Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2024 – 05:24 PM EST

PDB ID	:	6D8A
Title	:	RsAgo Ternary Complex with guide RNA and Target DNA Containing A-A Bulge Within the Seed Segment of the Target Strand
Authors	:	Liu, Y.; Esyunina, D.; Olovnikov, I.; Teplova, M.; Patel, D.J.
Deposited on	:	2018-04-26
Resolution	:	2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

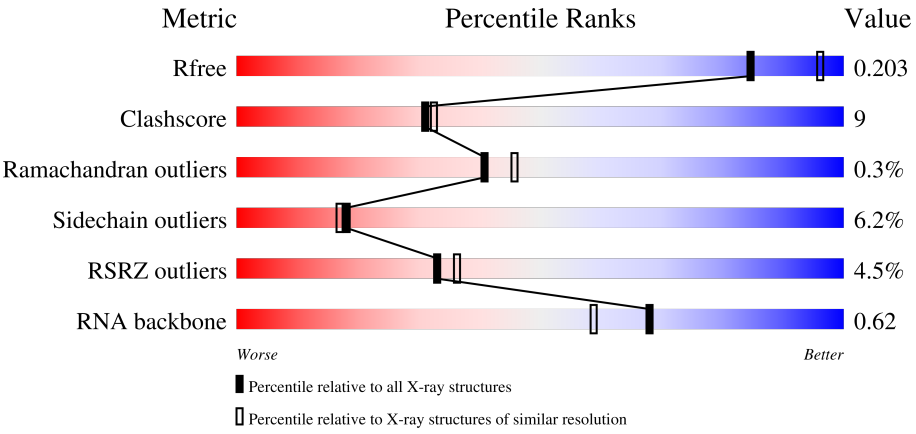
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)
RNA backbone	3102	1016 (2.66-1.86)

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	4% 79% 15%
1	F	791	5% 74% 19%
2	C	18	83% 17%
2	H	18	44% 44% 11%

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Mol	Chain	Length	Quality of chain
3	G	26	8% 50% 31% 19%
3	J	26	4% 46% 31% 8% 15%

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
4	MPD	A	801	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 25923 atoms, of which 12227 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	C	H	N	O	S	0	0	0
			11580	3718	5733	1047	1066	16			
1	F	758	Total	C	H	N	O	S	0	0	0
			11323	3665	5563	1019	1060	16			

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
F	-13	MET	-	initiating methionine	UNP A4WYU7
F	-12	HIS	-	expression tag	UNP A4WYU7
F	-11	HIS	-	expression tag	UNP A4WYU7
F	-10	HIS	-	expression tag	UNP A4WYU7
F	-9	HIS	-	expression tag	UNP A4WYU7
F	-8	HIS	-	expression tag	UNP A4WYU7
F	-7	HIS	-	expression tag	UNP A4WYU7
F	-6	ASP	-	expression tag	UNP A4WYU7
F	-5	TYR	-	expression tag	UNP A4WYU7
F	-4	LYS	-	expression tag	UNP A4WYU7

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

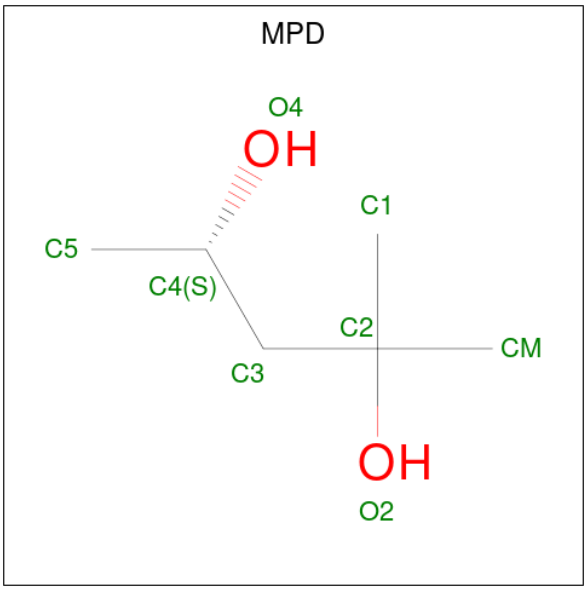
- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*GP*UP*GP*AP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	18	Total	C	H	N	O	P	0	0	0
			581	172	195	70	126	18			
2	H	18	Total	C	H	N	O	P	0	0	0
			581	172	195	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*AP*AP*TP*AP*AP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	21	Total	C	H	N	O	P	0	0	0
			636	195	226	70	124	21			
3	J	22	Total	C	H	N	O	P	0	0	0
			682	209	242	78	131	22			

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

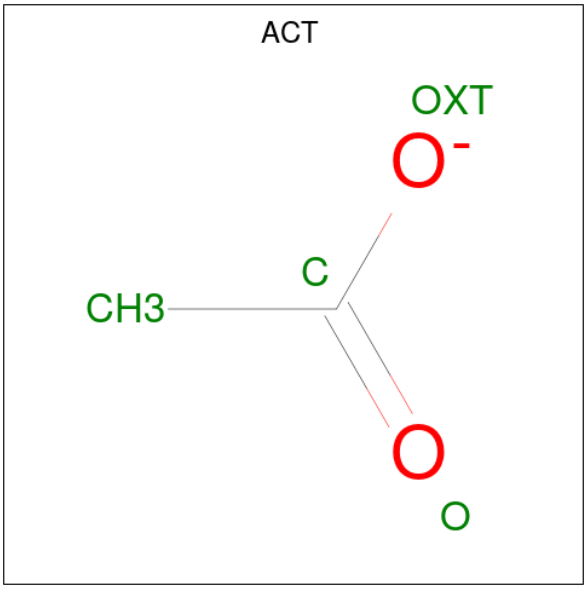


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 22 6 14 2	0	0
4	G	1	Total C H O 22 6 14 2	0	0
4	F	1	Total C H O 22 6 14 2	0	0
4	F	1	Total C H O 22 6 14 2	0	0
4	J	1	Total C H O 22 6 14 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Mg 1 1	0	0
5	H	1	Total Mg 1 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C H O 7 2 3 2	0	0

- Molecule 7 is water.

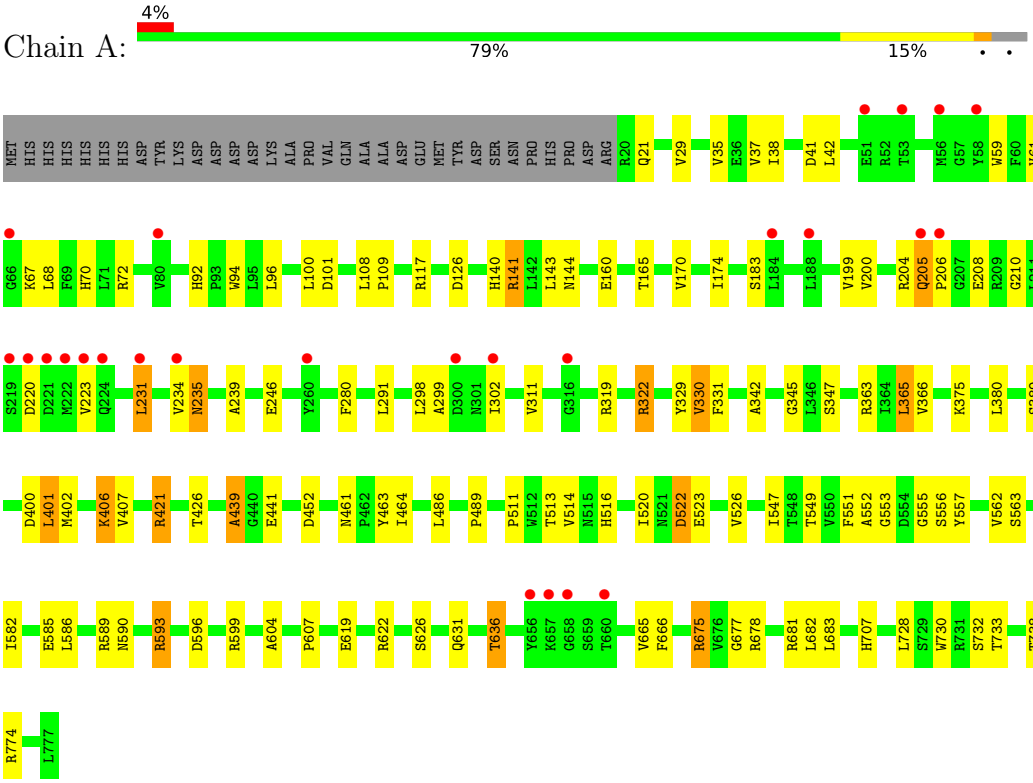
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	163	Total O 163 163	0	0
7	C	20	Total O 20 20	0	0
7	G	19	Total O 19 19	0	0
7	F	173	Total O 173 173	0	0
7	H	29	Total O 29 29	0	0
7	J	17	Total O 17 17	0	0

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.

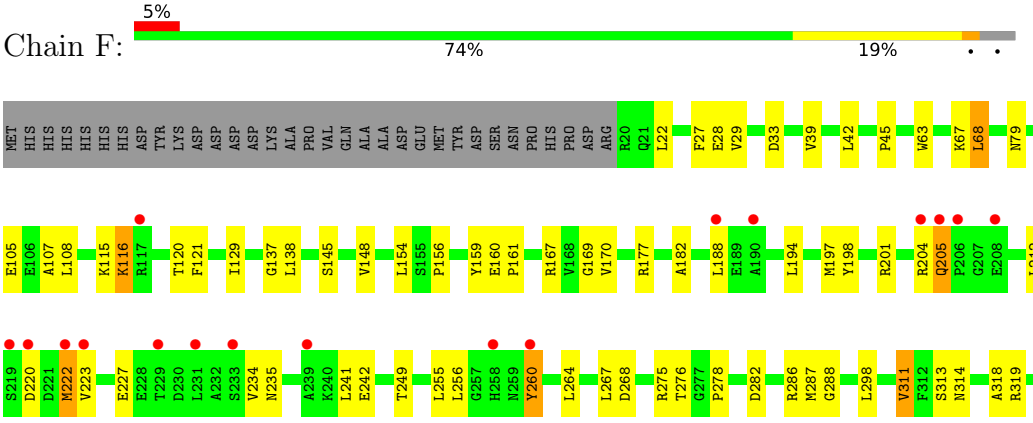
• Molecule 1: Uncharacterized protein

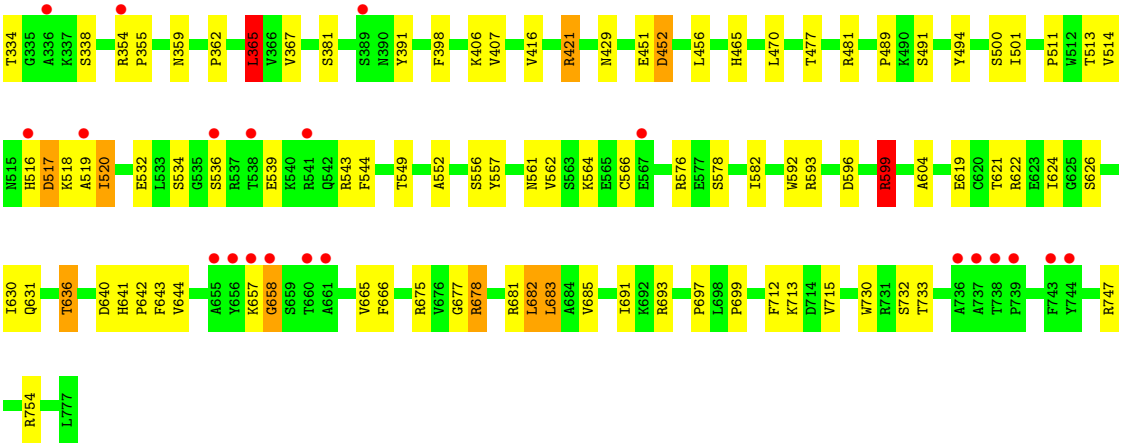
Chain A:



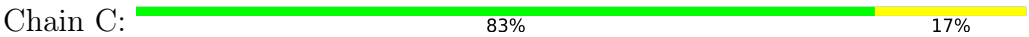
• Molecule 1: Uncharacterized protein

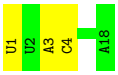
Chain F:



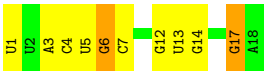


• Molecule 2: RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*GP*UP*GP*AP*CP*GP*A)-3')

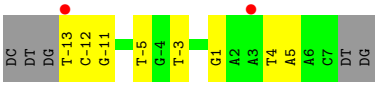




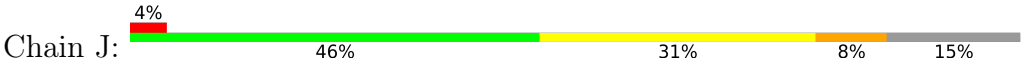
• Molecule 2: RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*GP*UP*GP*AP*CP*GP*A)-3')

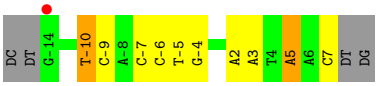


• Molecule 3: DNA (5'-D(P*TP*CP*GP*TP*CP*AP*CP*CP*TP*GP*TP*GP*CP*AP*GP*AP*AP*TP*AP*AP*C)-3')



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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.41Å 118.98Å 118.82Å 90.00° 95.51° 90.00°	Depositor
Resolution (Å)	42.66 – 2.25 42.67 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.66-2.25) 93.1 (42.67-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.24Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.239 0.202 , 0.203	Depositor DCC
R_{free} test set	4414 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	25923	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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: MPD, MG, ACT

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	0.38	0/5976	0.59	1/8120 (0.0%)
1	F	0.39	0/5888	0.60	3/8014 (0.0%)
2	C	0.67	1/431 (0.2%)	0.94	0/668
2	H	0.75	1/431 (0.2%)	1.05	1/668 (0.1%)
3	G	1.18	1/458 (0.2%)	1.21	2/703 (0.3%)
3	J	1.26	2/492 (0.4%)	1.26	1/756 (0.1%)
All	All	0.51	5/13676 (0.0%)	0.70	8/18929 (0.0%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	U	OP3-P	-11.10	1.47	1.61
2	C	1	U	OP3-P	-9.81	1.49	1.61
3	G	-13	DT	C5-C7	-5.82	1.46	1.50
3	J	5	DA	C3'-O3'	5.45	1.51	1.44
3	J	-10	DT	C5-C7	-5.03	1.47	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	599	ARG	NE-CZ-NH1	7.83	124.22	120.30
3	G	5	DA	O4'-C4'-C3'	-7.73	101.36	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	599	ARG	CG-CD-NE	-7.54	95.97	111.80
3	J	-5	DT	O4'-C1'-N1	6.12	112.28	108.00
1	A	365	LEU	CA-CB-CG	5.78	128.60	115.30
1	F	365	LEU	CA-CB-CG	5.50	127.94	115.30
2	H	6	G	N3-C4-N9	-5.23	122.86	126.00
3	G	-3	DT	C4'-C3'-C2'	5.12	107.71	103.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	599	ARG	Sidechain

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	5847	5733	5743	90	0
1	F	5760	5563	5574	120	0
2	C	386	195	195	3	0
2	H	386	195	195	8	0
3	G	410	226	227	5	0
3	J	440	242	243	8	0
4	A	8	14	14	14	0
4	F	16	28	28	5	0
4	G	8	14	14	4	0
4	J	8	14	14	1	0
5	C	1	0	0	0	0
5	H	1	0	0	0	0
6	F	4	3	3	0	0
7	A	163	0	0	7	0
7	C	20	0	0	0	0
7	F	173	0	0	11	0
7	G	19	0	0	1	0
7	H	29	0	0	0	0
7	J	17	0	0	1	0
All	All	13696	12227	12250	231	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 9.

All (231) 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:707:HIS:HB2	4:A:801:MPD:H53	1.49	0.94
1:F:513:THR:HG21	1:F:556:SER:HB2	1.49	0.94
1:A:61:VAL:HG13	1:A:68:LEU:HD21	1.48	0.93
1:F:129:ILE:HG12	1:F:148:VAL:HG12	1.49	0.93
1:A:707:HIS:HA	4:A:801:MPD:H31	1.50	0.93
1:F:513:THR:HG23	1:F:557:TYR:O	1.76	0.86
1:A:513:THR:HG21	1:A:556:SER:HB3	1.60	0.81
1:F:223:VAL:HB	1:F:234:VAL:O	1.82	0.80
1:A:607:PRO:HB3	4:A:801:MPD:H4	1.64	0.79
1:F:624:ILE:HD11	1:F:630:ILE:HG13	1.65	0.78
1:A:421:ARG:HH21	1:A:421:ARG:HG3	1.50	0.77
1:A:513:THR:HG23	1:A:557:TYR:O	1.86	0.76
1:F:624:ILE:HD11	1:F:630:ILE:CG1	2.17	0.74
1:A:516:HIS:O	1:A:555:GLY:HA2	1.87	0.74
1:F:268:ASP:OD2	1:F:693:ARG:NH2	2.22	0.73
1:A:421:ARG:HG3	1:A:421:ARG:NH2	2.03	0.73
3:J:-6:DC:OP1	7:J:201:HOH:O	2.09	0.71
1:A:774:ARG:NH2	7:A:902:HOH:O	2.24	0.70
1:F:513:THR:HG22	1:F:514:VAL:N	2.07	0.68
1:A:513:THR:HG21	1:A:556:SER:CB	2.24	0.67
1:F:631:GLN:HB3	1:F:712:PHE:HB2	1.77	0.66
1:A:707:HIS:CA	4:A:801:MPD:H31	2.24	0.65
1:F:242:GLU:OE1	7:F:901:HOH:O	2.15	0.64
4:G:101:MPD:H12	4:G:101:MPD:H53	1.81	0.63
1:F:311:VAL:HG12	4:F:802:MPD:H4	1.80	0.63
1:F:161:PRO:HB3	4:F:802:MPD:O2	1.99	0.62
1:A:375:LYS:HG2	1:A:486:LEU:HD21	1.80	0.62
1:F:85:ARG:NH1	7:F:906:HOH:O	2.28	0.62
2:C:3:A:N6	4:G:101:MPD:H51	2.14	0.61
1:A:585:GLU:O	1:A:589:ARG:HG2	2.00	0.61
1:F:501:ILE:HD11	1:F:733:THR:HG22	1.82	0.60
1:F:260:TYR:OH	1:F:264:LEU:HD11	2.02	0.60
1:A:549:THR:HG21	1:A:582:ILE:CD1	2.31	0.60
1:F:276:THR:HG23	7:F:1048:HOH:O	2.01	0.59
1:F:576:ARG:HD3	1:F:619:GLU:HG3	1.84	0.59
1:A:101:ASP:OD2	1:A:117:ARG:NH2	2.35	0.59
1:A:29:VAL:HG11	1:A:100:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:LEU:HD22	1:F:197:MET:HE1	1.85	0.58
1:F:494:TYR:CE2	3:J:5:DA:H2'	2.38	0.58
1:A:322:ARG:NH1	7:A:913:HOH:O	2.36	0.58
1:A:363:ARG:NH1	1:A:441:GLU:O	2.36	0.58
1:F:311:VAL:HG12	4:F:802:MPD:C4	2.33	0.58
1:F:222:MET:N	7:F:915:HOH:O	2.38	0.57
1:A:174:ILE:HD12	1:A:280:PHE:HD1	1.69	0.57
1:A:513:THR:HG22	1:A:514:VAL:N	2.18	0.57
1:F:643:PHE:HB3	1:F:682:LEU:HD21	1.86	0.56
3:G:1:DG:O6	4:G:101:MPD:H52	2.05	0.56
4:F:802:MPD:H52	4:F:802:MPD:CM	2.35	0.56
1:A:607:PRO:HB3	4:A:801:MPD:H11	1.89	0.55
1:F:513:THR:HG22	1:F:514:VAL:H	1.70	0.55
1:F:160:GLU:HB2	1:F:677:GLY:HA2	1.88	0.55
1:A:21:GLN:HG3	1:A:311:VAL:CG1	2.37	0.55
1:A:607:PRO:HB2	4:A:801:MPD:HM2	1.89	0.54
1:F:421:ARG:HG2	1:F:456:LEU:HD21	1.89	0.54
1:A:576:ARG:HG2	1:A:576:ARG:HH11	1.72	0.54
1:A:217:ALA:O	1:A:223:VAL:HG23	2.07	0.54
1:F:681:ARG:CZ	1:F:715:VAL:HG13	2.38	0.54
1:A:636:THR:CG2	4:A:801:MPD:C4	2.85	0.53
2:H:12:G:H2'	2:H:13:U:O4'	2.08	0.53
1:F:599:ARG:NH1	1:F:631:GLN:OE1	2.42	0.53
1:A:174:ILE:HD12	1:A:280:PHE:CD1	2.44	0.53
1:A:604:ALA:O	1:A:636:THR:HA	2.09	0.53
1:F:255:LEU:C	1:F:256:LEU:HD12	2.28	0.53
1:A:599:ARG:HD3	1:A:631:GLN:OE1	2.08	0.53
1:F:513:THR:HG21	1:F:556:SER:CB	2.29	0.53
1:A:607:PRO:CB	4:A:801:MPD:HM2	2.40	0.52
1:A:513:THR:HG22	1:A:514:VAL:H	1.74	0.52
1:F:314:ASN:HA	1:F:318:ALA:O	2.09	0.52
1:F:520:ILE:HD13	1:F:599:ARG:NH2	2.25	0.52
1:F:79:ASN:ND2	7:F:921:HOH:O	2.43	0.52
1:A:391:TYR:CE1	1:A:489:PRO:HB2	2.45	0.51
1:F:624:ILE:HD11	1:F:630:ILE:HG12	1.92	0.51
1:A:439:ALA:N	7:A:916:HOH:O	2.44	0.51
1:F:161:PRO:HG3	1:F:167:ARG:HE	1.75	0.51
1:F:543:ARG:NH2	2:H:14:G:OP1	2.41	0.51
3:J:7:DC:H2'	3:J:7:DC:O2	2.09	0.51
1:F:513:THR:CG2	1:F:556:SER:HB2	2.31	0.51
1:A:707:HIS:HD2	4:A:801:MPD:H52	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:HIS:CD2	4:A:801:MPD:H52	2.45	0.51
1:F:362:PRO:HG2	1:F:407:VAL:HG22	1.93	0.51
1:A:319:ARG:NH1	7:A:920:HOH:O	2.44	0.50
1:F:513:THR:CG2	1:F:514:VAL:N	2.74	0.50
1:A:523:GLU:HB3	1:A:552:ALA:HB2	1.94	0.50
1:A:200:VAL:HG23	1:A:210:GLY:C	2.32	0.50
2:H:6:G:H2'	2:H:7:C:O4'	2.12	0.50
1:F:148:VAL:HA	1:F:177:ARG:O	2.11	0.49
1:A:636:THR:HG23	4:A:801:MPD:O4	2.12	0.49
1:A:421:ARG:HH21	1:A:421:ARG:CG	2.20	0.49
1:F:194:LEU:HD22	1:F:197:MET:CE	2.42	0.49
1:F:249:THR:HG22	1:F:260:TYR:OH	2.11	0.49
1:F:641:HIS:HB2	1:F:642:PRO:HD2	1.93	0.49
1:A:553:GLY:N	1:A:556:SER:O	2.36	0.49
1:F:145:SER:OG	1:F:182:ALA:HB2	2.11	0.49
1:A:331:PHE:CE1	1:A:345:GLY:HA3	2.48	0.49
1:F:42:LEU:HD13	1:F:68:LEU:HG	1.94	0.49
1:F:578:SER:O	1:F:582:ILE:HD12	2.12	0.49
1:A:665:VAL:O	1:A:666:PHE:HB2	2.13	0.48
1:A:707:HIS:CB	4:A:801:MPD:H53	2.34	0.48
1:F:593:ARG:N	1:F:596:ASP:OD2	2.42	0.48
1:A:68:LEU:HD22	1:A:70:HIS:CE1	2.48	0.48
1:F:29:VAL:CG2	1:F:170:VAL:HG23	2.43	0.48
1:A:299:ALA:HB3	1:A:302:ILE:HG12	1.95	0.48
1:A:299:ALA:HB3	1:A:302:ILE:CD1	2.44	0.48
1:A:636:THR:CG2	4:A:801:MPD:O4	2.60	0.48
3:J:7:DC:O2	3:J:7:DC:C2'	2.62	0.48
1:A:212:LEU:HD13	1:A:234:VAL:HG21	1.96	0.48
1:A:747:ARG:HD2	7:A:939:HOH:O	2.11	0.48
1:F:121:PHE:HZ	1:F:287:MET:HE2	1.78	0.48
1:F:452:ASP:OD1	1:F:452:ASP:N	2.45	0.48
4:F:802:MPD:H52	4:F:802:MPD:HM1	1.95	0.47
1:A:576:ARG:HD2	1:A:619:GLU:HG3	1.96	0.47
1:F:544:PHE:HB3	1:F:566:CYS:HB2	1.95	0.47
1:F:516:HIS:CE1	1:F:518:LYS:HG2	2.50	0.47
1:F:604:ALA:O	1:F:636:THR:HA	2.15	0.47
1:F:275:ARG:CD	7:F:924:HOH:O	2.62	0.47
1:A:21:GLN:HG3	1:A:311:VAL:HG11	1.97	0.47
1:A:406:LYS:HG2	1:A:407:VAL:N	2.29	0.47
1:F:105:GLU:OE1	1:F:116:LYS:HE2	2.15	0.47
1:F:197:MET:HE3	1:F:241:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:599:ARG:NH1	1:F:712:PHE:CE1	2.83	0.47
1:F:282:ASP:O	1:F:286:ARG:HG3	2.15	0.47
1:A:235:ASN:OD1	1:A:235:ASN:N	2.47	0.47
1:F:640:ASP:O	3:J:-7:DC:H3'	2.14	0.47
3:G:1:DG:O6	4:G:101:MPD:C5	2.64	0.46
1:F:197:MET:HE3	1:F:241:LEU:CD2	2.45	0.46
1:F:501:ILE:CD1	1:F:733:THR:HG22	2.43	0.46
3:G:1:DG:H2"	3:G:4:DT:OP2	2.15	0.46
1:F:275:ARG:HB3	1:F:697:PRO:HB3	1.97	0.46
2:H:3:A:H2'	2:H:4:C:C6	2.50	0.46
1:A:329:TYR:CE2	1:A:342:ALA:HB2	2.50	0.46
1:A:520:ILE:HD13	1:A:599:ARG:CZ	2.45	0.46
1:A:92:HIS:HB3	1:A:94:TRP:NE1	2.30	0.46
1:A:108:LEU:HD11	1:A:291:LEU:HD21	1.97	0.46
1:A:160:GLU:HB2	1:A:677:GLY:HA2	1.96	0.46
1:F:222:MET:HA	1:F:222:MET:CE	2.46	0.46
1:A:636:THR:CG2	4:A:801:MPD:H4	2.46	0.46
1:F:516:HIS:HB3	1:F:557:TYR:CE2	2.50	0.46
2:H:17:G:H8	2:H:17:G:H5"	1.81	0.46
1:A:366:VAL:HG11	1:A:380:LEU:HD11	1.97	0.45
1:F:549:THR:HG21	1:F:582:ILE:CD1	2.47	0.45
1:F:275:ARG:NE	7:F:924:HOH:O	2.49	0.45
1:A:29:VAL:HG21	1:A:170:VAL:HG23	1.99	0.45
1:A:330:VAL:HG22	1:A:513:THR:HB	1.98	0.45
1:A:522:ASP:OD2	1:A:590:ASN:ND2	2.46	0.45
1:F:747:ARG:HA	1:F:747:ARG:NE	2.32	0.45
1:F:29:VAL:HG21	1:F:170:VAL:HG23	1.99	0.45
1:F:154:LEU:HD11	1:F:287:MET:CE	2.46	0.45
1:F:513:THR:CG2	1:F:514:VAL:H	2.30	0.45
1:F:234:VAL:CG1	1:F:235:ASN:N	2.80	0.45
1:A:675:ARG:HG3	1:A:681:ARG:CZ	2.47	0.44
1:F:201:ARG:NH1	1:F:212:LEU:HD21	2.32	0.44
7:F:968:HOH:O	2:H:5:U:H4'	2.17	0.44
1:F:561:ASN:ND2	7:F:928:HOH:O	2.50	0.44
1:F:154:LEU:HD11	1:F:287:MET:HE2	1.99	0.44
1:A:738:THR:OG1	1:A:739:PRO:HD2	2.18	0.44
1:A:547:ILE:HB	1:A:563:SER:HB3	1.99	0.44
1:F:516:HIS:CE1	1:F:552:ALA:HB1	2.52	0.44
1:A:143:LEU:HD23	1:A:143:LEU:HA	1.84	0.44
1:A:205:GLN:O	1:A:208:GLU:N	2.51	0.44
1:F:391:TYR:CE2	1:F:489:PRO:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:HIS:ND1	1:A:141:ARG:N	2.65	0.44
1:A:96:LEU:HD22	1:A:298:LEU:HD13	1.99	0.43
1:F:657:LYS:N	1:F:658:GLY:HA2	2.33	0.43
1:A:678:ARG:NH2	1:A:678:ARG:HB3	2.33	0.43
1:F:665:VAL:O	1:F:666:PHE:HB2	2.18	0.43
1:A:37:VAL:CG1	1:A:38:ILE:N	2.81	0.43
1:F:218:ILE:CG2	1:F:218:ILE:O	2.65	0.43
1:A:205:GLN:H	1:A:205:GLN:HG2	1.63	0.43
3:G:-12:DC:H2'	3:G:-11:DG:C8	2.52	0.43
1:F:188:LEU:HG	1:F:218:ILE:HG21	2.00	0.43
1:F:107:ALA:C	1:F:108:LEU:HD12	2.39	0.43
1:F:148:VAL:HG11	1:F:267:LEU:HD11	2.01	0.43
1:F:691:ILE:HD11	1:F:699:PRO:HG3	1.99	0.43
1:F:429:ASN:HD21	1:F:465:HIS:HB3	1.83	0.43
1:F:532:GLU:O	3:J:-4:DG:H5"	2.19	0.42
1:A:401:LEU:HD13	1:A:402:MET:HE2	2.01	0.42
1:F:198:TYR:CZ	1:F:214:ARG:HD3	2.54	0.42
1:F:362:PRO:HD2	1:F:406:LYS:O	2.18	0.42
1:F:549:THR:HG21	1:F:582:ILE:HD13	2.02	0.42
3:J:2:DA:H2"	3:J:3:DA:OP1	2.18	0.42
1:A:551:PHE:CD2	1:A:586:LEU:HD11	2.54	0.42
1:F:354:ARG:N	1:F:355:PRO:CD	2.82	0.42
1:F:683:LEU:HD13	1:F:685:VAL:CG1	2.49	0.42
1:F:365:LEU:HD13	1:F:367:VAL:CG2	2.50	0.42
1:F:137:GLY:C	1:F:138:LEU:HD12	2.40	0.42
1:F:543:ARG:HH22	2:H:14:G:P	2.42	0.42
1:F:276:THR:HG22	1:F:278:PRO:HD2	2.01	0.42
1:F:398:PHE:HD1	1:F:500:SER:HB3	1.85	0.42
1:A:439:ALA:HA	7:A:916:HOH:O	2.19	0.42
1:F:732:SER:HB3	2:H:3:A:O2'	2.20	0.42
4:J:101:MPD:H11	4:J:101:MPD:O4	2.19	0.42
1:A:59:TRP:CZ3	1:A:72:ARG:HB2	2.55	0.42
1:A:732:SER:HB3	2:C:3:A:O2'	2.20	0.42
1:F:39:VAL:CG1	1:F:67:LYS:HG2	2.50	0.42
1:F:27:PHE:CZ	1:F:288:GLY:HA3	2.55	0.41
1:F:197:MET:HE1	1:F:241:LEU:HD11	2.02	0.41
1:F:314:ASN:OD1	1:F:319:ARG:HA	2.19	0.41
1:F:28:GLU:HG2	1:F:159:TYR:OH	2.19	0.41
1:F:198:TYR:CE1	1:F:214:ARG:HD3	2.55	0.41
1:F:330:VAL:CG2	1:F:513:THR:HB	2.50	0.41
1:F:470:LEU:HD13	1:F:477:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:-10:DT:C4	3:J:-9:DC:N4	2.87	0.41
1:F:204:ARG:O	1:F:205:GLN:CB	2.67	0.41
1:F:511:PRO:HD2	1:F:730:TRP:CE2	2.55	0.41
3:G:-5:DT:H5'	7:G:212:HOH:O	2.20	0.41
1:F:39:VAL:HG12	1:F:67:LYS:HG2	2.03	0.41
1:A:461:ASN:OD1	1:A:463:TYR:HB3	2.20	0.41
1:F:451:GLU:OE2	1:F:481:ARG:NH1	2.51	0.41
1:A:322:ARG:CZ	7:A:913:HOH:O	2.68	0.41
1:A:593:ARG:N	1:A:596:ASP:OD2	2.41	0.41
1:F:45:PRO:HG3	1:F:63:TRP:CZ2	2.56	0.41
1:F:416:VAL:HA	7:F:978:HOH:O	2.20	0.41
1:F:621:THR:HG23	1:F:630:ILE:HD13	2.03	0.41
1:F:754:ARG:NH1	7:F:919:HOH:O	2.40	0.41
1:A:199:VAL:HG13	1:A:239:ALA:HB1	2.01	0.41
1:F:156:PRO:HA	1:F:169:GLY:O	2.21	0.41
1:F:517:ASP:O	1:F:519:ALA:N	2.53	0.41
1:F:592:TRP:HZ3	1:F:624:ILE:HB	1.85	0.41
1:A:421:ARG:HH12	1:A:452:ASP:HB3	1.85	0.41
1:A:464:ILE:HD12	1:A:464:ILE:HA	1.91	0.41
1:A:619:GLU:OE1	1:A:622:ARG:NH1	2.54	0.41
1:F:218:ILE:O	1:F:218:ILE:HG22	2.22	0.40
1:F:332:ASP:OD1	1:F:334:THR:N	2.53	0.40
1:A:549:THR:HG21	1:A:582:ILE:HD11	2.01	0.40
2:C:3:A:H2'	2:C:4:C:C6	2.56	0.40
1:F:227:GLU:OE1	1:F:536:SER:HB2	2.22	0.40
1:F:678:ARG:HH12	1:F:713:LYS:HE2	1.86	0.40
1:A:42:LEU:HD22	1:A:68:LEU:HD12	2.03	0.40
1:A:511:PRO:HD2	1:A:730:TRP:CE2	2.56	0.40
1:F:96:LEU:HD22	1:F:298:LEU:HD13	2.02	0.40
1:F:520:ILE:HD12	1:F:599:ARG:HB3	2.03	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	756/791 (96%)	729 (96%)	24 (3%)	3 (0%)	34	37
1	F	756/791 (96%)	724 (96%)	30 (4%)	2 (0%)	41	46
All	All	1512/1582 (96%)	1453 (96%)	54 (4%)	5 (0%)	41	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	ALA
1	A	231	LEU
1	F	205	GLN
1	A	206	PRO
1	F	658	GLY

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	602/672 (90%)	563 (94%)	39 (6%)	17	16
1	F	583/672 (87%)	549 (94%)	34 (6%)	20	20
All	All	1185/1344 (88%)	1112 (94%)	73 (6%)	18	17

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	41	ASP
1	A	67	LYS
1	A	109	PRO
1	A	126	ASP
1	A	141	ARG
1	A	144	ASN
1	A	165	THR

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Mol	Chain	Res	Type
1	A	183	SER
1	A	204	ARG
1	A	205	GLN
1	A	218	ILE
1	A	220	ASP
1	A	231	LEU
1	A	235	ASN
1	A	246	GLU
1	A	322	ARG
1	A	330	VAL
1	A	347	SER
1	A	365	LEU
1	A	389	SER
1	A	395	SER
1	A	400	ASP
1	A	401	LEU
1	A	406	LYS
1	A	421	ARG
1	A	426	THR
1	A	522	ASP
1	A	526	VAL
1	A	562	VAL
1	A	578	SER
1	A	593	ARG
1	A	626	SER
1	A	636	THR
1	A	675	ARG
1	A	682	LEU
1	A	683	LEU
1	A	728	LEU
1	A	733	THR
1	F	22	LEU
1	F	33	ASP
1	F	68	LEU
1	F	115	LYS
1	F	116	LYS
1	F	120	THR
1	F	214	ARG
1	F	218	ILE
1	F	220	ASP
1	F	222	MET
1	F	260	TYR

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Mol	Chain	Res	Type
1	F	311	VAL
1	F	313	SER
1	F	338	SER
1	F	359	ASN
1	F	365	LEU
1	F	381	SER
1	F	421	ARG
1	F	452	ASP
1	F	491	SER
1	F	517	ASP
1	F	520	ILE
1	F	534	SER
1	F	539	GLU
1	F	562	VAL
1	F	564	LYS
1	F	622	ARG
1	F	626	SER
1	F	636	THR
1	F	644	VAL
1	F	675	ARG
1	F	678	ARG
1	F	682	LEU
1	F	683	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	17/18 (94%)	0	0
2	H	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	H	17	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
6	ACT	F	803	-	3,3,3	0.97	0	3,3,3	1.49	0
4	MPD	F	801	-	7,7,7	0.26	0	9,10,10	0.61	0
4	MPD	J	101	-	7,7,7	0.26	0	9,10,10	0.23	0
4	MPD	G	101	-	7,7,7	0.20	0	9,10,10	0.62	0
4	MPD	A	801	-	7,7,7	0.14	0	9,10,10	1.32	1 (11%)
4	MPD	F	802	-	7,7,7	0.23	0	9,10,10	1.06	1 (11%)

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
4	MPD	F	801	-	-	1/5/5/5	-
4	MPD	J	101	-	-	0/5/5/5	-
4	MPD	G	101	-	-	1/5/5/5	-
4	MPD	A	801	-	-	2/5/5/5	-
4	MPD	F	802	-	-	1/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	802	MPD	O2-C2-C3	-2.44	100.64	109.80
4	A	801	MPD	C5-C4-C3	2.16	121.85	111.69

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	MPD	C2-C3-C4-O4
4	A	801	MPD	C2-C3-C4-C5
4	G	101	MPD	C2-C3-C4-C5
4	F	802	MPD	C2-C3-C4-O4
4	F	801	MPD	C2-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	101	MPD	1	0
4	G	101	MPD	4	0
4	A	801	MPD	14	0
4	F	802	MPD	5	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%)	0.15	29 (3%) 40 43	26, 47, 81, 122	1 (0%)
1	F	758/791 (95%)	0.33	40 (5%) 26 29	29, 51, 85, 131	2 (0%)
2	C	18/18 (100%)	0.05	0 100 100	31, 39, 67, 95	0
2	H	18/18 (100%)	0.27	0 100 100	35, 42, 58, 67	0
3	G	21/26 (80%)	0.14	2 (9%) 8 8	37, 52, 100, 113	0
3	J	22/26 (84%)	0.24	1 (4%) 33 36	38, 53, 93, 125	0
All	All	1595/1670 (95%)	0.23	72 (4%) 33 36	26, 49, 83, 131	3 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	658	GLY	6.8
1	F	218	ILE	6.3
1	F	656	TYR	5.8
1	A	658	GLY	5.8
1	A	188	LEU	5.3
1	F	222	MET	4.8
1	F	655	ALA	4.4
1	F	260	TYR	4.4
1	F	231	LEU	4.3
1	F	208	GLU	4.2
1	F	661	ALA	4.2
1	A	220	ASP	4.2
1	A	660	THR	4.1
1	F	737	ALA	3.9
1	F	538	THR	3.9
1	A	234	VAL	3.8
1	A	231	LEU	3.8
1	F	660	THR	3.7
1	A	206	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	656	TYR	3.6
1	F	657	LYS	3.6
1	F	223	VAL	3.6
1	F	567	GLU	3.4
1	F	188	LEU	3.4
1	A	218	ILE	3.3
1	A	66	GLY	3.3
1	A	219	SER	3.3
1	F	204	ARG	3.3
3	G	-13	DT	3.3
1	A	657	LYS	3.2
1	F	233	SER	3.0
1	F	541	ARG	3.0
1	A	221	ASP	2.9
1	F	744	TYR	2.9
1	A	260	TYR	2.8
1	F	220	ASP	2.7
1	F	516	HIS	2.7
1	A	63	TRP	2.7
1	A	300	ASP	2.6
1	A	316	GLY	2.6
1	A	224	GLN	2.6
1	A	53	THR	2.6
1	F	736	ALA	2.6
1	F	519	ALA	2.5
1	F	743	PHE	2.5
1	A	222	MET	2.5
1	A	56	MET	2.4
1	F	258	HIS	2.4
1	F	389	SER	2.4
1	A	58	TYR	2.4
1	A	223	VAL	2.3
3	J	-14	DG	2.3
1	A	184	LEU	2.3
1	F	336	ALA	2.3
1	F	229	THR	2.3
1	F	190	ALA	2.3
1	F	239	ALA	2.3
1	F	117	ARG	2.3
1	A	51	GLU	2.2
3	G	3	DA	2.2
1	F	536	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	205	GLN	2.2
1	F	738	THR	2.1
1	F	739	PRO	2.1
1	A	80	VAL	2.1
1	F	330	VAL	2.1
1	F	354	ARG	2.1
1	F	206	PRO	2.1
1	F	205	GLN	2.1
1	A	64	PHE	2.1
1	F	219	SER	2.0
1	A	302	ILE	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
6	ACT	F	803	4/4	0.67	0.21	56,58,67,67	0
4	MPD	G	101	8/8	0.81	0.38	50,79,100,100	0
4	MPD	F	802	8/8	0.83	0.38	60,72,85,85	0
4	MPD	A	801	8/8	0.85	0.32	36,46,72,73	0
4	MPD	J	101	8/8	0.92	0.24	63,80,94,94	0
4	MPD	F	801	8/8	0.94	0.20	54,67,81,81	0
5	MG	C	101	1/1	0.97	0.09	28,28,28,28	0
5	MG	H	101	1/1	0.98	0.23	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.