Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:07 AM GMT

PDB ID	:	2ZNJ
Title	:	Crystal structure of Pyrrolysyl-tRNA synthetase from Desulfitobacterium hafniense
Authors	:	Nozawa, K.; Araiso, Y.; Soll, D.; Ishitani, R.; Nureki, O.
Deposited on	:	2008-04-25
Resolution	:	2.50 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

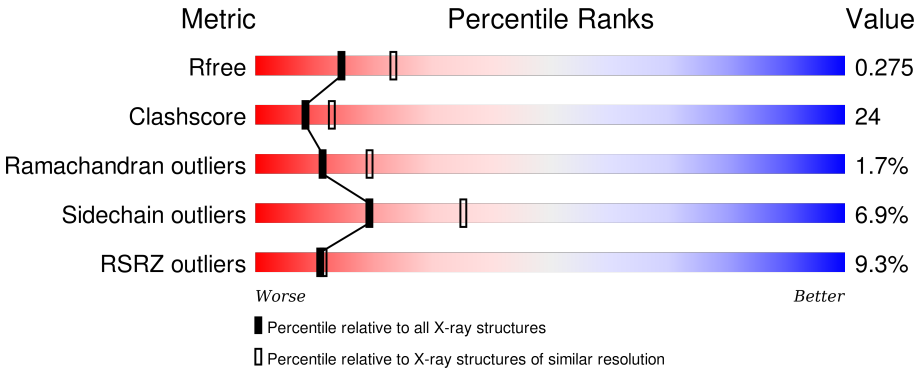
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	308	10%, 56%, 31%, •, 10%
1	B	308	11%, 57%, 28%, • •, 9%
1	C	308	4%, 58%, 30%, •, 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7189 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 uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2255	1434	396	413	12			
1	B	279	Total	C	N	O	S	0	0	0
			2263	1440	397	414	12			
1	C	278	Total	C	N	O	S	0	0	0
			2255	1434	396	413	12			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP B0S4P3
A	-18	GLY	-	EXPRESSION TAG	UNP B0S4P3
A	-17	SER	-	EXPRESSION TAG	UNP B0S4P3
A	-16	SER	-	EXPRESSION TAG	UNP B0S4P3
A	-15	HIS	-	EXPRESSION TAG	UNP B0S4P3
A	-14	HIS	-	EXPRESSION TAG	UNP B0S4P3
A	-13	HIS	-	EXPRESSION TAG	UNP B0S4P3
A	-12	HIS	-	EXPRESSION TAG	UNP B0S4P3
A	-11	HIS	-	EXPRESSION TAG	UNP B0S4P3
A	-10	HIS	-	EXPRESSION TAG	UNP B0S4P3
A	-9	SER	-	EXPRESSION TAG	UNP B0S4P3
A	-8	SER	-	EXPRESSION TAG	UNP B0S4P3
A	-7	GLY	-	EXPRESSION TAG	UNP B0S4P3
A	-6	LEU	-	EXPRESSION TAG	UNP B0S4P3
A	-5	VAL	-	EXPRESSION TAG	UNP B0S4P3
A	-4	PRO	-	EXPRESSION TAG	UNP B0S4P3
A	-3	ARG	-	EXPRESSION TAG	UNP B0S4P3
A	-2	GLY	-	EXPRESSION TAG	UNP B0S4P3
A	-1	SER	-	EXPRESSION TAG	UNP B0S4P3
A	0	HIS	-	EXPRESSION TAG	UNP B0S4P3
B	-19	MET	-	EXPRESSION TAG	UNP B0S4P3
B	-18	GLY	-	EXPRESSION TAG	UNP B0S4P3
B	-17	SER	-	EXPRESSION TAG	UNP B0S4P3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP B0S4P3
B	-15	HIS	-	EXPRESSION TAG	UNP B0S4P3
B	-14	HIS	-	EXPRESSION TAG	UNP B0S4P3
B	-13	HIS	-	EXPRESSION TAG	UNP B0S4P3
B	-12	HIS	-	EXPRESSION TAG	UNP B0S4P3
B	-11	HIS	-	EXPRESSION TAG	UNP B0S4P3
B	-10	HIS	-	EXPRESSION TAG	UNP B0S4P3
B	-9	SER	-	EXPRESSION TAG	UNP B0S4P3
B	-8	SER	-	EXPRESSION TAG	UNP B0S4P3
B	-7	GLY	-	EXPRESSION TAG	UNP B0S4P3
B	-6	LEU	-	EXPRESSION TAG	UNP B0S4P3
B	-5	VAL	-	EXPRESSION TAG	UNP B0S4P3
B	-4	PRO	-	EXPRESSION TAG	UNP B0S4P3
B	-3	ARG	-	EXPRESSION TAG	UNP B0S4P3
B	-2	GLY	-	EXPRESSION TAG	UNP B0S4P3
B	-1	SER	-	EXPRESSION TAG	UNP B0S4P3
B	0	HIS	-	EXPRESSION TAG	UNP B0S4P3
C	-19	MET	-	EXPRESSION TAG	UNP B0S4P3
C	-18	GLY	-	EXPRESSION TAG	UNP B0S4P3
C	-17	SER	-	EXPRESSION TAG	UNP B0S4P3
C	-16	SER	-	EXPRESSION TAG	UNP B0S4P3
C	-15	HIS	-	EXPRESSION TAG	UNP B0S4P3
C	-14	HIS	-	EXPRESSION TAG	UNP B0S4P3
C	-13	HIS	-	EXPRESSION TAG	UNP B0S4P3
C	-12	HIS	-	EXPRESSION TAG	UNP B0S4P3
C	-11	HIS	-	EXPRESSION TAG	UNP B0S4P3
C	-10	HIS	-	EXPRESSION TAG	UNP B0S4P3
C	-9	SER	-	EXPRESSION TAG	UNP B0S4P3
C	-8	SER	-	EXPRESSION TAG	UNP B0S4P3
C	-7	GLY	-	EXPRESSION TAG	UNP B0S4P3
C	-6	LEU	-	EXPRESSION TAG	UNP B0S4P3
C	-5	VAL	-	EXPRESSION TAG	UNP B0S4P3
C	-4	PRO	-	EXPRESSION TAG	UNP B0S4P3
C	-3	ARG	-	EXPRESSION TAG	UNP B0S4P3
C	-2	GLY	-	EXPRESSION TAG	UNP B0S4P3
C	-1	SER	-	EXPRESSION TAG	UNP B0S4P3
C	0	HIS	-	EXPRESSION TAG	UNP B0S4P3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	125	Total O 125 125	0	0

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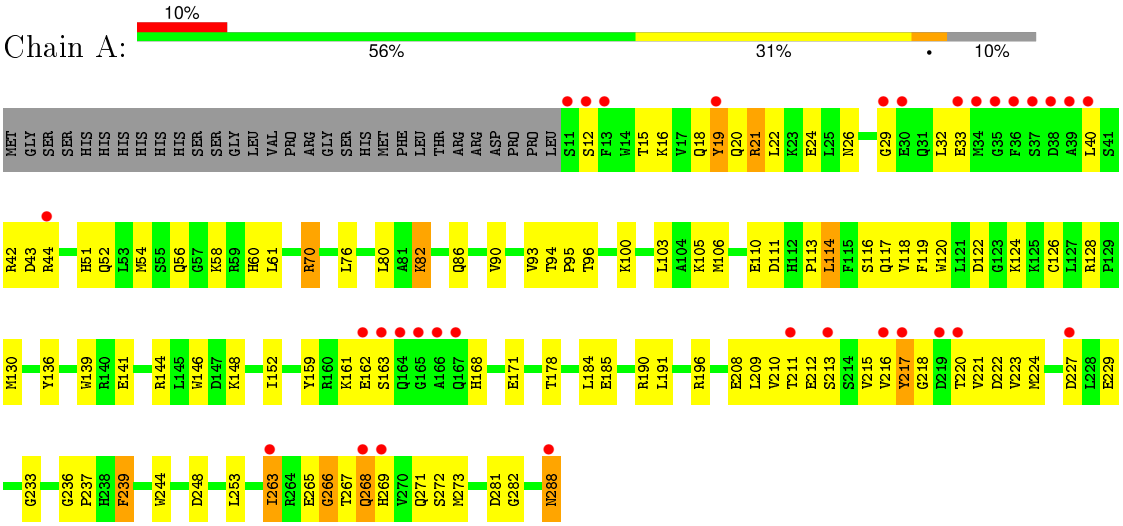
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	123	Total O 123 123	0	0
2	C	168	Total O 168 168	0	0

3 Residue-property plots (i)

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

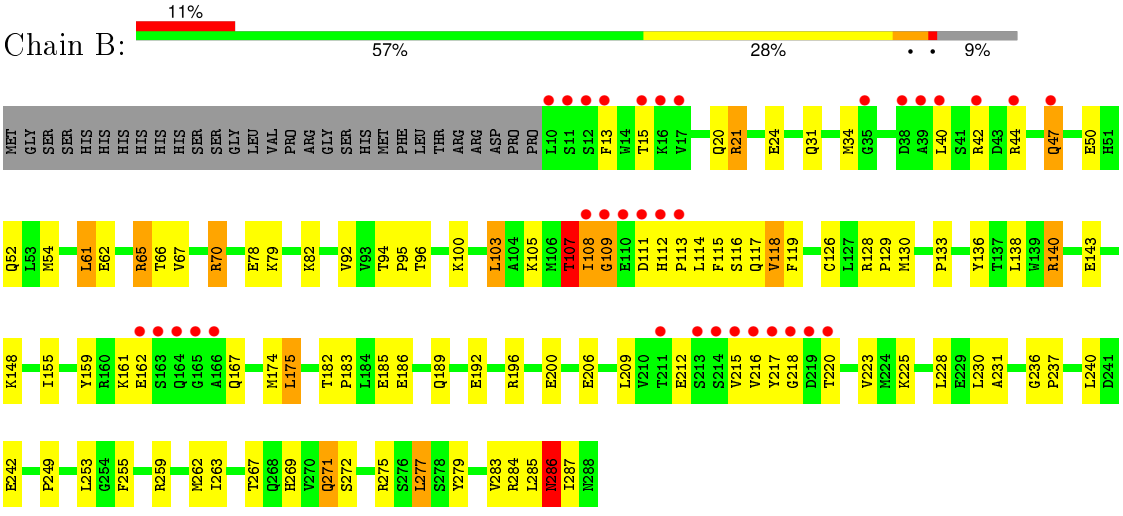
- Molecule 1: Putative uncharacterized protein

Chain A:



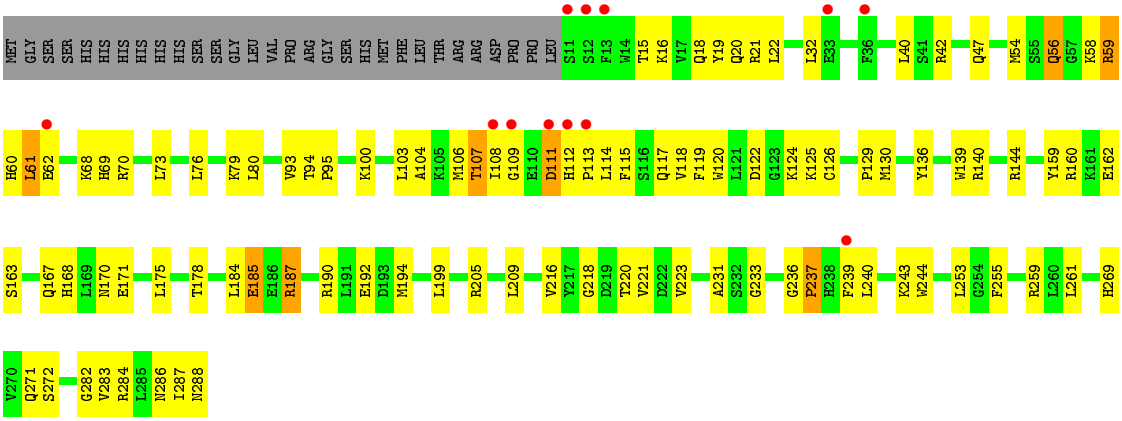
- Molecule 1: Putative uncharacterized protein

Chain B:



- Molecule 1: Putative uncharacterized protein

Chain C:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET PHE LEU THR ARG ARG ASP PRO PRO LEU S11 S12 F13 W14 T15 K16 V17 Q18 Y19 Q20 R21 L22 L32 E33 F36 L40 S41 R42 Q47 M54 S55 Q56 G57 K58 R59
H60 L61 E62 K68 H69 R70 L73 L76 K79 L80 V93 T94 P95 K100 L103 A104 K105 M106 T107 I108 G109 E110 D111 H112 P113 L114 F115 S116 Q117 V118 F119 W120 L121 D122 G123 K124 K125 C126 P129 M130 Y136 W139 R140 R144 Y159 R160 K161 E162
S163 Q167 H168 L169 N170 E171 L175 T178 L184 E185 E186 R187 R190 L191 E192 D193 M194 L199 R205 L209 V216 Y217 G218 D219 T220 V221 D222 V223 A231 S232 G233 G236 P237 H238 F239 L240 K243 W244 L253 G254 F255 R259 L260 L261 H269
V270 Q271 S272 G282 V283 R284 L285 N286 I287 N288

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	124.92Å 128.56Å 124.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.67 – 2.50 44.67 – 2.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.67-2.50) 99.5 (44.67-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.08Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.214 , 0.275 0.214 , 0.275	Depositor DCC
R_{free} test set	1768 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.2	EDS
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 59243 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7189	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.37	0/2303	0.61	0/3105
1	B	0.36	0/2311	0.62	1/3116 (0.0%)
1	C	0.38	0/2303	0.63	0/3105
All	All	0.37	0/6917	0.62	1/9326 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	109	GLY	N-CA-C	-5.31	99.83	113.10

There are no chirality outliers.

There are no planarity outliers.

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	2255	0	2249	97	0
1	B	2263	0	2260	126	0
1	C	2255	0	2249	105	0
2	A	125	0	0	13	0
2	B	123	0	0	7	0
2	C	168	0	0	13	0
All	All	7189	0	6758	324	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 24.

All (324) 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:C:104:ALA:HA	1:C:108:ILE:HB	1.32	1.10
1:B:108:ILE:HG12	1:B:109:GLY:H	1.00	1.06
1:C:107:THR:HG23	1:C:240:LEU:HD21	1.33	1.06
1:C:108:ILE:HG12	1:C:112:HIS:HB3	1.44	1.00
1:C:108:ILE:HD11	1:C:114:LEU:HB3	1.46	0.97
1:B:140:ARG:HH11	1:B:140:ARG:HB3	1.29	0.96
1:B:108:ILE:HG12	1:B:109:GLY:N	1.81	0.93
1:A:216:VAL:HG13	1:A:217:TYR:H	1.34	0.92
1:B:103:LEU:HD11	1:B:114:LEU:HD22	1.49	0.92
1:B:108:ILE:CG1	1:B:109:GLY:H	1.85	0.89
1:B:15:THR:HG23	1:B:42:ARG:HH12	1.39	0.86
1:B:228:LEU:HD13	1:B:263:ILE:HD12	1.58	0.84
1:C:112:HIS:ND1	1:C:113:PRO:HD2	1.93	0.84
1:A:52:GLN:HE21	1:A:56:GLN:HE21	1.26	0.83
1:B:54:MET:HE2	1:B:287:ILE:HA	1.60	0.82
1:C:21:ARG:HH21	1:C:54:MET:HE3	1.44	0.81
1:C:58:LYS:HE3	1:C:288:ASN:HB2	1.62	0.81
1:B:113:PRO:O	1:B:117:GLN:HG3	1.82	0.79
1:C:107:THR:CG2	1:C:240:LEU:HD21	2.12	0.78
1:C:100:LYS:HD3	2:C:433:HOH:O	1.83	0.77
1:B:15:THR:HG23	1:B:42:ARG:NH1	1.99	0.77
1:B:112:HIS:ND1	1:B:113:PRO:HD2	1.99	0.76
1:A:58:LYS:HD2	1:A:288:ASN:HB2	1.66	0.76
1:A:233:GLY:HA3	1:A:253:LEU:HD12	1.67	0.75
1:B:108:ILE:CD1	1:B:114:LEU:HB3	2.17	0.75
1:C:112:HIS:HD2	1:C:114:LEU:HB2	1.51	0.75
1:C:118:VAL:CG1	1:C:126:CYS:HB2	2.17	0.74
1:A:269:HIS:ND1	1:A:271:GLN:HG2	2.01	0.74
1:C:112:HIS:HE1	1:C:216:VAL:HG22	1.52	0.73
1:B:209:LEU:CD2	1:B:223:VAL:HG22	2.19	0.73
1:C:108:ILE:HG21	1:C:115:PHE:CE2	2.25	0.72
1:A:162:GLU:HA	2:A:410:HOH:O	1.88	0.71
1:C:112:HIS:CE1	1:C:216:VAL:HG22	2.25	0.71
1:C:61:LEU:CD2	1:C:283:VAL:HG11	2.22	0.70
1:B:108:ILE:HD12	1:B:114:LEU:HB3	1.72	0.70
1:B:269:HIS:HB3	1:B:271:GLN:HE21	1.57	0.69
1:C:112:HIS:CG	1:C:113:PRO:HD2	2.28	0.69
1:B:40:LEU:HB2	2:B:429:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HG11	1:A:126:CYS:SG	2.33	0.68
1:B:112:HIS:HD2	1:B:114:LEU:HB2	1.59	0.67
1:C:104:ALA:HA	1:C:108:ILE:CB	2.18	0.67
1:B:284:ARG:NH1	1:B:286:ASN:HB2	2.09	0.67
1:C:56:GLN:HA	1:C:59:ARG:HD2	1.75	0.67
1:A:26:ASN:OD1	1:A:267:THR:HG23	1.95	0.66
1:A:263:ILE:O	1:A:263:ILE:HG22	1.96	0.65
1:C:117:GLN:HE21	1:C:160:ARG:HH12	1.42	0.65
1:C:54:MET:HE2	1:C:287:ILE:HA	1.78	0.65
1:C:112:HIS:HB2	2:C:401:HOH:O	1.97	0.65
1:B:108:ILE:HG13	1:B:112:HIS:HB3	1.76	0.65
1:B:259:ARG:O	1:B:263:ILE:HG12	1.96	0.65
1:C:113:PRO:O	1:C:117:GLN:HG2	1.98	0.64
1:B:114:LEU:HA	1:B:117:GLN:OE1	1.97	0.64
1:A:213:SER:HA	1:A:218:GLY:O	1.98	0.64
1:C:184:LEU:HA	1:C:187:ARG:HD3	1.80	0.64
1:B:103:LEU:HD12	1:B:115:PHE:CE1	2.32	0.64
1:B:112:HIS:CD2	1:B:114:LEU:HB2	2.32	0.64
1:B:117:GLN:HG2	1:B:162:GLU:OE1	1.98	0.64
1:A:52:GLN:HE21	1:A:56:GLN:NE2	1.96	0.64
1:C:54:MET:CE	1:C:287:ILE:HA	2.28	0.63
1:C:61:LEU:HD21	1:C:283:VAL:HG11	1.80	0.63
1:A:163:SER:HB2	1:A:168:HIS:HB3	1.79	0.63
1:B:107:THR:HG22	1:B:107:THR:O	1.99	0.62
1:C:218:GLY:HA3	1:C:239:PHE:HE2	1.64	0.62
1:A:119:PHE:CZ	1:A:161:LYS:HA	2.34	0.62
1:A:95:PRO:HD2	1:B:277:LEU:HD13	1.80	0.62
1:A:224:MET:HG2	1:A:229:GLU:HA	1.81	0.62
1:A:148:LYS:HE2	1:A:248:ASP:CG	2.20	0.62
1:A:19:TYR:CE1	1:A:32:LEU:HD11	2.35	0.61
1:B:54:MET:HE2	1:B:287:ILE:CA	2.31	0.61
1:B:262:MET:HG3	1:B:267:THR:HG23	1.83	0.60
1:B:140:ARG:HH11	1:B:140:ARG:CB	2.07	0.60
1:A:148:LYS:HE2	1:A:248:ASP:OD2	2.01	0.60
1:A:273:MET:HB2	2:A:320:HOH:O	2.01	0.60
1:C:93:VAL:HG13	1:C:93:VAL:O	2.02	0.60
1:C:205:ARG:HG2	2:C:345:HOH:O	2.02	0.60
1:A:32:LEU:HD23	1:A:32:LEU:O	2.02	0.59
1:B:47:GLN:C	1:B:47:GLN:HE21	2.05	0.59
1:A:141:GLU:HG2	2:A:325:HOH:O	2.03	0.59
1:C:118:VAL:HG11	1:C:126:CYS:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:SER:HA	1:A:168:HIS:HD2	1.67	0.58
1:C:175:LEU:C	1:C:175:LEU:HD23	2.23	0.58
1:A:191:LEU:HD13	1:A:221:VAL:HG21	1.85	0.58
1:C:21:ARG:NH2	1:C:54:MET:HE3	2.16	0.58
1:A:21:ARG:HH21	1:A:54:MET:CE	2.17	0.58
1:B:21:ARG:HH21	1:B:54:MET:HE1	1.68	0.57
1:B:108:ILE:HD11	1:B:112:HIS:O	2.04	0.57
1:A:216:VAL:HG13	1:A:217:TYR:N	2.14	0.57
1:A:114:LEU:HD21	1:A:130:MET:CE	2.32	0.57
1:B:225:LYS:HB2	1:B:230:LEU:HD11	1.86	0.57
1:C:20:GLN:HG2	2:C:337:HOH:O	2.04	0.57
1:B:107:THR:O	1:B:108:ILE:HB	2.05	0.57
1:C:112:HIS:NE2	1:C:216:VAL:HG13	2.19	0.56
1:C:117:GLN:HB3	1:C:160:ARG:NH1	2.20	0.56
1:B:40:LEU:C	1:B:40:LEU:HD13	2.25	0.56
1:B:62:GLU:CD	1:B:65:ARG:HH12	2.09	0.56
1:B:231:ALA:HB2	1:B:255:PHE:CD2	2.40	0.56
1:A:163:SER:HA	1:A:168:HIS:CD2	2.41	0.56
1:C:112:HIS:CE1	1:C:113:PRO:HD2	2.41	0.56
1:B:167:GLN:HE21	1:B:259:ARG:NH2	2.04	0.56
1:B:212:GLU:CG	1:B:220:THR:HB	2.36	0.55
1:C:59:ARG:O	1:C:62:GLU:HG2	2.06	0.55
1:A:139:TRP:HZ2	1:A:178:THR:HB	1.71	0.55
1:A:191:LEU:HD22	1:A:253:LEU:HD13	1.89	0.55
1:C:184:LEU:HA	1:C:187:ARG:CD	2.36	0.55
1:B:62:GLU:CD	1:B:65:ARG:NH1	2.60	0.55
1:A:265:GLU:O	1:A:266:GLY:O	2.25	0.55
1:A:236:GLY:HA2	1:A:237:PRO:C	2.27	0.55
1:B:31:GLN:HA	1:B:34:MET:CE	2.37	0.55
1:C:106:MET:O	1:C:107:THR:OG1	2.22	0.54
1:A:216:VAL:O	1:A:239:PHE:CE2	2.60	0.54
1:C:117:GLN:NE2	1:C:160:ARG:HH12	2.04	0.54
1:B:183:PRO:HG2	1:B:186:GLU:HB2	1.88	0.54
1:A:15:THR:HG22	1:A:18:GLN:CG	2.38	0.54
1:B:108:ILE:HG13	1:B:112:HIS:H	1.73	0.54
1:B:277:LEU:HD22	2:B:473:HOH:O	2.07	0.54
1:C:19:TYR:CE1	1:C:32:LEU:HD22	2.43	0.54
1:B:21:ARG:HH21	1:B:54:MET:CE	2.20	0.54
1:C:140:ARG:HB2	2:C:392:HOH:O	2.07	0.54
1:A:58:LYS:HD2	1:A:288:ASN:CB	2.38	0.54
1:A:106:MET:HE1	1:A:244:TRP:NE1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ALA:HB2	1:C:255:PHE:CD2	2.43	0.54
1:C:236:GLY:HA2	1:C:237:PRO:C	2.28	0.54
1:B:96:THR:HA	1:B:128:ARG:HD3	1.90	0.53
1:C:220:THR:HG23	1:C:233:GLY:O	2.09	0.53
1:B:108:ILE:HD13	1:B:115:PHE:HD1	1.73	0.53
1:C:108:ILE:HD11	1:C:114:LEU:CB	2.30	0.53
1:B:108:ILE:CG1	1:B:112:HIS:HB3	2.38	0.53
1:C:190:ARG:O	1:C:194:MET:HG3	2.08	0.53
1:C:122:ASP:OD1	1:C:125:LYS:HE2	2.08	0.53
1:B:108:ILE:HD12	1:B:114:LEU:CB	2.37	0.53
1:A:21:ARG:HH21	1:A:54:MET:HE2	1.74	0.53
1:B:20:GLN:NE2	1:B:20:GLN:HA	2.24	0.53
1:C:58:LYS:HE3	1:C:288:ASN:CB	2.37	0.52
1:A:19:TYR:HD1	1:A:32:LEU:HD21	1.74	0.52
1:C:120:TRP:CE3	1:C:126:CYS:HB3	2.45	0.52
1:B:107:THR:HB	1:B:240:LEU:HD21	1.90	0.52
1:A:267:THR:HG22	1:A:268:GLN:N	2.25	0.52
1:B:217:TYR:HD1	1:B:217:TYR:O	1.93	0.52
1:A:42:ARG:HG2	2:A:315:HOH:O	2.10	0.52
1:B:47:GLN:C	1:B:47:GLN:NE2	2.62	0.52
1:A:19:TYR:CD1	1:A:32:LEU:HD21	2.45	0.51
1:A:114:LEU:HD21	1:A:130:MET:HE3	1.91	0.51
1:B:212:GLU:HG2	1:B:220:THR:O	2.10	0.51
1:C:269:HIS:HB3	1:C:271:GLN:HG2	1.91	0.51
1:C:118:VAL:HG11	1:C:126:CYS:CB	2.41	0.51
1:B:262:MET:HG3	1:B:267:THR:CG2	2.40	0.51
1:C:108:ILE:O	1:C:108:ILE:CG2	2.59	0.51
1:B:31:GLN:O	1:B:34:MET:HG2	2.11	0.51
1:C:21:ARG:NH2	1:C:54:MET:CE	2.74	0.51
1:B:206:GLU:HG3	1:B:225:LYS:HD2	1.93	0.51
1:B:13:PHE:O	1:B:42:ARG:HD2	2.11	0.51
1:A:20:GLN:O	1:A:24:GLU:HG3	2.11	0.51
1:A:263:ILE:O	1:A:263:ILE:CG2	2.59	0.51
1:C:94:THR:HB	1:C:95:PRO:CD	2.41	0.51
1:C:220:THR:HG22	1:C:221:VAL:N	2.26	0.50
1:A:29:GLY:O	1:A:33:GLU:HG3	2.11	0.50
1:A:70:ARG:HD3	2:A:358:HOH:O	2.12	0.50
1:C:61:LEU:HD22	1:C:283:VAL:HG21	1.94	0.50
1:A:40:LEU:O	1:A:44:ARG:HG3	2.12	0.50
1:A:265:GLU:O	1:A:266:GLY:C	2.49	0.50
1:C:163:SER:OG	1:C:168:HIS:HD2	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:THR:H	1:C:18:GLN:HE21	1.60	0.49
1:B:119:PHE:CZ	1:B:161:LYS:HB3	2.47	0.49
1:C:108:ILE:HD13	1:C:115:PHE:CD2	2.48	0.49
1:B:65:ARG:NH1	1:B:66:THR:HG23	2.27	0.49
1:A:94:THR:HB	1:A:95:PRO:CD	2.42	0.49
1:C:259:ARG:HG2	2:C:353:HOH:O	2.12	0.49
1:B:212:GLU:HG3	1:B:212:GLU:O	2.12	0.49
1:C:160:ARG:NH1	1:C:162:GLU:O	2.46	0.49
1:C:59:ARG:HD3	1:C:60:HIS:N	2.27	0.49
1:A:95:PRO:CD	1:B:277:LEU:HD13	2.42	0.49
1:B:143:GLU:HG2	1:B:148:LYS:HE3	1.94	0.49
1:B:108:ILE:HD13	1:B:115:PHE:CD1	2.48	0.49
1:B:206:GLU:O	1:B:225:LYS:HD3	2.13	0.49
1:B:70:ARG:HH22	1:B:78:GLU:CD	2.16	0.49
1:B:114:LEU:HD23	1:B:114:LEU:O	2.13	0.49
1:A:215:VAL:HG13	1:A:216:VAL:N	2.26	0.49
1:B:228:LEU:CD1	1:B:263:ILE:HD12	2.38	0.49
1:B:284:ARG:CZ	1:B:286:ASN:HB2	2.43	0.48
1:B:20:GLN:HE21	1:B:20:GLN:HA	1.77	0.48
1:B:40:LEU:HD11	1:B:44:ARG:HE	1.78	0.48
1:B:262:MET:HA	1:B:267:THR:HG22	1.93	0.48
1:C:112:HIS:CE1	1:C:216:VAL:HG13	2.48	0.48
1:B:31:GLN:HA	1:B:34:MET:HE2	1.94	0.48
1:B:40:LEU:HD11	2:B:404:HOH:O	2.12	0.48
1:C:54:MET:CE	1:C:288:ASN:H	2.26	0.48
1:B:189:GLN:O	1:B:192:GLU:HB2	2.13	0.48
1:C:61:LEU:HD21	1:C:283:VAL:CG1	2.43	0.48
1:A:15:THR:HG22	1:A:18:GLN:CD	2.34	0.48
1:C:68:LYS:O	1:C:69:HIS:HB2	2.14	0.48
1:C:21:ARG:HH21	1:C:54:MET:CE	2.19	0.48
1:B:206:GLU:HG3	1:B:225:LYS:CD	2.44	0.48
1:B:79:LYS:HD2	2:B:416:HOH:O	2.14	0.48
1:A:15:THR:HG22	1:A:18:GLN:HB2	1.94	0.48
1:A:82:LYS:HE2	2:A:313:HOH:O	2.14	0.48
1:B:70:ARG:HG2	1:B:70:ARG:O	2.14	0.47
1:A:116:SER:O	1:A:161:LYS:HE2	2.15	0.47
1:A:106:MET:CE	1:A:244:TRP:NE1	2.78	0.47
1:B:236:GLY:HA2	1:B:237:PRO:C	2.34	0.47
1:C:108:ILE:HA	1:C:112:HIS:HB2	1.97	0.47
1:B:105:LYS:C	1:B:107:THR:H	2.19	0.47
1:B:107:THR:CG2	1:B:107:THR:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:VAL:HG11	1:C:126:CYS:SG	2.54	0.47
1:A:216:VAL:O	1:A:239:PHE:HE2	1.98	0.47
1:B:167:GLN:NE2	1:B:259:ARG:NH2	2.63	0.47
1:A:15:THR:HG22	1:A:18:GLN:NE2	2.30	0.47
1:B:215:VAL:HG22	1:B:215:VAL:O	2.15	0.47
1:B:65:ARG:HB3	1:B:65:ARG:HH11	1.79	0.46
1:C:168:HIS:HE1	1:C:170:ASN:OD1	1.97	0.46
1:A:106:MET:HE1	1:A:244:TRP:HE1	1.80	0.46
1:A:51:HIS:HD2	2:A:335:HOH:O	1.97	0.46
1:A:269:HIS:CG	1:A:271:GLN:HG2	2.50	0.46
1:A:209:LEU:HD12	1:A:223:VAL:HG22	1.97	0.46
1:A:217:TYR:HB3	1:A:220:THR:OG1	2.15	0.46
1:A:272:SER:O	1:A:282:GLY:HA2	2.15	0.46
1:B:50:GLU:O	1:B:54:MET:HG3	2.16	0.46
1:B:209:LEU:HD23	1:B:223:VAL:HG22	1.96	0.46
1:B:108:ILE:HG23	1:B:115:PHE:CE1	2.51	0.46
1:B:228:LEU:HD13	1:B:263:ILE:CD1	2.38	0.46
1:A:229:GLU:O	1:A:229:GLU:HG3	2.14	0.46
1:A:33:GLU:HG2	2:A:374:HOH:O	2.16	0.46
1:C:54:MET:HE1	1:C:288:ASN:N	2.31	0.46
1:B:20:GLN:O	1:B:24:GLU:HG3	2.16	0.46
1:A:118:VAL:CG1	1:A:126:CYS:HB2	2.46	0.46
1:A:267:THR:CG2	1:A:268:GLN:N	2.79	0.45
1:A:146:TRP:CZ2	1:B:65:ARG:HB2	2.51	0.45
1:A:122:ASP:HB3	1:A:124:LYS:H	1.82	0.45
1:B:108:ILE:HG13	1:B:112:HIS:CB	2.46	0.45
1:B:167:GLN:HE21	1:B:259:ARG:HH21	1.63	0.45
1:A:114:LEU:HD21	1:A:130:MET:HE1	1.99	0.45
1:B:40:LEU:C	1:B:42:ARG:N	2.66	0.45
1:A:106:MET:CE	1:A:244:TRP:HE1	2.29	0.45
1:B:275:ARG:HG3	2:B:433:HOH:O	2.16	0.45
1:C:122:ASP:OD2	1:C:124:LYS:N	2.47	0.45
1:B:216:VAL:HG13	1:B:217:TYR:CD2	2.51	0.45
1:B:94:THR:HB	1:B:95:PRO:HD2	1.97	0.45
1:A:163:SER:CB	1:A:168:HIS:HB3	2.45	0.45
1:A:111:ASP:O	1:A:113:PRO:HD3	2.17	0.45
1:C:167:GLN:HE22	1:C:269:HIS:HA	1.81	0.45
1:B:116:SER:HA	2:B:434:HOH:O	2.16	0.45
1:C:159:TYR:CE2	1:C:171:GLU:HG2	2.52	0.45
1:C:218:GLY:HA3	1:C:239:PHE:CE2	2.50	0.45
1:C:107:THR:HG21	1:C:239:PHE:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:MET:HE1	1:C:244:TRP:NE1	2.32	0.45
1:A:93:VAL:HG13	1:A:93:VAL:O	2.17	0.45
1:C:76:LEU:O	1:C:80:LEU:HG	2.17	0.44
1:B:182:THR:O	1:B:249:PRO:HB2	2.18	0.44
1:A:12:SER:HA	2:A:339:HOH:O	2.17	0.44
1:C:108:ILE:HA	2:C:401:HOH:O	2.17	0.44
1:C:272:SER:OG	1:C:282:GLY:HA2	2.17	0.44
1:A:96:THR:HA	1:A:128:ARG:HD3	1.99	0.44
1:C:40:LEU:HD12	1:C:40:LEU:N	2.33	0.44
1:C:108:ILE:HG23	2:C:442:HOH:O	2.17	0.44
1:C:185:GLU:CD	1:C:185:GLU:H	2.07	0.44
1:A:43:ASP:HA	2:A:315:HOH:O	2.17	0.44
1:C:129:PRO:HG2	1:C:130:MET:HE1	2.00	0.44
1:C:122:ASP:HA	2:C:360:HOH:O	2.17	0.44
1:A:190:ARG:HH11	1:A:190:ARG:HA	1.83	0.44
1:A:120:TRP:CE3	1:A:126:CYS:HB3	2.52	0.44
1:C:40:LEU:C	1:C:42:ARG:N	2.71	0.43
1:C:113:PRO:HD3	2:C:396:HOH:O	2.17	0.43
1:A:40:LEU:HG	1:A:44:ARG:CZ	2.48	0.43
1:A:196:ARG:HD3	2:A:388:HOH:O	2.18	0.43
1:B:108:ILE:CD1	1:B:112:HIS:HB3	2.49	0.43
1:C:185:GLU:N	1:C:185:GLU:OE1	2.28	0.43
1:C:73:LEU:HA	1:C:261:LEU:HD11	2.00	0.43
1:C:243:LYS:HB2	2:C:438:HOH:O	2.17	0.43
1:B:40:LEU:O	1:B:42:ARG:N	2.51	0.43
1:A:144:ARG:NH2	1:B:287:ILE:O	2.51	0.43
1:B:155:ILE:HG12	1:B:175:LEU:HD13	2.00	0.43
1:B:100:LYS:HE2	1:B:115:PHE:HE2	1.83	0.43
1:C:139:TRP:HZ2	1:C:178:THR:HB	1.84	0.43
1:C:192:GLU:OE2	1:C:209:LEU:HD13	2.18	0.43
1:A:216:VAL:O	1:A:218:GLY:N	2.52	0.43
1:A:159:TYR:CE2	1:A:171:GLU:HG2	2.54	0.43
1:B:62:GLU:OE1	1:B:65:ARG:NH1	2.52	0.42
1:A:208:GLU:HG2	1:A:209:LEU:N	2.34	0.42
1:B:155:ILE:HA	1:B:174:MET:O	2.18	0.42
1:B:118:VAL:HG13	1:B:126:CYS:HB2	2.01	0.42
1:B:103:LEU:HD12	1:B:115:PHE:HE1	1.81	0.42
1:A:161:LYS:HE3	2:A:385:HOH:O	2.18	0.42
1:C:199:LEU:HD11	1:C:223:VAL:HG11	2.01	0.42
1:B:209:LEU:HD21	1:B:223:VAL:HG22	1.98	0.42
1:B:206:GLU:HG3	1:B:206:GLU:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:HD21	1:B:129:PRO:HG3	2.00	0.42
1:C:271:GLN:NE2	2:C:463:HOH:O	2.52	0.42
1:B:272:SER:HA	1:B:279:TYR:CG	2.55	0.42
1:C:54:MET:HE1	1:C:287:ILE:HA	2.02	0.42
1:C:129:PRO:HG2	1:C:130:MET:CE	2.50	0.42
1:A:60:HIS:HE1	1:A:281:ASP:OD2	2.02	0.42
1:B:54:MET:CE	1:B:287:ILE:HG22	2.49	0.42
1:A:19:TYR:HE1	1:A:32:LEU:HD11	1.82	0.42
1:B:217:TYR:CD1	1:B:217:TYR:O	2.71	0.42
1:B:117:GLN:NE2	1:B:162:GLU:OE2	2.53	0.42
1:B:231:ALA:HB2	1:B:255:PHE:CE2	2.54	0.42
1:B:20:GLN:HE21	1:B:20:GLN:CA	2.29	0.41
1:A:90:VAL:O	1:A:152:ILE:HA	2.20	0.41
1:C:79:LYS:HE3	2:C:467:HOH:O	2.20	0.41
1:C:106:MET:HE1	1:C:244:TRP:HE1	1.85	0.41
1:C:284:ARG:HG3	1:C:286:ASN:OD1	2.19	0.41
1:A:191:LEU:HA	1:A:191:LEU:HD23	1.94	0.41
1:C:220:THR:CG2	1:C:221:VAL:N	2.83	0.41
1:B:159:TYR:N	1:B:159:TYR:CD1	2.88	0.41
1:C:106:MET:CE	1:C:244:TRP:HE1	2.33	0.41
1:B:196:ARG:O	1:B:200:GLU:HB2	2.21	0.41
1:B:133:PRO:HG2	2:B:511:HOH:O	2.20	0.41
1:A:105:LYS:HB2	1:A:244:TRP:CZ2	2.56	0.41
1:B:108:ILE:HD11	1:B:115:PHE:H	1.86	0.41
1:A:70:ARG:HG2	1:A:70:ARG:O	2.19	0.41
1:A:44:ARG:HG2	1:A:44:ARG:HH11	1.86	0.41
1:A:184:LEU:HG	2:A:318:HOH:O	2.20	0.41
1:A:110:GLU:OE1	1:A:110:GLU:HA	2.21	0.41
1:A:76:LEU:O	1:A:80:LEU:HG	2.21	0.41
1:B:61:LEU:HD13	1:B:283:VAL:HG21	2.03	0.41
1:B:253:LEU:HD12	1:B:253:LEU:HA	1.92	0.41
1:C:109:GLY:C	1:C:111:ASP:H	2.24	0.41
1:B:54:MET:HE3	1:B:287:ILE:HG22	2.02	0.41
1:C:118:VAL:CG1	1:C:119:PHE:N	2.84	0.41
1:C:16:LYS:HE2	1:C:20:GLN:OE1	2.21	0.41
1:B:206:GLU:CG	1:B:225:LYS:HE2	2.51	0.40
1:C:19:TYR:CD1	1:C:32:LEU:HD22	2.55	0.40
1:B:103:LEU:HD12	1:B:115:PHE:CD1	2.56	0.40
1:B:92:VAL:HG21	1:B:138:LEU:HD12	2.03	0.40
1:A:211:THR:HG22	1:A:212:GLU:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	276/308 (90%)	249 (90%)	21 (8%)	6 (2%)	8 13
1	B	277/308 (90%)	253 (91%)	19 (7%)	5 (2%)	11 18
1	C	276/308 (90%)	264 (96%)	9 (3%)	3 (1%)	17 31
All	All	829/924 (90%)	766 (92%)	49 (6%)	14 (2%)	11 19

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	GLY
1	B	108	ILE
1	B	107	THR
1	B	218	GLY
1	B	286	ASN
1	C	111	ASP
1	A	217	TYR
1	A	268	GLN
1	A	210	VAL
1	A	16	LYS
1	B	111	ASP
1	C	107	THR
1	A	263	ILE
1	C	237	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/269 (90%)	225 (93%)	17 (7%)	19	34
1	B	243/269 (90%)	222 (91%)	21 (9%)	13	24
1	C	242/269 (90%)	230 (95%)	12 (5%)	30	53
All	All	727/807 (90%)	677 (93%)	50 (7%)	19	35

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	TYR
1	A	21	ARG
1	A	22	LEU
1	A	61	LEU
1	A	70	ARG
1	A	82	LYS
1	A	86	GLN
1	A	100	LYS
1	A	103	LEU
1	A	114	LEU
1	A	117	GLN
1	A	136	TYR
1	A	185	GLU
1	A	222	ASP
1	A	227	ASP
1	A	239	PHE
1	A	288	ASN
1	B	21	ARG
1	B	47	GLN
1	B	52	GLN
1	B	61	LEU
1	B	65	ARG
1	B	67	VAL
1	B	70	ARG
1	B	82	LYS
1	B	103	LEU
1	B	107	THR
1	B	118	VAL
1	B	130	MET
1	B	136	TYR
1	B	140	ARG
1	B	175	LEU
1	B	185	GLU
1	B	242	GLU

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Mol	Chain	Res	Type
1	B	271	GLN
1	B	277	LEU
1	B	285	LEU
1	B	286	ASN
1	C	22	LEU
1	C	47	GLN
1	C	56	GLN
1	C	59	ARG
1	C	61	LEU
1	C	70	ARG
1	C	103	LEU
1	C	136	TYR
1	C	144	ARG
1	C	185	GLU
1	C	187	ARG
1	C	253	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	56	GLN
1	A	60	HIS
1	A	63	GLN
1	A	117	GLN
1	A	164	GLN
1	A	189	GLN
1	A	271	GLN
1	A	288	ASN
1	B	18	GLN
1	B	20	GLN
1	B	26	ASN
1	B	47	GLN
1	B	167	GLN
1	B	238	HIS
1	B	271	GLN
1	B	286	ASN
1	B	288	ASN
1	C	18	GLN
1	C	26	ASN
1	C	47	GLN
1	C	52	GLN

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Mol	Chain	Res	Type
1	C	56	GLN
1	C	112	HIS
1	C	117	GLN
1	C	167	GLN
1	C	168	HIS
1	C	271	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	278/308 (90%)	0.27	32 (11%)	6	6	17, 37, 77, 86	0
1	B	279/308 (90%)	0.38	34 (12%)	5	5	14, 36, 78, 88	0
1	C	278/308 (90%)	-0.13	12 (4%)	39	44	11, 34, 66, 78	0
All	All	835/924 (90%)	0.17	78 (9%)	11	11	11, 36, 76, 88	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	VAL	18.8
1	B	215	VAL	17.9
1	B	218	GLY	11.7
1	B	165	GLY	11.5
1	C	109	GLY	9.6
1	B	217	TYR	8.4
1	A	164	GLN	7.1
1	A	13	PHE	6.6
1	A	11	SER	6.5
1	B	214	SER	6.4
1	B	219	ASP	6.3
1	B	163	SER	6.0
1	B	166	ALA	6.0
1	B	113	PRO	6.0
1	B	164	GLN	5.7
1	B	108	ILE	5.5
1	B	110	GLU	5.5
1	A	30	GLU	5.4
1	A	166	ALA	5.4
1	A	163	SER	5.4
1	C	111	ASP	5.4
1	B	213	SER	5.3
1	A	213	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	39	ALA	5.3
1	A	216	VAL	4.8
1	A	165	GLY	4.6
1	C	113	PRO	4.5
1	C	108	ILE	4.4
1	B	162	GLU	4.3
1	B	40	LEU	4.3
1	A	36	PHE	4.2
1	C	36	PHE	4.2
1	A	19	TYR	4.0
1	A	34	MET	4.0
1	B	109	GLY	4.0
1	A	38	ASP	3.9
1	B	112	HIS	3.9
1	A	219	ASP	3.8
1	A	39	ALA	3.8
1	B	16	LYS	3.8
1	A	40	LEU	3.7
1	A	37	SER	3.7
1	B	10	LEU	3.7
1	A	217	TYR	3.6
1	A	35	GLY	3.5
1	A	44	ARG	3.5
1	A	268	GLN	3.5
1	C	112	HIS	3.5
1	B	47	GLN	3.4
1	B	220	THR	3.4
1	A	211	THR	3.4
1	A	162	GLU	3.3
1	A	12	SER	3.2
1	B	111	ASP	3.1
1	B	11	SER	3.0
1	A	33	GLU	3.0
1	B	44	ARG	2.9
1	A	167	GLN	2.9
1	A	227	ASP	2.8
1	A	220	THR	2.7
1	B	38	ASP	2.7
1	C	33	GLU	2.7
1	A	288	ASN	2.5
1	A	269	HIS	2.4
1	B	13	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	12	SER	2.4
1	A	263	ILE	2.3
1	C	11	SER	2.3
1	A	29	GLY	2.3
1	C	239	PHE	2.3
1	B	15	THR	2.3
1	B	35	GLY	2.3
1	B	42	ARG	2.3
1	C	13	PHE	2.3
1	B	17	VAL	2.3
1	B	211	THR	2.2
1	C	12	SER	2.1
1	C	62	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.