



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:38 AM GMT

PDB ID : 2RHB
Title : Crystal structure of Nsp15-H234A mutant- Hexamer in asymmetric unit
Authors : Palaninathan, S.; Bhardwaj, K.; Alcantara, J.M.O.; Guarino, L.; Yi, L.L.;
Kao, C.C.; Sacchettini, J.
Deposited on : 2007-10-08
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

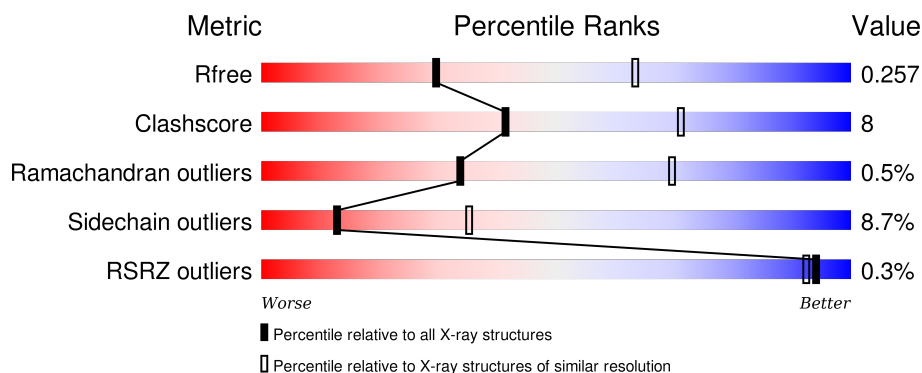
1 Overall quality at a glance

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	353	 76% 17% . .
1	B	353	 79% 16% . .
1	C	353	 78% 16% . .
1	D	353	 78% 18% . .
1	E	353	 77% 18% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	353	<div><div><div>%</div><div><div></div></div></div><div><div></div><div>75%</div><div>20%</div><div><div></div><div></div></div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16512 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 Uridylate-specific endoribonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	1	0
			2688	1717	437	522	12			
1	B	346	Total	C	N	O	S	0	0	0
			2689	1719	439	519	12			
1	C	345	Total	C	N	O	S	0	1	0
			2696	1723	439	522	12			
1	D	346	Total	C	N	O	S	0	0	0
			2681	1714	436	519	12			
1	E	346	Total	C	N	O	S	0	1	0
			2637	1676	436	513	12			
1	F	344	Total	C	N	O	S	0	1	0
			2680	1713	437	519	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	expression tag	UNP P59641
A	-5	HIS	-	expression tag	UNP P59641
A	-4	HIS	-	expression tag	UNP P59641
A	-3	HIS	-	expression tag	UNP P59641
A	-2	HIS	-	expression tag	UNP P59641
A	-1	HIS	-	expression tag	UNP P59641
A	0	MET	-	expression tag	UNP P59641
A	234	ALA	HIS	engineered	UNP P59641
B	-6	HIS	-	expression tag	UNP P59641
B	-5	HIS	-	expression tag	UNP P59641
B	-4	HIS	-	expression tag	UNP P59641
B	-3	HIS	-	expression tag	UNP P59641
B	-2	HIS	-	expression tag	UNP P59641
B	-1	HIS	-	expression tag	UNP P59641
B	0	MET	-	expression tag	UNP P59641
B	234	ALA	HIS	engineered	UNP P59641
C	-6	HIS	-	expression tag	UNP P59641

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP P59641
C	-4	HIS	-	expression tag	UNP P59641
C	-3	HIS	-	expression tag	UNP P59641
C	-2	HIS	-	expression tag	UNP P59641
C	-1	HIS	-	expression tag	UNP P59641
C	0	MET	-	expression tag	UNP P59641
C	234	ALA	HIS	engineered	UNP P59641
D	-6	HIS	-	expression tag	UNP P59641
D	-5	HIS	-	expression tag	UNP P59641
D	-4	HIS	-	expression tag	UNP P59641
D	-3	HIS	-	expression tag	UNP P59641
D	-2	HIS	-	expression tag	UNP P59641
D	-1	HIS	-	expression tag	UNP P59641
D	0	MET	-	expression tag	UNP P59641
D	234	ALA	HIS	engineered	UNP P59641
E	-6	HIS	-	expression tag	UNP P59641
E	-5	HIS	-	expression tag	UNP P59641
E	-4	HIS	-	expression tag	UNP P59641
E	-3	HIS	-	expression tag	UNP P59641
E	-2	HIS	-	expression tag	UNP P59641
E	-1	HIS	-	expression tag	UNP P59641
E	0	MET	-	expression tag	UNP P59641
E	234	ALA	HIS	engineered	UNP P59641
F	-6	HIS	-	expression tag	UNP P59641
F	-5	HIS	-	expression tag	UNP P59641
F	-4	HIS	-	expression tag	UNP P59641
F	-3	HIS	-	expression tag	UNP P59641
F	-2	HIS	-	expression tag	UNP P59641
F	-1	HIS	-	expression tag	UNP P59641
F	0	MET	-	expression tag	UNP P59641
F	234	ALA	HIS	engineered	UNP P59641

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	107	Total O 107 107	0	0
2	B	111	Total O 111 111	0	0
2	C	77	Total O 77 77	0	0
2	D	52	Total O 52 52	0	0

Continued on next page...

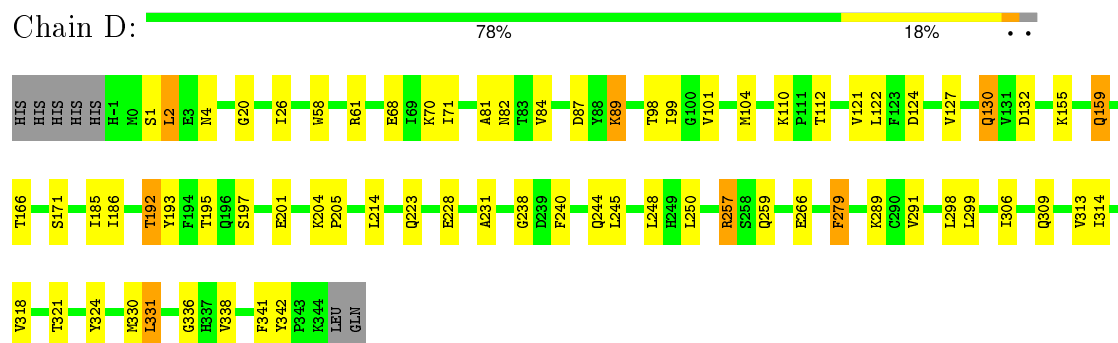
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	48	Total	O	0	0
			48	48		
2	F	46	Total	O	0	0
			46	46		

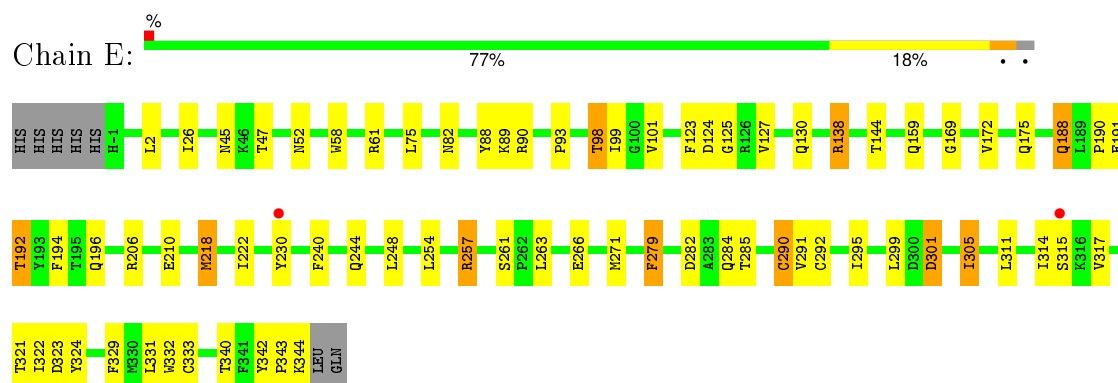
- Molecule 1: Uridylate-specific endoribonuclease



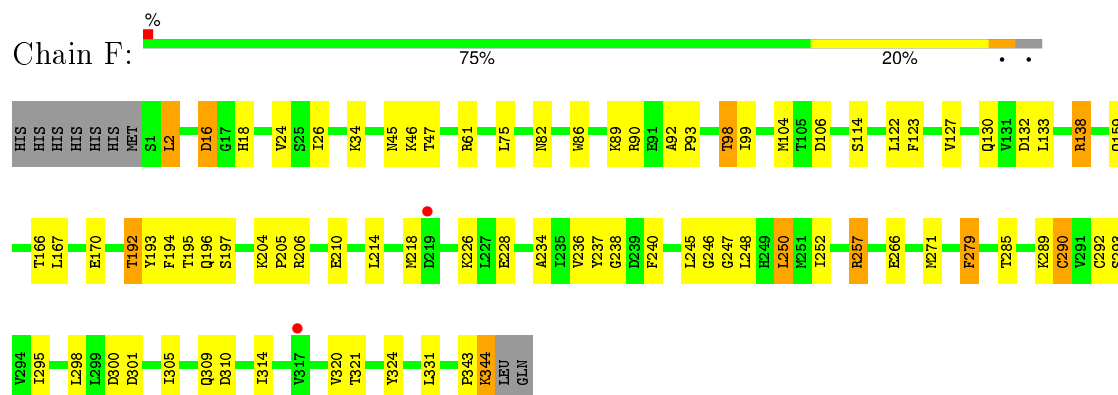
- Molecule 1: Uridylate-specific endoribonuclease



- Molecule 1: Uridylate-specific endoribonuclease



- Molecule 1: Uridylate-specific endoribonuclease



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	305.76 Å 305.76 Å 88.74 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 34.01 – 2.65	Depositor EDS
% Data completeness (in resolution range)	92.0 (50.00-2.80) 86.7 (34.01-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.65 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.260 0.206 , 0.257	Depositor DCC
R_{free} test set	3507 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 41.3	EDS
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 78182 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16512	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.34	0/2745	0.53	0/3725
1	B	0.34	0/2742	0.55	0/3720
1	C	0.35	0/2753	0.56	0/3733
1	D	0.34	0/2733	0.53	0/3709
1	E	0.35	0/2691	0.51	0/3654
1	F	0.34	0/2738	0.53	0/3715
All	All	0.34	0/16402	0.53	0/22256

There are no bond length outliers.

There are no bond angle outliers.

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	2688	0	2659	41	0
1	B	2689	0	2668	54	0
1	C	2696	0	2681	46	0
1	D	2681	0	2654	53	0
1	E	2637	0	2564	45	0
1	F	2680	0	2659	51	0
2	A	107	0	0	0	0
2	B	111	0	0	1	0
2	C	77	0	0	1	0
2	D	52	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	48	0	0	1	0
2	F	46	0	0	0	0
All	All	16512	0	15885	270	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 8.

All (270) 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:192:THR:HG21	1:D:324:TYR:H	1.23	1.02
1:D:98:THR:HG21	1:D:101:VAL:HB	1.40	1.01
1:F:192:THR:HG21	1:F:324:TYR:H	1.24	1.00
1:B:98:THR:HG22	1:B:106:ASP:OD1	1.62	0.99
1:E:192:THR:HG21	1:E:324:TYR:H	1.26	0.99
1:D:98:THR:CG2	1:D:101:VAL:HB	1.96	0.94
1:D:2:LEU:HD11	1:D:26:ILE:HD11	1.49	0.93
1:B:245:LEU:HB3	1:B:289:LYS:HB2	1.52	0.92
1:A:192:THR:HG21	1:A:324:TYR:H	1.34	0.91
1:C:295:ILE:HG23	1:C:296:ASP:H	1.36	0.89
1:C:295:ILE:CG2	1:C:296:ASP:H	1.89	0.85
1:B:192:THR:HG22	1:B:321:THR:HG22	1.58	0.84
1:F:192:THR:HG23	1:F:321:THR:HG22	1.57	0.84
1:C:192:THR:HG21	1:C:324:TYR:H	1.42	0.84
1:B:124:ASP:H	1:B:130:GLN:NE2	1.76	0.83
1:E:196:GLN:HG3	1:E:206:ARG:HH11	1.44	0.82
1:A:124:ASP:H	1:A:130:GLN:NE2	1.78	0.81
1:B:98:THR:CG2	1:B:101:VAL:HB	2.10	0.81
1:E:196:GLN:HG3	1:E:206:ARG:NH1	1.96	0.80
1:F:138:ARG:HH11	1:F:138:ARG:HG3	1.48	0.79
1:F:343:PRO:O	1:F:344:LYS:HB2	1.85	0.76
1:A:240:PHE:CZ	1:A:257:ARG:HG3	2.20	0.76
1:C:266:GLU:HB2	1:C:279:PHE:HB3	1.65	0.76
1:B:98:THR:HG21	1:B:101:VAL:HB	1.67	0.76
1:B:124:ASP:H	1:B:130:GLN:HE21	1.34	0.76
1:D:159:GLN:HE21	1:D:159:GLN:H	1.34	0.75
1:B:301:ASP:O	1:B:305:ILE:HG12	1.87	0.75
1:C:34:LYS:HE2	1:F:104:MET:HE2	1.70	0.74
1:C:104:MET:HE1	1:F:34:LYS:HB2	1.71	0.73
1:F:2:LEU:HD11	1:F:26:ILE:HD11	1.71	0.72
1:A:58:TRP:O	1:A:61:ARG:HB3	1.90	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:THR:HB	1:B:323:ASP:OD2	1.89	0.71
1:E:2:LEU:HD21	1:E:26:ILE:HD11	1.73	0.70
1:B:192:THR:HG21	1:B:324:TYR:HA	1.74	0.69
1:F:301:ASP:O	1:F:305:ILE:HG12	1.92	0.69
1:F:240:PHE:CE2	1:F:257:ARG:HG3	2.28	0.69
1:C:192:THR:HG21	1:C:324:TYR:N	2.08	0.69
1:D:266:GLU:HB2	1:D:279:PHE:HB3	1.74	0.68
1:B:98:THR:CG2	1:B:106:ASP:OD1	2.39	0.68
1:B:23:PRO:HB2	1:D:104:MET:HE2	1.75	0.68
1:C:295:ILE:CG2	1:C:296:ASP:N	2.56	0.67
1:C:125:GLY:HA3	1:C:144:THR:HG22	1.77	0.67
1:B:192:THR:HG22	1:B:321:THR:CG2	2.25	0.66
1:D:214:LEU:HB3	1:D:259:GLN:HE22	1.60	0.66
1:E:279:PHE:CD1	1:E:290:CYS:HB3	2.30	0.66
1:C:2:LEU:HD11	1:C:26:ILE:HD11	1.77	0.65
1:A:295:ILE:HD11	1:A:297:LEU:HG	1.79	0.65
1:D:192:THR:HG23	1:D:321:THR:HG22	1.79	0.65
1:E:301:ASP:O	1:E:305:ILE:HG12	1.97	0.65
1:A:5:VAL:HG21	1:A:56:GLU:HG3	1.77	0.64
1:F:192:THR:CG2	1:F:324:TYR:H	2.06	0.64
1:F:289:LYS:HD3	1:F:292:CYS:HB3	1.78	0.64
1:A:240:PHE:HB3	1:A:285:THR:HG21	1.79	0.64
1:F:196:GLN:HG3	1:F:206:ARG:HH11	1.63	0.63
1:B:98:THR:HG23	1:B:101:VAL:HB	1.81	0.63
1:D:309:GLN:HG2	1:D:331:LEU:HD13	1.80	0.63
1:B:34:LYS:HE2	1:D:104:MET:HE1	1.81	0.62
1:C:138:ARG:HH11	1:C:138:ARG:HG3	1.63	0.62
1:A:315:SER:HA	1:A:331:LEU:O	1.98	0.62
1:B:238:GLY:HA3	1:B:248:LEU:HD13	1.80	0.62
1:C:192:THR:HG21	1:C:324:TYR:HA	1.81	0.62
1:D:192:THR:HG21	1:D:324:TYR:N	2.07	0.62
1:A:301:ASP:O	1:A:305:ILE:HG12	2.00	0.62
1:A:84:VAL:HG23	1:A:101:VAL:HG11	1.82	0.61
1:F:16:ASP:HB3	1:F:18:HIS:HD2	1.64	0.61
1:B:240:PHE:CE2	1:B:257:ARG:HG3	2.35	0.61
1:A:124:ASP:H	1:A:130:GLN:HE21	1.46	0.61
1:D:192:THR:CG2	1:D:324:TYR:H	2.07	0.61
1:A:285:THR:CG2	1:A:287:SER:H	2.13	0.61
1:B:138:ARG:HH11	1:B:138:ARG:CG	2.15	0.60
1:F:234:ALA:O	1:F:247:GLY:HA3	2.02	0.59
1:D:70:LYS:NZ	1:D:197:SER:HB3	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:PRO:HG3	1:B:214:LEU:HD12	1.85	0.59
1:D:195:THR:HG22	1:D:197:SER:H	1.68	0.59
1:F:238:GLY:HA3	1:F:248:LEU:HG	1.85	0.58
1:E:125:GLY:HA3	1:E:144:THR:HG22	1.86	0.58
1:B:23:PRO:HB2	1:D:104:MET:CE	2.33	0.58
1:C:159:GLN:HA	1:C:167:LEU:O	2.03	0.58
1:D:231:ALA:HB2	1:D:338:VAL:O	2.03	0.57
1:B:257:ARG:HH12	1:B:284:GLN:HB3	1.69	0.57
1:D:2:LEU:HD11	1:D:26:ILE:CD1	2.30	0.57
1:F:266:GLU:HB3	1:F:279:PHE:HB3	1.85	0.57
1:A:125:GLY:HA3	1:A:144:THR:HG22	1.86	0.56
1:A:285:THR:HG23	1:A:287:SER:H	1.68	0.56
1:A:266:GLU:HB2	1:A:279:PHE:HB3	1.85	0.56
1:B:240:PHE:CZ	1:B:257:ARG:HG3	2.41	0.56
1:E:295:ILE:HD11	1:E:322:ILE:HD13	1.87	0.56
1:C:104:MET:HE2	1:F:34:LYS:HE2	1.88	0.56
1:B:138:ARG:HH11	1:B:138:ARG:HG3	1.70	0.56
1:D:309:GLN:HE22	1:D:318:VAL:HG11	1.71	0.56
1:E:266:GLU:HB2	1:E:279:PHE:HB3	1.88	0.56
1:A:195:THR:HG22	1:A:295:ILE:CD1	2.36	0.55
1:D:84:VAL:HG23	1:D:101:VAL:HG11	1.88	0.55
1:B:45:ASN:ND2	1:B:47:THR:H	2.04	0.55
1:D:68:GLU:HB2	1:D:71:ILE:HD12	1.89	0.55
1:E:188:GLN:HG2	1:E:188:GLN:O	2.07	0.55
1:E:82:ASN:HA	1:E:99:ILE:O	2.08	0.54
1:C:192:THR:HG21	1:C:324:TYR:CA	2.38	0.54
1:D:70:LYS:HZ1	1:D:197:SER:HB3	1.71	0.54
1:A:70:LYS:HZ1	1:A:197:SER:HB3	1.73	0.54
1:B:125:GLY:HA3	1:B:144:THR:HG22	1.89	0.54
1:F:245:LEU:HD21	1:F:248:LEU:HD12	1.89	0.54
1:E:190:PRO:HB2	1:E:321:THR:HG21	1.88	0.54
1:A:245:LEU:HB3	1:A:287:SER:OG	2.08	0.53
1:D:240:PHE:CZ	1:D:257:ARG:HG3	2.43	0.53
1:C:240:PHE:CZ	1:C:257:ARG:HG3	2.44	0.53
1:C:294:VAL:HG12	1:C:295:ILE:N	2.24	0.53
1:D:309:GLN:NE2	1:D:318:VAL:HG11	2.24	0.53
1:B:218:MET:HG3	1:B:237:TYR:CE2	2.43	0.53
1:E:138:ARG:HB3	1:E:138:ARG:HH11	1.74	0.53
1:B:70:LYS:HZ2	1:B:195:THR:HG21	1.73	0.53
1:B:218:MET:HG3	1:B:237:TYR:CZ	2.44	0.52
1:B:305:ILE:HD12	1:B:320:VAL:HG11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LYS:HB2	1:D:104:MET:HE3	1.91	0.52
1:D:58:TRP:O	1:D:61:ARG:HG3	2.09	0.52
1:E:98:THR:CG2	1:E:101:VAL:HB	2.40	0.52
1:F:210:GLU:HG3	1:F:252:ILE:HD12	1.92	0.51
1:D:87:ASP:OD1	1:D:89:LYS:HG2	2.10	0.51
1:C:23:PRO:HB2	1:F:104:MET:CE	2.41	0.51
1:D:110:LYS:C	1:D:112:THR:H	2.15	0.51
1:F:192:THR:HG22	1:F:193:TYR:O	2.11	0.50
1:E:315:SER:HA	1:E:331:LEU:O	2.11	0.50
1:B:127:VAL:HG22	1:B:130:GLN:HG3	1.92	0.50
1:F:138:ARG:HH11	1:F:138:ARG:CG	2.19	0.50
1:E:98:THR:HG23	1:E:101:VAL:HB	1.93	0.50
1:F:192:THR:HG21	1:F:324:TYR:N	2.08	0.50
1:A:204:LYS:HD3	1:A:205:PRO:HD2	1.93	0.50
1:E:279:PHE:HA	1:E:290:CYS:HA	1.94	0.49
1:F:123:PHE:HA	1:F:130:GLN:NE2	2.28	0.49
1:E:192:THR:HG21	1:E:324:TYR:N	2.11	0.49
1:E:169:GLY:HA3	1:E:172:VAL:O	2.12	0.49
1:E:90:ARG:NH2	1:E:93:PRO:O	2.46	0.49
1:B:249:HIS:O	1:B:294:VAL:HA	2.13	0.48
1:A:61:ARG:HD3	1:A:88:TYR:OH	2.13	0.48
1:A:193:TYR:CE1	1:A:305:ILE:HD11	2.48	0.48
1:E:58:TRP:O	1:E:61:ARG:HG3	2.13	0.48
1:E:240:PHE:CE2	1:E:257:ARG:HG3	2.49	0.48
1:F:240:PHE:CZ	1:F:257:ARG:HG3	2.48	0.48
1:D:205:PRO:HG3	1:D:214:LEU:HD12	1.95	0.48
1:E:343:PRO:O	1:E:344:LYS:CB	2.61	0.48
1:C:214:LEU:HB3	1:C:259:GLN:HE22	1.79	0.48
1:F:195:THR:HG22	1:F:197:SER:H	1.79	0.48
1:C:23:PRO:HB2	1:F:104:MET:HE3	1.95	0.48
1:E:248:LEU:HD11	1:E:254:LEU:HA	1.96	0.47
1:A:170:GLU:HB2	1:C:285:THR:HA	1.96	0.47
1:C:294:VAL:O	1:C:295:ILE:HB	2.14	0.47
1:E:230:TYR:CE1	1:E:311:LEU:HD11	2.49	0.47
1:F:90:ARG:NH2	1:F:93:PRO:O	2.47	0.47
1:B:127:VAL:CG2	1:B:130:GLN:HG3	2.44	0.47
1:D:240:PHE:CE2	1:D:257:ARG:HG3	2.49	0.47
1:F:218:MET:HG3	1:F:237:TYR:CE2	2.49	0.47
1:E:285:THR:HA	1:F:170:GLU:HB2	1.96	0.47
1:C:195:THR:HB	1:C:323:ASP:OD2	2.15	0.47
1:C:104:MET:CE	1:F:34:LYS:HE2	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLN:HA	1:A:133:LEU:HD12	1.97	0.47
1:B:138:ARG:HB3	1:B:138:ARG:HH11	1.79	0.47
1:C:45:ASN:ND2	1:C:47:THR:H	2.13	0.47
1:B:1:SER:HB2	1:D:1:SER:HB2	1.96	0.47
1:B:284:GLN:HA	1:B:284:GLN:HE21	1.78	0.47
1:E:194:PHE:HA	1:E:323:ASP:OD2	2.14	0.47
1:F:98:THR:HG23	1:F:106:ASP:OD1	2.15	0.47
1:C:315:SER:HA	1:C:331:LEU:O	2.15	0.46
1:F:343:PRO:O	1:F:344:LYS:CB	2.62	0.46
1:E:314:ILE:O	1:E:333:CYS:N	2.46	0.46
1:D:313:VAL:HG12	1:D:314:ILE:N	2.30	0.46
1:B:265:LEU:HG	1:B:280:ILE:HG12	1.98	0.46
1:D:124:ASP:H	1:D:130:GLN:NE2	2.13	0.46
1:D:306:ILE:HD11	1:D:338:VAL:HG11	1.98	0.46
1:F:218:MET:HG3	1:F:237:TYR:CZ	2.51	0.46
1:E:45:ASN:ND2	1:E:47:THR:H	2.13	0.46
1:B:34:LYS:HB2	1:D:104:MET:CE	2.45	0.46
1:B:245:LEU:CB	1:B:289:LYS:HB2	2.36	0.45
1:C:34:LYS:HB2	1:F:104:MET:HE1	1.98	0.45
1:D:331:LEU:HB2	1:D:341:PHE:HD2	1.81	0.45
1:A:305:ILE:HD12	1:A:320:VAL:HG11	1.98	0.45
1:E:124:ASP:HB3	1:E:127:VAL:HG12	1.99	0.45
1:B:315:SER:HB3	1:B:332:TRP:CE3	2.51	0.45
1:E:329:PHE:HA	1:E:343:PRO:HA	1.98	0.45
1:A:210:GLU:HG2	1:A:299:LEU:HB2	1.98	0.45
1:D:4:ASN:HA	1:D:20:GLY:O	2.17	0.45
1:C:240:PHE:CE2	1:C:257:ARG:HG3	2.52	0.45
1:C:295:ILE:HG23	1:C:296:ASP:N	2.17	0.45
1:B:138:ARG:NH1	1:B:138:ARG:HG3	2.32	0.45
1:A:82:ASN:HA	1:A:99:ILE:O	2.17	0.44
1:C:264:LYS:O	1:C:280:ILE:HA	2.16	0.44
1:A:61:ARG:HB3	1:A:61:ARG:HE	1.50	0.44
1:E:61:ARG:HD2	1:E:88:TYR:OH	2.17	0.44
1:C:98:THR:HG23	1:C:106:ASP:OD1	2.17	0.44
1:C:245:LEU:HD21	1:C:248:LEU:HD12	1.98	0.44
1:C:0:MET:N	2:C:836:HOH:O	2.47	0.44
1:E:314:ILE:O	1:E:332:TRP:HA	2.18	0.44
1:E:2:LEU:HD13	1:E:52:ASN:HB2	2.00	0.44
1:F:279:PHE:CD1	1:F:290:CYS:HB3	2.52	0.44
1:A:159:GLN:NE2	1:A:159:GLN:H	2.15	0.44
1:F:82:ASN:HA	1:F:99:ILE:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ASP:H	1:C:130:GLN:NE2	2.16	0.44
1:D:309:GLN:HE22	1:D:318:VAL:CG1	2.31	0.44
1:F:61:ARG:HG2	1:F:86:TRP:HB2	2.00	0.44
1:B:6:ALA:O	1:B:10:VAL:HG22	2.18	0.44
1:A:8:ASN:HB3	1:A:15:PHE:HA	1.98	0.44
1:D:192:THR:HG22	1:D:193:TYR:O	2.17	0.43
1:A:332:TRP:HB2	1:A:340:THR:HG22	2.00	0.43
1:B:16:ASP:HB3	1:B:18:HIS:HD2	1.82	0.43
1:D:238:GLY:HA3	1:D:248:LEU:HG	1.99	0.43
1:C:8:ASN:HB3	1:C:15:PHE:HA	2.00	0.43
1:C:65:PRO:HG3	1:C:172:VAL:HG11	2.00	0.43
1:C:34:LYS:HD3	1:C:39:ASP:OD1	2.17	0.43
1:B:266:GLU:HB2	1:B:279:PHE:HB3	2.00	0.43
1:B:187:GLN:HB3	1:B:187:GLN:HE21	1.65	0.43
1:A:10:VAL:HG11	1:A:33:THR:HG21	2.00	0.43
1:F:196:GLN:HG3	1:F:206:ARG:NH1	2.32	0.43
1:B:138:ARG:HH11	1:B:138:ARG:CB	2.32	0.43
1:F:130:GLN:HA	1:F:133:LEU:HD12	2.00	0.43
1:E:123:PHE:HD2	1:E:130:GLN:HE21	1.66	0.43
1:C:2:LEU:HD12	1:F:2:LEU:HD12	2.01	0.43
1:F:123:PHE:HA	1:F:130:GLN:HE22	1.84	0.43
1:C:141:VAL:HG22	1:C:180:LYS:HG3	1.99	0.43
1:D:81:ALA:HB2	1:D:121:VAL:HG12	2.00	0.43
1:F:305:ILE:HD12	1:F:320:VAL:HG11	1.99	0.43
1:A:195:THR:HG22	1:A:295:ILE:HD12	2.00	0.43
1:C:110:LYS:HA	1:C:111:PRO:HD3	1.88	0.43
1:E:263:LEU:HD23	1:E:282:ASP:HA	1.99	0.43
1:A:238:GLY:HA2	1:A:246:GLY:O	2.18	0.43
1:E:210:GLU:HG2	1:E:299:LEU:HB2	1.99	0.43
1:B:279:PHE:C	1:B:279:PHE:HD2	2.22	0.42
1:B:279:PHE:CD1	1:B:290:CYS:HB3	2.54	0.42
1:D:130:GLN:HB3	1:D:130:GLN:HE21	1.56	0.42
1:E:196:GLN:HE21	1:E:206:ARG:HD2	1.83	0.42
1:E:89:LYS:HD3	2:E:394:HOH:O	2.19	0.42
1:D:82:ASN:HA	1:D:99:ILE:O	2.19	0.42
1:C:104:MET:HE1	1:F:34:LYS:CB	2.47	0.42
1:F:138:ARG:CG	1:F:138:ARG:NH1	2.82	0.42
1:B:-1:HIS:N	2:B:431:HOH:O	2.53	0.42
1:D:171:SER:OG	1:F:285:THR:HB	2.20	0.42
1:F:194:PHE:HE2	1:F:324:TYR:CE1	2.37	0.42
1:E:261:SER:HB3	1:E:284:GLN:HE21	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:GLN:CG	1:E:206:ARG:HH11	2.22	0.42
1:A:313:VAL:HG12	1:A:315:SER:H	1.84	0.42
1:B:315:SER:HA	1:B:331:LEU:O	2.20	0.42
1:D:330:MET:HB3	1:D:342:TYR:CE2	2.55	0.42
1:C:143:ILE:HA	1:C:177:ASN:O	2.20	0.42
1:A:285:THR:HG22	1:A:287:SER:H	1.84	0.42
1:F:236:VAL:HG13	1:F:250:LEU:HB2	2.01	0.42
1:F:47:THR:HG22	1:F:92:ALA:HA	2.00	0.42
1:E:218:MET:O	1:E:222:ILE:HG13	2.19	0.41
1:F:238:GLY:HA2	1:F:246:GLY:O	2.19	0.41
1:B:279:PHE:CD2	1:B:279:PHE:C	2.92	0.41
1:A:45:ASN:ND2	1:A:47:THR:H	2.18	0.41
1:D:159:GLN:NE2	1:D:159:GLN:H	2.09	0.41
1:C:279:PHE:CD2	1:C:290:CYS:HA	2.55	0.41
1:B:248:LEU:HG	1:B:254:LEU:HD12	2.03	0.41
1:D:84:VAL:CG2	1:D:101:VAL:HG11	2.51	0.41
1:D:331:LEU:HB2	1:D:341:PHE:CD2	2.56	0.41
1:C:65:PRO:HG2	1:C:172:VAL:HG13	2.02	0.41
1:A:238:GLY:HA3	1:A:248:LEU:HG	2.03	0.41
1:E:192:THR:HG23	1:E:321:THR:HG22	2.03	0.41
1:C:295:ILE:HA	1:C:295:ILE:HD13	1.99	0.41
1:A:240:PHE:CE2	1:A:257:ARG:HG3	2.55	0.41
1:D:245:LEU:HD21	1:D:248:LEU:HD12	2.01	0.41
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.88	0.41
1:A:2:LEU:HD12	1:E:2:LEU:HD22	2.03	0.40
1:E:317:VAL:HA	1:E:329:PHE:O	2.21	0.40
1:A:138:ARG:NH1	1:A:183:ASP:HA	2.36	0.40
1:B:26:ILE:HG21	1:D:26:ILE:HG21	2.04	0.40
1:D:204:LYS:HA	1:D:205:PRO:HD3	1.95	0.40
1:F:204:LYS:HA	1:F:205:PRO:HD2	1.96	0.40
1:D:110:LYS:HB2	1:D:112:THR:HG22	2.03	0.40
1:D:245:LEU:HB3	1:D:289:LYS:HB2	2.04	0.40
1:C:293:SER:HB2	1:C:343:PRO:HG2	2.03	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	344/353 (98%)	330 (96%)	12 (4%)	2 (1%)	30	65
1	B	344/353 (98%)	330 (96%)	13 (4%)	1 (0%)	46	79
1	C	344/353 (98%)	326 (95%)	15 (4%)	3 (1%)	21	55
1	D	344/353 (98%)	325 (94%)	17 (5%)	2 (1%)	30	65
1	E	345/353 (98%)	325 (94%)	18 (5%)	2 (1%)	30	65
1	F	343/353 (97%)	326 (95%)	17 (5%)	0	100	100
All	All	2064/2118 (98%)	1962 (95%)	92 (4%)	10 (0%)	34	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	295	ILE
1	D	336	GLY
1	C	128	GLU
1	D	291	VAL
1	A	226	LYS
1	E	218	MET
1	C	61	ARG
1	A	291	VAL
1	B	291	VAL
1	E	291	VAL

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	299/309 (97%)	267 (89%)	32 (11%)	8	24
1	B	298/309 (96%)	277 (93%)	21 (7%)	19	47
1	C	301/309 (97%)	273 (91%)	28 (9%)	11	32
1	D	296/309 (96%)	274 (93%)	22 (7%)	17	43
1	E	285/309 (92%)	267 (94%)	18 (6%)	22	53
1	F	298/309 (96%)	264 (89%)	34 (11%)	7	21
All	All	1777/1854 (96%)	1622 (91%)	155 (9%)	13	35

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	12	LYS
1	A	21	GLU
1	A	25	SER
1	A	35	VAL
1	A	36	ASP
1	A	40	VAL
1	A	56	GLU
1	A	61	ARG
1	A	75	LEU
1	A	104	MET
1	A	127	VAL
1	A	132[A]	ASP
1	A	132[B]	ASP
1	A	138	ARG
1	A	159	GLN
1	A	166	THR
1	A	192	THR
1	A	197	SER
1	A	228	GLU
1	A	244	GLN
1	A	257	ARG
1	A	271	MET
1	A	279	PHE
1	A	285	THR
1	A	295	ILE
1	A	298	LEU
1	A	299	LEU
1	A	300	ASP
1	A	311	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	316	LYS
1	A	331	LEU
1	B	40	VAL
1	B	75	LEU
1	B	89	LYS
1	B	103	THR
1	B	122	LEU
1	B	127	VAL
1	B	138	ARG
1	B	147	SER
1	B	159	GLN
1	B	166	THR
1	B	187	GLN
1	B	195	THR
1	B	220	GLU
1	B	257	ARG
1	B	271	MET
1	B	279	PHE
1	B	284	GLN
1	B	290	CYS
1	B	293	SER
1	B	299	LEU
1	B	313	VAL
1	C	0	MET
1	C	1	SER
1	C	2	LEU
1	C	12	LYS
1	C	56	GLU
1	C	75	LEU
1	C	91	GLU
1	C	97	SER
1	C	98	THR
1	C	104	MET
1	C	127	VAL
1	C	159	GLN
1	C	167	LEU
1	C	192	THR
1	C	195	THR
1	C	220	GLU
1	C	224	ARG
1	C	257	ARG
1	C	269	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	279	PHE
1	C	290	CYS
1	C	298	LEU
1	C	299	LEU
1	C	300	ASP
1	C	311	LEU
1	C	321	THR
1	C	331	LEU
1	C	335	ASP
1	D	2	LEU
1	D	89	LYS
1	D	122	LEU
1	D	127	VAL
1	D	130	GLN
1	D	132	ASP
1	D	155	LYS
1	D	159	GLN
1	D	166	THR
1	D	185	ILE
1	D	186	ILE
1	D	192	THR
1	D	201	GLU
1	D	223	GLN
1	D	228	GLU
1	D	244	GLN
1	D	250	LEU
1	D	257	ARG
1	D	279	PHE
1	D	298	LEU
1	D	299	LEU
1	D	331	LEU
1	E	75	LEU
1	E	98	THR
1	E	138	ARG
1	E	159	GLN
1	E	175	GLN
1	E	188	GLN
1	E	191	GLU
1	E	192	THR
1	E	244	GLN
1	E	257	ARG
1	E	271	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	279	PHE
1	E	290	CYS
1	E	292	CYS
1	E	301	ASP
1	E	305	ILE
1	E	340	THR
1	E	342	TYR
1	F	2	LEU
1	F	16	ASP
1	F	24	VAL
1	F	45	ASN
1	F	46	LYS
1	F	75	LEU
1	F	89	LYS
1	F	98	THR
1	F	114	SER
1	F	122	LEU
1	F	127	VAL
1	F	132	ASP
1	F	138	ARG
1	F	159	GLN
1	F	166	THR
1	F	167	LEU
1	F	192	THR
1	F	214	LEU
1	F	226	LYS
1	F	228	GLU
1	F	250	LEU
1	F	257	ARG
1	F	271	MET
1	F	279	PHE
1	F	290	CYS
1	F	293	SER
1	F	295	ILE
1	F	298	LEU
1	F	300	ASP
1	F	309	GLN
1	F	310	ASP
1	F	314	ILE
1	F	331	LEU
1	F	344	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	130	GLN
1	A	159	GLN
1	A	175	GLN
1	A	208	GLN
1	B	4	ASN
1	B	18	HIS
1	B	45	ASN
1	B	130	GLN
1	B	187	GLN
1	B	259	GLN
1	B	284	GLN
1	C	45	ASN
1	C	130	GLN
1	C	159	GLN
1	C	175	GLN
1	C	244	GLN
1	C	259	GLN
1	C	337	HIS
1	D	45	ASN
1	D	130	GLN
1	D	159	GLN
1	D	175	GLN
1	D	259	GLN
1	D	284	GLN
1	D	309	GLN
1	E	4	ASN
1	E	18	HIS
1	E	45	ASN
1	E	130	GLN
1	E	159	GLN
1	E	175	GLN
1	E	196	GLN
1	E	284	GLN
1	F	4	ASN
1	F	18	HIS
1	F	45	ASN
1	F	130	GLN
1	F	136	ASN
1	F	159	GLN
1	F	196	GLN
1	F	223	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	284	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	345/353 (97%)	-0.62	0 100 100	35, 50, 68, 74	0
1	B	346/353 (98%)	-0.57	3 (0%) 85 79	34, 47, 75, 93	0
1	C	345/353 (97%)	-0.50	0 100 100	38, 54, 73, 79	0
1	D	346/353 (98%)	-0.48	0 100 100	37, 63, 86, 92	0
1	E	346/353 (98%)	-0.28	2 (0%) 90 86	38, 70, 99, 107	0
1	F	344/353 (97%)	-0.22	2 (0%) 90 86	39, 76, 99, 104	0
All	All	2072/2118 (97%)	-0.44	7 (0%) 94 92	34, 59, 91, 107	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	230	TYR	3.0
1	B	242	HIS	2.9
1	E	315	SER	2.7
1	B	241	SER	2.6
1	F	219	ASP	2.5
1	B	248	LEU	2.5
1	F	317	VAL	2.3

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.