Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 09:03 AM 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
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:

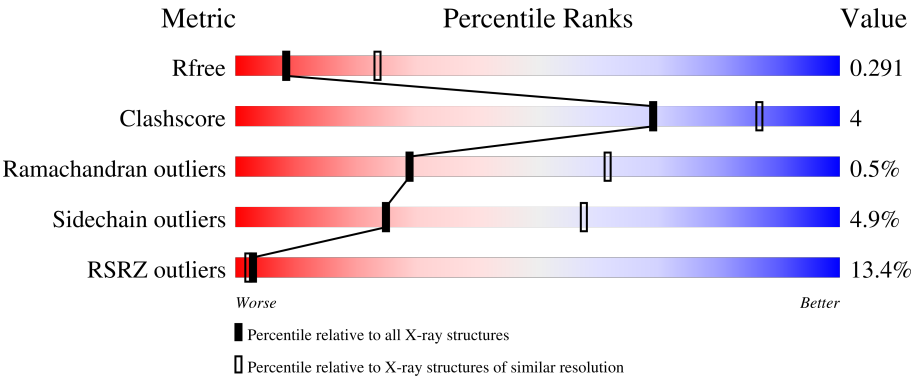
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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 <=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	10% 80% 10% • 8%
2	B	748	12% 84% 13% ••
3	C	157	25% 75% 10% • 13%

2 Entry composition (i)

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	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

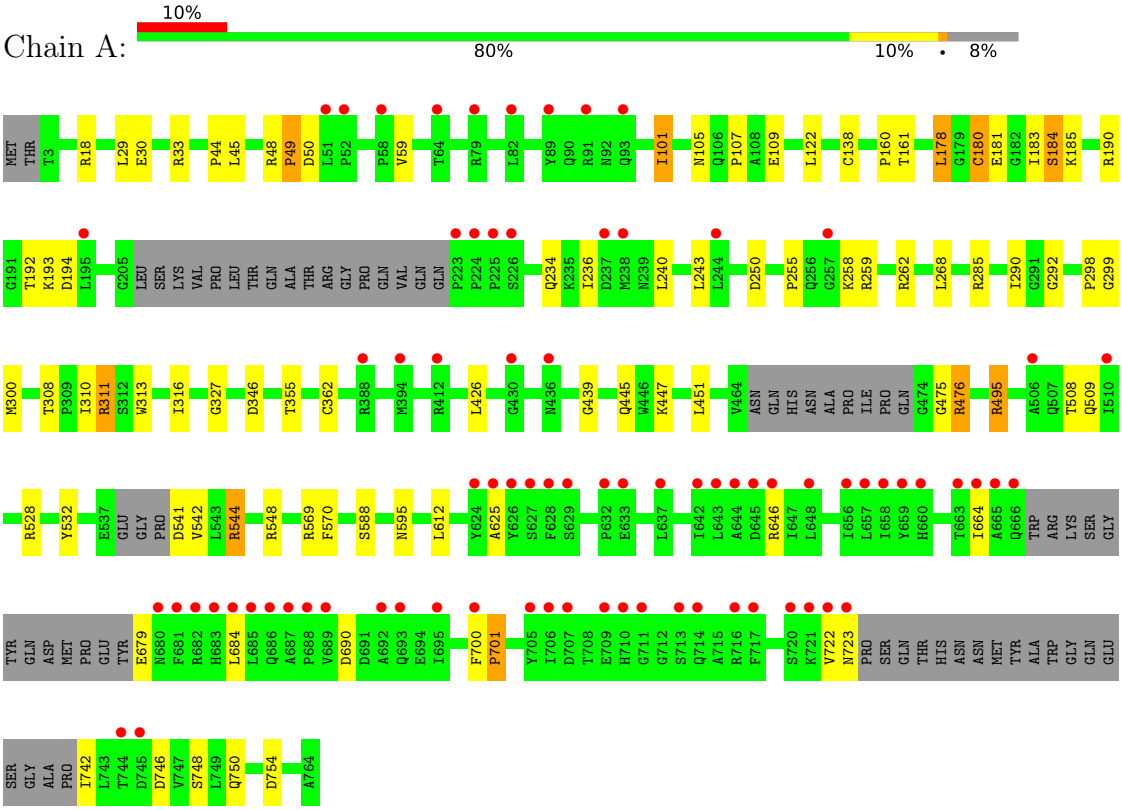
- Molecule 5 is water.

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

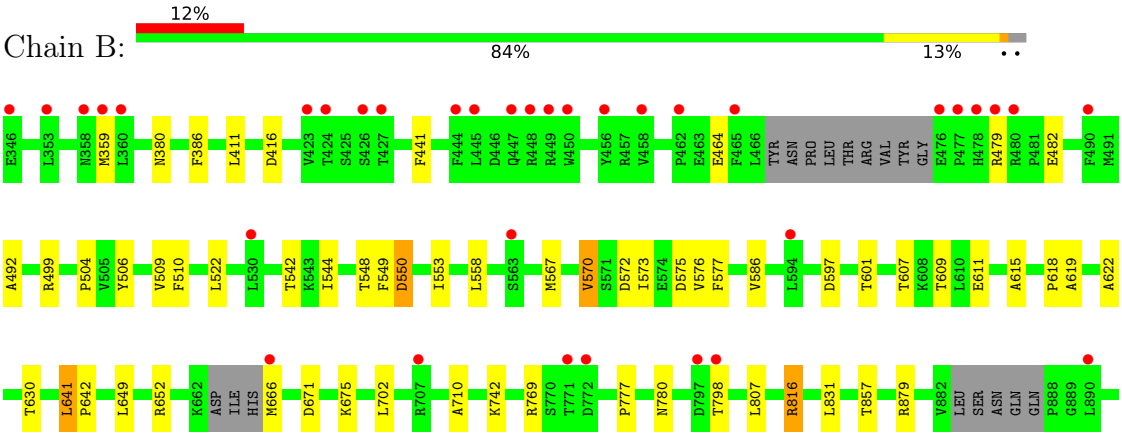
3 Residue-property plots (i)

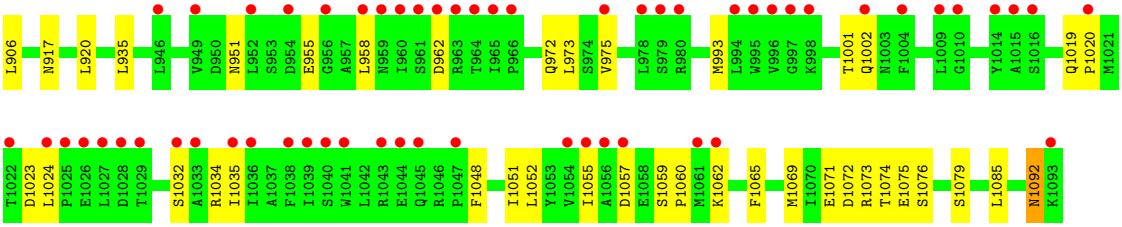
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein transport protein Sec23A

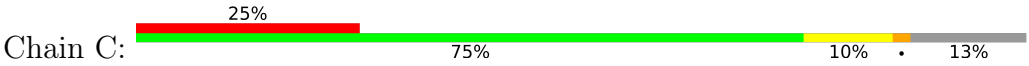


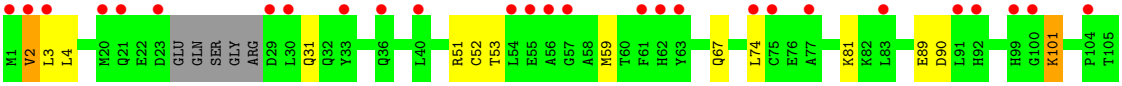
• Molecule 2: Protein transport protein Sec24A

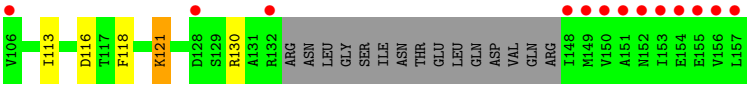




• Molecule 3: Vesicle-trafficking protein SEC22b







4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.00 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.244 , 0.298 0.241 , 0.291	Depositor DCC
R_{free} test set	2017 reflections (4.79%)	wwPDB-VP
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 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical 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

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:H	1:A:178:LEU:HD12	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:951:ASN:N	2:B:951:ASN:OD1	2.50	0.45
2:B:1055:ILE:HG21	2:B:1062:LYS:HD2	1.98	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:190:ARG:HH21	2:B:577:PHE:HB3	1.84	0.43
1:A:255:PRO:HG2	1:A:258:LYS:HG3	2.00	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:972:GLN:HB3	2:B:1071:GLU:OE2	2.19	0.41
2:B:1032:SER:HA	2:B:1035:ILE:HG22	2.03	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:710:ALA:HB3	2:B:777:PRO:HD2	2.02	0.41
2:B:975:VAL:HG23	2:B:1072:ASP:OD2	2.21	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:OD2	1:A:746:ASP:N	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: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:1020:PRO:HA	2:B:1055:ILE:HG12	2.03	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%)	22	54
2	B	723/748 (97%)	671 (93%)	50 (7%)	2 (0%)	41	71
3	C	131/157 (83%)	119 (91%)	11 (8%)	1 (1%)	19	51
All	All	1545/1669 (93%)	1445 (94%)	92 (6%)	8 (0%)	29	61

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 (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	612/666 (92%)	583 (95%)	29 (5%)	26	59
2	B	662/678 (98%)	632 (96%)	30 (4%)	27	61
3	C	119/138 (86%)	110 (92%)	9 (8%)	13	36
All	All	1393/1482 (94%)	1325 (95%)	68 (5%)	25	57

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

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

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)

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 (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, 95^{th} 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	79 (11%)	5 4	46, 82, 198, 390	0
2	B	731/748 (97%)	0.58	92 (12%)	3 3	43, 89, 214, 302	0
3	C	137/157 (87%)	1.32	40 (29%)	0 0	82, 138, 202, 264	0
All	All	1571/1669 (94%)	0.66	211 (13%)	3 2	43, 88, 209, 390	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	685	LEU	15.2
1	A	684	LEU	14.8
1	A	659	TYR	10.5
2	B	1022	THR	10.2
1	A	717	PHE	9.7
1	A	706	ILE	8.6
1	A	680	ASN	8.5
1	A	657	LEU	7.8
1	A	688	PRO	7.8
1	A	642	ILE	7.7
1	A	628	PHE	7.7
2	B	1035	ILE	7.7
3	C	23	ASP	7.6
3	C	1	MET	7.4
1	A	648	LEU	7.4
2	B	476	GLU	6.9
2	B	958	LEU	6.8
2	B	1009	LEU	6.8
3	C	149	MET	6.8
1	A	714	GLN	6.5
2	B	772	ASP	6.3
1	A	64	THR	6.3
2	B	949	VAL	6.2

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Mol	Chain	Res	Type	RSRZ
2	B	1024	LEU	6.2
1	A	682	ARG	5.9
1	A	711	GLY	5.8
3	C	29	ASP	5.8
1	A	716	ARG	5.7
1	A	643	LEU	5.5
1	A	689	VAL	5.5
1	A	722	VAL	5.4
1	A	644	ALA	5.3
2	B	956	GLY	5.3
3	C	153	ILE	5.3
2	B	445	LEU	5.1
1	A	663	THR	5.1
3	C	157	LEU	5.0
1	A	692	ALA	4.9
2	B	1039	ILE	4.9
1	A	709	GLU	4.9
2	B	1028	ASP	4.9
2	B	962	ASP	4.9
2	B	477	PRO	4.8
2	B	1056	ALA	4.7
3	C	57	GLY	4.7
2	B	980	ARG	4.7
3	C	99	HIS	4.6
2	B	979	SER	4.6
2	B	996	VAL	4.6
1	A	665	ALA	4.6
2	B	1027	LEU	4.6
1	A	658	ILE	4.5
1	A	664	ILE	4.5
2	B	1025	PRO	4.4
1	A	93	GLN	4.4
1	A	710	HIS	4.4
1	A	223	PRO	4.4
2	B	1055	ILE	4.3
2	B	1020	PRO	4.2
1	A	625	ALA	4.2
1	A	721	LYS	4.0
1	A	629	SER	4.0
1	A	666	GLN	4.0
2	B	1010	GLY	3.9
3	C	62	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	128	ASP	3.8
3	C	152	ASN	3.8
2	B	797	ASP	3.8
2	B	1036	ILE	3.8
2	B	961	SER	3.8
1	A	436	ASN	3.8
2	B	965	ILE	3.7
2	B	1093	LYS	3.7
1	A	52	PRO	3.6
2	B	1061	MET	3.6
1	A	686	GLN	3.6
2	B	1054	VAL	3.5
3	C	61	PHE	3.5
1	A	720	SER	3.5
3	C	156	VAL	3.5
1	A	394	MET	3.5
2	B	424	THR	3.5
2	B	479	ARG	3.5
3	C	104	PRO	3.5
3	C	55	GLU	3.5
1	A	707	ASP	3.5
2	B	966	PRO	3.5
2	B	771	THR	3.4
1	A	89	TYR	3.4
2	B	478	HIS	3.4
3	C	33	TYR	3.4
2	B	1043	ARG	3.4
2	B	1047	PRO	3.3
1	A	237	ASP	3.3
2	B	465	PHE	3.3
2	B	353	LEU	3.2
1	A	681	PHE	3.2
3	C	150	VAL	3.2
2	B	666	MET	3.2
2	B	798	THR	3.1
2	B	450	TRP	3.1
1	A	506	ALA	3.1
2	B	1057	ASP	3.1
2	B	1038	PHE	3.1
1	A	713	SER	3.1
1	A	693	GLN	3.1
3	C	63	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	447	GLN	3.0
2	B	1014	TYR	3.0
2	B	978	LEU	3.0
2	B	1032	SER	3.0
1	A	624	TYR	3.0
2	B	1026	GLU	3.0
3	C	154	GLU	2.9
1	A	705	TYR	2.9
2	B	963	ARG	2.9
3	C	56	ALA	2.9
1	A	744	THR	2.8
1	A	224	PRO	2.8
2	B	1029	THR	2.8
2	B	448	ARG	2.8
3	C	3	LEU	2.8
3	C	21	GLN	2.8
2	B	1044	GLU	2.8
1	A	510	ILE	2.8
3	C	151	ALA	2.8
2	B	444	PHE	2.8
2	B	1002	GLN	2.8
1	A	656	ILE	2.8
1	A	79	ARG	2.8
1	A	646	ARG	2.8
2	B	530	LEU	2.8
2	B	1045	GLN	2.8
3	C	100	GLY	2.7
1	A	225	PRO	2.7
1	A	645	ASP	2.7
2	B	462	PRO	2.7
2	B	359	MET	2.7
1	A	257	GLY	2.7
2	B	449	ARG	2.7
2	B	1004	PHE	2.6
1	A	723	ASN	2.6
2	B	458	VAL	2.6
1	A	632	PRO	2.6
3	C	30	LEU	2.6
3	C	36	GLN	2.6
1	A	226	SER	2.6
1	A	700	PHE	2.6
2	B	427	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	890	LEU	2.5
3	C	148	ILE	2.5
2	B	946	LEU	2.5
1	A	660	HIS	2.5
3	C	20	MET	2.5
1	A	244	LEU	2.5
3	C	40	LEU	2.4
3	C	132	ARG	2.4
2	B	959	ASN	2.4
2	B	995	TRP	2.4
1	A	627	SER	2.4
3	C	77	ALA	2.4
2	B	1015	ALA	2.4
2	B	952	LEU	2.4
2	B	960	ILE	2.4
1	A	683	HIS	2.4
1	A	238	MET	2.4
2	B	346	GLU	2.3
3	C	106	VAL	2.3
2	B	563	SER	2.3
3	C	92	HIS	2.3
2	B	423	VAL	2.3
1	A	82	LEU	2.3
3	C	83	LEU	2.3
2	B	964	THR	2.3
1	A	430	GLY	2.3
2	B	707	ARG	2.3
2	B	358	ASN	2.3
2	B	426	SER	2.3
2	B	456	TYR	2.3
2	B	994	LEU	2.2
3	C	91	LEU	2.2
3	C	155	GLU	2.2
1	A	58	PRO	2.2
1	A	695	ILE	2.2
2	B	480	ARG	2.2
2	B	360	LEU	2.2
1	A	687	ALA	2.2
2	B	1062	LYS	2.2
2	B	997	GLY	2.1
1	A	745	ASP	2.1
1	A	91	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	388	ARG	2.1
1	A	626	TYR	2.1
3	C	54	LEU	2.1
2	B	1033	ALA	2.1
1	A	637	LEU	2.1
3	C	75	CYS	2.1
2	B	975	VAL	2.1
3	C	2	VAL	2.1
1	A	195	LEU	2.1
3	C	74	LEU	2.1
2	B	1016	SER	2.1
2	B	1041	TRP	2.0
1	A	412	ARG	2.0
1	A	51	LEU	2.0
2	B	998	LYS	2.0
1	A	633	GLU	2.0
2	B	954	ASP	2.0
2	B	1040	SER	2.0
2	B	490	PHE	2.0
2	B	594	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, 95^{th} 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
4	ZN	A	801	1/1	0.96	0.12	122,122,122,122	0
4	ZN	B	1101	1/1	0.98	0.12	110,110,110,110	0

6.5 Other polymers (i)

There are no such residues in this entry.