



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:44 AM UTC

PDB ID : 5SU4 / pdb_00005su4
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 ⓘ 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

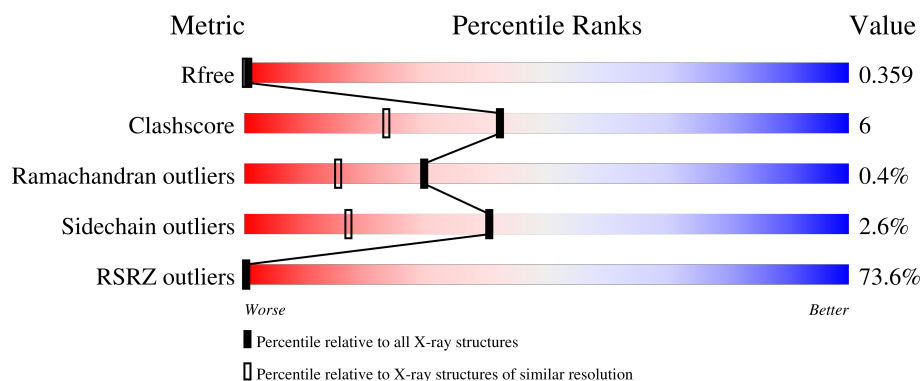
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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}	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	66% 74% 16% • 8%
2	B	308	73% 83% 13% • •

2 Entry composition

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
			Total	C	N	O	S			
1	A	237	2008	1287	336	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
			Total	C	N	O	S			
2	B	300	2571	1649	419	483	20	0	8	0

There are 20 discrepancies between the modelled and reference sequences:

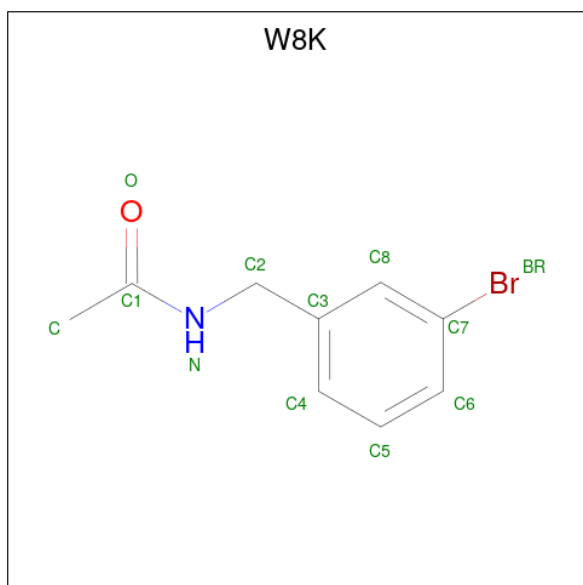
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN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

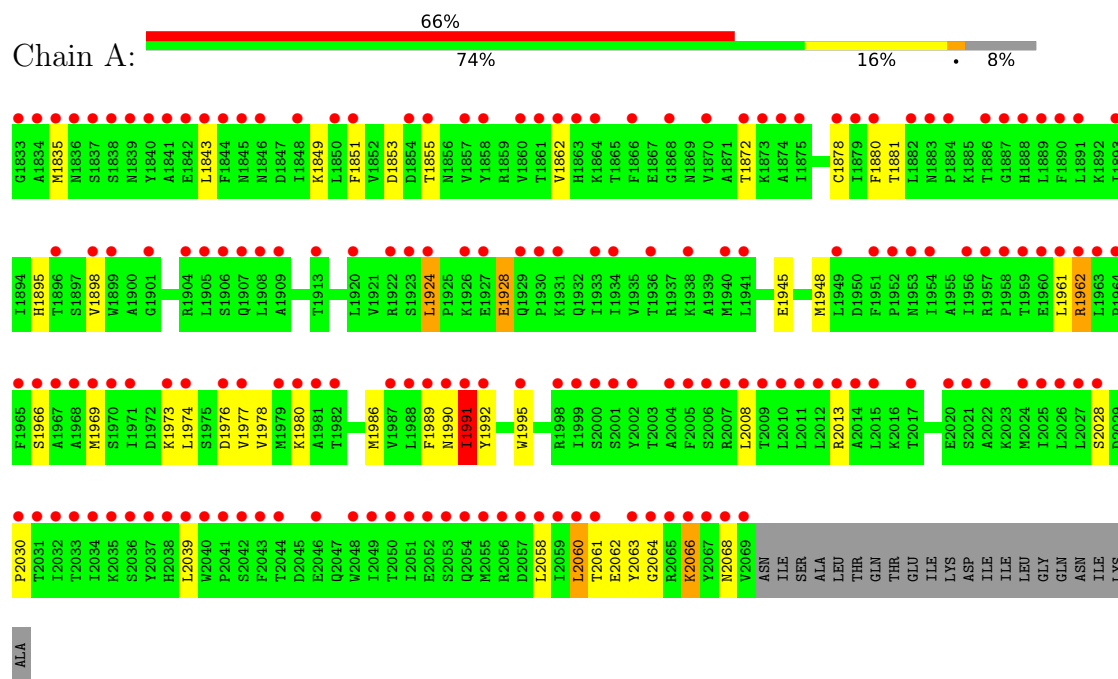
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	31	Total	O	0	0
			31	31		

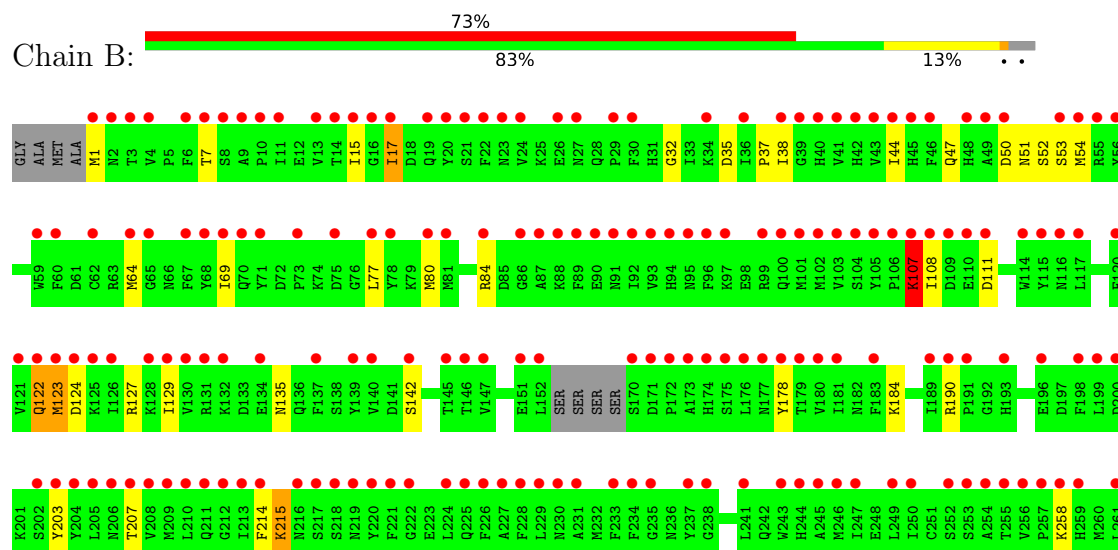
3 Residue-property plots [i](#)

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



• Molecule 2: A1 cistron-splicing factor AAR2



D262	K263	L264	D265	E266	I267	L268	Y269	Y270	Q271	I272	K273	T274	L275	F276	E277	Q278	Y279	S280	D281	I282	L283	L284	N285	E286	R287	V288	W289	N290	I291	C292	L293	Y294	S295	S296	F297	Q298	S301	L302	H303	N304	T305	E306	K307	I308	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	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) 98.8 (44.24-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 1.66Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.346 , 0.357 0.345 , 0.359	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)	0.36 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	0.88	4/2055 (0.2%)	0.99	6/2784 (0.2%)
2	B	0.87	4/2642 (0.2%)	1.16	11/3569 (0.3%)
All	All	0.87	8/4697 (0.2%)	1.09	17/6353 (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	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	15.68	1.53	1.33
2	B	123	MET	N-CA	8.25	1.57	1.46
1	A	1991	ILE	C-O	-7.08	1.13	1.24
2	B	122	GLN	C-N	6.39	1.43	1.33
1	A	1928	GLU	C-O	-6.35	1.15	1.24
2	B	17	ILE	C-O	-5.85	1.17	1.24
1	A	1974	LEU	C-N	-5.10	1.27	1.33
2	B	32	GLY	C-O	-5.03	1.18	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	GLN	CA-C-N	-7.87	107.38	121.14
2	B	122	GLN	C-N-CA	-7.87	107.38	121.14
2	B	15	ILE	CA-C-N	-7.76	116.66	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	15	ILE	C-N-CA	-7.76	116.66	122.33
2	B	124	ASP	CB-CA-C	7.44	123.50	110.85
1	A	1924	LEU	CA-C-N	6.89	127.29	119.92
1	A	1924	LEU	C-N-CA	6.89	127.29	119.92
1	A	1990	ASN	N-CA-C	-6.89	98.72	109.25
2	B	214	PHE	CA-C-N	6.77	134.47	121.54
2	B	214	PHE	C-N-CA	6.77	134.47	121.54
2	B	124	ASP	CA-CB-CG	6.73	119.33	112.60
2	B	214	PHE	O-C-N	6.73	129.36	122.09
1	A	1977	VAL	CB-CA-C	5.99	119.64	111.97
2	B	7	THR	CA-C-O	-5.96	114.23	120.55
1	A	1986	MET	CA-C-N	5.45	130.12	123.10
1	A	1986	MET	C-N-CA	5.45	130.12	123.10
2	B	122	GLN	CA-C-O	-5.01	115.24	121.06

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

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	30	0
2	B	2571	0	2443	28	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	57	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 (57) 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
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.20	0.82
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
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
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:2058:LEU:C	1:A:2058:LEU:HD23	2.39	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
1:A:1945:GLU:OE1	2:B:184:LYS:NZ	2.47	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
1:A:1835:MET:HE1	1:A:1961:LEU:HD12	1.97	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:1969:MET:HE1	1:A:1978:VAL:HG21	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:SER:O	2:B:54[A]:MET:HB3	2.15	0.44
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
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
1:A:1992:TYR:O	1:A:1995:TRP:CG	2.73	0.41
1:A:1851:PHE:O	1:A:1881:THR:HA	2.21	0.41
1:A:1835:MET:HE3	1:A:1835:MET:HB3	1.98	0.41
1:A:2028:SER:O	1:A:2030:PRO:HD3	2.21	0.40
1:A:1948:MET:HB3	1:A:1948:MET:HE3	1.87	0.40
1:A:2060:LEU:HG	1:A:2061:THR:N	2.34	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%)	18	6
All	All	553/566 (98%)	534 (97%)	17 (3%)	2 (0%)	30	15

All (2) Ramachandran outliers are listed below:

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

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	228/233 (98%)	223 (98%)	5 (2%)	45	23
2	B	286/284 (101%)	278 (97%)	8 (3%)	38	15
All	All	514/517 (99%)	501 (98%)	13 (2%)	40	18

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

Mol	Chain	Res	Type
1	A	1962	ARG
1	A	1973	LYS
1	A	1991	ILE
1	A	2060	LEU
1	A	2066	LYS
2	B	77	LEU
2	B	84	ARG
2	B	107	LYS
2	B	142	SER
2	B	281	ASP
2	B	282	ILE
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	1856	ASN
1	A	1947	HIS
2	B	135	ASN
2	B	259	HIS

5.3.3 RNA ⓘ

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](#)

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	A	2101	-	12,12,12	2.82	5 (41%)	15,15,15	3.38	6 (40%)
3	W8K	B	402	-	12,12,12	2.55	5 (41%)	15,15,15	1.27	1 (6%)
3	W8K	B	403	-	12,12,12	2.07	5 (41%)	15,15,15	2.87	7 (46%)
3	W8K	B	401	-	12,12,12	2.76	3 (25%)	15,15,15	2.23	8 (53%)

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	W8K	BR-C7	-8.32	1.73	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2101	W8K	C2-N	-6.05	1.34	1.46
3	B	402	W8K	BR-C7	-5.65	1.79	1.90
3	A	2101	W8K	C8-C3	-4.51	1.31	1.39
3	B	403	W8K	C6-C7	-3.64	1.31	1.38
3	A	2101	W8K	C2-C3	-3.60	1.43	1.51
3	B	402	W8K	O-C1	-3.55	1.15	1.23
3	B	402	W8K	C2-N	-3.26	1.39	1.46
3	B	403	W8K	BR-C7	-3.24	1.83	1.90
3	B	402	W8K	C5-C4	-3.22	1.33	1.38
3	A	2101	W8K	C5-C4	-3.08	1.33	1.38
3	B	401	W8K	C5-C6	-3.08	1.33	1.38
3	A	2101	W8K	C8-C7	-2.68	1.33	1.38
3	B	403	W8K	C5-C4	-2.63	1.34	1.38
3	B	403	W8K	C2-N	-2.53	1.41	1.46
3	B	401	W8K	C2-N	-2.47	1.41	1.46
3	B	402	W8K	C8-C7	-2.37	1.33	1.38
3	B	403	W8K	C5-C6	-2.23	1.35	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	-8.41	101.77	116.12
3	B	403	W8K	BR-C7-C6	-7.14	109.57	119.30
3	A	2101	W8K	C3-C2-N	-6.25	99.90	113.07
3	B	401	W8K	BR-C7-C6	-4.82	112.73	119.30
3	A	2101	W8K	O-C1-C	4.35	129.81	122.05
3	B	403	W8K	C3-C8-C7	-4.06	113.51	119.41
3	B	403	W8K	BR-C7-C8	3.78	124.59	119.23
3	A	2101	W8K	C4-C3-C8	3.71	123.67	118.55
3	B	401	W8K	C3-C8-C7	-3.67	114.09	119.41
3	B	403	W8K	C2-C3-C4	-3.23	114.34	120.94
3	B	403	W8K	C6-C7-C8	2.96	125.80	121.53
3	B	403	W8K	C3-C2-N	-2.70	107.39	113.07
3	B	402	W8K	C4-C3-C8	2.60	122.13	118.55
3	B	401	W8K	C2-C3-C4	-2.58	115.67	120.94
3	A	2101	W8K	O-C1-N	2.53	128.42	121.78
3	A	2101	W8K	C3-C8-C7	-2.52	115.75	119.41
3	B	401	W8K	O-C1-C	2.43	126.38	122.05
3	B	401	W8K	C3-C2-N	-2.39	108.04	113.07
3	B	401	W8K	C6-C7-C8	2.33	124.89	121.53
3	B	403	W8K	O-C1-C	2.29	126.14	122.05
3	B	401	W8K	BR-C7-C8	2.22	122.37	119.23

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	401	W8K	C4-C3-C8	2.12	121.47	118.55

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

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%)	2.97	171 (72%) 0 0	26, 74, 121, 200	12 (5%)
2	B	300/308 (97%)	3.01	224 (74%) 0 0	26, 75, 126, 178	8 (2%)
All	All	537/566 (94%)	2.99	395 (73%) 0 0	26, 75, 123, 200	20 (3%)

All (395) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	283	LEU	10.3
2	B	203[A]	TYR	8.9
1	A	1878	CYS	8.8
2	B	77	LEU	8.1
1	A	1940	MET	7.8
1	A	1979[A]	MET	7.7
2	B	267	ILE	7.5
2	B	114	TRP	6.8
2	B	268	LEU	6.7
2	B	101	MET	6.7
1	A	2069	VAL	6.7
2	B	291	ILE	6.6
1	A	2060	LEU	6.5
2	B	41[A]	VAL	6.5
1	A	2051	ILE	6.3
2	B	80	MET	6.2
1	A	1989	PHE	6.2
2	B	108	ILE	6.1
1	A	2026	LEU	6.1
2	B	275	LEU	6.0
1	A	2059	ILE	5.9
2	B	254	ALA	5.8
1	A	2010	LEU	5.8
1	A	1834	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	2017[A]	THR	5.6
2	B	289	TRP	5.6
1	A	2015	LEU	5.5
2	B	247	ILE	5.4
2	B	246	MET	5.4
2	B	199	LEU	5.4
2	B	7	THR	5.4
1	A	2037	TYR	5.3
2	B	233	PHE	5.3
1	A	2048	TRP	5.3
1	A	1862	VAL	5.2
2	B	227	ALA	5.2
1	A	2068	ASN	5.2
1	A	2012	LEU	5.2
2	B	152	LEU	5.2
1	A	1840	TYR	5.2
1	A	1970	SER	5.2
1	A	2034	ILE	5.1
2	B	234	PHE	5.1
1	A	2063	TYR	5.1
1	A	1924	LEU	5.1
1	A	1988	LEU	5.1
2	B	221	PHE	5.1
1	A	1866	PHE	5.0
2	B	54[A]	MET	5.0
2	B	279	TYR	5.0
2	B	147	VAL	5.0
2	B	288	VAL	5.0
1	A	1860	VAL	4.9
2	B	270	TYR	4.9
1	A	2040	TRP	4.9
2	B	17	ILE	4.8
2	B	213	ILE	4.8
2	B	129	ILE	4.8
1	A	1934	ILE	4.7
2	B	92	ILE	4.7
1	A	1913	THR	4.7
1	A	1991	ILE	4.7
1	A	2043	PHE	4.7
2	B	305	THR	4.7
1	A	2064	GLY	4.7
2	B	292	CYS	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	68	TYR	4.6
1	A	2039	LEU	4.6
1	A	1846	ASN	4.6
2	B	49	ALA	4.6
2	B	313	TYR	4.5
1	A	1851	PHE	4.5
2	B	316	LEU	4.5
2	B	174	HIS	4.5
2	B	173	ALA	4.5
2	B	170	SER	4.4
2	B	284	LEU	4.4
1	A	2025	ILE	4.4
2	B	282	ILE	4.4
2	B	121	VAL	4.4
2	B	274	THR	4.4
1	A	1901	GLY	4.4
2	B	269	TYR	4.4
2	B	261	LEU	4.4
1	A	1963	LEU	4.3
1	A	1833	GLY	4.3
1	A	1930	PRO	4.3
1	A	2067	TYR	4.3
1	A	1848	ILE	4.3
2	B	111	ASP	4.3
1	A	2061	THR	4.2
1	A	2027	LEU	4.2
2	B	59	TRP	4.2
2	B	226	PHE	4.2
1	A	1835	MET	4.2
2	B	126	ILE	4.2
2	B	308	ILE	4.2
2	B	205	LEU	4.2
1	A	2005	PHE	4.2
2	B	24	VAL	4.2
2	B	172	PRO	4.2
2	B	271	GLN	4.2
2	B	67	PHE	4.2
2	B	130	VAL	4.2
2	B	134	GLU	4.2
2	B	16	GLY	4.2
2	B	109	ASP	4.1
2	B	73	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	177[A]	ASN	4.1
2	B	103	VAL	4.1
1	A	1875	ILE	4.1
1	A	2011	LEU	4.1
2	B	193	HIS	4.1
2	B	245	ALA	4.0
1	A	2030	PRO	4.0
1	A	1936	THR	4.0
1	A	1951	PHE	4.0
2	B	13	VAL	4.0
1	A	2014	ALA	3.9
2	B	123	MET	3.9
1	A	1968	ALA	3.9
2	B	107	LYS	3.9
1	A	1987	VAL	3.8
2	B	272	ILE	3.8
1	A	2002	TYR	3.8
2	B	214	PHE	3.8
2	B	211[A]	GLN	3.8
1	A	2032	ILE	3.8
2	B	220	TYR	3.8
2	B	89	PHE	3.7
2	B	120	PHE	3.7
2	B	224	LEU	3.7
1	A	2058	LEU	3.7
2	B	259	HIS	3.7
2	B	115	TYR	3.7
1	A	1880	PHE	3.7
1	A	1886	THR	3.7
2	B	48	HIS	3.7
2	B	139	TYR	3.7
1	A	2056[A]	ARG	3.6
1	A	1961	LEU	3.6
2	B	217	SER	3.6
1	A	2041	PRO	3.6
2	B	258	LYS	3.6
1	A	1908	LEU	3.6
1	A	1965	PHE	3.5
2	B	30	PHE	3.5
2	B	244	HIS	3.5
1	A	1922	ARG	3.5
2	B	69	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1857	VAL	3.5
1	A	1898[A]	VAL	3.5
2	B	140	VAL	3.5
2	B	294	TYR	3.5
2	B	222	GLY	3.5
1	A	1863	HIS	3.5
1	A	1909	ALA	3.5
2	B	11	ILE	3.5
2	B	298	GLN	3.5
1	A	1958	PRO	3.5
2	B	1	MET	3.5
2	B	55	ARG	3.5
2	B	257	PRO	3.5
1	A	1971	ILE	3.4
1	A	1882	LEU	3.4
1	A	1920	LEU	3.4
1	A	1941	LEU	3.4
2	B	229	LEU	3.4
1	A	1977	VAL	3.4
1	A	1956	ILE	3.4
2	B	297	PHE	3.4
1	A	1874	ALA	3.4
1	A	1967	ALA	3.4
1	A	2044	THR	3.4
2	B	14	THR	3.4
2	B	276	PRO	3.4
1	A	2065	ARG	3.4
2	B	125	LYS	3.3
1	A	1888	HIS	3.3
2	B	15	ILE	3.3
2	B	249	LEU	3.3
2	B	198	PHE	3.3
2	B	43	VAL	3.3
2	B	64[A]	MET	3.3
1	A	2004	ALA	3.3
2	B	38	ILE	3.3
2	B	290	ASN	3.3
2	B	145	THR	3.3
2	B	304	ASN	3.3
1	A	1999	ILE	3.3
2	B	44[A]	ILE	3.3
1	A	1980	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	29	PRO	3.2
2	B	124	ASP	3.2
2	B	99	ARG	3.2
2	B	60	PHE	3.2
2	B	86	GLY	3.2
2	B	106	PRO	3.2
2	B	181	ILE	3.2
1	A	1995	TRP	3.2
2	B	26	GLU	3.2
1	A	2066	LYS	3.2
1	A	2022	ALA	3.2
2	B	253	SER	3.2
2	B	256	VAL	3.2
2	B	303	HIS	3.2
1	A	1954	ILE	3.2
1	A	2049	ILE	3.2
2	B	293	LEU	3.2
1	A	1957	ARG	3.2
2	B	301	SER	3.2
2	B	22	PHE	3.2
2	B	230[A]	ASN	3.1
1	A	1933	ILE	3.1
2	B	62	CYS	3.1
2	B	102	MET	3.1
2	B	104	SER	3.1
1	A	1891	LEU	3.1
2	B	117	LEU	3.1
2	B	176	LEU	3.1
1	A	2009	THR	3.1
2	B	179	THR	3.1
2	B	93	VAL	3.1
1	A	1964	PRO	3.1
2	B	204	TYR	3.1
1	A	1962	ARG	3.1
1	A	1890	PHE	3.1
2	B	225	GLN	3.0
2	B	2	ASN	3.0
1	A	1841	ALA	3.0
2	B	207	THR	3.0
2	B	96	PHE	3.0
2	B	131	ARG	3.0
2	B	132	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	122	GLN	3.0
1	A	1855[A]	THR	3.0
1	A	1864	LYS	3.0
2	B	70	GLN	2.9
1	A	1969	MET	2.9
1	A	1868	GLY	2.9
1	A	2007	ARG	2.9
1	A	2024[A]	MET	2.9
2	B	266	GLU	2.9
2	B	146	THR	2.9
2	B	95	ASN	2.9
2	B	235	GLY	2.9
2	B	183	PHE	2.9
2	B	255	THR	2.9
2	B	264	LEU	2.9
1	A	1854	ASP	2.9
2	B	10	PRO	2.9
2	B	189	ILE	2.9
2	B	9	ALA	2.8
1	A	1976	ASP	2.8
1	A	2038	HIS	2.8
2	B	53	SER	2.8
2	B	175	SER	2.8
1	A	1861	THR	2.8
2	B	128	LYS	2.8
2	B	171	ASP	2.8
1	A	1870	VAL	2.8
2	B	317	LEU	2.8
1	A	2033	THR	2.8
2	B	75	ASP	2.8
1	A	1990	ASN	2.8
1	A	1960[A]	GLU	2.8
1	A	2046	GLU	2.8
2	B	50	ASP	2.8
2	B	19	GLN	2.7
1	A	1931[A]	LYS	2.7
1	A	1949	LEU	2.7
2	B	105	TYR	2.7
1	A	1893	ILE	2.7
1	A	1998	ARG	2.7
2	B	243	TRP	2.7
2	B	302	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	190	ARG	2.7
1	A	1906	SER	2.7
2	B	8	SER	2.7
2	B	262	ASP	2.7
1	A	1952	PRO	2.7
2	B	228	PHE	2.7
2	B	151	GLU	2.7
1	A	2042	SER	2.7
2	B	210	LEU	2.7
1	A	1887	GLY	2.7
1	A	1953	ASN	2.7
2	B	285	ASN	2.6
1	A	1850	LEU	2.6
2	B	56	TYR	2.6
2	B	237	TYR	2.6
2	B	191	PRO	2.6
1	A	2021	SER	2.6
1	A	1844	PHE	2.6
2	B	3	THR	2.6
2	B	90	GLU	2.6
2	B	180	VAL	2.6
1	A	2006	SER	2.6
2	B	88	LYS	2.6
2	B	27	ASN	2.6
2	B	46	PHE	2.6
1	A	1858	TYR	2.6
2	B	20	TYR	2.6
2	B	142	SER	2.6
1	A	1839	ASN	2.6
2	B	110	GLU	2.6
1	A	1929	GLN	2.5
1	A	1889	LEU	2.5
2	B	273	LYS	2.5
1	A	1836	ASN	2.5
2	B	91	ASN	2.5
2	B	84	ARG	2.5
1	A	1959	THR	2.5
2	B	208	VAL	2.5
2	B	278	GLN	2.5
1	A	2055	MET	2.5
1	A	1966	SER	2.5
2	B	202	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	34	LYS	2.5
2	B	45	HIS	2.5
1	A	1927	GLU	2.5
1	A	1843	LEU	2.4
1	A	1905	LEU	2.4
1	A	1981	ALA	2.4
1	A	1926	LYS	2.4
2	B	40	HIS	2.4
2	B	212	GLY	2.4
2	B	6	PHE	2.4
1	A	2053[A]	SER	2.4
2	B	21	SER	2.4
2	B	206	ASN	2.4
1	A	2036	SER	2.4
1	A	1896	THR	2.4
1	A	1992	TYR	2.4
1	A	2013	ARG	2.4
2	B	71	TYR	2.4
1	A	1879	ILE	2.4
1	A	2031	THR	2.3
1	A	2057[A]	ASP	2.3
2	B	87	ALA	2.3
2	B	97	LYS	2.3
1	A	1899	TRP	2.3
2	B	36	ILE	2.3
2	B	216	ASN	2.3
1	A	2001[A]	SER	2.3
1	A	2028	SER	2.3
2	B	218	SER	2.3
2	B	252	SER	2.3
2	B	307	LYS	2.3
2	B	250	ILE	2.3
1	A	2035	LYS	2.3
2	B	116	ASN	2.3
1	A	1973	LYS	2.3
2	B	39	GLY	2.3
2	B	231	ALA	2.2
1	A	1845	ASN	2.2
1	A	1837	SER	2.2
1	A	1873	LYS	2.2
2	B	81	MET	2.2
2	B	100	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2050	THR	2.2
1	A	1883	ASN	2.2
2	B	241	LEU	2.2
2	B	65	GLY	2.2
2	B	137	PHE	2.2
2	B	314	PRO	2.2
1	A	1923	SER	2.2
1	A	2020	GLU	2.2
1	A	2052	GLU	2.2
2	B	277	GLU	2.2
1	A	1974	LEU	2.2
2	B	78	TYR	2.2
1	A	2000	SER	2.2
1	A	1842	GLU	2.1
2	B	196	GLU	2.1
1	A	1904	ARG	2.1
2	B	178	TYR	2.1
1	A	1938	LYS	2.1
2	B	219	ASN	2.1
2	B	315	GLU	2.1
1	A	1872	THR	2.1
1	A	1982	THR	2.1
2	B	238	GLY	2.1
1	A	1907	GLN	2.1
2	B	295	SER	2.1
1	A	2008	LEU	2.1
1	A	1884	PRO	2.1
2	B	42	HIS	2.1
2	B	94	HIS	2.1
2	B	23	ASN	2.0
2	B	209	MET	2.0
2	B	200	ASP	2.0
1	A	1838	SER	2.0
1	A	2054	GLN	2.0
2	B	4	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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($\text{\AA}^2$)	Q<0.9
3	W8K	A	2101	12/12	0.88	0.21	28,28,28,28	12
3	W8K	B	403	12/12	0.94	0.20	28,28,28,28	12
3	W8K	B	401	12/12	0.95	0.18	28,28,28,28	0
3	W8K	B	402	12/12	0.97	0.16	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.