Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 07:49 PM EDT

PDB ID	:	5VNF
Title	:	Crystal structure of Sec23a/Sec24a/Sec22 complexed with a C-terminal VV sorting motif
Authors	:	Ma, W.; Goldberg, J.
Deposited on	:	2017-04-30
Resolution	:	2.41 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:

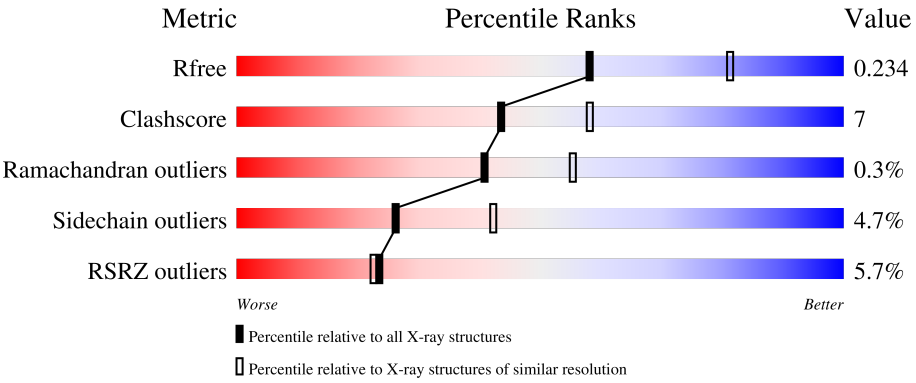
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.41 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	5% 77% 14% • 7%
2	B	748	3% 81% 15% • •
3	C	157	17% 68% 16% • 14%
4	D	5	80% 20%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12585 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
			5612	3575	967	1030	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
			5749	3667	980	1068	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
			1084	696	177	203	8			

- Molecule 4 is a protein called C-terminal VV Sorting motif: VAL-THR-SER-VAL-VAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	5	Total	C	N	O	0	0	0
			31	19	5	7			

- 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.

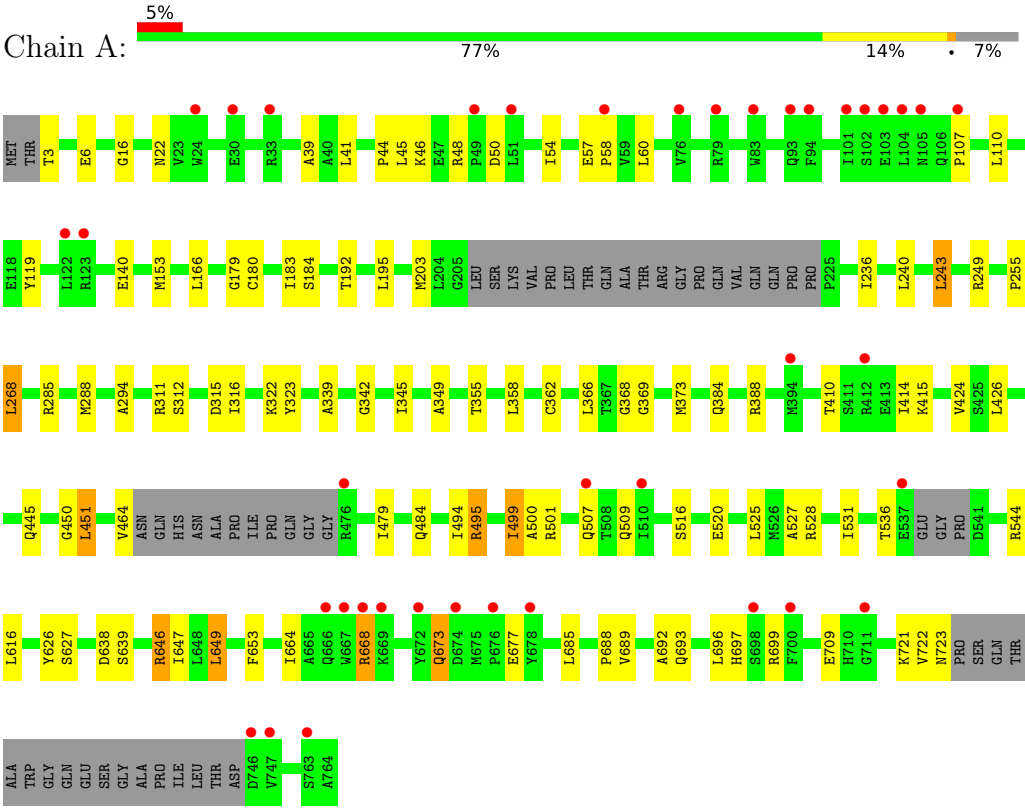
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	40	Total O 40 40	0	0
6	B	63	Total O 63 63	0	0
6	C	4	Total O 4 4	0	0

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.

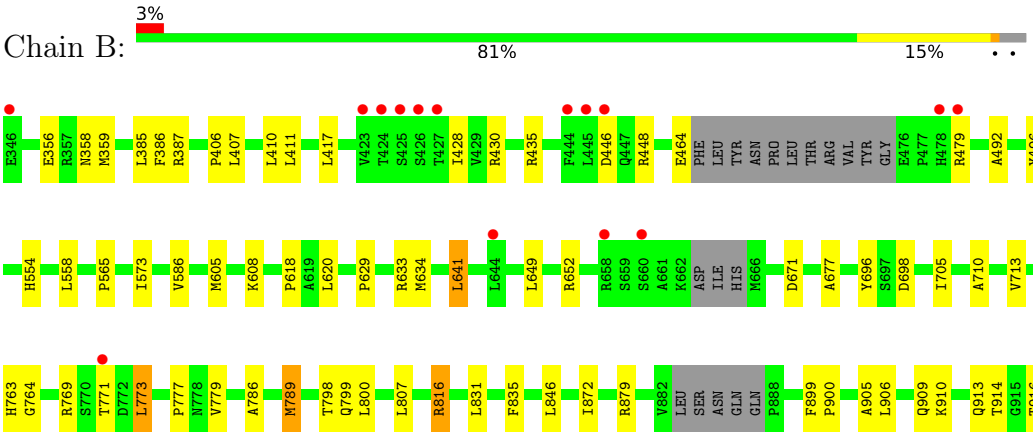
• Molecule 1: Protein transport protein Sec23A

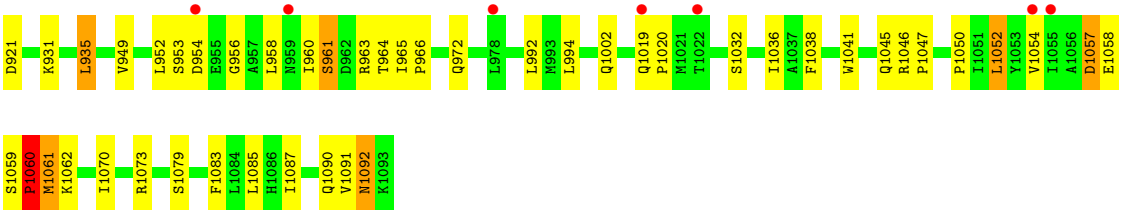
Chain A:



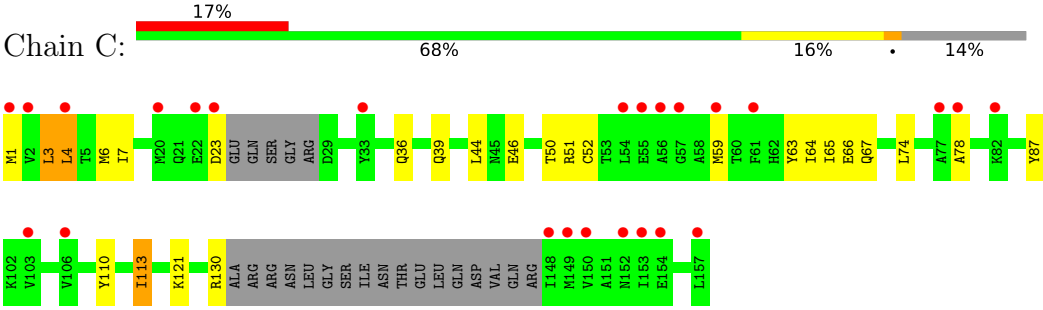
• Molecule 2: Protein transport protein Sec24A

Chain B:

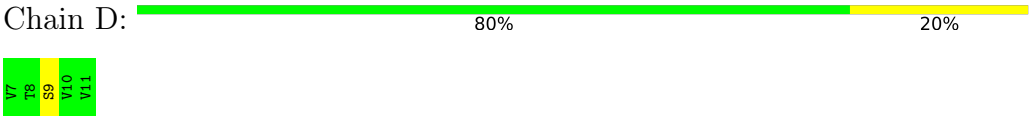




• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: C-terminal VV Sorting motif: VAL-THR-SER-VAL-VAL



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	147.82Å 97.08Å 129.82Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	48.82 – 2.41 48.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.5 (48.82-2.41) 98.5 (48.82-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.204 , 0.241 0.200 , 0.234	Depositor DCC
R_{free} test set	1668 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12585	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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	0.45	0/5742	0.49	0/7774
2	B	0.41	0/5872	0.52	0/7981
3	C	0.34	0/1103	0.48	0/1485
4	D	0.29	0/30	0.61	0/39
All	All	0.42	0/12747	0.50	0/17279

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	5612	0	5560	66	0
2	B	5749	0	5791	82	0
3	C	1084	0	1082	24	0
4	D	31	0	26	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	40	0	0	4	0
6	B	63	0	0	8	0
6	C	4	0	0	0	0
All	All	12585	0	12459	168	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 7.

All (168) 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:342:GLY:O	6:A:901:HOH:O	2.00	0.80
1:A:183:ILE:HG23	1:A:184:SER:N	1.95	0.79
3:C:3:LEU:CB	3:C:74:LEU:O	2.32	0.77
1:A:183:ILE:CG2	1:A:184:SER:N	2.45	0.77
2:B:741:ARG:O	6:B:1201:HOH:O	2.01	0.76
2:B:464:GLU:O	6:B:1202:HOH:O	2.02	0.76
2:B:629:PRO:HG3	3:C:23:ASP:HB2	1.66	0.76
3:C:3:LEU:HD22	3:C:3:LEU:N	2.00	0.75
3:C:3:LEU:HD22	3:C:3:LEU:H	1.52	0.74
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.71	0.73
1:A:721:LYS:NZ	6:A:903:HOH:O	2.21	0.73
2:B:1060:PRO:HD2	2:B:1061:MET:N	2.04	0.72
2:B:994:LEU:HB3	2:B:1054:VAL:HG22	1.71	0.72
3:C:4:LEU:O	3:C:4:LEU:HD23	1.89	0.71
3:C:1:MET:HE2	3:C:78:ALA:HB3	1.74	0.70
1:A:114:PHE:HB3	1:A:117:ILE:HD12	1.74	0.69
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.74	0.68
2:B:1060:PRO:O	2:B:1062:LYS:HG3	1.92	0.68
1:A:484:GLN:OE1	6:A:902:HOH:O	2.11	0.68
2:B:1060:PRO:O	2:B:1062:LYS:N	2.26	0.68
2:B:1060:PRO:HG2	2:B:1062:LYS:H	1.58	0.68
2:B:931:LYS:NZ	6:B:1210:HOH:O	2.26	0.68
3:C:3:LEU:HB2	3:C:74:LEU:O	1.93	0.67
2:B:921:ASP:OD2	6:B:1203:HOH:O	2.13	0.67
2:B:954:ASP:CB	2:B:964:THR:HG21	2.25	0.67
1:A:647:ILE:HG21	1:A:688:PRO:HG3	1.78	0.65
2:B:410:LEU:HD22	2:B:935:LEU:HG	1.78	0.64
2:B:779:VAL:HG21	2:B:807:LEU:HD21	1.79	0.64
2:B:872:ILE:HD12	2:B:1090:GLN:HB2	1.78	0.63
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.82	0.62
3:C:4:LEU:CD2	3:C:74:LEU:HB3	2.29	0.62
2:B:1060:PRO:CD	2:B:1061:MET:N	2.57	0.62
3:C:1:MET:HE2	3:C:78:ALA:CB	2.29	0.62
1:A:183:ILE:HD13	2:B:605:MET:CE	2.30	0.61
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.83	0.60
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.83	0.60
1:A:195:LEU:HD13	1:A:203:MET:HE1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLU:HA	1:A:249:ARG:HH21	1.67	0.59
1:A:668:ARG:NH1	1:A:709:GLU:OE2	2.36	0.58
2:B:1054:VAL:O	2:B:1054:VAL:HG12	2.03	0.57
3:C:4:LEU:HD22	3:C:74:LEU:HB3	1.87	0.57
1:A:22:ASN:HB2	1:A:516:SER:HB2	1.88	0.56
2:B:913:GLN:HE21	2:B:918:ALA:HB2	1.72	0.55
1:A:183:ILE:CG2	1:A:184:SER:H	2.17	0.55
3:C:36:GLN:HA	3:C:39:GLN:HG3	1.89	0.55
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.90	0.54
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.89	0.54
1:A:484:GLN:HG2	1:A:494:ILE:HG12	1.89	0.54
2:B:966:PRO:HG2	2:B:1038:PHE:HB2	1.90	0.54
2:B:759:ILE:HG13	2:B:789:MET:HE3	1.90	0.53
2:B:1060:PRO:HD2	2:B:1061:MET:H	1.74	0.53
1:A:3:THR:HG22	1:A:6:GLU:H	1.73	0.53
1:A:44:PRO:O	1:A:495:ARG:NH1	2.40	0.53
1:A:183:ILE:HD13	2:B:605:MET:HE2	1.89	0.53
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.44	0.53
1:A:653:PHE:HA	1:A:699:ARG:NH1	2.24	0.52
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.90	0.52
3:C:3:LEU:HB3	3:C:74:LEU:O	2.08	0.52
1:A:166:LEU:HD23	1:A:243:LEU:HD13	1.92	0.52
1:A:500:ALA:O	1:A:501:ARG:NH1	2.39	0.51
2:B:1060:PRO:O	2:B:1061:MET:C	2.46	0.51
1:A:626:TYR:HB2	1:A:647:ILE:HB	1.93	0.51
1:A:410:THR:HB	1:A:414:ILE:HB	1.93	0.50
2:B:1057:ASP:O	2:B:1060:PRO:HD3	2.12	0.50
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.93	0.50
1:A:183:ILE:HG22	1:A:184:SER:H	1.76	0.50
2:B:1060:PRO:C	2:B:1062:LYS:N	2.63	0.50
2:B:498:LEU:N	6:B:1209:HOH:O	2.26	0.49
2:B:879:ARG:HD2	2:B:1091:VAL:HG12	1.94	0.49
1:A:183:ILE:O	1:A:184:SER:OG	2.16	0.49
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.93	0.49
3:C:51:ARG:NH2	3:C:66:GLU:OE2	2.46	0.49
2:B:909:GLN:HG2	2:B:910:LYS:N	2.28	0.49
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.95	0.49
2:B:1083:PHE:O	2:B:1087:ILE:HG12	2.12	0.48
3:C:51:ARG:HD3	3:C:64:ILE:HG22	1.95	0.48
2:B:1060:PRO:C	2:B:1062:LYS:H	2.15	0.48
3:C:4:LEU:HD23	3:C:74:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HD22	1:A:203:MET:HE2	1.97	0.47
1:A:368:GLY:HA3	1:A:450:GLY:O	2.14	0.47
1:A:384:GLN:O	1:A:388:ARG:HG3	2.14	0.47
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.96	0.47
1:A:312:SER:H	1:A:315:ASP:HB2	1.80	0.47
1:A:673:GLN:HG2	1:A:685:LEU:HD12	1.97	0.47
2:B:1041:TRP:O	2:B:1045:GLN:HG2	2.15	0.47
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.50	0.47
2:B:407:LEU:HG	2:B:789:MET:HG3	1.97	0.46
2:B:633:ARG:NH2	6:B:1216:HOH:O	2.45	0.46
1:A:312:SER:O	1:A:316:ILE:HG12	2.14	0.46
1:A:415:LYS:HD2	1:A:464:VAL:HG21	1.97	0.46
2:B:769:ARG:HB2	2:B:773:LEU:HB3	1.97	0.46
1:A:46:LYS:O	1:A:495:ARG:NH2	2.45	0.46
1:A:339:ALA:HB1	1:A:424:VAL:HG21	1.98	0.45
1:A:345:ILE:O	1:A:369:GLY:HA3	2.15	0.45
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.98	0.45
1:A:692:ALA:O	1:A:696:LEU:HB2	2.17	0.45
3:C:44:LEU:HD13	3:C:65:ILE:HD11	1.98	0.45
1:A:649:LEU:C	1:A:649:LEU:HD12	2.36	0.45
3:C:1:MET:HE1	3:C:78:ALA:O	2.17	0.45
2:B:1059:SER:O	2:B:1059:SER:OG	2.27	0.45
1:A:500:ALA:N	6:A:904:HOH:O	2.24	0.45
1:A:527:ALA:O	1:A:531:ILE:HG12	2.17	0.45
2:B:953:SER:O	6:B:1204:HOH:O	2.21	0.45
3:C:3:LEU:C	3:C:3:LEU:CD2	2.86	0.45
3:C:110:TYR:HB3	3:C:113:ILE:HG23	1.99	0.44
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.98	0.44
2:B:963:ARG:HB3	2:B:965:ILE:HD11	2.00	0.44
1:A:16:GLY:HA2	1:A:46:LYS:HD3	1.99	0.44
1:A:366:LEU:HD22	1:A:424:VAL:HG22	1.99	0.44
2:B:992:LEU:O	2:B:1052:LEU:HA	2.17	0.44
2:B:464:GLU:O	6:B:1205:HOH:O	2.21	0.44
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.98	0.44
3:C:59:MET:HB3	3:C:74:LEU:HD11	1.99	0.44
1:A:113:GLN:C	1:A:114:PHE:CD1	2.90	0.44
2:B:1057:ASP:O	2:B:1058:GLU:C	2.54	0.44
1:A:358:LEU:HD22	1:A:597:PRO:HB3	1.99	0.44
1:A:114:PHE:CD1	1:A:114:PHE:N	2.81	0.43
1:A:54:ILE:O	1:A:119:TYR:HA	2.17	0.43
2:B:558:LEU:HD23	2:B:565:PRO:HB3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:TYR:CZ	3:C:91:LEU:HD11	2.54	0.43
2:B:1052:LEU:C	2:B:1052:LEU:HD23	2.39	0.43
1:A:322:LYS:HE3	1:A:323:TYR:CZ	2.53	0.43
2:B:446:ASP:C	2:B:448:ARG:H	2.21	0.43
1:A:107:PRO:HG2	1:A:110:LEU:HD12	2.00	0.43
2:B:558:LEU:HB2	2:B:586:VAL:HG11	2.01	0.43
1:A:696:LEU:O	1:A:697:HIS:ND1	2.51	0.43
2:B:677:ALA:HB2	2:B:705:ILE:HA	2.01	0.43
3:C:3:LEU:C	3:C:3:LEU:HD23	2.39	0.43
1:A:48:ARG:O	1:A:50:ASP:N	2.46	0.43
2:B:385:LEU:HD21	2:B:417:LEU:HD21	1.99	0.43
2:B:492:ALA:HB1	2:B:496:TYR:HB2	2.00	0.43
2:B:764:GLY:HA2	2:B:931:LYS:O	2.19	0.43
2:B:428:ILE:HG22	2:B:430:ARG:HG3	2.01	0.42
2:B:641:LEU:HD22	2:B:649:LEU:HB2	2.01	0.42
2:B:799:GLN:O	2:B:800:LEU:HD23	2.19	0.42
2:B:956:GLY:HA3	2:B:965:ILE:O	2.20	0.42
1:A:45:LEU:HD11	1:A:451:LEU:HD13	2.02	0.42
2:B:949:VAL:HA	2:B:952:LEU:HD21	2.02	0.42
1:A:689:VAL:O	1:A:693:GLN:HG2	2.19	0.42
2:B:831:LEU:HD22	2:B:835:PHE:CE2	2.54	0.41
2:B:430:ARG:HD3	2:B:435:ARG:HH21	1.85	0.41
2:B:958:LEU:HA	2:B:964:THR:HA	2.01	0.41
1:A:479:ILE:HB	1:A:499:ILE:HD11	2.02	0.41
2:B:671:ASP:OD1	2:B:671:ASP:N	2.48	0.41
2:B:1052:LEU:HD23	2:B:1052:LEU:O	2.20	0.41
2:B:879:ARG:CZ	2:B:1092:ASN:HB3	2.51	0.41
2:B:909:GLN:HG2	2:B:910:LYS:H	1.85	0.41
2:B:905:ALA:HB2	2:B:1070:ILE:HD13	2.02	0.41
1:A:349:ALA:O	1:A:373:MET:HA	2.21	0.41
1:A:520:GLU:HB3	1:A:616:LEU:HD11	2.02	0.41
1:A:638:ASP:HA	1:A:723:ASN:H	1.86	0.41
2:B:913:GLN:NE2	2:B:918:ALA:HB2	2.33	0.41
1:A:249:ARG:NH1	3:C:130:ARG:HB3	2.36	0.41
2:B:387:ARG:HD2	2:B:935:LEU:HD12	2.04	0.41
2:B:620:LEU:HD22	2:B:634:MET:CE	2.51	0.41
1:A:268:LEU:HG	1:A:288:MET:SD	2.61	0.40
2:B:773:LEU:HD11	4:D:9:SER:HB3	2.03	0.40
2:B:1060:PRO:CD	2:B:1061:MET:H	2.30	0.40
2:B:963:ARG:HB3	2:B:965:ILE:CD1	2.52	0.40
2:B:1032:SER:O	2:B:1036:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLY:CA	1:A:236:ILE:HD11	2.52	0.40
1:A:638:ASP:OD1	1:A:639:SER:N	2.55	0.40
2:B:356:GLU:C	2:B:358:ASN:H	2.25	0.40
2:B:1046:ARG:HD2	2:B:1050:PRO:HG3	2.03	0.40
2:B:406:PRO:HB2	2:B:846:LEU:HD23	2.04	0.40
2:B:710:ALA:HB3	2:B:777:PRO:HD2	2.03	0.40
2:B:954:ASP:CB	2:B:964:THR:CG2	2.98	0.40
2:B:1052:LEU:HD21	2:B:1054:VAL:HG23	2.03	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%)	664 (95%)	33 (5%)	0	100	100
2	B	721/748 (96%)	681 (94%)	36 (5%)	4 (1%)	25	36
3	C	129/157 (82%)	122 (95%)	7 (5%)	0	100	100
4	D	3/5 (60%)	3 (100%)	0	0	100	100
All	All	1550/1674 (93%)	1470 (95%)	76 (5%)	4 (0%)	41	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1047	PRO
2	B	1061	MET
2	B	961	SER
2	B	1060	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	617/666 (93%)	590 (96%)	27 (4%)	28 45
2	B	656/678 (97%)	627 (96%)	29 (4%)	28 45
3	C	118/138 (86%)	108 (92%)	10 (8%)	10 16
4	D	3/5 (60%)	3 (100%)	0	100 100
All	All	1394/1487 (94%)	1328 (95%)	66 (5%)	26 42

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

Mol	Chain	Res	Type
1	A	41	LEU
1	A	60	LEU
1	A	115	SER
1	A	153	MET
1	A	180	CYS
1	A	192	THR
1	A	240	LEU
1	A	243	LEU
1	A	268	LEU
1	A	285	ARG
1	A	311	ARG
1	A	362	CYS
1	A	451	LEU
1	A	495	ARG
1	A	499	ILE
1	A	507	GLN
1	A	509	GLN
1	A	528	ARG
1	A	536	THR
1	A	544	ARG
1	A	570	PHE
1	A	646	ARG
1	A	649	LEU
1	A	668	ARG

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Mol	Chain	Res	Type
1	A	673	GLN
1	A	677	GLU
1	A	722	VAL
2	B	359	MET
2	B	386	PHE
2	B	411	LEU
2	B	479	ARG
2	B	498	LEU
2	B	522	LEU
2	B	554	HIS
2	B	608	LYS
2	B	641	LEU
2	B	713	VAL
2	B	771	THR
2	B	773	LEU
2	B	789	MET
2	B	798	THR
2	B	816	ARG
2	B	906	LEU
2	B	914	THR
2	B	916	THR
2	B	920	LEU
2	B	935	LEU
2	B	960	ILE
2	B	961	SER
2	B	972	GLN
2	B	1002	GLN
2	B	1052	LEU
2	B	1057	ASP
2	B	1060	PRO
2	B	1085	LEU
2	B	1092	ASN
3	C	3	LEU
3	C	4	LEU
3	C	6	MET
3	C	7	ILE
3	C	46	GLU
3	C	50	THR
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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
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

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

5.5 Carbohydrates

There are no monosaccharides 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, 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%)	0.42	42 (5%) 22 21	40, 72, 113, 142	0
2	B	729/748 (97%)	0.24	22 (3%) 50 49	36, 58, 97, 123	0
3	C	135/157 (85%)	0.99	26 (19%) 1 0	55, 94, 128, 137	0
4	D	5/5 (100%)	0.54	0 100 100	74, 80, 97, 97	0
All	All	1576/1674 (94%)	0.39	90 (5%) 23 22	36, 67, 113, 142	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1	MET	7.1
2	B	1055	ILE	7.1
3	C	153	ILE	6.1
1	A	674	ASP	6.0
2	B	445	LEU	5.2
1	A	94	PHE	5.2
2	B	959	ASN	4.7
3	C	78	ALA	4.6
2	B	1019	GLN	4.1
3	C	33	TYR	4.1
1	A	49	PRO	4.1
1	A	105	ASN	3.9
1	A	123	ARG	3.9
2	B	478	HIS	3.9
1	A	476	ARG	3.8
3	C	57	GLY	3.8
3	C	157	LEU	3.7
2	B	644	LEU	3.5
2	B	771	THR	3.5
3	C	150	VAL	3.5
2	B	423	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	669	LYS	3.4
1	A	51	LEU	3.3
2	B	424	THR	3.3
3	C	54	LEU	3.3
1	A	104	LEU	3.2
1	A	678	TYR	3.2
3	C	149	MET	3.2
3	C	61	PHE	3.2
1	A	700	PHE	3.1
3	C	56	ALA	3.1
1	A	436	ASN	3.0
1	A	122	LEU	3.0
1	A	668	ARG	3.0
1	A	667	TRP	2.9
3	C	23	ASP	2.9
2	B	346	GLU	2.9
2	B	427	THR	2.9
2	B	426	SER	2.8
1	A	672	TYR	2.8
1	A	510	ILE	2.7
2	B	479	ARG	2.7
3	C	148	ILE	2.7
3	C	103	VAL	2.7
2	B	446	ASP	2.7
1	A	30	GLU	2.6
2	B	954	ASP	2.6
1	A	103	GLU	2.6
1	A	79	ARG	2.6
1	A	746	ASP	2.6
3	C	55	GLU	2.6
1	A	58	PRO	2.5
1	A	537	GLU	2.5
1	A	83	TRP	2.5
1	A	33	ARG	2.5
1	A	431	PRO	2.5
2	B	1054	VAL	2.5
2	B	425	SER	2.4
1	A	107	PRO	2.4
1	A	24	TRP	2.4
1	A	666	GLN	2.4
3	C	77	ALA	2.4
1	A	438	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	154	GLU	2.4
1	A	76	VAL	2.4
3	C	82	LYS	2.4
2	B	1022	THR	2.4
3	C	4	LEU	2.4
3	C	152	ASN	2.3
1	A	93	GLN	2.3
2	B	444	PHE	2.2
1	A	102	SER	2.2
1	A	507	GLN	2.2
3	C	22	GLU	2.2
1	A	711	GLY	2.2
2	B	978	LEU	2.2
3	C	106	VAL	2.2
1	A	698	SER	2.2
1	A	747	VAL	2.1
1	A	763	SER	2.1
2	B	658	ARG	2.1
1	A	676	PRO	2.1
3	C	101	LYS	2.1
3	C	2	VAL	2.0
1	A	101	ILE	2.0
1	A	412	ARG	2.0
2	B	660	SER	2.0
1	A	394	MET	2.0
3	C	20	MET	2.0
3	C	59	MET	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	A	801	1/1	0.84	0.20	156,156,156,156	0
5	ZN	B	1101	1/1	0.90	0.24	104,104,104,104	0

6.5 Other polymers (i)

There are no such residues in this entry.