Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:54 AM UTC

PDB ID	:	7FMM / pdb_00007fmm
Title	:	PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P06D09 from the F2X-Universal Library
Authors	:	Barthel, T.; Wollenhaupt, J.; Lima, G.M.A.; Wahl, M.C.; Weiss, M.S.
Deposited on	:	2022-08-26
Resolution	:	1.69 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:

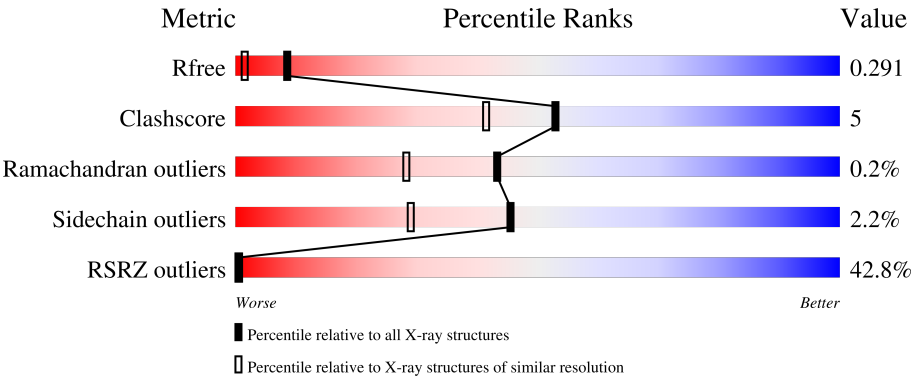
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	258	36% 82% 9% 8%
2	B	308	45% 82% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9210 atoms, of which 4524 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	237	Total	C	H	N	O	S	0	21	0
			4068	1287	2060	336	373	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1833	GLY	-	expression tag	UNP P33334
A	1834	ALA	-	expression tag	UNP P33334
A	1835	MET	-	expression tag	UNP P33334

- Molecule 2 is a protein called A1 cistron-splicing factor AAR2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	300	Total	C	H	N	O	S	22	17	0
			5044	1654	2464	421	485	20			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	GLY	deletion	UNP P32357
B	?	-	SER	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357

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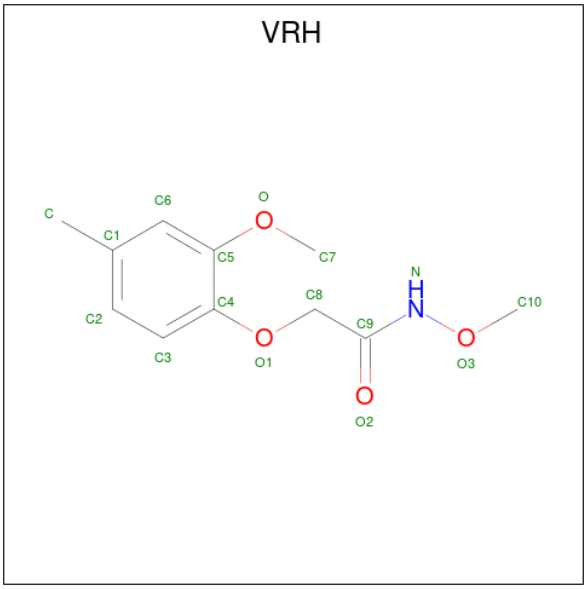
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	MET	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ASN	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	170	SER	ASP	conflict	UNP P32357

- Molecule 3 is N-methoxy-2-(2-methoxy-4-methylphenoxy)acetamide (CCD ID: VRH) (formula: $C_{11}H_{15}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 16 11 1 4	0	0
3	B	1	Total C N O 16 11 1 4	0	0

- Molecule 4 is water.

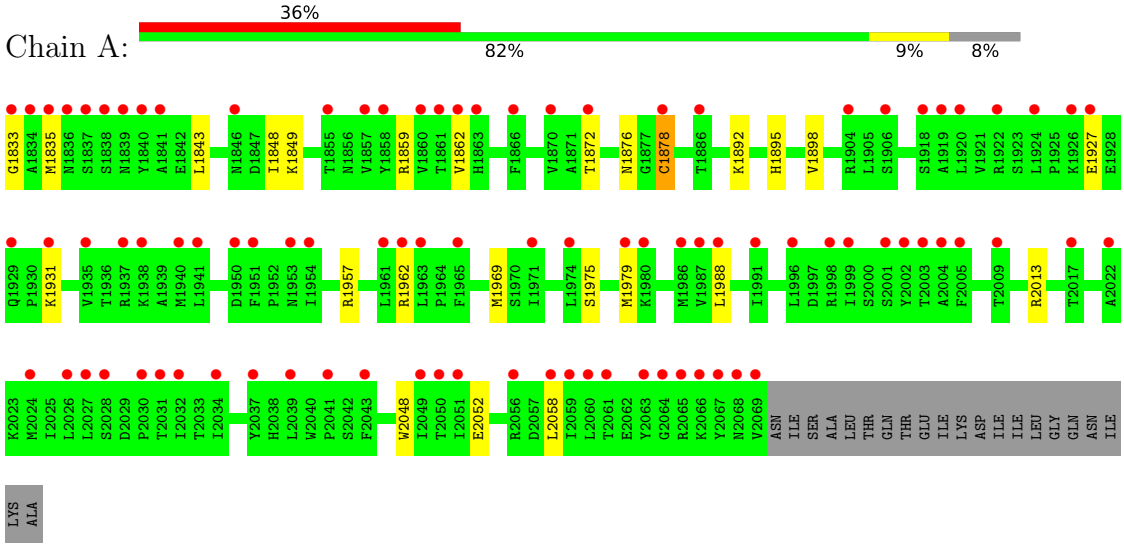
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	35	Total O 35 35	0	0
4	B	31	Total O 31 31	0	0

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.

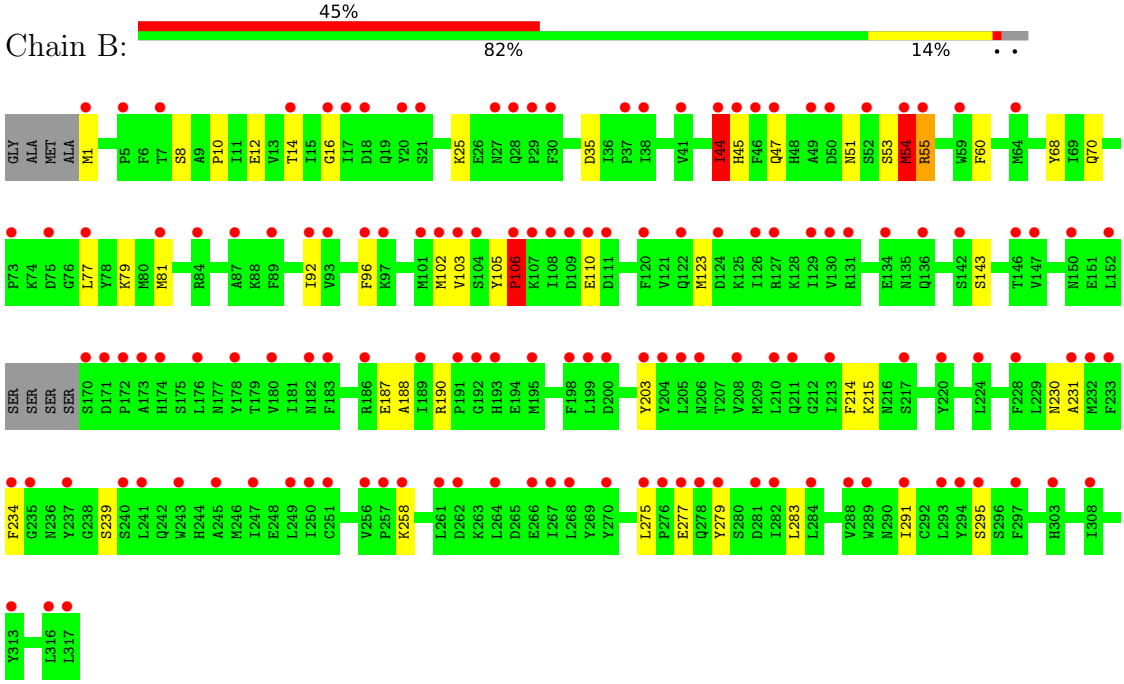
• Molecule 1: Pre-mRNA-splicing factor 8

Chain A:



• Molecule 2: A1 cistron-splicing factor AAR2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	89.34Å 81.38Å 93.42Å 90.00° 108.27° 90.00°	Depositor
Resolution (Å)	44.01 – 1.69 44.01 – 1.69	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.01-1.69) 98.3 (44.01-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 1.69Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.257 , 0.287 0.267 , 0.291	Depositor DCC
R_{free} test set	2100 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9210	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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: VRH

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	0.67	1/2149 (0.0%)	0.74	1/2911 (0.0%)
2	B	0.82	10/2739 (0.4%)	1.03	20/3699 (0.5%)
All	All	0.76	11/4888 (0.2%)	0.91	21/6610 (0.3%)

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
2	B	0	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	55[A]	ARG	N-CA	7.80	1.55	1.45
2	B	55[B]	ARG	N-CA	7.80	1.55	1.45
2	B	45[A]	HIS	N-CA	7.38	1.55	1.45
2	B	45[B]	HIS	N-CA	7.38	1.55	1.45
2	B	54[A]	MET	C-N	7.16	1.42	1.33
2	B	54[B]	MET	C-N	7.16	1.42	1.33
2	B	44[A]	ILE	C-N	6.49	1.41	1.33
2	B	44[B]	ILE	C-N	6.49	1.41	1.33
1	A	1876	ASN	CB-CG	-5.26	1.38	1.52
2	B	231	ALA	C-O	-5.13	1.18	1.24
2	B	105	TYR	C-O	-5.03	1.17	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	54[A]	MET	CA-C-N	-9.52	106.00	120.94
2	B	54[A]	MET	C-N-CA	-9.52	106.00	120.94
2	B	54[B]	MET	CA-C-N	-9.52	106.00	120.94
2	B	54[B]	MET	C-N-CA	-9.52	106.00	120.94
2	B	44[A]	ILE	CA-C-N	-8.42	107.18	121.75
2	B	44[A]	ILE	C-N-CA	-8.42	107.18	121.75
2	B	44[B]	ILE	CA-C-N	-8.42	107.18	121.75
2	B	44[B]	ILE	C-N-CA	-8.42	107.18	121.75
2	B	45[A]	HIS	CA-CB-CG	6.59	120.39	113.80
2	B	45[B]	HIS	CA-CB-CG	6.59	120.39	113.80
2	B	105	TYR	CB-CA-C	5.63	118.09	109.60
2	B	106	PRO	CA-N-CD	-5.59	104.17	112.00
2	B	14	THR	CB-CA-C	5.32	119.10	110.22
2	B	105	TYR	N-CA-C	-5.31	102.17	109.71
1	A	1878	CYS	N-CA-C	-5.24	100.48	108.76
2	B	44[A]	ILE	N-CA-C	-5.17	100.96	108.97
2	B	44[B]	ILE	N-CA-C	-5.17	100.96	108.97
2	B	44[A]	ILE	CA-C-O	-5.16	114.92	121.48
2	B	44[B]	ILE	CA-C-O	-5.16	114.92	121.48
2	B	103	VAL	N-CA-C	-5.16	104.42	110.05
2	B	16	GLY	O-C-N	-5.09	119.69	123.61

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	44[A]	ILE	Mainchain
2	B	44[B]	ILE	Mainchain
2	B	54[A]	MET	Mainchain
2	B	54[B]	MET	Mainchain

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	2008	2060	1974	15	0
2	B	2580	2464	2398	30	0
3	B	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	35	0	0	0	0
4	B	31	0	0	1	0
All	All	4686	4524	4372	45	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 (45) 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)
2:B:44[B]:ILE:HG13	2:B:60:PHE:HE1	1.27	0.98
2:B:44[B]:ILE:HG13	2:B:60:PHE:CE1	2.08	0.88
2:B:70:GLN:HB3	2:B:81:MET:HE2	1.64	0.80
2:B:1:MET:N	4:B:501:HOH:O	2.24	0.69
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.38	0.68
2:B:230[B]:ASN:ND2	2:B:239:SER:OG	2.27	0.67
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.76	0.66
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.78	0.66
2:B:44[B]:ILE:CG1	2:B:60:PHE:CE1	2.80	0.65
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.22	0.64
2:B:68:TYR:CE2	2:B:81:MET:HE3	2.32	0.64
2:B:44[B]:ILE:CG1	2:B:60:PHE:HE1	2.08	0.62
2:B:1:MET:HB3	2:B:35:ASP:HA	1.82	0.60
1:A:1895:HIS:O	1:A:1898[A]:VAL:HG22	2.04	0.58
2:B:258:LYS:HD2	2:B:258:LYS:H	1.71	0.55
1:A:1979[B]:MET:HA	1:A:1979[B]:MET:HE2	1.89	0.55
2:B:96:PHE:CB	2:B:102:MET:HE3	2.37	0.54
2:B:70:GLN:CB	2:B:81:MET:HE2	2.38	0.52
1:A:1969:MET:HA	1:A:1969:MET:HE2	1.92	0.52
2:B:1:MET:HE3	2:B:35:ASP:O	2.11	0.50
2:B:12:GLU:HG3	2:B:25:LYS:HA	1.93	0.50
2:B:110:GLU:HG2	2:B:110:GLU:O	2.12	0.49
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.95	0.49
1:A:1833:GLY:O	1:A:1957:ARG:HB3	2.15	0.47
2:B:230[B]:ASN:OD1	2:B:234:PHE:HD2	1.99	0.46
2:B:214:PHE:O	2:B:215:LYS:HB2	2.16	0.45
1:A:1862:VAL:HG22	1:A:1872:THR:HG22	1.99	0.45
2:B:187:GLU:H	2:B:187:GLU:CD	2.24	0.45
1:A:1878:CYS:HA	1:A:1892:LYS:O	2.16	0.45
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.51	0.44
1:A:1859:ARG:NH1	1:A:1979[B]:MET:HE3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54[B]:MET:HE1	2:B:143:SER:HB3	2.00	0.44
1:A:2048:TRP:O	1:A:2052:GLU:HG3	2.18	0.43
2:B:77:LEU:HD21	2:B:79:LYS:CE	2.48	0.42
2:B:44[A]:ILE:O	2:B:44[A]:ILE:HG23	2.19	0.42
2:B:190:ARG:HG3	2:B:203[B]:TYR:CE2	2.54	0.42
2:B:8:SER:C	2:B:10:PRO:HD3	2.44	0.42
2:B:44[B]:ILE:CD1	2:B:60:PHE:CE1	3.02	0.42
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.60	0.42
2:B:54[A]:MET:HE2	2:B:54[A]:MET:HB3	1.82	0.41
1:A:1975:SER:O	1:A:1979[A]:MET:SD	2.79	0.41
2:B:51:ASN:OD1	2:B:53:SER:HB2	2.20	0.41
2:B:279:TYR:HB3	2:B:283:LEU:HD12	2.03	0.41

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	258/258 (100%)	250 (97%)	8 (3%)	0	100	100
2	B	315/308 (102%)	300 (95%)	14 (4%)	1 (0%)	36	22
All	All	573/566 (101%)	550 (96%)	22 (4%)	1 (0%)	43	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	106	PRO

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	237/233 (102%)	235 (99%)	2 (1%)	73 65
2	B	294/284 (104%)	283 (96%)	11 (4%)	30 14
All	All	531/517 (103%)	518 (98%)	13 (2%)	45 26

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1927	GLU
1	A	1988	LEU
2	B	47	GLN
2	B	55[A]	ARG
2	B	55[B]	ARG
2	B	92	ILE
2	B	106	PRO
2	B	123[A]	MET
2	B	123[B]	MET
2	B	275	LEU
2	B	277	GLU
2	B	291	ILE
2	B	295	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2038	HIS
2	B	40	HIS
2	B	150	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	VRH	B	402	-	16,16,16	4.90	9 (56%)	18,20,20	1.74	4 (22%)
3	VRH	B	401	-	16,16,16	2.57	5 (31%)	18,20,20	2.28	6 (33%)

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
3	VRH	B	402	-	-	3/9/10/10	0/1/1/1
3	VRH	B	401	-	-	5/9/10/10	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	VRH	O3-N	-17.15	1.25	1.40
3	B	402	VRH	O2-C9	-5.75	1.11	1.23
3	B	401	VRH	C9-N	5.75	1.41	1.32
3	B	401	VRH	O3-N	-5.57	1.35	1.40
3	B	401	VRH	O-C7	-4.09	1.31	1.42
3	B	402	VRH	C2-C3	-3.46	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	VRH	O1-C4	-3.36	1.31	1.37
3	B	402	VRH	C9-N	3.17	1.37	1.32
3	B	401	VRH	C4-C5	-2.73	1.35	1.40
3	B	402	VRH	C3-C4	-2.20	1.35	1.39
3	B	401	VRH	O1-C4	-2.13	1.33	1.37
3	B	402	VRH	C6-C1	-2.12	1.35	1.39
3	B	402	VRH	O-C7	-2.03	1.37	1.42
3	B	402	VRH	O1-C8	-2.02	1.38	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	VRH	C8-O1-C4	-4.65	107.90	117.60
3	B	401	VRH	C7-O-C5	-4.45	110.99	117.51
3	B	401	VRH	C10-O3-N	4.30	114.15	109.60
3	B	402	VRH	C7-O-C5	3.68	122.92	117.51
3	B	402	VRH	O2-C9-N	-3.41	119.03	123.30
3	B	402	VRH	O-C5-C4	3.38	119.99	115.40
3	B	401	VRH	O-C5-C4	2.74	119.12	115.40
3	B	401	VRH	O-C5-C6	-2.43	119.89	124.08
3	B	401	VRH	O2-C9-C8	2.35	126.12	119.65
3	B	402	VRH	C10-O3-N	-2.18	107.30	109.60

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	VRH	O2-C9-N-O3
3	B	402	VRH	O2-C9-N-O3
3	B	401	VRH	C4-C5-O-C7
3	B	401	VRH	C6-C5-O-C7
3	B	401	VRH	C5-C4-O1-C8
3	B	401	VRH	C3-C4-O1-C8
3	B	402	VRH	C5-C4-O1-C8
3	B	402	VRH	C9-C8-O1-C4

There are no ring outliers.

No monomer is involved in short contacts.

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	237/258 (91%)	1.79	92 (38%)	1	0	22, 62, 112, 214	12 (5%)
2	B	300/308 (97%)	2.09	138 (46%)	0	0	24, 67, 120, 188	9 (3%)
All	All	537/566 (94%)	1.96	230 (42%)	0	0	22, 64, 115, 214	21 (3%)

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	106	PRO	7.3
1	A	2069	VAL	6.6
2	B	101	MET	6.4
2	B	203[A]	TYR	6.4
1	A	1979[A]	MET	6.4
2	B	279	TYR	6.1
2	B	54[A]	MET	6.0
2	B	152	LEU	5.8
1	A	1919[A]	ALA	5.5
2	B	316	LEU	5.4
2	B	275	LEU	5.4
2	B	122[A]	GLN	5.3
2	B	170	SER	5.2
1	A	2059	ILE	5.1
2	B	111	ASP	5.0
2	B	261	LEU	5.0
1	A	1834	ALA	5.0
2	B	282	ILE	5.0
1	A	1940	MET	4.7
1	A	2060	LEU	4.7
2	B	1	MET	4.5
2	B	174	HIS	4.5
2	B	204[A]	TYR	4.5
2	B	198	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	2061	THR	4.4
1	A	1866	PHE	4.3
2	B	297	PHE	4.2
1	A	1833	GLY	4.2
2	B	45[A]	HIS	4.2
2	B	228	PHE	4.2
2	B	172	PRO	4.0
1	A	2063	TYR	4.0
1	A	1878	CYS	4.0
2	B	49	ALA	4.0
2	B	173	ALA	4.0
2	B	276	PRO	3.9
2	B	317	LEU	3.8
1	A	1927	GLU	3.8
2	B	130	VAL	3.8
2	B	267	ILE	3.8
2	B	205	LEU	3.8
1	A	1840	TYR	3.7
1	A	1961[A]	LEU	3.7
2	B	191	PRO	3.7
2	B	46	PHE	3.7
2	B	268	LEU	3.7
1	A	2065	ARG	3.6
1	A	1857	VAL	3.5
1	A	1860	VAL	3.5
2	B	20	TYR	3.5
2	B	16	GLY	3.5
2	B	257	PRO	3.5
1	A	1904	ARG	3.5
2	B	44[A]	ILE	3.5
2	B	243	TRP	3.5
1	A	1991	ILE	3.4
1	A	2027	LEU	3.4
2	B	108	ILE	3.4
2	B	129	ILE	3.3
2	B	176	LEU	3.3
2	B	233	PHE	3.3
2	B	50	ASP	3.3
2	B	213	ILE	3.3
1	A	1862	VAL	3.3
2	B	183	PHE	3.2
1	A	1855[A]	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	189	ILE	3.2
1	A	1974	LEU	3.2
2	B	38	ILE	3.1
2	B	77	LEU	3.1
1	A	2066	LYS	3.1
2	B	92	ILE	3.1
1	A	1963	LEU	3.1
2	B	249	LEU	3.1
2	B	7	THR	3.1
2	B	126	ILE	3.1
2	B	29	PRO	3.0
1	A	2067	TYR	3.0
2	B	21	SER	3.0
1	A	1841	ALA	3.0
1	A	1922	ARG	3.0
2	B	103	VAL	3.0
2	B	235	GLY	3.0
2	B	89	PHE	3.0
2	B	237	TYR	2.9
2	B	250	ILE	2.9
2	B	171	ASP	2.9
2	B	134	GLU	2.9
1	A	1870	VAL	2.9
1	A	1924	LEU	2.9
2	B	199	LEU	2.9
1	A	1837	SER	2.9
2	B	109	ASP	2.8
1	A	2037	TYR	2.8
2	B	55[A]	ARG	2.8
1	A	1965	PHE	2.8
2	B	102	MET	2.8
2	B	241	LEU	2.8
1	A	1835	MET	2.8
1	A	2024[A]	MET	2.8
2	B	146	THR	2.8
1	A	1838	SER	2.8
1	A	1951	PHE	2.8
2	B	120	PHE	2.8
1	A	2068	ASN	2.8
1	A	2028	SER	2.8
2	B	28	GLN	2.7
1	A	2032	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	208	VAL	2.7
2	B	178[A]	TYR	2.7
2	B	291	ILE	2.7
2	B	193	HIS	2.7
2	B	150	ASN	2.7
1	A	1986	MET	2.7
2	B	127	ARG	2.6
2	B	231	ALA	2.6
1	A	1953	ASN	2.6
1	A	2056[A]	ARG	2.6
2	B	303	HIS	2.6
1	A	1861	THR	2.6
2	B	192	GLY	2.6
2	B	251	CYS	2.6
2	B	52	SER	2.6
2	B	107	LYS	2.6
2	B	142	SER	2.6
2	B	195	MET	2.6
2	B	87	ALA	2.6
2	B	37	PRO	2.6
1	A	1962	ARG	2.6
2	B	14	THR	2.5
2	B	75	ASP	2.5
2	B	30	PHE	2.5
2	B	240	SER	2.5
1	A	1846	ASN	2.5
2	B	27	ASN	2.5
2	B	180	VAL	2.5
1	A	2041	PRO	2.5
2	B	245	ALA	2.5
2	B	59	TRP	2.5
1	A	1996	LEU	2.5
2	B	147	VAL	2.5
1	A	2034	ILE	2.5
1	A	1886	THR	2.5
2	B	232	MET	2.5
2	B	266	GLU	2.5
1	A	2022	ALA	2.5
1	A	1926	LYS	2.5
1	A	2064	GLY	2.5
1	A	1999	ILE	2.5
2	B	217	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1988	LEU	2.4
1	A	1935	VAL	2.4
1	A	1920	LEU	2.4
1	A	2009	THR	2.4
2	B	308	ILE	2.4
1	A	1938	LYS	2.4
1	A	2003	THR	2.4
2	B	281	ASP	2.4
2	B	211[A]	GLN	2.3
1	A	2017[A]	THR	2.3
1	A	1863	HIS	2.3
1	A	1987	VAL	2.3
2	B	182	ASN	2.3
2	B	206	ASN	2.3
1	A	1931[A]	LYS	2.3
1	A	1872	THR	2.3
2	B	64[A]	MET	2.3
2	B	270	TYR	2.3
2	B	289	TRP	2.3
2	B	73	PRO	2.3
1	A	2031	THR	2.3
2	B	210	LEU	2.3
1	A	1918[A]	SER	2.3
2	B	96	PHE	2.3
1	A	2051	ILE	2.3
2	B	200	ASP	2.3
2	B	256	VAL	2.3
1	A	1836	ASN	2.2
2	B	84	ARG	2.2
1	A	2026	LEU	2.2
2	B	124	ASP	2.2
2	B	262	ASP	2.2
1	A	1954	ILE	2.2
2	B	278	GLN	2.2
2	B	258	LYS	2.2
2	B	18	ASP	2.2
2	B	47	GLN	2.2
1	A	2043	PHE	2.2
1	A	2049	ILE	2.2
2	B	5	PRO	2.2
1	A	1950	ASP	2.2
1	A	2004	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	110	GLU	2.2
1	A	1941	LEU	2.2
2	B	224	LEU	2.2
1	A	1937	ARG	2.2
2	B	234	PHE	2.2
1	A	2030	PRO	2.2
2	B	104	SER	2.2
1	A	2058	LEU	2.1
2	B	293	LEU	2.1
1	A	2001[A]	SER	2.1
2	B	17	ILE	2.1
2	B	313	TYR	2.1
1	A	2039	LEU	2.1
2	B	277	GLU	2.1
1	A	1971	ILE	2.1
2	B	294	TYR	2.1
2	B	97	LYS	2.1
2	B	41[A]	VAL	2.1
2	B	288	VAL	2.1
2	B	81	MET	2.1
1	A	1998	ARG	2.1
2	B	264	LEU	2.1
2	B	284	LEU	2.1
1	A	1980[A]	LYS	2.1
1	A	1858	TYR	2.1
1	A	2002[A]	TYR	2.1
1	A	2005	PHE	2.1
2	B	247	ILE	2.1
1	A	1839	ASN	2.0
1	A	1929	GLN	2.0
1	A	1906	SER	2.0
2	B	93	VAL	2.0
2	B	131	ARG	2.0
2	B	295	SER	2.0
1	A	2050	THR	2.0
2	B	136	GLN	2.0
2	B	186	ARG	2.0
2	B	220	TYR	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 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, 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
3	VRH	B	401	16/16	0.66	0.19	20,20,20,20	16
3	VRH	B	402	16/16	0.81	0.15	20,20,20,20	16

6.5 Other polymers (i)

There are no such residues in this entry.