	VAL
1	E	739	VAL
1	E	740	ARG
1	E	746	ARG
1	E	748	ARG
1	E	751	SER
1	E	752	LEU
2	F	49	LEU
2	F	69	VAL
2	F	72	THR
2	F	88	LYS
2	F	114	SER
2	F	117	THR
2	F	118	PHE
2	F	133	GLU
2	F	145	LEU
2	F	150	SER
2	F	152	VAL
2	F	164	VAL

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Mol	Chain	Res	Type
2	F	171	THR
2	F	175	LEU
2	F	187	THR
3	G	10	GLN
3	G	17	ASN
3	G	20	HIS
3	G	39	LEU
3	G	40	LYS
3	G	64	TRP
3	G	66	GLU
3	G	74	THR
3	G	88	ILE
3	G	113	ARG
3	G	129	TYR
3	G	136	VAL
3	G	139	ASN
3	G	144	ASN
3	G	154	THR
3	G	162	LEU
3	G	167	LYS
3	G	192	THR
3	G	196	GLU
3	G	204	GLU
3	G	215	LEU
3	G	240	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	71	ASN
1	A	83	GLN
1	A	192	HIS
1	A	209	HIS
1	A	220	GLN
1	A	247	HIS
1	A	322	HIS
1	A	367	GLN
1	A	441	ASN
1	A	470	GLN
1	A	509	HIS
1	A	533	GLN

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Mol	Chain	Res	Type
1	A	595	GLN
1	A	602	HIS
1	A	603	GLN
1	A	647	ASN
1	A	671	ASN
1	A	672	GLN
1	A	717	ASN
2	B	27	ASN
2	B	35	ASN
2	B	57	GLN
2	B	77	GLN
2	B	179	ASN
3	C	9	ASN
3	C	11	GLN
3	C	21	HIS
3	C	39	HIS
3	C	84	HIS
3	C	140	ASN
3	C	145	ASN
3	C	201	HIS
3	C	249	GLN
1	E	60	ASN
1	E	71	ASN
1	E	83	GLN
1	E	192	HIS
1	E	209	HIS
1	E	218	GLN
1	E	220	GLN
1	E	247	HIS
1	E	292	HIS
1	E	322	HIS
1	E	396	HIS
1	E	418	GLN
1	E	441	ASN
1	E	470	GLN
1	E	509	HIS
1	E	533	GLN
1	E	602	HIS
1	E	603	GLN
1	E	635	GLN
1	E	647	ASN
1	E	671	ASN

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Mol	Chain	Res	Type
1	E	672	GLN
1	E	717	ASN
2	F	27	ASN
2	F	35	ASN
2	F	57	GLN
2	F	77	GLN
2	F	179	ASN
3	G	8	ASN
3	G	38	HIS
3	G	137	ASN
3	G	139	ASN
3	G	248	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SF4	A	1764	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	A	1765	6	38,52,52	1.91	5 (13%)	43,81,81	3.14	18 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MGD	A	1766	6	38,52,52	1.73	8 (21%)	43,81,81	2.82	12 (27%)
4	SF4	B	1194	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	1195	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	1196	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	1197	2	0,12,12	0.00	-	0,24,24	0.00	-
7	PCI	C	1252	-	12,12,12	1.17	0	18,18,18	1.25	3 (16%)
4	SF4	E	1764	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	E	1765	6	38,52,52	1.55	6 (15%)	43,81,81	2.61	17 (39%)
5	MGD	E	1766	6	38,52,52	1.97	12 (31%)	43,81,81	2.51	14 (32%)
4	SF4	F	1194	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	F	1195	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	F	1196	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	F	1197	2	0,12,12	0.00	-	0,24,24	0.00	-
7	PCI	G	1251	-	12,12,12	1.08	0	18,18,18	1.09	1 (5%)

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
4	SF4	A	1764	1	-	0/0/48/48	0/6/5/5
5	MGD	A	1765	6	-	0/18/66/66	0/6/6/6
5	MGD	A	1766	6	-	0/18/66/66	0/6/6/6
4	SF4	B	1194	2	-	0/0/48/48	0/6/5/5
4	SF4	B	1195	2	-	0/0/48/48	0/6/5/5
4	SF4	B	1196	2	-	0/0/48/48	0/6/5/5
4	SF4	B	1197	2	-	0/0/48/48	0/6/5/5
7	PCI	C	1252	-	-	0/0/0/0	0/1/1/1
4	SF4	E	1764	1	-	0/0/48/48	0/6/5/5
5	MGD	E	1765	6	-	0/18/66/66	0/6/6/6
5	MGD	E	1766	6	-	0/18/66/66	0/6/6/6
4	SF4	F	1194	2	-	0/0/48/48	0/6/5/5
4	SF4	F	1195	2	-	0/0/48/48	0/6/5/5
4	SF4	F	1196	2	-	0/0/48/48	0/6/5/5
4	SF4	F	1197	2	-	0/0/48/48	0/6/5/5
7	PCI	G	1251	-	-	0/0/0/0	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1765	MGD	C23-C14	-7.07	1.48	1.53
5	A	1766	MGD	C23-C14	-4.70	1.50	1.53
5	E	1765	MGD	C23-C14	-4.31	1.50	1.53
5	E	1766	MGD	C23-C14	-3.94	1.50	1.53
5	E	1766	MGD	C21-N22	-3.91	1.27	1.35
5	A	1766	MGD	C14-N15	-3.50	1.40	1.45
5	E	1766	MGD	C19-N19	-3.27	1.27	1.34
5	E	1766	MGD	C19-N18	-3.17	1.29	1.35
5	E	1766	MGD	C16-N15	-3.03	1.31	1.38
5	A	1766	MGD	PB-O2B	-2.73	1.43	1.54
5	E	1766	MGD	C14-N15	-2.62	1.41	1.45
5	A	1766	MGD	PA-O2A	-2.49	1.44	1.54
5	E	1766	MGD	O11-C11	-2.21	1.40	1.43
5	E	1766	MGD	O4'-C4'	-2.21	1.39	1.45
5	E	1765	MGD	C3'-C4'	-2.21	1.47	1.53
5	E	1765	MGD	C19-N18	-2.13	1.31	1.35
5	A	1766	MGD	C21-N22	-2.01	1.31	1.35
5	A	1765	MGD	C16-C21	2.28	1.46	1.41
5	E	1766	MGD	C16-C21	2.33	1.46	1.41
5	E	1766	MGD	C6-C5	2.58	1.46	1.41
5	E	1765	MGD	C6-C5	2.61	1.46	1.41
5	A	1766	MGD	C6-C5	2.69	1.46	1.41
5	A	1765	MGD	O4'-C1'	3.07	1.45	1.41
5	E	1765	MGD	C5-C4	3.17	1.47	1.40
5	A	1766	MGD	C5-C4	3.27	1.47	1.40
5	E	1765	MGD	C16-C21	3.29	1.48	1.41
5	E	1766	MGD	O3'-C3'	3.36	1.51	1.43
5	A	1765	MGD	C5-C4	3.38	1.48	1.40
5	A	1766	MGD	O11-C23	3.50	1.48	1.43
5	E	1766	MGD	C5-C4	4.28	1.50	1.40
5	A	1765	MGD	C6-C5	5.23	1.51	1.41

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1765	MGD	O11-C23-C14	-7.31	103.97	108.96
5	E	1765	MGD	C4-C5-N7	-6.04	103.92	109.48
5	A	1765	MGD	C5-C6-N1	-5.96	115.44	123.59
5	A	1765	MGD	C4-C5-N7	-5.04	104.84	109.48
5	A	1765	MGD	N3-C2-N1	-4.46	120.65	127.44
5	E	1766	MGD	C4'-O4'-C1'	-4.38	104.91	109.72
5	E	1765	MGD	C5-C6-N1	-4.37	117.61	123.59
5	E	1766	MGD	C5-C6-N1	-4.23	117.81	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1765	MGD	C1'-N9-C4	-3.77	121.25	126.94
5	E	1765	MGD	C6-C5-C4	-3.71	116.47	120.90
5	E	1765	MGD	N3-C2-N1	-3.55	122.03	127.44
5	A	1766	MGD	C5-C6-N1	-3.40	118.94	123.59
5	A	1766	MGD	N3-C2-N1	-3.36	122.33	127.44
5	A	1766	MGD	C6-C5-C4	-3.35	116.89	120.90
5	A	1765	MGD	N18-C19-N20	-3.19	120.30	125.53
5	E	1766	MGD	C4-C5-N7	-3.05	106.67	109.48
7	C	1252	PCI	C1-C2-C3	-2.69	118.87	121.21
5	A	1766	MGD	O5'-C5'-C4'	-2.60	99.52	109.12
5	E	1765	MGD	O3'-C3'-C4'	-2.59	103.28	111.05
5	A	1765	MGD	C6-C5-C4	-2.57	117.83	120.90
5	E	1765	MGD	C16-N15-C14	-2.52	111.86	118.65
5	A	1765	MGD	O4'-C4'-C5'	-2.45	100.57	109.32
7	G	1251	PCI	C1-C2-C3	-2.25	119.25	121.21
5	A	1766	MGD	C16-C21-N22	-2.18	116.06	118.34
5	A	1766	MGD	O4'-C4'-C5'	-2.02	102.09	109.32
5	E	1765	MGD	C16-C21-N22	2.07	120.50	118.34
5	A	1765	MGD	C16-C21-N22	2.09	120.53	118.34
5	E	1765	MGD	O2B-PB-O1B	2.15	124.19	112.53
5	E	1766	MGD	O3B-PB-O5'	2.23	108.86	102.94
5	A	1765	MGD	C4'-O4'-C1'	2.43	112.39	109.72
5	A	1766	MGD	O2B-PB-O3B	2.44	116.16	105.09
5	E	1765	MGD	N2-C2-N1	2.44	121.25	117.20
5	A	1765	MGD	N22-C21-N20	2.52	120.63	116.62
5	E	1766	MGD	N19-C19-N20	2.52	121.38	117.20
5	A	1765	MGD	O2B-PB-O3B	2.54	116.60	105.09
5	E	1766	MGD	O3'-C3'-C4'	2.54	118.67	111.05
5	E	1766	MGD	O2A-PA-O1A	2.56	126.39	112.53
7	C	1252	PCI	C1-C6-CL5	2.58	120.75	117.99
7	C	1252	PCI	C6-C1-C2	2.63	120.18	117.64
5	E	1766	MGD	C19-N20-C21	2.70	120.61	114.54
5	A	1765	MGD	PA-O3B-PB	2.89	140.84	132.73
5	A	1765	MGD	N19-C19-N18	3.03	122.22	117.20
5	E	1765	MGD	O3B-PA-O3A	3.04	111.00	102.94
5	E	1766	MGD	C17-N18-C19	3.11	120.26	115.94
5	A	1766	MGD	C2'-C1'-N9	3.17	119.13	114.29
5	E	1766	MGD	C6-N1-C2	3.20	120.38	115.94
5	A	1765	MGD	C2'-C1'-N9	3.21	119.20	114.29
5	E	1765	MGD	N22-C21-N20	3.31	121.88	116.62
5	E	1765	MGD	O3B-PB-O5'	3.37	111.88	102.94
5	E	1766	MGD	C21-C16-N15	3.39	123.12	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1766	MGD	N22-C21-N20	3.64	122.41	116.62
5	E	1765	MGD	C17-N18-C19	3.75	121.15	115.94
5	E	1766	MGD	O4'-C1'-N9	3.80	116.05	108.10
5	A	1765	MGD	N2-C2-N1	3.80	123.50	117.20
5	A	1765	MGD	C19-N20-C21	3.83	123.14	114.54
5	E	1765	MGD	C19-N20-C21	4.19	123.95	114.54
5	A	1766	MGD	C6-N1-C2	4.52	122.22	115.94
5	E	1766	MGD	N22-C21-N20	4.93	124.47	116.62
5	E	1765	MGD	C6-N1-C2	5.12	123.04	115.94
5	A	1766	MGD	O4'-C1'-N9	5.56	119.74	108.10
5	A	1765	MGD	C17-N18-C19	5.57	123.67	115.94
5	A	1765	MGD	C6-N1-C2	6.16	124.49	115.94
5	E	1766	MGD	O11-C23-C14	9.95	115.77	108.96
5	A	1765	MGD	O11-C23-C14	12.04	117.19	108.96
5	A	1766	MGD	O11-C23-C14	13.33	118.07	108.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1765	MGD	4	0
5	A	1766	MGD	3	0
4	B	1194	SF4	1	0
4	B	1195	SF4	1	0
4	B	1196	SF4	2	0
7	C	1252	PCI	11	0
4	E	1764	SF4	1	0
5	E	1765	MGD	5	0
5	E	1766	MGD	7	0
4	F	1194	SF4	3	0
4	F	1195	SF4	2	0
4	F	1196	SF4	1	0
7	G	1251	PCI	10	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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	A	735/765 (96%)	1.09	121 (16%)	2 2	27, 53, 85, 139	0
1	E	735/765 (96%)	0.94	104 (14%)	4 3	27, 52, 83, 141	0
2	B	194/195 (99%)	0.69	15 (7%)	16 18	29, 46, 70, 94	0
2	F	194/195 (99%)	0.95	17 (8%)	12 13	34, 51, 72, 93	0
3	C	251/253 (99%)	1.08	39 (15%)	3 3	35, 59, 85, 103	0
3	G	251/253 (99%)	1.57	72 (28%)	1 0	37, 68, 97, 111	0
All	All	2360/2426 (97%)	1.05	368 (15%)	3 2	27, 54, 86, 141	0

All (368) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	764	ARG	23.3
3	G	251	GLY	19.5
3	C	111	GLY	15.3
3	C	252	GLY	15.1
1	A	607	VAL	14.9
2	F	194	HIS	13.9
1	E	394	GLY	13.8
2	F	1	MET	12.5
1	E	398	PRO	11.5
1	E	396	HIS	11.1
2	B	1	MET	10.9
1	E	389	SER	10.8
1	E	393	GLY	10.5
1	A	389	SER	10.3
1	E	607	VAL	10.1
1	E	397	GLU	9.8
1	E	392	SER	9.5
3	C	223	GLN	9.4
1	E	764	ARG	9.1

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Mol	Chain	Res	Type	RSRZ
1	A	586	ALA	8.6
1	A	401	PHE	8.3
1	A	583	PHE	8.1
1	E	592	LEU	7.9
1	E	600	ALA	7.9
3	G	111	SER	7.7
1	A	284	VAL	7.6
1	A	393	GLY	7.6
3	G	221	TRP	7.5
1	E	390	GLY	7.4
2	B	193	HIS	7.2
3	C	222	TRP	7.1
1	A	397	GLU	6.8
1	E	388	CYS	6.6
1	A	398	PRO	6.6
3	G	110	GLY	6.6
3	G	104	LEU	6.5
2	F	193	HIS	6.5
1	E	400	GLY	6.4
1	E	594	CYS	6.4
1	A	396	HIS	6.4
1	A	592	LEU	6.3
1	A	606	PRO	6.2
3	G	224	ARG	6.2
3	C	226	LEU	6.0
3	G	225	LEU	5.9
1	A	388	CYS	5.8
1	E	395	ASP	5.8
3	G	107	LEU	5.7
3	G	63	LEU	5.5
1	E	401	PHE	5.5
3	G	76	ILE	5.5
1	A	392	SER	5.5
1	A	597	PHE	5.4
1	A	632	ALA	5.3
1	E	599	GLU	5.3
3	C	110	LYS	5.3
2	F	2	PRO	5.2
3	G	49	THR	5.2
1	A	385	ALA	5.1
1	A	390	GLY	5.0
3	G	50	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	362	GLY	4.9
3	G	163	ALA	4.9
3	C	224	GLU	4.8
1	E	34	ALA	4.8
1	A	538	LYS	4.8
2	B	46	TYR	4.8
3	G	69	ALA	4.8
1	E	595	GLN	4.6
1	E	133	GLU	4.5
2	B	79	LYS	4.5
1	A	207	GLY	4.5
3	G	73	PHE	4.5
2	F	16	CYS	4.4
1	A	399	GLU	4.4
3	G	109	LYS	4.3
1	E	391	PRO	4.2
1	E	323	LYS	4.1
1	E	47	CYS	4.1
1	A	594	CYS	4.1
1	A	599	GLU	4.1
2	F	79	LYS	4.1
3	C	70	ALA	4.1
1	A	384	ALA	4.0
1	E	608	PHE	4.0
1	A	34	ALA	4.0
1	E	385	ALA	4.0
1	A	567	ARG	4.0
3	G	77	TRP	3.9
1	E	597	PHE	3.9
1	A	561	MET	3.9
1	E	591	GLU	3.9
3	C	108	LEU	3.9
1	E	567	ARG	3.8
3	G	112	GLN	3.8
3	C	208	PHE	3.8
1	E	468	LEU	3.8
3	C	64	LEU	3.8
1	A	370	TYR	3.7
1	A	608	PHE	3.7
3	G	45	ALA	3.7
1	E	399	GLU	3.7
1	A	335	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
3	G	82	PHE	3.6
1	A	277	GLU	3.6
1	E	113	ARG	3.6
1	A	570	PRO	3.6
1	E	554	ASP	3.6
1	A	383	PRO	3.6
1	A	364	TYR	3.6
1	E	572	LEU	3.6
3	C	40	LEU	3.6
1	E	606	PRO	3.5
2	B	2	PRO	3.5
3	C	105	LEU	3.5
1	E	370	TYR	3.5
2	B	124	GLU	3.5
2	F	68	PRO	3.5
3	C	114	ARG	3.5
3	G	114	ALA	3.5
1	E	628	VAL	3.5
1	E	630	THR	3.4
1	E	384	ALA	3.4
1	A	571	TRP	3.4
3	G	41	GLY	3.4
1	E	214	THR	3.4
1	E	622	LEU	3.4
1	E	372	GLU	3.4
3	G	101	THR	3.4
3	G	117	TRP	3.4
2	B	146	GLU	3.4
1	A	42	GLN	3.3
2	F	110	ALA	3.3
3	G	149	GLY	3.3
3	C	112	SER	3.3
1	A	36	GLU	3.3
1	A	596	ARG	3.2
1	E	469	PRO	3.2
1	A	595	GLN	3.2
1	A	40	VAL	3.2
1	E	590	ILE	3.2
1	E	173	CYS	3.2
3	C	75	THR	3.2
1	A	537	TRP	3.2
1	E	632	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	36	GLU	3.2
1	E	508	ALA	3.1
3	G	38	HIS	3.1
3	G	146	LEU	3.1
1	A	431	PRO	3.1
1	A	38	LYS	3.1
3	G	53	LEU	3.1
3	G	64	TRP	3.1
3	G	106	TYR	3.1
2	F	170	GLY	3.0
1	A	281	LYS	3.0
3	G	71	PHE	3.0
1	A	47	CYS	3.0
2	B	194	HIS	3.0
1	A	48	PHE	3.0
3	C	71	ARG	3.0
3	G	206	GLY	3.0
1	E	478	VAL	3.0
3	G	39	LEU	3.0
3	C	94	TRP	3.0
3	G	127	LEU	2.9
1	A	557	THR	2.9
1	A	590	ILE	2.9
2	F	149	GLU	2.9
3	G	153	LEU	2.9
2	B	16	CYS	2.9
1	A	548	LEU	2.9
1	A	591	GLU	2.9
1	E	324	PRO	2.9
3	G	228	TRP	2.9
2	F	46	TYR	2.9
3	C	69	PRO	2.9
1	A	579	GLY	2.9
3	G	57	ALA	2.9
1	E	748	ARG	2.8
3	G	207	PHE	2.8
1	A	295	ASP	2.8
1	A	346	ALA	2.8
3	C	149	ALA	2.8
1	A	102	VAL	2.8
3	G	15	TRP	2.8
1	A	573	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
3	G	169	PRO	2.8
1	A	337	TYR	2.8
3	G	46	ARG	2.8
3	G	74	THR	2.8
3	G	105	LEU	2.8
3	G	162	LEU	2.8
1	A	400	GLY	2.8
3	C	109	GLY	2.8
1	A	748	ARG	2.8
1	A	151	TRP	2.7
3	G	150	LEU	2.7
2	F	17	ALA	2.7
1	A	296	PHE	2.7
3	G	100	LEU	2.7
3	G	166	LEU	2.7
1	E	467	VAL	2.7
1	E	536	PRO	2.7
3	G	129	TYR	2.7
1	E	634	THR	2.7
1	A	577	LYS	2.7
3	C	79	LEU	2.7
3	G	122	PHE	2.7
1	A	560	GLY	2.7
1	A	585	THR	2.7
1	E	578	GLU	2.7
3	G	171	ALA	2.7
1	A	359	ARG	2.6
1	A	527	LEU	2.6
1	A	685	THR	2.6
3	G	118	ALA	2.6
1	A	515	THR	2.6
3	C	78	TRP	2.6
1	A	600	ALA	2.6
1	E	48	PHE	2.6
1	A	602	HIS	2.6
3	C	170	PRO	2.6
1	E	386	GLY	2.6
2	B	81	GLY	2.6
3	G	28	GLY	2.6
1	E	580	ARG	2.6
3	G	167	LYS	2.6
3	G	70	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	484	THR	2.6
3	C	95	GLY	2.5
1	A	428	GLU	2.5
3	C	179	LEU	2.5
3	G	154	THR	2.5
1	A	580	ARG	2.5
2	B	120	ALA	2.5
1	E	286	PHE	2.5
1	E	635	GLN	2.5
1	A	628	VAL	2.5
3	C	186	LEU	2.5
1	E	584	GLY	2.5
1	E	631	PHE	2.5
1	A	285	GLY	2.5
2	F	14	VAL	2.5
1	E	457	LYS	2.5
1	E	574	ASP	2.5
1	A	129	LEU	2.5
1	E	549	GLN	2.5
3	G	34	ALA	2.5
1	E	114	VAL	2.4
1	E	605	LEU	2.4
3	G	52	ALA	2.4
1	A	569	LYS	2.4
1	A	656	ALA	2.4
1	E	596	ARG	2.4
2	F	71	PRO	2.4
1	E	546	THR	2.4
1	E	685	THR	2.4
1	E	603	GLN	2.4
1	E	355	GLY	2.4
1	E	553	LEU	2.4
1	A	206	ILE	2.4
3	G	56	ILE	2.4
3	C	113	GLN	2.4
1	A	430	TYR	2.4
1	A	510	GLU	2.4
1	E	579	GLY	2.4
1	A	117	TRP	2.4
1	A	575	TRP	2.4
1	E	575	TRP	2.4
3	C	147	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	57	ALA	2.4
1	E	629	HIS	2.4
2	B	149	GLU	2.4
1	E	383	PRO	2.3
1	A	427	GLY	2.3
1	A	678	GLY	2.3
1	A	553	LEU	2.3
1	A	556	GLU	2.3
1	E	561	MET	2.3
3	C	77	ILE	2.3
3	G	27	ALA	2.3
1	A	584	GLY	2.3
1	E	151	TRP	2.3
1	A	349	TYR	2.3
1	A	605	LEU	2.3
3	C	68	SER	2.3
1	E	577	LYS	2.3
1	A	763	ARG	2.3
1	A	761	ASP	2.3
1	A	173	CYS	2.3
1	A	59	GLY	2.3
3	C	229	TRP	2.3
1	E	331	THR	2.3
3	G	131	GLY	2.3
1	A	375	PRO	2.3
1	A	205	LEU	2.3
2	B	134	THR	2.3
1	A	361	GLY	2.3
3	G	93	TRP	2.3
1	E	50	ARG	2.3
1	A	70	ALA	2.2
1	E	532	GLU	2.2
1	A	593	TYR	2.2
1	A	587	SER	2.2
1	A	554	ASP	2.2
2	F	70	CYS	2.2
1	A	465	ILE	2.2
1	E	336	TRP	2.2
1	E	537	TRP	2.2
1	A	360	PRO	2.2
3	G	42	ASP	2.2
1	A	601	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	123	LEU	2.2
1	A	54	VAL	2.2
3	G	157	VAL	2.2
1	A	325	ARG	2.2
1	E	295	ASP	2.2
3	C	227	ALA	2.2
1	E	292	HIS	2.2
3	C	219	GLY	2.2
1	A	63	TYR	2.2
1	A	270	TYR	2.2
1	A	43	ILE	2.2
1	E	79	CYS	2.2
1	E	662	LYS	2.2
3	C	241	LEU	2.2
1	E	176	PRO	2.2
1	A	467	VAL	2.1
3	G	148	ALA	2.1
2	F	88	LYS	2.1
1	E	224	LEU	2.1
3	G	178	LEU	2.1
3	G	130	PRO	2.1
1	E	569	LYS	2.1
3	G	180	GLY	2.1
1	E	335	VAL	2.1
1	A	208	HIS	2.1
3	G	72	ARG	2.1
1	A	576	GLU	2.1
1	A	342	TYR	2.1
1	E	759	PRO	2.1
3	G	67	SER	2.1
3	C	204	GLU	2.1
1	A	153	VAL	2.1
2	B	135	CYS	2.1
2	F	67	VAL	2.1
1	A	282	TYR	2.1
1	A	50	ARG	2.1
1	A	146	GLY	2.1
3	C	173	LEU	2.1
3	G	185	LEU	2.1
1	E	66	GLU	2.1
1	E	593	TYR	2.1
1	E	31	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	585	THR	2.1
1	A	240	SER	2.1
1	A	568	GLY	2.0
1	E	498	LYS	2.0
1	E	44	CYS	2.0
1	E	172	LEU	2.0
3	G	48	TYR	2.0
3	C	82	SER	2.0
1	E	106	GLN	2.0
1	E	174	THR	2.0
3	G	222	GLN	2.0
3	C	211	GLY	2.0
1	E	421	ILE	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, 95th 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
7	PCI	C	1252	12/12	0.91	0.23	0.26	34,37,38,41	0
7	PCI	G	1251	12/12	0.70	0.27	0.14	48,49,50,50	0
5	MGD	E	1766	47/47	0.95	0.23	-0.24	25,34,40,42	0
5	MGD	E	1765	47/47	0.96	0.23	-0.26	35,41,46,48	0
5	MGD	A	1765	47/47	0.95	0.21	-0.27	33,42,44,45	0
4	SF4	B	1196	8/8	0.82	0.16	-0.35	47,53,56,58	0
5	MGD	A	1766	47/47	0.96	0.18	-1.02	29,36,41,42	0
4	SF4	A	1764	8/8	0.96	0.16	-1.18	35,41,42,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SF4	F	1196	8/8	0.90	0.14	-1.25	42,45,47,48	0
4	SF4	F	1194	8/8	0.88	0.14	-1.27	75,78,79,81	0
4	SF4	B	1194	8/8	0.83	0.15	-1.48	70,71,72,73	0
4	SF4	E	1764	8/8	0.96	0.16	-1.60	37,42,46,46	0
4	SF4	B	1197	8/8	0.97	0.10	-1.69	39,40,43,45	0
4	SF4	F	1197	8/8	0.93	0.12	-2.62	49,51,53,55	0
4	SF4	F	1195	8/8	0.93	0.10	-2.77	38,43,44,44	0
4	SF4	B	1195	8/8	0.93	0.11	-4.58	47,50,52,53	0
6	MO	A	1767	1/1	0.98	0.13	-	42,42,42,42	0
6	MO	E	1767	1/1	0.98	0.14	-	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.