



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:27 PM UTC

PDB ID : 5VNH / pdb_00005vnh
Title : Crystal structure of Sec23a/Sec24a/Sec22 complexed with a C-terminal SV sorting motif
Authors : Ma, W.; Goldberg, J.
Deposited on : 2017-04-30
Resolution : 2.60 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
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

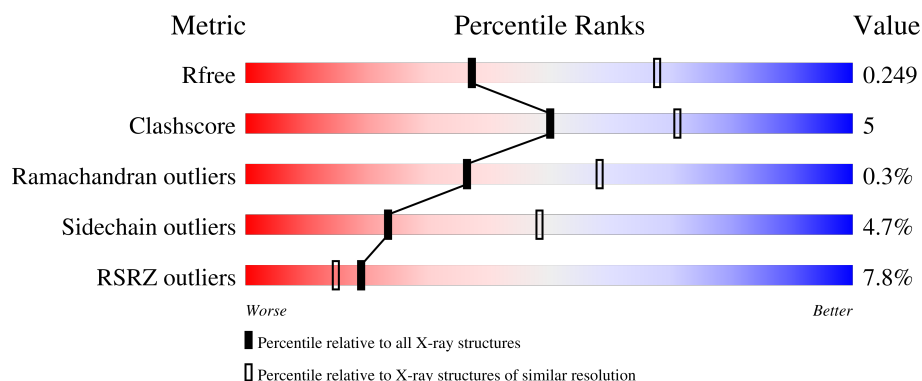
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	764	8% 78% 13% • 7%
2	B	748	7% 80% 16% • •
3	C	157	6% 70% 13% • 14%
4	D	6	50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12569 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	707	Total	C	N	O	S	0	0	0
			5623	3583	967	1033	40			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	729	Total	C	N	O	S	0	0	0
			5758	3672	981	1071	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	135	Total	C	N	O	S	0	0	0
			1087	699	177	203	8			

- Molecule 4 is a protein called C-terminal SV motif.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			19	11	3	5			

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

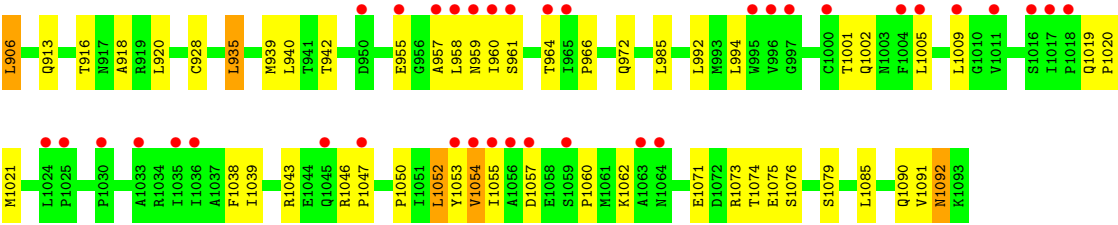
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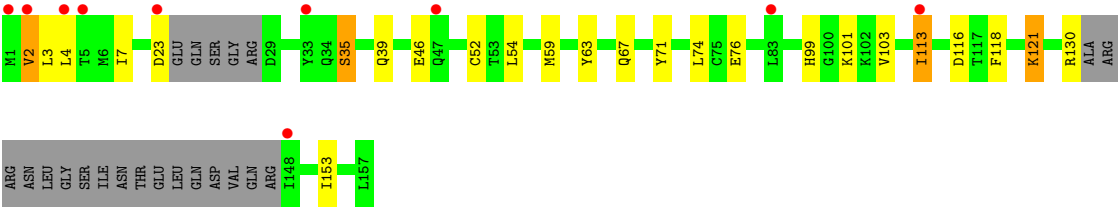
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Zn 1	0	0

- Molecule 6 is water.

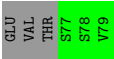
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	43	Total 43	O 43	0	0
6	B	36	Total 36	O 36	0	0
6	C	1	Total 1	O 1	0	0



• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: C-terminal SV motif



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.94Å 96.89Å 127.34Å 90.00° 91.61° 90.00°	Depositor
Resolution (Å)	48.88 – 2.60 48.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.88-2.60) 99.5 (48.88-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.212 , 0.250 0.212 , 0.249	Depositor DCC
R_{free} test set	2011 reflections (3.25%)	wwPDB-VP
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12569	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.20	0/5754	0.33	0/7790
2	B	0.11	0/5881	0.32	1/7993 (0.0%)
3	C	0.11	0/1106	0.33	0/1489
4	D	0.14	0/18	0.19	0/22
All	All	0.16	0/12759	0.32	1/17294 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1054	VAL	N-CA-C	-5.61	107.02	112.29

There are no chirality outliers.

There are no planarity outliers.

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	5623	0	5571	59	0
2	B	5758	0	5806	63	0
3	C	1087	0	1091	13	0
4	D	19	0	15	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	43	0	0	2	0
6	B	36	0	0	2	0
6	C	1	0	0	0	0
All	All	12569	0	12483	133	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 5.

All (133) 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:629:PRO:HG3	3:C:23:ASP:HB2	1.63	0.80
1:A:3:THR:HG22	1:A:6:GLU:H	1.52	0.74
3:C:54:LEU:HD13	3:C:153:ILE:HD13	1.69	0.74
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.73	0.71
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.74	0.69
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.74	0.68
2:B:666:MET:HE2	2:B:860:LEU:HB2	1.74	0.68
2:B:666:MET:HE3	2:B:855:SER:HB3	1.76	0.67
2:B:928:CYS:SG	6:B:1216:HOH:O	2.53	0.66
2:B:872:ILE:HD12	2:B:1090:GLN:HB2	1.79	0.64
1:A:528:ARG:HA	1:A:608:MET:HE1	1.78	0.64
1:A:626:TYR:HB2	1:A:647:ILE:HB	1.80	0.63
1:A:44:PRO:O	1:A:495:ARG:NH1	2.31	0.63
2:B:972:GLN:NE2	2:B:1071:GLU:OE2	2.32	0.62
1:A:259:ARG:NH2	1:A:308:THR:O	2.32	0.62
1:A:240:LEU:HD22	1:A:244:LEU:HG	1.82	0.61
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.83	0.61
2:B:788:GLN:OE1	6:B:1201:HOH:O	2.16	0.60
2:B:1074:THR:HG23	2:B:1076:SER:H	1.67	0.59
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.84	0.58
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.84	0.57
1:A:67:ARG:O	1:A:409:LYS:NZ	2.38	0.57
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.86	0.57
1:A:548:ARG:NH1	6:A:903:HOH:O	2.37	0.57
2:B:494:SER:HA	2:B:497:MET:HE3	1.86	0.57
2:B:906:LEU:HD13	2:B:942:THR:HG21	1.87	0.56
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.88	0.56
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.86	0.56
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.70	0.56
1:A:415:LYS:HB3	1:A:434:SER:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:O	1:A:50:ASP:N	2.39	0.55
1:A:398:PHE:HB3	1:A:400:MET:HG3	1.88	0.55
2:B:436:THR:HG21	2:B:454:LEU:HD13	1.88	0.55
2:B:913:GLN:HE21	2:B:918:ALA:HB2	1.73	0.54
1:A:153:MET:SD	1:A:387:GLN:HB3	2.48	0.54
1:A:626:TYR:N	1:A:647:ILE:O	2.40	0.53
2:B:1046:ARG:HD2	2:B:1050:PRO:HG3	1.90	0.53
2:B:1055:ILE:HG21	2:B:1062:LYS:HD2	1.88	0.53
3:C:35:SER:O	3:C:39:GLN:HG2	2.09	0.53
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.91	0.52
2:B:759:ILE:HG13	2:B:789:MET:HE3	1.92	0.52
1:A:140:GLU:HA	1:A:249:ARG:HH21	1.74	0.52
2:B:966:PRO:HG2	2:B:1038:PHE:HB2	1.90	0.52
1:A:370:TYR:HE2	1:A:389:VAL:HG13	1.74	0.51
1:A:310:ILE:HG22	1:A:311:ARG:HD3	1.93	0.51
1:A:410:THR:HB	1:A:414:ILE:HB	1.93	0.51
2:B:558:LEU:HD23	2:B:565:PRO:HB3	1.91	0.51
1:A:527:ALA:O	1:A:531:ILE:HG12	2.10	0.51
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.92	0.51
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.93	0.50
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.47	0.50
3:C:4:LEU:HB3	3:C:74:LEU:HB3	1.93	0.50
2:B:779:VAL:HG21	2:B:807:LEU:HD21	1.92	0.50
1:A:312:SER:O	1:A:316:ILE:HG12	2.12	0.50
2:B:482:GLU:N	2:B:482:GLU:OE1	2.44	0.49
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.95	0.49
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.93	0.49
2:B:446:ASP:HB2	2:B:449:ARG:HB2	1.94	0.49
2:B:985:LEU:HD11	2:B:992:LEU:HB3	1.95	0.48
2:B:633:ARG:HB2	2:B:778:ASN:HD21	1.78	0.48
3:C:7:ILE:HD12	3:C:71:TYR:CD2	2.48	0.48
2:B:642:PRO:HG2	2:B:702:LEU:HD21	1.96	0.48
1:A:98:TYR:OH	1:A:109:GLU:OE1	2.26	0.47
2:B:841:GLN:HG2	2:B:939:MET:HE2	1.95	0.47
1:A:673:GLN:HG2	1:A:685:LEU:HD12	1.96	0.47
1:A:638:ASP:OD1	1:A:639:SER:N	2.48	0.47
2:B:504:PRO:HG2	2:B:542:THR:HA	1.96	0.47
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.97	0.47
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	1.96	0.47
2:B:992:LEU:HB2	2:B:1052:LEU:HB2	1.95	0.47
2:B:769:ARG:HB2	2:B:773:LEU:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:710:ALA:HB3	2:B:777:PRO:HD2	1.96	0.46
2:B:631:GLY:HA2	2:B:685:VAL:HG22	1.98	0.46
2:B:346:GLU:N	2:B:346:GLU:OE1	2.49	0.46
2:B:1005:LEU:HD23	2:B:1009:LEU:HD12	1.97	0.46
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.50	0.46
1:A:51:LEU:HD22	1:A:114:PHE:HE1	1.81	0.46
1:A:48:ARG:HB2	1:A:49:PRO:HD2	1.98	0.45
3:C:118:PHE:HA	3:C:121:LYS:HG2	1.98	0.45
2:B:525:VAL:HG22	2:B:735:LEU:HD11	1.98	0.45
1:A:18:ARG:HH21	1:A:518:ASP:CG	2.25	0.45
2:B:879:ARG:CZ	2:B:1092:ASN:HB3	2.46	0.45
2:B:351:VAL:HG13	2:B:356:GLU:HG3	1.98	0.45
2:B:446:ASP:C	2:B:448:ARG:H	2.24	0.45
2:B:1039:ILE:O	2:B:1043:ARG:HG2	2.17	0.45
1:A:268:LEU:HG	1:A:288:MET:SD	2.57	0.45
1:A:583:HIS:HA	1:A:586:ARG:HD3	1.98	0.45
3:C:59:MET:HE1	3:C:76:GLU:HG2	1.99	0.45
2:B:994:LEU:HB3	2:B:1054:VAL:HG13	1.98	0.44
1:A:236:ILE:HD13	1:A:236:ILE:HA	1.72	0.44
1:A:262:ARG:NH2	6:A:905:HOH:O	2.48	0.44
1:A:722:VAL:HG22	1:A:723:ASN:H	1.81	0.44
2:B:780:ASN:HD21	2:B:783:ALA:HB2	1.81	0.44
2:B:876:SER:HA	2:B:1091:VAL:HG13	1.99	0.44
1:A:618:MET:HE2	1:A:653:PHE:CD2	2.53	0.44
3:C:7:ILE:HD12	3:C:71:TYR:HD2	1.83	0.43
1:A:677:GLU:H	1:A:677:GLU:HG3	1.62	0.43
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.99	0.43
2:B:957:ALA:C	2:B:959:ASN:H	2.26	0.43
1:A:162:ALA:O	1:A:233:VAL:HG23	2.19	0.43
1:A:249:ARG:CZ	3:C:130:ARG:HB2	2.49	0.43
2:B:1060:PRO:HG2	2:B:1062:LYS:H	1.84	0.43
2:B:416:ASP:OD1	2:B:742:LYS:NZ	2.49	0.43
3:C:113:ILE:O	3:C:116:ASP:HB2	2.19	0.42
1:A:199:GLN:HB3	1:A:203:MET:HE2	2.01	0.42
2:B:960:ILE:C	2:B:961:SER:HG	2.27	0.42
1:A:643:LEU:HD12	1:A:646:ARG:HD3	2.01	0.42
2:B:1053:TYR:CD1	2:B:1055:ILE:HB	2.54	0.42
1:A:310:ILE:H	1:A:310:ILE:HD12	1.85	0.42
1:A:180:CYS:SG	1:A:185:LYS:HD3	2.60	0.42
2:B:955:GLU:N	2:B:955:GLU:OE1	2.52	0.42
3:C:59:MET:HB3	3:C:74:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:616:LEU:O	2:B:620:LEU:HG	2.20	0.42
2:B:1019:GLN:O	2:B:1055:ILE:HG23	2.19	0.42
1:A:368:GLY:HA3	1:A:450:GLY:O	2.20	0.42
1:A:148:LYS:HE3	1:A:244:LEU:O	2.20	0.41
2:B:492:ALA:HB1	2:B:496:TYR:HB2	2.02	0.41
2:B:412:HIS:CE1	2:B:415:LYS:HB2	2.56	0.41
1:A:664:ILE:HG23	1:A:681:PHE:HE1	1.86	0.41
3:C:99:HIS:O	3:C:103:VAL:HG23	2.20	0.41
1:A:381:LEU:HA	1:A:702:MET:HE2	2.03	0.41
2:B:609:THR:HG22	2:B:611:GLU:H	1.85	0.41
1:A:51:LEU:HD22	1:A:114:PHE:CE1	2.56	0.41
1:A:546:LEU:HD12	1:A:546:LEU:HA	1.92	0.41
1:A:311:ARG:NH2	1:A:358:LEU:HB3	2.36	0.41
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.86	0.41
1:A:673:GLN:HG3	1:A:681:PHE:CE2	2.55	0.40
2:B:555:PHE:HZ	2:B:622:ALA:HB1	1.86	0.40
1:A:300:MET:HB3	1:A:300:MET:HE2	1.71	0.40
1:A:673:GLN:CD	1:A:673:GLN:H	2.28	0.40
2:B:423:VAL:HG23	2:B:488:ILE:HD11	2.03	0.40
2:B:410:LEU:HD22	2:B:935:LEU:HG	2.04	0.40
1:A:517:PHE:HB3	1:A:573:THR:HG22	2.02	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	697/764 (91%)	661 (95%)	34 (5%)	2 (0%)	36	58
2	B	721/748 (96%)	685 (95%)	34 (5%)	2 (0%)	36	58
3	C	129/157 (82%)	118 (92%)	10 (8%)	1 (1%)	16	34
4	D	1/6 (17%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1548/1675 (92%)	1465 (95%)	78 (5%)	5 (0%)	36 58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	PRO
2	B	463	GLU
1	A	184	SER
3	C	2	VAL
2	B	1047	PRO

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	619/666 (93%)	595 (96%)	24 (4%)	28 55
2	B	659/678 (97%)	625 (95%)	34 (5%)	21 44
3	C	119/138 (86%)	111 (93%)	8 (7%)	15 33
4	D	2/6 (33%)	2 (100%)	0	100 100
All	All	1399/1488 (94%)	1333 (95%)	66 (5%)	23 48

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	30	GLU
1	A	41	LEU
1	A	116	SER
1	A	141	ASP
1	A	153	MET
1	A	192	THR
1	A	236	ILE
1	A	240	LEU
1	A	243	LEU

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Mol	Chain	Res	Type
1	A	268	LEU
1	A	400	MET
1	A	424	VAL
1	A	437	GLU
1	A	451	LEU
1	A	499	ILE
1	A	508	THR
1	A	544	ARG
1	A	566	SER
1	A	569	ARG
1	A	570	PHE
1	A	637	LEU
1	A	673	GLN
1	A	677	GLU
2	B	346	GLU
2	B	349	ARG
2	B	359	MET
2	B	411	LEU
2	B	497	MET
2	B	522	LEU
2	B	554	HIS
2	B	573	ILE
2	B	608	LYS
2	B	609	THR
2	B	641	LEU
2	B	650	LYS
2	B	679	ASP
2	B	713	VAL
2	B	771	THR
2	B	773	LEU
2	B	787	VAL
2	B	816	ARG
2	B	856	MET
2	B	857	THR
2	B	861	SER
2	B	906	LEU
2	B	916	THR
2	B	920	LEU
2	B	935	LEU
2	B	940	LEU
2	B	958	LEU
2	B	964	THR

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Mol	Chain	Res	Type
2	B	1001	THR
2	B	1002	GLN
2	B	1052	LEU
2	B	1075	GLU
2	B	1085	LEU
2	B	1092	ASN
3	C	2	VAL
3	C	3	LEU
3	C	35	SER
3	C	46	GLU
3	C	67	GLN
3	C	101	LYS
3	C	113	ILE
3	C	121	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	281	ASN
1	A	579	GLN
1	A	606	HIS
1	A	614	GLN
2	B	515	ASN
2	B	613	GLN
2	B	727	GLN
2	B	729	GLN
2	B	780	ASN
2	B	913	GLN
2	B	917	ASN
2	B	967	GLN
2	B	1064	ASN
3	C	152	ASN

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](#)

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, 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	707/764 (92%)	0.38	63 (8%)	15	12	42, 70, 182, 266	0
2	B	729/748 (97%)	0.33	50 (6%)	23	18	41, 74, 180, 265	0
3	C	135/157 (85%)	0.81	10 (7%)	20	16	81, 143, 200, 223	0
4	D	3/6 (50%)	0.95	0	100	100	112, 112, 113, 124	0
All	All	1574/1675 (93%)	0.39	123 (7%)	19	15	41, 75, 185, 266	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	625	ALA	5.0
2	B	1053	TYR	4.8
2	B	957	ALA	4.8
1	A	628	PHE	4.7
2	B	1004	PHE	4.5
2	B	1024	LEU	4.4
1	A	122	LEU	4.2
2	B	1005	LEU	4.1
3	C	2	VAL	4.1
2	B	1036	ILE	4.0
1	A	659	TYR	4.0
1	A	658	ILE	3.9
2	B	661	ALA	3.9
2	B	1009	LEU	3.9
1	A	631	PRO	3.8
1	A	688	PRO	3.8
1	A	124	GLY	3.7
1	A	238	MET	3.7
2	B	965	ILE	3.7
2	B	1055	ILE	3.7
1	A	665	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	722	VAL	3.5
1	A	746	ASP	3.5
1	A	626	TYR	3.4
2	B	1047	PRO	3.4
2	B	958	LEU	3.4
2	B	1030	PRO	3.4
1	A	706	ILE	3.3
2	B	996	VAL	3.3
1	A	684	LEU	3.3
2	B	562	LEU	3.3
2	B	1054	VAL	3.3
1	A	680	ASN	3.3
1	A	689	VAL	3.3
2	B	1064	ASN	3.3
1	A	627	SER	3.2
2	B	881	SER	3.2
2	B	1056	ALA	3.1
1	A	632	PRO	3.1
2	B	1035	ILE	3.1
1	A	718	LEU	3.1
3	C	4	LEU	3.1
3	C	113	ILE	3.0
1	A	506	ALA	3.0
1	A	717	PHE	3.0
2	B	1018	PRO	3.0
2	B	959	ASN	3.0
3	C	23	ASP	3.0
1	A	664	ILE	3.0
2	B	960	ILE	3.0
1	A	681	PHE	2.9
2	B	1063	ALA	2.9
1	A	225	PRO	2.9
2	B	559	GLN	2.9
1	A	643	LEU	2.8
2	B	1025	PRO	2.8
1	A	205	GLY	2.8
2	B	997	GLY	2.8
2	B	1000	CYS	2.7
1	A	715	ALA	2.7
2	B	1057	ASP	2.7
2	B	1011	VAL	2.7
2	B	1033	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	888	PRO	2.7
1	A	4	TYR	2.6
1	A	49	PRO	2.6
1	A	701	PRO	2.5
1	A	362	CYS	2.5
1	A	104	LEU	2.5
1	A	646	ARG	2.5
1	A	683	HIS	2.5
2	B	666	MET	2.5
1	A	695	ILE	2.5
2	B	1045	GLN	2.5
3	C	47	GLN	2.5
1	A	548	ARG	2.4
2	B	445	LEU	2.4
1	A	94	PHE	2.4
1	A	687	ALA	2.4
2	B	798	THR	2.4
3	C	148	ILE	2.4
1	A	62	SER	2.4
1	A	363	CYS	2.4
1	A	667	TRP	2.4
1	A	700	PHE	2.4
1	A	34	MET	2.4
3	C	1	MET	2.4
1	A	676	PRO	2.4
1	A	234	GLN	2.4
1	A	195	LEU	2.4
1	A	685	LEU	2.4
2	B	961	SER	2.4
2	B	433	SER	2.3
2	B	995	TRP	2.3
1	A	719	LEU	2.3
1	A	65	THR	2.3
1	A	320	ASN	2.3
2	B	770	SER	2.3
1	A	674	ASP	2.2
1	A	634	PRO	2.2
1	A	657	LEU	2.2
2	B	423	VAL	2.2
2	B	955	GLU	2.2
1	A	648	LEU	2.2
1	A	645	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1017	ILE	2.2
1	A	652	THR	2.1
3	C	5	THR	2.1
1	A	239	ASN	2.1
1	A	237	ASP	2.1
2	B	964	THR	2.1
1	A	721	LYS	2.1
1	A	48	ARG	2.1
1	A	244	LEU	2.1
2	B	1059	SER	2.1
3	C	33	TYR	2.1
2	B	950	ASP	2.0
1	A	155	LEU	2.0
2	B	347	GLY	2.0
2	B	1016	SER	2.0
2	B	447	GLN	2.0
3	C	83	LEU	2.0
2	B	882	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	A	801	1/1	0.98	0.08	105,105,105,105	0
5	ZN	B	1101	1/1	0.98	0.10	129,129,129,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.