Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 06:39 AM EDT

PDB ID	:	5VNG
Title	:	Crystal structure of Sec23a/Sec24a/Sec22 complexed with a C-terminal II 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:

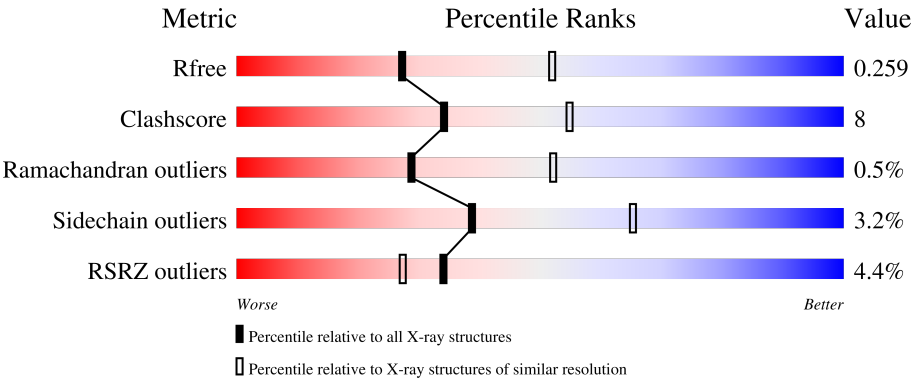
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.60 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	4% 75% 15% • 9%
2	B	748	3% 78% 18% • •
3	C	157	13% 62% 22% • 14%
4	D	6	50% 17% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ZN	B	1101	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12409 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	696	Total	C	N	O	S	0	0	0
			5509	3509	947	1014	39			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	728	Total	C	N	O	S	0	0	0
			5728	3655	975	1065	33			

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 ILE-ILE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			28	18	4	6			

- 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

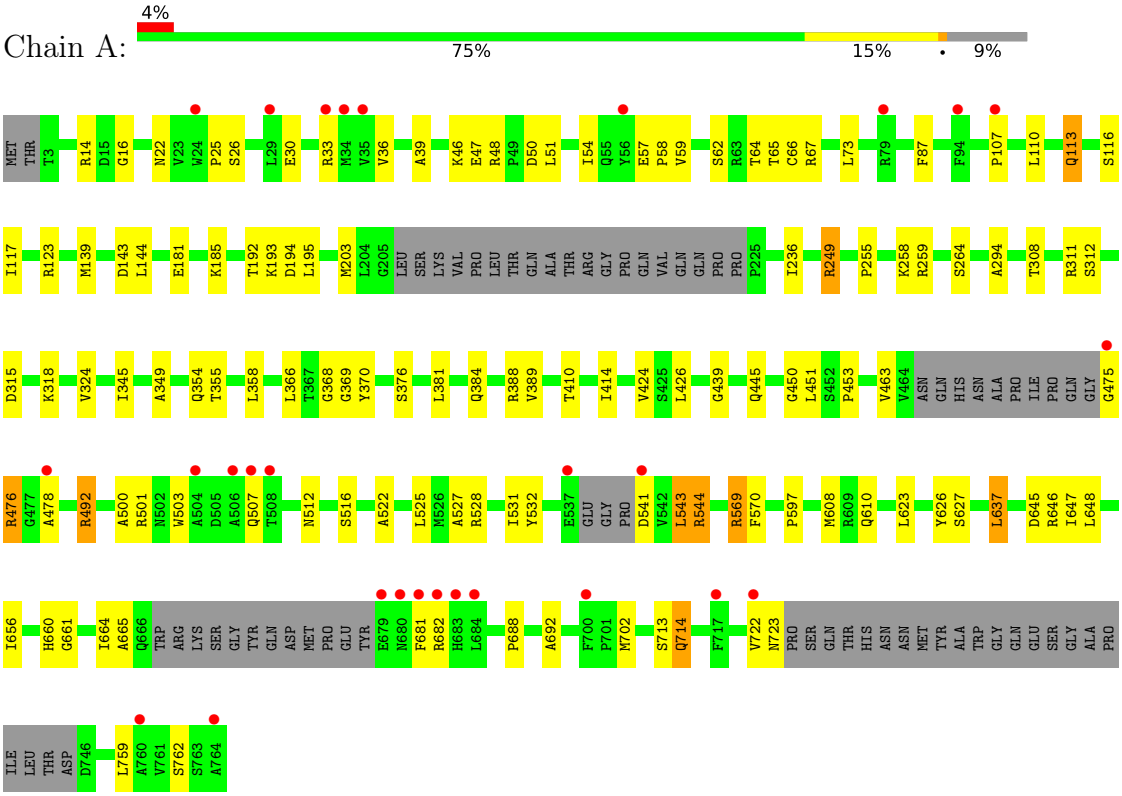
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	19	Total O 19 19	0	0
6	B	36	Total O 36 36	0	0
6	C	1	Total O 1 1	0	0
6	D	2	Total O 2 2	0	0

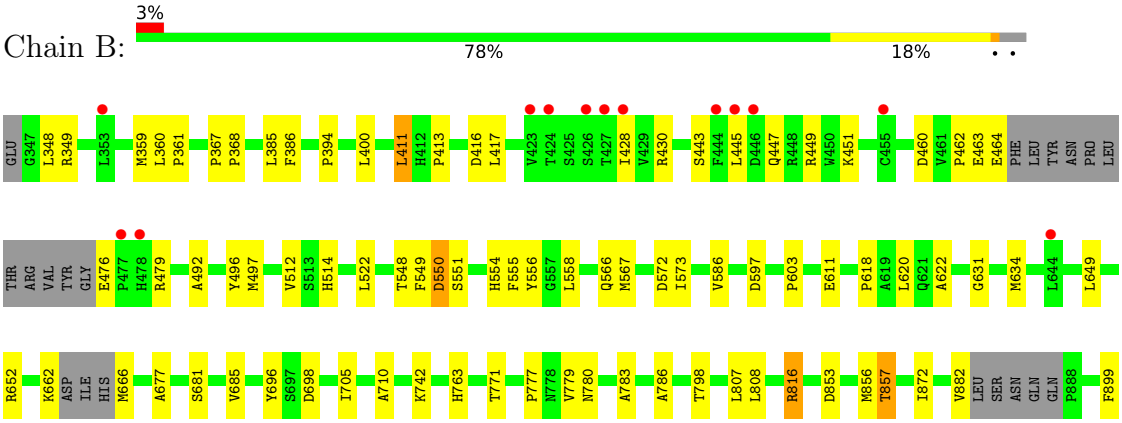
3 Residue-property plots (i)

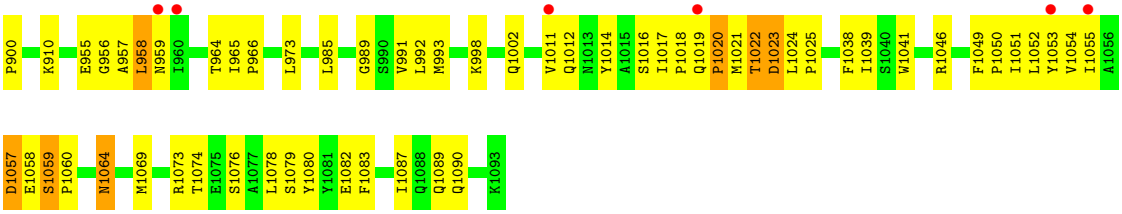
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

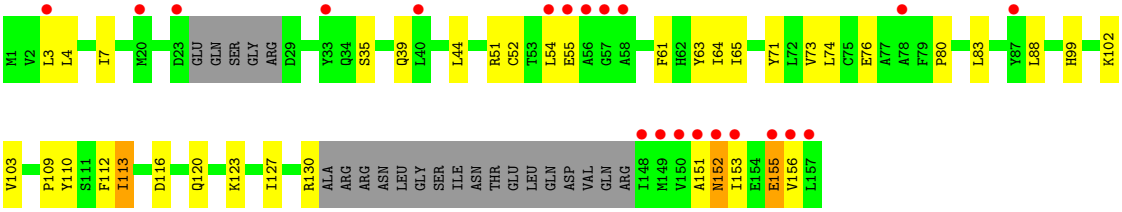


• Molecule 2: Protein transport protein Sec24A





• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: C-terminal ILE-ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.26Å 97.10Å 130.03Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	48.96 – 2.60 48.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.0 (48.96-2.60) 92.0 (48.96-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.199 , 0.257 0.202 , 0.259	Depositor DCC
R_{free} test set	1802 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å^2)	64.9	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12409	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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	0.30	0/5634	0.46	0/7627
2	B	0.46	0/5851	0.49	0/7957
3	C	0.25	0/1103	0.43	0/1485
4	D	0.20	0/27	0.39	0/34
All	All	0.38	0/12615	0.47	0/17103

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	5509	0	5457	78	0
2	B	5728	0	5760	110	0
3	C	1084	0	1082	24	0
4	D	28	0	31	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	19	0	0	1	0
6	B	36	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	2	0	0	0	0
All	All	12409	0	12330	208	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 8.

All (208) 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:1019:GLN:HB3	2:B:1020:PRO:HD3	1.49	0.91
2:B:550:ASP:OD1	2:B:551:SER:N	2.09	0.86
2:B:1057:ASP:O	2:B:1060:PRO:CD	2.25	0.85
1:A:759:LEU:HA	1:A:762:SER:OG	1.77	0.84
1:A:64:THR:O	1:A:67:ARG:HG2	1.80	0.82
2:B:965:ILE:HD13	2:B:1041:TRP:HB2	1.66	0.77
1:A:475:GLY:O	1:A:476:ARG:HB2	1.84	0.77
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.50	0.77
3:C:55:GLU:O	3:C:152:ASN:ND2	2.17	0.76
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.68	0.76
1:A:759:LEU:O	1:A:762:SER:OG	2.03	0.76
2:B:1057:ASP:O	2:B:1060:PRO:HD2	1.87	0.75
2:B:1022:THR:O	2:B:1052:LEU:O	2.04	0.75
3:C:110:TYR:HB3	3:C:113:ILE:HG23	1.68	0.75
2:B:1039:ILE:HD13	2:B:1052:LEU:CD1	2.16	0.74
2:B:991:VAL:CG2	2:B:1053:TYR:HE2	2.01	0.73
3:C:3:LEU:HD12	3:C:123:LYS:HG3	1.69	0.73
1:A:626:TYR:HB2	1:A:647:ILE:HB	1.71	0.72
2:B:1057:ASP:N	2:B:1060:PRO:HG3	2.04	0.72
2:B:991:VAL:HG22	2:B:1053:TYR:HE2	1.55	0.72
1:A:87:PHE:HE1	1:A:478:ALA:O	1.73	0.71
2:B:991:VAL:HG22	2:B:1053:TYR:CE2	2.26	0.71
1:A:30:GLU:HB3	1:A:33:ARG:HE	1.56	0.70
2:B:1057:ASP:C	2:B:1060:PRO:HD3	2.11	0.70
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.74	0.69
2:B:991:VAL:CG2	2:B:1053:TYR:CE2	2.75	0.69
2:B:1064:ASN:N	2:B:1064:ASN:OD1	2.21	0.69
2:B:1069:MET:HA	2:B:1069:MET:HE2	1.75	0.69
2:B:1002:GLN:NE2	2:B:1012:GLN:O	2.27	0.66
1:A:259:ARG:NH2	1:A:308:THR:O	2.29	0.65
1:A:87:PHE:CE1	1:A:478:ALA:O	2.49	0.65
2:B:1052:LEU:C	2:B:1052:LEU:HD23	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:993:MET:HB3	2:B:1053:TYR:CE1	2.31	0.64
1:A:759:LEU:CA	1:A:762:SER:OG	2.45	0.64
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.25	0.63
2:B:476:GLU:OE1	2:B:479:ARG:NH1	2.31	0.63
1:A:647:ILE:HG21	1:A:688:PRO:HG3	1.81	0.63
2:B:551:SER:OG	2:B:611:GLU:OE1	2.16	0.62
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.82	0.62
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.82	0.62
3:C:4:LEU:HB3	3:C:74:LEU:HB3	1.82	0.62
3:C:51:ARG:HG2	3:C:64:ILE:HG22	1.82	0.62
2:B:1039:ILE:HD13	2:B:1052:LEU:HD13	1.83	0.61
2:B:1054:VAL:O	2:B:1054:VAL:HG12	2.01	0.60
2:B:1057:ASP:HB3	2:B:1060:PRO:HD3	1.84	0.60
2:B:1078:LEU:HD22	2:B:1082:GLU:HB3	1.83	0.60
2:B:497:MET:HG2	2:B:816:ARG:HG3	1.84	0.60
2:B:779:VAL:HG21	2:B:807:LEU:HD21	1.83	0.59
2:B:631:GLY:HA2	2:B:685:VAL:HG22	1.85	0.59
2:B:872:ILE:HD12	2:B:1090:GLN:HB2	1.84	0.59
2:B:497:MET:HE3	3:C:109:PRO:HB2	1.84	0.59
3:C:44:LEU:HD13	3:C:65:ILE:HD11	1.86	0.58
1:A:426:LEU:HD12	1:A:445:GLN:HG2	1.86	0.57
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.86	0.57
2:B:958:LEU:HA	2:B:964:THR:HA	1.86	0.57
1:A:661:GLY:O	1:A:665:ALA:N	2.38	0.56
2:B:359:MET:SD	2:B:1080:TYR:OH	2.58	0.56
2:B:808:LEU:HB2	4:D:4:ILE:HD13	1.88	0.56
2:B:956:GLY:HA3	2:B:965:ILE:O	2.06	0.55
1:A:123:ARG:HD2	1:A:492:ARG:HE	1.71	0.55
1:A:759:LEU:C	1:A:762:SER:OG	2.44	0.55
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.88	0.55
3:C:102:LYS:HE2	3:C:112:PHE:HE1	1.71	0.55
1:A:25:PRO:HG2	1:A:463:VAL:HG21	1.89	0.55
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.89	0.55
2:B:1069:MET:HA	2:B:1069:MET:CE	2.36	0.55
2:B:1074:THR:HG23	2:B:1076:SER:H	1.72	0.54
2:B:416:ASP:OD1	2:B:742:LYS:NZ	2.40	0.54
2:B:1057:ASP:C	2:B:1060:PRO:CD	2.73	0.54
1:A:30:GLU:HB3	1:A:33:ARG:NE	2.22	0.54
2:B:1059:SER:N	2:B:1060:PRO:CD	2.70	0.54
3:C:54:LEU:O	3:C:61:PHE:N	2.39	0.53
1:A:370:TYR:HE2	1:A:389:VAL:HG13	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1059:SER:N	2:B:1060:PRO:HD3	2.24	0.53
1:A:22:ASN:HB2	1:A:516:SER:HB2	1.92	0.52
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.92	0.52
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.92	0.52
1:A:143:ASP:OD1	1:A:376:SER:OG	2.21	0.51
2:B:993:MET:CB	2:B:1053:TYR:CE1	2.90	0.51
2:B:991:VAL:HG21	2:B:1053:TYR:CE2	2.46	0.51
2:B:447:GLN:HG2	2:B:447:GLN:O	2.09	0.51
1:A:312:SER:H	1:A:315:ASP:HB2	1.74	0.51
1:A:500:ALA:O	1:A:501:ARG:NH1	2.38	0.51
1:A:647:ILE:HD13	1:A:660:HIS:HA	1.93	0.51
2:B:1057:ASP:CB	2:B:1060:PRO:HD3	2.40	0.51
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.46	0.51
2:B:966:PRO:HG2	2:B:1038:PHE:HB2	1.92	0.50
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.94	0.50
3:C:113:ILE:O	3:C:116:ASP:HB2	2.11	0.50
2:B:1083:PHE:O	2:B:1087:ILE:HG12	2.10	0.50
1:A:410:THR:HB	1:A:414:ILE:HB	1.94	0.49
2:B:1019:GLN:HB3	2:B:1020:PRO:CD	2.34	0.49
1:A:249:ARG:HH12	3:C:130:ARG:HB3	1.76	0.49
2:B:1058:GLU:OE2	2:B:1058:GLU:HA	2.11	0.49
1:A:541:ASP:HB3	1:A:544:ARG:HG3	1.94	0.48
1:A:714:GLN:H	1:A:714:GLN:HG2	1.48	0.48
2:B:853:ASP:O	2:B:857:THR:HB	2.14	0.48
3:C:54:LEU:HD23	3:C:151:ALA:HB3	1.94	0.48
2:B:1014:TYR:C	2:B:1014:TYR:CD1	2.85	0.48
1:A:107:PRO:HG2	1:A:110:LEU:HD12	1.95	0.48
1:A:193:LYS:NZ	2:B:572:ASP:OD2	2.33	0.48
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.96	0.48
2:B:1011:VAL:HG13	2:B:1016:SER:HB2	1.94	0.48
1:A:384:GLN:O	1:A:388:ARG:HG3	2.13	0.47
1:A:36:VAL:HG11	1:A:522:ALA:HB1	1.96	0.47
2:B:991:VAL:HG21	2:B:1053:TYR:HE2	1.75	0.47
2:B:1021:MET:HB3	2:B:1054:VAL:HB	1.97	0.47
1:A:62:SER:O	1:A:62:SER:OG	2.27	0.47
2:B:360:LEU:HD12	2:B:361:PRO:HD2	1.95	0.47
2:B:496:TYR:O	2:B:816:ARG:NH1	2.46	0.47
2:B:411:LEU:HD12	2:B:413:PRO:HD3	1.96	0.47
2:B:1046:ARG:HD2	2:B:1050:PRO:HG3	1.95	0.47
1:A:30:GLU:HB3	1:A:33:ARG:HB3	1.97	0.47
1:A:366:LEU:HD22	1:A:424:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:973:LEU:HB3	2:B:1069:MET:HE2	1.97	0.47
2:B:666:MET:HB3	2:B:856:MET:CE	2.45	0.47
1:A:368:GLY:HA3	1:A:450:GLY:O	2.15	0.46
1:A:722:VAL:HG22	1:A:723:ASN:H	1.81	0.46
1:A:48:ARG:O	1:A:50:ASP:N	2.47	0.46
1:A:185:LYS:HB3	2:B:567:MET:HB3	1.97	0.46
2:B:958:LEU:HB3	2:B:964:THR:OG1	2.15	0.46
1:A:311:ARG:O	1:A:354:GLN:NE2	2.48	0.46
3:C:7:ILE:HD12	3:C:71:TYR:HD2	1.80	0.46
3:C:7:ILE:HD12	3:C:71:TYR:CD2	2.51	0.46
3:C:35:SER:O	3:C:39:GLN:HG2	2.16	0.46
2:B:385:LEU:HD21	2:B:417:LEU:HD21	1.97	0.46
3:C:80:PRO:HB2	3:C:83:LEU:HG	1.97	0.46
2:B:1055:ILE:O	2:B:1060:PRO:HG3	2.16	0.46
1:A:475:GLY:HA2	1:A:503:TRP:HD1	1.80	0.46
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.98	0.46
2:B:989:GLY:O	2:B:1046:ARG:NH1	2.49	0.45
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.50	0.45
1:A:664:ILE:HG23	1:A:681:PHE:CZ	2.51	0.45
3:C:3:LEU:HG	3:C:127:ILE:HD12	1.98	0.45
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.98	0.45
1:A:194:ASP:OD1	1:A:195:LEU:N	2.49	0.45
2:B:556:TYR:HA	2:B:566:GLN:O	2.16	0.45
1:A:73:LEU:HD13	1:A:478:ALA:HB2	1.98	0.45
1:A:656:ILE:HG21	1:A:692:ALA:HB1	1.99	0.45
2:B:428:ILE:HG22	2:B:430:ARG:HG3	1.99	0.44
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.98	0.44
1:A:645:ASP:HA	1:A:664:ILE:HG12	1.99	0.44
3:C:120:GLN:HA	3:C:123:LYS:HB3	1.98	0.44
3:C:155:GLU:H	3:C:155:GLU:HG2	1.49	0.44
1:A:311:ARG:HD3	1:A:324:VAL:HG22	2.00	0.44
1:A:528:ARG:NH2	1:A:610:GLN:O	2.50	0.44
2:B:1024:LEU:HB3	2:B:1025:PRO:HD2	1.99	0.44
1:A:637:LEU:HD23	1:A:637:LEU:HA	1.78	0.44
2:B:957:ALA:C	2:B:959:ASN:H	2.22	0.43
2:B:998:LYS:HA	2:B:1014:TYR:CE2	2.52	0.43
1:A:349:ALA:HB1	1:A:355:THR:HG21	2.00	0.43
2:B:677:ALA:HB2	2:B:705:ILE:HA	2.00	0.43
1:A:47:GLU:HG3	1:A:453:PRO:HB3	2.00	0.43
2:B:443:SER:HB2	2:B:451:LYS:HB3	2.00	0.43
2:B:1049:PHE:C	2:B:1049:PHE:CD1	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:LEU:HD23	1:A:543:LEU:HA	1.82	0.43
2:B:394:PRO:HG2	2:B:400:LEU:HD13	2.01	0.43
3:C:99:HIS:O	3:C:103:VAL:HG23	2.18	0.43
2:B:1052:LEU:C	2:B:1052:LEU:CD2	2.86	0.43
1:A:315:ASP:OD1	1:A:318:LYS:NZ	2.51	0.43
2:B:549:PHE:CD1	2:B:549:PHE:N	2.87	0.43
2:B:555:PHE:HZ	2:B:622:ALA:HB1	1.84	0.43
3:C:73:VAL:HB	3:C:88:LEU:HD21	2.00	0.43
2:B:958:LEU:H	2:B:958:LEU:HG	1.54	0.42
2:B:681:SER:HA	2:B:777:PRO:HG3	2.01	0.42
2:B:985:LEU:HD11	2:B:992:LEU:HB3	2.01	0.42
2:B:992:LEU:O	2:B:1052:LEU:HA	2.19	0.42
2:B:462:PRO:O	2:B:464:GLU:N	2.46	0.42
3:C:3:LEU:HD23	3:C:3:LEU:HA	1.82	0.42
3:C:113:ILE:H	3:C:113:ILE:HG13	1.52	0.42
2:B:573:ILE:HD13	2:B:573:ILE:HA	1.86	0.42
1:A:48:ARG:CZ	1:A:51:LEU:HD11	2.49	0.42
1:A:14:ARG:O	1:A:48:ARG:NH1	2.53	0.42
1:A:358:LEU:HD22	1:A:597:PRO:HB3	2.02	0.42
2:B:780:ASN:ND2	2:B:783:ALA:HB2	2.34	0.42
1:A:16:GLY:HA2	1:A:46:LYS:HD3	2.00	0.42
1:A:381:LEU:HD12	1:A:702:MET:HE2	2.01	0.42
1:A:682:ARG:HD3	1:A:682:ARG:HA	1.81	0.42
2:B:620:LEU:HD22	2:B:634:MET:HE3	2.02	0.42
1:A:531:ILE:HB	1:A:608:MET:HE1	2.02	0.42
2:B:522:LEU:HD23	2:B:603:PRO:HA	2.02	0.42
1:A:569:ARG:NH1	6:A:902:HOH:O	2.32	0.41
1:A:623:LEU:HD11	1:A:648:LEU:HB3	2.01	0.41
2:B:710:ALA:HB3	2:B:777:PRO:HD2	2.02	0.41
2:B:1055:ILE:O	2:B:1060:PRO:CB	2.67	0.41
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.55	0.41
1:A:664:ILE:HG23	1:A:681:PHE:HZ	1.86	0.41
2:B:1069:MET:CE	2:B:1069:MET:CA	2.98	0.41
1:A:14:ARG:HG3	1:A:48:ARG:HH12	1.86	0.41
2:B:514:HIS:N	2:B:611:GLU:O	2.49	0.41
1:A:264:SER:HB2	1:A:294:ALA:HB2	2.03	0.41
2:B:1014:TYR:CD1	2:B:1014:TYR:O	2.73	0.41
2:B:367:PRO:HA	2:B:368:PRO:HD3	1.97	0.41
2:B:449:ARG:HD3	2:B:460:ASP:HA	2.02	0.41
2:B:1058:GLU:OE2	2:B:1058:GLU:CA	2.69	0.41
1:A:139:MET:HG3	1:A:144:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.55	0.41
2:B:1022:THR:HG22	2:B:1023:ASP:HB2	2.03	0.41
2:B:1017:ILE:HA	2:B:1018:PRO:HD3	1.90	0.40
1:A:73:LEU:CD1	1:A:478:ALA:HB2	2.51	0.40
1:A:345:ILE:O	1:A:369:GLY:HA3	2.21	0.40
2:B:512:VAL:HG22	2:B:549:PHE:O	2.21	0.40
2:B:958:LEU:HD23	2:B:964:THR:HG23	2.04	0.40
1:A:527:ALA:O	1:A:531:ILE:HG12	2.22	0.40
2:B:548:THR:OG1	2:B:554:HIS:HB2	2.22	0.40
2:B:1089:GLN:HE21	2:B:1090:GLN:HE21	1.68	0.40
1:A:113:GLN:H	1:A:113:GLN:HG3	1.52	0.40
2:B:1054:VAL:O	2:B:1054:VAL:CG1	2.68	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	684/764 (90%)	641 (94%)	40 (6%)	3 (0%)	34	57
2	B	720/748 (96%)	688 (96%)	28 (4%)	4 (1%)	25	47
3	C	129/157 (82%)	122 (95%)	6 (5%)	1 (1%)	19	39
4	D	2/6 (33%)	2 (100%)	0	0	100	100
All	All	1535/1675 (92%)	1453 (95%)	74 (5%)	8 (0%)	29	52

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	ARG
1	A	66	CYS
2	B	1020	PRO

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Mol	Chain	Res	Type
2	B	463	GLU
2	B	550	ASP
3	C	153	ILE
1	A	59	VAL
2	B	1059	SER

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	606/666 (91%)	587 (97%)	19 (3%)	40	66
2	B	653/678 (96%)	633 (97%)	20 (3%)	40	66
3	C	118/138 (86%)	113 (96%)	5 (4%)	30	55
4	D	3/6 (50%)	3 (100%)	0	100	100
All	All	1380/1488 (93%)	1336 (97%)	44 (3%)	39	65

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	65	THR
1	A	113	GLN
1	A	116	SER
1	A	181	GLU
1	A	192	THR
1	A	236	ILE
1	A	249	ARG
1	A	451	LEU
1	A	492	ARG
1	A	507	GLN
1	A	512	ASN
1	A	543	LEU
1	A	544	ARG
1	A	569	ARG
1	A	570	PHE

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Mol	Chain	Res	Type
1	A	637	LEU
1	A	713	SER
1	A	714	GLN
2	B	348	LEU
2	B	349	ARG
2	B	386	PHE
2	B	411	LEU
2	B	445	LEU
2	B	597	ASP
2	B	662	LYS
2	B	771	THR
2	B	798	THR
2	B	816	ARG
2	B	857	THR
2	B	882	VAL
2	B	910	LYS
2	B	955	GLU
2	B	958	LEU
2	B	1022	THR
2	B	1023	ASP
2	B	1051	ILE
2	B	1057	ASP
2	B	1064	ASN
3	C	76	GLU
3	C	113	ILE
3	C	152	ASN
3	C	155	GLU
3	C	156	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1089	GLN
3	C	21	GLN
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 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	696/764 (91%)	0.28	28 (4%) 38 31	49, 85, 135, 197	0
2	B	728/748 (97%)	0.13	19 (2%) 56 50	43, 72, 118, 167	0
3	C	135/157 (85%)	0.79	21 (15%) 2 1	64, 109, 166, 222	0
4	D	4/6 (66%)	-0.06	0 100 100	104, 106, 108, 110	0
All	All	1563/1675 (93%)	0.25	68 (4%) 34 27	43, 80, 138, 222	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	424	THR	7.0
1	A	764	ALA	5.7
3	C	150	VAL	4.9
2	B	960	ILE	4.8
3	C	33	TYR	4.8
1	A	681	PHE	4.7
3	C	56	ALA	4.6
3	C	23	ASP	4.6
2	B	959	ASN	4.6
2	B	1019	GLN	4.5
1	A	478	ALA	4.5
3	C	54	LEU	4.4
3	C	148	ILE	4.4
3	C	152	ASN	4.3
1	A	33	ARG	4.2
2	B	423	VAL	4.1
1	A	29	LEU	4.0
3	C	157	LEU	4.0
3	C	149	MET	3.9
1	A	684	LEU	3.9
2	B	1055	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	700	PHE	3.7
1	A	508	THR	3.7
3	C	20	MET	3.7
1	A	679	GLU	3.6
2	B	1053	TYR	3.5
3	C	151	ALA	3.5
3	C	156	VAL	3.4
2	B	445	LEU	3.4
1	A	537	GLU	3.3
1	A	56	TYR	3.2
3	C	57	GLY	3.2
1	A	34	MET	3.1
1	A	682	ARG	3.1
1	A	717	PHE	3.1
2	B	478	HIS	3.0
3	C	87	TYR	3.0
2	B	353	LEU	3.0
3	C	155	GLU	2.9
3	C	78	ALA	2.9
3	C	40	LEU	2.8
1	A	475	GLY	2.7
1	A	24	TRP	2.7
2	B	427	THR	2.6
3	C	153	ILE	2.5
1	A	35	VAL	2.5
2	B	1011	VAL	2.5
3	C	58	ALA	2.5
2	B	446	ASP	2.4
2	B	444	PHE	2.4
1	A	506	ALA	2.4
1	A	94	PHE	2.4
1	A	107	PRO	2.4
1	A	722	VAL	2.3
3	C	3	LEU	2.3
1	A	680	ASN	2.3
1	A	683	HIS	2.2
2	B	477	PRO	2.2
3	C	55	GLU	2.2
2	B	428	ILE	2.1
1	A	79	ARG	2.1
2	B	455	CYS	2.1
1	A	541	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	644	LEU	2.1
2	B	426	SER	2.1
1	A	507	GLN	2.0
1	A	504	ALA	2.0
1	A	760	ALA	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	0.35	0.41	201,201,201,201	0
5	ZN	A	801	1/1	0.93	0.19	119,119,119,119	0

6.5 Other polymers (i)

There are no such residues in this entry.