



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:04 AM UTC

PDB ID : 5SU7 / pdb_00005su7
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P03E12 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 : 1.81 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

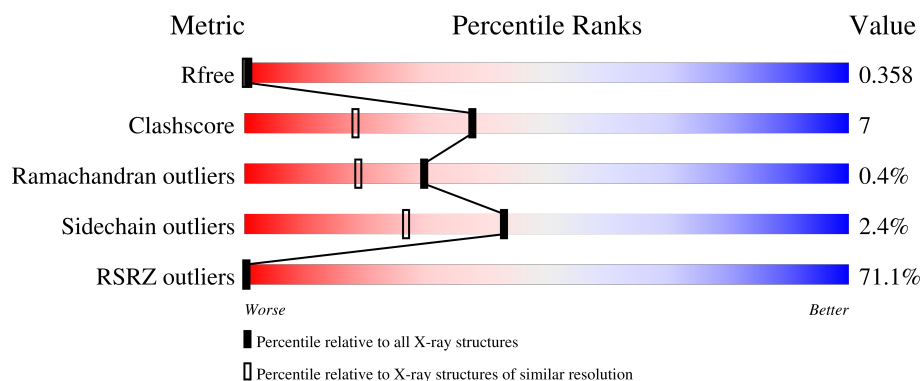
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	69% 76% 15% 8%
2	B	308	66% 82% 14% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9164 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:

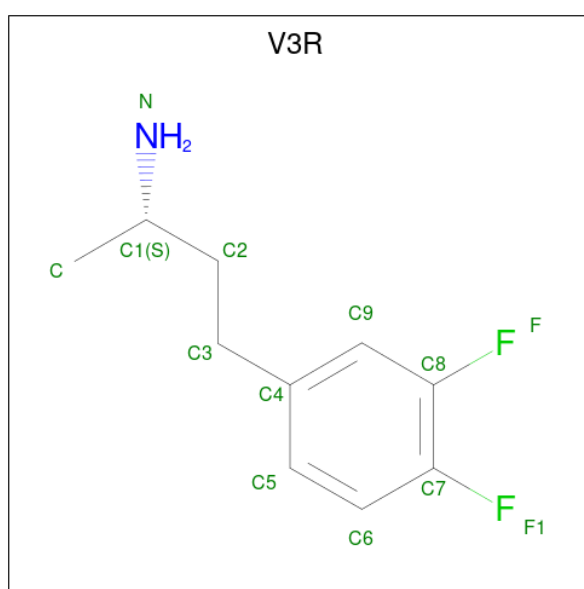
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	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 (2S)-4-(3,4-difluorophenyl)butan-2-amine (CCD ID: V3R) (formula: C₁₀H₁₃F₂N).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	F	N	0	0
			13	10	2	1		

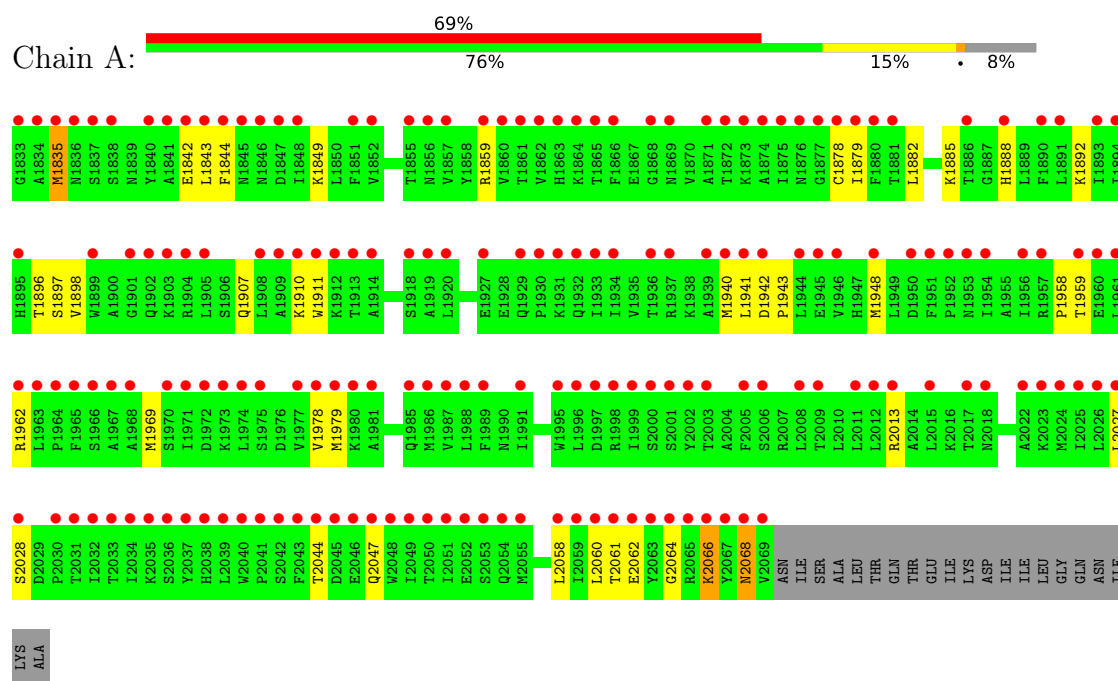
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	16	Total	O	0	0
			16	16		

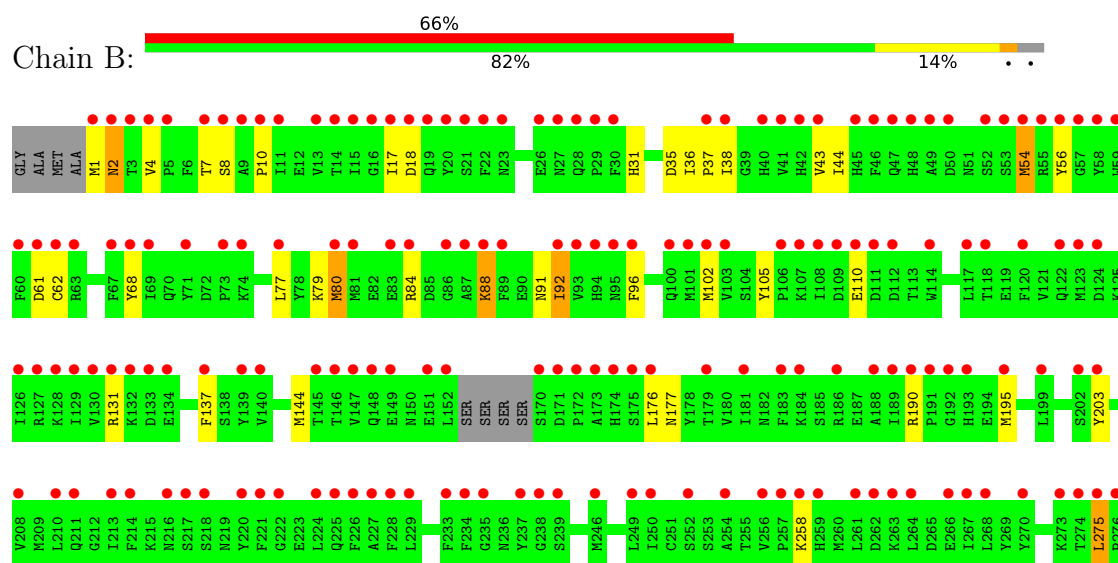
3 Residue-property plots

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



E277	Q278	Y279	S280	D281	I282	L283	R287	V288	W289	N290	I291	C292	L293	Y294	S295	S296	F297	Q298	K299	N300	S301	L302	T305	E306	K307	I308	N309	E310	N311	K312	Y313	P314	E315	L316	L317
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.39Å 81.82Å 93.72Å 90.00° 108.03° 90.00°	Depositor
Resolution (Å)	44.75 – 1.81 44.75 – 1.81	Depositor EDS
% Data completeness (in resolution range)	97.8 (44.75-1.81) 98.0 (44.75-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.318 , 0.346 0.331 , 0.358	Depositor DCC
R_{free} test set	2100 reflections (3.70%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 71.6	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	0.91	EDS
Total number of atoms	9164	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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: V3R

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	0.82	3/2149 (0.1%)	0.84	1/2911 (0.0%)
2	B	0.86	0/2739	0.98	3/3699 (0.1%)
All	All	0.85	3/4888 (0.1%)	0.92	4/6610 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1879	ILE	CB-CG2	6.29	1.73	1.52
1	A	1978	VAL	CA-C	5.04	1.58	1.52
1	A	1907	GLN	C-O	5.03	1.30	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	THR	CA-C-O	-10.39	108.36	120.10
1	A	1896	THR	N-CA-C	7.13	121.61	112.34
2	B	7	THR	O-C-N	5.95	129.19	122.22
2	B	88	LYS	N-CA-CB	5.23	118.38	110.28

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	24	0
2	B	2580	2464	2396	41	0
3	B	13	0	0	1	0
4	A	23	0	0	0	0
4	B	16	0	0	1	0
All	All	4640	4524	4370	64	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 (64) 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:88:LYS:HD3	2:B:92:ILE:HD11	1.18	1.09
2:B:88:LYS:CD	2:B:92:ILE:HD11	1.99	0.92
2:B:287:ARG:O	2:B:291:ILE:HD13	1.79	0.83
2:B:88:LYS:HD3	2:B:92:ILE:CD1	2.07	0.81
2:B:4:VAL:HG11	2:B:44[B]:ILE:CD1	2.19	0.72
1:A:2061:THR:O	1:A:2064:GLY:N	2.21	0.71
2:B:4:VAL:HG11	2:B:44[B]:ILE:HD12	1.72	0.71
2:B:80:MET:HG2	2:B:137:PHE:CE2	2.29	0.68
2:B:88:LYS:O	2:B:92:ILE:HG12	1.97	0.65
1:A:1979[B]:MET:HA	1:A:1979[B]:MET:HE2	1.81	0.62
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.33	0.62
2:B:80:MET:HG2	2:B:137:PHE:CD2	2.35	0.62
2:B:4:VAL:HG23	2:B:36:ILE:CD1	2.30	0.61
2:B:31:HIS:O	2:B:102:MET:HE2	2.04	0.57
2:B:80:MET:HG2	2:B:137:PHE:CZ	2.41	0.56
2:B:1:MET:HB3	2:B:35:ASP:HA	1.87	0.55
2:B:54[A]:MET:HE1	4:B:507:HOH:O	2.07	0.55
2:B:4:VAL:HG23	2:B:36:ILE:HD12	1.90	0.54
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.73	0.53
2:B:258:LYS:HD2	2:B:258:LYS:H	1.73	0.53
2:B:56:TYR:CZ	2:B:77:LEU:HB2	2.44	0.53
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.91	0.53
2:B:1:MET:H2	2:B:38:ILE:HD11	1.75	0.50
2:B:8:SER:C	2:B:10:PRO:HD3	2.36	0.50
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.93	0.50
1:A:1910:LYS:O	1:A:1940:MET:HE1	2.11	0.50
2:B:80:MET:HG2	2:B:137:PHE:CG	2.46	0.50
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.48	0.49
2:B:277:GLU:CD	2:B:277:GLU:H	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.55	0.47
2:B:110:GLU:HG2	2:B:110:GLU:O	2.16	0.46
2:B:68:TYR:OH	3:B:401:V3R:C	2.63	0.46
2:B:2:ASN:HB3	2:B:62:CYS:SG	2.56	0.46
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.98	0.46
1:A:2064:GLY:O	1:A:2068:ASN:N	2.48	0.46
1:A:2062:GLU:O	1:A:2066:LYS:HB2	2.15	0.46
2:B:80:MET:SD	2:B:137:PHE:CG	3.10	0.45
1:A:1941:LEU:HD11	1:A:1958:PRO:HB3	1.99	0.44
2:B:56:TYR:CE2	2:B:77:LEU:HB2	2.53	0.44
1:A:2044:THR:OG1	1:A:2047:GLN:HG3	2.17	0.44
1:A:1911:TRP:CD1	2:B:195:MET:HE3	2.54	0.43
1:A:1835:MET:HE3	1:A:1835:MET:HB3	1.90	0.43
2:B:43:VAL:HG13	2:B:43:VAL:O	2.19	0.42
2:B:144:MET:HE2	2:B:176:LEU:HG	2.01	0.42
1:A:1844:PHE:O	1:A:1885:LYS:NZ	2.34	0.42
1:A:1948:MET:HE3	1:A:1948:MET:HB3	1.94	0.42
2:B:17:ILE:O	2:B:18:ASP:C	2.63	0.42
1:A:1878:CYS:HA	1:A:1892:LYS:O	2.19	0.42
1:A:1842:GLU:O	1:A:1849:LYS:NZ	2.52	0.41
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.45	0.41
2:B:77:LEU:N	2:B:77:LEU:HD23	2.34	0.41
1:A:1897:SER:O	1:A:1898[B]:VAL:C	2.64	0.41
1:A:1942:ASP:HB2	1:A:1943:PRO:HD3	2.02	0.41
1:A:1859:ARG:HH12	1:A:1979[A]:MET:CE	2.33	0.41
1:A:1882:LEU:HD12	1:A:1888:HIS:O	2.21	0.41
2:B:80:MET:HG2	2:B:137:PHE:CE1	2.56	0.40
2:B:190:ARG:HG3	2:B:203[B]:TYR:CE2	2.57	0.40
2:B:61:ASP:OD1	2:B:61:ASP:C	2.65	0.40
2:B:131:ARG:HH21	2:B:177[B]:ASN:ND2	2.19	0.40
1:A:1835:MET:H	1:A:1959:THR:HA	1.87	0.40
1:A:2027:LEU:O	1:A:2028:SER:C	2.64	0.40
2:B:1:MET:N	2:B:38:ILE:HD11	2.36	0.40
2:B:80:MET:HG2	2:B:137:PHE:CD1	2.57	0.40
2:B:275:LEU:HD21	2:B:283:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	243 (94%)	14 (5%)	1 (0%)	30	19
2	B	315/308 (102%)	299 (95%)	14 (4%)	2 (1%)	21	11
All	All	573/566 (101%)	542 (95%)	28 (5%)	3 (0%)	30	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2068	ASN
2	B	54[A]	MET
2	B	54[B]	MET

5.3.2 Protein sidechains

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	50
2	B	294/284 (104%)	285 (97%)	9 (3%)	35	17
All	All	531/517 (103%)	519 (98%)	12 (2%)	43	28

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	2060	LEU
1	A	2066	LYS

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Mol	Chain	Res	Type
2	B	2	ASN
2	B	80	MET
2	B	84	ARG
2	B	91	ASN
2	B	92	ILE
2	B	275	LEU
2	B	281	ASP
2	B	295	SER
2	B	315	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1947	HIS
2	B	23	ASN
2	B	47	GLN
2	B	259	HIS

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	V3R	B	401	-	13,13,13	1.29	2 (15%)	17,17,17	1.24	2 (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
3	V3R	B	401	-	-	5/5/5/5	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	V3R	C1-N	2.70	1.56	1.49
3	B	401	V3R	F1-C7	-2.15	1.29	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	401	V3R	C3-C2-C1	-2.96	107.39	113.42
3	B	401	V3R	C4-C9-C8	-2.82	117.53	119.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	V3R	C1-C2-C3-C4
3	B	401	V3R	N-C1-C2-C3
3	B	401	V3R	C-C1-C2-C3
3	B	401	V3R	C2-C3-C4-C9
3	B	401	V3R	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	V3R	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	3.25	179 (75%) 0 0	28, 98, 190, 276	12 (5%)
2	B	300/308 (97%)	3.17	203 (67%) 0 0	29, 96, 201, 306	9 (3%)
All	All	537/566 (94%)	3.20	382 (71%) 0 0	28, 98, 200, 306	21 (3%)

All (382) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2039	LEU	10.9
1	A	2040	TRP	10.7
2	B	77	LEU	10.1
2	B	54[A]	MET	9.5
2	B	316	LEU	8.7
1	A	1956	ILE	8.7
2	B	62	CYS	8.5
1	A	2060	LEU	8.4
1	A	2048	TRP	7.9
1	A	1964	PRO	7.9
1	A	2041	PRO	7.8
2	B	17	ILE	7.8
1	A	1979[A]	MET	7.7
1	A	1875	ILE	7.7
2	B	103	VAL	7.6
2	B	291	ILE	7.4
2	B	293	LEU	7.2
1	A	2059	ILE	7.1
2	B	38	ILE	6.9
2	B	152	LEU	6.8
1	A	1879	ILE	6.7
2	B	276	PRO	6.6
1	A	1848	ILE	6.6
2	B	93	VAL	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	1894	ILE	6.5
2	B	20	TYR	6.5
2	B	254	ALA	6.5
2	B	122[A]	GLN	6.5
1	A	1888	HIS	6.4
2	B	214	PHE	6.4
1	A	1944	LEU	6.4
1	A	2017[A]	THR	6.3
2	B	41[A]	VAL	6.3
2	B	101	MET	6.2
2	B	19	GLN	6.2
1	A	1862	VAL	6.2
1	A	1941	LEU	6.1
2	B	130	VAL	6.1
2	B	246	MET	6.1
2	B	43	VAL	6.1
2	B	15	ILE	6.0
2	B	279	TYR	6.0
2	B	129	ILE	6.0
1	A	1946	VAL	5.9
2	B	46	PHE	5.9
1	A	1977	VAL	5.9
2	B	74	LYS	5.8
1	A	1840	TYR	5.8
2	B	283	LEU	5.8
1	A	2032	ILE	5.8
1	A	1909	ALA	5.8
2	B	55[A]	ARG	5.7
2	B	9	ALA	5.7
1	A	2051	ILE	5.7
2	B	1	MET	5.6
2	B	81	MET	5.6
2	B	126	ILE	5.6
2	B	282	ILE	5.6
1	A	1965	PHE	5.6
2	B	13	VAL	5.6
2	B	114	TRP	5.6
2	B	45[A]	HIS	5.6
2	B	49	ALA	5.6
2	B	267	ILE	5.6
2	B	222	GLY	5.5
2	B	80	MET	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	67	PHE	5.5
1	A	1963	LEU	5.4
1	A	1866	PHE	5.4
1	A	2058	LEU	5.4
1	A	1966	SER	5.4
2	B	83	GLU	5.3
1	A	1833	GLY	5.3
2	B	239	SER	5.3
1	A	2068	ASN	5.2
2	B	10	PRO	5.2
2	B	124	ASP	5.2
1	A	1951	PHE	5.2
1	A	1913	THR	5.1
2	B	213	ILE	5.1
2	B	128	LYS	5.1
2	B	275	LEU	5.1
1	A	2063	TYR	5.0
2	B	22	PHE	5.0
2	B	189	ILE	5.0
2	B	288	VAL	4.9
2	B	8	SER	4.9
2	B	170	SER	4.9
1	A	1959	THR	4.9
1	A	1978	VAL	4.9
1	A	1940	MET	4.9
1	A	1901	GLY	4.8
1	A	2049	ILE	4.8
2	B	18	ASP	4.8
2	B	89	PHE	4.8
2	B	217	SER	4.8
2	B	14	THR	4.8
2	B	56	TYR	4.7
1	A	1834	ALA	4.7
1	A	1841	ALA	4.7
1	A	2069	VAL	4.7
1	A	1970	SER	4.7
2	B	234	PHE	4.6
1	A	2002[A]	TYR	4.6
1	A	1857	VAL	4.6
2	B	317	LEU	4.6
1	A	2043	PHE	4.6
2	B	313	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	256	VAL	4.6
2	B	108	ILE	4.6
2	B	28	GLN	4.6
2	B	220	TYR	4.6
1	A	2027	LEU	4.6
2	B	203[A]	TYR	4.5
1	A	2067	TYR	4.5
2	B	4	VAL	4.5
1	A	2052	GLU	4.5
2	B	102	MET	4.5
2	B	37	PRO	4.5
1	A	1902	GLN	4.4
1	A	1973	LYS	4.3
1	A	1878	CYS	4.3
1	A	1860	VAL	4.3
2	B	147	VAL	4.2
1	A	1991	ILE	4.2
2	B	107	LYS	4.2
1	A	1856[A]	ASN	4.2
2	B	221	PHE	4.2
2	B	106	PRO	4.2
2	B	109	ASP	4.2
1	A	2038	HIS	4.2
2	B	16	GLY	4.2
2	B	192	GLY	4.2
2	B	127	ARG	4.2
1	A	2061	THR	4.2
1	A	1961[A]	LEU	4.2
2	B	264	LEU	4.2
2	B	173	ALA	4.1
2	B	47	GLN	4.1
1	A	1880	PHE	4.1
2	B	176	LEU	4.1
2	B	290	ASN	4.1
2	B	294	TYR	4.1
2	B	73	PRO	4.1
1	A	2028	SER	4.1
1	A	2005	PHE	4.0
1	A	2037	TYR	4.0
1	A	1846	ASN	4.0
2	B	50	ASP	4.0
1	A	1838	SER	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	145	THR	4.0
2	B	92	ILE	4.0
2	B	199	LEU	4.0
1	A	1835	MET	3.9
2	B	29	PRO	3.9
2	B	193	HIS	3.9
2	B	95	ASN	3.9
2	B	211[A]	GLN	3.9
1	A	2050	THR	3.9
1	A	1852	VAL	3.8
1	A	2030	PRO	3.8
1	A	1975	SER	3.8
2	B	175	SER	3.8
2	B	139	TYR	3.8
2	B	123[A]	MET	3.8
2	B	249	LEU	3.8
1	A	1903	LYS	3.8
1	A	1910	LYS	3.8
2	B	280	SER	3.8
1	A	2065	ARG	3.8
2	B	131	ARG	3.8
2	B	42[A]	HIS	3.7
2	B	174	HIS	3.7
2	B	117	LEU	3.7
1	A	1968	ALA	3.7
2	B	233	PHE	3.7
1	A	1988	LEU	3.7
1	A	1918[A]	SER	3.7
1	A	2064	GLY	3.7
1	A	2003	THR	3.7
2	B	146	THR	3.6
2	B	305	THR	3.6
1	A	1876	ASN	3.6
1	A	1971	ILE	3.6
1	A	2022	ALA	3.6
1	A	2055	MET	3.6
2	B	30	PHE	3.6
2	B	216	ASN	3.5
1	A	2042	SER	3.5
1	A	2053[A]	SER	3.5
2	B	60	PHE	3.5
1	A	1843	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	2025	ILE	3.5
1	A	2066	LYS	3.5
2	B	23	ASN	3.5
1	A	2001[A]	SER	3.4
1	A	1914	ALA	3.4
2	B	172	PRO	3.4
2	B	57	GLY	3.4
1	A	2054[A]	GLN	3.4
1	A	1957	ARG	3.4
2	B	63	ARG	3.4
1	A	2044	THR	3.4
2	B	195	MET	3.4
2	B	100	GLN	3.3
2	B	58	TYR	3.3
1	A	1987	VAL	3.3
2	B	7	THR	3.3
1	A	1952	PRO	3.3
2	B	5	PRO	3.3
2	B	171	ASP	3.3
2	B	261	LEU	3.3
2	B	61	ASP	3.2
2	B	268	LEU	3.2
2	B	120	PHE	3.2
1	A	1932[A]	GLN	3.2
1	A	1954	ILE	3.2
1	A	2062	GLU	3.2
2	B	281	ASP	3.2
2	B	188	ALA	3.2
1	A	1931[A]	LYS	3.2
1	A	1837	SER	3.2
1	A	1844	PHE	3.2
2	B	133	ASP	3.2
2	B	59	TRP	3.1
2	B	68	TYR	3.1
1	A	1972	ASP	3.1
1	A	1851	PHE	3.1
1	A	1936	THR	3.1
1	A	2009	THR	3.1
1	A	2036	SER	3.1
2	B	53	SER	3.1
2	B	257	PRO	3.1
2	B	277	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	208	VAL	3.1
1	A	1890	PHE	3.1
2	B	226	PHE	3.1
1	A	1893	ILE	3.0
1	A	1933	ILE	3.0
2	B	262	ASP	3.0
1	A	1996	LEU	3.0
2	B	263	LYS	3.0
1	A	1861	THR	3.0
2	B	299	LYS	3.0
1	A	1999	ILE	3.0
1	A	1905	LEU	3.0
2	B	186	ARG	3.0
2	B	237	TYR	3.0
2	B	110	GLU	3.0
1	A	1899[A]	TRP	3.0
2	B	52	SER	3.0
2	B	3	THR	3.0
1	A	1967	ALA	3.0
1	A	2008	LEU	3.0
1	A	1895	HIS	3.0
1	A	1998	ARG	3.0
1	A	2013	ARG	3.0
2	B	250	ILE	3.0
1	A	1891	LEU	2.9
1	A	1842	GLU	2.9
1	A	1874	ALA	2.9
2	B	11	ILE	2.9
1	A	1929	GLN	2.9
1	A	1985	GLN	2.9
2	B	27	ASN	2.9
1	A	2023	LYS	2.9
2	B	184	LYS	2.9
1	A	1881	THR	2.8
2	B	300	ASN	2.8
1	A	1980[A]	LYS	2.8
1	A	1960[A]	GLU	2.8
1	A	2046	GLU	2.8
1	A	2024[A]	MET	2.8
1	A	1911	TRP	2.8
2	B	274	THR	2.8
1	A	1904	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	266	GLU	2.8
1	A	1865	THR	2.8
2	B	21	SER	2.8
1	A	1981	ALA	2.8
2	B	292	CYS	2.8
1	A	1872	THR	2.8
1	A	2011	LEU	2.8
2	B	302	LEU	2.8
2	B	134	GLU	2.7
1	A	1995	TRP	2.7
1	A	2047	GLN	2.7
1	A	1912	LYS	2.7
1	A	1974	LEU	2.7
2	B	308	ILE	2.7
2	B	84	ARG	2.7
2	B	218	SER	2.7
2	B	278	GLN	2.7
2	B	258	LYS	2.7
2	B	40	HIS	2.7
2	B	112	ASP	2.7
2	B	179	THR	2.7
1	A	1908	LEU	2.7
2	B	229	LEU	2.7
2	B	140	VAL	2.7
2	B	225	GLN	2.6
2	B	71	TYR	2.6
1	A	2000	SER	2.6
1	A	2015	LEU	2.6
1	A	1859	ARG	2.6
1	A	1986	MET	2.6
2	B	148	GLN	2.6
2	B	149	GLU	2.6
2	B	306	GLU	2.6
2	B	2	ASN	2.6
2	B	259	HIS	2.6
1	A	1962	ARG	2.6
2	B	111	ASP	2.6
1	A	1953	ASN	2.6
1	A	1855[A]	THR	2.6
2	B	137	PHE	2.5
2	B	224	LEU	2.5
2	B	289	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	88	LYS	2.5
2	B	190	ARG	2.5
1	A	1948	MET	2.5
2	B	311	ASN	2.5
2	B	228	PHE	2.5
1	A	1845	ASN	2.5
2	B	295	SER	2.5
1	A	1939	ALA	2.5
2	B	118	THR	2.5
1	A	1877	GLY	2.4
2	B	132	LYS	2.4
1	A	1847	ASP	2.4
2	B	191	PRO	2.4
1	A	1868	GLY	2.4
2	B	202	SER	2.4
1	A	1942	ASP	2.4
1	A	1950	ASP	2.4
2	B	210	LEU	2.4
1	A	1871	ALA	2.4
1	A	1919[A]	ALA	2.4
1	A	1934	ILE	2.3
2	B	314	PRO	2.3
2	B	96	PHE	2.3
1	A	1836	ASN	2.3
2	B	48	HIS	2.3
2	B	227	ALA	2.3
1	A	1945	GLU	2.3
1	A	2035	LYS	2.3
1	A	2034	ILE	2.3
2	B	235	GLY	2.3
1	A	1997	ASP	2.3
1	A	1869	ASN	2.3
2	B	94	HIS	2.3
1	A	2026	LEU	2.3
2	B	307	LYS	2.3
2	B	270	TYR	2.2
2	B	310	GLU	2.2
1	A	1937	ARG	2.2
2	B	69	ILE	2.2
1	A	1863	HIS	2.2
1	A	2033	THR	2.2
1	A	1920	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	238	GLY	2.2
2	B	87	ALA	2.2
2	B	183	PHE	2.2
2	B	151	GLU	2.2
1	A	2031	THR	2.2
1	A	1927	GLU	2.1
1	A	1989	PHE	2.1
1	A	2018[A]	ASN	2.1
2	B	181	ILE	2.1
2	B	26	GLU	2.1
1	A	2045	ASP	2.1
1	A	2006	SER	2.1
1	A	1873	LYS	2.1
1	A	1930	PRO	2.1
2	B	301	SER	2.1
1	A	1864	LYS	2.1
1	A	2012	LEU	2.1
2	B	273	LYS	2.0
2	B	297	PHE	2.0
2	B	252	SER	2.0
1	A	1886	THR	2.0
2	B	86	GLY	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	V3R	B	401	13/13	0.79	0.14	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.