Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:17 PM BST

PDB ID	:	4FQU
Title	:	Glutathionyl-Hydroquinone Reductase PcpF of Sphingobium chlorophenolicum
Authors	:	Green, A.R.; Hayes, R.P.; Xun, L.; Kang, C.
Deposited on	:	2012-06-25
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/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:

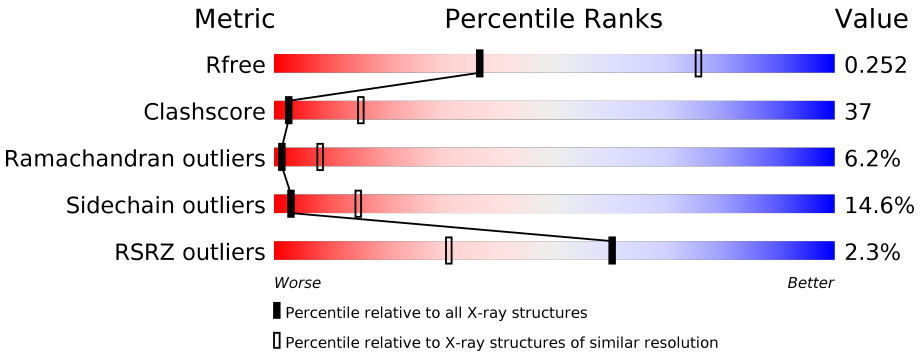
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	313	2% 55% 33% 10%
1	B	313	2% 52% 35% 8%
1	C	313	2% 45% 43% 9%
1	D	313	3% 41% 46% 12%
1	E	313	3% 45% 40% 13%
1	F	313	2% 55% 33% 7%

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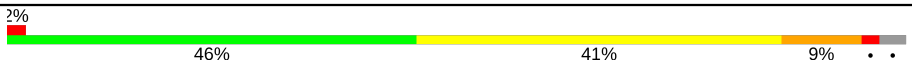
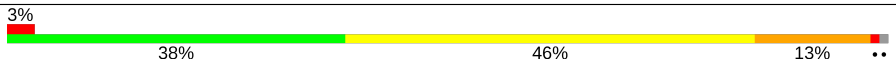
Mol	Chain	Length	Quality of chain
1	G	313	
1	H	313	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19729 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 Putative glutathione transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2491	1592	435	458	6			
1	B	303	Total	C	N	O	S	0	0	0
			2420	1549	424	441	6			
1	C	312	Total	C	N	O	S	0	0	0
			2482	1584	435	457	6			
1	D	312	Total	C	N	O	S	0	0	0
			2481	1586	432	457	6			
1	E	312	Total	C	N	O	S	0	0	0
			2484	1587	435	456	6			
1	F	308	Total	C	N	O	S	0	0	0
			2444	1559	429	450	6			
1	G	305	Total	C	N	O	S	0	0	0
			2428	1551	426	445	6			
1	H	309	Total	C	N	O	S	0	0	0
			2444	1561	430	447	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	5	Total	O	0	0
			5	5		
2	C	9	Total	O	0	0
			9	9		
2	D	3	Total	O	0	0
			3	3		
2	E	1	Total	O	0	0
			1	1		
2	F	13	Total	O	0	0
			13	13		

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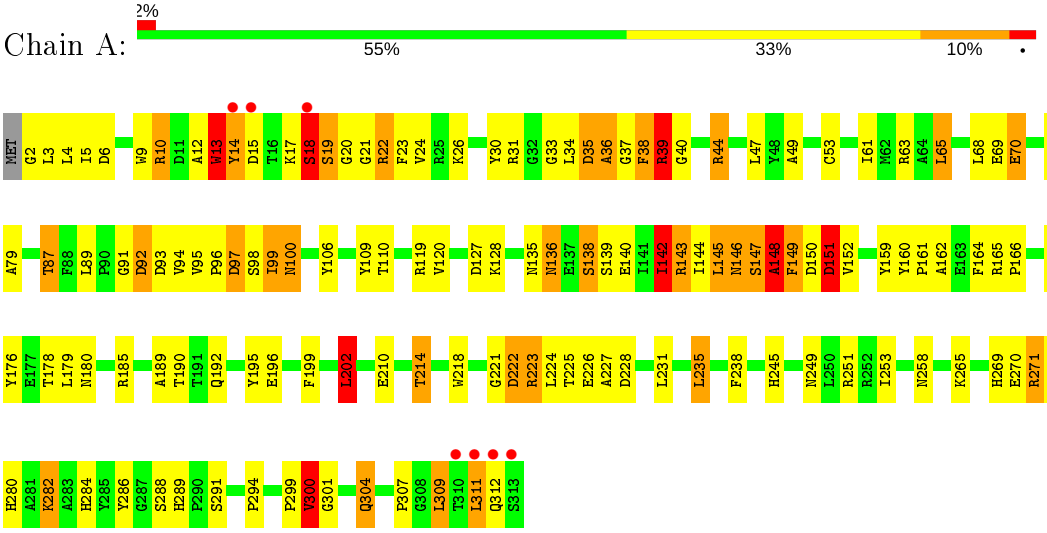
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total O 2 2	0	0
2	H	1	Total O 1 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

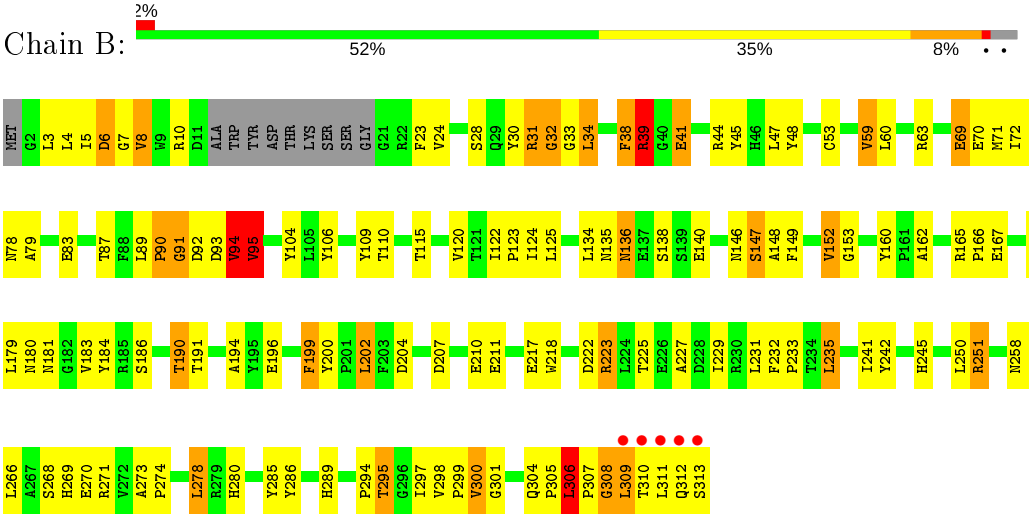
- Molecule 1: Putative glutathione transferase

Chain A:



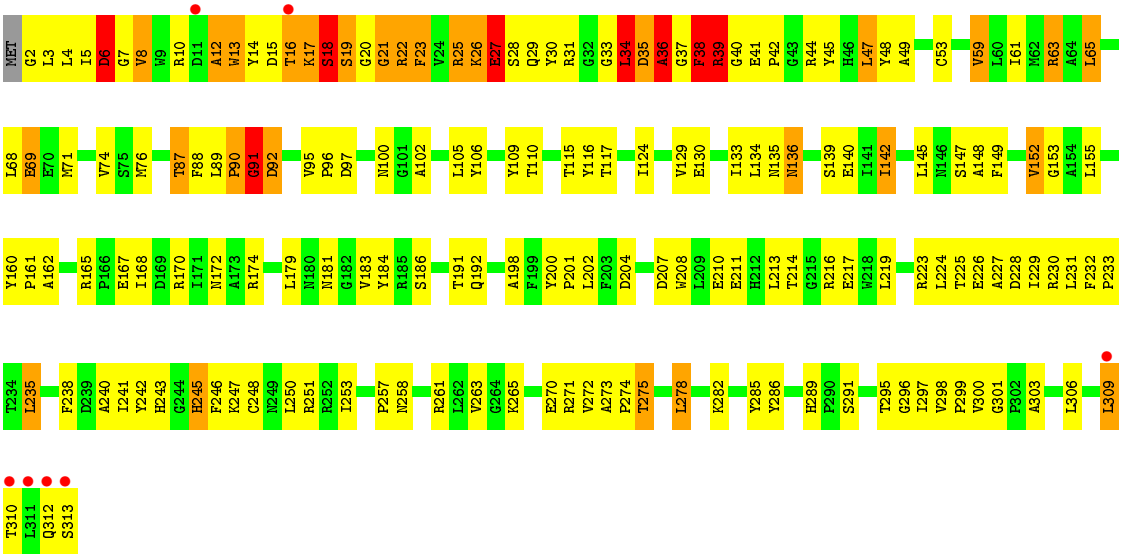
- Molecule 1: Putative glutathione transferase

Chain B:

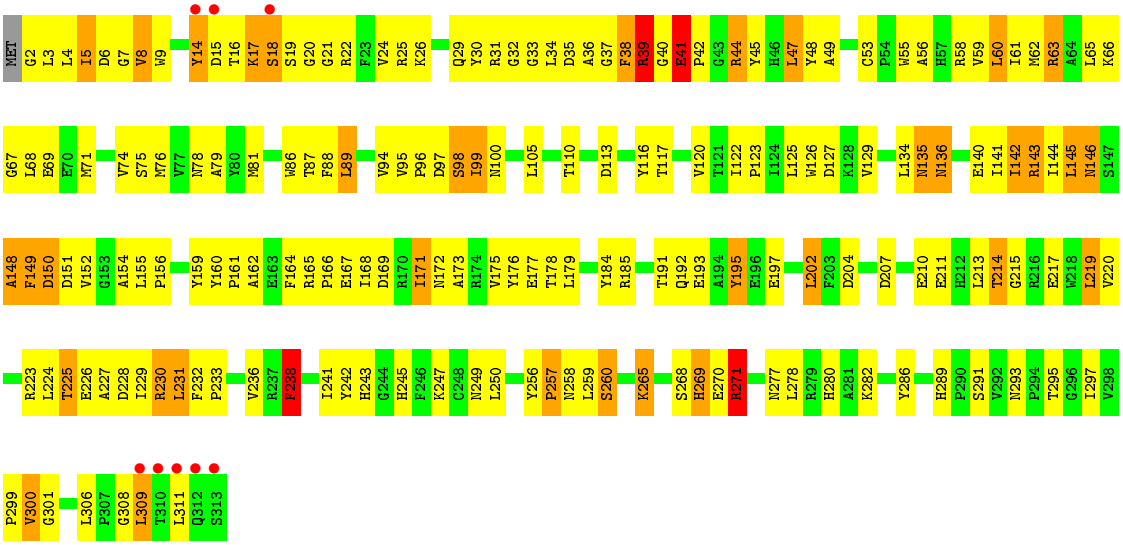


- Molecule 1: Putative glutathione transferase

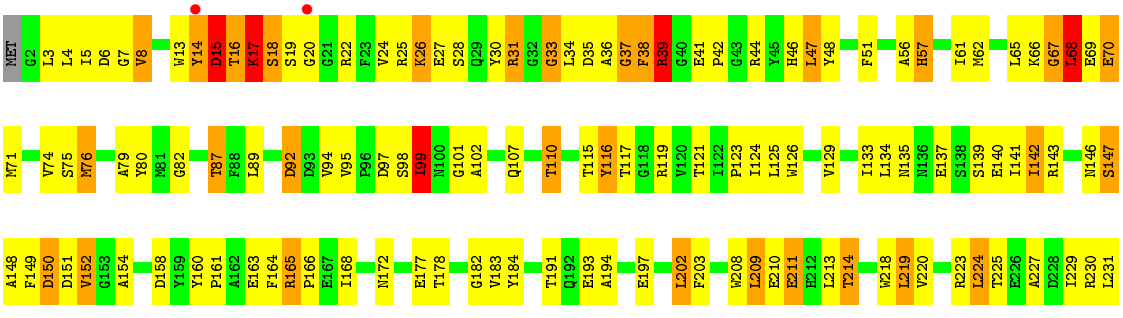
Chain C:

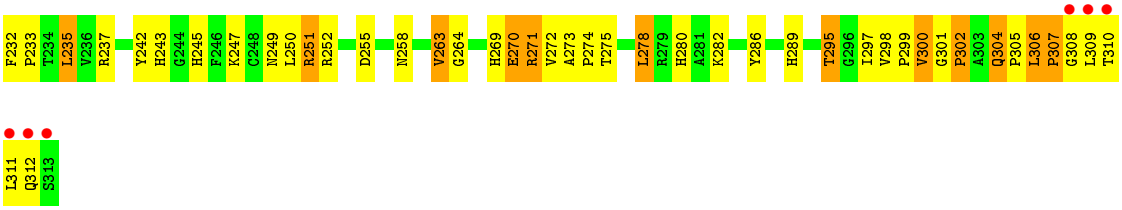


• Molecule 1: Putative glutathione transferase

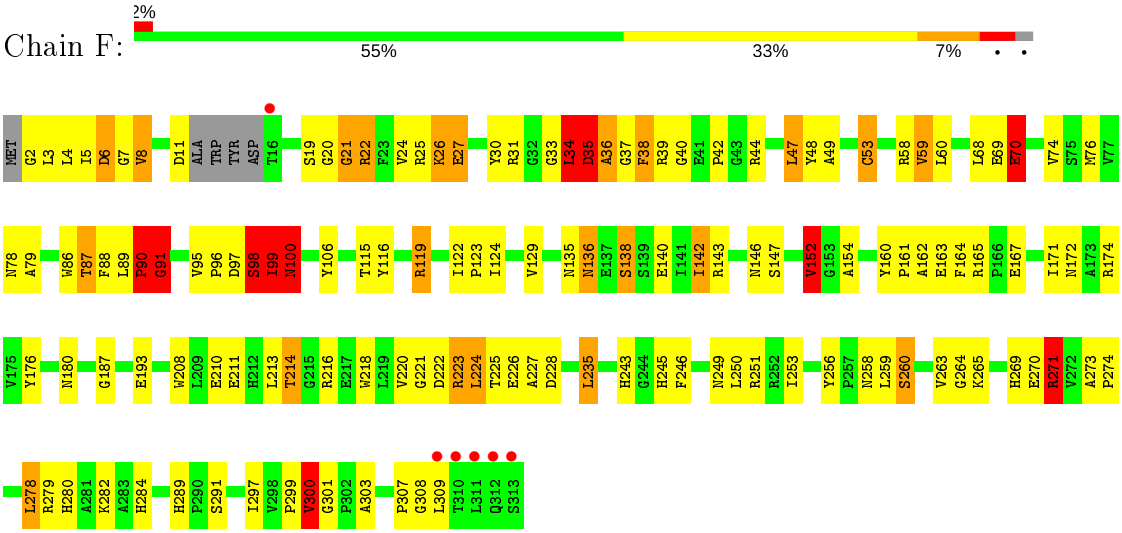


• Molecule 1: Putative glutathione transferase

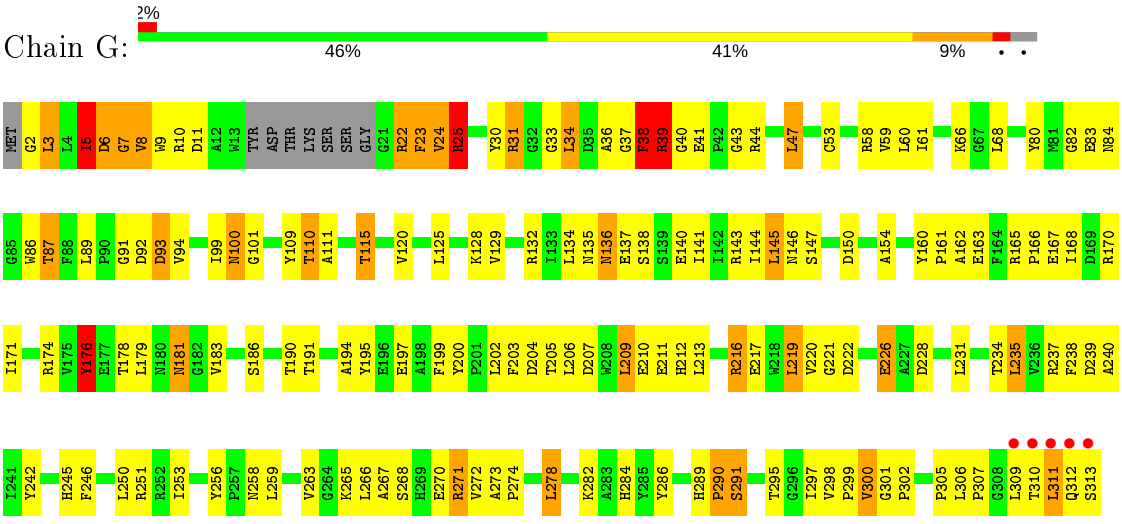




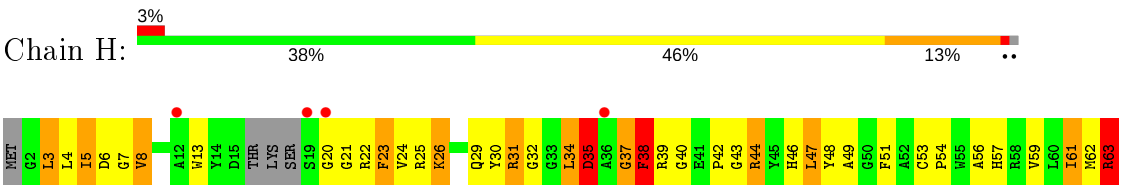
• Molecule 1: Putative glutathione transferase

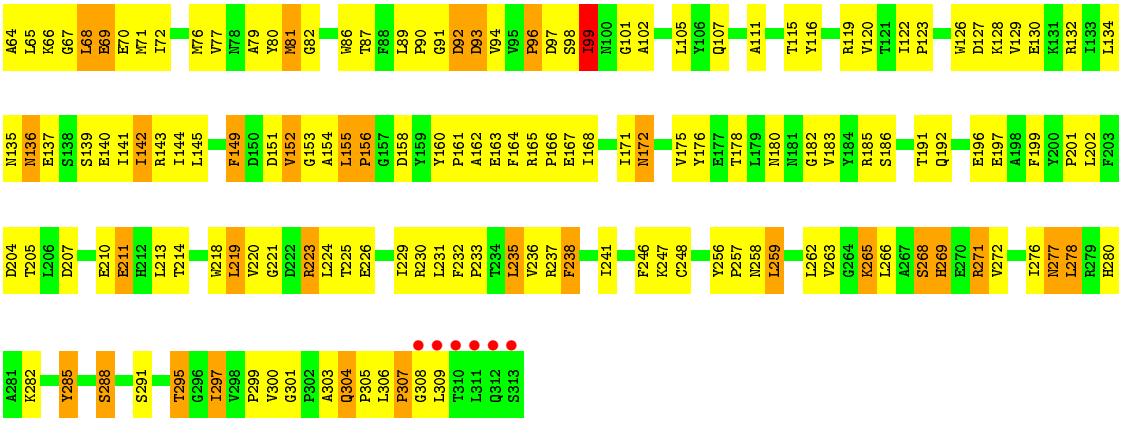


• Molecule 1: Putative glutathione transferase



• Molecule 1: Putative glutathione transferase




A64 L65 K66 G67 L68 E69 E70 M71 I72 M76 V77 N78 A79 Y80 M81 G82 W86 T87 F88 L89 P90 G91 D92 D93 V94 V95 P96 D97 S98 I99 N100 G101 A102 L105 Y106 Q107 A111 T115 Y116 R119 V120 T121 I122 P123 W126 D127 K128 V129 E130 K131 R132 I133 L134
N135 N136 E137 S138 S139 E140 I141 I142 R143 I144 L145 F149 D150 D151 V152 G153 A154 L155 P156 G157 D158 Y159 Y160 P161 A162 E163 F164 R165 P166 E167 I168 I171 N172 V175 Y176 E177 T178 L179 N180 N181 G182 V183 Y184 R185 S186 T191 Q192 E196 E197 A198 F199 Y200 P201 L202 F203
D204 T205 L206 D207 E210 E211 H212 L213 T214 W218 L219 V220 G221 D222 R223 L224 T225 E226 I229 R230 L231 F232 P233 T234 L235 V236 R237 F238 I241 F246 K247 C248 Y256 P257 N258 L259 L262 V263 G264 K265 L266 A267 S268 H269 E270 R271 V272 I276 N277 L278 R279 H280
A281 K282 Y285 S288 S291 T295 G296 I297 V298 P299 V300 G301 P302 A303 Q304 P305 L306 P307 G308 L309 T310 L311 Q312 S313

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	242.84Å 242.84Å 242.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 3.00 49.57 – 2.83	Depositor EDS
% Data completeness (in resolution range)	87.9 (49.57-3.00) 84.0 (49.57-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.36 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.202 , 0.256 0.195 , 0.252	Depositor DCC
R_{free} test set	2007 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19729	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.94	5/2562 (0.2%)	0.97	4/3490 (0.1%)
1	B	0.82	1/2488 (0.0%)	0.94	6/3387 (0.2%)
1	C	0.80	2/2552 (0.1%)	0.95	4/3476 (0.1%)
1	D	0.72	1/2552 (0.0%)	0.88	3/3478 (0.1%)
1	E	0.80	0/2554	0.92	4/3479 (0.1%)
1	F	0.93	2/2511 (0.1%)	0.95	2/3418 (0.1%)
1	G	0.68	0/2495	0.84	2/3397 (0.1%)
1	H	0.63	0/2511	0.79	0/3419
All	All	0.80	11/20225 (0.1%)	0.91	25/27544 (0.1%)

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	A	0	3
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	2
All	All	0	9

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	SER	CB-OG	6.75	1.51	1.42
1	B	53	CYS	CB-SG	-6.33	1.71	1.82
1	A	53	CYS	CB-SG	-6.18	1.71	1.82
1	F	70	GLU	CG-CD	6.14	1.61	1.51
1	A	70	GLU	CG-CD	5.71	1.60	1.51
1	A	148	ALA	CA-CB	5.68	1.64	1.52
1	F	53	CYS	CB-SG	-5.49	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	SER	CB-OG	5.40	1.49	1.42
1	C	53	CYS	CB-SG	-5.17	1.73	1.81
1	D	41	GLU	CG-CD	5.14	1.59	1.51
1	C	38	PHE	CB-CG	5.12	1.60	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	39	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	E	76	MET	CG-SD-CE	-7.11	88.83	100.20
1	F	91	GLY	N-CA-C	6.47	129.29	113.10
1	C	91	GLY	N-CA-C	6.35	128.98	113.10
1	B	306	LEU	CA-CB-CG	6.27	129.72	115.30
1	B	39	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	89	LEU	CA-CB-CG	6.05	129.21	115.30
1	E	33	GLY	N-CA-C	-5.85	98.47	113.10
1	C	39	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	E	165	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	E	251	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	D	179	LEU	CA-CB-CG	5.59	128.15	115.30
1	B	94	VAL	N-CA-C	5.42	125.64	111.00
1	B	95	VAL	N-CA-C	5.41	125.60	111.00
1	A	97	ASP	CB-CG-OD2	5.39	123.16	118.30
1	A	142	ILE	CG1-CB-CG2	-5.37	99.58	111.40
1	F	34	LEU	CA-CB-CG	5.36	127.63	115.30
1	C	6	ASP	N-CA-C	-5.27	96.78	111.00
1	G	91	GLY	N-CA-C	-5.24	100.01	113.10
1	A	149	PHE	N-CA-C	-5.21	96.94	111.00
1	D	39	ARG	CB-CA-C	-5.16	100.09	110.40
1	G	7	GLY	N-CA-C	-5.11	100.33	113.10
1	B	31	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	C	142	ILE	CG1-CB-CG2	-5.07	100.24	111.40
1	A	202	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ALA	Peptide
1	A	39	ARG	Peptide
1	A	40	GLY	Peptide
1	C	36	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	C	6	ASP	Peptide
1	D	300	VAL	Peptide
1	E	6	ASP	Peptide
1	F	21	GLY	Peptide
1	F	6	ASP	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	2491	0	2406	178	0
1	B	2420	0	2340	152	0
1	C	2482	0	2392	196	0
1	D	2481	0	2383	236	0
1	E	2484	0	2385	189	0
1	F	2444	0	2354	147	0
1	G	2428	0	2344	153	0
1	H	2444	0	2351	207	0
2	A	21	0	0	3	0
2	B	5	0	0	0	0
2	C	9	0	0	4	0
2	D	3	0	0	1	0
2	E	1	0	0	0	0
2	F	13	0	0	1	0
2	G	2	0	0	0	0
2	H	1	0	0	0	0
All	All	19729	0	18955	1412	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (1412) 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:39:ARG:HE	1:A:148:ALA:C	1.39	1.27
1:A:143:ARG:HH11	1:A:143:ARG:HG3	1.06	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLY:HA3	2:A:401:HOH:O	1.46	1.12
1:C:213:LEU:HD21	1:C:219:LEU:HD23	1.29	1.12
1:H:23:PHE:CB	1:H:24:VAL:HA	1.73	1.12
1:B:39:ARG:NH1	1:B:39:ARG:HB3	1.63	1.11
1:A:37:GLY:HA2	1:A:38:PHE:CB	1.76	1.11
1:A:23:PHE:CE2	1:F:26:LYS:HB2	1.86	1.09
1:E:7:GLY:HA3	1:E:8:VAL:CB	1.82	1.08
1:D:214:THR:HG23	1:D:215:GLY:H	1.16	1.06
1:E:31:ARG:HH11	1:E:31:ARG:HG2	1.11	1.06
1:H:23:PHE:HB3	1:H:24:VAL:HA	1.12	1.06
1:A:39:ARG:NE	1:A:148:ALA:C	2.10	1.05
1:B:39:ARG:HH22	1:B:44:ARG:CZ	1.69	1.05
1:F:119:ARG:HG3	1:F:119:ARG:HH11	1.17	1.05
1:B:39:ARG:HH11	1:B:39:ARG:CB	1.69	1.04
1:C:152:VAL:HG12	1:C:153:GLY:H	0.88	1.04
1:F:19:SER:HB3	1:F:20:GLY:HA2	1.38	1.04
1:C:152:VAL:HG12	1:C:153:GLY:N	1.63	1.03
1:D:39:ARG:HG3	1:D:40:GLY:N	1.71	1.03
1:D:143:ARG:HH11	1:D:143:ARG:HG3	1.19	1.02
1:A:37:GLY:CA	1:A:38:PHE:HB3	1.89	1.01
1:D:37:GLY:HA2	1:D:38:PHE:HB3	1.38	1.00
1:A:17:LYS:HA	1:A:18:SER:HB3	1.41	1.00
1:C:152:VAL:CG1	1:C:153:GLY:H	1.75	1.00
1:C:38:PHE:CD1	1:C:38:PHE:O	2.15	1.00
1:D:87:THR:HG21	1:D:89:LEU:HG	1.41	0.99
1:A:270:GLU:O	1:A:271:ARG:HB2	1.62	0.98
1:F:87:THR:HG23	1:F:89:LEU:H	1.24	0.98
1:A:49:ALA:HB3	1:A:76:MET:HE1	1.45	0.98
1:F:270:GLU:O	1:F:271:ARG:HB2	1.61	0.98
1:A:39:ARG:HH21	1:A:149:PHE:H	1.01	0.98
1:A:143:ARG:CG	1:A:143:ARG:HH11	1.76	0.98
1:G:167:GLU:HG3	1:G:170:ARG:NH1	1.78	0.98
1:B:245:HIS:HE1	1:B:289:HIS:HD2	1.08	0.98
1:H:271:ARG:HH11	1:H:271:ARG:HG2	1.29	0.98
1:D:71:MET:SD	1:D:149:PHE:CZ	2.58	0.97
1:H:23:PHE:HB3	1:H:24:VAL:CA	1.94	0.97
1:C:38:PHE:O	1:C:38:PHE:HD1	1.45	0.96
1:D:63:ARG:HG2	1:D:63:ARG:HH11	1.27	0.96
1:H:6:ASP:H	1:H:7:GLY:HA2	1.29	0.96
1:A:19:SER:N	1:A:20:GLY:HA2	1.81	0.96
1:G:39:ARG:HA	1:G:39:ARG:NE	1.82	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:HH11	1:B:39:ARG:HB3	0.79	0.95
1:C:7:GLY:HA2	1:C:8:VAL:O	1.66	0.95
1:G:174:ARG:O	1:G:178:THR:HG22	1.65	0.94
1:A:245:HIS:HE1	1:A:289:HIS:CD2	1.86	0.94
1:E:87:THR:HG23	1:E:89:LEU:H	1.29	0.94
1:D:136:ASN:C	1:D:136:ASN:HD22	1.68	0.93
1:A:22:ARG:HG2	1:A:22:ARG:HH11	1.30	0.93
1:B:78:ASN:ND2	1:B:91:GLY:HA3	1.82	0.93
1:G:191:THR:HG23	1:G:194:ALA:H	1.33	0.93
1:A:39:ARG:HG2	1:A:148:ALA:O	1.68	0.92
1:A:14:TYR:N	1:A:15:ASP:HA	1.84	0.92
1:B:38:PHE:HB2	1:B:39:ARG:O	1.69	0.92
1:B:38:PHE:HB2	1:B:39:ARG:CA	2.00	0.91
1:A:222:ASP:N	2:A:401:HOH:O	2.04	0.91
1:D:37:GLY:HA2	1:D:38:PHE:CB	1.98	0.91
1:A:143:ARG:NH1	1:A:143:ARG:HG3	1.78	0.90
1:F:37:GLY:HA2	1:F:39:ARG:H	1.34	0.90
1:G:167:GLU:HG3	1:G:170:ARG:HH12	1.36	0.90
1:D:143:ARG:CG	1:D:143:ARG:HH11	1.84	0.90
1:E:300:VAL:HG12	1:F:250:LEU:HD13	1.51	0.90
1:F:99:ILE:O	1:F:99:ILE:HD12	1.71	0.89
1:A:37:GLY:HA2	1:A:38:PHE:HB3	0.94	0.89
1:B:270:GLU:O	1:B:271:ARG:HB2	1.73	0.89
1:B:38:PHE:HB2	1:B:39:ARG:C	1.92	0.89
1:A:245:HIS:HE1	1:A:289:HIS:HD2	1.15	0.89
1:C:27:GLU:CD	1:C:28:SER:H	1.75	0.89
1:H:42:PRO:HD3	1:H:152:VAL:HG11	1.55	0.89
1:D:47:LEU:HB3	1:D:74:VAL:HG12	1.53	0.88
1:H:34:LEU:H	1:H:144:ILE:HD11	1.36	0.88
1:H:38:PHE:HD2	1:H:38:PHE:O	1.56	0.88
1:A:223:ARG:CB	1:A:223:ARG:HH11	1.87	0.88
1:E:270:GLU:O	1:E:271:ARG:HB2	1.74	0.88
1:E:300:VAL:CG1	1:F:250:LEU:HD13	2.03	0.88
1:C:49:ALA:HB3	1:C:76:MET:CE	2.03	0.87
1:D:150:ASP:HA	1:D:154:ALA:HB3	1.55	0.87
1:A:39:ARG:NH1	1:A:147:SER:N	2.21	0.87
1:A:39:ARG:NH2	1:A:149:PHE:H	1.73	0.87
1:B:199:PHE:HD2	1:B:199:PHE:H	1.22	0.87
1:G:213:LEU:HD21	1:G:219:LEU:HD23	1.55	0.86
1:A:22:ARG:CG	1:A:22:ARG:HH11	1.87	0.86
1:C:210:GLU:OE2	1:C:257:PRO:HD2	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:THR:HG22	1:D:89:LEU:H	1.38	0.86
1:E:31:ARG:NH1	1:E:31:ARG:HG2	1.87	0.86
1:C:87:THR:CG2	1:C:89:LEU:H	1.88	0.86
1:A:19:SER:H	1:A:20:GLY:HA2	1.37	0.85
1:A:5:ILE:HG21	1:A:10:ARG:HH11	1.41	0.85
1:B:41:GLU:CD	1:B:41:GLU:H	1.77	0.85
1:D:217:GLU:HB3	1:D:265:LYS:NZ	1.90	0.85
1:F:37:GLY:HA2	1:F:39:ARG:HG3	1.59	0.85
1:H:155:LEU:HB3	1:H:156:PRO:HD2	1.56	0.85
1:D:87:THR:CG2	1:D:89:LEU:HG	2.05	0.85
1:H:306:LEU:HB3	1:H:307:PRO:HD2	1.56	0.85
1:B:245:HIS:HE1	1:B:289:HIS:CD2	1.95	0.85
1:H:226:GLU:HA	1:H:229:ILE:HD12	1.58	0.85
1:H:37:GLY:N	1:H:38:PHE:HB3	1.91	0.85
1:B:191:THR:HG23	1:B:194:ALA:H	1.42	0.85
1:E:31:ARG:HH11	1:E:31:ARG:CG	1.90	0.84
1:A:17:LYS:HA	1:A:18:SER:CB	2.04	0.84
1:H:63:ARG:HH11	1:H:63:ARG:HG2	1.39	0.84
1:D:282:LYS:NZ	1:D:301:GLY:HA3	1.92	0.84
1:H:6:ASP:O	1:H:115:THR:HA	1.77	0.84
1:H:271:ARG:CG	1:H:271:ARG:HH11	1.90	0.84
1:C:33:GLY:O	1:C:34:LEU:HB2	1.79	0.83
1:H:304:GLN:NE2	1:H:304:GLN:H	1.76	0.83
1:F:224:LEU:HD12	1:F:225:THR:N	1.92	0.83
1:A:39:ARG:HE	1:A:149:PHE:N	1.75	0.83
1:D:59:VAL:HG12	1:D:142:ILE:HD13	1.60	0.83
1:A:23:PHE:HE2	1:F:26:LYS:HB2	1.43	0.83
1:H:304:GLN:HE21	1:H:304:GLN:H	1.26	0.83
1:C:42:PRO:HG3	1:C:152:VAL:HG11	1.60	0.83
1:C:39:ARG:HB3	1:C:41:GLU:OE1	1.78	0.82
1:D:269:HIS:ND1	1:D:270:GLU:O	2.11	0.82
1:A:223:ARG:HH11	1:A:223:ARG:HB3	1.44	0.82
1:G:31:ARG:CG	1:G:31:ARG:HH11	1.92	0.82
1:H:79:ALA:HB2	1:H:280:HIS:CE1	2.14	0.82
1:E:14:TYR:O	1:E:15:ASP:HB3	1.79	0.82
1:H:91:GLY:O	1:H:94:VAL:HG23	1.80	0.82
1:E:245:HIS:HE1	1:E:289:HIS:HD2	1.26	0.82
1:E:13:TRP:O	1:E:14:TYR:HB2	1.78	0.82
1:G:22:ARG:HD3	1:G:23:PHE:H	1.43	0.82
1:D:63:ARG:CG	1:D:63:ARG:HH11	1.92	0.81
1:B:38:PHE:HB2	1:B:39:ARG:HA	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:GLY:O	1:E:34:LEU:HB2	1.78	0.81
1:C:63:ARG:HG2	1:C:63:ARG:HH11	1.46	0.81
1:H:241:ILE:HD13	1:H:285:TYR:CD1	2.15	0.81
1:B:41:GLU:OE1	1:B:44:ARG:HD2	1.80	0.81
1:B:30:TYR:O	1:B:135:ASN:HA	1.81	0.80
1:H:6:ASP:N	1:H:7:GLY:HA2	1.94	0.80
1:A:299:PRO:C	1:A:301:GLY:H	1.83	0.80
1:E:152:VAL:HG12	1:E:152:VAL:O	1.78	0.80
1:B:312:GLN:HG2	1:B:313:SER:H	1.45	0.80
1:C:136:ASN:HD22	1:C:136:ASN:H	1.29	0.80
1:C:16:THR:HG21	1:C:20:GLY:O	1.82	0.80
1:D:38:PHE:O	2:D:402:HOH:O	1.99	0.80
1:A:39:ARG:HH12	1:A:147:SER:N	1.80	0.80
1:G:213:LEU:HD12	1:G:259:LEU:HD23	1.62	0.80
1:H:20:GLY:HA3	1:H:22:ARG:H	1.47	0.79
1:C:87:THR:HG23	1:C:89:LEU:H	1.47	0.79
1:D:122:ILE:HB	1:D:123:PRO:HA	1.65	0.79
1:A:39:ARG:HH21	1:A:149:PHE:N	1.79	0.79
1:A:99:ILE:O	1:A:99:ILE:HD12	1.82	0.79
1:D:270:GLU:O	1:D:271:ARG:HB2	1.81	0.79
1:E:17:LYS:HA	1:E:18:SER:CB	2.12	0.79
1:F:214:THR:HA	1:F:258:ASN:ND2	1.97	0.79
1:F:37:GLY:CA	1:F:39:ARG:H	1.96	0.79
1:D:214:THR:HA	1:D:258:ASN:ND2	1.98	0.79
1:H:166:PRO:HG2	1:H:167:GLU:H	1.48	0.78
1:D:214:THR:CG2	1:D:215:GLY:H	1.96	0.78
1:D:256:TYR:O	1:D:260:SER:HB2	1.83	0.78
1:F:87:THR:CG2	1:F:89:LEU:H	1.96	0.78
1:F:245:HIS:HE1	1:F:289:HIS:HD2	1.31	0.78
1:G:39:ARG:NH2	1:G:41:GLU:OE1	2.16	0.78
1:D:202:LEU:HD12	1:D:202:LEU:C	2.04	0.78
1:D:87:THR:CG2	1:D:89:LEU:H	1.97	0.78
1:E:150:ASP:N	1:E:154:ALA:HB3	1.99	0.78
1:H:282:LYS:NZ	1:H:301:GLY:HA3	1.99	0.77
1:G:204:ASP:O	1:G:207:ASP:HB2	1.84	0.77
1:B:7:GLY:HA2	1:B:8:VAL:CB	2.15	0.77
1:C:265:LYS:HA	1:C:310:THR:HG21	1.67	0.77
1:C:49:ALA:HB3	1:C:76:MET:HE2	1.67	0.77
1:D:164:PHE:C	1:D:166:PRO:HD2	2.03	0.77
1:G:34:LEU:HD11	1:G:140:GLU:HB3	1.65	0.77
1:B:76:MET:HB2	1:B:95:VAL:HG13	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:GLY:HA2	1:G:8:VAL:CB	2.14	0.77
1:H:162:ALA:HA	1:H:165:ARG:HD2	1.66	0.77
1:H:218:TRP:CZ2	1:H:265:LYS:HE2	2.20	0.77
1:D:226:GLU:HA	1:D:229:ILE:HG13	1.65	0.77
1:E:150:ASP:H	1:E:154:ALA:HB3	1.48	0.77
1:E:282:LYS:NZ	1:E:301:GLY:HA3	1.99	0.77
1:B:39:ARG:NH2	1:B:44:ARG:CZ	2.47	0.76
1:C:30:TYR:O	1:C:135:ASN:HA	1.84	0.76
1:H:94:VAL:HG12	1:H:96:PRO:HD3	1.68	0.76
1:H:105:LEU:HD21	1:H:122:ILE:HG23	1.65	0.76
1:D:214:THR:HG23	1:D:215:GLY:N	1.96	0.76
1:E:125:LEU:HD23	1:E:134:LEU:HD23	1.68	0.76
1:F:22:ARG:HH11	1:F:22:ARG:HB3	1.50	0.76
1:G:33:GLY:O	1:G:34:LEU:HB2	1.85	0.76
1:A:300:VAL:HB	1:B:199:PHE:CZ	2.21	0.75
1:G:5:ILE:O	1:G:6:ASP:HB2	1.85	0.75
1:B:196:GLU:HA	1:B:199:PHE:HE2	1.52	0.75
1:F:245:HIS:HE1	1:F:289:HIS:CD2	2.03	0.75
1:C:37:GLY:HA2	1:C:38:PHE:CB	2.17	0.75
1:C:49:ALA:HB3	1:C:76:MET:HE1	1.68	0.74
1:C:87:THR:HG23	1:C:89:LEU:HG	1.67	0.74
1:G:286:TYR:HB2	1:G:298:VAL:HG22	1.69	0.74
1:H:149:PHE:HD1	1:H:149:PHE:N	1.86	0.74
1:A:223:ARG:NH1	1:A:223:ARG:HB3	2.01	0.74
1:H:164:PHE:O	1:H:168:ILE:HG13	1.88	0.74
1:B:245:HIS:CE1	1:B:289:HIS:HD2	2.00	0.74
1:G:6:ASP:O	1:G:115:THR:HA	1.87	0.74
1:E:224:LEU:HD12	1:E:225:THR:N	2.03	0.74
1:A:245:HIS:CE1	1:A:289:HIS:HD2	2.02	0.74
1:B:79:ALA:HB2	1:B:280:HIS:CE1	2.23	0.74
1:D:136:ASN:C	1:D:136:ASN:ND2	2.42	0.73
1:E:56:ALA:HA	1:E:123:PRO:HG3	1.70	0.73
1:G:179:LEU:O	1:G:183:VAL:HG13	1.88	0.73
1:E:202:LEU:HD12	1:E:202:LEU:C	2.07	0.73
1:H:176:TYR:HA	1:H:180:ASN:HB2	1.69	0.73
1:H:37:GLY:H	1:H:38:PHE:CB	2.01	0.73
1:B:38:PHE:HB3	1:B:148:ALA:HB1	1.70	0.73
1:A:20:GLY:HA3	1:A:21:GLY:C	2.09	0.73
1:C:39:ARG:HB3	1:C:41:GLU:CD	2.09	0.73
1:E:46:HIS:HB3	1:E:126:TRP:HB3	1.70	0.73
1:G:37:GLY:HA2	1:G:38:PHE:CD2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:HIS:HE1	1:D:289:HIS:CD2	2.06	0.73
1:F:22:ARG:HG2	1:F:22:ARG:O	1.87	0.73
1:D:41:GLU:HG2	1:D:42:PRO:HD2	1.70	0.73
1:G:231:LEU:HG	1:G:235:LEU:HD22	1.71	0.73
1:F:269:HIS:ND1	1:F:270:GLU:O	2.22	0.73
1:B:6:ASP:H	1:B:7:GLY:HA2	1.53	0.72
1:C:37:GLY:HA2	1:C:38:PHE:CG	2.24	0.72
1:D:15:ASP:C	1:D:17:LYS:H	1.93	0.72
1:H:51:PHE:CD1	1:H:277:ASN:HB3	2.24	0.72
1:E:19:SER:CB	1:E:20:GLY:HA3	2.19	0.72
1:H:192:GLN:O	1:H:196:GLU:HG3	1.89	0.72
1:D:5:ILE:CG2	1:D:6:ASP:N	2.52	0.72
1:H:37:GLY:HA2	1:H:39:ARG:HG3	1.71	0.72
1:D:245:HIS:HE1	1:D:289:HIS:HD2	1.35	0.72
1:G:38:PHE:HD1	1:G:39:ARG:O	1.71	0.72
1:C:270:GLU:O	1:C:271:ARG:HB2	1.87	0.72
1:D:193:GLU:O	1:D:197:GLU:HG3	1.90	0.72
1:D:38:PHE:HD1	1:D:39:ARG:H	1.35	0.72
1:F:270:GLU:O	1:F:271:ARG:CB	2.35	0.72
1:E:37:GLY:HA3	1:E:38:PHE:CD2	2.24	0.72
1:E:37:GLY:HA3	1:E:38:PHE:HD2	1.53	0.72
1:H:5:ILE:HG22	1:H:8:VAL:CB	2.20	0.71
1:A:218:TRP:CZ2	1:A:265:LYS:HE3	2.25	0.71
1:B:93:ASP:O	1:B:94:VAL:HG13	1.90	0.71
1:D:5:ILE:HG22	1:D:8:VAL:CB	2.20	0.71
1:B:33:GLY:H	1:B:134:LEU:HD11	1.55	0.71
1:C:5:ILE:CG2	1:C:6:ASP:H	2.03	0.71
1:D:162:ALA:HA	1:D:165:ARG:HG3	1.73	0.71
1:G:216:ARG:HH11	1:G:216:ARG:HG2	1.56	0.71
1:B:305:PRO:HB2	1:B:306:LEU:HD13	1.72	0.70
1:D:49:ALA:O	1:D:76:MET:HA	1.91	0.70
1:D:143:ARG:HG3	1:D:143:ARG:NH1	1.96	0.70
1:A:282:LYS:HE2	1:A:301:GLY:HA3	1.73	0.70
1:D:63:ARG:HG2	1:D:63:ARG:NH1	2.01	0.70
1:A:39:ARG:NH1	1:A:144:ILE:O	2.25	0.70
1:E:37:GLY:HA2	1:E:38:PHE:HB3	1.73	0.70
1:F:36:ALA:C	1:F:38:PHE:HB3	2.12	0.70
1:H:172:ASN:HB3	1:H:230:ARG:HH21	1.57	0.70
1:D:144:ILE:HG22	1:D:145:LEU:HD23	1.73	0.70
1:D:39:ARG:NH1	1:D:149:PHE:CD1	2.60	0.70
1:B:90:PRO:O	1:B:91:GLY:O	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:THR:O	1:E:202:LEU:HB2	1.92	0.69
1:B:39:ARG:HG3	1:H:207:ASP:OD2	1.92	0.69
1:A:170:ARG:HH11	1:A:170:ARG:HG3	1.56	0.69
1:C:23:PHE:CE2	1:E:27:GLU:HB3	2.27	0.69
1:E:163:GLU:HG2	1:E:164:PHE:CD1	2.26	0.69
1:H:89:LEU:HB3	1:H:90:PRO:HD2	1.73	0.69
1:B:39:ARG:HH22	1:B:44:ARG:NE	1.90	0.69
1:A:39:ARG:HD3	1:A:148:ALA:H	1.57	0.69
1:A:39:ARG:NE	1:A:148:ALA:N	2.39	0.69
1:G:136:ASN:HD22	1:G:136:ASN:H	1.40	0.69
1:D:202:LEU:HD12	1:D:202:LEU:O	1.93	0.69
1:B:23:PHE:CG	1:B:23:PHE:O	2.45	0.69
1:H:37:GLY:C	1:H:39:ARG:H	1.93	0.69
1:C:5:ILE:HG23	1:C:6:ASP:N	2.07	0.69
1:E:117:THR:O	1:E:117:THR:HG22	1.93	0.69
1:F:30:TYR:H	1:F:136:ASN:HD21	1.41	0.69
1:H:241:ILE:HD13	1:H:285:TYR:HD1	1.57	0.69
1:A:5:ILE:CG2	1:A:10:ARG:HH11	2.06	0.69
1:D:38:PHE:HD1	1:D:39:ARG:N	1.90	0.69
1:G:212:HIS:O	1:G:216:ARG:HD2	1.93	0.69
1:G:216:ARG:HG2	1:G:216:ARG:NH1	2.07	0.69
1:C:200:TYR:CZ	1:D:300:VAL:HG21	2.29	0.68
1:E:147:SER:O	1:E:149:PHE:N	2.27	0.68
1:A:39:ARG:NE	1:A:148:ALA:CA	2.56	0.68
1:F:264:GLY:HA3	1:F:308:GLY:O	1.92	0.68
1:G:286:TYR:CZ	1:G:299:PRO:HG2	2.27	0.68
1:E:307:PRO:HG2	1:E:308:GLY:H	1.58	0.68
1:A:39:ARG:CZ	1:A:147:SER:C	2.62	0.68
1:G:38:PHE:CD1	1:G:39:ARG:O	2.47	0.68
1:H:40:GLY:HA3	1:H:149:PHE:CE1	2.29	0.68
1:D:60:LEU:HD21	1:D:76:MET:CE	2.24	0.68
1:F:143:ARG:NH2	1:F:226:GLU:OE2	2.27	0.68
1:F:19:SER:HB3	1:F:20:GLY:CA	2.21	0.68
1:D:207:ASP:HB3	1:G:37:GLY:O	1.92	0.68
1:B:39:ARG:HG2	1:B:41:GLU:OE2	1.93	0.68
1:F:22:ARG:NH1	1:F:22:ARG:HB3	2.07	0.68
1:C:20:GLY:N	1:C:21:GLY:CA	2.56	0.68
1:F:119:ARG:CG	1:F:119:ARG:HH11	1.98	0.68
1:H:38:PHE:O	1:H:38:PHE:CD2	2.43	0.68
1:H:66:LYS:O	1:H:68:LEU:HD12	1.93	0.68
1:D:5:ILE:CG2	1:D:6:ASP:H	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:VAL:CG1	1:E:152:VAL:O	2.42	0.67
1:F:19:SER:CB	1:F:20:GLY:HA2	2.13	0.67
1:H:149:PHE:CD1	1:H:149:PHE:N	2.58	0.67
1:H:87:THR:OG1	1:H:89:LEU:HG	1.94	0.67
1:B:270:GLU:O	1:B:271:ARG:CB	2.43	0.67
1:D:60:LEU:HD21	1:D:76:MET:HE1	1.75	0.67
1:G:39:ARG:HE	1:G:40:GLY:HA2	1.60	0.67
1:G:87:THR:HG23	1:G:89:LEU:H	1.60	0.67
1:D:217:GLU:HB3	1:D:265:LYS:HZ2	1.57	0.67
1:G:31:ARG:HG3	1:G:31:ARG:HH11	1.60	0.67
1:H:37:GLY:N	1:H:38:PHE:CB	2.57	0.67
1:A:22:ARG:HG2	1:A:22:ARG:NH1	2.08	0.67
1:C:241:ILE:HD13	1:C:285:TYR:CD1	2.30	0.67
1:B:196:GLU:HA	1:B:199:PHE:CE2	2.29	0.66
1:C:213:LEU:HD21	1:C:219:LEU:CD2	2.18	0.66
1:A:30:TYR:HB2	1:A:136:ASN:ND2	2.10	0.66
1:C:39:ARG:H	1:C:39:ARG:NH1	1.94	0.66
1:D:5:ILE:HG23	1:D:6:ASP:N	2.10	0.66
1:E:183:VAL:HG11	1:E:242:TYR:CD2	2.31	0.66
1:B:199:PHE:HA	1:B:202:LEU:HB3	1.76	0.66
1:B:41:GLU:CD	1:B:41:GLU:N	2.48	0.66
1:H:158:ASP:O	1:H:161:PRO:HD3	1.95	0.66
1:B:136:ASN:H	1:B:136:ASN:HD22	1.43	0.66
1:B:89:LEU:O	1:B:91:GLY:N	2.28	0.66
1:C:243:HIS:HA	1:C:248:CYS:O	1.95	0.66
1:A:299:PRO:C	1:A:301:GLY:N	2.50	0.65
1:D:165:ARG:N	1:D:166:PRO:HD2	2.11	0.65
1:C:5:ILE:CG2	1:C:6:ASP:N	2.58	0.65
1:C:7:GLY:HA2	1:C:8:VAL:C	2.16	0.65
1:D:79:ALA:HB2	1:D:280:HIS:CE1	2.31	0.65
1:H:63:ARG:NH1	1:H:63:ARG:HG2	2.06	0.65
1:H:304:GLN:HE21	1:H:304:GLN:N	1.94	0.65
1:E:237:ARG:HG3	1:E:237:ARG:HH11	1.61	0.65
1:H:23:PHE:CB	1:H:24:VAL:CA	2.63	0.65
1:C:37:GLY:HA2	1:C:38:PHE:HB3	1.77	0.65
1:F:34:LEU:O	1:F:35:ASP:CB	2.45	0.65
1:F:34:LEU:O	1:F:35:ASP:OD2	2.15	0.65
1:D:220:VAL:HB	1:D:225:THR:HG21	1.78	0.65
1:D:232:PHE:O	1:D:236:VAL:HG12	1.97	0.65
1:F:4:LEU:HD21	1:F:106:TYR:HB2	1.78	0.65
1:G:270:GLU:O	1:G:271:ARG:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:172:ASN:HB3	1:H:230:ARG:NH2	2.12	0.65
1:F:228:ASP:OD1	2:F:405:HOH:O	2.14	0.65
1:C:39:ARG:H	1:C:39:ARG:CZ	2.09	0.65
1:E:124:ILE:HG23	1:E:133:ILE:HG23	1.78	0.65
1:E:191:THR:HG22	1:E:193:GLU:N	2.12	0.64
1:E:107:GLN:HA	1:E:110:THR:HG22	1.80	0.64
1:B:6:ASP:N	1:B:7:GLY:HA2	2.11	0.64
1:D:99:ILE:HG13	1:D:100:ASN:N	2.13	0.64
1:E:95:VAL:HG12	1:E:95:VAL:O	1.98	0.64
1:G:245:HIS:HE1	1:G:289:HIS:HD2	1.44	0.64
1:H:165:ARG:N	1:H:166:PRO:HD2	2.12	0.64
1:C:20:GLY:N	1:C:21:GLY:HA3	2.12	0.64
1:F:97:ASP:C	1:F:98:SER:O	2.34	0.64
1:B:199:PHE:CD2	1:B:200:TYR:N	2.65	0.64
1:E:158:ASP:O	1:E:161:PRO:HD3	1.97	0.64
1:G:150:ASP:HA	1:G:154:ALA:HB3	1.78	0.64
1:G:68:LEU:HD12	1:G:145:LEU:HD13	1.80	0.64
1:H:213:LEU:HD12	1:H:258:ASN:HB3	1.78	0.64
1:A:30:TYR:O	1:A:135:ASN:HA	1.98	0.64
1:A:49:ALA:CB	1:A:76:MET:HE1	2.25	0.64
1:C:231:LEU:O	1:C:231:LEU:HG	1.95	0.64
1:A:300:VAL:HB	1:B:199:PHE:HZ	1.62	0.64
1:C:18:SER:O	1:C:19:SER:HB2	1.98	0.64
1:H:271:ARG:NH1	1:H:271:ARG:HG2	2.07	0.64
1:H:51:PHE:HD1	1:H:277:ASN:HB3	1.61	0.64
1:A:61:ILE:HG22	1:A:65:LEU:HD22	1.80	0.64
1:H:42:PRO:CD	1:H:152:VAL:HG11	2.26	0.64
1:B:31:ARG:HD2	1:B:140:GLU:OE1	1.98	0.63
1:B:78:ASN:HD22	1:B:91:GLY:HA3	1.63	0.63
1:C:217:GLU:OE1	1:C:265:LYS:HE2	1.97	0.63
1:B:271:ARG:HG2	1:B:271:ARG:NH1	2.13	0.63
1:E:79:ALA:HB2	1:E:280:HIS:CE1	2.33	0.63
1:C:14:TYR:N	1:C:15:ASP:HA	2.12	0.63
1:F:31:ARG:NH1	1:F:140:GLU:OE2	2.31	0.63
1:B:162:ALA:HA	1:B:165:ARG:NE	2.12	0.63
1:B:93:ASP:HB3	1:B:280:HIS:ND1	2.13	0.63
1:D:25:ARG:HH12	1:D:29:GLN:HG2	1.64	0.63
1:E:164:PHE:C	1:E:166:PRO:HD2	2.18	0.63
1:F:38:PHE:O	1:F:38:PHE:HD1	1.79	0.63
1:E:68:LEU:HD12	1:E:68:LEU:N	2.13	0.63
1:F:7:GLY:HA2	1:F:8:VAL:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ASN:OD1	1:B:301:GLY:HA3	1.99	0.63
1:C:61:ILE:HG22	1:C:65:LEU:HD22	1.81	0.63
1:D:172:ASN:HA	1:D:175:VAL:HG12	1.81	0.63
1:H:136:ASN:HD22	1:H:136:ASN:H	1.45	0.63
1:B:199:PHE:HD2	1:B:199:PHE:N	1.94	0.62
1:E:245:HIS:CE1	1:E:289:HIS:HD2	2.15	0.62
1:F:48:TYR:HB2	1:F:124:ILE:HB	1.79	0.62
1:E:295:THR:OG1	1:E:297:ILE:HG13	2.00	0.62
1:G:168:ILE:HG12	1:G:220:VAL:HG21	1.80	0.62
1:A:39:ARG:CZ	1:A:148:ALA:N	2.62	0.62
1:F:172:ASN:HD21	1:F:227:ALA:HA	1.64	0.62
1:G:197:GLU:OE2	1:H:115:THR:HG21	1.98	0.62
1:H:305:PRO:HB2	1:H:306:LEU:HD12	1.82	0.62
1:B:39:ARG:NH2	1:B:44:ARG:NE	2.46	0.62
1:F:87:THR:HG23	1:F:89:LEU:HG	1.80	0.62
1:G:245:HIS:HE1	1:G:289:HIS:CD2	2.17	0.62
1:H:155:LEU:HB3	1:H:156:PRO:CD	2.25	0.62
1:H:299:PRO:C	1:H:301:GLY:H	2.02	0.62
1:C:44:ARG:HD3	1:C:45:TYR:CE2	2.33	0.62
1:C:48:TYR:HB2	1:C:124:ILE:HB	1.80	0.62
1:F:38:PHE:C	1:F:40:GLY:H	2.01	0.62
1:G:22:ARG:HD3	1:G:23:PHE:N	2.15	0.62
1:D:38:PHE:CD1	1:D:39:ARG:N	2.65	0.62
1:H:120:VAL:HG12	1:H:120:VAL:O	1.97	0.62
1:H:37:GLY:H	1:H:38:PHE:HB3	1.60	0.62
1:B:165:ARG:N	1:B:166:PRO:HD2	2.15	0.62
1:D:56:ALA:O	1:D:60:LEU:HD12	1.99	0.62
1:F:245:HIS:CE1	1:F:289:HIS:HD2	2.17	0.62
1:A:148:ALA:HA	1:A:150:ASP:H	1.65	0.61
1:F:37:GLY:CA	1:F:39:ARG:HG3	2.29	0.61
1:C:238:PHE:CD1	1:C:253:ILE:HG12	2.35	0.61
1:H:202:LEU:C	1:H:202:LEU:HD23	2.20	0.61
1:A:99:ILE:O	1:A:100:ASN:HB2	1.99	0.61
1:D:309:LEU:HD12	1:D:311:LEU:HD12	1.81	0.61
1:B:300:VAL:H	1:B:301:GLY:HA3	1.64	0.61
1:E:191:THR:HG22	1:E:193:GLU:H	1.64	0.61
1:E:47:LEU:HD22	1:E:47:LEU:C	2.21	0.61
1:F:3:LEU:HD13	1:F:24:VAL:HG11	1.81	0.61
1:G:31:ARG:NH1	1:G:31:ARG:CG	2.59	0.61
1:C:27:GLU:CD	1:C:28:SER:N	2.49	0.61
1:E:150:ASP:H	1:E:154:ALA:CB	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:ARG:HG2	1:F:27:GLU:HG2	1.83	0.61
1:F:37:GLY:HA2	1:F:39:ARG:N	2.10	0.61
1:G:37:GLY:HA2	1:G:38:PHE:CB	2.31	0.61
1:G:210:GLU:HB2	1:G:256:TYR:HD1	1.66	0.61
1:H:6:ASP:N	1:H:7:GLY:CA	2.64	0.61
1:B:271:ARG:HG2	1:B:271:ARG:HH11	1.66	0.61
1:A:106:TYR:HA	1:A:120:VAL:HG11	1.83	0.60
1:A:165:ARG:N	1:A:166:PRO:HD2	2.15	0.60
1:B:176:TYR:HA	1:B:180:ASN:HB2	1.82	0.60
1:F:136:ASN:H	1:F:136:ASN:HD22	1.49	0.60
1:F:299:PRO:C	1:F:301:GLY:H	2.04	0.60
1:G:39:ARG:HA	1:G:39:ARG:CZ	2.30	0.60
1:H:98:SER:O	1:H:99:ILE:HG12	2.02	0.60
1:D:97:ASP:OD2	1:D:100:ASN:HB2	2.00	0.60
1:D:39:ARG:HD3	1:D:149:PHE:HA	1.82	0.60
1:G:132:ARG:HG3	1:G:132:ARG:HH11	1.66	0.60
1:G:213:LEU:HD21	1:G:219:LEU:CD2	2.29	0.60
1:C:172:ASN:ND2	2:C:407:HOH:O	2.33	0.60
1:C:23:PHE:C	1:C:23:PHE:CD1	2.73	0.60
1:D:14:TYR:CD2	1:D:14:TYR:C	2.75	0.60
1:D:71:MET:SD	1:D:149:PHE:CE2	2.95	0.60
1:D:39:ARG:CD	1:D:149:PHE:HA	2.31	0.60
1:D:5:ILE:HG22	1:D:6:ASP:H	1.67	0.60
1:B:38:PHE:CB	1:B:39:ARG:HA	2.27	0.60
1:E:149:PHE:O	1:E:151:ASP:N	2.34	0.60
1:E:87:THR:HG23	1:E:89:LEU:N	2.11	0.60
1:F:33:GLY:O	1:F:34:LEU:HB2	2.02	0.60
1:G:310:THR:O	1:G:311:LEU:HB2	2.01	0.60
1:G:31:ARG:HG2	1:G:31:ARG:HH11	1.65	0.60
1:C:5:ILE:HG23	1:C:6:ASP:H	1.63	0.60
1:E:37:GLY:HA2	1:E:38:PHE:CB	2.29	0.60
1:G:87:THR:HG23	1:G:89:LEU:HG	1.84	0.60
1:D:39:ARG:HH11	1:D:149:PHE:HB2	1.65	0.60
1:D:39:ARG:CZ	1:D:149:PHE:CD1	2.84	0.59
1:D:211:GLU:O	1:D:214:THR:HB	2.01	0.59
1:C:271:ARG:HH11	1:C:271:ARG:HG2	1.67	0.59
1:C:200:TYR:OH	1:D:300:VAL:CG2	2.50	0.59
1:C:152:VAL:CG1	1:C:153:GLY:N	2.40	0.59
1:D:229:ILE:O	1:D:233:PRO:HD3	2.01	0.59
1:F:99:ILE:O	1:F:99:ILE:CD1	2.47	0.59
1:B:95:VAL:O	1:B:95:VAL:HG22	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:GLU:HG2	1:E:164:PHE:CE1	2.38	0.59
1:G:37:GLY:HA2	1:G:38:PHE:CG	2.38	0.59
1:A:231:LEU:HG	1:A:235:LEU:HD22	1.83	0.59
1:B:218:TRP:CZ2	1:B:265:LYS:HD3	2.37	0.59
1:B:93:ASP:OD2	1:B:93:ASP:O	2.21	0.59
1:C:39:ARG:HG2	1:C:44:ARG:NH1	2.16	0.59
1:C:192:GLN:HA	1:D:297:ILE:HG12	1.84	0.59
1:H:56:ALA:HA	1:H:123:PRO:HD3	1.84	0.59
1:F:2:GLY:O	1:F:3:LEU:HD23	2.03	0.59
1:D:178:THR:O	1:D:202:LEU:HB2	2.02	0.59
1:E:213:LEU:HD21	1:E:219:LEU:HD23	1.85	0.59
1:D:39:ARG:NH1	1:D:149:PHE:HB2	2.17	0.59
1:C:38:PHE:O	1:C:39:ARG:O	2.20	0.58
1:A:300:VAL:HB	1:B:199:PHE:CE1	2.38	0.58
1:C:295:THR:HG23	2:C:405:HOH:O	2.02	0.58
1:C:282:LYS:NZ	1:C:301:GLY:HA3	2.18	0.58
1:G:132:ARG:HG3	1:G:132:ARG:NH1	2.17	0.58
1:B:273:ALA:HB3	1:B:274:PRO:HD3	1.85	0.58
1:C:12:ALA:HB1	1:E:13:TRP:CE3	2.38	0.58
1:A:39:ARG:CG	1:A:148:ALA:O	2.48	0.58
1:C:97:ASP:OD1	1:C:102:ALA:HB3	2.04	0.58
1:E:3:LEU:HD13	1:E:24:VAL:HG11	1.84	0.58
1:H:40:GLY:CA	1:H:149:PHE:CE1	2.86	0.58
1:C:179:LEU:HD12	1:C:202:LEU:CD2	2.33	0.58
1:H:137:GLU:HB3	1:H:140:GLU:HG3	1.84	0.58
1:H:34:LEU:N	1:H:144:ILE:HD11	2.11	0.58
1:H:304:GLN:NE2	1:H:304:GLN:N	2.51	0.58
1:H:42:PRO:HB3	1:H:71:MET:HG3	1.86	0.58
1:E:67:GLY:O	1:E:69:GLU:N	2.35	0.58
1:G:22:ARG:HG2	1:H:185:ARG:NH2	2.18	0.58
1:H:136:ASN:N	1:H:136:ASN:HD22	1.99	0.58
1:B:6:ASP:N	1:B:7:GLY:CA	2.67	0.58
1:C:63:ARG:NH1	1:C:63:ARG:HG2	2.10	0.58
1:E:66:LYS:O	1:E:68:LEU:N	2.32	0.58
1:A:143:ARG:CG	1:A:143:ARG:NH1	2.47	0.58
1:A:49:ALA:HB3	1:A:76:MET:CE	2.26	0.58
1:D:68:LEU:HD22	1:D:149:PHE:CD1	2.39	0.58
1:E:282:LYS:HZ1	1:E:301:GLY:HA3	1.65	0.58
1:F:42:PRO:HD3	1:F:152:VAL:HG11	1.86	0.58
1:A:87:THR:OG1	1:A:89:LEU:HG	2.03	0.58
1:B:199:PHE:CD2	1:B:199:PHE:N	2.65	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LEU:HB2	1:D:228:ASP:OD2	2.04	0.57
1:D:4:LEU:HD22	1:D:7:GLY:HA2	1.86	0.57
1:E:286:TYR:HB2	1:E:298:VAL:HG22	1.86	0.57
1:F:30:TYR:H	1:F:136:ASN:ND2	2.02	0.57
1:G:140:GLU:O	1:G:144:ILE:HG13	2.04	0.57
1:D:15:ASP:O	1:D:17:LYS:N	2.37	0.57
1:E:92:ASP:N	1:E:92:ASP:OD1	2.37	0.57
1:F:119:ARG:NH1	1:F:119:ARG:HG3	1.97	0.57
1:C:191:THR:C	1:D:297:ILE:HD11	2.25	0.57
1:D:30:TYR:O	1:D:135:ASN:HA	2.05	0.57
1:G:7:GLY:CA	1:G:8:VAL:CB	2.82	0.57
1:C:309:LEU:HD22	1:C:310:THR:H	1.70	0.57
1:E:38:PHE:HD1	1:E:39:ARG:H	1.51	0.57
1:H:67:GLY:O	1:H:69:GLU:N	2.38	0.57
1:E:62:MET:HB2	1:E:142:ILE:HD11	1.87	0.57
1:H:168:ILE:HG12	1:H:220:VAL:HG21	1.86	0.57
1:B:152:VAL:CG1	1:B:152:VAL:O	2.52	0.57
1:A:109:TYR:CD1	1:A:120:VAL:HG13	2.39	0.57
1:A:39:ARG:HH12	1:A:146:ASN:N	2.03	0.57
1:E:107:GLN:O	1:E:110:THR:HG22	2.04	0.57
1:C:47:LEU:HB3	1:C:74:VAL:HG12	1.87	0.57
1:A:39:ARG:HH12	1:A:146:ASN:C	2.08	0.57
1:B:217:GLU:OE1	1:B:311:LEU:HD21	2.05	0.57
1:G:216:ARG:CG	1:G:216:ARG:HH11	2.16	0.57
1:A:245:HIS:CE1	1:A:289:HIS:CD2	2.79	0.57
1:C:224:LEU:HD12	1:C:225:THR:N	2.20	0.57
1:C:172:ASN:HD21	1:C:227:ALA:HA	1.70	0.57
1:A:162:ALA:HA	1:A:165:ARG:HG3	1.87	0.56
1:C:167:GLU:HG3	1:C:170:ARG:NH1	2.20	0.56
1:D:299:PRO:C	1:D:301:GLY:N	2.56	0.56
1:D:149:PHE:O	1:D:154:ALA:HB2	2.05	0.56
1:E:300:VAL:CG1	1:E:300:VAL:O	2.54	0.56
1:E:307:PRO:CG	1:E:308:GLY:H	2.16	0.56
1:E:61:ILE:HD13	1:E:272:VAL:HG13	1.86	0.56
1:G:61:ILE:HG23	1:G:272:VAL:HG22	1.85	0.56
1:C:4:LEU:HD21	1:C:106:TYR:HB2	1.87	0.56
1:D:39:ARG:NH1	1:D:149:PHE:CG	2.73	0.56
1:E:229:ILE:O	1:E:233:PRO:HD3	2.05	0.56
1:G:30:TYR:H	1:G:136:ASN:HD21	1.54	0.56
1:G:39:ARG:HE	1:G:39:ARG:HA	1.65	0.56
1:H:59:VAL:HG11	1:H:141:ILE:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASN:HD21	1:B:91:GLY:HA3	1.63	0.56
1:F:68:LEU:HD21	1:F:154:ALA:HB2	1.87	0.56
1:G:110:THR:HG22	1:G:111:ALA:N	2.20	0.56
1:E:160:TYR:CE1	1:E:165:ARG:HG3	2.39	0.56
1:H:213:LEU:HD23	1:H:219:LEU:HD23	1.87	0.56
1:H:81:MET:HB3	1:H:288:SER:HB2	1.86	0.56
1:A:19:SER:H	1:A:20:GLY:CA	2.13	0.56
1:E:245:HIS:HE1	1:E:289:HIS:CD2	2.16	0.56
1:F:143:ARG:O	1:F:146:ASN:HB3	2.04	0.56
1:F:36:ALA:O	1:F:38:PHE:HB3	2.04	0.56
1:G:31:ARG:NH1	1:G:31:ARG:HG2	2.20	0.56
1:H:164:PHE:C	1:H:166:PRO:HD2	2.25	0.56
1:B:106:TYR:HA	1:B:120:VAL:HG11	1.88	0.56
1:B:23:PHE:O	1:B:23:PHE:CD2	2.59	0.56
1:D:44:ARG:HG2	1:D:45:TYR:CE2	2.40	0.56
1:E:160:TYR:CZ	1:E:165:ARG:HG3	2.40	0.56
1:G:210:GLU:CD	1:G:258:ASN:HB2	2.26	0.56
1:B:122:ILE:HB	1:B:123:PRO:HA	1.87	0.56
1:C:87:THR:HG22	1:C:89:LEU:H	1.69	0.56
1:D:282:LYS:HZ2	1:D:301:GLY:HA3	1.71	0.56
1:G:2:GLY:HA3	1:G:11:ASP:HA	1.88	0.56
1:H:163:GLU:C	1:H:164:PHE:HD2	2.09	0.56
1:E:62:MET:HE2	1:E:142:ILE:O	2.06	0.56
1:H:22:ARG:HB2	1:H:23:PHE:HA	1.88	0.56
1:H:91:GLY:O	1:H:94:VAL:CG2	2.52	0.56
1:A:159:TYR:HE1	1:A:224:LEU:HD23	1.71	0.55
1:D:2:GLY:HA3	1:D:9:TRP:CZ2	2.41	0.55
1:F:37:GLY:C	1:F:39:ARG:H	2.09	0.55
1:F:97:ASP:OD2	1:F:100:ASN:HB3	2.05	0.55
1:H:172:ASN:ND2	1:H:230:ARG:HE	2.04	0.55
1:A:192:GLN:O	1:A:196:GLU:HG3	2.06	0.55
1:A:299:PRO:O	1:A:301:GLY:N	2.39	0.55
1:D:172:ASN:HD21	1:D:227:ALA:HA	1.69	0.55
1:A:271:ARG:HG2	1:A:271:ARG:HH11	1.69	0.55
1:A:304:GLN:HA	1:A:304:GLN:HE21	1.72	0.55
1:A:98:SER:O	1:A:99:ILE:HG13	2.05	0.55
1:D:14:TYR:CD1	1:D:26:LYS:HE2	2.41	0.55
1:D:286:TYR:CZ	1:D:299:PRO:HG2	2.42	0.55
1:E:191:THR:HG22	1:E:194:ALA:H	1.71	0.55
1:G:167:GLU:CG	1:G:170:ARG:HH12	2.14	0.55
1:C:27:GLU:OE1	1:C:28:SER:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:VAL:O	1:D:192:GLN:NE2	2.39	0.55
1:D:87:THR:CG2	1:D:88:PHE:N	2.69	0.55
1:E:282:LYS:HZ2	1:E:301:GLY:HA3	1.68	0.55
1:F:79:ALA:HB2	1:F:280:HIS:CE1	2.41	0.55
1:A:284:HIS:O	1:A:288:SER:HB2	2.06	0.55
1:C:136:ASN:HD22	1:C:136:ASN:N	1.94	0.55
1:D:231:LEU:O	1:D:231:LEU:HG	2.05	0.55
1:E:16:THR:O	1:E:17:LYS:HB2	2.07	0.55
1:G:136:ASN:N	1:G:136:ASN:HD22	2.00	0.55
1:G:213:LEU:CD1	1:G:259:LEU:HD23	2.36	0.55
1:G:59:VAL:HG21	1:G:141:ILE:HG21	1.87	0.55
1:H:37:GLY:C	1:H:39:ARG:N	2.60	0.55
1:A:199:PHE:O	1:A:202:LEU:HB3	2.07	0.55
1:A:282:LYS:HE2	1:A:301:GLY:CA	2.35	0.55
1:B:89:LEU:HB3	1:B:90:PRO:HD2	1.89	0.55
1:C:240:ALA:HB1	1:C:282:LYS:HD2	1.89	0.55
1:A:39:ARG:HD3	1:A:148:ALA:N	2.21	0.55
1:D:2:GLY:O	1:D:3:LEU:HD23	2.07	0.55
1:D:44:ARG:HD3	1:D:129:VAL:HG21	1.89	0.55
1:H:5:ILE:CG2	1:H:6:ASP:N	2.69	0.55
1:E:160:TYR:N	1:E:161:PRO:HD3	2.22	0.55
1:F:58:ARG:HD2	1:F:138:SER:OG	2.07	0.55
1:A:44:ARG:O	1:A:128:LYS:HG3	2.07	0.54
1:B:202:LEU:HD12	1:B:202:LEU:C	2.27	0.54
1:C:59:VAL:HA	1:C:142:ILE:HD11	1.88	0.54
1:D:241:ILE:CG1	1:D:282:LYS:HG2	2.38	0.54
1:G:312:GLN:HG2	1:G:313:SER:H	1.72	0.54
1:H:160:TYR:N	1:H:161:PRO:CD	2.70	0.54
1:H:162:ALA:HA	1:H:165:ARG:CD	2.37	0.54
1:H:68:LEU:H	1:H:68:LEU:HD12	1.71	0.54
1:A:170:ARG:NH1	1:A:170:ARG:HG3	2.20	0.54
1:C:245:HIS:NE2	1:C:289:HIS:HD2	2.05	0.54
1:D:145:LEU:HD23	1:D:145:LEU:N	2.22	0.54
1:F:78:ASN:HD21	1:F:91:GLY:HA3	1.72	0.54
1:H:63:ARG:O	1:H:65:LEU:N	2.35	0.54
1:D:270:GLU:O	1:D:271:ARG:CB	2.54	0.54
1:G:44:ARG:HG3	1:G:129:VAL:HG23	1.90	0.54
1:H:30:TYR:H	1:H:136:ASN:HD21	1.55	0.54
1:H:57:HIS:CD2	1:H:237:ARG:HH22	2.25	0.54
1:B:76:MET:HB2	1:B:94:VAL:HB	1.89	0.54
1:C:13:TRP:HE1	1:E:13:TRP:HA	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:PRO:HG3	1:D:247:LYS:HD3	1.90	0.54
1:D:47:LEU:HD22	1:D:48:TYR:N	2.22	0.54
1:H:164:PHE:HE1	1:H:221:GLY:HA3	1.72	0.54
1:C:26:LYS:HB2	1:C:27:GLU:OE2	2.07	0.54
1:C:265:LYS:CA	1:C:310:THR:HG21	2.36	0.54
1:D:282:LYS:HZ1	1:D:301:GLY:HA3	1.73	0.54
1:E:13:TRP:HZ2	1:E:17:LYS:HZ2	1.55	0.54
1:H:256:TYR:HB3	1:H:259:LEU:HB2	1.90	0.54
1:H:282:LYS:NZ	1:H:301:GLY:CA	2.71	0.54
1:C:162:ALA:HA	1:C:165:ARG:CD	2.38	0.54
1:E:44:ARG:HG2	1:E:129:VAL:HG23	1.89	0.54
1:E:286:TYR:CZ	1:E:299:PRO:HG2	2.43	0.54
1:H:271:ARG:CG	1:H:271:ARG:NH1	2.58	0.54
1:A:160:TYR:N	1:A:161:PRO:HD3	2.22	0.54
1:C:19:SER:HB3	1:C:20:GLY:HA3	1.89	0.54
1:C:27:GLU:OE1	1:C:28:SER:N	2.41	0.54
1:A:39:ARG:NE	1:A:149:PHE:N	2.46	0.54
1:B:178:THR:O	1:B:202:LEU:HB2	2.08	0.54
1:C:167:GLU:HG3	1:C:170:ARG:HH11	1.73	0.54
1:D:150:ASP:O	1:D:152:VAL:N	2.39	0.54
1:E:62:MET:HB2	1:E:142:ILE:CD1	2.37	0.54
1:E:66:LYS:HD2	1:E:146:ASN:HA	1.90	0.54
1:E:15:ASP:CG	1:E:15:ASP:O	2.46	0.54
1:E:37:GLY:CA	1:E:38:PHE:CD2	2.91	0.54
1:D:210:GLU:OE2	1:D:257:PRO:HG2	2.08	0.54
1:G:58:ARG:HD2	1:G:138:SER:OG	2.08	0.54
1:A:136:ASN:HD22	1:A:136:ASN:N	2.07	0.53
1:B:32:GLY:HA3	1:B:134:LEU:HD12	1.89	0.53
1:D:159:TYR:HD1	1:D:224:LEU:O	1.92	0.53
1:E:70:GLU:N	1:E:70:GLU:CD	2.62	0.53
1:F:256:TYR:O	1:F:260:SER:HB2	2.08	0.53
1:B:232:PHE:HB3	1:B:233:PRO:HD3	1.90	0.53
1:E:13:TRP:NE1	1:E:16:THR:HG22	2.23	0.53
1:G:210:GLU:OE1	1:G:256:TYR:HB3	2.08	0.53
1:A:39:ARG:NH2	1:A:149:PHE:N	2.47	0.53
1:D:53:CYS:HG	1:D:55:TRP:HD1	1.56	0.53
1:F:30:TYR:O	1:F:135:ASN:HA	2.09	0.53
1:F:36:ALA:C	1:F:38:PHE:CB	2.77	0.53
1:B:286:TYR:HB2	1:B:298:VAL:HG22	1.90	0.53
1:D:268:SER:HB2	1:D:309:LEU:HD22	1.89	0.53
1:E:160:TYR:N	1:E:161:PRO:CD	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:ASN:ND2	1:F:91:GLY:HA3	2.24	0.53
1:A:151:ASP:HB3	1:A:152:VAL:HG13	1.89	0.53
1:E:150:ASP:CA	1:E:154:ALA:HB3	2.39	0.53
1:C:87:THR:CG2	1:C:89:LEU:HG	2.35	0.53
1:F:5:ILE:C	1:F:7:GLY:N	2.60	0.53
1:G:312:GLN:HG2	1:G:313:SER:N	2.23	0.53
1:C:16:THR:HG22	1:C:18:SER:H	1.74	0.53
1:E:210:GLU:CD	1:E:258:ASN:HB2	2.29	0.53
1:A:97:ASP:OD2	1:A:100:ASN:HB3	2.08	0.53
1:B:269:HIS:ND1	1:B:270:GLU:O	2.35	0.53
1:G:31:ARG:NH1	1:G:140:GLU:OE2	2.41	0.53
1:A:39:ARG:CD	1:A:148:ALA:N	2.72	0.53
1:B:93:ASP:CB	1:B:280:HIS:ND1	2.72	0.53
1:B:268:SER:CB	1:B:309:LEU:HG	2.39	0.53
1:B:38:PHE:CB	1:B:39:ARG:O	2.52	0.53
1:C:251:ARG:NH2	2:C:401:HOH:O	2.19	0.53
1:H:97:ASP:O	1:H:101:GLY:HA2	2.09	0.53
1:E:210:GLU:OE2	1:E:258:ASN:HB2	2.08	0.53
1:H:226:GLU:O	1:H:230:ARG:HG3	2.08	0.53
1:H:47:LEU:C	1:H:47:LEU:HD22	2.28	0.53
1:B:44:ARG:NH1	1:B:45:TYR:OH	2.41	0.52
1:C:23:PHE:CD2	1:E:27:GLU:HB3	2.44	0.52
1:H:213:LEU:CD1	1:H:258:ASN:HB3	2.39	0.52
1:A:13:TRP:C	1:A:15:ASP:HA	2.28	0.52
1:C:20:GLY:HA2	1:E:184:TYR:CB	2.38	0.52
1:E:172:ASN:HD21	1:E:227:ALA:HA	1.73	0.52
1:G:34:LEU:HD21	1:G:140:GLU:OE1	2.08	0.52
1:D:136:ASN:ND2	1:D:136:ASN:O	2.42	0.52
1:D:98:SER:O	1:D:100:ASN:N	2.42	0.52
1:E:142:ILE:O	1:E:142:ILE:HD13	2.10	0.52
1:G:213:LEU:CD2	1:G:219:LEU:HD23	2.34	0.52
1:C:25:ARG:CZ	1:C:29:GLN:HG2	2.40	0.52
1:E:202:LEU:HD12	1:E:203:PHE:N	2.25	0.52
1:A:172:ASN:HD21	1:A:227:ALA:HA	1.75	0.52
1:C:23:PHE:HD1	1:C:23:PHE:O	1.93	0.52
1:D:113:ASP:OD1	1:D:113:ASP:C	2.48	0.52
1:D:44:ARG:HD3	1:D:129:VAL:CG2	2.38	0.52
1:D:66:LYS:HE3	1:D:146:ASN:HA	1.91	0.52
1:E:97:ASP:CB	1:E:102:ALA:HB3	2.39	0.52
1:H:81:MET:H	1:H:288:SER:HB3	1.74	0.52
1:A:282:LYS:CE	1:A:301:GLY:HA3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:VAL:CG1	1:B:123:PRO:HG3	2.39	0.52
1:D:214:THR:CG2	1:D:215:GLY:N	2.65	0.52
1:E:34:LEU:HD11	1:E:140:GLU:HB3	1.92	0.52
1:F:214:THR:HA	1:F:258:ASN:HD21	1.73	0.52
1:A:136:ASN:H	1:A:136:ASN:HD22	1.56	0.52
1:A:5:ILE:HG21	1:A:10:ARG:NH1	2.19	0.52
1:D:25:ARG:NH1	1:D:29:GLN:HG2	2.25	0.52
1:E:308:GLY:O	1:E:309:LEU:HG	2.10	0.52
1:G:238:PHE:CD1	1:G:253:ILE:HG12	2.44	0.52
1:H:81:MET:HB3	1:H:288:SER:CB	2.39	0.52
1:C:286:TYR:CE2	1:C:299:PRO:HD2	2.45	0.52
1:D:143:ARG:CG	1:D:143:ARG:NH1	2.54	0.52
1:D:97:ASP:C	1:D:98:SER:O	2.47	0.52
1:F:224:LEU:HD12	1:F:224:LEU:C	2.30	0.52
1:H:97:ASP:HB3	1:H:102:ALA:H	1.75	0.52
1:B:231:LEU:HG	1:B:235:LEU:HD22	1.91	0.52
1:B:94:VAL:HG12	1:B:95:VAL:HG12	1.92	0.52
1:D:14:TYR:CG	1:D:14:TYR:O	2.63	0.52
1:D:230:ARG:O	1:D:233:PRO:HD2	2.10	0.52
1:F:7:GLY:HA2	1:F:8:VAL:C	2.30	0.52
1:H:266:LEU:O	1:H:272:VAL:HG21	2.09	0.52
1:H:4:LEU:HD12	1:H:116:TYR:CD2	2.45	0.52
1:D:269:HIS:CE1	1:D:271:ARG:HB2	2.46	0.52
1:F:34:LEU:O	1:F:35:ASP:CG	2.48	0.52
1:F:37:GLY:N	1:F:38:PHE:HB3	2.25	0.52
1:G:282:LYS:NZ	1:G:301:GLY:HA3	2.25	0.52
1:B:30:TYR:H	1:B:136:ASN:HD21	1.58	0.51
1:D:135:ASN:HD21	1:D:140:GLU:HB2	1.74	0.51
1:F:59:VAL:HA	1:F:142:ILE:HD11	1.92	0.51
1:H:31:ARG:HG3	1:H:140:GLU:OE1	2.10	0.51
1:A:160:TYR:CE2	1:A:165:ARG:HD3	2.45	0.51
1:C:162:ALA:HA	1:C:165:ARG:HD2	1.92	0.51
1:C:201:PRO:O	1:C:202:LEU:C	2.49	0.51
1:G:203:PHE:CE1	1:G:250:LEU:HB3	2.46	0.51
1:H:47:LEU:HD22	1:H:48:TYR:N	2.25	0.51
1:C:179:LEU:HD12	1:C:202:LEU:HD21	1.92	0.51
1:E:214:THR:HG23	1:E:258:ASN:HD21	1.75	0.51
1:G:240:ALA:HA	1:G:302:PRO:HG2	1.92	0.51
1:H:56:ALA:CA	1:H:123:PRO:HD3	2.39	0.51
1:H:67:GLY:C	1:H:69:GLU:H	2.14	0.51
1:A:147:SER:O	1:A:150:ASP:CG	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:PHE:HB3	1:E:154:ALA:HB2	1.93	0.51
1:E:232:PHE:N	1:E:233:PRO:HD2	2.26	0.51
1:E:31:ARG:HH12	1:E:137:GLU:HG2	1.75	0.51
1:F:300:VAL:HG13	1:F:300:VAL:O	2.09	0.51
1:H:164:PHE:CE1	1:H:221:GLY:HA3	2.45	0.51
1:A:68:LEU:HD12	1:A:145:LEU:HD13	1.92	0.51
1:F:162:ALA:HA	1:F:165:ARG:NE	2.26	0.51
1:D:269:HIS:CE1	1:D:270:GLU:O	2.63	0.51
1:E:26:LYS:HD3	1:E:26:LYS:C	2.31	0.51
1:F:163:GLU:HB2	1:F:164:PHE:CD1	2.45	0.51
1:F:47:LEU:HB3	1:F:74:VAL:HG12	1.92	0.51
1:A:161:PRO:HB2	1:A:164:PHE:HD1	1.76	0.51
1:B:39:ARG:CZ	1:B:41:GLU:CD	2.79	0.51
1:C:44:ARG:HG3	1:C:129:VAL:HG23	1.93	0.51
1:E:31:ARG:NH1	1:E:137:GLU:HG2	2.25	0.51
1:F:7:GLY:HA2	1:F:8:VAL:CB	2.41	0.51
1:G:31:ARG:HG3	1:G:140:GLU:OE1	2.10	0.51
1:B:191:THR:CG2	1:B:194:ALA:H	2.21	0.51
1:D:15:ASP:C	1:D:17:LYS:N	2.63	0.51
1:D:257:PRO:HG2	1:D:258:ASN:H	1.76	0.51
1:E:99:ILE:HD13	1:E:99:ILE:C	2.31	0.51
1:C:37:GLY:HA2	1:C:38:PHE:CD2	2.46	0.50
1:D:81:MET:CE	1:D:86:TRP:CE2	2.94	0.50
1:E:247:LYS:HG2	1:F:299:PRO:HB3	1.93	0.50
1:H:137:GLU:HG3	1:H:139:SER:OG	2.10	0.50
1:A:2:GLY:HA3	1:A:9:TRP:CZ2	2.47	0.50
1:B:186:SER:OG	1:B:199:PHE:HB3	2.10	0.50
1:B:179:LEU:CD1	1:B:202:LEU:HD13	2.42	0.50
1:C:286:TYR:O	1:C:296:GLY:HA2	2.11	0.50
1:G:176:TYR:HE1	1:G:181:ASN:ND2	2.09	0.50
1:D:41:GLU:HA	1:D:152:VAL:HG11	1.94	0.50
1:G:205:THR:HG22	1:G:209:LEU:HD23	1.93	0.50
1:H:127:ASP:OD1	1:H:130:GLU:HG3	2.11	0.50
1:H:182:GLY:O	1:H:183:VAL:C	2.49	0.50
1:C:42:PRO:CG	1:C:152:VAL:HG11	2.37	0.50
1:D:149:PHE:CD2	1:D:149:PHE:O	2.64	0.50
1:E:68:LEU:HD12	1:E:68:LEU:H	1.76	0.50
1:H:178:THR:O	1:H:182:GLY:HA3	2.11	0.50
1:H:282:LYS:HZ2	1:H:301:GLY:HA3	1.77	0.50
1:C:5:ILE:HG13	1:C:22:ARG:HD2	1.93	0.50
1:D:3:LEU:HD13	1:D:24:VAL:HG11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:ARG:N	1:E:166:PRO:HD2	2.26	0.50
1:E:177:GLU:HG2	1:E:177:GLU:O	2.11	0.50
1:H:211:GLU:O	1:H:214:THR:HB	2.10	0.50
1:H:80:TYR:CE2	1:H:82:GLY:HA3	2.46	0.50
1:A:37:GLY:CA	1:A:38:PHE:CB	2.61	0.50
1:D:210:GLU:OE2	1:D:257:PRO:HD2	2.12	0.50
1:D:44:ARG:HG2	1:D:45:TYR:CZ	2.46	0.50
1:E:115:THR:O	1:E:116:TYR:C	2.50	0.50
1:F:161:PRO:HB3	1:F:223:ARG:NH2	2.26	0.50
1:F:265:LYS:HB2	1:F:309:LEU:HD13	1.93	0.50
1:H:166:PRO:HG2	1:H:167:GLU:N	2.23	0.50
1:H:166:PRO:CG	1:H:167:GLU:H	2.20	0.50
1:H:232:PHE:O	1:H:236:VAL:HG12	2.12	0.50
1:B:93:ASP:C	1:B:94:VAL:HG22	2.32	0.50
1:C:63:ARG:HH11	1:C:63:ARG:CG	2.17	0.50
1:F:37:GLY:N	1:F:38:PHE:CB	2.75	0.50
1:H:22:ARG:HH11	1:H:23:PHE:HD2	1.60	0.50
1:E:107:GLN:HA	1:E:110:THR:CG2	2.41	0.50
1:E:243:HIS:CD2	1:E:249:ASN:HA	2.47	0.50
1:F:78:ASN:HB2	1:F:87:THR:HG22	1.92	0.50
1:A:79:ALA:HB2	1:A:280:HIS:CE1	2.46	0.50
1:E:168:ILE:HG13	1:E:220:VAL:HG11	1.94	0.50
1:E:36:ALA:O	1:E:37:GLY:O	2.30	0.50
1:H:44:ARG:HH11	1:H:129:VAL:HB	1.76	0.50
1:D:122:ILE:HB	1:D:123:PRO:CA	2.39	0.49
1:E:202:LEU:CD1	1:E:202:LEU:C	2.79	0.49
1:E:42:PRO:HA	1:E:71:MET:HB3	1.93	0.49
1:H:59:VAL:HG11	1:H:141:ILE:HG21	1.93	0.49
1:H:172:ASN:CB	1:H:230:ARG:HH21	2.24	0.49
1:D:269:HIS:CE1	1:D:271:ARG:CB	2.95	0.49
1:F:90:PRO:O	1:F:91:GLY:O	2.31	0.49
1:C:226:GLU:O	1:C:230:ARG:HG2	2.12	0.49
1:C:2:GLY:N	1:E:19:SER:CB	2.75	0.49
1:E:208:TRP:O	1:E:211:GLU:N	2.46	0.49
1:E:44:ARG:CG	1:E:129:VAL:HG23	2.41	0.49
1:F:220:VAL:CG1	1:F:221:GLY:N	2.74	0.49
1:H:231:LEU:HD11	1:H:235:LEU:CD2	2.42	0.49
1:H:268:SER:O	1:H:269:HIS:C	2.51	0.49
1:G:24:VAL:HG23	1:H:26:LYS:HD3	1.94	0.49
1:C:16:THR:HG22	1:C:18:SER:N	2.27	0.49
1:C:272:VAL:O	1:C:275:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:GLU:HG2	1:D:171:ILE:HD12	1.94	0.49
1:B:231:LEU:HG	1:B:235:LEU:CD2	2.43	0.49
1:D:34:LEU:O	1:D:36:ALA:N	2.46	0.49
1:E:150:ASP:HA	1:E:154:ALA:HB3	1.93	0.49
1:E:273:ALA:HB3	1:E:274:PRO:HD3	1.93	0.49
1:H:299:PRO:C	1:H:301:GLY:N	2.66	0.49
1:A:294:PRO:HG3	1:B:294:PRO:HG3	1.94	0.49
1:D:152:VAL:O	1:D:152:VAL:HG12	2.12	0.49
1:E:67:GLY:O	1:E:69:GLU:HG2	2.12	0.49
1:G:235:LEU:HB3	1:G:263:VAL:CG2	2.42	0.49
1:H:49:ALA:O	1:H:77:VAL:HG22	2.12	0.49
1:A:106:TYR:CA	1:A:120:VAL:HG11	2.42	0.49
1:B:190:THR:HG23	1:D:6:ASP:OD1	2.12	0.49
1:D:162:ALA:HB2	1:D:165:ARG:CZ	2.43	0.49
1:H:142:ILE:HD11	1:H:226:GLU:HB2	1.95	0.49
1:A:269:HIS:C	1:A:270:GLU:O	2.44	0.49
1:H:143:ARG:NH1	1:H:160:TYR:CZ	2.81	0.49
1:A:218:TRP:CZ3	1:A:224:LEU:HD13	2.48	0.49
1:D:126:TRP:C	1:D:126:TRP:CD1	2.85	0.49
1:E:208:TRP:O	1:E:209:LEU:C	2.50	0.49
1:G:109:TYR:CD1	1:G:120:VAL:HG13	2.47	0.49
1:A:178:THR:O	1:A:202:LEU:HD22	2.13	0.49
1:B:295:THR:OG1	1:B:297:ILE:HG12	2.13	0.49
1:C:31:ARG:HD2	1:C:140:GLU:OE1	2.13	0.49
1:E:98:SER:O	1:E:99:ILE:HG22	2.13	0.49
1:F:160:TYR:CE1	1:F:165:ARG:HG2	2.48	0.49
1:H:271:ARG:CB	1:H:271:ARG:HH11	2.25	0.49
1:A:143:ARG:NH1	1:A:226:GLU:OE1	2.45	0.48
1:F:218:TRP:CZ2	1:F:265:LYS:HD3	2.48	0.48
1:H:20:GLY:HA3	1:H:22:ARG:N	2.20	0.48
1:H:63:ARG:CG	1:H:63:ARG:HH11	2.16	0.48
1:A:14:TYR:CG	1:A:14:TYR:O	2.67	0.48
1:C:37:GLY:CA	1:C:38:PHE:HB3	2.42	0.48
1:D:243:HIS:CD2	1:D:249:ASN:HA	2.48	0.48
1:F:220:VAL:HG12	1:F:221:GLY:N	2.28	0.48
1:F:273:ALA:N	1:F:274:PRO:HD2	2.28	0.48
1:B:33:GLY:O	1:B:34:LEU:HB2	2.12	0.48
1:C:136:ASN:H	1:C:136:ASN:ND2	2.06	0.48
1:C:42:PRO:HD3	1:C:152:VAL:HG21	1.95	0.48
1:E:97:ASP:OD2	1:E:102:ALA:HB3	2.13	0.48
1:G:237:ARG:HG3	1:G:237:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ARG:O	1:C:27:GLU:N	2.45	0.48
1:D:191:THR:O	1:D:192:GLN:C	2.50	0.48
1:F:42:PRO:HD3	1:F:152:VAL:CG1	2.44	0.48
1:A:31:ARG:NH1	1:A:140:GLU:OE2	2.46	0.48
1:D:66:LYS:HB2	1:D:68:LEU:HG	1.95	0.48
1:E:183:VAL:HG21	1:E:242:TYR:CE2	2.48	0.48
1:E:263:VAL:HG12	1:E:264:GLY:N	2.29	0.48
1:F:6:ASP:HA	1:F:115:THR:O	2.14	0.48
1:H:231:LEU:HD11	1:H:235:LEU:HD22	1.96	0.48
1:H:92:ASP:N	1:H:92:ASP:OD1	2.36	0.48
1:F:34:LEU:O	1:F:35:ASP:HB3	2.13	0.48
1:F:70:GLU:CD	1:F:70:GLU:H	2.16	0.48
1:F:60:LEU:HD21	1:F:76:MET:HE1	1.95	0.48
1:A:22:ARG:CG	1:A:22:ARG:NH1	2.58	0.48
1:A:238:PHE:CD1	1:A:253:ILE:HG12	2.48	0.48
1:H:306:LEU:HB3	1:H:307:PRO:CD	2.29	0.48
1:H:44:ARG:O	1:H:128:LYS:HB2	2.13	0.48
1:H:57:HIS:O	1:H:61:ILE:HG12	2.13	0.48
1:H:66:LYS:C	1:H:68:LEU:HD12	2.34	0.48
1:C:10:ARG:HG2	1:C:15:ASP:CG	2.34	0.48
1:D:39:ARG:HB2	1:D:148:ALA:HB1	1.96	0.48
1:D:150:ASP:C	1:D:152:VAL:H	2.17	0.48
1:E:68:LEU:HD23	1:E:149:PHE:CD2	2.48	0.48
1:F:119:ARG:CG	1:F:119:ARG:NH1	2.65	0.48
1:F:99:ILE:O	1:F:100:ASN:HB2	2.14	0.48
1:G:213:LEU:HD12	1:G:259:LEU:CD2	2.36	0.48
1:G:39:ARG:CA	1:G:39:ARG:NE	2.59	0.48
1:A:95:VAL:HA	1:A:96:PRO:HD3	1.63	0.48
1:C:282:LYS:HZ1	1:C:301:GLY:HA3	1.79	0.48
1:E:191:THR:CG2	1:E:194:ALA:H	2.27	0.48
1:E:35:ASP:O	1:E:36:ALA:C	2.52	0.48
1:G:299:PRO:C	1:G:301:GLY:N	2.66	0.48
1:G:39:ARG:HE	1:G:40:GLY:CA	2.27	0.48
1:H:7:GLY:HA2	1:H:8:VAL:CB	2.44	0.48
1:C:19:SER:N	1:C:20:GLY:HA3	2.28	0.47
1:C:229:ILE:O	1:C:233:PRO:HD3	2.14	0.47
1:D:105:LEU:HD21	1:D:122:ILE:HG23	1.96	0.47
1:D:175:VAL:O	1:D:175:VAL:HG22	2.13	0.47
1:E:178:THR:O	1:E:182:GLY:HA3	2.14	0.47
1:F:269:HIS:CE1	1:F:270:GLU:O	2.66	0.47
1:E:229:ILE:O	1:E:233:PRO:CD	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:PRO:O	1:E:305:PRO:HD3	2.14	0.47
1:F:299:PRO:C	1:F:301:GLY:N	2.68	0.47
1:G:299:PRO:O	1:G:301:GLY:N	2.47	0.47
1:H:259:LEU:O	1:H:263:VAL:HG23	2.14	0.47
1:C:160:TYR:N	1:C:161:PRO:HD3	2.28	0.47
1:C:47:LEU:HD21	1:C:59:VAL:HG21	1.96	0.47
1:D:17:LYS:HG3	1:D:21:GLY:H	1.80	0.47
1:H:171:ILE:O	1:H:175:VAL:HG23	2.15	0.47
1:H:229:ILE:O	1:H:233:PRO:HD3	2.14	0.47
1:A:35:ASP:O	1:A:36:ALA:C	2.52	0.47
1:A:92:ASP:O	1:A:93:ASP:HB2	2.13	0.47
1:B:307:PRO:O	1:B:308:GLY:O	2.32	0.47
1:H:46:HIS:HB2	1:H:128:LYS:HE3	1.96	0.47
1:A:270:GLU:O	1:A:271:ARG:CB	2.38	0.47
1:D:238:PHE:HA	1:D:242:TYR:HB2	1.97	0.47
1:B:309:LEU:HD22	1:B:310:THR:N	2.30	0.47
1:C:38:PHE:H	1:C:39:ARG:NH1	2.12	0.47
1:F:243:HIS:CD2	1:F:249:ASN:HA	2.50	0.47
1:H:24:VAL:O	1:H:25:ARG:HB2	2.15	0.47
1:H:63:ARG:C	1:H:65:LEU:H	2.18	0.47
1:C:20:GLY:HA2	1:E:184:TYR:HB2	1.97	0.47
1:D:202:LEU:CD1	1:D:202:LEU:C	2.76	0.47
1:D:87:THR:CG2	1:D:89:LEU:CG	2.87	0.47
1:F:210:GLU:OE2	1:F:258:ASN:HB2	2.13	0.47
1:F:44:ARG:HG3	1:F:129:VAL:HG23	1.96	0.47
1:H:266:LEU:O	1:H:272:VAL:CG2	2.63	0.47
1:C:179:LEU:HA	1:C:202:LEU:CD2	2.44	0.47
1:F:152:VAL:O	1:F:152:VAL:CG1	2.61	0.47
1:G:30:TYR:O	1:G:135:ASN:HA	2.15	0.47
1:G:302:PRO:O	1:G:305:PRO:HG3	2.15	0.47
1:A:223:ARG:CB	1:A:223:ARG:NH1	2.62	0.47
1:D:4:LEU:HD12	1:D:116:TYR:CD2	2.50	0.47
1:E:224:LEU:C	1:E:224:LEU:HD12	2.34	0.47
1:E:278:LEU:HA	1:E:278:LEU:HD12	1.66	0.47
1:E:47:LEU:HD22	1:E:48:TYR:N	2.29	0.47
1:F:167:GLU:O	1:F:171:ILE:HG13	2.14	0.47
1:H:44:ARG:O	1:H:44:ARG:HG3	2.13	0.47
1:C:61:ILE:CG2	1:C:65:LEU:HD22	2.45	0.47
1:D:78:ASN:OD1	1:D:79:ALA:N	2.47	0.47
1:E:97:ASP:HB3	1:E:102:ALA:HB3	1.96	0.47
1:F:33:GLY:O	1:F:34:LEU:HD22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:GLY:HA2	1:G:38:PHE:HB3	1.97	0.47
1:H:30:TYR:O	1:H:135:ASN:HA	2.15	0.47
1:C:179:LEU:HD12	1:C:202:LEU:HD22	1.96	0.46
1:C:174:ARG:HD3	1:C:208:TRP:CE3	2.50	0.46
1:C:25:ARG:NH1	1:C:29:GLN:HG2	2.29	0.46
1:C:33:GLY:O	1:C:34:LEU:CB	2.55	0.46
1:D:39:ARG:HB3	1:D:148:ALA:O	2.15	0.46
1:C:23:PHE:HE2	1:E:27:GLU:HB3	1.80	0.46
1:E:310:THR:HG22	1:E:311:LEU:N	2.30	0.46
1:G:134:LEU:HD12	1:G:134:LEU:O	2.15	0.46
1:G:295:THR:HB	1:G:297:ILE:HG12	1.96	0.46
1:G:8:VAL:CB	1:G:10:ARG:HH11	2.28	0.46
1:G:9:TRP:NE1	1:G:84:ASN:HA	2.30	0.46
1:H:165:ARG:N	1:H:166:PRO:CD	2.78	0.46
1:A:304:GLN:CA	1:A:304:GLN:HE21	2.27	0.46
1:B:147:SER:O	1:B:149:PHE:N	2.48	0.46
1:B:204:ASP:O	1:B:207:ASP:HB2	2.15	0.46
1:B:69:GLU:HG2	1:B:69:GLU:H	1.59	0.46
1:B:79:ALA:HB2	1:B:280:HIS:NE2	2.30	0.46
1:C:35:ASP:O	1:C:36:ALA:HB2	2.14	0.46
1:D:165:ARG:N	1:D:166:PRO:CD	2.77	0.46
1:G:137:GLU:HG3	1:G:140:GLU:HG3	1.97	0.46
1:G:176:TYR:C	1:G:176:TYR:CD1	2.88	0.46
1:G:3:LEU:C	1:G:3:LEU:CD1	2.84	0.46
1:F:210:GLU:OE1	1:F:256:TYR:HB3	2.16	0.46
1:G:38:PHE:O	1:G:39:ARG:CB	2.64	0.46
1:A:39:ARG:NH1	1:A:147:SER:CA	2.78	0.46
1:B:312:GLN:HG2	1:B:313:SER:N	2.22	0.46
1:D:37:GLY:HA2	1:D:38:PHE:CG	2.51	0.46
1:E:7:GLY:CA	1:E:8:VAL:CB	2.72	0.46
1:G:210:GLU:OE2	1:G:258:ASN:HB2	2.15	0.46
1:A:5:ILE:HA	1:A:5:ILE:HD12	1.81	0.46
1:B:218:TRP:CH2	1:B:265:LYS:HD3	2.50	0.46
1:D:149:PHE:HD2	1:D:149:PHE:O	1.99	0.46
1:D:19:SER:N	1:D:20:GLY:HA3	2.30	0.46
1:H:68:LEU:HD21	1:H:149:PHE:HD2	1.80	0.46
1:A:39:ARG:HD2	1:A:144:ILE:O	2.14	0.46
1:D:14:TYR:CE2	1:D:24:VAL:HB	2.50	0.46
1:D:78:ASN:HA	1:D:94:VAL:HG22	1.97	0.46
1:E:75:SER:HA	1:E:95:VAL:HG12	1.98	0.46
1:A:311:LEU:O	1:A:311:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:TYR:C	1:D:176:TYR:CD2	2.89	0.46
1:F:187:GLY:HA3	1:F:246:PHE:CD1	2.51	0.46
1:A:210:GLU:CD	1:A:258:ASN:HB2	2.35	0.46
1:A:33:GLY:O	1:A:34:LEU:CB	2.60	0.46
1:B:258:ASN:CG	1:B:261:ARG:HH21	2.19	0.46
1:B:90:PRO:O	1:B:91:GLY:C	2.55	0.46
1:C:17:LYS:O	1:C:18:SER:HB2	2.16	0.46
1:C:69:GLU:H	1:C:69:GLU:HG2	1.50	0.46
1:G:171:ILE:O	1:G:174:ARG:N	2.40	0.46
1:H:57:HIS:CG	1:H:237:ARG:HH22	2.34	0.46
1:H:37:GLY:HA2	1:H:39:ARG:N	2.30	0.46
1:A:91:GLY:O	1:A:94:VAL:HG23	2.16	0.46
1:C:204:ASP:O	1:C:207:ASP:HB2	2.16	0.46
1:C:37:GLY:CA	1:C:38:PHE:CB	2.93	0.46
1:C:90:PRO:O	1:C:91:GLY:O	2.33	0.46
1:E:214:THR:HG23	1:E:258:ASN:ND2	2.30	0.46
1:H:271:ARG:CB	1:H:271:ARG:NH1	2.78	0.46
1:C:26:LYS:C	1:C:27:GLU:HG3	2.37	0.46
1:D:81:MET:HE3	1:D:86:TRP:CE2	2.50	0.46
1:F:37:GLY:C	1:F:39:ARG:N	2.69	0.46
1:G:160:TYR:CE2	1:G:165:ARG:HD3	2.51	0.46
1:A:179:LEU:HA	1:A:202:LEU:HD22	1.97	0.45
1:C:136:ASN:ND2	1:C:136:ASN:N	2.63	0.45
1:C:23:PHE:O	1:C:23:PHE:CD1	2.69	0.45
1:C:258:ASN:O	1:C:261:ARG:N	2.49	0.45
1:H:277:ASN:OD1	1:H:277:ASN:C	2.54	0.45
1:D:167:GLU:OE1	1:D:220:VAL:HG22	2.16	0.45
1:G:245:HIS:CE1	1:G:289:HIS:HD2	2.30	0.45
1:H:151:ASP:O	1:H:153:GLY:N	2.47	0.45
1:H:232:PHE:N	1:H:233:PRO:HD2	2.31	0.45
1:A:37:GLY:CA	1:A:38:PHE:HD1	2.30	0.45
1:A:5:ILE:CG2	1:A:6:ASP:N	2.79	0.45
1:D:184:TYR:O	1:D:185:ARG:C	2.54	0.45
1:D:241:ILE:HG13	1:D:282:LYS:HG2	1.98	0.45
1:F:211:GLU:O	1:F:214:THR:HB	2.15	0.45
1:F:37:GLY:CA	1:F:38:PHE:HB3	2.45	0.45
1:G:191:THR:HG23	1:G:194:ALA:N	2.15	0.45
1:H:163:GLU:O	1:H:164:PHE:HD2	2.00	0.45
1:C:105:LEU:HA	1:C:105:LEU:HD12	1.76	0.45
1:C:174:ARG:HD3	1:C:208:TRP:CZ3	2.51	0.45
1:C:232:PHE:N	1:C:233:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ARG:HD3	1:C:45:TYR:CZ	2.52	0.45
1:C:47:LEU:HD11	1:C:59:VAL:CG2	2.46	0.45
1:E:97:ASP:OD2	1:E:102:ALA:CB	2.64	0.45
1:G:165:ARG:N	1:G:166:PRO:HD2	2.32	0.45
1:H:218:TRP:CZ3	1:H:224:LEU:HD13	2.52	0.45
1:C:5:ILE:HG22	1:C:6:ASP:H	1.78	0.45
1:D:120:VAL:O	1:D:120:VAL:HG12	2.17	0.45
1:E:44:ARG:HG3	1:E:129:VAL:CG2	2.46	0.45
1:G:231:LEU:HG	1:G:235:LEU:CD2	2.45	0.45
1:G:266:LEU:O	1:G:268:SER:N	2.50	0.45
1:B:160:TYR:CZ	1:B:165:ARG:HG2	2.52	0.45
1:D:63:ARG:NH2	1:D:74:VAL:HG13	2.31	0.45
1:E:172:ASN:ND2	1:E:230:ARG:HD3	2.31	0.45
1:E:231:LEU:HG	1:E:235:LEU:HD22	1.98	0.45
1:H:163:GLU:C	1:H:164:PHE:CD2	2.90	0.45
1:A:12:ALA:O	1:A:13:TRP:O	2.34	0.45
1:B:223:ARG:O	1:B:225:THR:HG23	2.17	0.45
1:A:249:ASN:OD1	1:B:301:GLY:CA	2.63	0.45
1:C:59:VAL:HA	1:C:142:ILE:CD1	2.47	0.45
1:A:63:ARG:NH2	1:A:74:VAL:HG23	2.32	0.45
1:C:136:ASN:C	1:C:136:ASN:ND2	2.69	0.45
1:C:235:LEU:HB3	1:C:263:VAL:HG21	1.98	0.45
1:D:14:TYR:CE1	1:D:26:LYS:HE2	2.52	0.45
1:D:161:PRO:HG3	1:D:223:ARG:NH2	2.31	0.45
1:A:13:TRP:HB2	1:A:15:ASP:HA	1.99	0.45
1:A:17:LYS:C	1:A:21:GLY:HA3	2.37	0.45
1:A:221:GLY:CA	2:A:401:HOH:O	2.21	0.45
1:A:5:ILE:CG2	1:A:10:ARG:NH1	2.77	0.45
1:C:241:ILE:HD13	1:C:285:TYR:HD1	1.81	0.45
1:D:204:ASP:O	1:D:207:ASP:HB2	2.17	0.45
1:E:57:HIS:NE2	1:E:275:THR:O	2.48	0.45
1:E:250:LEU:CD1	1:F:303:ALA:HB2	2.47	0.45
1:G:290:PRO:HD2	1:G:291:SER:H	1.82	0.45
1:G:92:ASP:O	1:G:94:VAL:N	2.50	0.45
1:H:160:TYR:CZ	1:H:165:ARG:HG2	2.52	0.45
1:B:39:ARG:CZ	1:B:41:GLU:OE2	2.65	0.45
1:D:142:ILE:HA	1:D:142:ILE:HD12	1.47	0.45
1:D:162:ALA:HA	1:D:165:ARG:CG	2.43	0.45
1:D:33:GLY:HA3	1:D:144:ILE:HD11	1.98	0.45
1:E:62:MET:HG2	1:E:142:ILE:HD13	1.98	0.45
1:F:33:GLY:O	1:F:34:LEU:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:86:TRP:HB2	1:H:105:LEU:CD2	2.46	0.45
1:H:99:ILE:CG1	1:H:99:ILE:O	2.65	0.45
1:A:2:GLY:O	1:A:3:LEU:HD23	2.17	0.44
1:C:76:MET:H	1:C:95:VAL:HB	1.81	0.44
1:D:39:ARG:NH1	1:D:149:PHE:CB	2.79	0.44
1:E:51:PHE:HB2	1:E:280:HIS:CD2	2.52	0.44
1:F:142:ILE:HA	1:F:142:ILE:HD13	1.32	0.44
1:F:250:LEU:HA	1:F:250:LEU:HD12	1.63	0.44
1:D:81:MET:HE1	1:D:86:TRP:CE2	2.52	0.44
1:G:270:GLU:O	1:G:271:ARG:CB	2.61	0.44
1:A:19:SER:HB3	1:F:3:LEU:HD21	1.99	0.44
1:B:152:VAL:HG13	1:B:152:VAL:O	2.15	0.44
1:B:210:GLU:OE1	1:B:259:LEU:HG	2.16	0.44
1:B:278:LEU:HD12	1:B:278:LEU:HA	1.59	0.44
1:B:93:ASP:O	1:B:94:VAL:CG1	2.64	0.44
1:D:71:MET:HB3	1:D:149:PHE:HZ	1.82	0.44
1:H:201:PRO:HA	1:H:204:ASP:HB2	2.00	0.44
1:B:232:PHE:N	1:B:233:PRO:CD	2.80	0.44
1:B:5:ILE:CG2	1:B:6:ASP:N	2.81	0.44
1:C:245:HIS:CD2	1:C:246:PHE:CE1	3.06	0.44
1:C:278:LEU:HD12	1:C:278:LEU:HA	1.55	0.44
1:C:286:TYR:CD2	1:C:299:PRO:HD2	2.52	0.44
1:C:39:ARG:HB2	1:C:40:GLY:H	1.46	0.44
1:D:53:CYS:SG	1:D:55:TRP:HD1	2.41	0.44
1:D:66:LYS:O	1:D:68:LEU:N	2.51	0.44
1:G:286:TYR:CD2	1:G:299:PRO:HD2	2.52	0.44
1:G:39:ARG:HE	1:G:39:ARG:CA	2.24	0.44
1:A:138:SER:O	1:A:139:SER:C	2.55	0.44
1:B:266:LEU:HA	1:B:266:LEU:HD23	1.59	0.44
1:D:135:ASN:HD21	1:D:140:GLU:CB	2.31	0.44
1:D:37:GLY:HA2	1:D:38:PHE:CD2	2.53	0.44
1:E:30:TYR:O	1:E:135:ASN:HA	2.17	0.44
1:G:278:LEU:HA	1:G:278:LEU:HD12	1.85	0.44
1:A:176:TYR:HA	1:A:180:ASN:HB2	1.98	0.44
1:B:48:TYR:HB2	1:B:124:ILE:HB	2.00	0.44
1:A:300:VAL:CB	1:B:199:PHE:HZ	2.30	0.44
1:C:106:TYR:CD1	1:C:106:TYR:C	2.91	0.44
1:D:68:LEU:HD12	1:D:145:LEU:HD13	2.00	0.44
1:D:66:LYS:C	1:D:68:LEU:H	2.20	0.44
1:G:60:LEU:HA	1:G:60:LEU:HD23	1.55	0.44
1:H:30:TYR:H	1:H:136:ASN:ND2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:GLN:HG3	1:H:192:GLN:O	2.16	0.44
1:H:278:LEU:HA	1:H:278:LEU:HD12	1.54	0.44
1:H:295:THR:OG1	1:H:297:ILE:HG13	2.17	0.44
1:H:7:GLY:CA	1:H:8:VAL:O	2.66	0.44
1:A:214:THR:HA	1:A:258:ASN:ND2	2.33	0.44
1:A:79:ALA:HB2	1:A:280:HIS:NE2	2.33	0.44
1:D:269:HIS:HE1	1:D:271:ARG:CB	2.30	0.44
1:E:252:ARG:O	1:E:255:ASP:HB2	2.17	0.44
1:F:3:LEU:CD1	1:F:24:VAL:HG11	2.47	0.44
1:B:34:LEU:HD21	1:B:140:GLU:HG2	2.00	0.44
1:C:147:SER:O	1:C:149:PHE:N	2.50	0.44
1:C:18:SER:O	1:C:19:SER:CB	2.64	0.44
1:D:14:TYR:O	1:D:18:SER:HB3	2.18	0.44
1:D:61:ILE:HG21	1:D:229:ILE:HG23	2.00	0.44
1:F:122:ILE:HB	1:F:123:PRO:HA	2.00	0.44
1:G:219:LEU:HG	1:G:228:ASP:OD2	2.17	0.44
1:H:44:ARG:HH12	1:H:130:GLU:HG3	1.83	0.44
1:H:235:LEU:HA	1:H:235:LEU:HD12	1.71	0.44
1:B:3:LEU:HD12	1:B:24:VAL:HG11	1.99	0.44
1:D:53:CYS:HB3	1:D:56:ALA:HB3	1.99	0.44
1:E:218:TRP:CB	1:E:223:ARG:O	2.66	0.44
1:G:205:THR:O	1:G:209:LEU:HB2	2.18	0.44
1:H:68:LEU:HD21	1:H:149:PHE:CD2	2.53	0.44
1:A:37:GLY:CA	1:A:38:PHE:CD1	3.01	0.43
1:B:183:VAL:HG23	1:B:184:TYR:N	2.33	0.43
1:E:304:GLN:HA	1:E:305:PRO:HD2	1.69	0.43
1:G:203:PHE:CZ	1:G:250:LEU:N	2.86	0.43
1:G:86:TRP:CH2	1:G:284:HIS:CD2	3.06	0.43
1:G:5:ILE:O	1:G:6:ASP:CB	2.59	0.43
1:H:241:ILE:HG21	1:H:285:TYR:CD1	2.53	0.43
1:B:4:LEU:HA	1:B:4:LEU:HD23	1.72	0.43
1:B:63:ARG:NH2	1:B:72:ILE:O	2.42	0.43
1:C:168:ILE:CD1	1:C:225:THR:HB	2.48	0.43
1:D:39:ARG:CB	1:D:148:ALA:HB1	2.48	0.43
1:D:58:ARG:O	1:D:61:ILE:HB	2.18	0.43
1:F:47:LEU:C	1:F:47:LEU:CD2	2.87	0.43
1:G:80:TYR:CE2	1:G:82:GLY:HA3	2.52	0.43
1:B:104:TYR:HD2	1:B:106:TYR:CZ	2.36	0.43
1:D:4:LEU:HA	1:D:4:LEU:HD23	1.92	0.43
1:E:300:VAL:HG13	1:E:300:VAL:O	2.19	0.43
1:E:42:PRO:N	1:E:152:VAL:HG11	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:ARG:CG	1:F:22:ARG:O	2.63	0.43
1:H:231:LEU:CD1	1:H:235:LEU:HD22	2.49	0.43
1:A:99:ILE:O	1:A:99:ILE:CD1	2.61	0.43
1:B:172:ASN:HD21	1:B:227:ALA:HA	1.82	0.43
1:E:98:SER:C	1:E:99:ILE:HG22	2.38	0.43
1:G:160:TYR:N	1:G:161:PRO:HD3	2.32	0.43
1:E:237:ARG:HG3	1:E:237:ARG:NH1	2.31	0.43
1:E:270:GLU:O	1:E:271:ARG:CB	2.48	0.43
1:C:87:THR:CG2	1:C:88:PHE:N	2.80	0.43
1:D:61:ILE:O	1:D:62:MET:C	2.56	0.43
1:E:191:THR:HB	1:E:194:ALA:HB3	2.01	0.43
1:G:24:VAL:O	1:G:25:ARG:HG2	2.19	0.43
1:G:37:GLY:CA	1:G:38:PHE:CB	2.96	0.43
1:H:40:GLY:HA2	1:H:149:PHE:CE1	2.54	0.43
1:H:91:GLY:C	1:H:94:VAL:HG23	2.39	0.43
1:A:26:LYS:HB3	1:A:119:ARG:HD2	1.99	0.43
1:A:17:LYS:HB3	1:F:291:SER:CB	2.48	0.43
1:A:14:TYR:CD1	1:A:24:VAL:HB	2.53	0.43
1:C:161:PRO:O	1:C:165:ARG:HG3	2.19	0.43
1:D:5:ILE:HD12	1:D:117:THR:HG23	2.00	0.43
1:D:122:ILE:HD13	1:D:122:ILE:HG21	1.71	0.43
1:D:175:VAL:HG21	1:D:231:LEU:HB2	2.01	0.43
1:D:225:THR:HG23	1:D:228:ASP:OD1	2.19	0.43
1:E:94:VAL:HG12	1:E:95:VAL:N	2.33	0.43
1:G:99:ILE:HG22	1:G:100:ASN:N	2.33	0.43
1:G:282:LYS:NZ	1:G:301:GLY:CA	2.82	0.43
1:A:304:GLN:HA	1:A:304:GLN:NE2	2.33	0.43
1:A:309:LEU:HD12	1:A:309:LEU:N	2.34	0.43
1:A:74:VAL:HG12	1:A:75:SER:N	2.33	0.43
1:B:109:TYR:CD1	1:B:120:VAL:HG13	2.53	0.43
1:B:160:TYR:CE1	1:B:165:ARG:HG2	2.53	0.43
1:C:300:VAL:HG23	1:D:195:TYR:CE2	2.54	0.43
1:D:39:ARG:HD2	1:D:149:PHE:HA	1.98	0.43
1:D:65:LEU:HD21	1:D:224:LEU:HD21	2.01	0.43
1:E:46:HIS:CD2	1:E:99:ILE:HG21	2.53	0.43
1:E:47:LEU:CD2	1:E:47:LEU:C	2.87	0.43
1:G:199:PHE:O	1:G:202:LEU:HB3	2.18	0.43
1:G:38:PHE:O	1:G:39:ARG:HG2	2.18	0.43
1:A:218:TRP:CE2	1:A:265:LYS:HE3	2.53	0.43
1:C:20:GLY:HA2	1:E:184:TYR:HB3	2.01	0.43
1:D:167:GLU:O	1:D:168:ILE:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ARG:HH11	1:D:149:PHE:CB	2.30	0.43
1:G:66:LYS:NZ	1:G:146:ASN:O	2.51	0.43
1:G:251:ARG:HG3	1:G:256:TYR:HE2	1.82	0.43
1:G:273:ALA:N	1:G:274:PRO:CD	2.82	0.43
1:H:24:VAL:O	1:H:24:VAL:HG22	2.18	0.43
1:A:97:ASP:OD2	1:A:100:ASN:CB	2.67	0.43
1:B:89:LEU:C	1:B:91:GLY:N	2.71	0.43
1:C:183:VAL:HG11	1:C:242:TYR:CD2	2.54	0.43
1:D:105:LEU:CD2	1:D:122:ILE:HG23	2.49	0.43
1:F:235:LEU:HD23	1:F:263:VAL:HG23	2.01	0.43
1:F:299:PRO:O	1:F:301:GLY:N	2.51	0.43
1:F:49:ALA:HB3	1:F:76:MET:HE1	2.01	0.43
1:H:31:ARG:HD2	1:H:140:GLU:CD	2.39	0.43
1:A:98:SER:O	1:A:99:ILE:CG1	2.65	0.42
1:B:300:VAL:N	1:B:301:GLY:HA3	2.31	0.42
1:C:109:TYR:CE1	1:C:124:ILE:HD11	2.53	0.42
1:C:12:ALA:HB1	1:E:13:TRP:HE3	1.82	0.42
1:C:183:VAL:HG23	1:C:184:TYR:N	2.34	0.42
1:D:269:HIS:HE1	1:D:271:ARG:HB2	1.83	0.42
1:D:5:ILE:HA	1:D:5:ILE:HD12	1.43	0.42
1:G:200:TYR:C	1:G:202:LEU:N	2.72	0.42
1:G:217:GLU:HB3	1:G:265:LYS:NZ	2.34	0.42
1:G:266:LEU:C	1:G:268:SER:H	2.22	0.42
1:H:183:VAL:O	1:H:186:SER:HB2	2.19	0.42
1:A:300:VAL:CB	1:B:199:PHE:CZ	2.97	0.42
1:B:241:ILE:HG21	1:B:285:TYR:CG	2.53	0.42
1:C:19:SER:HB3	1:C:20:GLY:CA	2.49	0.42
1:C:68:LEU:HA	1:C:68:LEU:HD23	1.56	0.42
1:D:176:TYR:CD2	1:D:177:GLU:N	2.87	0.42
1:D:37:GLY:CA	1:D:38:PHE:CB	2.83	0.42
1:E:80:TYR:CE2	1:E:82:GLY:HA3	2.53	0.42
1:F:38:PHE:O	1:F:38:PHE:CD1	2.64	0.42
1:G:125:LEU:HA	1:G:125:LEU:HD12	1.84	0.42
1:G:203:PHE:CZ	1:G:250:LEU:HB3	2.53	0.42
1:H:151:ASP:C	1:H:153:GLY:H	2.22	0.42
1:A:61:ILE:HG23	1:A:272:VAL:HG22	2.01	0.42
1:D:210:GLU:CD	1:D:258:ASN:HB2	2.39	0.42
1:E:75:SER:C	1:E:76:MET:HG2	2.38	0.42
1:F:38:PHE:C	1:F:40:GLY:N	2.71	0.42
1:F:87:THR:CG2	1:F:88:PHE:N	2.81	0.42
1:G:5:ILE:O	1:G:7:GLY:CA	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASP:C	1:A:127:ASP:OD1	2.58	0.42
1:A:223:ARG:O	1:A:225:THR:HG23	2.19	0.42
1:A:34:LEU:HA	1:A:34:LEU:HD12	1.80	0.42
1:A:39:ARG:NH1	1:A:147:SER:H	2.11	0.42
1:B:136:ASN:HD22	1:B:136:ASN:N	2.07	0.42
1:B:199:PHE:C	1:B:202:LEU:H	2.23	0.42
1:C:219:LEU:HG	1:C:228:ASP:OD2	2.19	0.42
1:D:214:THR:HA	1:D:258:ASN:HD21	1.80	0.42
1:D:217:GLU:HB3	1:D:265:LYS:HZ1	1.78	0.42
1:D:32:GLY:HA3	1:D:134:LEU:CD1	2.49	0.42
1:E:47:LEU:HD23	1:E:124:ILE:O	2.19	0.42
1:F:174:ARG:HD3	1:F:208:TRP:CZ3	2.54	0.42
1:F:210:GLU:CD	1:F:258:ASN:HB2	2.38	0.42
1:F:99:ILE:O	1:F:99:ILE:CG1	2.68	0.42
1:G:299:PRO:C	1:G:301:GLY:H	2.22	0.42
1:H:304:GLN:HA	1:H:305:PRO:HD3	1.81	0.42
1:H:35:ASP:O	1:H:38:PHE:CD1	2.73	0.42
1:C:133:ILE:HG22	1:C:134:LEU:N	2.33	0.42
1:D:127:ASP:OD1	1:D:129:VAL:HB	2.19	0.42
1:D:14:TYR:CD2	1:D:14:TYR:O	2.72	0.42
1:D:3:LEU:CD1	1:D:24:VAL:HG11	2.49	0.42
1:D:76:MET:N	1:D:95:VAL:HB	2.35	0.42
1:C:12:ALA:CB	1:E:13:TRP:CE3	3.02	0.42
1:F:31:ARG:HD2	1:F:140:GLU:OE1	2.19	0.42
1:G:242:TYR:HA	1:G:246:PHE:HB2	2.01	0.42
1:G:6:ASP:HB2	1:G:7:GLY:HA2	2.02	0.42
1:H:161:PRO:HG3	1:H:223:ARG:NH1	2.34	0.42
1:A:195:TYR:OH	1:B:300:VAL:HB	2.19	0.42
1:C:160:TYR:N	1:C:161:PRO:CD	2.82	0.42
1:D:229:ILE:O	1:D:233:PRO:CD	2.67	0.42
1:E:168:ILE:HD11	1:E:225:THR:HB	2.00	0.42
1:A:159:TYR:CE1	1:A:224:LEU:HD23	2.53	0.42
1:A:286:TYR:CD1	1:A:299:PRO:HD3	2.54	0.42
1:B:75:SER:HA	1:B:95:VAL:HG22	2.02	0.42
1:D:165:ARG:O	1:D:169:ASP:HB2	2.20	0.42
1:E:57:HIS:HB3	1:E:233:PRO:HB3	2.02	0.42
1:C:270:GLU:O	1:C:271:ARG:CB	2.54	0.42
1:E:44:ARG:CG	1:E:129:VAL:CG2	2.98	0.42
1:A:17:LYS:HB3	1:F:291:SER:HB3	2.01	0.42
1:H:43:GLY:O	1:H:128:LYS:HD2	2.20	0.42
1:H:61:ILE:O	1:H:62:MET:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:LEU:HD12	1:C:250:LEU:HA	1.70	0.42
1:C:300:VAL:HG23	1:D:195:TYR:HE2	1.85	0.42
1:D:37:GLY:CA	1:D:38:PHE:CD2	3.03	0.42
1:F:6:ASP:CA	1:F:115:THR:O	2.67	0.42
1:C:273:ALA:N	1:C:274:PRO:CD	2.82	0.42
1:D:277:ASN:OD1	1:D:277:ASN:C	2.57	0.42
1:D:31:ARG:NH1	1:D:140:GLU:OE2	2.53	0.42
1:D:47:LEU:HD22	1:D:47:LEU:C	2.40	0.42
1:D:75:SER:C	1:D:76:MET:HG2	2.39	0.42
1:E:245:HIS:HB2	1:E:286:TYR:CZ	2.54	0.42
1:F:213:LEU:HD12	1:F:259:LEU:HD23	2.02	0.42
1:G:47:LEU:CD2	1:G:47:LEU:C	2.88	0.42
1:H:126:TRP:C	1:H:126:TRP:CD1	2.93	0.42
1:A:37:GLY:HA3	1:A:38:PHE:HD1	1.85	0.41
1:C:312:GLN:O	1:C:313:SER:HB3	2.20	0.41
1:D:81:MET:HE3	1:D:86:TRP:CD2	2.55	0.41
1:F:7:GLY:CA	1:F:8:VAL:O	2.65	0.41
1:A:17:LYS:HD2	1:A:18:SER:HB3	2.00	0.41
1:C:5:ILE:HD12	1:C:5:ILE:HA	1.46	0.41
1:E:310:THR:HG22	1:E:311:LEU:H	1.85	0.41
1:E:4:LEU:O	1:E:5:ILE:HD13	2.20	0.41
1:B:7:GLY:CA	1:B:8:VAL:CB	2.92	0.41
1:C:5:ILE:O	1:C:117:THR:HG23	2.20	0.41
1:D:39:ARG:HD3	1:D:149:PHE:CD2	2.56	0.41
1:D:33:GLY:O	1:D:34:LEU:HB2	2.20	0.41
1:F:31:ARG:HA	1:F:135:ASN:ND2	2.35	0.41
1:F:37:GLY:CA	1:F:38:PHE:CB	2.98	0.41
1:A:44:ARG:NH1	1:A:127:ASP:OD2	2.53	0.41
1:B:6:ASP:O	1:B:115:THR:HA	2.19	0.41
1:B:78:ASN:OD1	1:B:79:ALA:N	2.54	0.41
1:C:16:THR:C	1:C:18:SER:N	2.73	0.41
1:C:303:ALA:HB2	1:D:250:LEU:CD1	2.50	0.41
1:D:44:ARG:HH11	1:D:129:VAL:HB	1.86	0.41
1:E:299:PRO:C	1:E:301:GLY:N	2.73	0.41
1:E:44:ARG:HG3	1:E:129:VAL:HG21	2.02	0.41
1:F:49:ALA:HB3	1:F:76:MET:CE	2.51	0.41
1:F:86:TRP:CH2	1:F:284:HIS:CE1	3.08	0.41
1:H:23:PHE:H	1:H:24:VAL:HB	1.86	0.41
1:A:39:ARG:CZ	1:A:149:PHE:N	2.83	0.41
1:A:74:VAL:CG1	1:A:76:MET:HE3	2.51	0.41
1:C:210:GLU:OE2	1:C:257:PRO:CD	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:TRP:CD1	1:D:126:TRP:O	2.73	0.41
1:E:135:ASN:OD1	1:E:141:ILE:HG13	2.19	0.41
1:E:218:TRP:HB2	1:E:223:ARG:O	2.21	0.41
1:G:34:LEU:HD21	1:G:140:GLU:CD	2.41	0.41
1:G:195:TYR:CE1	1:G:199:PHE:HB2	2.56	0.41
1:H:175:VAL:HG12	1:H:180:ASN:OD1	2.20	0.41
1:B:172:ASN:HD22	1:B:172:ASN:HA	1.65	0.41
1:B:229:ILE:O	1:B:233:PRO:CD	2.69	0.41
1:C:139:SER:HB2	1:C:230:ARG:NH1	2.35	0.41
1:C:282:LYS:HZ2	1:C:301:GLY:HA3	1.85	0.41
1:G:167:GLU:CG	1:G:170:ARG:NH1	2.67	0.41
1:H:32:GLY:HA3	1:H:134:LEU:HD12	2.02	0.41
1:H:72:ILE:HD11	1:H:149:PHE:HE2	1.86	0.41
1:H:199:PHE:O	1:H:202:LEU:HB3	2.20	0.41
1:H:262:LEU:HD12	1:H:262:LEU:O	2.20	0.41
1:H:93:ASP:OD2	1:H:93:ASP:N	2.53	0.41
1:A:235:LEU:HA	1:A:235:LEU:HD12	1.84	0.41
1:B:162:ALA:HA	1:B:165:ARG:CD	2.50	0.41
1:B:245:HIS:CE1	1:B:289:HIS:CD2	2.88	0.41
1:B:89:LEU:CB	1:B:90:PRO:HD2	2.47	0.41
1:C:155:LEU:HD23	1:C:155:LEU:HA	1.83	0.41
1:C:89:LEU:HB3	1:C:90:PRO:HD2	2.02	0.41
1:F:297:ILE:H	1:F:297:ILE:HG12	1.74	0.41
1:G:92:ASP:C	1:G:94:VAL:H	2.24	0.41
1:A:17:LYS:HB3	1:F:291:SER:OG	2.20	0.41
1:A:269:HIS:ND1	1:A:270:GLU:O	2.47	0.41
1:B:71:MET:HE1	1:B:153:GLY:HA3	2.01	0.41
1:C:142:ILE:HD13	1:C:142:ILE:HA	1.75	0.41
1:D:210:GLU:CD	1:D:257:PRO:HD2	2.41	0.41
1:D:293:ASN:O	1:D:293:ASN:CG	2.59	0.41
1:E:139:SER:O	1:E:142:ILE:HG22	2.20	0.41
1:G:220:VAL:HG12	1:G:221:GLY:N	2.35	0.41
1:G:282:LYS:HZ1	1:G:301:GLY:HA3	1.86	0.41
1:H:282:LYS:HZ1	1:H:301:GLY:HA3	1.79	0.41
1:H:91:GLY:N	1:H:94:VAL:HG21	2.36	0.41
1:A:300:VAL:O	1:A:300:VAL:HG13	2.20	0.41
1:B:87:THR:HG23	1:B:89:LEU:H	1.86	0.41
1:D:87:THR:HG22	1:D:88:PHE:N	2.36	0.41
1:E:36:ALA:O	1:E:37:GLY:C	2.59	0.41
1:F:7:GLY:CA	1:F:8:VAL:C	2.89	0.41
1:G:43:GLY:O	1:G:128:LYS:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:246:PHE:O	1:H:248:CYS:N	2.54	0.41
1:H:53:CYS:HA	1:H:54:PRO:HD3	1.89	0.41
1:B:183:VAL:HG11	1:B:242:TYR:CD2	2.55	0.41
1:C:214:THR:C	1:C:216:ARG:H	2.24	0.41
1:C:224:LEU:C	1:C:224:LEU:HD12	2.41	0.41
1:C:265:LYS:HA	1:C:310:THR:CG2	2.45	0.41
1:C:95:VAL:HA	1:C:96:PRO:HD3	1.91	0.41
1:D:4:LEU:HD12	1:D:116:TYR:HD2	1.86	0.41
1:E:68:LEU:CD1	1:E:68:LEU:N	2.82	0.41
1:F:253:ILE:H	1:F:253:ILE:HG12	1.64	0.41
1:F:95:VAL:HA	1:F:96:PRO:HD3	1.75	0.41
1:G:282:LYS:HZ1	1:G:301:GLY:CA	2.34	0.41
1:A:17:LYS:CE	1:A:18:SER:OG	2.68	0.41
1:B:60:LEU:HA	1:B:60:LEU:HD23	1.80	0.41
1:C:235:LEU:HB3	1:C:263:VAL:CG2	2.50	0.41
1:C:312:GLN:O	1:C:313:SER:CB	2.69	0.41
1:D:160:TYR:N	1:D:161:PRO:CD	2.84	0.41
1:D:245:HIS:HB2	1:D:286:TYR:CZ	2.55	0.41
1:D:63:ARG:HH21	1:D:74:VAL:HG13	1.86	0.41
1:E:17:LYS:CA	1:E:18:SER:CB	2.93	0.41
1:E:87:THR:CG2	1:E:89:LEU:HG	2.51	0.41
1:F:6:ASP:C	1:F:115:THR:O	2.59	0.41
1:F:278:LEU:HD12	1:F:278:LEU:HA	1.94	0.41
1:G:161:PRO:O	1:G:162:ALA:C	2.59	0.41
1:G:99:ILE:HG22	1:G:100:ASN:OD1	2.21	0.41
1:C:186:SER:HB3	1:C:198:ALA:HB3	2.02	0.40
1:E:306:LEU:HA	1:E:306:LEU:HD12	1.88	0.40
1:F:176:TYR:HA	1:F:180:ASN:HB2	2.04	0.40
1:A:4:LEU:HA	1:A:4:LEU:HD23	1.90	0.40
1:B:273:ALA:N	1:B:274:PRO:CD	2.84	0.40
1:C:87:THR:N	2:C:402:HOH:O	2.54	0.40
1:F:87:THR:HG23	1:F:88:PHE:N	2.36	0.40
1:G:38:PHE:O	1:G:39:ARG:HB2	2.21	0.40
1:H:3:LEU:HD22	1:H:3:LEU:HA	1.61	0.40
1:C:89:LEU:HA	1:C:90:PRO:HD3	1.94	0.40
1:D:135:ASN:OD1	1:D:135:ASN:C	2.59	0.40
1:E:143:ARG:O	1:E:146:ASN:HB3	2.21	0.40
1:H:307:PRO:HB2	1:H:308:GLY:H	1.71	0.40
1:B:306:LEU:HD13	1:B:306:LEU:N	2.36	0.40
1:C:4:LEU:HD12	1:C:116:TYR:HD2	1.87	0.40
1:D:125:LEU:HB2	1:D:141:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:HIS:CE1	1:D:271:ARG:HB3	2.57	0.40
1:E:41:GLU:HA	1:E:152:VAL:HG11	2.03	0.40
1:H:139:SER:C	1:H:142:ILE:HG22	2.42	0.40
1:H:160:TYR:CD2	1:H:165:ARG:NE	2.90	0.40
1:H:220:VAL:HG23	1:H:225:THR:HG21	2.04	0.40
1:H:5:ILE:HA	1:H:5:ILE:HD12	1.55	0.40
1:A:185:ARG:O	1:A:189:ALA:HB2	2.21	0.40
1:A:300:VAL:CG2	1:B:199:PHE:HZ	2.34	0.40
1:B:250:LEU:O	1:B:251:ARG:HB3	2.21	0.40
1:D:68:LEU:HD22	1:D:149:PHE:CE1	2.56	0.40
1:E:235:LEU:HB3	1:E:263:VAL:CG2	2.51	0.40
1:E:307:PRO:CG	1:E:308:GLY:N	2.83	0.40
1:F:37:GLY:HA2	1:F:38:PHE:HB3	2.02	0.40
1:G:143:ARG:HE	1:G:226:GLU:CD	2.24	0.40
1:H:210:GLU:O	1:H:210:GLU:HG3	2.20	0.40
1:H:21:GLY:O	1:H:22:ARG:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	310/313 (99%)	263 (85%)	33 (11%)	14 (4%)	2 14
1	B	299/313 (96%)	252 (84%)	39 (13%)	8 (3%)	5 26
1	C	310/313 (99%)	238 (77%)	52 (17%)	20 (6%)	1 7
1	D	310/313 (99%)	238 (77%)	52 (17%)	20 (6%)	1 7
1	E	310/313 (99%)	247 (80%)	41 (13%)	22 (7%)	1 5
1	F	304/313 (97%)	262 (86%)	27 (9%)	15 (5%)	2 13
1	G	301/313 (96%)	241 (80%)	39 (13%)	21 (7%)	1 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	305/313 (97%)	213 (70%)	60 (20%)	32 (10%)	0 2
All	All	2449/2504 (98%)	1954 (80%)	343 (14%)	152 (6%)	1 8

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	TRP
1	A	36	ALA
1	A	38	PHE
1	A	147	SER
1	A	307	PRO
1	B	91	GLY
1	B	92	ASP
1	B	308	GLY
1	C	13	TRP
1	C	18	SER
1	C	19	SER
1	C	26	LYS
1	C	27	GLU
1	C	35	ASP
1	C	38	PHE
1	C	39	ARG
1	C	91	GLY
1	C	92	ASP
1	D	16	THR
1	D	35	ASP
1	D	38	PHE
1	D	98	SER
1	D	214	THR
1	D	271	ARG
1	E	18	SER
1	E	68	LEU
1	E	99	ILE
1	E	148	ALA
1	E	150	ASP
1	E	307	PRO
1	E	312	GLN
1	F	36	ALA
1	F	90	PRO
1	F	91	GLY
1	F	100	ASN
1	F	116	TYR

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Mol	Chain	Res	Type
1	F	152	VAL
1	G	6	ASP
1	G	36	ALA
1	G	38	PHE
1	G	39	ARG
1	G	176	TYR
1	G	307	PRO
1	G	309	LEU
1	H	38	PHE
1	H	68	LEU
1	H	96	PRO
1	H	152	VAL
1	H	219	LEU
1	H	238	PHE
1	H	247	LYS
1	H	257	PRO
1	H	303	ALA
1	A	18	SER
1	A	99	ILE
1	A	100	ASN
1	A	142	ILE
1	A	300	VAL
1	B	95	VAL
1	C	36	ALA
1	C	148	ALA
1	D	151	ASP
1	D	173	ALA
1	D	265	LYS
1	D	308	GLY
1	E	8	VAL
1	E	15	ASP
1	E	16	THR
1	E	37	GLY
1	E	38	PHE
1	E	39	ARG
1	E	67	GLY
1	E	116	TYR
1	E	152	VAL
1	F	98	SER
1	F	271	ARG
1	G	93	ASP
1	H	26	LYS

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Mol	Chain	Res	Type
1	H	35	ASP
1	H	61	ILE
1	H	64	ALA
1	H	111	ALA
1	H	155	LEU
1	H	269	HIS
1	H	276	ILE
1	H	297	ILE
1	H	300	VAL
1	A	151	ASP
1	B	299	PRO
1	C	34	LEU
1	C	100	ASN
1	D	148	ALA
1	D	269	HIS
1	E	17	LYS
1	E	271	ARG
1	F	35	ASP
1	G	5	ILE
1	G	83	GLU
1	G	311	LEU
1	H	8	VAL
1	H	13	TRP
1	H	63	ARG
1	H	268	SER
1	A	39	ARG
1	A	271	ARG
1	B	90	PRO
1	C	8	VAL
1	D	96	PRO
1	D	238	PHE
1	D	257	PRO
1	D	309	LEU
1	E	209	LEU
1	E	219	LEU
1	E	269	HIS
1	F	21	GLY
1	F	138	SER
1	F	300	VAL
1	G	163	GLU
1	G	219	LEU
1	G	267	ALA

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Mol	Chain	Res	Type
1	G	300	VAL
1	H	99	ILE
1	H	154	ALA
1	H	285	TYR
1	H	307	PRO
1	H	309	LEU
1	C	12	ALA
1	C	245	HIS
1	D	8	VAL
1	D	150	ASP
1	F	8	VAL
1	G	8	VAL
1	G	271	ARG
1	H	156	PRO
1	A	312	GLN
1	B	8	VAL
1	C	152	VAL
1	D	67	GLY
1	G	25	ARG
1	G	101	GLY
1	G	290	PRO
1	H	34	LEU
1	H	259	LEU
1	D	156	PRO
1	H	37	GLY
1	B	32	GLY
1	C	90	PRO
1	E	101	GLY
1	G	306	LEU
1	C	21	GLY
1	F	99	ILE
1	F	307	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	258/260 (99%)	223 (86%)	35 (14%)	3 17
1	B	250/260 (96%)	212 (85%)	38 (15%)	3 14
1	C	256/260 (98%)	221 (86%)	35 (14%)	3 17
1	D	255/260 (98%)	217 (85%)	38 (15%)	3 14
1	E	254/260 (98%)	216 (85%)	38 (15%)	3 14
1	F	252/260 (97%)	216 (86%)	36 (14%)	3 15
1	G	250/260 (96%)	214 (86%)	36 (14%)	3 15
1	H	249/260 (96%)	209 (84%)	40 (16%)	2 12
All	All	2024/2080 (97%)	1728 (85%)	296 (15%)	3 15

All (296) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	13	TRP
1	A	14	TYR
1	A	22	ARG
1	A	35	ASP
1	A	44	ARG
1	A	47	LEU
1	A	65	LEU
1	A	69	GLU
1	A	70	GLU
1	A	87	THR
1	A	92	ASP
1	A	110	THR
1	A	136	ASN
1	A	138	SER
1	A	142	ILE
1	A	143	ARG
1	A	145	LEU
1	A	146	ASN
1	A	151	ASP
1	A	190	THR
1	A	202	LEU
1	A	214	THR
1	A	222	ASP
1	A	223	ARG
1	A	228	ASP
1	A	235	LEU

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Mol	Chain	Res	Type
1	A	251	ARG
1	A	278	LEU
1	A	282	LYS
1	A	291	SER
1	A	300	VAL
1	A	304	GLN
1	A	309	LEU
1	A	311	LEU
1	B	6	ASP
1	B	10	ARG
1	B	28	SER
1	B	34	LEU
1	B	38	PHE
1	B	39	ARG
1	B	41	GLU
1	B	47	LEU
1	B	59	VAL
1	B	69	GLU
1	B	70	GLU
1	B	73	SER
1	B	83	GLU
1	B	94	VAL
1	B	95	VAL
1	B	110	THR
1	B	125	LEU
1	B	136	ASN
1	B	138	SER
1	B	146	ASN
1	B	147	SER
1	B	152	VAL
1	B	167	GLU
1	B	181	ASN
1	B	190	THR
1	B	199	PHE
1	B	202	LEU
1	B	211	GLU
1	B	222	ASP
1	B	223	ARG
1	B	235	LEU
1	B	251	ARG
1	B	278	LEU
1	B	295	THR

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Mol	Chain	Res	Type
1	B	300	VAL
1	B	304	GLN
1	B	306	LEU
1	B	309	LEU
1	C	3	LEU
1	C	16	THR
1	C	17	LYS
1	C	18	SER
1	C	22	ARG
1	C	23	PHE
1	C	25	ARG
1	C	27	GLU
1	C	34	LEU
1	C	38	PHE
1	C	39	ARG
1	C	47	LEU
1	C	59	VAL
1	C	63	ARG
1	C	65	LEU
1	C	69	GLU
1	C	71	MET
1	C	87	THR
1	C	92	ASP
1	C	110	THR
1	C	115	THR
1	C	130	GLU
1	C	136	ASN
1	C	145	LEU
1	C	181	ASN
1	C	211	GLU
1	C	223	ARG
1	C	235	LEU
1	C	247	LYS
1	C	275	THR
1	C	278	LEU
1	C	291	SER
1	C	297	ILE
1	C	306	LEU
1	C	309	LEU
1	D	5	ILE
1	D	14	TYR
1	D	17	LYS

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Mol	Chain	Res	Type
1	D	18	SER
1	D	22	ARG
1	D	39	ARG
1	D	41	GLU
1	D	44	ARG
1	D	47	LEU
1	D	60	LEU
1	D	63	ARG
1	D	69	GLU
1	D	99	ILE
1	D	110	THR
1	D	135	ASN
1	D	136	ASN
1	D	142	ILE
1	D	143	ARG
1	D	145	LEU
1	D	146	ASN
1	D	149	PHE
1	D	155	LEU
1	D	171	ILE
1	D	195	TYR
1	D	202	LEU
1	D	213	LEU
1	D	219	LEU
1	D	225	THR
1	D	230	ARG
1	D	231	LEU
1	D	238	PHE
1	D	259	LEU
1	D	260	SER
1	D	271	ARG
1	D	278	LEU
1	D	291	SER
1	D	295	THR
1	D	306	LEU
1	E	14	TYR
1	E	15	ASP
1	E	17	LYS
1	E	22	ARG
1	E	25	ARG
1	E	26	LYS
1	E	28	SER

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Mol	Chain	Res	Type
1	E	31	ARG
1	E	39	ARG
1	E	47	LEU
1	E	57	HIS
1	E	65	LEU
1	E	68	LEU
1	E	70	GLU
1	E	74	VAL
1	E	87	THR
1	E	92	ASP
1	E	99	ILE
1	E	110	THR
1	E	119	ARG
1	E	121	THR
1	E	142	ILE
1	E	147	SER
1	E	197	GLU
1	E	202	LEU
1	E	211	GLU
1	E	214	THR
1	E	224	LEU
1	E	235	LEU
1	E	251	ARG
1	E	263	VAL
1	E	270	GLU
1	E	278	LEU
1	E	295	THR
1	E	300	VAL
1	E	302	PRO
1	E	304	GLN
1	E	306	LEU
1	F	11	ASP
1	F	22	ARG
1	F	26	LYS
1	F	27	GLU
1	F	34	LEU
1	F	35	ASP
1	F	38	PHE
1	F	47	LEU
1	F	53	CYS
1	F	59	VAL
1	F	69	GLU

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Mol	Chain	Res	Type
1	F	70	GLU
1	F	87	THR
1	F	90	PRO
1	F	98	SER
1	F	99	ILE
1	F	100	ASN
1	F	119	ARG
1	F	136	ASN
1	F	142	ILE
1	F	147	SER
1	F	152	VAL
1	F	193	GLU
1	F	214	THR
1	F	216	ARG
1	F	222	ASP
1	F	223	ARG
1	F	224	LEU
1	F	235	LEU
1	F	251	ARG
1	F	260	SER
1	F	271	ARG
1	F	278	LEU
1	F	279	ARG
1	F	282	LYS
1	F	300	VAL
1	G	3	LEU
1	G	5	ILE
1	G	22	ARG
1	G	23	PHE
1	G	24	VAL
1	G	25	ARG
1	G	31	ARG
1	G	34	LEU
1	G	38	PHE
1	G	39	ARG
1	G	47	LEU
1	G	53	CYS
1	G	87	THR
1	G	93	ASP
1	G	100	ASN
1	G	110	THR
1	G	115	THR

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Mol	Chain	Res	Type
1	G	136	ASN
1	G	145	LEU
1	G	147	SER
1	G	176	TYR
1	G	181	ASN
1	G	186	SER
1	G	190	THR
1	G	206	LEU
1	G	209	LEU
1	G	211	GLU
1	G	216	ARG
1	G	222	ASP
1	G	226	GLU
1	G	234	THR
1	G	235	LEU
1	G	239	ASP
1	G	278	LEU
1	G	291	SER
1	G	300	VAL
1	H	3	LEU
1	H	5	ILE
1	H	23	PHE
1	H	29	GLN
1	H	31	ARG
1	H	35	ASP
1	H	38	PHE
1	H	44	ARG
1	H	47	LEU
1	H	63	ARG
1	H	69	GLU
1	H	70	GLU
1	H	76	MET
1	H	81	MET
1	H	92	ASP
1	H	93	ASP
1	H	99	ILE
1	H	107	GLN
1	H	119	ARG
1	H	132	ARG
1	H	136	ASN
1	H	142	ILE
1	H	145	LEU

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Mol	Chain	Res	Type
1	H	149	PHE
1	H	172	ASN
1	H	191	THR
1	H	197	GLU
1	H	205	THR
1	H	211	GLU
1	H	223	ARG
1	H	235	LEU
1	H	238	PHE
1	H	265	LYS
1	H	271	ARG
1	H	277	ASN
1	H	278	LEU
1	H	288	SER
1	H	291	SER
1	H	295	THR
1	H	304	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	136	ASN
1	A	172	ASN
1	A	180	ASN
1	A	245	HIS
1	A	289	HIS
1	A	304	GLN
1	B	84	ASN
1	B	136	ASN
1	B	172	ASN
1	B	245	HIS
1	B	289	HIS
1	B	312	GLN
1	C	84	ASN
1	C	136	ASN
1	C	172	ASN
1	C	289	HIS
1	C	312	GLN
1	D	136	ASN
1	D	172	ASN
1	D	245	HIS

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Mol	Chain	Res	Type
1	D	289	HIS
1	D	293	ASN
1	E	29	GLN
1	E	172	ASN
1	E	180	ASN
1	E	243	HIS
1	E	245	HIS
1	E	289	HIS
1	E	304	GLN
1	F	29	GLN
1	F	100	ASN
1	F	136	ASN
1	F	172	ASN
1	F	180	ASN
1	F	245	HIS
1	F	289	HIS
1	G	29	GLN
1	G	136	ASN
1	G	172	ASN
1	G	180	ASN
1	G	212	HIS
1	G	245	HIS
1	G	289	HIS
1	G	304	GLN
1	H	136	ASN
1	H	172	ASN
1	H	192	GLN
1	H	245	HIS
1	H	280	HIS
1	H	304	GLN
1	H	312	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	312/313 (99%)	-0.57	7 (2%)	62	33	15, 25, 76, 137	0
1	B	303/313 (96%)	-0.52	5 (1%)	70	41	20, 38, 68, 147	0
1	C	312/313 (99%)	-0.55	7 (2%)	62	33	21, 36, 90, 132	0
1	D	312/313 (99%)	-0.44	8 (2%)	56	27	26, 45, 94, 153	0
1	E	312/313 (99%)	-0.46	8 (2%)	56	27	19, 41, 87, 146	0
1	F	308/313 (98%)	-0.60	6 (1%)	66	37	17, 29, 78, 139	0
1	G	305/313 (97%)	-0.42	5 (1%)	72	44	32, 49, 86, 154	0
1	H	309/313 (98%)	-0.15	10 (3%)	47	20	36, 63, 99, 164	0
All	All	2473/2504 (98%)	-0.46	56 (2%)	60	31	15, 41, 88, 164	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	310	THR	10.2
1	G	312	GLN	10.1
1	B	310	THR	8.5
1	F	310	THR	7.9
1	G	310	THR	7.7
1	D	313	SER	7.2
1	G	313	SER	6.6
1	H	309	LEU	6.5
1	G	311	LEU	6.4
1	H	311	LEU	6.4
1	F	312	GLN	6.2
1	D	310	THR	6.2
1	E	313	SER	5.7
1	B	311	LEU	5.3
1	B	309	LEU	5.0
1	C	311	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	313	SER	5.0
1	G	309	LEU	4.9
1	E	310	THR	4.9
1	F	309	LEU	4.9
1	A	311	LEU	4.7
1	F	313	SER	4.6
1	C	309	LEU	4.5
1	C	312	GLN	4.3
1	A	312	GLN	4.2
1	H	313	SER	3.9
1	B	313	SER	3.9
1	E	309	LEU	3.8
1	H	312	GLN	3.7
1	A	310	THR	3.7
1	C	310	THR	3.6
1	D	312	GLN	3.6
1	A	313	SER	3.6
1	E	312	GLN	3.6
1	D	15	ASP	3.5
1	D	18	SER	3.4
1	H	19	SER	3.4
1	E	311	LEU	3.3
1	E	308	GLY	3.3
1	D	309	LEU	3.1
1	H	36	ALA	3.0
1	H	20	GLY	2.9
1	H	308	GLY	2.8
1	B	312	GLN	2.7
1	F	311	LEU	2.6
1	E	20	GLY	2.6
1	D	311	LEU	2.5
1	C	11	ASP	2.3
1	F	16	THR	2.3
1	A	18	SER	2.3
1	A	14	TYR	2.1
1	H	12	ALA	2.1
1	A	15	ASP	2.1
1	E	14	TYR	2.0
1	D	14	TYR	2.0
1	C	16	THR	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.