



Full wwPDB X-ray Structure Validation Report i

Oct 25, 2022 – 04:21 PM EDT

PDB ID : 5SU4
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P03E02 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 : 1.66 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

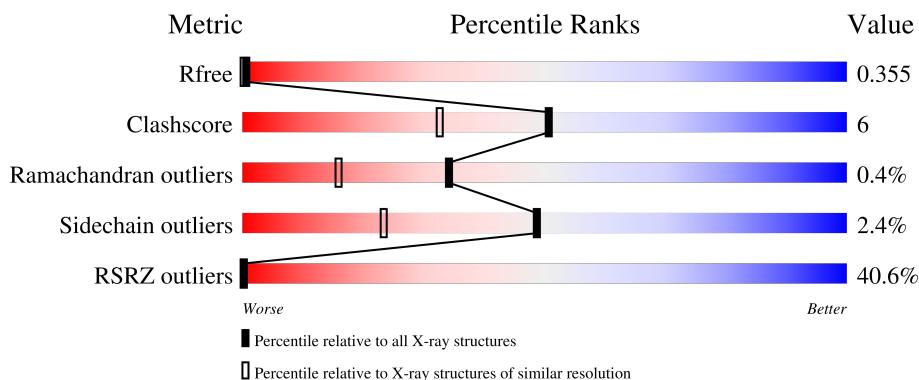
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

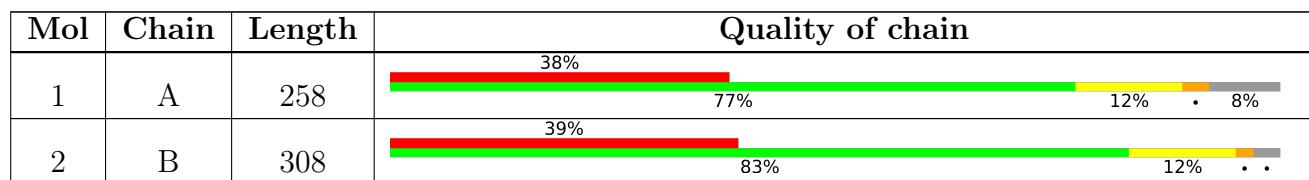
The reported resolution of this entry is 1.66 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (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.



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4687 atoms, of which 0 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 2008	N 1287	O 336	S 373	12	8	12	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	
2	B	300	Total	C 2571	N 1649	O 419	S 483	20	0	8	0

There are 20 discrepancies between the modelled and reference sequences:

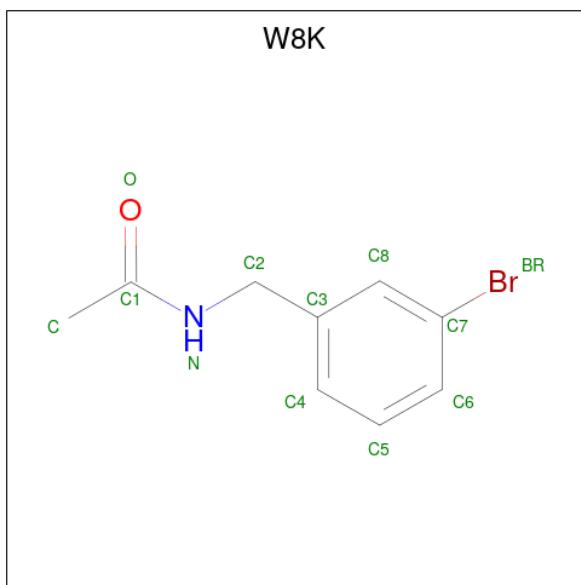
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	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 N-[(3-bromophenyl)methyl]acetamide (three-letter code: W8K) (formula: C₉H₁₀BrNO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			12	1	9	1	1		
3	B	1	Total	Br	C	N	O	0	0
			12	1	9	1	1		
3	B	1	Total	Br	C	N	O	0	0
			12	1	9	1	1		
3	B	1	Total	Br	C	N	O	0	0
			12	1	9	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		

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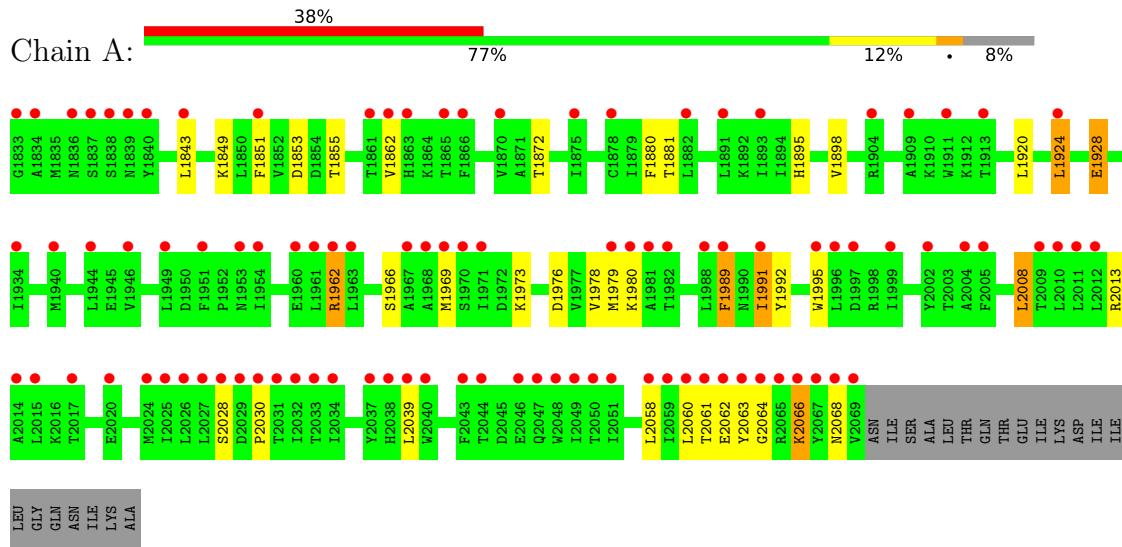
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	31	Total O 31 31	0	0

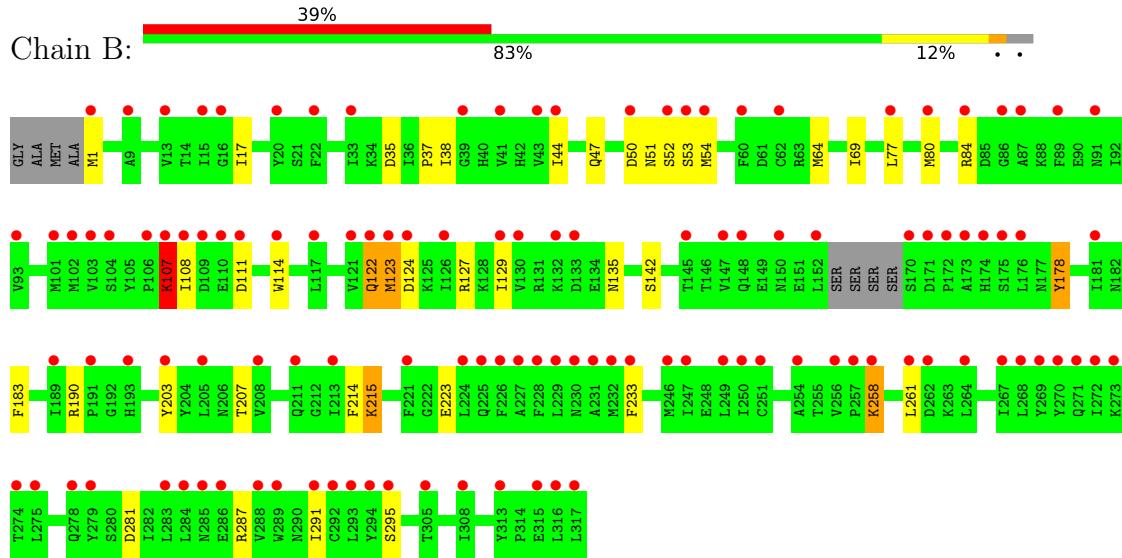
3 Residue-property plots

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 i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.38Å 81.64Å 93.60Å 90.00° 109.05° 90.00°	Depositor
Resolution (Å)	44.24 – 1.66 44.24 – 1.66	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.24-1.66) 98.9 (44.24-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	0.97 (at 1.66Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R , R_{free}	0.346 , 0.357 0.342 , 0.355	Depositor DCC
R_{free} test set	2101 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.8	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4687	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section: W8K

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	0.79	2/2055 (0.1%)	0.88	3/2784 (0.1%)
2	B	0.81	6/2642 (0.2%)	0.92	4/3569 (0.1%)
All	All	0.80	8/4697 (0.2%)	0.90	7/6353 (0.1%)

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	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1924	LEU	C-N	10.07	1.53	1.34
2	B	223	GLU	CD-OE2	-6.62	1.18	1.25
2	B	114	TRP	CE3-CZ3	6.49	1.49	1.38
2	B	183	PHE	CB-CG	5.57	1.60	1.51
1	A	1928	GLU	CD-OE2	-5.52	1.19	1.25
2	B	178	TYR	CE2-CZ	-5.43	1.31	1.38
2	B	123	MET	N-CA	5.38	1.57	1.46
2	B	233	PHE	CE1-CZ	5.36	1.47	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2008	LEU	CB-CG-CD1	-8.13	97.18	111.00
2	B	124	ASP	CB-CA-C	6.55	123.50	110.40
2	B	122	GLN	C-N-CA	-5.73	107.38	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	261	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	A	1920	LEU	CB-CG-CD1	-5.28	102.02	111.00
2	B	214	PHE	C-N-CA	5.11	134.47	121.70
1	A	1989	PHE	CB-CA-C	-5.05	100.31	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	122	GLN	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	0	2041	25	0
2	B	2571	0	2443	27	0
3	A	12	0	0	0	0
3	B	36	0	0	0	0
4	A	29	0	0	0	0
4	B	31	0	0	1	0
All	All	4687	0	4484	52	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 6.

All (52) 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:1962:ARG:O	1:A:2013:ARG:NH2	2.07	0.87
2:B:37:PRO:HG3	2:B:107:LYS:HG3	1.65	0.77
2:B:1:MET:N	4:B:501:HOH:O	2.18	0.76
2:B:17:ILE:HD13	2:B:44[B]:ILE:HG12	1.70	0.73
2:B:127:ARG:NH2	2:B:135:ASN:O	2.22	0.73
2:B:17:ILE:HD13	2:B:44[B]:ILE:CG1	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1989:PHE:CD1	1:A:2039:LEU:HD21	2.32	0.65
1:A:2061:THR:O	1:A:2064:GLY:N	2.30	0.64
1:A:2064:GLY:O	1:A:2068:ASN:N	2.33	0.61
2:B:108:ILE:HG22	2:B:111:ASP:H	1.68	0.59
1:A:1895:HIS:O	1:A:1898[A]:VAL:HG22	2.04	0.58
2:B:287:ARG:O	2:B:291:ILE:HD13	2.04	0.57
1:A:1853:ASP:HB3	1:A:1880:PHE:HB3	1.88	0.55
2:B:64[A]:MET:SD	2:B:123:MET:HB2	2.47	0.55
2:B:1:MET:HB3	2:B:35:ASP:HA	1.86	0.55
1:A:1969:MET:HE3	1:A:1978:VAL:HG21	1.88	0.54
2:B:50:ASP:OD1	2:B:51:ASN:N	2.42	0.53
2:B:258:LYS:HD2	2:B:258:LYS:H	1.74	0.52
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.91	0.52
2:B:108:ILE:HB	2:B:111:ASP:HB3	1.91	0.52
1:A:2062:GLU:O	1:A:2066:LYS:HB2	2.10	0.52
1:A:1991:ILE:HG21	1:A:2008:LEU:HD22	1.92	0.51
2:B:17:ILE:O	2:B:17:ILE:HG23	2.12	0.50
1:A:1991:ILE:HG21	1:A:2008:LEU:CD2	2.42	0.50
1:A:1991:ILE:HG23	1:A:2008:LEU:HD13	1.94	0.49
2:B:37:PRO:CG	2:B:107:LYS:HG3	2.38	0.49
2:B:108:ILE:HG21	2:B:111:ASP:HB2	1.94	0.48
1:A:1991:ILE:CG2	1:A:2008:LEU:HD22	2.45	0.47
2:B:190:ARG:HG3	2:B:203[B]:TYR:CZ	2.49	0.47
2:B:69:ILE:HD13	2:B:80:MET:HA	1.95	0.47
2:B:108:ILE:CG2	2:B:111:ASP:HB2	2.45	0.47
2:B:203[A]:TYR:CZ	2:B:207:THR:HG21	2.50	0.47
2:B:53:SER:O	2:B:54[A]:MET:HB3	2.15	0.46
2:B:47:GLN:NE2	2:B:52:SER:O	2.47	0.46
1:A:1924:LEU:HD13	1:A:1928:GLU:O	2.17	0.45
2:B:1:MET:H2	2:B:38:ILE:HD11	1.82	0.45
1:A:2060:LEU:O	1:A:2063:TYR:HB3	2.16	0.45
1:A:1855[A]:THR:HG21	1:A:1966:SER:HB2	1.97	0.45
1:A:1976:ASP:O	1:A:1980:LYS:HG3	2.17	0.45
1:A:1862:VAL:HG22	1:A:1872:THR:HG22	2.00	0.43
2:B:108:ILE:HG22	2:B:111:ASP:N	2.31	0.43
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.39	0.43
2:B:1:MET:N	2:B:38:ILE:HD11	2.32	0.43
1:A:1991:ILE:CG2	1:A:1991:ILE:O	2.67	0.43
2:B:129:ILE:HD13	2:B:178:TYR:CD1	2.54	0.42
1:A:1924:LEU:HD23	1:A:1924:LEU:HA	1.83	0.42
2:B:51:ASN:OD1	2:B:53:SER:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1992:TYR:O	1:A:1995:TRP:CG	2.73	0.41
1:A:2060:LEU:HG	1:A:2061:THR:N	2.34	0.41
1:A:1851:PHE:O	1:A:1881:THR:HA	2.21	0.41
1:A:2028:SER:O	1:A:2030:PRO:HD3	2.21	0.40
2:B:215:LYS:HD3	2:B:215:LYS:HA	1.73	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	248/258 (96%)	241 (97%)	7 (3%)	0	100 100
2	B	305/308 (99%)	293 (96%)	10 (3%)	2 (1%)	22 6
All	All	553/566 (98%)	534 (97%)	17 (3%)	2 (0%)	34 16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	107	LYS
2	B	215	LYS

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	228/233 (98%)	221 (97%)	7 (3%)	40 14
2	B	286/284 (101%)	279 (98%)	7 (2%)	49 23
All	All	514/517 (99%)	500 (97%)	14 (3%)	49 19

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1962	ARG
1	A	1973	LYS
1	A	1979[A]	MET
1	A	1979[B]	MET
1	A	1979[C]	MET
1	A	1991	ILE
1	A	2066	LYS
2	B	77	LEU
2	B	84	ARG
2	B	107	LYS
2	B	142	SER
2	B	258	LYS
2	B	281	ASP
2	B	295	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1947	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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

4 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	W8K	B	401	-	12,12,12	2.65	3 (25%)	15,15,15	2.15	8 (53%)
3	W8K	B	403	-	12,12,12	1.94	4 (33%)	15,15,15	2.76	7 (46%)
3	W8K	A	2101	-	12,12,12	2.76	5 (41%)	15,15,15	3.28	6 (40%)
3	W8K	B	402	-	12,12,12	2.44	5 (41%)	15,15,15	1.22	1 (6%)

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	W8K	B	401	-	-	2/5/5/5	0/1/1/1
3	W8K	B	403	-	-	0/5/5/5	0/1/1/1
3	W8K	A	2101	-	-	0/5/5/5	0/1/1/1
3	W8K	B	402	-	-	2/5/5/5	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	W8K	BR-C7	-8.11	1.73	1.90
3	A	2101	W8K	C2-N	-6.17	1.34	1.46
3	B	402	W8K	BR-C7	-5.50	1.79	1.90
3	A	2101	W8K	C8-C3	-4.45	1.31	1.39
3	A	2101	W8K	C2-C3	-3.67	1.43	1.51
3	B	402	W8K	O-C1	-3.51	1.15	1.23
3	B	403	W8K	C6-C7	-3.38	1.31	1.38
3	B	402	W8K	C2-N	-3.31	1.39	1.46
3	B	403	W8K	BR-C7	-3.15	1.83	1.90
3	B	402	W8K	C5-C4	-2.63	1.33	1.38
3	A	2101	W8K	C8-C7	-2.58	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	W8K	C2-N	-2.56	1.41	1.46
3	A	2101	W8K	C5-C4	-2.51	1.33	1.38
3	B	401	W8K	C5-C6	-2.51	1.33	1.38
3	B	401	W8K	C2-N	-2.50	1.41	1.46
3	B	402	W8K	C8-C7	-2.28	1.33	1.38
3	B	403	W8K	C5-C4	-2.14	1.34	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2101	W8K	C-C1-N	-8.08	101.77	116.09
3	B	403	W8K	BR-C7-C6	-6.69	109.57	119.30
3	A	2101	W8K	C3-C2-N	-6.14	99.90	113.05
3	B	401	W8K	BR-C7-C6	-4.52	112.73	119.30
3	A	2101	W8K	O-C1-C	4.17	129.81	122.06
3	B	403	W8K	C3-C8-C7	-3.88	113.51	119.44
3	B	403	W8K	BR-C7-C8	3.83	124.59	119.27
3	A	2101	W8K	C4-C3-C8	3.66	123.67	118.54
3	B	401	W8K	C3-C8-C7	-3.50	114.09	119.44
3	B	403	W8K	C2-C3-C4	-3.17	114.34	120.91
3	B	403	W8K	C6-C7-C8	2.98	125.80	121.48
3	B	403	W8K	C3-C2-N	-2.64	107.39	113.05
3	B	402	W8K	C4-C3-C8	2.57	122.13	118.54
3	B	401	W8K	C2-C3-C4	-2.53	115.67	120.91
3	A	2101	W8K	C3-C8-C7	-2.42	115.75	119.44
3	A	2101	W8K	O-C1-N	2.37	128.42	121.74
3	B	401	W8K	C6-C7-C8	2.36	124.89	121.48
3	B	401	W8K	C3-C2-N	-2.34	108.04	113.05
3	B	401	W8K	O-C1-C	2.33	126.38	122.06
3	B	401	W8K	BR-C7-C8	2.23	122.37	119.27
3	B	403	W8K	O-C1-C	2.20	126.14	122.06
3	B	401	W8K	C4-C3-C8	2.09	121.47	118.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	W8K	O-C1-N-C2
3	B	401	W8K	C-C1-N-C2
3	B	402	W8K	O-C1-N-C2
3	B	402	W8K	C-C1-N-C2

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 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	237/258 (91%)	2.15	99 (41%) 0 0	44, 76, 121, 200	0
2	B	300/308 (97%)	2.12	119 (39%) 0 0	45, 75, 126, 178	0
All	All	537/566 (94%)	2.13	218 (40%) 0 0	44, 76, 123, 200	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	53	SER	13.0
2	B	152	LEU	12.9
1	A	2068	ASN	12.5
1	A	2069	VAL	10.0
2	B	52	SER	9.9
2	B	108	ILE	9.8
1	A	2064	GLY	8.5
1	A	2066	LYS	7.7
1	A	2063	TYR	7.7
2	B	171	ASP	7.5
1	A	1866	PHE	7.4
1	A	2028	SER	7.0
2	B	109	ASP	6.8
1	A	2027	LEU	6.3
2	B	170	SER	6.1
2	B	173	ALA	6.1
1	A	2059	ILE	6.0
2	B	279	TYR	6.0
2	B	283	LEU	6.0
1	A	2017[A]	THR	5.9
2	B	316	LEU	5.9
1	A	2060	LEU	5.7
2	B	101	MET	5.6
1	A	1962	ARG	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	1878	CYS	5.4
1	A	2032	ILE	5.3
2	B	293	LEU	5.3
1	A	2015	LEU	5.2
1	A	1953	ASN	5.1
1	A	2025	ILE	4.9
2	B	1	MET	4.8
2	B	291	ILE	4.8
2	B	229	LEU	4.8
1	A	1949	LEU	4.7
2	B	80	MET	4.7
2	B	147	VAL	4.6
2	B	305	THR	4.6
2	B	103	VAL	4.6
1	A	2065	ARG	4.5
2	B	284	LEU	4.5
1	A	1836	ASN	4.5
2	B	114	TRP	4.4
2	B	246	MET	4.4
1	A	1940	MET	4.4
2	B	77	LEU	4.4
1	A	2051	ILE	4.3
1	A	1989	PHE	4.3
1	A	1870	VAL	4.3
1	A	2012	LEU	4.2
2	B	172	PRO	4.2
2	B	87	ALA	4.1
2	B	268	LEU	4.1
2	B	181	ILE	4.1
1	A	2067	TYR	4.1
2	B	270	TYR	4.0
1	A	2040	TRP	4.0
2	B	43	VAL	3.9
2	B	247	ILE	3.9
2	B	275	LEU	3.9
2	B	274	THR	3.9
2	B	110	GLU	3.9
1	A	2010	LEU	3.9
1	A	2046	GLU	3.9
1	A	2039	LEU	3.8
1	A	1967	ALA	3.8
2	B	313	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	1861	THR	3.7
2	B	189	ILE	3.7
2	B	123	MET	3.7
1	A	1971	ILE	3.7
1	A	2031	THR	3.7
1	A	2026	LEU	3.7
2	B	256	VAL	3.7
1	A	2034	ILE	3.7
2	B	174	HIS	3.7
1	A	1979[A]	MET	3.7
1	A	2014	ALA	3.6
2	B	203[A]	TYR	3.6
1	A	1961	LEU	3.6
2	B	317	LEU	3.6
2	B	228	PHE	3.6
2	B	264	LEU	3.6
1	A	1924	LEU	3.5
2	B	41[A]	VAL	3.5
2	B	133	ASP	3.5
1	A	1865	THR	3.5
1	A	1882	LEU	3.5
1	A	1963	LEU	3.5
1	A	1988	LEU	3.5
1	A	1913	THR	3.4
2	B	132	LYS	3.4
1	A	1999	ILE	3.4
1	A	2044	THR	3.4
2	B	249	LEU	3.4
2	B	213	ILE	3.3
2	B	267	ILE	3.3
1	A	1951	PHE	3.3
2	B	230[A]	ASN	3.3
2	B	62	CYS	3.3
1	A	2049	ILE	3.3
2	B	224	LEU	3.3
1	A	1991	ILE	3.3
2	B	271	GLN	3.3
2	B	121	VAL	3.3
2	B	124	ASP	3.3
2	B	272	ILE	3.3
2	B	117	LEU	3.2
2	B	292	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	2061	THR	3.2
2	B	227	ALA	3.2
1	A	2005	PHE	3.2
1	A	2048	TRP	3.2
2	B	148	GLN	3.2
1	A	1837	SER	3.2
2	B	295	SER	3.2
2	B	50	ASP	3.1
1	A	2024[A]	MET	3.1
2	B	15	ILE	3.1
2	B	308	ILE	3.1
2	B	107	LYS	3.1
2	B	84	ARG	3.1
1	A	1833	GLY	3.1
2	B	211[A]	GLN	3.1
2	B	269	TYR	3.0
1	A	1970	SER	3.0
2	B	130	VAL	3.0
1	A	2011	LEU	3.0
1	A	2058	LEU	3.0
2	B	13	VAL	3.0
2	B	250	ILE	3.0
2	B	208	VAL	3.0
2	B	150	ASN	2.9
2	B	294	TYR	2.9
1	A	1995	TRP	2.9
2	B	254	ALA	2.9
1	A	2002	TYR	2.9
2	B	145	THR	2.9
1	A	1996	LEU	2.8
2	B	288	VAL	2.8
1	A	2043	PHE	2.8
2	B	258	LYS	2.8
2	B	233	PHE	2.8
1	A	2037	TYR	2.8
1	A	1862	VAL	2.8
2	B	221	PHE	2.8
2	B	54[A]	MET	2.7
1	A	2062	GLU	2.7
2	B	193	HIS	2.7
2	B	102	MET	2.7
1	A	1934	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1891	LEU	2.7
2	B	205	LEU	2.7
2	B	285	ASN	2.6
2	B	315	GLU	2.6
2	B	122	GLN	2.6
1	A	1954	ILE	2.6
1	A	1909	ALA	2.6
2	B	191	PRO	2.6
1	A	2030	PRO	2.6
2	B	86	GLY	2.5
2	B	91	ASN	2.5
1	A	2009	THR	2.5
2	B	33	ILE	2.5
2	B	126	ILE	2.5
1	A	1840	TYR	2.5
2	B	231	ALA	2.5
2	B	278	GLN	2.4
2	B	232	MET	2.4
2	B	20	TYR	2.4
1	A	2033	THR	2.4
2	B	225	GLN	2.4
2	B	104	SER	2.4
2	B	226	PHE	2.4
2	B	111	ASP	2.4
2	B	257	PRO	2.3
1	A	2029	ASP	2.3
1	A	2050	THR	2.3
2	B	262	ASP	2.3
1	A	1851	PHE	2.3
1	A	1904	ARG	2.3
1	A	1980	LYS	2.3
2	B	106	PRO	2.3
1	A	1863	HIS	2.3
2	B	9	ALA	2.3
2	B	60	PHE	2.3
2	B	286	GLU	2.3
2	B	93	VAL	2.3
1	A	1875	ILE	2.3
2	B	273	LYS	2.3
1	A	1960[A]	GLU	2.2
1	A	1946	VAL	2.2
1	A	2004	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	175	SER	2.2
1	A	2047	GLN	2.2
2	B	22	PHE	2.2
2	B	251	CYS	2.2
2	B	176	LEU	2.2
2	B	44[A]	ILE	2.1
2	B	16	GLY	2.1
1	A	2020	GLU	2.1
1	A	1981	ALA	2.1
2	B	129	ILE	2.1
2	B	89	PHE	2.1
1	A	1839	ASN	2.1
1	A	1982	THR	2.1
1	A	1997	ASP	2.1
1	A	1968	ALA	2.1
2	B	39	GLY	2.1
1	A	1834	ALA	2.1
1	A	1843	LEU	2.1
1	A	1838	SER	2.1
1	A	1893	ILE	2.1
1	A	1969	MET	2.0
1	A	1911	TRP	2.0
1	A	2038	HIS	2.0
2	B	289	TRP	2.0
1	A	1944	LEU	2.0
2	B	261	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	W8K	A	2101	12/12	0.89	0.28	28,28,28,28	12
3	W8K	B	401	12/12	0.97	0.27	28,28,28,28	0
3	W8K	B	403	12/12	0.97	0.29	28,28,28,28	12
3	W8K	B	402	12/12	0.98	0.19	28,28,28,28	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.