Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 06:17 PM EST

PDB ID	:	6D8P
Title	:	Ternary RsAgo Complex Containing Guide RNA Paired with Target DNA
Authors	:	Liu, Y.; Esyunina, D.; Olovnikov, I.; Teplova, M.; Patel, D.J.
Deposited on	:	2018-04-26
Resolution	:	2.10 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

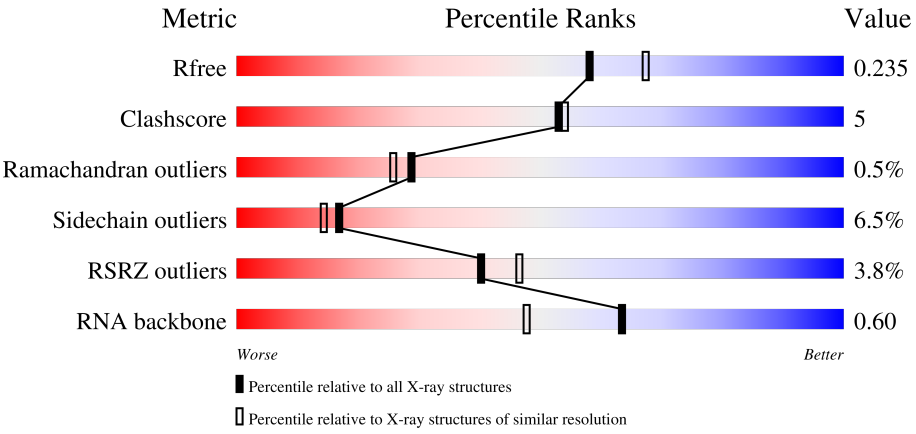
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)
RNA backbone	3102	1000 (2.54-1.66)

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 of 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	791	2% 80% 14%
1	B	791	5% 80% 12% 5%
2	C	18	72% 28%
2	E	18	56% 39% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	24	54% 25% 17%
3	J	24	4% 54% 21% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	E	102	-	-	-	X
5	ACT	E	103	-	-	-	X
5	ACT	G	101	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14004 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	758	Total 5918	C 3755	N 1067	O 1080	S 16	0	5	0
1	B	752	Total 5685	C 3630	N 992	O 1047	S 16	0	2	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A4WYU7
A	-12	HIS	-	expression tag	UNP A4WYU7
A	-11	HIS	-	expression tag	UNP A4WYU7
A	-10	HIS	-	expression tag	UNP A4WYU7
A	-9	HIS	-	expression tag	UNP A4WYU7
A	-8	HIS	-	expression tag	UNP A4WYU7
A	-7	HIS	-	expression tag	UNP A4WYU7
A	-6	ASP	-	expression tag	UNP A4WYU7
A	-5	TYR	-	expression tag	UNP A4WYU7
A	-4	LYS	-	expression tag	UNP A4WYU7
A	-3	ASP	-	expression tag	UNP A4WYU7
A	-2	ASP	-	expression tag	UNP A4WYU7
A	-1	ASP	-	expression tag	UNP A4WYU7
A	0	ASP	-	expression tag	UNP A4WYU7
A	1	LYS	-	expression tag	UNP A4WYU7
B	-13	MET	-	initiating methionine	UNP A4WYU7
B	-12	HIS	-	expression tag	UNP A4WYU7
B	-11	HIS	-	expression tag	UNP A4WYU7
B	-10	HIS	-	expression tag	UNP A4WYU7
B	-9	HIS	-	expression tag	UNP A4WYU7
B	-8	HIS	-	expression tag	UNP A4WYU7
B	-7	HIS	-	expression tag	UNP A4WYU7
B	-6	ASP	-	expression tag	UNP A4WYU7
B	-5	TYR	-	expression tag	UNP A4WYU7
B	-4	LYS	-	expression tag	UNP A4WYU7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	ASP	-	expression tag	UNP A4WYU7
B	-2	ASP	-	expression tag	UNP A4WYU7
B	-1	ASP	-	expression tag	UNP A4WYU7
B	0	ASP	-	expression tag	UNP A4WYU7
B	1	LYS	-	expression tag	UNP A4WYU7

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*AP*CP*AP *GP*GP*UP*GP*AP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			386	172	70	126	18			
2	C	18	Total	C	N	O	P	0	0	0
			386	172	70	126	18			

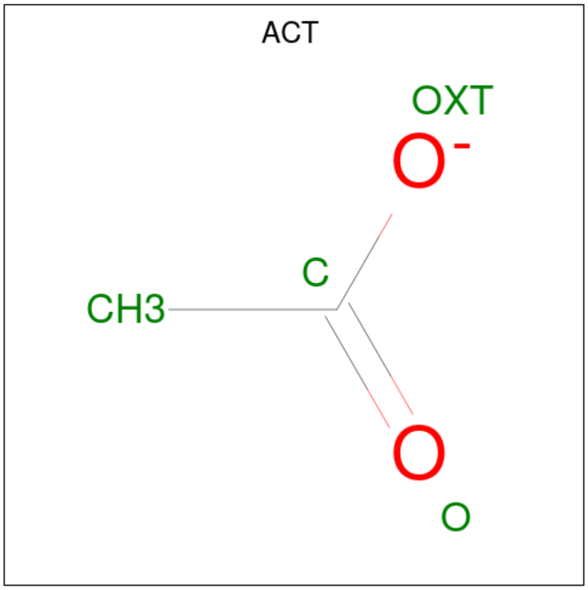
- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*CP*GP*TP*CP*AP*CP*CP*TP*GP *TP*GP*CP*AP*GP*TP*AP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	19	Total	C	N	O	P	0	0	0
			386	184	68	115	19			
3	G	20	Total	C	N	O	P	0	0	0
			408	194	73	121	20			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Mg	0	0
			5	5		
4	E	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



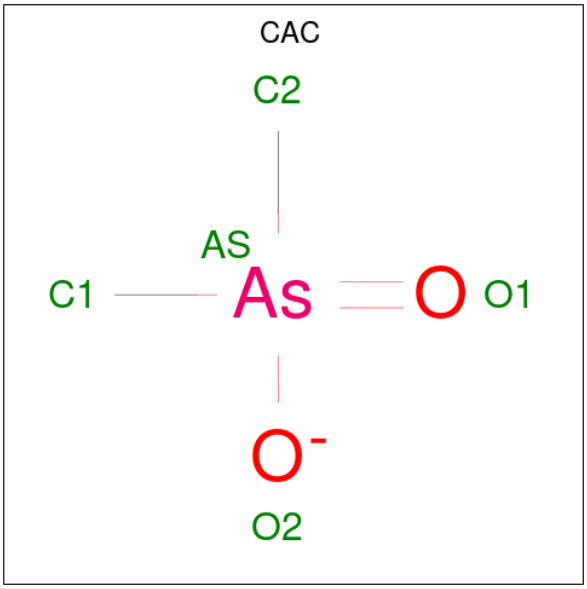
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

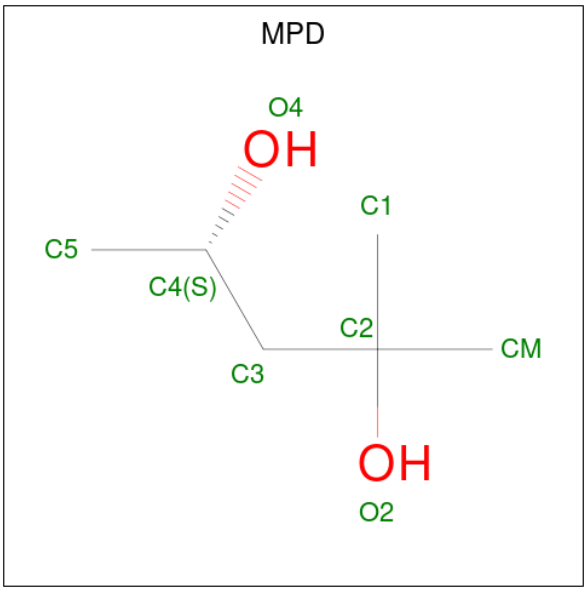
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0

- Molecule 6 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total As C O 5 1 2 2	0	0
6	A	1	Total As C O 5 1 2 2	0	0
6	A	1	Total As C O 5 1 2 2	0	0
6	B	1	Total As C O 5 1 2 2	0	0

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 8 6 2	0	0

- Molecule 8 is water.

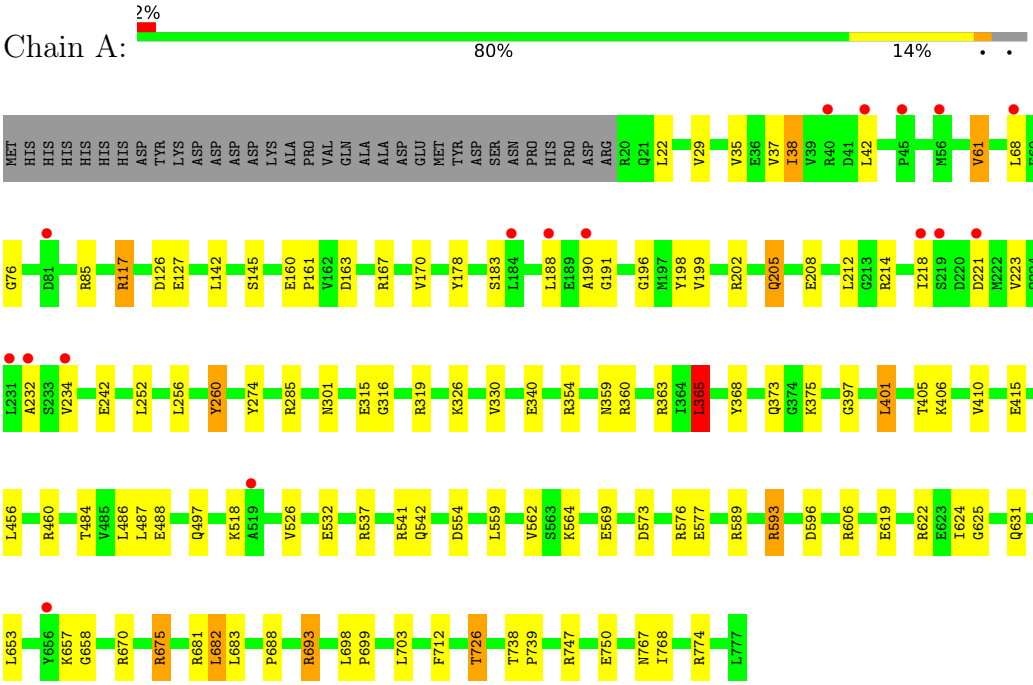
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	354	Total O 354 354	0	0
8	E	52	Total O 52 52	0	0
8	J	38	Total O 38 38	0	0
8	B	217	Total O 217 217	0	0
8	C	34	Total O 34 34	0	0
8	G	25	Total O 25 25	0	0

3 Residue-property plots (i)

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

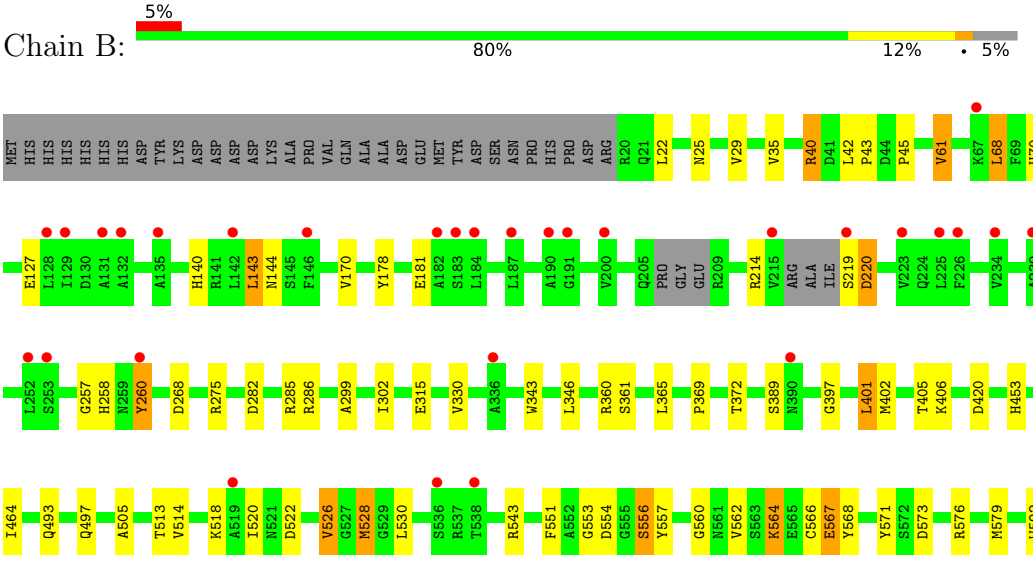
• Molecule 1: Uncharacterized protein

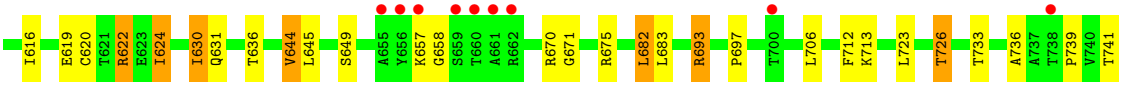
Chain A:



• Molecule 1: Uncharacterized protein

Chain B:



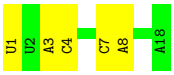


• Molecule 2: RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*GP*UP*GP*AP*CP*GP*A)-3')

Chain E:

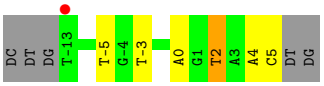
• Molecule 2: RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*GP*UP*GP*AP*CP*GP*A)-3')

Chain C:



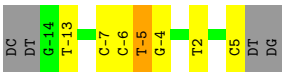
• Molecule 3: DNA (5'-D(P*TP*CP*GP*TP*CP*AP*CP*CP*TP*GP*TP*GP*CP*AP*GP*TP*AP*AP*C)-3')

Chain J:



• Molecule 3: DNA (5'-D(P*TP*CP*GP*TP*CP*AP*CP*CP*TP*GP*TP*GP*CP*AP*GP*TP*AP*AP*C)-3')

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.23Å 119.22Å 117.65Å 90.00° 95.62° 90.00°	Depositor
Resolution (Å)	42.34 – 2.10 42.34 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.4 (42.34-2.10) 89.3 (42.34-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.182 , 0.235 0.182 , 0.235	Depositor DCC
R_{free} test set	5085 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14004	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MPD, ACT, CAC

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	0.40	0/6059	0.58	1/8223 (0.0%)
1	B	0.37	0/5817	0.56	1/7920 (0.0%)
2	C	0.69	1/431 (0.2%)	0.90	0/668
2	E	0.71	1/431 (0.2%)	1.02	1/668 (0.1%)
3	G	0.74	0/456	1.42	5/701 (0.7%)
3	J	0.75	0/431	1.38	5/662 (0.8%)
All	All	0.45	2/13625 (0.0%)	0.70	13/18842 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	U	OP3-P	-9.74	1.49	1.61
2	E	1	U	OP3-P	-9.39	1.49	1.61

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	-5	DT	O4'-C1'-N1	8.85	114.19	108.00
3	G	-6	DC	O4'-C1'-N1	7.88	113.52	108.00
3	G	-4	DG	O4'-C1'-N9	7.59	113.31	108.00
3	G	5	DC	O4'-C4'-C3'	-6.54	101.89	104.50
3	J	2	DT	O4'-C1'-N1	-6.38	103.53	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	365	LEU	CA-CB-CG	6.10	129.33	115.30
3	G	-5	DT	O4'-C1'-N1	5.68	111.97	108.00
3	J	-5	DT	C5-C4-O4	-5.49	121.06	124.90
2	E	4	C	N1-C2-O2	-5.34	115.69	118.90
3	G	-13	DT	O4'-C1'-N1	5.28	111.69	108.00
1	B	567	GLU	N-CA-C	5.28	125.25	111.00
3	J	-3	DT	N3-C4-O4	5.25	123.05	119.90
3	J	4	DA	O4'-C1'-N9	5.18	111.62	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	566	CYS	Peptide

5.2 Too-close contacts (i)

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	5918	0	5850	62	0
1	B	5685	0	5462	66	0
2	C	386	0	195	2	0
2	E	386	0	195	5	0
3	G	408	0	226	3	0
3	J	386	0	215	3	0
4	A	5	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	48	0	36	1	0
5	B	16	0	12	0	0
5	E	8	0	6	0	0
5	G	4	0	3	1	0
5	J	4	0	3	0	0
6	A	15	0	0	0	0
6	B	5	0	0	0	0
7	C	8	0	14	1	0
8	A	354	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	217	0	0	5	0
8	C	34	0	0	0	0
8	E	52	0	0	1	0
8	G	25	0	0	0	0
8	J	38	0	0	0	0
All	All	14004	0	12217	137	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 5.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576[B]:ARG:HD2	1:A:619:GLU:HG3	1.59	0.83
1:B:258:HIS:HA	1:B:260:TYR:H	1.44	0.83
1:A:421:ARG:HG2	1:A:456:LEU:HD21	1.64	0.78
1:B:88:ARG:NH1	8:B:902:HOH:O	2.16	0.78
1:B:268:ASP:OD2	1:B:693:ARG:NH2	2.18	0.77
1:B:603:HIS:ND1	1:B:741:THR:HG21	2.02	0.75
1:B:282:ASP:OD1	1:B:285:ARG:NH1	2.18	0.75
1:B:726:THR:OG1	1:B:736:ALA:O	2.09	0.70
1:B:61:VAL:HG13	1:B:68:LEU:HD21	1.74	0.70
1:A:365:LEU:HD23	1:A:410:VAL:HG22	1.72	0.70
1:B:573:ASP:OD1	1:B:576:ARG:NH2	2.27	0.67
1:A:693:ARG:HG2	3:J:2:DT:H5'	1.78	0.66
1:B:178:TYR:O	8:B:901:HOH:O	2.13	0.66
1:A:576[B]:ARG:NH1	1:A:577:GLU:OE2	2.29	0.65
1:B:543:ARG:NH2	1:B:568:TYR:OH	2.29	0.65
1:A:360:ARG:HB3	1:A:405:THR:HG23	1.80	0.64
1:A:117:ARG:NH2	8:A:905:HOH:O	2.32	0.63
1:B:513:THR:HG23	1:B:557:TYR:O	1.98	0.63
1:A:573:ASP:OD1	1:A:576[A]:ARG:NH2	2.32	0.63
1:A:698:LEU:HD12	1:A:699:PRO:HD2	1.83	0.61
1:B:723:LEU:O	1:B:726:THR:HG22	2.00	0.60
1:B:360:ARG:HB3	1:B:405:THR:HG23	1.84	0.60
1:A:242:GLU:OE1	1:A:537:ARG:NH2	2.35	0.59
1:A:198:TYR:CZ	1:A:214:ARG:HD2	2.37	0.59
1:B:553:GLY:N	1:B:556:SER:O	2.27	0.59
1:A:161:PRO:HG3	1:A:167:ARG:HD2	1.85	0.58
1:B:40:ARG:HG2	1:B:70:HIS:HE1	1.67	0.58
1:B:513:THR:HG21	1:B:556:SER:HB3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ARG:HH22	1:A:726:THR:CG2	2.17	0.57
3:G:-5:DT:H3'	5:G:101:ACT:H2	1.86	0.57
2:C:3:A:H2'	2:C:4:C:C6	2.39	0.57
2:E:3:A:H2'	2:E:4:C:C6	2.40	0.56
3:J:5:DC:C6	3:J:5:DC:H5'	2.41	0.56
1:B:513:THR:HG22	1:B:514:VAL:N	2.21	0.55
1:B:315:GLU:O	8:B:903:HOH:O	2.18	0.55
1:B:219:SER:OG	1:B:220:ASP:N	2.39	0.55
1:B:670:ARG:HH22	1:B:726:THR:CG2	2.20	0.55
1:A:38:ILE:HG22	1:A:70:HIS:HB2	1.89	0.54
1:A:363:ARG:NH1	1:A:441:GLU:O	2.40	0.54
1:A:670:ARG:HH22	1:A:726:THR:HG22	1.71	0.54
1:B:576:ARG:HD3	1:B:616:ILE:HD13	1.88	0.53
1:B:530:LEU:HD11	1:B:543:ARG:HB3	1.88	0.53
1:A:205:GLN:HG3	1:A:208:GLU:CB	2.39	0.53
1:A:368:TYR:HE2	1:A:373:GLN:HG2	1.74	0.53
1:B:258:HIS:HA	1:B:260:TYR:N	2.17	0.52
1:A:61:VAL:HG13	1:A:68:LEU:HD21	1.91	0.52
1:A:260:TYR:OH	3:J:0:DA:OP1	2.27	0.52
1:B:513:THR:HG21	1:B:556:SER:CB	2.39	0.52
1:B:693:ARG:HG2	3:G:2:DT:H5'	1.92	0.52
1:A:593:ARG:N	1:A:596:ASP:OD2	2.40	0.52
1:B:564:LYS:HG2	1:B:767:ASN:ND2	2.26	0.51
1:B:513:THR:HG22	1:B:514:VAL:H	1.75	0.51
2:C:7:C:H2'	2:C:8:A:C8	2.46	0.51
1:B:576:ARG:HD2	1:B:619:GLU:HG3	1.93	0.50
1:B:275:ARG:HB3	1:B:697:PRO:HB3	1.94	0.50
1:A:126:ASP:OD2	1:A:274:TYR:OH	2.30	0.49
1:A:142:LEU:O	1:A:145:SER:OG	2.29	0.49
1:B:620:CYS:O	1:B:624:ILE:HG23	2.11	0.49
2:E:7:C:H2'	2:E:8:A:C8	2.48	0.49
1:B:299:ALA:HB3	1:B:302:ILE:HB	1.95	0.49
1:A:196:GLY:O	1:A:214:ARG:HG2	2.13	0.49
1:A:375:LYS:HD2	1:A:486:LEU:HD21	1.94	0.49
1:B:612:ASP:O	1:B:616:ILE:HG12	2.11	0.48
1:A:212:LEU:HD22	1:A:234:VAL:HG21	1.96	0.48
1:A:38:ILE:CG2	1:A:70:HIS:HB2	2.43	0.48
1:B:706:LEU:HD21	1:B:713:LYS:HA	1.95	0.48
1:A:326:LYS:NZ	8:A:914:HOH:O	2.42	0.48
1:A:675:ARG:HG3	1:A:681:ARG:CZ	2.44	0.48
1:A:228:GLU:HG2	1:A:232:ALA:HA	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:GLY:O	1:B:401:LEU:HB2	2.14	0.47
1:B:526:VAL:HG11	1:B:579:MET:HG2	1.97	0.47
1:B:671:GLY:HA2	1:B:723:LEU:HD22	1.97	0.47
1:A:72:ARG:NH2	1:A:76:GLY:O	2.48	0.47
1:A:397:GLY:O	1:A:401:LEU:HB2	2.15	0.47
1:B:286:ARG:NH1	8:B:915:HOH:O	2.47	0.46
1:A:218:ILE:HG12	1:A:223:VAL:HG12	1.96	0.46
1:B:747:ARG:HH22	1:B:750:GLU:CD	2.19	0.46
1:A:205:GLN:H	1:A:205:GLN:HG2	1.32	0.45
1:A:559:LEU:HD23	1:A:774[A]:ARG:NE	2.32	0.45
1:B:564:LYS:HG2	1:B:767:ASN:HD21	1.81	0.45
1:B:257:GLY:HA2	1:B:260:TYR:HB3	1.98	0.45
1:A:624:ILE:HG13	1:A:625:GLY:N	2.31	0.45
1:B:739:PRO:HB2	1:B:741:THR:HG22	1.99	0.45
1:A:767:ASN:HB2	8:A:987:HOH:O	2.16	0.44
1:B:631:GLN:HB3	1:B:712:PHE:HB2	2.00	0.44
1:B:140:HIS:HB3	1:B:143:LEU:HB2	1.99	0.44
1:A:631:GLN:HB3	1:A:712:PHE:HB2	2.00	0.44
7:C:102:MPD:H53	3:G:-7:DC:C4	2.52	0.44
2:E:18:A:OP2	8:E:201:HOH:O	2.21	0.44
1:B:461:ASN:HB3	1:B:464:ILE:HG22	1.99	0.43
1:A:223:VAL:HG22	1:A:234:VAL:O	2.18	0.43
1:B:505:ALA:HB1	1:B:774:ARG:HG3	2.00	0.43
1:A:738:THR:OG1	1:A:739:PRO:HD2	2.18	0.43
1:B:624:ILE:HG12	1:B:630:ILE:HD12	2.01	0.43
1:A:747:ARG:HH22	1:A:750:GLU:CD	2.23	0.43
1:B:257:GLY:HA2	1:B:258:HIS:HA	1.86	0.43
1:B:43:PRO:O	1:B:45:PRO:HD3	2.19	0.42
1:B:361:SER:HG	1:B:405:THR:HG1	1.67	0.42
1:A:68:LEU:HD22	1:A:70:HIS:NE2	2.34	0.42
1:A:242:GLU:CD	1:A:537:ARG:HH22	2.20	0.42
1:A:252:LEU:O	1:A:256:LEU:HB2	2.18	0.42
1:A:657:LYS:HA	1:A:658:GLY:HA2	1.69	0.42
1:A:484:THR:HA	1:A:487:LEU:HG	2.00	0.42
1:B:670:ARG:HH22	1:B:726:THR:HG23	1.84	0.42
1:A:163:ASP:HB2	8:A:1140:HOH:O	2.17	0.42
1:B:346:LEU:HD21	1:B:402:MET:HE1	2.02	0.42
1:A:214:ARG:O	1:A:225:LEU:HA	2.20	0.42
1:A:421:ARG:O	1:A:460[B]:ARG:HD2	2.20	0.42
1:B:551:PHE:HE2	1:B:560:GLY:HA3	1.85	0.42
1:B:369:PRO:HB2	1:B:372:THR:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:LEU:HD13	1:A:703:LEU:HD13	2.02	0.41
1:B:401:LEU:HD13	1:B:402:MET:HE1	2.01	0.41
1:A:354:ARG:NH1	8:A:909:HOH:O	2.33	0.41
1:B:29:VAL:HG21	1:B:170:VAL:HG23	2.02	0.41
1:B:459:ASP:OD1	1:B:460[B]:ARG:HG2	2.21	0.41
1:B:592:TRP:HZ3	1:B:624:ILE:HB	1.86	0.41
1:B:657:LYS:HA	1:B:658:GLY:HA2	1.75	0.41
1:A:160:GLU:HA	1:A:161:PRO:HD2	1.90	0.41
1:A:653:LEU:HD13	1:A:688:PRO:HB2	2.03	0.41
1:B:25:ASN:CG	1:B:644:VAL:HG13	2.41	0.41
1:B:343:TRP:CZ3	1:B:401:LEU:HD11	2.55	0.41
1:A:178:TYR:CD1	2:E:8:A:H4'	2.56	0.41
1:A:315:GLU:HA	1:A:316:GLY:HA2	1.69	0.41
1:A:183:SER:HA	1:A:202:ARG:NH2	2.36	0.41
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.88	0.41
1:A:190:ALA:HA	1:A:191:GLY:HA2	1.77	0.41
1:A:326:LYS:NZ	1:A:340:GLU:OE1	2.54	0.41
1:A:497:GLN:OE1	5:A:814:ACT:H1	2.21	0.41
2:E:6:G:H2'	2:E:7:C:O4'	2.21	0.41
1:B:144:ASN:HB2	8:B:1000:HOH:O	2.20	0.41
1:B:528:MET:HE3	1:B:571:TYR:HB2	2.02	0.41
1:A:532:GLU:HB3	1:A:541[B]:ARG:HB3	2.02	0.40
1:B:493:GLN:O	1:B:497:GLN:HG3	2.21	0.40
1:B:645:LEU:HD21	1:B:682:LEU:HD23	2.03	0.40
1:A:29:VAL:HG21	1:A:170:VAL:HG23	2.03	0.40
1:B:420:ASP:O	1:B:453:HIS:NE2	2.54	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	761/791 (96%)	740 (97%)	18 (2%)	3 (0%)	34	32
1	B	748/791 (95%)	711 (95%)	33 (4%)	4 (0%)	29	26
All	All	1509/1582 (95%)	1451 (96%)	51 (3%)	7 (0%)	29	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	LYS
1	B	220	ASP
1	B	518	LYS
1	A	554	ASP
1	B	554	ASP
1	B	567	GLU
1	A	768	ILE

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	617/672 (92%)	576 (93%)	41 (7%)	16	14
1	B	568/672 (84%)	532 (94%)	36 (6%)	18	15
All	All	1185/1344 (88%)	1108 (94%)	77 (6%)	17	14

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	35	VAL
1	A	37	VAL
1	A	38	ILE
1	A	42	LEU
1	A	61	VAL
1	A	85	ARG
1	A	117	ARG
1	A	127	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	199	VAL
1	A	205	GLN
1	A	221	ASP
1	A	228	GLU
1	A	260	TYR
1	A	285	ARG
1	A	301	ASN
1	A	319	ARG
1	A	330	VAL
1	A	359	ASN
1	A	365	LEU
1	A	401	LEU
1	A	406	LYS
1	A	415	GLU
1	A	421	ARG
1	A	488	GLU
1	A	526	VAL
1	A	542	GLN
1	A	562	VAL
1	A	564	LYS
1	A	569	GLU
1	A	589	ARG
1	A	593	ARG
1	A	606	ARG
1	A	622	ARG
1	A	636	THR
1	A	644	VAL
1	A	675	ARG
1	A	682	LEU
1	A	683	LEU
1	A	693	ARG
1	A	726	THR
1	B	22	LEU
1	B	35	VAL
1	B	40	ARG
1	B	42	LEU
1	B	61	VAL
1	B	68	LEU
1	B	127	GLU
1	B	143	LEU
1	B	181	GLU
1	B	214	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	245	LYS
1	B	260	TYR
1	B	330	VAL
1	B	365	LEU
1	B	389	SER
1	B	401	LEU
1	B	406	LYS
1	B	520	ILE
1	B	522	ASP
1	B	526	VAL
1	B	528	MET
1	B	556	SER
1	B	562	VAL
1	B	564	LYS
1	B	622	ARG
1	B	624	ILE
1	B	630	ILE
1	B	636	THR
1	B	644	VAL
1	B	649	SER
1	B	675	ARG
1	B	682	LEU
1	B	683	LEU
1	B	693	ARG
1	B	726	THR
1	B	733	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	GLN
1	B	767	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	17/18 (94%)	0	0
2	E	17/18 (94%)	1 (5%)	0
All	All	34/36 (94%)	1 (2%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	12	G

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 7 are monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ACT	A	811	-	3,3,3	0.83	0	3,3,3	1.28	0
5	ACT	A	806	-	3,3,3	0.75	0	3,3,3	1.27	0
5	ACT	A	808	-	3,3,3	0.78	0	3,3,3	1.34	0
6	CAC	A	819	-	0,4,4	-	-	0,6,6	-	-
5	ACT	B	802	-	3,3,3	0.77	0	3,3,3	1.33	0
5	ACT	A	807	-	3,3,3	0.74	0	3,3,3	1.27	0
5	ACT	A	812	-	3,3,3	0.78	0	3,3,3	1.28	0
5	ACT	E	102	-	3,3,3	0.73	0	3,3,3	1.32	0
5	ACT	B	801	-	3,3,3	0.77	0	3,3,3	1.38	0
5	ACT	J	101	-	3,3,3	0.79	0	3,3,3	1.28	0
5	ACT	A	815	-	3,3,3	0.75	0	3,3,3	1.28	0
5	ACT	A	814	-	3,3,3	0.76	0	3,3,3	1.09	0
6	CAC	A	818	-	0,4,4	-	-	0,6,6	-	-
5	ACT	E	103	-	3,3,3	0.78	0	3,3,3	1.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CAC	A	820	-	0,4,4	-	-	0,6,6	-	-
7	MPD	C	102	-	7,7,7	0.25	0	9,10,10	0.26	0
5	ACT	B	804	-	3,3,3	0.79	0	3,3,3	1.18	0
5	ACT	A	816	-	3,3,3	0.73	0	3,3,3	1.33	0
5	ACT	B	803	-	3,3,3	0.76	0	3,3,3	1.24	0
5	ACT	A	809	-	3,3,3	0.78	0	3,3,3	1.37	0
6	CAC	B	805	-	0,4,4	-	-	0,6,6	-	-
5	ACT	A	810	-	3,3,3	0.81	0	3,3,3	1.84	2 (66%)
5	ACT	A	817	-	3,3,3	0.79	0	3,3,3	1.44	0
5	ACT	A	813	-	3,3,3	0.79	0	3,3,3	1.30	0
5	ACT	G	101	-	3,3,3	0.80	0	3,3,3	1.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MPD	C	102	-	-	3/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	810	ACT	OXT-C-O	-2.34	113.44	122.05
5	A	810	ACT	OXT-C-CH3	2.16	124.09	115.18

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	102	MPD	C2-C3-C4-C5
7	C	102	MPD	C1-C2-C3-C4
7	C	102	MPD	O2-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	814	ACT	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	102	MPD	1	0
5	G	101	ACT	1	0

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

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	758/791 (95%)	-0.10	17 (2%) 62 66	14, 30, 66, 104	0
1	B	752/791 (95%)	0.17	42 (5%) 24 29	15, 37, 72, 128	0
2	C	18/18 (100%)	-0.75	0 100 100	20, 32, 42, 45	0
2	E	18/18 (100%)	-0.82	0 100 100	18, 23, 49, 96	0
3	G	20/24 (83%)	-0.31	0 100 100	20, 38, 69, 93	0
3	J	19/24 (79%)	-0.33	1 (5%) 26 32	21, 28, 76, 135	0
All	All	1585/1666 (95%)	0.01	60 (3%) 40 46	14, 33, 69, 135	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	660	THR	5.9
1	B	661	ALA	5.6
1	B	187	LEU	5.3
1	B	656	TYR	4.7
1	B	132	ALA	4.3
1	B	223	VAL	4.3
1	A	188	LEU	4.1
1	A	218	ILE	4.0
1	B	519	ALA	3.6
1	B	135	ALA	3.5
1	B	191	GLY	3.5
1	B	219	SER	3.5
1	B	260	TYR	3.5
1	B	536	SER	3.4
1	B	146	PHE	3.4
1	A	234	VAL	3.4
1	B	226	PHE	3.3
1	A	42	LEU	3.1
1	A	184	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	184	LEU	3.0
1	B	538	THR	3.0
1	B	215	VAL	2.8
1	B	128	LEU	2.7
1	B	253	SER	2.7
1	B	131	ALA	2.6
1	B	183	SER	2.6
1	A	81	ASP	2.6
1	A	219	SER	2.6
1	B	657	LYS	2.6
1	B	142	LEU	2.6
1	A	190	ALA	2.5
3	J	-13	DT	2.5
1	B	129	ILE	2.5
1	A	45	PRO	2.4
1	A	231	LEU	2.4
1	B	662	ARG	2.3
1	B	190	ALA	2.3
1	B	659	SER	2.3
1	B	123	ALA	2.3
1	B	655	ALA	2.2
1	B	738	THR	2.2
1	B	743	PHE	2.2
1	B	234	VAL	2.2
1	A	56	MET	2.2
1	A	232	ALA	2.2
1	B	336	ALA	2.2
1	A	656	TYR	2.2
1	B	67	LYS	2.2
1	B	200	VAL	2.1
1	A	519	ALA	2.1
1	B	225	LEU	2.1
1	A	68	LEU	2.1
1	B	700	THR	2.1
1	B	390	ASN	2.1
1	B	239	ALA	2.1
1	A	221	ASP	2.1
1	A	40	ARG	2.0
1	B	182	ALA	2.0
1	B	252	LEU	2.0
1	B	249	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	A	811	4/4	0.56	0.30	50,61,61,61	0
4	MG	A	802	1/1	0.65	0.20	63,63,63,63	0
5	ACT	J	101	4/4	0.67	0.27	54,59,61,62	0
5	ACT	E	103	4/4	0.71	0.47	63,70,71,72	0
5	ACT	E	102	4/4	0.75	0.40	50,59,60,62	0
5	ACT	A	817	4/4	0.76	0.17	61,66,68,70	0
5	ACT	G	101	4/4	0.78	0.42	41,49,49,53	0
5	ACT	A	816	4/4	0.84	0.14	66,72,72,72	0
5	ACT	A	815	4/4	0.84	0.25	89,89,91,91	0
5	ACT	A	813	4/4	0.85	0.21	60,67,68,71	0
5	ACT	A	812	4/4	0.86	0.16	60,64,64,64	0
6	CAC	B	805	5/5	0.86	0.27	70,109,152,160	0
5	ACT	A	809	4/4	0.88	0.23	56,63,64,67	0
6	CAC	A	820	5/5	0.89	0.21	48,75,96,177	0
5	ACT	B	804	4/4	0.90	0.22	37,47,51,65	0
5	ACT	A	814	4/4	0.90	0.36	50,51,58,62	0
6	CAC	A	818	5/5	0.91	0.18	60,62,147,151	0
5	ACT	A	807	4/4	0.91	0.28	52,58,58,64	0
5	ACT	B	801	4/4	0.91	0.15	81,82,83,83	0
7	MPD	C	102	8/8	0.92	0.17	52,56,61,66	0
5	ACT	A	810	4/4	0.93	0.14	24,30,35,36	0
5	ACT	A	808	4/4	0.93	0.11	74,76,76,77	0
4	MG	A	803	1/1	0.94	0.10	56,56,56,56	0
5	ACT	A	806	4/4	0.95	0.10	64,69,69,71	0
5	ACT	B	802	4/4	0.95	0.11	50,50,53,54	0
6	CAC	A	819	5/5	0.96	0.12	66,115,129,160	0
5	ACT	B	803	4/4	0.96	0.19	36,51,52,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	804	1/1	0.98	0.12	26,26,26,26	0
4	MG	A	805	1/1	0.98	0.10	23,23,23,23	0
4	MG	A	801	1/1	0.98	0.12	30,30,30,30	0
4	MG	C	101	1/1	0.99	0.15	19,19,19,19	0
4	MG	E	101	1/1	0.99	0.11	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.