Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:04 pm BST

PDB ID	:	5H2T
Title	:	Structure of trehalose synthase
Authors	:	Wang, D.; Huang, H.; Zhou, J.; Jiang, L.
Deposited on	:	2016-10-18
Resolution	:	2.80 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 ①) were used in the production of this report:

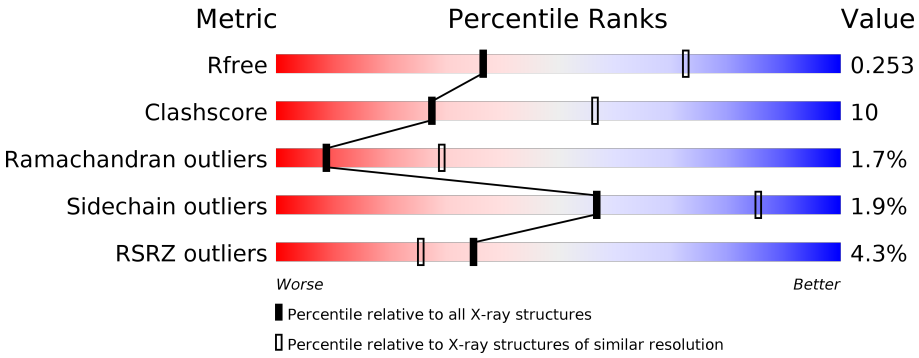
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.80 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.



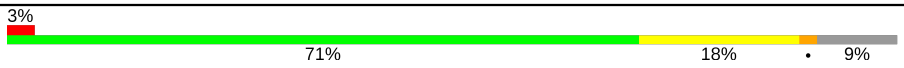
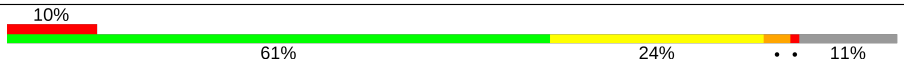
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	601	75% 15% 9%
1	B	601	2% 75% 15% 9%
1	C	601	2% 70% 19% 9%
1	D	601	4% 72% 16% 9%
1	E	601	4% 69% 19% 9%
1	F	601	5% 67% 20% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	601	
1	H	601	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 35620 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 Trehalose synthase.

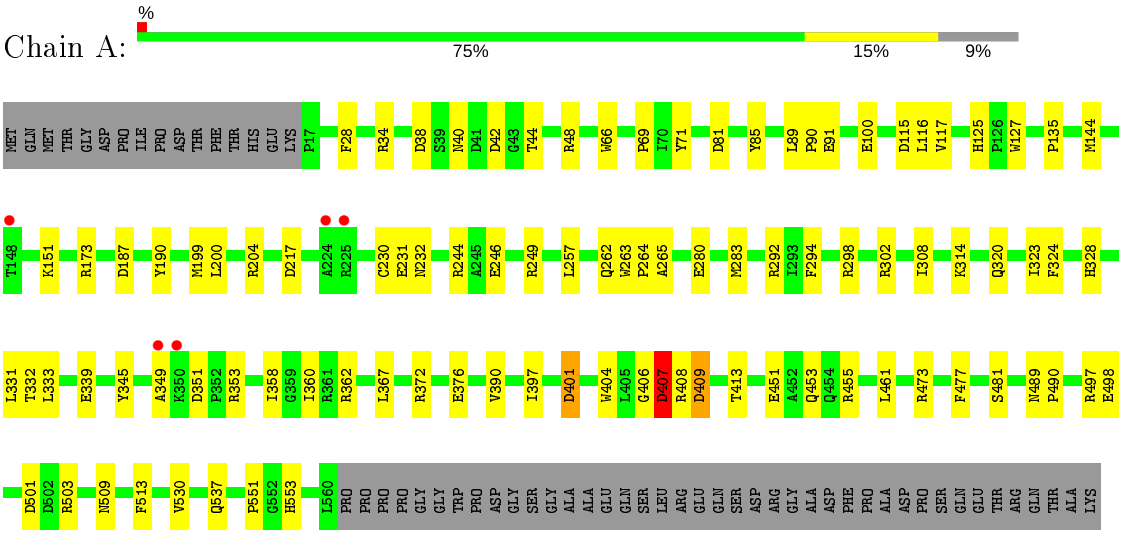
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	B	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	C	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	D	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	E	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	F	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	G	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	H	536	Total	C	N	O	S	0	0	0
			4386	2810	748	805	23			

3 Residue-property plots (i)

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

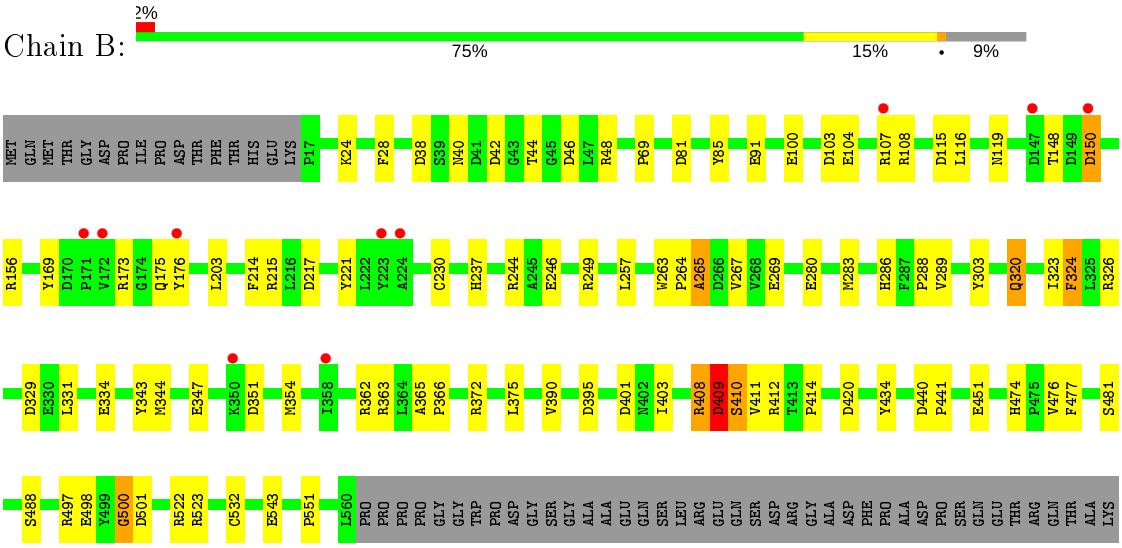
- Molecule 1: Trehalose synthase

Chain A:



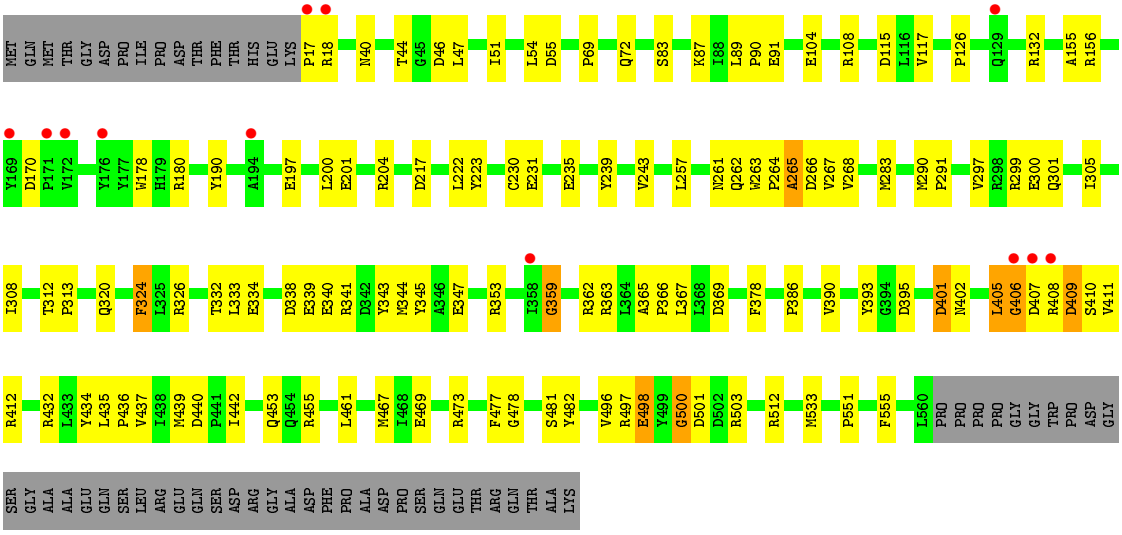
- Molecule 1: Trehalose synthase

Chain B:



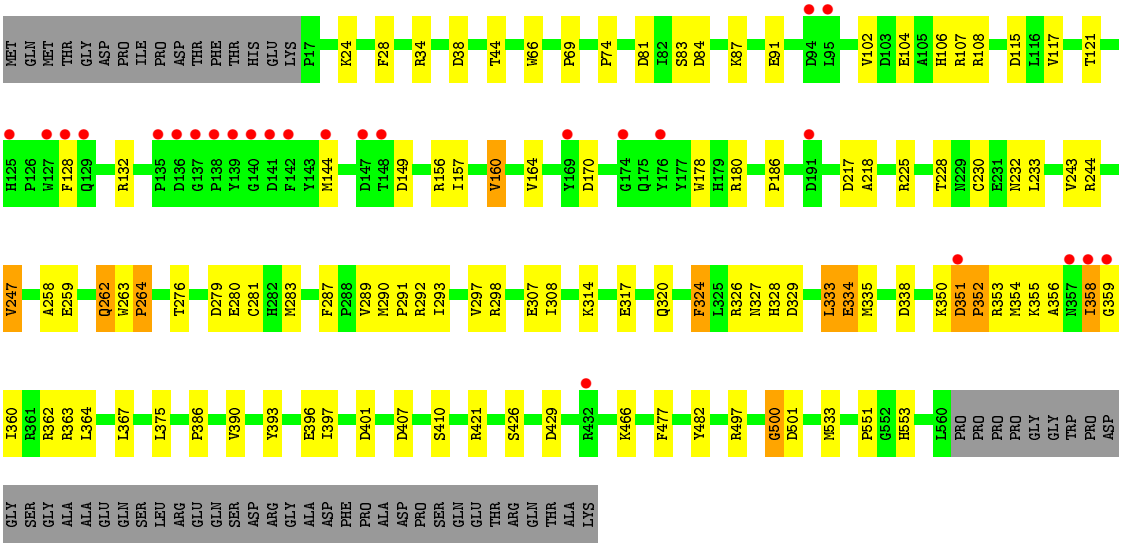
- Molecule 1: Trehalose synthase

Chain C:



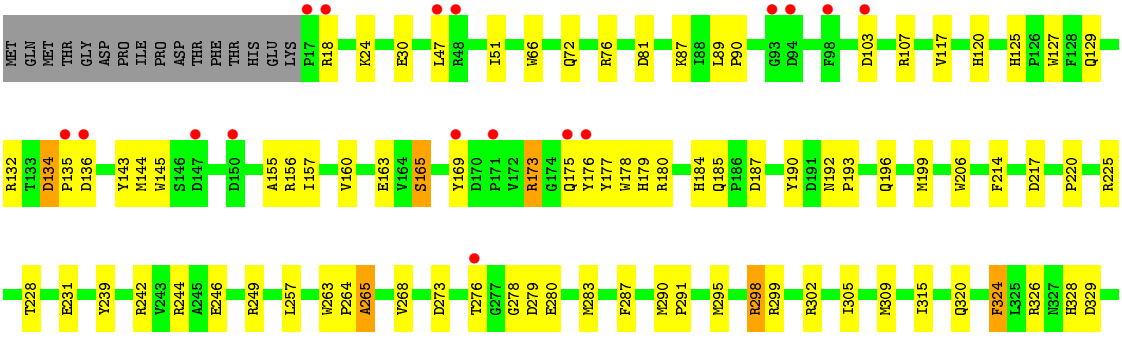
• Molecule 1: Trehalose synthase

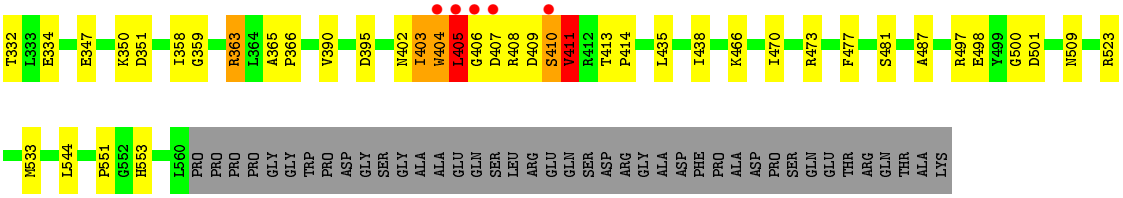
Chain D:



• Molecule 1: Trehalose synthase

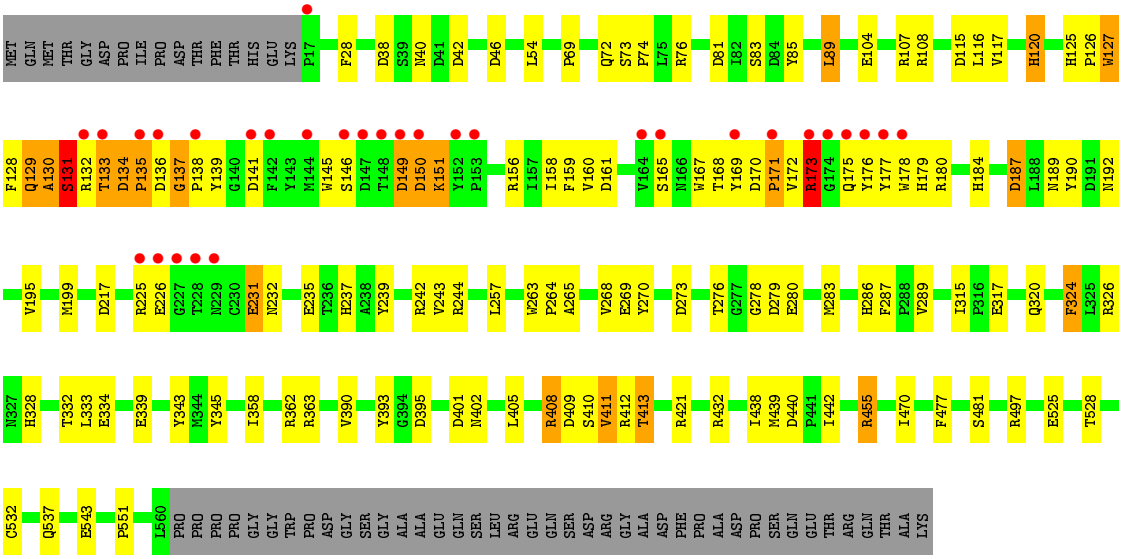
Chain E:





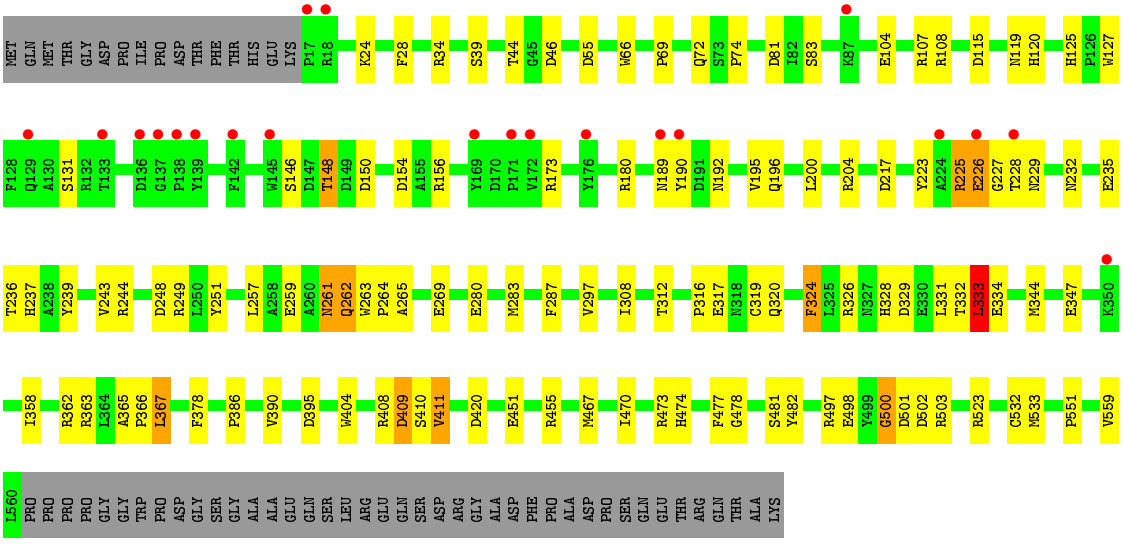
• Molecule 1: Trehalose synthase

Chain F:



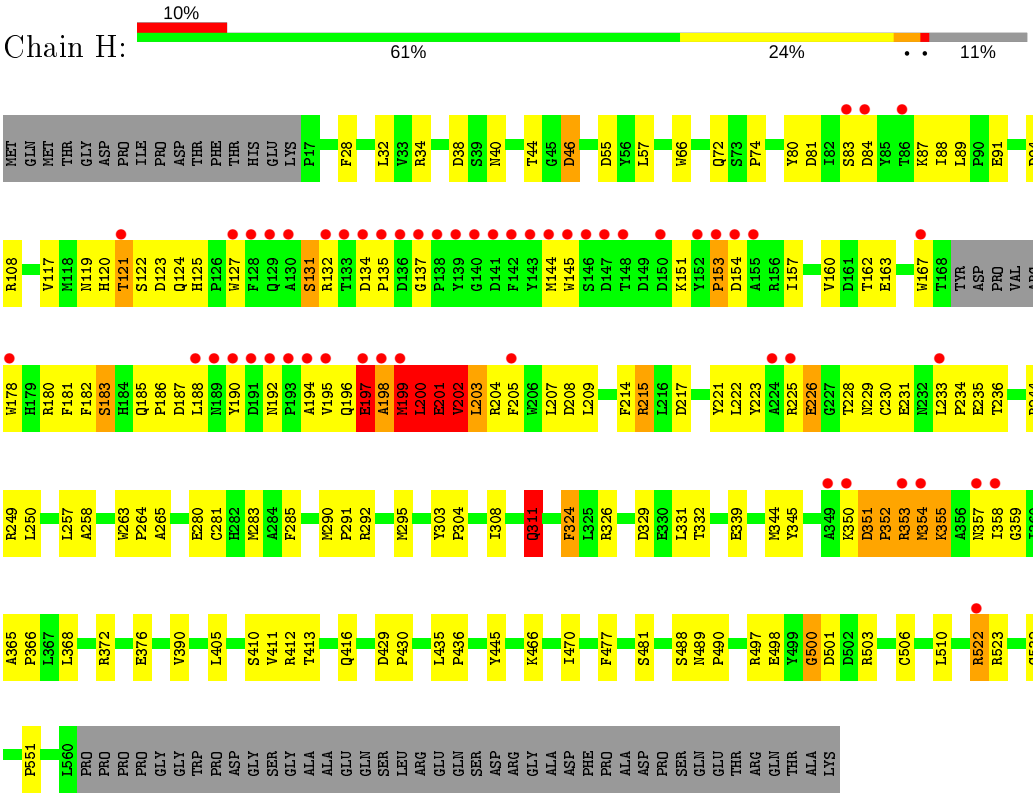
• Molecule 1: Trehalose synthase

Chain G:



• Molecule 1: Trehalose synthase

Chain H:


10%
61%
24%
11%
MET GLN MET THR GLY ASP PRO ILE PRO ASP THR PHE THR HIS GLU LYS P17 F28 L32 V33 R34 D38 S39 N40 T44 G45 D46 D55 Y56 L57 W66 Q72 S73 P74 Y80 D81 I82 S83 D84 Y85 T86 K87 I88 L89 P90 E91 D94 L95 E104
R108 V117 M118 N119 H120 T121 S122 D123 Q124 H125 P126 W127 F128 Q129 A130 S131 R132 T133 D134 P135 D136 G137 P138 Y139 G140 D141 F142 Y143 M144 W145 S146 D147 T148 D149 D150 K151 Y152 P153 D154 A155 R156 I157 V160 D161 T162 E163 W167 T168 TYR ASP PRO VAL ARG GLY GLN TYR Y177
W178 H179 R180 F181 F182 S183 H184 Q185 P186 D187 L188 N189 Y190 D191 N192 P193 A194 V195 Q196 E197 A198 M199 L200 E201 V202 L203 R204 P205 W206 L207 D208 L209 F214 R215 L216 D217 Y221 L222 Y223 A224 R225 E226 G227 T228 N229 C230 E231 N232 L233 P234 E235 T236 R244 A245 E246 V247 D248
R249 L250 L257 A258 W263 P264 A265 E280 C281 H282 M283 A284 F285 M290 P291 R292 M295 Y303 P304 I308 Q311 F324 L325 R326 D329 E330 L331 T332 E339 M344 Y345 A349 K350 D351 P352 R353 M354 K355 A356 N357 I358 G359 I360 R361 R362 R363 L364
A365 P366 L367 L368 R372 E376 V390 L405 S410 V411 R412 T413 Q416 D429 P430 L435 P436 Y445 K466 I470 F477 S481 S488 N489 P490 R497 E498 Y499 G500 D501 D502 R503 C506 L510 R522 R523 C532 G542 E543 L544
P551 L560 PRO PRO PRO PRO GLY GLY TRP PRO ASP GLY SER GLY ALA ALA GLU GLN SER LEU ARG GLU GLN SER ASP ARG GLY ALA ASP PHE PRO ALA ASP PRO SER GLN GLU THR ARG GLN THR ALA LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	248.76Å 133.12Å 211.78Å 90.00° 112.54° 90.00°	Depositor
Resolution (Å)	43.57 – 2.80 49.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.57-2.80) 99.2 (49.18-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1-2155	Depositor
R, R_{free}	0.205 , 0.252 0.207 , 0.253	Depositor DCC
R_{free} test set	7745 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	35620	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% 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	0.65	0/4599	0.69	1/6269 (0.0%)
1	B	0.63	1/4599 (0.0%)	0.68	2/6269 (0.0%)
1	C	0.59	0/4599	0.67	1/6269 (0.0%)
1	D	0.59	0/4599	0.69	1/6269 (0.0%)
1	E	0.59	0/4599	0.69	4/6269 (0.1%)
1	F	0.61	0/4599	0.76	6/6269 (0.1%)
1	G	0.59	1/4599 (0.0%)	0.70	4/6269 (0.1%)
1	H	0.61	1/4519 (0.0%)	0.78	6/6159 (0.1%)
All	All	0.61	3/36712 (0.0%)	0.71	25/50042 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	9
All	All	0	18

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	404	TRP	CD2-CE2	7.18	1.50	1.41
1	H	506	CYS	CB-SG	-5.55	1.72	1.81
1	B	532	CYS	CB-SG	-5.33	1.73	1.81

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	200	LEU	CA-CB-CG	11.07	140.76	115.30
1	G	333	LEU	CA-CB-CG	9.66	137.52	115.30
1	G	404	TRP	CG-CD2-CE3	7.93	141.03	133.90
1	H	311	GLN	CA-CB-CG	6.89	128.57	113.40
1	F	89	LEU	CA-CB-CG	6.70	130.70	115.30
1	H	201	GLU	N-CA-C	-6.67	92.99	111.00
1	E	134	ASP	CB-CG-OD1	6.06	123.75	118.30
1	H	197	GLU	CA-CB-CG	5.91	126.39	113.40
1	G	404	TRP	CD1-CG-CD2	5.76	110.91	106.30
1	C	359	GLY	N-CA-C	-5.57	99.17	113.10
1	H	510	LEU	CA-CB-CG	-5.54	102.56	115.30
1	B	409	ASP	N-CA-C	-5.50	96.14	111.00
1	F	408	ARG	N-CA-C	-5.49	96.19	111.00
1	A	332	THR	N-CA-C	-5.46	96.25	111.00
1	E	363	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	F	411	VAL	N-CA-C	-5.38	96.47	111.00
1	E	411	VAL	N-CA-C	-5.34	96.58	111.00
1	F	173	ARG	CB-CG-CD	5.34	125.48	111.60
1	B	408	ARG	N-CA-C	-5.30	96.70	111.00
1	F	137	GLY	C-N-CD	-5.25	109.05	120.60
1	G	404	TRP	CE2-CD2-CG	-5.23	103.12	107.30
1	D	333	LEU	CB-CA-C	5.19	120.07	110.20
1	H	202	VAL	CA-C-N	-5.18	105.80	117.20
1	F	131	SER	N-CA-C	5.14	124.87	111.00
1	E	405	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	ASP	Peptide
1	D	351	ASP	Peptide
1	D	352	PRO	Peptide
1	E	165	SER	Peptide
1	E	410	SER	Peptide
1	F	131	SER	Peptide
1	F	149	ASP	Peptide
1	G	225	ARG	Peptide
1	G	333	LEU	Peptide
1	H	131	SER	Peptide
1	H	196	GLN	Peptide
1	H	199	MET	Peptide
1	H	200	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	H	202	VAL	Peptide
1	H	350	LYS	Peptide
1	H	352	PRO	Peptide
1	H	353	ARG	Peptide
1	H	543	GLU	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	4462	0	4252	59	0
1	B	4462	0	4252	64	0
1	C	4462	0	4252	81	0
1	D	4462	0	4252	78	0
1	E	4462	0	4252	90	0
1	F	4462	0	4252	114	0
1	G	4462	0	4252	79	0
1	H	4386	0	4178	141	0
All	All	35620	0	33942	692	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 10.

All (692) 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:D:356:ALA:HB1	1:D:360:ILE:H	0.99	1.13
1:D:334:GLU:N	1:D:358:ILE:O	1.99	0.94
1:D:356:ALA:HB1	1:D:360:ILE:N	1.83	0.94
1:H:201:GLU:O	1:H:204:ARG:N	2.04	0.91
1:A:125:HIS:HD2	1:A:127:TRP:H	1.20	0.90
1:F:133:THR:HG23	1:F:134:ASP:HA	1.54	0.90
1:D:352:PRO:HA	1:D:354:MET:HG2	1.56	0.87
1:E:196:GLN:OE1	1:E:242:ARG:NH1	2.07	0.87
1:D:333:LEU:HB3	1:D:359:GLY:H	1.40	0.85
1:G:332:THR:HG23	1:G:334:GLU:H	1.38	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:PHE:O	1:D:497:ARG:NH2	2.10	0.85
1:F:137:GLY:N	1:F:139:TYR:H	1.76	0.84
1:E:407:ASP:OD1	1:E:410:SER:N	2.09	0.83
1:A:232:ASN:ND2	1:A:262:GLN:HE22	1.76	0.83
1:B:119:ASN:HD21	1:B:221:TYR:HB2	1.43	0.82
1:H:197:GLU:O	1:H:200:LEU:N	2.09	0.82
1:F:137:GLY:H	1:F:139:TYR:H	1.28	0.82
1:G:477:PHE:O	1:G:497:ARG:NH2	2.12	0.82
1:C:551:PRO:HG3	1:E:551:PRO:HG3	1.61	0.82
1:C:72:GLN:HG3	1:C:87:LYS:HD3	1.62	0.81
1:B:119:ASN:ND2	1:B:221:TYR:HB2	1.94	0.81
1:A:372:ARG:NH1	1:A:376:GLU:OE2	2.13	0.81
1:F:170:ASP:HB2	1:F:173:ARG:HG3	1.63	0.80
1:F:332:THR:O	1:F:334:GLU:N	2.15	0.80
1:C:156:ARG:O	1:C:180:ARG:NH1	2.15	0.80
1:H:355:LYS:N	1:H:357:ASN:OD1	2.14	0.80
1:E:477:PHE:O	1:E:497:ARG:NH2	2.15	0.79
1:H:226:GLU:H	1:H:228:THR:H	1.28	0.78
1:B:551:PRO:HG3	1:D:551:PRO:HG3	1.66	0.77
1:F:117:VAL:HG11	1:F:120:HIS:CE1	2.19	0.77
1:H:522:ARG:HH22	1:H:544:LEU:HA	1.50	0.77
1:H:225:ARG:HG2	1:H:233:LEU:HD13	1.66	0.76
1:C:477:PHE:O	1:C:497:ARG:NH2	2.18	0.76
1:F:131:SER:HB3	1:F:173:ARG:HB3	1.67	0.76
1:B:363:ARG:HG3	1:B:395:ASP:OD1	1.86	0.76
1:F:551:PRO:HG3	1:G:551:PRO:HG3	1.68	0.76
1:H:200:LEU:O	1:H:201:GLU:HG3	1.87	0.75
1:B:477:PHE:O	1:B:497:ARG:NH2	2.19	0.75
1:F:165:SER:OG	1:F:167:TRP:O	2.05	0.75
1:F:363:ARG:HG2	1:F:395:ASP:OD1	1.87	0.74
1:F:455:ARG:HG3	1:F:455:ARG:HH11	1.51	0.74
1:A:498:GLU:OE2	1:A:503:ARG:NH1	2.20	0.73
1:A:246:GLU:OE2	1:A:249:ARG:NH1	2.22	0.73
1:G:244:ARG:HD3	1:G:280:GLU:O	1.88	0.73
1:E:470:ILE:HD13	1:E:473:ARG:HH21	1.54	0.73
1:C:406:GLY:O	1:C:407:ASP:HB3	1.89	0.72
1:C:408:ARG:O	1:C:409:ASP:HB2	1.89	0.72
1:F:170:ASP:N	1:F:170:ASP:OD1	2.19	0.72
1:G:226:GLU:O	1:G:228:THR:HG23	1.90	0.71
1:H:351:ASP:HB3	1:H:352:PRO:HA	1.72	0.71
1:H:498:GLU:OE2	1:H:523:ARG:NH2	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:THR:O	1:C:334:GLU:N	2.23	0.71
1:A:477:PHE:O	1:A:497:ARG:NH2	2.24	0.71
1:F:477:PHE:O	1:F:497:ARG:NH2	2.24	0.70
1:G:55:ASP:OD1	1:G:108:ARG:NH2	2.22	0.70
1:F:283:MET:HG2	1:F:320:GLN:HB3	1.72	0.70
1:F:156:ARG:O	1:F:180:ARG:NH1	2.24	0.70
1:H:83:SER:O	1:H:125:HIS:ND1	2.25	0.70
1:B:409:ASP:O	1:B:411:VAL:N	2.21	0.70
1:D:356:ALA:CB	1:D:360:ILE:H	1.93	0.69
1:F:409:ASP:O	1:F:410:SER:OG	2.06	0.69
1:C:362:ARG:HB2	1:C:367:LEU:HD13	1.73	0.69
1:E:72:GLN:HG3	1:E:87:LYS:HD3	1.75	0.69
1:E:184:HIS:HD2	1:E:185:GLN:HG3	1.58	0.69
1:F:40:ASN:ND2	1:F:42:ASP:OD1	2.26	0.69
1:A:551:PRO:HG3	1:H:551:PRO:HG3	1.74	0.69
1:G:328:HIS:NE2	1:G:358:ILE:O	2.25	0.69
1:A:406:GLY:O	1:A:408:ARG:N	2.25	0.68
1:E:156:ARG:O	1:E:180:ARG:NH1	2.27	0.68
1:C:467:MET:HE3	1:C:555:PHE:HZ	1.59	0.68
1:G:232:ASN:OD1	1:G:262:GLN:NE2	2.27	0.68
1:H:40:ASN:ND2	1:H:46:ASP:OD1	2.27	0.68
1:D:232:ASN:ND2	1:D:262:GLN:OE1	2.27	0.68
1:E:407:ASP:OD1	1:E:409:ASP:N	2.27	0.67
1:F:276:THR:HG23	1:F:278:GLY:H	1.59	0.67
1:C:353:ARG:NH1	1:C:369:ASP:OD2	2.28	0.67
1:H:372:ARG:NH1	1:H:376:GLU:OE2	2.27	0.67
1:C:363:ARG:HG2	1:C:395:ASP:OD1	1.94	0.67
1:H:200:LEU:HB3	1:H:202:VAL:N	2.10	0.67
1:E:405:LEU:HD23	1:E:435:LEU:HD22	1.77	0.67
1:F:128:PHE:O	1:F:130:ALA:N	2.28	0.66
1:F:104:GLU:OE1	1:F:108:ARG:NH1	2.27	0.66
1:E:145:TRP:CH2	1:E:173:ARG:HD3	2.30	0.66
1:H:229:ASN:O	1:H:231:GLU:N	2.29	0.66
1:F:130:ALA:HA	1:F:132:ARG:H	1.58	0.66
1:H:120:HIS:CD2	1:H:185:GLN:HB3	2.30	0.66
1:H:498:GLU:HG2	1:H:503:ARG:HG2	1.78	0.66
1:G:473:ARG:O	1:G:474:HIS:HD2	1.79	0.66
1:C:132:ARG:HD2	1:C:170:ASP:OD2	1.95	0.66
1:H:198:ALA:C	1:H:200:LEU:N	2.50	0.66
1:H:470:ILE:HD13	1:H:532:CYS:HB3	1.78	0.66
1:C:266:ASP:OD1	1:C:341:ARG:NH1	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:GLN:HA	1:F:89:LEU:HD13	1.77	0.65
1:E:295:MET:SD	1:E:298:ARG:NH1	2.69	0.65
1:H:500:GLY:O	1:H:501:ASP:HB2	1.96	0.65
1:H:257:LEU:HG	1:H:283:MET:HB2	1.77	0.65
1:B:498:GLU:OE2	1:B:523:ARG:NH1	2.30	0.65
1:C:409:ASP:HA	1:C:412:ARG:HB2	1.79	0.65
1:E:332:THR:O	1:E:334:GLU:N	2.30	0.65
1:D:354:MET:HG3	1:D:355:LYS:N	2.12	0.65
1:F:180:ARG:NH2	1:F:231:GLU:OE1	2.29	0.65
1:G:287:PHE:CE1	1:G:329:ASP:HB3	2.32	0.65
1:G:320:GLN:NE2	1:G:478:GLY:O	2.28	0.65
1:H:188:LEU:HD13	1:H:199:MET:HE3	1.77	0.65
1:D:156:ARG:O	1:D:180:ARG:NH1	2.30	0.64
1:H:194:ALA:C	1:H:197:GLU:HB3	2.16	0.64
1:A:44:THR:HG21	1:A:91:GLU:HG2	1.78	0.64
1:E:276:THR:HG21	1:E:279:ASP:HB3	1.78	0.64
1:H:95:LEU:HD23	1:H:205:PHE:HZ	1.61	0.64
1:B:40:ASN:ND2	1:B:42:ASP:OD1	2.31	0.64
1:D:355:LYS:HD2	1:D:362:ARG:HG3	1.80	0.64
1:D:354:MET:HG3	1:D:355:LYS:HG3	1.79	0.64
1:G:237:HIS:CE1	1:G:269:GLU:HG2	2.33	0.64
1:H:203:LEU:HD12	1:H:203:LEU:H	1.63	0.64
1:E:163:GLU:HG3	1:E:165:SER:HB3	1.79	0.64
1:F:363:ARG:NH1	1:F:393:TYR:O	2.31	0.63
1:C:104:GLU:OE1	1:C:108:ARG:NH1	2.31	0.63
1:H:95:LEU:HD23	1:H:205:PHE:CZ	2.34	0.63
1:B:522:ARG:HD3	1:B:543:GLU:HG3	1.80	0.63
1:E:295:MET:SD	1:E:298:ARG:NH2	2.72	0.63
1:E:283:MET:HG2	1:E:320:GLN:HB3	1.79	0.63
1:H:74:PRO:HD3	1:H:83:SER:OG	1.98	0.63
1:E:276:THR:HG23	1:E:278:GLY:H	1.64	0.63
1:F:273:ASP:O	1:F:276:THR:HG22	1.99	0.63
1:H:354:MET:HG3	1:H:357:ASN:OD1	1.98	0.62
1:D:334:GLU:H	1:D:358:ILE:C	2.02	0.62
1:H:477:PHE:O	1:H:497:ARG:NH2	2.33	0.62
1:H:134:ASP:HB3	1:H:137:GLY:HA3	1.82	0.62
1:D:132:ARG:HD2	1:D:170:ASP:OD2	1.99	0.62
1:B:173:ARG:NE	1:B:175:GLN:OE1	2.31	0.62
1:F:339:GLU:HG2	1:F:345:TYR:CZ	2.34	0.62
1:H:522:ARG:HH22	1:H:544:LEU:CA	2.12	0.62
1:F:131:SER:CB	1:F:173:ARG:HB3	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:ARG:O	1:G:180:ARG:NH2	2.29	0.62
1:A:360:ILE:HA	1:A:407:ASP:HB2	1.82	0.61
1:C:407:ASP:O	1:C:408:ARG:HG2	2.01	0.61
1:F:125:HIS:HD1	1:F:126:PRO:HD2	1.65	0.61
1:F:232:ASN:OD1	1:F:270:TYR:OH	2.11	0.61
1:F:328:HIS:NE2	1:F:358:ILE:O	2.33	0.61
1:G:263:TRP:CD2	1:G:264:PRO:HD2	2.35	0.61
1:D:28:PHE:HB2	1:D:390:VAL:HG22	1.83	0.61
1:E:145:TRP:HB3	1:E:175:GLN:NE2	2.15	0.61
1:E:328:HIS:NE2	1:E:358:ILE:O	2.33	0.61
1:H:225:ARG:O	1:H:228:THR:OG1	2.17	0.61
1:E:403:ILE:O	1:E:405:LEU:N	2.30	0.61
1:F:130:ALA:HA	1:F:132:ARG:N	2.15	0.61
1:A:257:LEU:HG	1:A:283:MET:HB2	1.82	0.60
1:H:190:TYR:HA	1:H:195:VAL:HG21	1.83	0.60
1:F:192:ASN:O	1:F:195:VAL:HG22	2.00	0.60
1:F:117:VAL:HA	1:F:217:ASP:HB2	1.81	0.60
1:E:295:MET:SD	1:E:298:ARG:CZ	2.90	0.60
1:A:190:TYR:OH	1:A:199:MET:HG3	2.01	0.60
1:C:55:ASP:OD1	1:C:108:ARG:NH2	2.29	0.60
1:D:355:LYS:HE3	1:D:367:LEU:HD23	1.83	0.60
1:E:134:ASP:HB2	1:E:136:ASP:OD1	2.02	0.60
1:H:339:GLU:HG3	1:H:345:TYR:CD2	2.36	0.60
1:F:40:ASN:N	1:F:40:ASN:OD1	2.34	0.60
1:C:434:TYR:O	1:C:435:LEU:HD12	2.02	0.60
1:D:354:MET:HG3	1:D:355:LYS:H	1.67	0.60
1:G:333:LEU:HD13	1:G:334:GLU:HG3	1.84	0.60
1:A:231:GLU:HB3	1:A:232:ASN:HD22	1.66	0.60
1:B:286:HIS:O	1:B:289:VAL:HG12	2.01	0.59
1:E:363:ARG:HG2	1:E:395:ASP:OD1	2.01	0.59
1:H:522:ARG:HH12	1:H:544:LEU:C	2.06	0.59
1:E:135:PRO:HB3	1:E:173:ARG:HH12	1.66	0.59
1:F:408:ARG:O	1:F:409:ASP:HB2	2.03	0.59
1:A:283:MET:HG2	1:A:320:GLN:HB3	1.84	0.59
1:D:283:MET:HG2	1:D:320:GLN:HB3	1.85	0.59
1:G:244:ARG:NH1	1:G:248:ASP:OD2	2.36	0.59
1:D:328:HIS:CE1	1:D:356:ALA:HB3	2.38	0.58
1:D:421:ARG:NH1	1:G:451:GLU:OE2	2.22	0.58
1:E:407:ASP:C	1:E:409:ASP:H	2.04	0.58
1:G:470:ILE:HD13	1:G:532:CYS:HB3	1.85	0.58
1:H:151:LYS:NZ	1:H:226:GLU:OE1	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:329:ASP:OD1	1:G:332:THR:HG22	2.04	0.58
1:B:169:TYR:HB2	1:B:176:TYR:CE1	2.38	0.58
1:D:24:LYS:NZ	1:D:317:GLU:O	2.26	0.58
1:E:225:ARG:O	1:E:228:THR:HG22	2.04	0.58
1:F:362:ARG:HD2	1:F:401:ASP:OD2	2.04	0.58
1:B:362:ARG:CZ	1:B:403:ILE:HD11	2.32	0.58
1:C:261:ASN:ND2	1:C:261:ASN:O	2.37	0.58
1:F:76:ARG:HD3	1:F:184:HIS:CD2	2.38	0.58
1:D:333:LEU:HB3	1:D:359:GLY:N	2.15	0.58
1:E:298:ARG:NH2	1:E:351:ASP:HB2	2.18	0.58
1:G:72:GLN:HG3	1:G:83:SER:HB2	1.85	0.58
1:A:232:ASN:HD21	1:A:262:GLN:HE22	1.49	0.58
1:G:257:LEU:HG	1:G:283:MET:HB2	1.86	0.58
1:H:292:ARG:NH1	1:H:308:ILE:HG23	2.19	0.57
1:B:148:THR:OG1	1:B:150:ASP:OD2	2.18	0.57
1:C:339:GLU:HG2	1:C:345:TYR:CE2	2.39	0.57
1:D:351:ASP:C	1:D:353:ARG:H	2.07	0.57
1:H:326:ARG:HB2	1:H:361:ARG:NH1	2.19	0.57
1:F:150:ASP:OD1	1:F:151:LYS:N	2.28	0.57
1:G:473:ARG:O	1:G:474:HIS:CD2	2.58	0.57
1:B:451:GLU:OE2	1:F:421:ARG:NH1	2.31	0.57
1:C:500:GLY:O	1:C:501:ASP:HB2	2.05	0.57
1:H:203:LEU:O	1:H:207:LEU:HB2	2.05	0.57
1:H:263:TRP:CD2	1:H:264:PRO:HD2	2.38	0.57
1:A:125:HIS:CD2	1:A:127:TRP:H	2.11	0.57
1:B:103:ASP:HB3	1:B:107:ARG:NH1	2.19	0.57
1:B:257:LEU:HG	1:B:283:MET:HB2	1.86	0.57
1:E:145:TRP:HB3	1:E:175:GLN:HE21	1.69	0.57
1:G:498:GLU:OE2	1:G:523:ARG:NH2	2.38	0.57
1:D:74:PRO:HD3	1:D:83:SER:OG	2.04	0.57
1:E:324:PHE:CD1	1:E:326:ARG:HG2	2.40	0.56
1:E:302:ARG:NH2	1:E:487:ALA:O	2.37	0.56
1:F:244:ARG:HD2	1:F:280:GLU:O	2.05	0.56
1:A:408:ARG:O	1:A:409:ASP:HB2	2.04	0.56
1:B:263:TRP:CD2	1:B:264:PRO:HD2	2.40	0.56
1:G:363:ARG:HG2	1:G:395:ASP:OD1	2.05	0.56
1:H:246:GLU:OE2	1:H:249:ARG:NH2	2.27	0.56
1:H:38:ASP:OD1	1:H:40:ASN:ND2	2.38	0.56
1:E:129:GLN:OE1	1:E:132:ARG:NE	2.36	0.56
1:G:225:ARG:HE	1:G:235:GLU:HG2	1.70	0.56
1:H:201:GLU:O	1:H:204:ARG:HG3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:THR:HG23	1:F:179:HIS:NE2	2.20	0.56
1:G:362:ARG:HB2	1:G:367:LEU:HD13	1.87	0.56
1:F:257:LEU:HG	1:F:283:MET:HB2	1.88	0.56
1:H:87:LYS:HD2	1:H:87:LYS:N	2.20	0.56
1:D:364:LEU:HG	1:D:375:LEU:HD23	1.86	0.56
1:D:500:GLY:O	1:D:501:ASP:HB2	2.05	0.56
1:F:263:TRP:CD2	1:F:264:PRO:HD2	2.41	0.56
1:A:292:ARG:HG3	1:A:308:ILE:HG12	1.88	0.56
1:C:320:GLN:NE2	1:C:478:GLY:O	2.35	0.56
1:E:402:ASN:ND2	1:E:405:LEU:HD11	2.20	0.56
1:A:44:THR:HG21	1:A:91:GLU:CG	2.36	0.55
1:F:409:ASP:HA	1:F:412:ARG:HB2	1.88	0.55
1:H:119:ASN:ND2	1:H:187:ASP:OD1	2.39	0.55
1:C:469:GLU:OE2	1:C:473:ARG:NH1	2.39	0.55
1:F:170:ASP:HB2	1:F:173:ARG:CG	2.36	0.55
1:F:402:ASN:O	1:F:410:SER:HB2	2.06	0.55
1:H:329:ASP:OD1	1:H:332:THR:OG1	2.20	0.55
1:D:225:ARG:O	1:D:228:THR:HG22	2.06	0.55
1:H:84:ASP:CG	1:H:87:LYS:HD3	2.27	0.55
1:A:481:SER:O	1:A:497:ARG:HD2	2.07	0.55
1:B:244:ARG:HD2	1:B:280:GLU:O	2.06	0.55
1:C:362:ARG:HD2	1:C:401:ASP:OD2	2.06	0.55
1:D:149:ASP:OD2	1:F:169:TYR:OH	2.25	0.55
1:B:156:ARG:NH2	1:B:334:GLU:OE1	2.40	0.55
1:F:134:ASP:N	1:F:135:PRO:CD	2.70	0.55
1:F:146:SER:O	1:F:175:GLN:HB2	2.07	0.55
1:E:103:ASP:HB3	1:E:107:ARG:HH21	1.72	0.54
1:E:145:TRP:CZ2	1:E:173:ARG:HD3	2.42	0.54
1:F:76:ARG:HD3	1:F:184:HIS:CG	2.42	0.54
1:H:104:GLU:OE1	1:H:108:ARG:NH1	2.39	0.54
1:A:48:ARG:NH2	1:A:100:GLU:OE1	2.38	0.54
1:D:421:ARG:NH2	1:G:420:ASP:OD2	2.35	0.54
1:H:311:GLN:HA	1:H:311:GLN:HE21	1.72	0.54
1:C:498:GLU:HB3	1:C:503:ARG:HG2	1.90	0.54
1:E:405:LEU:HD22	1:E:405:LEU:O	2.08	0.54
1:F:470:ILE:HD13	1:F:532:CYS:HB3	1.89	0.54
1:C:69:PRO:HD3	1:C:115:ASP:HB2	1.89	0.54
1:D:218:ALA:N	1:D:259:GLU:OE1	2.30	0.54
1:F:76:ARG:HG2	1:F:184:HIS:CE1	2.41	0.54
1:H:324:PHE:CD1	1:H:326:ARG:HG2	2.43	0.54
1:D:66:TRP:CD1	1:D:66:TRP:C	2.81	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:ILE:H	1:D:359:GLY:HA3	1.72	0.54
1:F:286:HIS:O	1:F:289:VAL:HG12	2.07	0.54
1:H:163:GLU:OE2	1:H:183:SER:N	2.40	0.54
1:B:500:GLY:O	1:B:501:ASP:HB2	2.08	0.53
1:C:338:ASP:OD2	1:C:341:ARG:NH2	2.31	0.53
1:F:190:TYR:OH	1:F:199:MET:HG3	2.07	0.53
1:F:481:SER:O	1:F:497:ARG:HD2	2.08	0.53
1:G:467:MET:HE2	1:G:533:MET:SD	2.47	0.53
1:C:363:ARG:NH1	1:C:393:TYR:O	2.42	0.53
1:D:69:PRO:HD3	1:D:115:ASP:HB2	1.91	0.53
1:D:363:ARG:NH1	1:D:393:TYR:O	2.42	0.53
1:F:239:TYR:O	1:F:243:VAL:HG23	2.09	0.53
1:B:40:ASN:OD1	1:B:40:ASN:N	2.41	0.53
1:D:324:PHE:CD1	1:D:326:ARG:HG2	2.44	0.53
1:E:144:MET:HB2	1:E:178:TRP:HB3	1.90	0.53
1:E:268:VAL:HG23	1:E:315:ILE:HG22	1.91	0.53
1:C:44:THR:HG21	1:C:91:GLU:CG	2.39	0.53
1:F:28:PHE:HB2	1:F:390:VAL:HG22	1.91	0.53
1:B:104:GLU:OE1	1:B:108:ARG:NH1	2.41	0.53
1:C:263:TRP:CD2	1:C:264:PRO:HD2	2.44	0.53
1:H:215:ARG:HD2	1:H:285:PHE:CE2	2.44	0.53
1:A:328:HIS:NE2	1:A:358:ILE:O	2.41	0.52
1:H:162:THR:HG22	1:H:163:GLU:HG3	1.91	0.52
1:H:192:ASN:OD1	1:H:194:ALA:N	2.36	0.52
1:E:246:GLU:OE2	1:E:249:ARG:NH1	2.42	0.52
1:D:44:THR:HG21	1:D:91:GLU:OE1	2.09	0.52
1:D:81:ASP:N	1:D:81:ASP:OD1	2.40	0.52
1:F:525:GLU:OE2	1:F:543:GLU:HG2	2.08	0.52
1:G:74:PRO:HD3	1:G:83:SER:OG	2.10	0.52
1:B:38:ASP:OD1	1:B:40:ASN:OD1	2.26	0.52
1:F:156:ARG:HH21	1:F:158:ILE:HA	1.74	0.52
1:A:263:TRP:CD2	1:A:264:PRO:HD2	2.44	0.52
1:A:362:ARG:HB2	1:A:367:LEU:HD13	1.92	0.52
1:D:358:ILE:H	1:D:359:GLY:CA	2.23	0.52
1:B:289:VAL:HG11	1:B:323:ILE:HG22	1.91	0.52
1:G:474:HIS:CE1	1:G:559:VAL:HG21	2.45	0.52
1:B:408:ARG:O	1:B:409:ASP:HB3	2.10	0.51
1:E:120:HIS:CD2	1:E:185:GLN:HB3	2.46	0.51
1:H:34:ARG:HG3	1:H:44:THR:HG23	1.93	0.51
1:D:34:ARG:HG3	1:D:44:THR:HG23	1.92	0.51
1:D:429:ASP:OD1	1:G:455:ARG:NH2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ARG:NH2	1:B:403:ILE:HD11	2.25	0.51
1:B:69:PRO:HD3	1:B:115:ASP:HB2	1.92	0.51
1:C:440:ASP:OD2	1:C:442:ILE:N	2.32	0.51
1:G:261:ASN:C	1:G:262:GLN:HG2	2.30	0.51
1:C:44:THR:HG21	1:C:91:GLU:HG2	1.92	0.51
1:C:200:LEU:O	1:C:204:ARG:HG3	2.10	0.51
1:C:434:TYR:CD2	1:C:435:LEU:HD13	2.45	0.51
1:D:355:LYS:HE3	1:D:367:LEU:CD2	2.41	0.51
1:E:470:ILE:HD13	1:E:473:ARG:NH2	2.25	0.51
1:F:117:VAL:HG11	1:F:120:HIS:HE1	1.72	0.51
1:F:276:THR:HG21	1:F:279:ASP:HB3	1.93	0.51
1:G:190:TYR:O	1:G:196:GLN:NE2	2.44	0.51
1:H:353:ARG:NH2	1:H:368:LEU:HA	2.25	0.51
1:H:95:LEU:N	1:H:95:LEU:HD12	2.25	0.51
1:E:117:VAL:HA	1:E:217:ASP:HB2	1.92	0.51
1:H:200:LEU:HG	1:H:202:VAL:HA	1.91	0.51
1:E:498:GLU:OE2	1:E:523:ARG:NH1	2.44	0.51
1:F:137:GLY:N	1:F:139:TYR:N	2.54	0.51
1:A:81:ASP:OD1	1:A:81:ASP:N	2.44	0.51
1:H:351:ASP:HB3	1:H:354:MET:O	2.10	0.51
1:H:66:TRP:CZ3	1:H:390:VAL:HG11	2.45	0.51
1:D:102:VAL:O	1:D:106:HIS:ND1	2.43	0.50
1:H:104:GLU:CD	1:H:108:ARG:HH12	2.14	0.50
1:H:80:TYR:CD1	1:H:331:LEU:HD21	2.46	0.50
1:D:117:VAL:HA	1:D:217:ASP:HB2	1.92	0.50
1:E:184:HIS:CD2	1:E:185:GLN:HG3	2.42	0.50
1:F:170:ASP:HB2	1:F:173:ARG:HE	1.76	0.50
1:G:232:ASN:CG	1:G:262:GLN:HE22	2.13	0.50
1:C:324:PHE:CD1	1:C:326:ARG:HG2	2.46	0.50
1:D:263:TRP:CD2	1:D:264:PRO:HD2	2.46	0.50
1:D:359:GLY:O	1:D:407:ASP:HB3	2.11	0.50
1:H:203:LEU:HB3	1:H:207:LEU:HD12	1.93	0.50
1:C:257:LEU:HG	1:C:283:MET:HB2	1.92	0.50
1:F:69:PRO:HD3	1:F:115:ASP:HB2	1.93	0.50
1:H:351:ASP:HB3	1:H:352:PRO:CA	2.41	0.50
1:C:17:PRO:C	1:C:18:ARG:HG3	2.32	0.50
1:G:196:GLN:O	1:G:200:LEU:HD13	2.11	0.50
1:C:339:GLU:HG2	1:C:345:TYR:CZ	2.46	0.50
1:G:259:GLU:HG3	1:G:331:LEU:HD13	1.93	0.50
1:E:481:SER:O	1:E:497:ARG:HD2	2.11	0.50
1:F:440:ASP:OD1	1:F:442:ILE:N	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ARG:CB	1:E:173:ARG:HG3	2.42	0.49
1:F:137:GLY:H	1:F:139:TYR:N	2.03	0.49
1:H:121:THR:HG22	1:H:122:SER:O	2.11	0.49
1:F:413:THR:HG21	1:F:438:ILE:HG13	1.94	0.49
1:H:215:ARG:HD2	1:H:285:PHE:HE2	1.77	0.49
1:E:257:LEU:HG	1:E:283:MET:HB2	1.94	0.49
1:E:404:TRP:CD1	1:H:436:PRO:HD3	2.48	0.49
1:F:129:GLN:O	1:F:132:ARG:HG3	2.12	0.49
1:B:362:ARG:HD2	1:B:401:ASP:OD2	2.13	0.49
1:E:135:PRO:HB3	1:E:173:ARG:NH1	2.27	0.49
1:F:324:PHE:CD1	1:F:326:ARG:HG2	2.47	0.49
1:H:201:GLU:HB3	1:H:204:ARG:HG2	1.93	0.49
1:E:239:TYR:O	1:E:242:ARG:HB2	2.12	0.49
1:H:199:MET:O	1:H:201:GLU:N	2.43	0.49
1:F:405:LEU:HB2	1:F:410:SER:HB3	1.95	0.49
1:A:28:PHE:HB2	1:A:390:VAL:HG22	1.95	0.49
1:F:190:TYR:HA	1:F:195:VAL:HG21	1.94	0.49
1:G:200:LEU:O	1:G:204:ARG:HG3	2.13	0.49
1:H:235:GLU:N	1:H:235:GLU:OE1	2.37	0.49
1:H:498:GLU:CD	1:H:523:ARG:HH21	2.16	0.48
1:A:360:ILE:HG23	1:A:407:ASP:HA	1.95	0.48
1:E:273:ASP:O	1:E:276:THR:HG22	2.13	0.48
1:G:28:PHE:HB2	1:G:390:VAL:HG22	1.94	0.48
1:H:132:ARG:HG3	1:H:135:PRO:HG3	1.95	0.48
1:H:200:LEU:HB3	1:H:201:GLU:C	2.34	0.48
1:H:88:ILE:HG22	1:H:95:LEU:HD12	1.95	0.48
1:G:125:HIS:HD2	1:G:127:TRP:HB2	1.77	0.48
1:E:298:ARG:HH11	1:E:299:ARG:HH21	1.62	0.48
1:H:223:TYR:HD2	1:H:236:THR:HG22	1.78	0.48
1:H:32:LEU:HD22	1:H:412:ARG:HB3	1.95	0.48
1:A:244:ARG:HD2	1:A:280:GLU:O	2.12	0.48
1:B:40:ASN:ND2	1:B:42:ASP:CG	2.67	0.48
1:E:169:TYR:HA	1:E:176:TYR:HA	1.96	0.48
1:G:498:GLU:OE1	1:G:523:ARG:NH1	2.40	0.48
1:H:416:GLN:HG2	1:H:445:TYR:HB3	1.95	0.48
1:A:530:VAL:HG22	1:A:537:GLN:HG2	1.94	0.48
1:F:74:PRO:HD3	1:F:83:SER:OG	2.13	0.48
1:G:217:ASP:HB3	1:G:331:LEU:HD21	1.96	0.48
1:H:258:ALA:HB2	1:H:281:CYS:SG	2.53	0.48
1:D:329:ASP:O	1:D:333:LEU:HA	2.14	0.48
1:D:386:PRO:HA	1:D:497:ARG:NH2	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:287:PHE:CE1	1:G:324:PHE:HZ	2.32	0.48
1:G:500:GLY:O	1:G:501:ASP:HB2	2.13	0.48
1:E:190:TYR:OH	1:E:199:MET:HG2	2.14	0.48
1:H:292:ARG:HG3	1:H:308:ILE:HG12	1.96	0.48
1:D:243:VAL:O	1:D:247:VAL:HG13	2.14	0.47
1:E:81:ASP:OD1	1:E:81:ASP:N	2.44	0.47
1:F:127:TRP:O	1:F:128:PHE:C	2.53	0.47
1:F:129:GLN:HE22	1:F:173:ARG:NH1	2.12	0.47
1:A:298:ARG:NH1	1:A:351:ASP:OD2	2.47	0.47
1:B:420:ASP:OD1	1:F:421:ARG:HB2	2.14	0.47
1:B:217:ASP:HB3	1:B:331:LEU:HD21	1.95	0.47
1:F:179:HIS:HA	1:F:187:ASP:OD1	2.13	0.47
1:F:83:SER:O	1:F:126:PRO:HD2	2.13	0.47
1:G:189:ASN:O	1:G:195:VAL:HG21	2.14	0.47
1:H:481:SER:O	1:H:497:ARG:HD2	2.14	0.47
1:B:409:ASP:C	1:B:411:VAL:H	2.11	0.47
1:C:362:ARG:CB	1:C:367:LEU:HD13	2.43	0.47
1:H:197:GLU:HG3	1:H:198:ALA:H	1.80	0.47
1:H:326:ARG:HB2	1:H:361:ARG:HH12	1.78	0.47
1:D:104:GLU:HG3	1:D:108:ARG:NH1	2.30	0.47
1:D:263:TRP:CG	1:D:264:PRO:HD2	2.49	0.47
1:G:474:HIS:CE1	1:G:559:VAL:CG2	2.98	0.47
1:H:167:TRP:CZ3	1:H:177:TYR:O	2.67	0.47
1:A:66:TRP:CD1	1:A:66:TRP:C	2.87	0.47
1:D:121:THR:O	1:D:186:PRO:HD2	2.15	0.47
1:E:134:ASP:HA	1:E:135:PRO:HD2	1.81	0.47
1:E:305:ILE:O	1:E:309:MET:HG2	2.15	0.47
1:B:351:ASP:HB3	1:B:354:MET:HB3	1.97	0.47
1:C:155:ALA:HB1	1:C:180:ARG:NH1	2.29	0.47
1:D:244:ARG:HD2	1:D:280:GLU:O	2.15	0.47
1:E:407:ASP:C	1:E:409:ASP:N	2.68	0.47
1:H:28:PHE:HB2	1:H:390:VAL:HG22	1.97	0.47
1:C:299:ARG:NH2	1:C:301:GLN:OE1	2.48	0.47
1:F:189:ASN:O	1:F:195:VAL:HG21	2.15	0.47
1:A:362:ARG:HD2	1:A:401:ASP:OD2	2.14	0.47
1:F:40:ASN:OD1	1:F:46:ASP:OD2	2.33	0.47
1:H:365:ALA:HB3	1:H:366:PRO:HD3	1.97	0.47
1:A:404:TRP:CD1	1:C:436:PRO:HD3	2.50	0.46
1:H:199:MET:O	1:H:202:VAL:HG23	2.15	0.46
1:C:197:GLU:O	1:C:201:GLU:HB2	2.14	0.46
1:F:145:TRP:CZ3	1:F:177:TYR:HB3	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:163:GLU:OE1	1:H:182:PHE:HA	2.15	0.46
1:H:225:ARG:HH21	1:H:234:PRO:HD2	1.80	0.46
1:E:298:ARG:CZ	1:E:351:ASP:HB2	2.46	0.46
1:G:239:TYR:O	1:G:243:VAL:HG23	2.15	0.46
1:H:190:TYR:OH	1:H:199:MET:HG2	2.15	0.46
1:H:244:ARG:HD3	1:H:280:GLU:O	2.15	0.46
1:H:72:GLN:HA	1:H:89:LEU:HD13	1.96	0.46
1:A:513:PHE:HE1	1:H:466:LYS:NZ	2.14	0.46
1:D:144:MET:HB2	1:D:178:TRP:HB3	1.97	0.46
1:A:117:VAL:HA	1:A:217:ASP:HB2	1.97	0.46
1:C:239:TYR:O	1:C:243:VAL:HG23	2.15	0.46
1:D:358:ILE:N	1:D:359:GLY:CA	2.79	0.46
1:D:421:ARG:HB2	1:G:420:ASP:OD1	2.15	0.46
1:H:81:ASP:OD1	1:H:81:ASP:N	2.48	0.46
1:C:117:VAL:HA	1:C:217:ASP:HB2	1.98	0.46
1:C:47:LEU:O	1:C:51:ILE:HG13	2.16	0.46
1:G:131:SER:O	1:G:173:ARG:NH1	2.47	0.46
1:H:119:ASN:ND2	1:H:221:TYR:HB2	2.31	0.46
1:B:324:PHE:CD1	1:B:326:ARG:HG2	2.50	0.46
1:C:324:PHE:HB3	1:C:390:VAL:HB	1.98	0.46
1:F:146:SER:O	1:F:176:TYR:N	2.49	0.45
1:A:397:ILE:HG22	1:A:461:LEU:HB2	1.97	0.45
1:F:128:PHE:O	1:F:129:GLN:C	2.54	0.45
1:F:167:TRP:CE2	1:F:178:TRP:HE3	2.34	0.45
1:F:237:HIS:CE1	1:F:269:GLU:HB3	2.51	0.45
1:A:367:LEU:HA	1:A:367:LEU:HD12	1.68	0.45
1:B:24:LYS:HG2	1:B:320:GLN:HG2	1.97	0.45
1:C:402:ASN:HB3	1:C:405:LEU:HD22	1.98	0.45
1:E:413:THR:HG23	1:E:414:PRO:HD2	1.97	0.45
1:H:357:ASN:O	1:H:357:ASN:ND2	2.50	0.45
1:E:413:THR:HG21	1:E:438:ILE:HG13	1.98	0.45
1:G:154:ASP:HB2	1:G:228:THR:O	2.16	0.45
1:G:69:PRO:HD3	1:G:115:ASP:HB2	1.98	0.45
1:D:396:GLU:HG2	1:D:397:ILE:HG23	1.99	0.45
1:G:498:GLU:OE2	1:G:503:ARG:NH1	2.50	0.45
1:B:246:GLU:OE2	1:B:249:ARG:NH1	2.50	0.45
1:C:300:GLU:OE2	1:C:512:ARG:NH1	2.48	0.45
1:C:453:GLN:HB3	1:C:461:LEU:HB3	1.99	0.45
1:G:237:HIS:NE2	1:G:269:GLU:HG2	2.32	0.45
1:G:308:ILE:O	1:G:312:THR:OG1	2.23	0.45
1:H:358:ILE:HD13	1:H:358:ILE:HA	1.88	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:PHE:CE2	1:D:132:ARG:HD3	2.52	0.45
1:F:136:ASP:HB2	1:F:137:GLY:C	2.37	0.45
1:F:171:PRO:HD2	1:F:173:ARG:NH2	2.31	0.45
1:F:279:ASP:OD1	1:F:279:ASP:N	2.50	0.45
1:F:268:VAL:HG23	1:F:315:ILE:HG22	1.98	0.45
1:F:362:ARG:HH11	1:F:401:ASP:CG	2.20	0.45
1:C:235:GLU:OE1	1:C:235:GLU:N	2.44	0.45
1:C:408:ARG:HG2	1:C:408:ARG:HH11	1.81	0.45
1:E:466:LYS:NZ	1:E:533:MET:O	2.24	0.45
1:F:128:PHE:C	1:F:130:ALA:N	2.67	0.45
1:F:134:ASP:C	1:F:134:ASP:OD1	2.56	0.45
1:H:200:LEU:HD12	1:H:204:ARG:HG3	1.99	0.45
1:H:117:VAL:HA	1:H:217:ASP:HB2	1.98	0.45
1:C:83:SER:O	1:C:126:PRO:HD2	2.17	0.45
1:G:473:ARG:C	1:G:474:HIS:CD2	2.91	0.45
1:H:290:MET:HB3	1:H:291:PRO:HD3	1.99	0.45
1:H:470:ILE:HG21	1:H:532:CYS:HB3	1.99	0.45
1:B:215:ARG:HD3	1:B:217:ASP:OD1	2.18	0.44
1:D:289:VAL:O	1:D:293:ILE:HG13	2.17	0.44
1:H:55:ASP:OD1	1:H:55:ASP:N	2.49	0.44
1:G:223:TYR:H	1:G:236:THR:HG22	1.82	0.44
1:H:522:ARG:CZ	1:H:543:GLU:HG2	2.47	0.44
1:B:48:ARG:NH1	1:B:100:GLU:OE2	2.46	0.44
1:E:157:ILE:O	1:E:160:VAL:HG22	2.17	0.44
1:A:69:PRO:HD3	1:A:115:ASP:HB2	1.99	0.44
1:B:237:HIS:CE1	1:B:269:GLU:HB3	2.53	0.44
1:D:298:ARG:NH2	1:D:350:LYS:O	2.50	0.44
1:E:407:ASP:OD1	1:E:408:ARG:N	2.49	0.44
1:G:192:ASN:O	1:G:195:VAL:HG22	2.18	0.44
1:G:409:ASP:C	1:G:411:VAL:N	2.69	0.44
1:D:355:LYS:HE2	1:D:355:LYS:HB2	1.48	0.44
1:E:145:TRP:CZ3	1:E:177:TYR:HB3	2.52	0.44
1:F:402:ASN:C	1:F:410:SER:HB2	2.37	0.44
1:H:40:ASN:HD22	1:H:46:ASP:CG	2.20	0.44
1:A:151:LYS:HB2	1:A:151:LYS:HE3	1.63	0.44
1:A:217:ASP:HB3	1:A:331:LEU:HD21	1.99	0.44
1:B:265:ALA:H	1:B:267:VAL:H	1.65	0.44
1:B:344:MET:HE1	1:B:347:GLU:HG3	2.00	0.44
1:B:409:ASP:HA	1:B:412:ARG:HD2	2.00	0.44
1:H:95:LEU:H	1:H:95:LEU:HD12	1.82	0.44
1:D:466:LYS:HD3	1:D:533:MET:CE	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:VAL:HG13	1:D:553:HIS:HE1	1.83	0.44
1:F:171:PRO:O	1:F:173:ARG:N	2.43	0.44
1:F:38:ASP:OD1	1:F:40:ASN:OD1	2.35	0.44
1:H:203:LEU:HG	1:H:214:PHE:CE1	2.53	0.44
1:A:89:LEU:HA	1:A:90:PRO:HD3	1.84	0.44
1:C:408:ARG:NH1	1:C:408:ARG:HG2	2.32	0.44
1:E:509:ASN:O	1:E:553:HIS:HA	2.18	0.44
1:H:125:HIS:HD2	1:H:127:TRP:HB2	1.82	0.44
1:C:40:ASN:N	1:C:40:ASN:OD1	2.50	0.44
1:E:30:GLU:OE1	1:E:326:ARG:NH2	2.38	0.44
1:E:359:GLY:HA3	1:E:408:ARG:NH1	2.33	0.44
1:F:125:HIS:ND1	1:F:126:PRO:HD2	2.30	0.44
1:G:386:PRO:HG3	1:G:482:TYR:HB2	1.99	0.44
1:H:295:MET:HG2	1:H:344:MET:SD	2.58	0.44
1:A:349:ALA:C	1:A:351:ASP:H	2.20	0.43
1:B:474:HIS:HB3	1:B:476:VAL:HG12	1.99	0.43
1:A:200:LEU:O	1:A:204:ARG:HG3	2.18	0.43
1:H:66:TRP:HZ3	1:H:390:VAL:HG11	1.82	0.43
1:C:405:LEU:O	1:C:406:GLY:O	2.37	0.43
1:E:324:PHE:HB3	1:E:390:VAL:HB	1.99	0.43
1:F:133:THR:CG2	1:F:134:ASP:HA	2.36	0.43
1:H:123:ASP:OD1	1:H:124:GLN:NE2	2.44	0.43
1:H:354:MET:HG3	1:H:357:ASN:CG	2.38	0.43
1:B:303:TYR:HD2	1:B:343:TYR:HH	1.67	0.43
1:B:40:ASN:OD1	1:B:46:ASP:OD2	2.36	0.43
1:E:244:ARG:HD3	1:E:280:GLU:O	2.19	0.43
1:E:24:LYS:HA	1:E:320:GLN:HE21	1.82	0.43
1:F:190:TYR:HA	1:F:195:VAL:CG2	2.49	0.43
1:F:528:THR:HG21	1:F:537:GLN:OE1	2.18	0.43
1:G:228:THR:HB	1:G:229:ASN:H	1.51	0.43
1:H:363:ARG:HG3	1:H:411:VAL:CG2	2.49	0.43
1:C:290:MET:HB3	1:C:291:PRO:HD3	2.01	0.43
1:D:132:ARG:NH1	1:D:170:ASP:OD1	2.52	0.43
1:D:327:ASN:O	1:D:335:MET:HG3	2.18	0.43
1:G:104:GLU:HA	1:G:107:ARG:HD2	2.01	0.43
1:H:192:ASN:O	1:H:195:VAL:HG22	2.18	0.43
1:A:38:ASP:OD1	1:A:40:ASN:OD1	2.36	0.43
1:C:496:VAL:HG12	1:C:498:GLU:HG2	2.01	0.43
1:E:179:HIS:HA	1:E:187:ASP:OD1	2.19	0.43
1:F:235:GLU:N	1:F:235:GLU:OE1	2.48	0.43
1:H:303:TYR:HB2	1:H:304:PRO:HD3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:354:MET:C	1:H:357:ASN:OD1	2.56	0.43
1:H:429:ASP:OD1	1:H:430:PRO:HD2	2.19	0.43
1:G:324:PHE:CD1	1:G:326:ARG:HG2	2.54	0.43
1:H:416:GLN:HE21	1:H:445:TYR:CA	2.31	0.43
1:H:91:GLU:HG2	1:H:91:GLU:H	1.39	0.43
1:D:290:MET:HB3	1:D:291:PRO:HD3	2.00	0.43
1:H:88:ILE:HG21	1:H:94:ASP:HA	2.01	0.43
1:A:333:LEU:HD21	1:A:408:ARG:HB2	2.00	0.43
1:A:509:ASN:O	1:A:553:HIS:HA	2.17	0.43
1:B:85:TYR:HD1	1:B:116:LEU:HD11	1.84	0.43
1:B:409:ASP:O	1:B:410:SER:HB3	2.19	0.43
1:C:408:ARG:O	1:C:409:ASP:CB	2.63	0.43
1:D:287:PHE:CE1	1:D:324:PHE:HZ	2.36	0.43
1:E:89:LEU:HA	1:E:90:PRO:HD3	1.83	0.43
1:F:54:LEU:HA	1:F:54:LEU:HD23	1.84	0.43
1:G:365:ALA:HB3	1:G:366:PRO:HD3	2.01	0.43
1:G:498:GLU:CD	1:G:523:ARG:HH22	2.22	0.43
1:B:103:ASP:HB3	1:B:107:ARG:HH12	1.83	0.42
1:B:203:LEU:HD22	1:B:214:PHE:CE1	2.54	0.42
1:C:437:VAL:O	1:C:439:MET:HG3	2.19	0.42
1:E:47:LEU:O	1:E:51:ILE:HG13	2.18	0.42
1:F:81:ASP:N	1:F:81:ASP:OD1	2.52	0.42
1:B:414:PRO:HG3	1:B:434:TYR:CE1	2.55	0.42
1:C:305:ILE:O	1:C:308:ILE:HG13	2.19	0.42
1:D:276:THR:HG21	1:D:279:ASP:HB3	2.00	0.42
1:E:365:ALA:HB3	1:E:366:PRO:HD3	2.01	0.42
1:E:402:ASN:C	1:E:403:ILE:O	2.57	0.42
1:H:204:ARG:O	1:H:208:ASP:N	2.43	0.42
1:B:286:HIS:CE1	1:B:288:PRO:HG2	2.54	0.42
1:E:143:TYR:HD1	1:E:187:ASP:O	2.02	0.42
1:F:134:ASP:N	1:F:135:PRO:HD3	2.33	0.42
1:H:205:PHE:O	1:H:209:LEU:HG	2.18	0.42
1:A:308:ILE:H	1:A:308:ILE:HG13	1.64	0.42
1:C:54:LEU:HA	1:C:54:LEU:HD23	1.91	0.42
1:D:228:THR:HG21	1:D:233:LEU:HD21	2.01	0.42
1:F:409:ASP:O	1:F:410:SER:CB	2.67	0.42
1:A:339:GLU:HG3	1:A:345:TYR:CD2	2.54	0.42
1:A:40:ASN:ND2	1:A:42:ASP:CG	2.73	0.42
1:B:481:SER:O	1:B:497:ARG:HD2	2.19	0.42
1:C:367:LEU:HA	1:C:367:LEU:HD12	1.91	0.42
1:E:220:PRO:O	1:E:231:GLU:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ARG:HE	1:A:473:ARG:HB2	1.67	0.42
1:C:200:LEU:HD21	1:C:243:VAL:HG22	2.02	0.42
1:F:151:LYS:HG3	1:F:167:TRP:HZ2	1.85	0.42
1:F:287:PHE:CE1	1:F:324:PHE:HZ	2.37	0.42
1:H:132:ARG:HG2	1:H:132:ARG:O	2.20	0.42
1:H:324:PHE:CE1	1:H:326:ARG:HG2	2.55	0.42
1:E:406:GLY:N	1:E:407:ASP:HA	2.35	0.42
1:E:66:TRP:C	1:E:66:TRP:CD1	2.93	0.42
1:G:119:ASN:HD22	1:G:120:HIS:HD2	1.66	0.42
1:H:489:ASN:HA	1:H:490:PRO:HD3	1.77	0.42
1:B:329:ASP:OD1	1:B:331:LEU:N	2.49	0.42
1:B:522:ARG:CD	1:B:543:GLU:HG3	2.47	0.42
1:C:340:GLU:HG2	1:C:341:ARG:HG3	2.00	0.42
1:D:157:ILE:O	1:D:160:VAL:HG22	2.19	0.42
1:D:84:ASP:OD2	1:D:87:LYS:HG3	2.20	0.42
1:E:155:ALA:HB1	1:E:180:ARG:NH1	2.34	0.42
1:D:228:THR:HG23	1:D:230:CYS:H	1.85	0.42
1:D:386:PRO:HG3	1:D:482:TYR:HB2	2.01	0.42
1:F:167:TRP:CH2	1:F:178:TRP:HB2	2.55	0.42
1:G:474:HIS:HE1	1:G:559:VAL:HG21	1.85	0.42
1:C:312:THR:HA	1:C:313:PRO:HD3	1.91	0.42
1:E:76:ARG:HB3	1:E:184:HIS:CE1	2.55	0.42
1:G:148:THR:HG23	1:G:150:ASP:OD1	2.20	0.42
1:H:180:ARG:HA	1:H:180:ARG:HD2	1.87	0.42
1:H:84:ASP:OD2	1:H:87:LYS:HD3	2.20	0.42
1:C:386:PRO:HG3	1:C:482:TYR:HB2	2.01	0.41
1:E:347:GLU:HA	1:E:350:LYS:HE2	2.01	0.41
1:G:204:ARG:HB3	1:G:251:TYR:OH	2.20	0.41
1:H:127:TRP:HZ3	1:H:199:MET:HE2	1.84	0.41
1:A:397:ILE:HB	1:A:453:GLN:HG3	2.02	0.41
1:B:115:ASP:OD1	1:B:215:ARG:HD2	2.20	0.41
1:D:258:ALA:HB2	1:D:281:CYS:SG	2.60	0.41
1:E:265:ALA:O	1:E:268:VAL:HG12	2.21	0.41
1:G:481:SER:O	1:G:497:ARG:HD2	2.19	0.41
1:H:200:LEU:O	1:H:201:GLU:CG	2.63	0.41
1:H:88:ILE:HG22	1:H:95:LEU:CD1	2.50	0.41
1:A:135:PRO:HG3	1:A:173:ARG:HD2	2.01	0.41
1:C:178:TRP:CZ2	1:C:180:ARG:HD3	2.55	0.41
1:C:265:ALA:O	1:C:268:VAL:HG12	2.21	0.41
1:G:217:ASP:HA	1:G:259:GLU:HB3	2.02	0.41
1:B:365:ALA:HB3	1:B:366:PRO:HD3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:MET:HE2	1:C:533:MET:SD	2.60	0.41
1:E:206:TRP:HB2	1:E:214:PHE:HZ	1.84	0.41
1:H:153:PRO:HB2	1:H:154:ASP:H	1.72	0.41
1:H:66:TRP:CD1	1:H:66:TRP:C	2.94	0.41
1:D:38:ASP:HB3	1:D:426:SER:HB2	2.02	0.41
1:F:159:PHE:C	1:F:161:ASP:H	2.24	0.41
1:H:194:ALA:CA	1:H:197:GLU:HB3	2.51	0.41
1:B:44:THR:HG21	1:B:91:GLU:HB2	2.02	0.41
1:C:297:VAL:HG21	1:C:378:PHE:CE1	2.55	0.41
1:D:292:ARG:HH12	1:D:307:GLU:HB3	1.86	0.41
1:D:283:MET:HA	1:D:320:GLN:O	2.21	0.41
1:E:263:TRP:CD2	1:E:264:PRO:HD2	2.56	0.41
1:F:137:GLY:CA	1:F:139:TYR:H	2.31	0.41
1:G:344:MET:HE1	1:G:347:GLU:HG3	2.02	0.41
1:G:81:ASP:OD1	1:G:81:ASP:N	2.49	0.41
1:H:488:SER:O	1:H:490:PRO:HD3	2.21	0.41
1:A:144:MET:HE3	1:A:187:ASP:HB3	2.02	0.41
1:A:451:GLU:OE2	1:A:455:ARG:NH1	2.54	0.41
1:E:192:ASN:HA	1:E:193:PRO:HD3	1.95	0.41
1:E:290:MET:HB3	1:E:291:PRO:HD3	2.02	0.41
1:F:73:SER:H	1:F:89:LEU:HD13	1.86	0.41
1:G:297:VAL:HG21	1:G:378:PHE:CE1	2.56	0.41
1:G:500:GLY:C	1:G:502:ASP:H	2.24	0.41
1:G:66:TRP:CZ3	1:G:390:VAL:HG11	2.56	0.41
1:H:194:ALA:HA	1:H:197:GLU:HB3	2.02	0.41
1:H:57:LEU:HA	1:H:57:LEU:HD23	1.84	0.41
1:B:440:ASP:HA	1:B:441:PRO:HD3	1.97	0.41
1:G:24:LYS:NZ	1:G:317:GLU:O	2.40	0.41
1:A:323:ILE:HG21	1:A:323:ILE:HD13	1.74	0.41
1:B:48:ARG:NH2	1:B:100:GLU:OE1	2.49	0.41
1:B:372:ARG:HA	1:B:375:LEU:HD12	2.03	0.41
1:C:481:SER:O	1:C:497:ARG:HD2	2.20	0.41
1:C:89:LEU:HA	1:C:90:PRO:HD3	1.83	0.41
1:F:85:TYR:HD1	1:F:116:LEU:HD11	1.86	0.41
1:H:181:PHE:HB3	1:H:182:PHE:H	1.76	0.41
1:B:28:PHE:HB2	1:B:390:VAL:HG22	2.03	0.41
1:C:222:LEU:HD23	1:C:222:LEU:HA	1.88	0.41
1:C:190:TYR:HB3	1:C:223:TYR:CZ	2.56	0.41
1:F:126:PRO:C	1:F:127:TRP:O	2.55	0.41
1:D:292:ARG:HG3	1:D:308:ILE:HG12	2.03	0.40
1:E:125:HIS:CD2	1:E:127:TRP:H	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:LYS:CG	1:F:167:TRP:CZ2	3.04	0.40
1:G:146:SER:C	1:G:148:THR:H	2.25	0.40
1:H:222:LEU:HB2	1:H:236:THR:HG22	2.03	0.40
1:H:405:LEU:HD13	1:H:435:LEU:HD22	2.03	0.40
1:A:489:ASN:HA	1:A:490:PRO:HD3	1.88	0.40
1:C:344:MET:HE1	1:C:347:GLU:HG3	2.03	0.40
1:C:40:ASN:OD1	1:C:46:ASP:OD1	2.40	0.40
1:G:192:ASN:O	1:G:196:GLN:HG3	2.21	0.40
1:H:144:MET:O	1:H:177:TYR:O	2.39	0.40
1:A:85:TYR:HD1	1:A:116:LEU:HD11	1.86	0.40
1:E:287:PHE:CE1	1:E:329:ASP:HB3	2.56	0.40
1:F:125:HIS:CD2	1:F:127:TRP:HB2	2.55	0.40
1:G:316:PRO:HB2	1:G:319:CYS:SG	2.61	0.40
1:G:34:ARG:HG3	1:G:44:THR:HG23	2.03	0.40
1:H:157:ILE:O	1:H:160:VAL:HG12	2.21	0.40
1:H:363:ARG:HG3	1:H:411:VAL:HG23	2.02	0.40
1:C:200:LEU:HA	1:C:200:LEU:HD23	1.90	0.40
1:C:231:GLU:OE1	1:C:262:GLN:NE2	2.54	0.40
1:C:365:ALA:HB3	1:C:366:PRO:HD3	2.04	0.40
1:A:71:TYR:CZ	1:A:116:LEU:HD13	2.57	0.40
1:A:294:PHE:O	1:A:298:ARG:HG2	2.21	0.40
1:B:408:ARG:HG2	1:B:409:ASP:H	1.86	0.40
1:B:81:ASP:N	1:B:81:ASP:OD1	2.51	0.40
1:C:265:ALA:H	1:C:267:VAL:H	1.68	0.40
1:F:129:GLN:HE22	1:F:173:ARG:HH12	1.68	0.40
1:H:121:THR:O	1:H:186:PRO:HD2	2.21	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	542/601 (90%)	521 (96%)	17 (3%)	4 (1%)	22 53
1	B	542/601 (90%)	522 (96%)	15 (3%)	5 (1%)	17 46
1	C	542/601 (90%)	513 (95%)	21 (4%)	8 (2%)	10 33
1	D	542/601 (90%)	516 (95%)	21 (4%)	5 (1%)	17 46
1	E	542/601 (90%)	515 (95%)	21 (4%)	6 (1%)	14 41
1	F	542/601 (90%)	496 (92%)	26 (5%)	20 (4%)	3 11
1	G	542/601 (90%)	518 (96%)	16 (3%)	8 (2%)	10 33
1	H	532/601 (88%)	491 (92%)	24 (4%)	17 (3%)	4 13
All	All	4326/4808 (90%)	4092 (95%)	161 (4%)	73 (2%)	9 29

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	ALA
1	A	407	ASP
1	B	150	ASP
1	D	358	ILE
1	E	403	ILE
1	E	411	VAL
1	F	127	TRP
1	F	129	GLN
1	F	131	SER
1	F	149	ASP
1	F	150	ASP
1	F	151	LYS
1	G	226	GLU
1	G	261	ASN
1	G	265	ALA
1	H	153	PRO
1	H	178	TRP
1	H	197	GLU
1	H	198	ALA
1	H	201	GLU
1	H	203	LEU
1	H	230	CYS
1	H	354	MET
1	H	355	LYS
1	H	410	SER
1	A	409	ASP
1	B	265	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	500	GLY
1	C	265	ALA
1	C	333	LEU
1	C	406	GLY
1	D	410	SER
1	E	18	ARG
1	E	265	ALA
1	F	160	VAL
1	F	172	VAL
1	F	265	ALA
1	F	333	LEU
1	G	409	ASP
1	G	410	SER
1	G	500	GLY
1	H	265	ALA
1	H	351	ASP
1	H	500	GLY
1	C	230	CYS
1	C	409	ASP
1	C	410	SER
1	E	500	GLY
1	F	135	PRO
1	F	141	ASP
1	F	187	ASP
1	F	225	ARG
1	G	227	GLY
1	G	408	ARG
1	H	226	GLU
1	B	230	CYS
1	B	409	ASP
1	C	359	GLY
1	D	334	GLU
1	F	173	ARG
1	F	226	GLU
1	H	183	SER
1	H	200	LEU
1	H	359	GLY
1	E	404	TRP
1	F	130	ALA
1	F	138	PRO
1	A	230	CYS
1	F	171	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	500	GLY
1	F	134	ASP
1	C	500	GLY
1	D	264	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	476/522 (91%)	468 (98%)	8 (2%)	60	87
1	B	476/522 (91%)	472 (99%)	4 (1%)	81	94
1	C	476/522 (91%)	468 (98%)	8 (2%)	60	87
1	D	476/522 (91%)	467 (98%)	9 (2%)	57	85
1	E	476/522 (91%)	469 (98%)	7 (2%)	65	89
1	F	476/522 (91%)	462 (97%)	14 (3%)	42	76
1	G	476/522 (91%)	467 (98%)	9 (2%)	57	85
1	H	468/522 (90%)	455 (97%)	13 (3%)	43	77
All	All	3800/4176 (91%)	3728 (98%)	72 (2%)	57	85

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	302	ARG
1	A	314	LYS
1	A	324	PHE
1	A	353	ARG
1	A	401	ASP
1	A	413	THR
1	A	501	ASP
1	B	320	GLN
1	B	324	PHE
1	B	410	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	488	SER
1	C	324	PHE
1	C	343	TYR
1	C	401	ASP
1	C	405	LEU
1	C	411	VAL
1	C	432	ARG
1	C	455	ARG
1	C	498	GLU
1	D	107	ARG
1	D	160	VAL
1	D	164	VAL
1	D	247	VAL
1	D	262	GLN
1	D	314	LYS
1	D	324	PHE
1	D	338	ASP
1	D	401	ASP
1	E	173	ARG
1	E	298	ARG
1	E	324	PHE
1	E	405	LEU
1	E	411	VAL
1	E	501	ASP
1	E	544	LEU
1	F	107	ARG
1	F	120	HIS
1	F	133	THR
1	F	173	ARG
1	F	231	GLU
1	F	242	ARG
1	F	317	GLU
1	F	324	PHE
1	F	343	TYR
1	F	411	VAL
1	F	413	THR
1	F	432	ARG
1	F	439	MET
1	F	455	ARG
1	G	39	SER
1	G	46	ASP
1	G	148	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	249	ARG
1	G	262	GLN
1	G	324	PHE
1	G	333	LEU
1	G	367	LEU
1	G	411	VAL
1	H	46	ASP
1	H	121	THR
1	H	131	SER
1	H	145	TRP
1	H	199	MET
1	H	200	LEU
1	H	215	ARG
1	H	248	ASP
1	H	250	LEU
1	H	311	GLN
1	H	324	PHE
1	H	413	THR
1	H	522	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	A	232	ASN
1	B	119	ASN
1	D	119	ASN
1	D	553	HIS
1	E	175	GLN
1	E	184	HIS
1	E	416	GLN
1	F	129	GLN
1	F	166	ASN
1	F	184	HIS
1	G	119	ASN
1	G	262	GLN
1	G	474	HIS
1	H	120	HIS
1	H	311	GLN
1	H	416	GLN
1	H	446	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 carbohydrates 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	544/601 (90%)	-0.31	5 (0%) 84 80	13, 24, 43, 71	0
1	B	544/601 (90%)	-0.25	10 (1%) 68 61	12, 25, 48, 72	0
1	C	544/601 (90%)	-0.22	12 (2%) 62 52	14, 31, 51, 102	0
1	D	544/601 (90%)	0.03	26 (4%) 30 21	15, 34, 54, 71	0
1	E	544/601 (90%)	-0.01	22 (4%) 38 28	15, 34, 68, 94	0
1	F	544/601 (90%)	0.07	31 (5%) 23 15	14, 31, 87, 103	0
1	G	544/601 (90%)	-0.07	21 (3%) 39 29	15, 36, 63, 87	0
1	H	536/601 (89%)	0.36	58 (10%) 5 3	16, 38, 80, 95	0
All	All	4344/4808 (90%)	-0.05	185 (4%) 35 25	12, 30, 65, 103	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	349	ALA	14.4
1	F	169	TYR	10.5
1	H	138	PRO	8.3
1	F	228	THR	8.2
1	D	358	ILE	7.8
1	F	227	GLY	6.6
1	D	357	ASN	6.4
1	H	225	ARG	6.2
1	F	138	PRO	5.8
1	H	139	TYR	5.8
1	F	153	PRO	5.7
1	F	174	GLY	5.5
1	H	198	ALA	5.2
1	C	406	GLY	5.2
1	H	133	THR	5.1
1	E	406	GLY	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	177	TYR	5.1
1	F	149	ASP	5.1
1	H	145	TRP	4.8
1	H	199	MET	4.8
1	H	137	GLY	4.7
1	F	136	ASP	4.7
1	G	136	ASP	4.7
1	H	143	TYR	4.7
1	H	144	MET	4.6
1	A	350	LYS	4.6
1	H	543	GLU	4.5
1	H	189	ASN	4.5
1	H	194	ALA	4.4
1	H	135	PRO	4.4
1	H	190	TYR	4.4
1	H	142	PHE	4.3
1	H	141	ASP	4.3
1	E	136	ASP	4.2
1	C	407	ASP	4.1
1	H	136	ASP	3.9
1	H	155	ALA	3.9
1	B	172	VAL	3.9
1	E	169	TYR	3.9
1	F	135	PRO	3.9
1	H	350	LYS	3.8
1	G	228	THR	3.7
1	D	359	GLY	3.7
1	C	358	ILE	3.7
1	H	542	GLY	3.7
1	D	139	TYR	3.6
1	E	410	SER	3.6
1	D	138	PRO	3.6
1	H	130	ALA	3.6
1	F	148	THR	3.6
1	F	152	TYR	3.6
1	F	133	THR	3.5
1	E	405	LEU	3.5
1	H	128	PHE	3.5
1	H	140	GLY	3.5
1	D	147	ASP	3.4
1	F	226	GLU	3.4
1	F	147	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	193	PRO	3.4
1	H	146	SER	3.4
1	H	147	ASP	3.4
1	C	169	TYR	3.3
1	H	353	ARG	3.3
1	D	176	TYR	3.3
1	H	154	ASP	3.3
1	H	153	PRO	3.3
1	H	191	ASP	3.3
1	G	169	TYR	3.3
1	D	135	PRO	3.2
1	E	407	ASP	3.2
1	G	171	PRO	3.2
1	H	167	TRP	3.1
1	G	224	ALA	3.1
1	H	522	ARG	3.1
1	F	175	GLN	3.1
1	F	225	ARG	3.1
1	G	17	PRO	3.0
1	F	141	ASP	3.0
1	H	358	ILE	3.0
1	D	136	ASP	3.0
1	H	195	VAL	3.0
1	B	350	LYS	3.0
1	F	146	SER	3.0
1	G	172	VAL	2.9
1	B	150	ASP	2.9
1	D	169	TYR	2.9
1	C	17	PRO	2.9
1	E	176	TYR	2.9
1	G	189	ASN	2.9
1	E	171	PRO	2.9
1	H	233	LEU	2.8
1	G	142	PHE	2.8
1	C	18	ARG	2.8
1	F	173	ARG	2.8
1	H	134	ASP	2.8
1	H	132	ARG	2.8
1	H	544	LEU	2.8
1	D	140	GLY	2.8
1	E	18	ARG	2.8
1	A	224	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	171	PRO	2.7
1	G	138	PRO	2.7
1	F	165	SER	2.7
1	E	47	LEU	2.7
1	H	83	SER	2.7
1	F	177	TYR	2.7
1	H	127	TRP	2.7
1	D	137	GLY	2.7
1	H	129	GLN	2.7
1	F	150	ASP	2.7
1	E	276	THR	2.7
1	E	147	ASP	2.6
1	H	152	TYR	2.6
1	H	178	TRP	2.6
1	F	144	MET	2.6
1	H	224	ALA	2.6
1	B	171	PRO	2.6
1	C	194	ALA	2.6
1	A	225	ARG	2.5
1	D	127	TRP	2.5
1	B	224	ALA	2.5
1	D	129	GLN	2.5
1	H	188	LEU	2.4
1	G	137	GLY	2.4
1	H	357	ASN	2.4
1	H	205	PHE	2.4
1	G	129	GLN	2.4
1	E	48	ARG	2.4
1	G	18	ARG	2.4
1	H	148	THR	2.4
1	E	103	ASP	2.4
1	B	147	ASP	2.3
1	G	350	LYS	2.3
1	C	172	VAL	2.3
1	G	133	THR	2.3
1	B	176	TYR	2.3
1	H	192	ASN	2.3
1	D	174	GLY	2.3
1	D	432	ARG	2.3
1	D	351	ASP	2.3
1	F	132	ARG	2.3
1	C	171	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	17	PRO	2.3
1	D	95	LEU	2.3
1	D	94	ASP	2.3
1	G	139	TYR	2.3
1	A	349	ALA	2.2
1	E	150	ASP	2.2
1	F	164	VAL	2.2
1	D	142	PHE	2.2
1	F	142	PHE	2.2
1	B	107	ARG	2.2
1	F	176	TYR	2.2
1	D	144	MET	2.2
1	B	358	ILE	2.1
1	D	125	HIS	2.1
1	A	148	THR	2.1
1	C	408	ARG	2.1
1	H	121	THR	2.1
1	G	190	TYR	2.1
1	H	86	THR	2.1
1	D	128	PHE	2.1
1	E	135	PRO	2.1
1	C	176	TYR	2.1
1	D	148	THR	2.1
1	H	354	MET	2.1
1	E	175	GLN	2.1
1	E	404	TRP	2.1
1	F	229	ASN	2.1
1	E	93	GLY	2.1
1	B	223	TYR	2.1
1	E	94	ASP	2.1
1	G	145	TRP	2.1
1	G	226	GLU	2.1
1	C	129	GLN	2.0
1	F	17	PRO	2.0
1	G	176	TYR	2.0
1	H	84	ASP	2.0
1	H	150	ASP	2.0
1	G	87	LYS	2.0
1	E	98	PHE	2.0
1	F	178	TRP	2.0
1	H	197	GLU	2.0
1	D	141	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	191	ASP	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 carbohydrates 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.