



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 07:26 AM UTC

PDB ID : 6D8A / pdb_00006d8a
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 wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

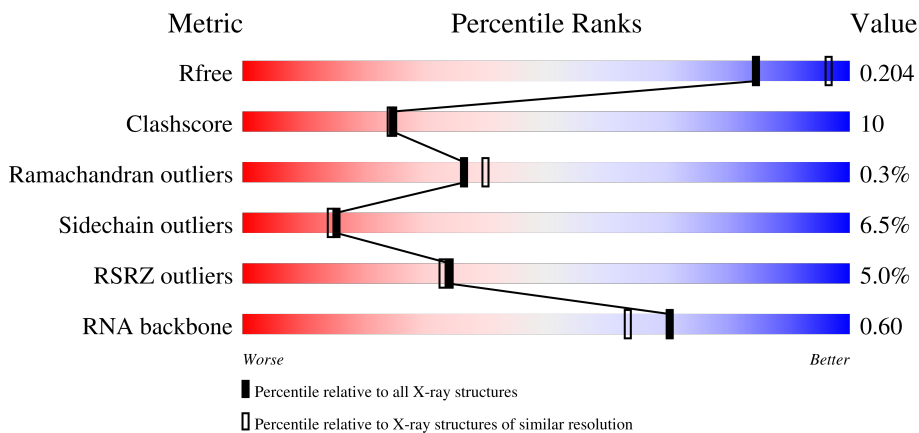
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)
RNA backbone	3983	1005 (2.56-1.96)

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 $\leq 5\%$. 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	791	 4% 77% 16% . .
1	F	791	 6% 73% 21% . .
2	C	18	 89% 11%
2	H	18	 50% 44% 6%

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Mol	Chain	Length	Quality of chain
3	G	26	
3	J	26	

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
			Total	C	H	N	O	S			
1	A	758	11580	3718	5733	1047	1066	16	0	0	0
1	F	758	11323	3665	5563	1019	1060	16	0	0	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
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

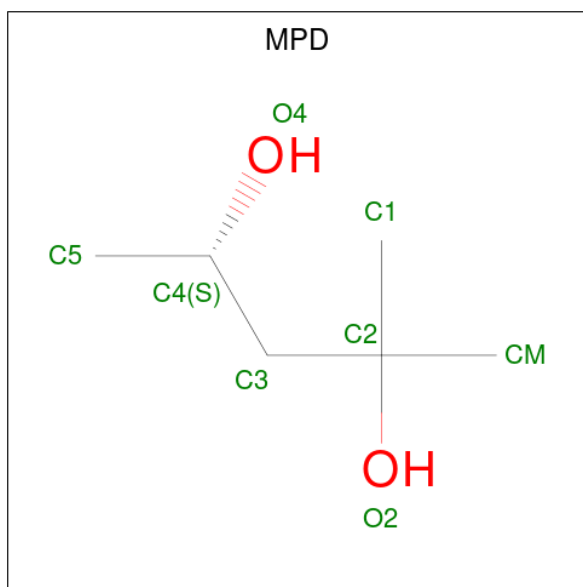
- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*GP*UP*GP*AP*CP*GP*A)-3').

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 (CCD ID: MPD) (formula: C₆H₁₄O₂).

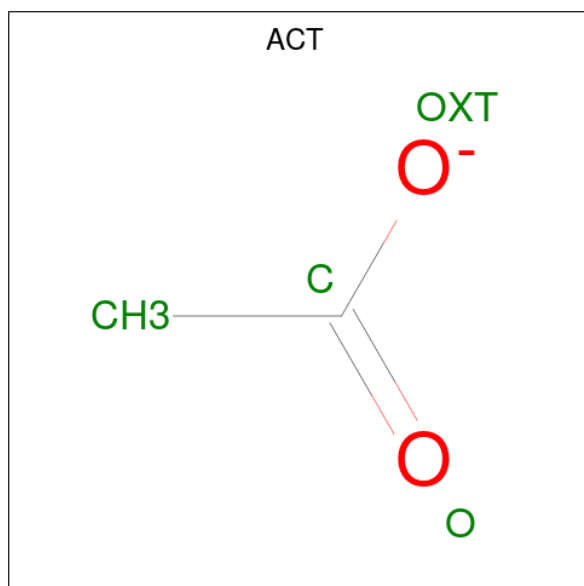


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			22	6	14	2		
4	G	1	Total	C	H	O	0	0
			22	6	14	2		
4	F	1	Total	C	H	O	0	0
			22	6	14	2		
4	F	1	Total	C	H	O	0	0
			22	6	14	2		
4	J	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

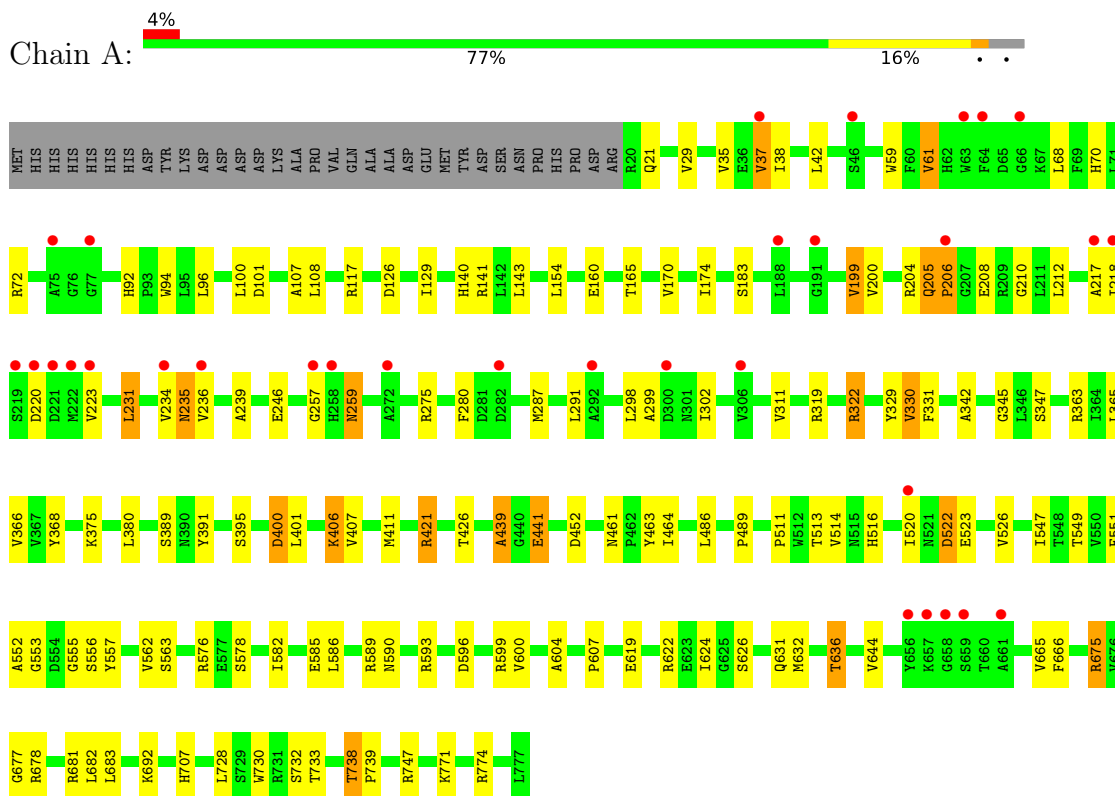
- Molecule 7 is water.

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

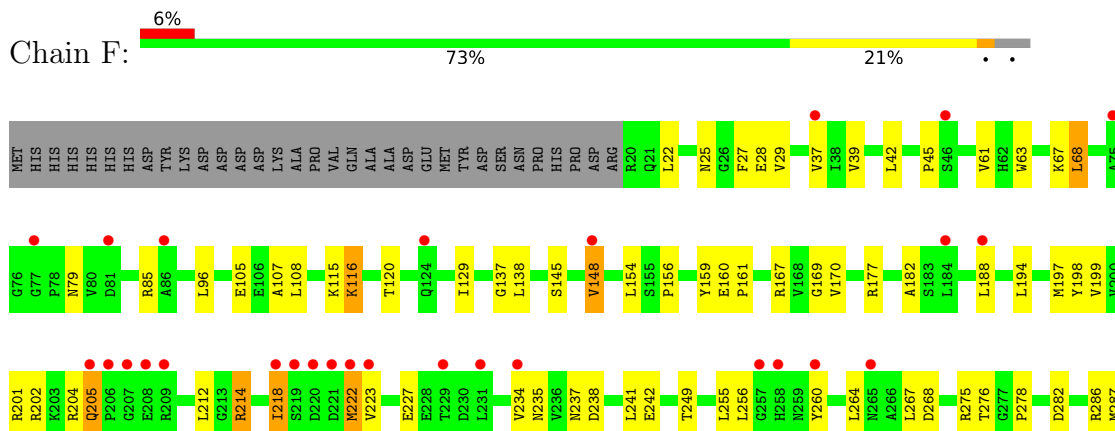
3 Residue-property plots [i](#)

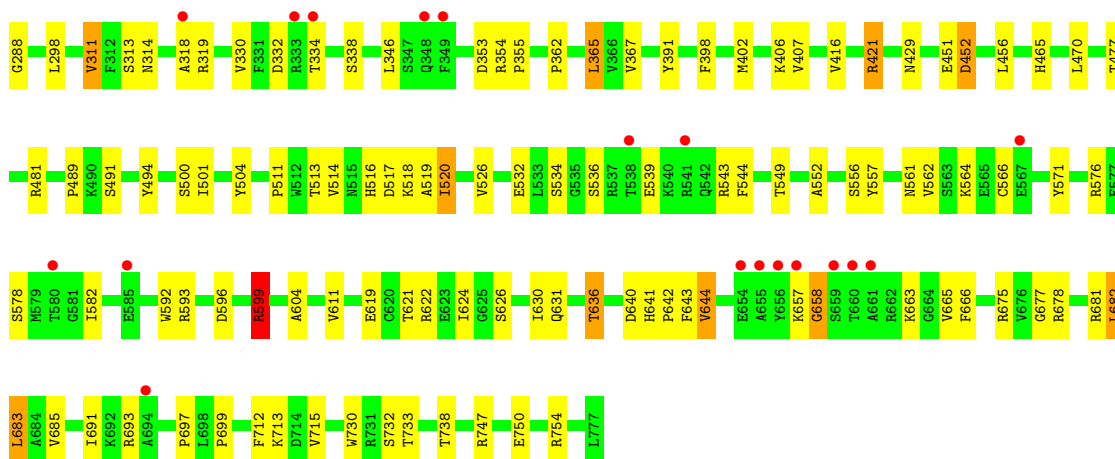
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



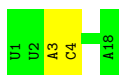
- Molecule 1: Uncharacterized protein





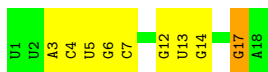
- Molecule 2: RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*GP*UP*GP*AP*C P*GP*A)-3')

Chain C: 89% 11%



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

Chain H: 50% 44% 6%



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

Chain G: 62% 19% 19%



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

Chain J: 4% 50% 35% 15%



4 Data and refinement statistics

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 42.66 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.66-2.25) 93.1 (42.66-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.24Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.239 0.203 , 0.204	Depositor DCC
R_{free} test set	4414 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtrriage
Anisotropy	0.297	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25923	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.31	0/5976	0.55	0/8120
1	F	0.34	1/5888 (0.0%)	0.55	1/8014 (0.0%)
2	C	0.27	0/431	0.50	0/668
2	H	0.28	0/431	0.55	0/668
3	G	0.62	0/458	0.80	0/703
3	J	0.64	0/492	0.87	0/756
All	All	0.35	1/13676 (0.0%)	0.57	1/18929 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	148	VAL	C-N	7.77	1.39	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	599	ARG	CG-CD-NE	-7.29	95.97	112.00

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	99	0
1	F	5760	5563	5574	130	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	10	0
7	C	20	0	0	0	0
7	F	173	0	0	12	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	250	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 250 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:HIS:HA	4:A:801:MPD:H31	1.50	0.93

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%)	30	31
1	F	756/791 (96%)	724 (96%)	30 (4%)	2 (0%)	36	40
All	All	1512/1582 (96%)	1453 (96%)	54 (4%)	5 (0%)	36	40

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	602/672 (90%)	558 (93%)	44 (7%)	13	12
1	F	583/672 (87%)	550 (94%)	33 (6%)	18	19
All	All	1185/1344 (88%)	1108 (94%)	77 (6%)	15	14

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	338	SER
1	F	636	THR
1	F	421	ARG
1	F	539	GLU
1	F	683	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	303	ASN
1	F	429	ASN
1	F	516	HIS
1	A	429	ASN
1	A	767	ASN

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 oligosaccharides 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	1.02	0	3,3,3	1.48	0
4	MPD	F	802	-	7,7,7	0.28	0	9,10,10	1.04	1 (11%)
4	MPD	J	101	-	7,7,7	0.29	0	9,10,10	0.19	0
4	MPD	A	801	-	7,7,7	0.16	0	9,10,10	1.33	2 (22%)
4	MPD	G	101	-	7,7,7	0.23	0	9,10,10	0.67	0
4	MPD	F	801	-	7,7,7	0.29	0	9,10,10	0.61	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
4	MPD	F	802	-	-	3/5/5/5	-
4	MPD	J	101	-	-	2/5/5/5	-
4	MPD	A	801	-	-	3/5/5/5	-
4	MPD	G	101	-	-	1/5/5/5	-
4	MPD	F	801	-	-	0/5/5/5	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	802	MPD	O2-C2-C3	-2.31	100.64	109.27
4	A	801	MPD	C5-C4-C3	2.19	121.85	111.67
4	A	801	MPD	C1-C2-C3	2.03	118.98	110.20

There are no chirality outliers.

5 of 9 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-C5
4	F	802	MPD	C2-C3-C4-O4

There are no ring outliers.

4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	802	MPD	5	0
4	J	101	MPD	1	0
4	A	801	MPD	14	0
4	G	101	MPD	4	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 [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	758/791 (95%)	0.33	32 (4%) 40 40	28, 51, 88, 129	1 (0%)
1	F	758/791 (95%)	0.49	46 (6%) 27 25	30, 56, 93, 144	2 (0%)
2	C	18/18 (100%)	-0.34	0 100 100	32, 42, 73, 104	0
2	H	18/18 (100%)	-0.33	0 100 100	37, 45, 63, 73	0
3	G	21/26 (80%)	0.14	0 100 100	39, 57, 109, 118	0
3	J	22/26 (84%)	0.13	1 (4%) 38 37	41, 57, 101, 133	0
All	All	1595/1670 (95%)	0.39	79 (4%) 34 33	28, 54, 90, 144	3 (0%)

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	221	ASP	4.8
1	F	231	LEU	4.7
1	F	656	TYR	4.2
1	F	209	ARG	4.1
1	F	188	LEU	4.1

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 oligosaccharides 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, 95th 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	0.71	0.20	56,58,67,67	0
4	MPD	A	801	8/8	0.72	0.18	36,46,72,73	0
4	MPD	F	802	8/8	0.75	0.18	60,72,85,85	0
4	MPD	G	101	8/8	0.77	0.18	50,79,100,100	0
4	MPD	J	101	8/8	0.87	0.12	63,80,94,94	0
4	MPD	F	801	8/8	0.89	0.10	54,67,81,81	0
5	MG	H	101	1/1	0.99	0.06	34,34,34,34	0
5	MG	C	101	1/1	0.99	0.03	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.