Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 01:44 AM EDT

PDB ID	:	5VNH
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:

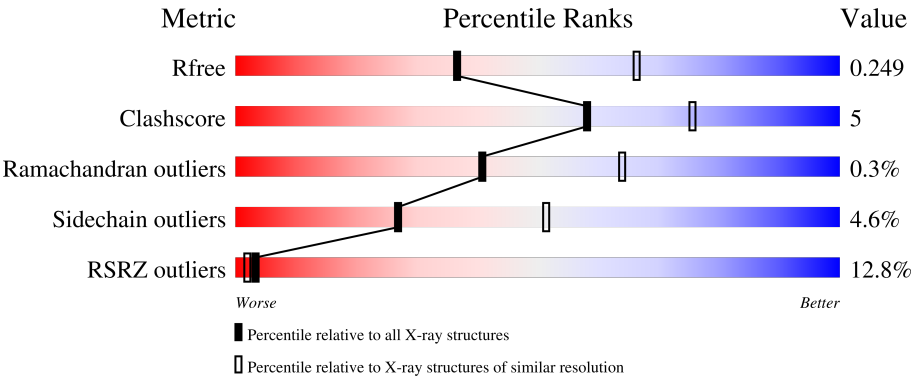
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	11% 79% 12% • 7%
2	B	748	11% 82% 15% • •
3	C	157	24% 70% 13% • 14%
4	D	6	50% 50%

2 Entry composition (i)

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 (three-letter code: 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 Zn 1 1	0	0

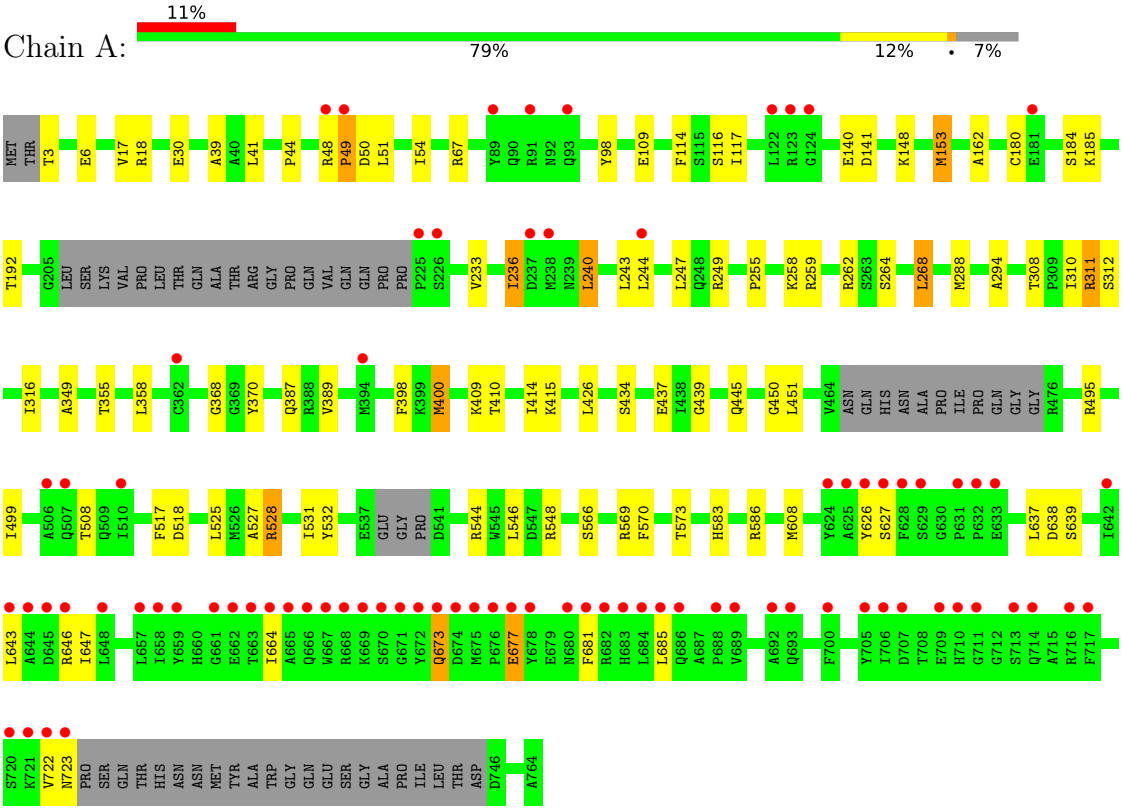
- Molecule 6 is water.

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

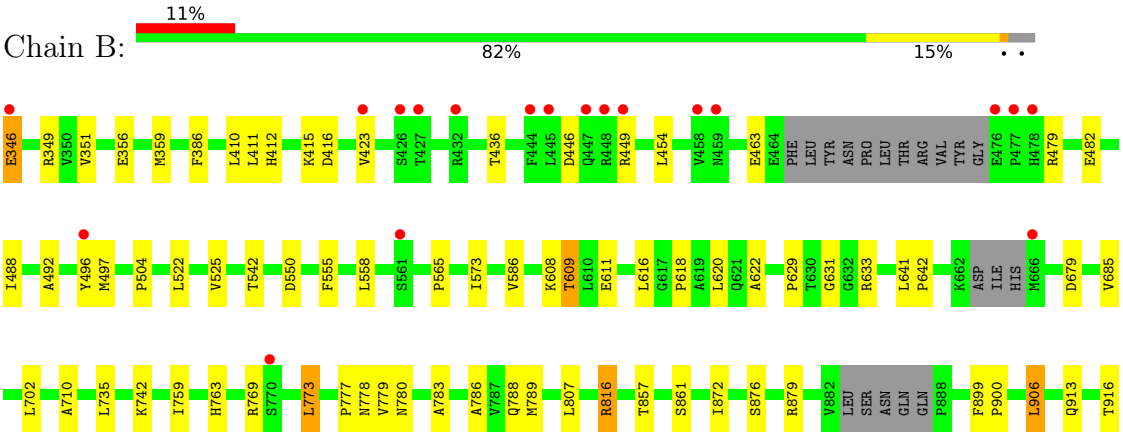
3 Residue-property plots (i)

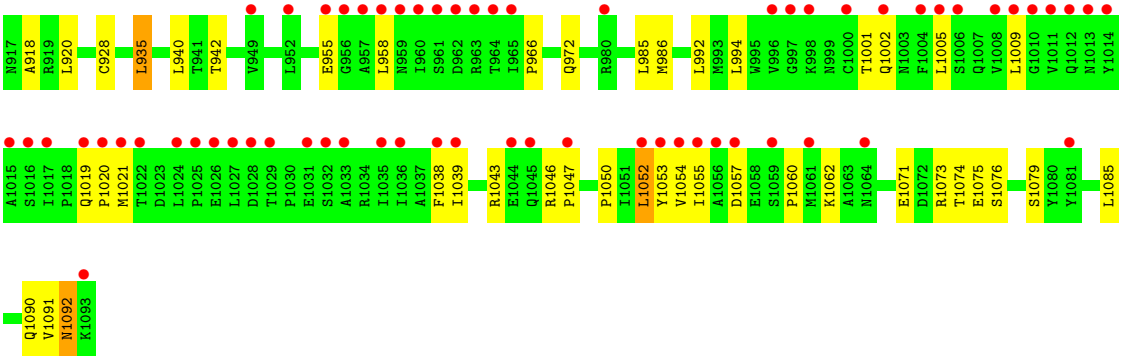
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



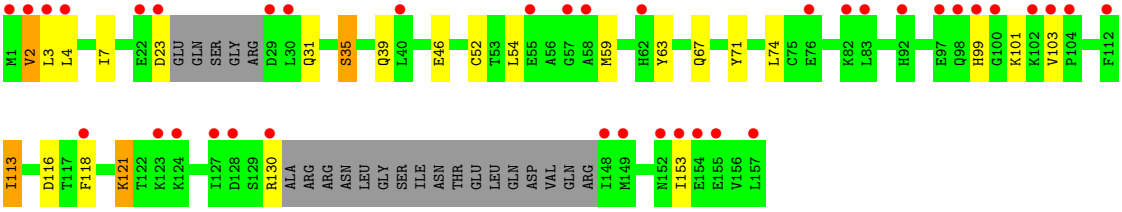
• Molecule 2: Protein transport protein Sec24A





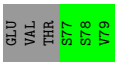
• Molecule 3: Vesicle-trafficking protein SEC22b

Chain C:



• Molecule 4: C-terminal SV motif

Chain D:



4 Data and refinement statistics (i)

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) 99.6 (48.88-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.212 , 0.250 0.211 , 0.249	Depositor DCC
R_{free} test set	1927 reflections (3.27%)	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 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[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	0/5754	0.43	0/7790
2	B	0.25	0/5881	0.43	0/7993
3	C	0.24	0/1106	0.41	0/1489
4	D	0.21	0/18	0.29	0/22
All	All	0.26	0/12759	0.43	0/17294

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	5623	0	5571	53	0
2	B	5758	0	5806	57	0
3	C	1087	0	1091	12	0
4	D	19	0	15	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
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	120	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 (120) 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
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: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: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
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
2:B:759:ILE:HG13	2:B:789:MET:HE3	1.88	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
1:A:140:GLU:HA	1:A:249:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:528:ARG:HA	1:A:608:MET:HE1	1.92	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
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:986:MET:HE3	2:B:986:MET:HB2	1.79	0.46
2:B:769:ARG:HB2	2:B:773:LEU:HB3	1.96	0.46
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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
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
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:18:ARG:HH21	1:A:518:ASP:CG	2.25	0.40
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	41	64
2	B	721/748 (96%)	685 (95%)	34 (5%)	2 (0%)	41	64
3	C	129/157 (82%)	118 (92%)	10 (8%)	1 (1%)	19	39
4	D	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1548/1675 (92%)	1465 (95%)	78 (5%)	5 (0%)	41	64

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 (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	619/666 (93%)	593 (96%)	26 (4%)	30 55
2	B	659/678 (97%)	630 (96%)	29 (4%)	28 53
3	C	119/138 (86%)	110 (92%)	9 (8%)	13 26
4	D	2/6 (33%)	2 (100%)	0	100 100
All	All	1399/1488 (94%)	1335 (95%)	64 (5%)	27 51

All (64) 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
1	A	247	LEU
1	A	268	LEU
1	A	311	ARG
1	A	400	MET
1	A	437	GLU
1	A	451	LEU
1	A	499	ILE
1	A	508	THR
1	A	528	ARG
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	386	PHE
2	B	411	LEU
2	B	479	ARG
2	B	497	MET

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Mol	Chain	Res	Type
2	B	522	LEU
2	B	550	ASP
2	B	608	LYS
2	B	609	THR
2	B	641	LEU
2	B	679	ASP
2	B	773	LEU
2	B	816	ARG
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	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	31	GLN
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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	606	HIS
2	B	913	GLN

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 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	707/764 (92%)	0.46	81 (11%) 4 3	42, 70, 182, 266	0
2	B	729/748 (97%)	0.44	82 (11%) 5 3	41, 74, 180, 265	0
3	C	135/157 (85%)	1.35	38 (28%) 0 0	81, 143, 200, 223	0
4	D	3/6 (50%)	0.37	0 100 100	112, 112, 113, 124	0
All	All	1574/1675 (93%)	0.52	201 (12%) 3 2	41, 75, 185, 266	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1055	ILE	12.4
1	A	684	LEU	12.4
1	A	685	LEU	12.0
2	B	958	LEU	11.1
3	C	1	MET	10.1
2	B	1009	LEU	9.6
1	A	717	PHE	9.3
1	A	682	ARG	8.5
1	A	628	PHE	8.5
1	A	680	ASN	8.3
1	A	688	PRO	8.2
1	A	677	GLU	8.2
3	C	29	ASP	8.0
1	A	122	LEU	7.6
1	A	675	MET	7.6
1	A	123	ARG	7.5
1	A	659	TYR	7.1
2	B	1002	GLN	7.0
3	C	128	ASP	7.0
2	B	1028	ASP	6.9
1	A	642	ILE	6.7

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Mol	Chain	Res	Type	RSRZ
2	B	1024	LEU	6.5
2	B	1035	ILE	6.3
1	A	714	GLN	6.2
1	A	625	ALA	6.2
2	B	1022	THR	6.2
3	C	23	ASP	6.2
1	A	648	LEU	6.2
1	A	678	TYR	6.2
1	A	716	ARG	6.1
2	B	1010	GLY	6.1
2	B	1061	MET	6.1
1	A	674	ASP	6.1
2	B	1004	PHE	6.0
1	A	689	VAL	6.0
2	B	1012	GLN	5.9
2	B	1016	SER	5.9
1	A	669	LYS	5.7
2	B	962	ASP	5.7
1	A	666	GLN	5.6
2	B	1014	TYR	5.6
1	A	676	PRO	5.6
1	A	672	TYR	5.5
3	C	153	ILE	5.4
1	A	667	TRP	5.4
2	B	1056	ALA	5.4
1	A	644	ALA	5.2
2	B	1005	LEU	5.2
1	A	629	SER	5.1
1	A	632	PRO	5.0
2	B	963	ARG	5.0
2	B	957	ALA	4.9
1	A	668	ARG	4.9
2	B	980	ARG	4.9
2	B	959	ASN	4.9
1	A	706	ILE	4.8
1	A	665	ALA	4.7
2	B	960	ILE	4.7
1	A	670	SER	4.7
1	A	49	PRO	4.7
3	C	83	LEU	4.6
2	B	1057	ASP	4.6
2	B	956	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	626	TYR	4.6
2	B	964	THR	4.6
1	A	713	SER	4.5
1	A	631	PRO	4.4
3	C	3	LEU	4.3
1	A	394	MET	4.2
1	A	658	ILE	4.2
1	A	646	ARG	4.2
2	B	961	SER	4.2
2	B	476	GLU	4.2
2	B	1017	ILE	4.2
1	A	693	GLN	4.2
3	C	55	GLU	4.0
2	B	998	LYS	4.0
2	B	1031	GLU	4.0
1	A	709	GLU	4.0
1	A	124	GLY	3.9
3	C	57	GLY	3.9
1	A	663	THR	3.9
2	B	1015	ALA	3.9
3	C	2	VAL	3.9
3	C	4	LEU	3.8
1	A	686	GLN	3.8
1	A	681	PHE	3.8
2	B	444	PHE	3.7
2	B	1011	VAL	3.7
2	B	346	GLU	3.7
2	B	1032	SER	3.7
1	A	645	ASP	3.6
2	B	1000	CYS	3.6
3	C	149	MET	3.6
3	C	155	GLU	3.6
2	B	1036	ILE	3.6
2	B	1053	TYR	3.6
1	A	507	GLN	3.5
2	B	1054	VAL	3.5
1	A	643	LEU	3.5
1	A	723	ASN	3.4
2	B	1025	PRO	3.4
1	A	711	GLY	3.4
3	C	152	ASN	3.3
1	A	633	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	627	SER	3.3
1	A	225	PRO	3.3
2	B	1039	ILE	3.2
2	B	965	ILE	3.2
3	C	148	ILE	3.2
1	A	673	GLN	3.2
3	C	127	ILE	3.2
3	C	99	HIS	3.2
3	C	157	LEU	3.2
2	B	1026	GLU	3.2
2	B	952	LEU	3.1
3	C	30	LEU	3.1
1	A	722	VAL	3.1
1	A	506	ALA	3.1
2	B	1029	THR	3.1
2	B	426	SER	3.0
3	C	154	GLU	3.0
2	B	1027	LEU	3.0
3	C	22	GLU	3.0
2	B	449	ARG	3.0
2	B	458	VAL	3.0
2	B	478	HIS	2.9
2	B	1045	GLN	2.9
3	C	82	LYS	2.9
1	A	244	LEU	2.9
2	B	949	VAL	2.8
1	A	705	TYR	2.8
2	B	1047	PRO	2.8
3	C	130	ARG	2.8
1	A	238	MET	2.7
3	C	123	LYS	2.7
1	A	707	ASP	2.7
1	A	91	ARG	2.7
3	C	104	PRO	2.7
1	A	510	ILE	2.7
2	B	1044	GLU	2.7
2	B	996	VAL	2.6
1	A	692	ALA	2.6
2	B	1093	LYS	2.6
2	B	1013	ASN	2.6
1	A	664	ILE	2.6
1	A	683	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	445	LEU	2.6
1	A	93	GLN	2.5
3	C	92	HIS	2.5
2	B	1021	MET	2.5
1	A	700	PHE	2.5
2	B	432	ARG	2.5
1	A	657	LEU	2.5
3	C	97	GLU	2.5
2	B	1052	LEU	2.4
2	B	423	VAL	2.4
2	B	770	SER	2.4
2	B	1008	VAL	2.4
2	B	1064	ASN	2.4
1	A	89	TYR	2.4
1	A	181	GLU	2.4
2	B	447	GLN	2.4
1	A	671	GLY	2.4
2	B	448	ARG	2.4
2	B	666	MET	2.4
2	B	477	PRO	2.4
2	B	1020	PRO	2.4
1	A	661	GLY	2.4
2	B	1033	ALA	2.3
2	B	496	TYR	2.3
1	A	624	TYR	2.3
3	C	118	PHE	2.3
1	A	237	ASP	2.3
3	C	100	GLY	2.3
2	B	561	SER	2.3
1	A	710	HIS	2.3
2	B	1038	PHE	2.3
3	C	103	VAL	2.3
3	C	112	PHE	2.2
2	B	1019	GLN	2.2
2	B	459	ASN	2.2
2	B	955	GLU	2.2
1	A	226	SER	2.2
3	C	102	LYS	2.2
2	B	997	GLY	2.2
2	B	427	THR	2.2
3	C	40	LEU	2.1
1	A	720	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	1081	TYR	2.1
3	C	98	GLN	2.1
2	B	1059	SER	2.1
1	A	48	ARG	2.1
3	C	76	GLU	2.1
1	A	362	CYS	2.0
1	A	662	GLU	2.0
3	C	62	HIS	2.0
3	C	58	ALA	2.0
2	B	1006	SER	2.0
3	C	124	LYS	2.0
1	A	721	LYS	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
5	ZN	B	1101	1/1	0.95	0.20	129,129,129,129	0
5	ZN	A	801	1/1	0.96	0.12	105,105,105,105	0

6.5 Other polymers (i)

There are no such residues in this entry.