



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 05:56 AM UTC

PDB ID : 7FM3 / pdb_00007fm3
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P05H09 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 : 1.65 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

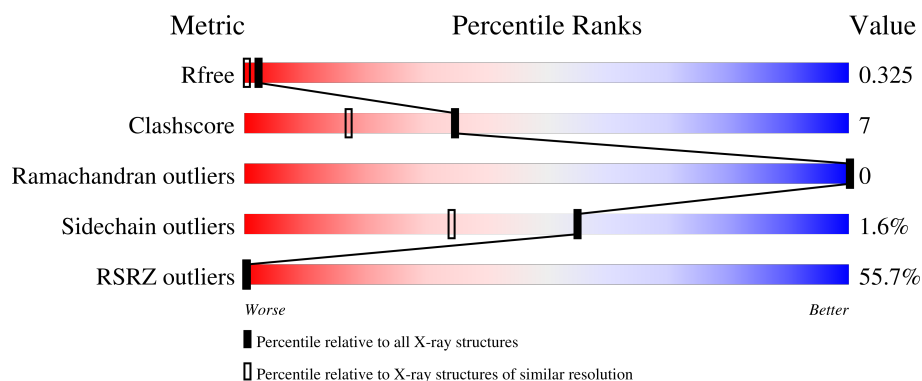
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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 $\leq 5\%$. 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	258	53% 72% 17% • 8%
2	B	308	53% 80% 17% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9193 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
			Total	C	H	N	O	S			
1	A	237	4068	1287	2060	336	373	12	0	21	0

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
			Total	C	H	N	O	S			
2	B	300	5044	1654	2464	421	485	20	11	17	0

There are 20 discrepancies between the modelled and reference sequences:

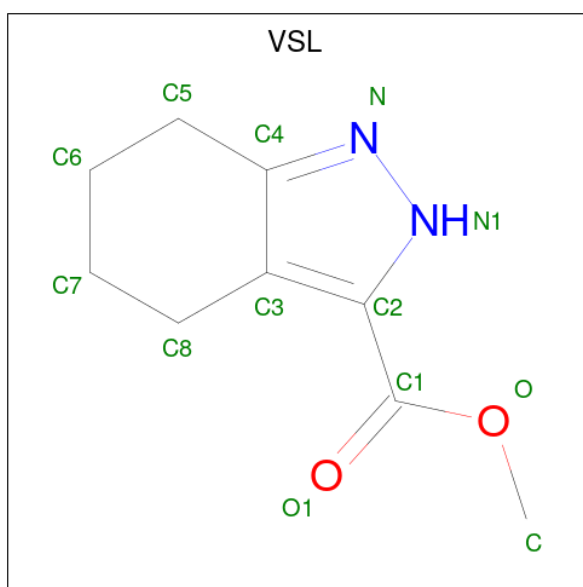
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	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 methyl 4,5,6,7-tetrahydro-2H-indazole-3-carboxylate (CCD ID: VSL) (formula: $C_9H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			13	9	2	2		

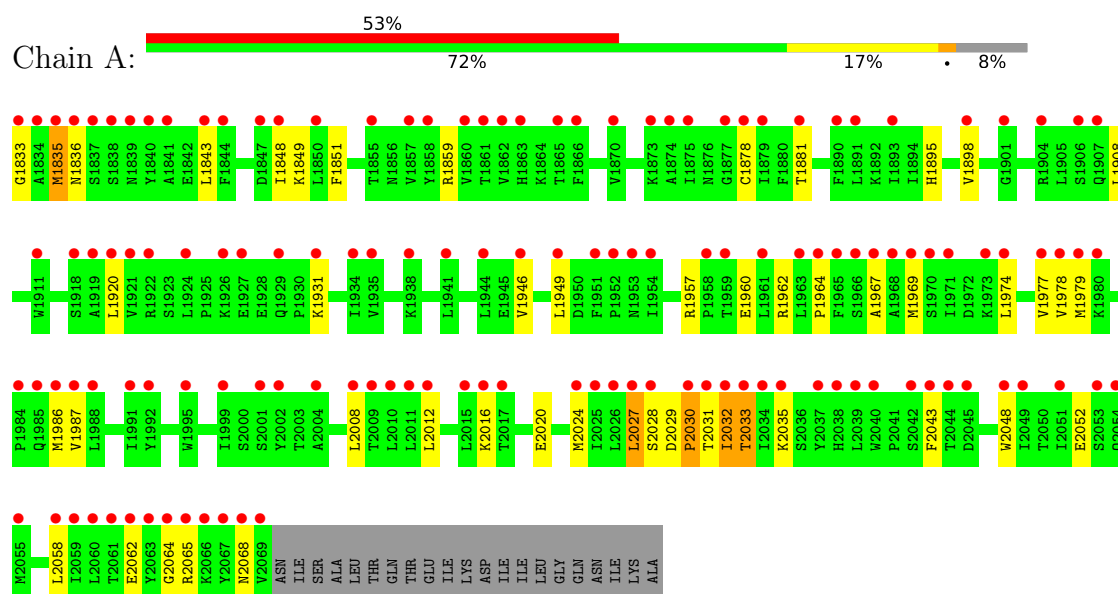
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	34	Total	O	0	0
			34	34		

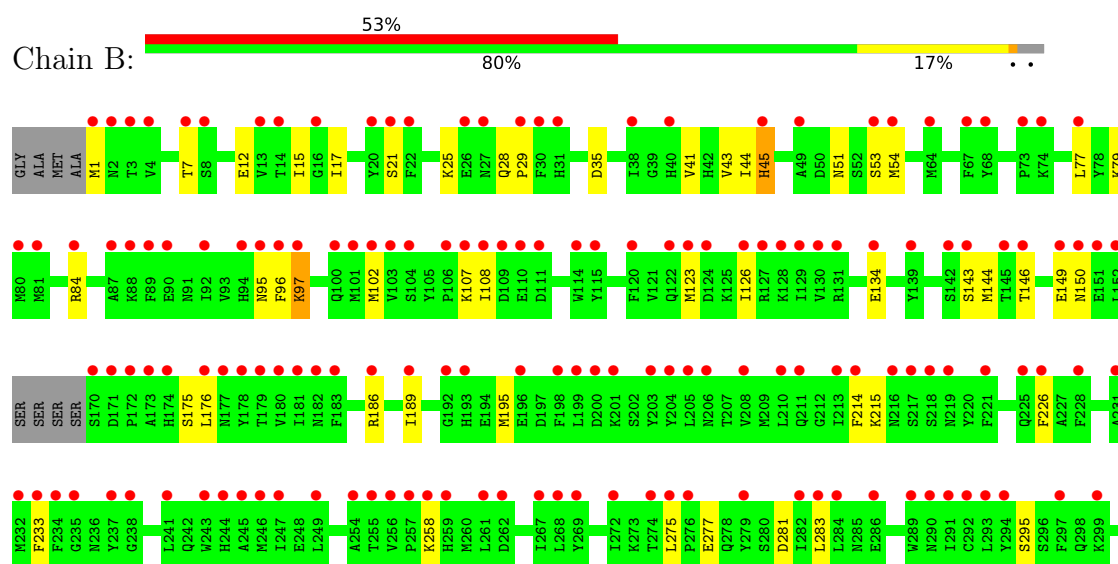
3 Residue-property plots

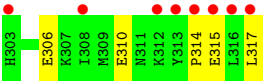
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: A1 cistron-splicing factor AAR2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.01Å 81.92Å 93.77Å 90.00° 108.44° 90.00°	Depositor
Resolution (Å)	44.73 – 1.65 44.73 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.7 (44.73-1.65) 97.0 (44.73-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.284 , 0.317 0.290 , 0.325	Depositor DCC
R_{free} test set	2100 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9193	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VSL

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	0.71	1/2149 (0.0%)	0.93	9/2911 (0.3%)
2	B	0.78	3/2739 (0.1%)	0.94	3/3699 (0.1%)
All	All	0.75	4/4888 (0.1%)	0.93	12/6610 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2027	LEU	C-O	6.50	1.30	1.23
2	B	7	THR	C-O	-5.51	1.17	1.24
2	B	45[A]	HIS	C-N	5.39	1.41	1.33
2	B	45[B]	HIS	C-N	5.39	1.41	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2030	PRO	CA-C-N	6.97	129.63	120.28
1	A	2030	PRO	C-N-CA	6.97	129.63	120.28
1	A	2030	PRO	CB-CA-C	-6.41	100.98	111.56
1	A	2028	SER	N-CA-C	-5.63	106.57	113.50
1	A	2027	LEU	N-CA-C	5.56	118.01	110.06
1	A	2031	THR	CA-C-N	5.39	129.10	122.37
1	A	2031	THR	C-N-CA	5.39	129.10	122.37
1	A	2033	THR	CA-CB-OG1	-5.39	101.52	109.60
2	B	123[A]	MET	CG-SD-CE	5.23	112.40	100.90
2	B	123[B]	MET	CG-SD-CE	5.23	112.40	100.90
1	A	2031	THR	CA-CB-OG1	5.18	117.37	109.60
2	B	84	ARG	CB-CA-C	5.04	119.98	109.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2008	2060	1974	31	0
2	B	2580	2464	2398	36	0
3	B	13	0	0	1	0
4	A	34	0	0	0	0
4	B	34	0	0	2	0
All	All	4669	4524	4372	67	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 7.

All (67) 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:258:LYS:HD2	2:B:258:LYS:H	1.54	0.72
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.70	0.72
2:B:96:PHE:CB	2:B:102:MET:HE3	2.25	0.66
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.45	0.64
2:B:54[A]:MET:HE2	4:B:523:HOH:O	1.99	0.61
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.82	0.61
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.67	0.59
2:B:277:GLU:CD	2:B:277:GLU:H	2.11	0.58
1:A:1895:HIS:O	1:A:1898[A]:VAL:HG22	2.03	0.57
1:A:1967:ALA:HB2	1:A:2016:LYS:HB2	1.86	0.56
2:B:17:ILE:HD13	2:B:44[B]:ILE:HG12	1.88	0.56
1:A:1979[B]:MET:HA	1:A:1979[B]:MET:HE2	1.88	0.55
2:B:51:ASN:OD1	2:B:53:SER:HB2	2.07	0.54
2:B:214:PHE:O	2:B:215:LYS:HB2	2.06	0.54
2:B:1:MET:N	4:B:502:HOH:O	2.40	0.54
1:A:1908:LEU:HA	2:B:195:MET:HE1	1.90	0.54
2:B:96:PHE:HB3	2:B:102:MET:HE3	1.89	0.54
1:A:1835:MET:O	1:A:1960[A]:GLU:N	2.32	0.53
1:A:1964:PRO:HG2	1:A:2012:LEU:HB2	1.88	0.53
1:A:1833:GLY:O	1:A:1957:ARG:HB3	2.10	0.52
1:A:1977:VAL:HG21	1:A:1987:VAL:HG21	1.92	0.51
1:A:2029:ASP:OD1	1:A:2030:PRO:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2033:THR:OG1	1:A:2035:LYS:NZ	2.45	0.49
2:B:186:ARG:NH1	2:B:189:ILE:O	2.44	0.49
2:B:77:LEU:CD2	2:B:79:LYS:HE3	2.42	0.49
2:B:1:MET:HE3	2:B:35:ASP:O	2.12	0.49
2:B:314:PRO:HD2	2:B:315:GLU:OE1	2.12	0.49
1:A:1859:ARG:NH1	1:A:1979[B]:MET:HE3	2.28	0.48
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.38	0.48
2:B:54[B]:MET:HE1	2:B:143:SER:HB3	1.94	0.48
1:A:2064:GLY:O	1:A:2068:ASN:N	2.43	0.48
2:B:126:ILE:HG12	2:B:226:PHE:CE1	2.49	0.47
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.96	0.47
1:A:2032:ILE:HG21	1:A:2043:PHE:CE1	2.50	0.46
2:B:144:MET:HE2	2:B:176:LEU:HG	1.98	0.46
1:A:1836:ASN:HB3	1:A:1960[A]:GLU:HB2	1.98	0.45
2:B:28:GLN:HG3	2:B:29:PRO:HD2	1.98	0.45
2:B:146:THR:OG1	2:B:149:GLU:HG3	2.16	0.45
2:B:12:GLU:HG3	2:B:25:LYS:HA	1.99	0.45
2:B:281:ASP:OD1	2:B:281:ASP:N	2.47	0.44
1:A:2032:ILE:HG21	1:A:2043:PHE:CD1	2.52	0.44
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.58	0.44
1:A:1974:LEU:O	1:A:1978:VAL:HG23	2.17	0.44
2:B:43:VAL:O	2:B:43:VAL:HG13	2.16	0.44
1:A:2008:LEU:O	1:A:2012:LEU:HG	2.18	0.44
2:B:214:PHE:O	2:B:215:LYS:CB	2.65	0.44
2:B:275:LEU:HD22	2:B:283:LEU:HD13	1.99	0.44
1:A:2062:GLU:OE2	1:A:2065:ARG:NH1	2.49	0.43
2:B:15:ILE:O	2:B:21:SER:HA	2.17	0.43
2:B:107:LYS:NZ	2:B:108:ILE:O	2.51	0.43
1:A:1859:ARG:HH11	1:A:1979[B]:MET:HE3	1.84	0.43
1:A:1946:VAL:O	1:A:1949:LEU:HG	2.19	0.43
2:B:28:GLN:CG	2:B:29:PRO:HD2	2.48	0.43
2:B:134:GLU:OE1	2:B:134:GLU:N	2.39	0.42
1:A:2020:GLU:OE1	1:A:2024[B]:MET:SD	2.78	0.42
2:B:17:ILE:HD13	2:B:44[B]:ILE:CG1	2.48	0.42
2:B:97:LYS:HE3	2:B:97:LYS:HB2	1.89	0.42
2:B:306:GLU:O	2:B:310:GLU:HG3	2.20	0.41
1:A:1835:MET:HE3	1:A:1835:MET:HB3	1.92	0.41
2:B:150:ASN:ND2	2:B:175:SER:OG	2.53	0.41
1:A:2048:TRP:O	1:A:2052:GLU:HG3	2.21	0.41
3:B:401:VSL:C8	3:B:401:VSL:O	2.69	0.40
1:A:1851:PHE:O	1:A:1881:THR:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1920:LEU:HD13	1:A:1986:MET:CE	2.52	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	258/258 (100%)	250 (97%)	8 (3%)	0	100	100
2	B	315/308 (102%)	303 (96%)	12 (4%)	0	100	100
All	All	573/566 (101%)	553 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	234 (99%)	3 (1%)	61	42
2	B	294/284 (104%)	288 (98%)	6 (2%)	48	26
All	All	531/517 (103%)	522 (98%)	9 (2%)	55	32

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	2027	LEU
1	A	2032	ILE
2	B	45[A]	HIS
2	B	45[B]	HIS
2	B	95	ASN
2	B	97	LYS
2	B	295	SER
2	B	317	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1947	HIS
1	A	2038	HIS
2	B	2	ASN
2	B	40	HIS
2	B	95	ASN
2	B	290	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](#)

1 ligand is 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	VSL	B	401	-	14,14,14	3.18	6 (42%)	18,19,19	2.32	10 (55%)

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	VSL	B	401	-	-	0/6/13/13	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	VSL	C2-N1	7.80	1.45	1.35
3	B	401	VSL	C8-C3	-4.85	1.42	1.51
3	B	401	VSL	N1-N	-4.02	1.28	1.36
3	B	401	VSL	C5-C4	-3.98	1.44	1.50
3	B	401	VSL	C2-C1	-3.32	1.38	1.46
3	B	401	VSL	O-C	-2.81	1.39	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	VSL	C1-C2-C3	-3.65	126.46	132.65
3	B	401	VSL	O-C1-C2	-3.32	107.55	111.92
3	B	401	VSL	C-O-C1	3.31	122.00	115.85
3	B	401	VSL	C4-N-N1	3.24	112.00	104.76
3	B	401	VSL	C8-C3-C2	3.13	133.50	129.91
3	B	401	VSL	C3-C4-N	-2.83	108.47	112.61
3	B	401	VSL	C1-C2-N1	2.75	126.36	120.75
3	B	401	VSL	C7-C8-C3	-2.50	106.48	111.85
3	B	401	VSL	C2-N1-N	-2.48	107.69	112.59
3	B	401	VSL	O1-C1-C2	2.47	128.61	123.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	VSL	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, 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	237/258 (91%)	2.48	136 (57%) 0 0	26, 79, 129, 199	12 (5%)
2	B	300/308 (97%)	2.36	163 (54%) 0 0	26, 76, 126, 235	9 (3%)
All	All	537/566 (94%)	2.41	299 (55%) 0 0	26, 77, 129, 235	21 (3%)

All (299) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	152	LEU	7.6
1	A	1967	ALA	7.2
2	B	49	ALA	7.2
2	B	198	PHE	6.7
2	B	92	ILE	6.3
2	B	316	LEU	6.2
1	A	1878	CYS	6.1
1	A	2069	VAL	6.0
2	B	203[A]	TYR	5.9
1	A	2017[A]	THR	5.9
2	B	180	VAL	5.9
2	B	54[A]	MET	5.8
1	A	1999	ILE	5.6
1	A	2040	TRP	5.4
1	A	2039	LEU	5.3
2	B	80	MET	5.3
1	A	1979[A]	MET	5.3
1	A	1965	PHE	5.2
1	A	1987	VAL	5.2
1	A	2009	THR	5.2
2	B	108	ILE	5.2
1	A	1834	ALA	5.2
1	A	2058	LEU	5.1
2	B	45[A]	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	1964	PRO	4.9
2	B	122[A]	GLN	4.8
2	B	77	LEU	4.8
1	A	1877	GLY	4.8
2	B	208	VAL	4.8
1	A	1866	PHE	4.8
2	B	275	LEU	4.7
2	B	308	ILE	4.7
2	B	103	VAL	4.7
2	B	294	TYR	4.7
2	B	1	MET	4.7
1	A	2027	LEU	4.6
2	B	104	SER	4.6
1	A	1974	LEU	4.6
2	B	192	GLY	4.6
2	B	313	TYR	4.5
2	B	101	MET	4.5
1	A	1857	VAL	4.5
1	A	1995	TRP	4.5
2	B	31	HIS	4.4
2	B	204[A]	TYR	4.4
1	A	2060	LEU	4.4
1	A	2051	ILE	4.4
1	A	1958	PRO	4.3
2	B	232	MET	4.3
1	A	1992	TYR	4.3
2	B	20	TYR	4.3
1	A	1935	VAL	4.3
2	B	172	PRO	4.3
1	A	1949	LEU	4.2
1	A	2015	LEU	4.2
2	B	170	SER	4.2
1	A	1986	MET	4.2
1	A	1840	TYR	4.2
1	A	2025	ILE	4.2
1	A	1861	THR	4.2
1	A	1835	MET	4.1
1	A	2063	TYR	4.1
2	B	269	TYR	4.1
1	A	2001[A]	SER	4.1
1	A	1984	PRO	4.1
2	B	178[A]	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	2033	THR	4.1
2	B	14	THR	4.1
2	B	174	HIS	4.1
2	B	283	LEU	4.0
2	B	261	LEU	4.0
1	A	1890	PHE	4.0
1	A	1968	ALA	4.0
2	B	257	PRO	4.0
2	B	89	PHE	4.0
2	B	173	ALA	4.0
2	B	279	TYR	3.9
2	B	193	HIS	3.9
2	B	241	LEU	3.9
1	A	1837	SER	3.9
2	B	291	ILE	3.9
1	A	1855[A]	THR	3.9
1	A	1988	LEU	3.9
1	A	2012	LEU	3.9
2	B	206	ASN	3.9
1	A	1961[A]	LEU	3.8
2	B	176	LEU	3.8
1	A	1971	ILE	3.8
1	A	1860	VAL	3.8
2	B	114	TRP	3.8
2	B	289	TRP	3.8
1	A	2037	TYR	3.8
2	B	181	ILE	3.7
2	B	297	PHE	3.7
1	A	1985	GLN	3.7
1	A	1953	ASN	3.7
1	A	1870	VAL	3.7
1	A	2061	THR	3.7
2	B	249	LEU	3.7
2	B	282	ILE	3.6
1	A	1946	VAL	3.6
2	B	96	PHE	3.6
2	B	233	PHE	3.6
2	B	237	TYR	3.6
2	B	276	PRO	3.5
2	B	3	THR	3.5
2	B	106	PRO	3.5
2	B	246	MET	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	214	PHE	3.5
1	A	1927	GLU	3.5
1	A	1833	GLY	3.5
2	B	38	ILE	3.4
1	A	1941	LEU	3.4
2	B	317	LEU	3.4
1	A	1951	PHE	3.4
1	A	1862	VAL	3.4
2	B	139	TYR	3.4
1	A	2048	TRP	3.4
1	A	1907	GLN	3.3
1	A	1954	ILE	3.3
1	A	2059	ILE	3.3
1	A	1836	ASN	3.3
2	B	95	ASN	3.3
1	A	2030	PRO	3.3
1	A	2024[A]	MET	3.3
2	B	218	SER	3.3
2	B	243	TRP	3.3
1	A	1924	LEU	3.3
1	A	2010	LEU	3.3
2	B	111	ASP	3.3
2	B	213	ILE	3.3
2	B	221	PHE	3.3
2	B	256	VAL	3.3
2	B	130	VAL	3.2
2	B	73	PRO	3.2
1	A	1963	LEU	3.2
2	B	299	LYS	3.2
1	A	1977	VAL	3.2
2	B	151	GLU	3.2
2	B	179	THR	3.2
1	A	2032	ILE	3.1
1	A	2049	ILE	3.1
2	B	231	ALA	3.1
2	B	22	PHE	3.1
1	A	1944	LEU	3.1
1	A	1874	ALA	3.1
1	A	2055	MET	3.1
2	B	87	ALA	3.1
1	A	1901	GLY	3.0
2	B	235	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	183	PHE	3.0
1	A	1952	PRO	3.0
2	B	210	LEU	3.0
1	A	1838	SER	3.0
2	B	21	SER	3.0
1	A	2008	LEU	3.0
2	B	225	GLN	3.0
2	B	217	SER	2.9
1	A	2034	ILE	2.9
2	B	27	ASN	2.9
1	A	2028	SER	2.9
2	B	142	SER	2.9
1	A	2067	TYR	2.9
1	A	2004	ALA	2.9
1	A	1922	ARG	2.9
2	B	293	LEU	2.9
1	A	2038	HIS	2.9
2	B	150	ASN	2.9
1	A	1906	SER	2.8
2	B	182	ASN	2.8
2	B	216	ASN	2.8
1	A	1938	LYS	2.8
2	B	254	ALA	2.8
1	A	1978	VAL	2.8
2	B	94	HIS	2.8
2	B	67	PHE	2.7
1	A	1931[A]	LYS	2.7
2	B	13	VAL	2.7
2	B	126	ILE	2.7
1	A	2064	GLY	2.7
2	B	26	GLU	2.7
2	B	109	ASP	2.7
2	B	199	LEU	2.7
2	B	100	GLN	2.7
1	A	1891	LEU	2.7
1	A	2044	THR	2.7
2	B	145	THR	2.7
1	A	2011	LEU	2.6
2	B	64[A]	MET	2.6
2	B	127	ARG	2.6
1	A	1863	HIS	2.6
2	B	40	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	131	ARG	2.6
1	A	2054[A]	GLN	2.6
2	B	259	HIS	2.6
2	B	303	HIS	2.6
2	B	245	ALA	2.6
2	B	177[A]	ASN	2.6
1	A	2043	PHE	2.6
1	A	1858	TYR	2.6
2	B	123[A]	MET	2.6
2	B	171	ASP	2.5
2	B	88	LYS	2.5
2	B	312	LYS	2.5
1	A	1969	MET	2.5
2	B	143	SER	2.5
2	B	292	CYS	2.5
2	B	205	LEU	2.5
2	B	284	LEU	2.5
1	A	1879	ILE	2.5
1	A	1839	ASN	2.5
1	A	1844	PHE	2.5
2	B	120	PHE	2.5
2	B	268	LEU	2.5
1	A	1893	ILE	2.5
2	B	97	LYS	2.5
2	B	244	HIS	2.5
1	A	1865	THR	2.5
1	A	1904	ARG	2.5
2	B	146	THR	2.5
2	B	186	ARG	2.5
1	A	2042	SER	2.5
2	B	200	ASP	2.4
1	A	1843	LEU	2.4
1	A	1920	LEU	2.4
2	B	16	GLY	2.4
1	A	2002[A]	TYR	2.4
1	A	1898[A]	VAL	2.4
2	B	219	ASN	2.4
2	B	258	LYS	2.4
1	A	2068	ASN	2.4
2	B	290	ASN	2.4
1	A	1881	THR	2.4
2	B	211[A]	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	274	THR	2.4
1	A	1991	ILE	2.4
1	A	1873	LYS	2.4
1	A	1970	SER	2.4
2	B	8	SER	2.4
2	B	228	PHE	2.4
1	A	2062	GLU	2.4
1	A	2066	LYS	2.4
1	A	1848	ILE	2.4
2	B	267	ILE	2.4
2	B	272	ILE	2.4
2	B	90	GLU	2.3
1	A	1841	ALA	2.3
2	B	68	TYR	2.3
2	B	2	ASN	2.3
2	B	53	SER	2.3
2	B	29	PRO	2.3
1	A	1911	TRP	2.3
1	A	2065	ARG	2.3
1	A	1973	LYS	2.3
1	A	1980[A]	LYS	2.3
2	B	128	LYS	2.3
1	A	1929	GLN	2.3
1	A	2016	LYS	2.3
1	A	1850	LEU	2.2
2	B	314	PRO	2.2
1	A	2031	THR	2.2
1	A	2045	ASP	2.2
2	B	196	GLU	2.2
2	B	286	GLU	2.2
2	B	30	PHE	2.2
2	B	129	ILE	2.2
2	B	255	THR	2.2
2	B	107	LYS	2.2
1	A	1966	SER	2.2
2	B	102	MET	2.2
2	B	110	GLU	2.2
1	A	1934	ILE	2.2
2	B	189	ILE	2.2
2	B	262	ASP	2.1
1	A	1919[A]	ALA	2.1
2	B	238	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2053[A]	SER	2.1
1	A	1921	VAL	2.1
1	A	2035	LYS	2.1
2	B	74	LYS	2.1
1	A	1918[A]	SER	2.1
2	B	124	ASP	2.1
2	B	234	PHE	2.1
1	A	1926	LYS	2.1
2	B	134	GLU	2.1
2	B	149	GLU	2.1
2	B	315	GLU	2.1
1	A	1847	ASP	2.1
1	A	2026	LEU	2.1
2	B	7	THR	2.1
1	A	1875	ILE	2.1
2	B	115	TYR	2.1
2	B	81	MET	2.0
2	B	4	VAL	2.0
2	B	84	ARG	2.0
1	A	1959	THR	2.0
2	B	201	LYS	2.0
2	B	226	PHE	2.0
2	B	247	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 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	VSL	B	401	13/13	0.76	0.14	20,20,20,20	13

6.5 Other polymers [i](#)

There are no such residues in this entry.