



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 29, 2017 – 05:39 PM EDT

PDB ID : 5VNO
Title : Crystal structure of Sec23a/Sec24a/Sec22
Authors : Ma, W.; Goldberg, J.
Deposited on : 2017-05-01
Resolution : 2.90 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

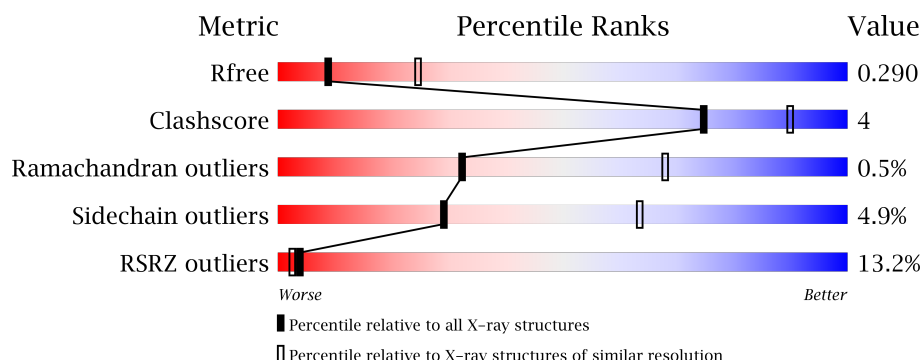
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	764	<div> <div>11%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>• 8%</div> </div> </div>
2	B	748	<div> <div>12%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>••</div> </div> </div>
3	C	157	<div> <div>25%</div> <div> <div></div> <div>75%</div> <div>10%</div> <div>• 13%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12507 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 Protein transport protein Sec23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	703	Total	C	N	O	S	0	0	0
			5561	3543	957	1022	39			

- Molecule 2 is a protein called Protein transport protein Sec24A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	731	Total	C	N	O	S	0	0	0
			5780	3690	983	1073	34			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1056	ALA	ARG	conflict	UNP O95486

- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	137	Total	C	N	O	S	0	0	0
			1102	708	181	205	8			

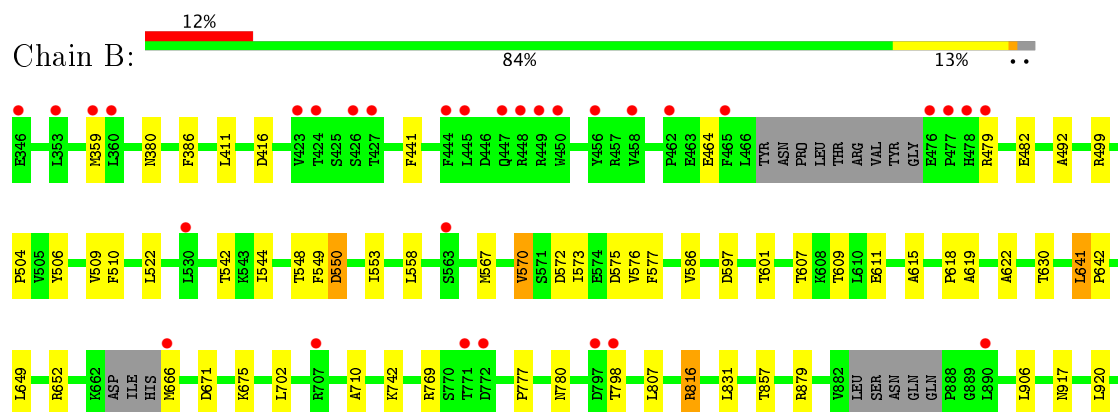
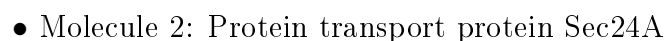
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

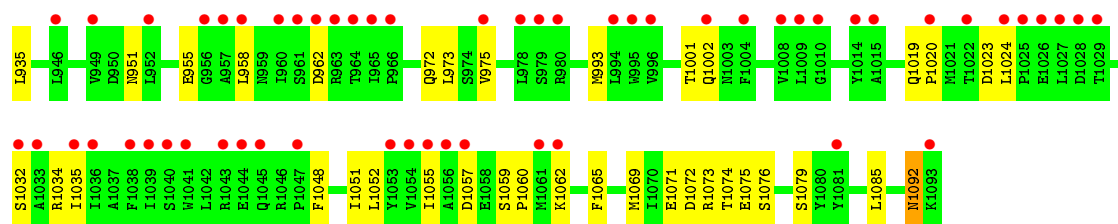
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

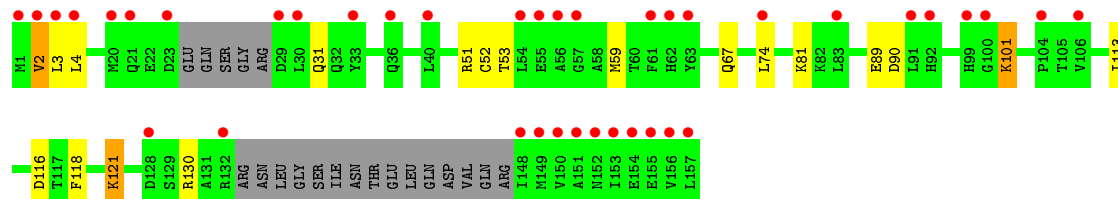
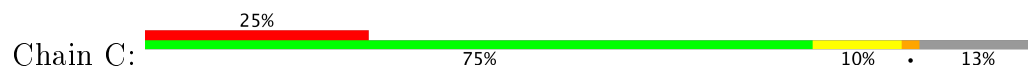
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total 12	O 12	0	0
5	B	47	Total 47	O 47	0	0
5	C	3	Total 3	O 3	0	0

- Molecule 1: Protein transport protein Sec23A





• Molecule 3: Vesicle-trafficking protein SEC22b



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.05Å 96.73Å 126.80Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	49.94 – 2.90 49.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.94-2.90) 99.6 (49.94-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.244 , 0.298 0.240 , 0.290	Depositor DCC
R_{free} test set	2018 reflections (4.79%)	DCC
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12507	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: ZN

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	0.28	0/5688	0.45	0/7702
2	B	0.27	0/5904	0.44	0/8024
3	C	0.25	0/1121	0.43	0/1508
All	All	0.27	0/12713	0.45	0/17234

There are no bond length outliers.

There are no bond angle outliers.

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	5561	0	5516	43	0
2	B	5780	0	5835	44	0
3	C	1102	0	1105	9	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	0	3	0
5	B	47	0	0	2	0
5	C	3	0	0	2	0
All	All	12507	0	12456	91	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 4.

All (91) 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:666:MET:N	5:B:1201:HOH:O	2.12	0.82
1:A:679:GLU:N	5:A:902:HOH:O	2.19	0.76
1:A:748:SER:OG	5:A:901:HOH:O	1.98	0.71
1:A:33:ARG:NH1	5:A:903:HOH:O	2.26	0.68
1:A:48:ARG:O	1:A:50:ASP:N	2.27	0.67
1:A:44:PRO:O	1:A:495:ARG:NH1	2.28	0.66
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.82	0.60
2:B:1023:ASP:OD1	2:B:1024:LEU:N	2.35	0.59
3:C:101:LYS:NZ	5:C:201:HOH:O	2.33	0.58
1:A:48:ARG:HB2	1:A:49:PRO:HD2	1.87	0.56
2:B:780:ASN:O	5:B:1202:HOH:O	2.18	0.55
1:A:250:ASP:O	3:C:130:ARG:NH2	2.29	0.55
2:B:955:GLU:N	2:B:955:GLU:OE1	2.40	0.55
1:A:541:ASP:OD1	1:A:542:VAL:N	2.41	0.54
3:C:59:MET:HB3	3:C:74:LEU:HD11	1.93	0.51
1:A:475:GLY:O	1:A:476:ARG:HB2	2.09	0.51
2:B:416:ASP:OD1	2:B:742:LYS:NZ	2.44	0.51
1:A:45:LEU:HA	1:A:495:ARG:NH1	2.25	0.50
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.93	0.50
3:C:52:CYS:SG	3:C:53:THR:N	2.84	0.50
2:B:973:LEU:HA	2:B:1069:MET:HE1	1.94	0.49
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.94	0.49
1:A:160:PRO:HB3	1:A:234:GLN:HB3	1.94	0.49
2:B:576:VAL:HG11	2:B:622:ALA:HB2	1.94	0.49
2:B:499:ARG:NH2	2:B:630:THR:O	2.40	0.49
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.48	0.48
2:B:482:GLU:N	2:B:482:GLU:OE1	2.45	0.48
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.94	0.48
1:A:193:LYS:NZ	2:B:572:ASP:OD2	2.35	0.48
1:A:750:GLN:OE1	1:A:750:GLN:N	2.45	0.48
1:A:190:ARG:NH1	2:B:575:ASP:OD2	2.46	0.48
2:B:609:THR:HG22	2:B:611:GLU:H	1.78	0.47
3:C:4:LEU:HB3	3:C:74:LEU:HB3	1.96	0.47
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.96	0.47
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.97	0.47
1:A:722:VAL:HG22	1:A:723:ASN:H	1.80	0.47
2:B:879:ARG:NH1	2:B:1092:ASN:OD1	2.48	0.47
2:B:553:ILE:HB	2:B:570:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:550:ASP:O	2:B:615:ALA:N	2.44	0.46
1:A:101:ILE:HD11	1:A:107:PRO:HD3	1.97	0.46
1:A:178:LEU:HD12	1:A:178:LEU:H	1.80	0.46
1:A:544:ARG:HG2	1:A:548:ARG:CZ	2.46	0.45
1:A:259:ARG:NH2	1:A:308:THR:O	2.49	0.45
2:B:1055:ILE:HG21	2:B:1062:LYS:HD2	1.98	0.45
2:B:951:ASN:N	2:B:951:ASN:OD1	2.50	0.45
1:A:285:ARG:NE	1:A:346:ASP:OD2	2.49	0.45
2:B:1074:THR:HG23	2:B:1076:SER:H	1.82	0.45
2:B:506:TYR:HB2	2:B:544:ILE:HD12	2.00	0.44
2:B:509:VAL:HG12	2:B:549:PHE:HE1	1.83	0.44
1:A:183:ILE:O	1:A:184:SER:OG	2.28	0.44
2:B:380:ASN:HA	2:B:441:PHE:HZ	1.81	0.44
1:A:255:PRO:HG2	1:A:258:LYS:HG3	2.00	0.43
1:A:190:ARG:HH21	2:B:577:PHE:HB3	1.84	0.43
1:A:664:ILE:HG22	1:A:664:ILE:O	2.18	0.43
3:C:118:PHE:HA	3:C:121:LYS:HG2	2.00	0.43
2:B:642:PRO:HG2	2:B:702:LEU:HD21	2.00	0.43
2:B:641:LEU:HD21	2:B:649:LEU:HB2	2.01	0.43
2:B:1055:ILE:O	2:B:1057:ASP:N	2.46	0.43
1:A:310:ILE:HG22	1:A:311:ARG:HD3	2.01	0.42
1:A:588:SER:OG	1:A:595:ASN:OD1	2.33	0.42
1:A:290:ILE:HG23	1:A:292:GLY:H	1.83	0.42
1:A:544:ARG:HH12	1:A:742:ILE:HA	1.84	0.42
2:B:993:MET:HE2	2:B:1065:PHE:HA	2.02	0.42
1:A:625:ALA:HB1	1:A:646:ARG:HD2	2.00	0.42
1:A:107:PRO:HB2	1:A:109:GLU:OE2	2.20	0.42
3:C:67:GLN:HG2	5:C:201:HOH:O	2.20	0.42
1:A:299:GLY:HA2	1:A:327:GLY:HA2	2.01	0.42
1:A:664:ILE:HD13	1:A:684:LEU:HD21	2.02	0.42
1:A:426:LEU:HD21	1:A:447:LYS:HB2	2.01	0.41
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.35	0.41
2:B:1032:SER:HA	2:B:1035:ILE:HG22	2.03	0.41
2:B:972:GLN:HB3	2:B:1071:GLU:OE2	2.19	0.41
3:C:51:ARG:NH2	3:C:89:GLU:OE2	2.53	0.41
1:A:180:CYS:SG	1:A:185:LYS:HE2	2.60	0.41
2:B:975:VAL:HG23	2:B:1072:ASP:OD2	2.21	0.41
2:B:710:ALA:HB3	2:B:777:PRO:HD2	2.02	0.41
1:A:313:TRP:HD1	1:A:595:ASN:O	2.03	0.41
2:B:597:ASP:O	2:B:601:THR:OG1	2.29	0.41
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:ASP:N	1:A:746:ASP:OD2	2.54	0.41
1:A:138:CYS:HB2	1:A:262:ARG:NH1	2.35	0.41
1:A:426:LEU:HD12	1:A:445:GLN:HB3	2.02	0.41
2:B:510:PHE:HB2	2:B:548:THR:HG22	2.02	0.41
3:C:4:LEU:HD23	3:C:74:LEU:HB3	2.03	0.41
1:A:185:LYS:HB3	2:B:567:MET:HB3	2.02	0.40
1:A:194:ASP:HB2	1:A:298:PRO:HG2	2.02	0.40
2:B:1059:SER:N	2:B:1060:PRO:HD3	2.36	0.40
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	2.03	0.40
2:B:553:ILE:HG12	2:B:619:ALA:HA	2.03	0.40
2:B:671:ASP:OD2	2:B:675:LYS:HE3	2.21	0.40
2:B:504:PRO:HG2	2:B:542:THR:HA	2.04	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	691/764 (90%)	655 (95%)	31 (4%)	5 (1%)	25	60
2	B	723/748 (97%)	671 (93%)	50 (7%)	2 (0%)	44	77
3	C	131/157 (83%)	119 (91%)	11 (8%)	1 (1%)	22	57
All	All	1545/1669 (93%)	1445 (94%)	92 (6%)	8 (0%)	32	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	GLU
2	B	769	ARG
1	A	184	SER
1	A	476	ARG
1	A	49	PRO

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Mol	Chain	Res	Type
1	A	59	VAL
2	B	550	ASP
3	C	2	VAL

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	612/666 (92%)	583 (95%)	29 (5%)	30	65
2	B	662/678 (98%)	632 (96%)	30 (4%)	32	66
3	C	119/138 (86%)	110 (92%)	9 (8%)	15	41
All	All	1393/1482 (94%)	1325 (95%)	68 (5%)	29	63

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	30	GLU
1	A	101	ILE
1	A	105	ASN
1	A	122	LEU
1	A	161	THR
1	A	178	LEU
1	A	180	CYS
1	A	192	THR
1	A	236	ILE
1	A	240	LEU
1	A	243	LEU
1	A	268	LEU
1	A	300	MET
1	A	311	ARG
1	A	316	ILE
1	A	355	THR
1	A	362	CYS
1	A	451	LEU

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Mol	Chain	Res	Type
1	A	495	ARG
1	A	508	THR
1	A	509	GLN
1	A	528	ARG
1	A	544	ARG
1	A	569	ARG
1	A	570	PHE
1	A	690	ASP
1	A	701	PRO
1	A	754	ASP
2	B	359	MET
2	B	386	PHE
2	B	411	LEU
2	B	464	GLU
2	B	479	ARG
2	B	522	LEU
2	B	570	VAL
2	B	607	THR
2	B	641	LEU
2	B	652	ARG
2	B	798	THR
2	B	807	LEU
2	B	816	ARG
2	B	831	LEU
2	B	857	THR
2	B	906	LEU
2	B	917	ASN
2	B	920	LEU
2	B	935	LEU
2	B	958	LEU
2	B	962	ASP
2	B	1001	THR
2	B	1002	GLN
2	B	1034	ARG
2	B	1048	PHE
2	B	1051	ILE
2	B	1052	LEU
2	B	1075	GLU
2	B	1085	LEU
2	B	1092	ASN
3	C	2	VAL
3	C	3	LEU

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Mol	Chain	Res	Type
3	C	31	GLN
3	C	81	LYS
3	C	90	ASP
3	C	101	LYS
3	C	113	ILE
3	C	116	ASP
3	C	121	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	703/764 (92%)	0.61	82 (11%) 5 4	46, 82, 198, 390	0
2	B	731/748 (97%)	0.58	87 (11%) 5 3	43, 89, 214, 302	0
3	C	137/157 (87%)	1.34	39 (28%) 1 0	82, 138, 202, 264	0
All	All	1571/1669 (94%)	0.66	208 (13%) 4 2	43, 88, 209, 390	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	685	LEU	16.0
1	A	684	LEU	14.9
1	A	659	TYR	10.5
2	B	1022	THR	10.0
1	A	706	ILE	8.9
1	A	717	PHE	8.8
2	B	1035	ILE	8.4
1	A	688	PRO	8.3
1	A	628	PHE	8.2
1	A	657	LEU	8.1
3	C	1	MET	7.9
1	A	642	ILE	7.9
1	A	648	LEU	7.8
1	A	680	ASN	7.8
3	C	23	ASP	7.6
2	B	958	LEU	7.5
2	B	1009	LEU	7.0
2	B	949	VAL	6.8
2	B	476	GLU	6.6
1	A	711	GLY	6.5
3	C	29	ASP	6.4
2	B	1024	LEU	6.3
3	C	149	MET	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	64	THR	6.2
1	A	682	ARG	6.1
1	A	689	VAL	6.1
2	B	772	ASP	6.0
1	A	714	GLN	6.0
2	B	1039	ILE	5.8
3	C	153	ILE	5.6
1	A	643	LEU	5.5
1	A	644	ALA	5.4
3	C	157	LEU	5.4
1	A	692	ALA	5.2
2	B	445	LEU	5.2
2	B	956	GLY	5.2
2	B	1028	ASP	5.2
1	A	716	ARG	5.1
1	A	722	VAL	4.9
3	C	99	HIS	4.8
2	B	1025	PRO	4.7
2	B	979	SER	4.7
1	A	709	GLU	4.6
2	B	477	PRO	4.6
2	B	980	ARG	4.6
1	A	663	THR	4.6
2	B	1027	LEU	4.6
1	A	223	PRO	4.6
2	B	996	VAL	4.5
2	B	962	ASP	4.5
1	A	664	ILE	4.5
1	A	710	HIS	4.5
1	A	658	ILE	4.4
1	A	665	ALA	4.4
2	B	1056	ALA	4.4
2	B	1010	GLY	4.4
3	C	57	GLY	4.4
1	A	93	GLN	4.4
2	B	1020	PRO	4.3
2	B	1036	ILE	4.3
1	A	625	ALA	4.2
2	B	1055	ILE	4.2
1	A	666	GLN	4.0
2	B	965	ILE	4.0
3	C	152	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	128	ASP	3.9
1	A	721	LYS	3.9
3	C	104	PRO	3.9
1	A	629	SER	3.8
1	A	705	TYR	3.8
1	A	52	PRO	3.8
2	B	966	PRO	3.7
2	B	1054	VAL	3.7
3	C	156	VAL	3.6
1	A	436	ASN	3.6
1	A	707	ASP	3.6
2	B	1093	LYS	3.5
2	B	1061	MET	3.5
2	B	797	ASP	3.5
3	C	62	HIS	3.5
2	B	961	SER	3.5
2	B	666	MET	3.5
1	A	720	SER	3.5
2	B	1047	PRO	3.4
3	C	33	TYR	3.4
1	A	89	TYR	3.4
3	C	154	GLU	3.4
1	A	394	MET	3.4
2	B	1038	PHE	3.4
2	B	424	THR	3.4
1	A	686	GLN	3.3
2	B	353	LEU	3.3
2	B	798	THR	3.3
2	B	465	PHE	3.3
3	C	61	PHE	3.2
2	B	479	ARG	3.2
2	B	478	HIS	3.2
2	B	963	ARG	3.2
1	A	224	PRO	3.2
3	C	55	GLU	3.2
2	B	771	THR	3.2
2	B	1014	TYR	3.1
2	B	450	TRP	3.1
2	B	1043	ARG	3.1
2	B	978	LEU	3.1
3	C	63	TYR	3.1
1	A	237	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	624	TYR	3.0
3	C	3	LEU	3.0
1	A	656	ILE	3.0
1	A	693	GLN	3.0
1	A	744	THR	2.9
3	C	150	VAL	2.9
3	C	36	GLN	2.9
1	A	681	PHE	2.9
3	C	151	ALA	2.9
2	B	458	VAL	2.9
2	B	1032	SER	2.9
3	C	100	GLY	2.9
2	B	448	ARG	2.9
2	B	449	ARG	2.9
1	A	257	GLY	2.9
1	A	226	SER	2.9
3	C	56	ALA	2.9
1	A	225	PRO	2.8
2	B	1057	ASP	2.8
2	B	530	LEU	2.8
2	B	890	LEU	2.8
1	A	646	ARG	2.8
2	B	359	MET	2.8
2	B	1004	PHE	2.8
2	B	1045	GLN	2.8
1	A	79	ARG	2.7
2	B	444	PHE	2.7
3	C	40	LEU	2.7
3	C	21	GLN	2.7
1	A	713	SER	2.6
1	A	700	PHE	2.6
1	A	645	ASP	2.6
1	A	506	ALA	2.6
1	A	683	HIS	2.6
3	C	148	ILE	2.6
2	B	1029	THR	2.6
2	B	447	GLN	2.6
3	C	30	LEU	2.6
1	A	510	ILE	2.6
3	C	91	LEU	2.6
1	A	632	PRO	2.6
1	A	627	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	430	GLY	2.5
1	A	82	LEU	2.5
2	B	426	SER	2.5
2	B	1026	GLU	2.5
1	A	660	HIS	2.5
2	B	427	THR	2.5
2	B	995	TRP	2.5
2	B	1015	ALA	2.4
2	B	346	GLU	2.4
2	B	707	ARG	2.4
3	C	132	ARG	2.4
2	B	964	THR	2.4
3	C	20	MET	2.4
3	C	106	VAL	2.4
2	B	423	VAL	2.4
1	A	723	ASN	2.4
3	C	83	LEU	2.3
2	B	1002	GLN	2.3
2	B	946	LEU	2.3
2	B	994	LEU	2.3
2	B	1044	GLU	2.3
1	A	626	TYR	2.3
2	B	952	LEU	2.3
3	C	92	HIS	2.3
2	B	957	ALA	2.3
3	C	2	VAL	2.3
3	C	155	GLU	2.3
2	B	1041	TRP	2.3
2	B	456	TYR	2.3
1	A	244	LEU	2.2
2	B	360	LEU	2.2
2	B	1062	LYS	2.2
1	A	633	GLU	2.2
1	A	695	ILE	2.2
1	A	58	PRO	2.2
2	B	960	ILE	2.2
1	A	91	ARG	2.2
2	B	462	PRO	2.2
2	B	1040	SER	2.2
3	C	74	LEU	2.1
1	A	687	ALA	2.1
1	A	388	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	563	SER	2.1
1	A	637	LEU	2.1
2	B	1033	ALA	2.1
1	A	238	MET	2.1
1	A	745	ASP	2.1
2	B	1008	VAL	2.1
2	B	975	VAL	2.1
1	A	99	ALA	2.1
3	C	54	LEU	2.1
1	A	696	LEU	2.0
1	A	3	THR	2.0
1	A	507	GLN	2.0
1	A	412	ARG	2.0
1	A	649	LEU	2.0
2	B	1053	TYR	2.0
2	B	1081	TYR	2.0
3	C	4	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	ZN	B	1101	1/1	0.98	0.12	-1.00	110,110,110,110	0
4	ZN	A	801	1/1	0.95	0.13	-1.14	122,122,122,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.