



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:59 PM UTC

PDB ID : 5VNG / pdb_00005vng
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	:	4-5-2 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

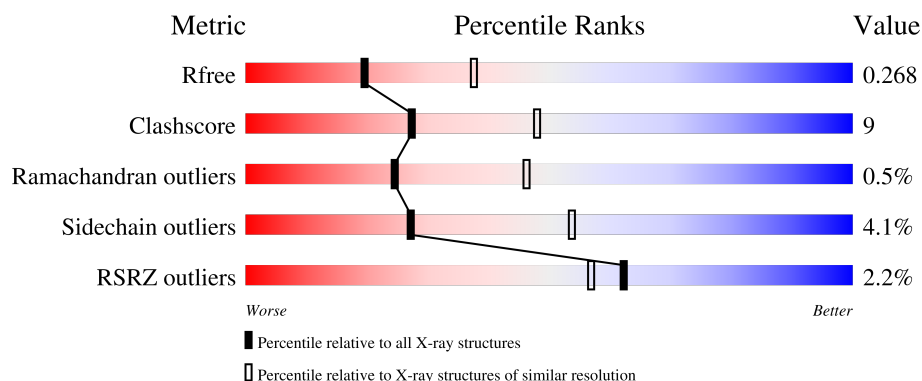
1 Overall quality at a glance

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	 2% 73% 16% 9%
2	B	748	 2% 76% 19% 4%
3	C	157	 3% 61% 24% 12%
4	D	6	 50% 17% 33%

2 Entry composition

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 (CCD ID: ZN) (formula: Zn).

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

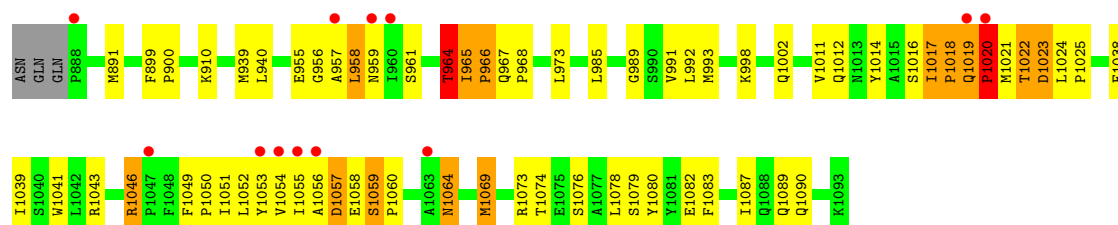
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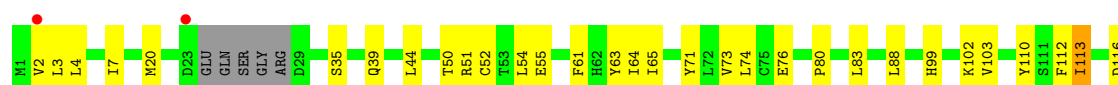
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Zn 1	0	0

- Molecule 6 is water.

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



• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: C-terminal ILE-ILE



4 Data and refinement statistics

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) 91.9 (48.96-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.199 , 0.257 0.218 , 0.268	Depositor DCC
R_{free} test set	2015 reflections (3.21%)	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 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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	0.27	0/5634	0.42	4/7627 (0.1%)
2	B	0.60	10/5851 (0.2%)	0.57	13/7957 (0.2%)
3	C	0.13	0/1103	0.35	0/1485
4	D	0.14	0/27	0.29	0/34
All	All	0.45	10/12615 (0.1%)	0.49	17/17103 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	968	PRO	C-O	-7.19	1.18	1.24
2	B	965	ILE	CA-C	-6.47	1.47	1.53
2	B	553	ILE	C-O	-5.73	1.17	1.24
2	B	964	THR	C-O	-5.59	1.17	1.24
2	B	966	PRO	C-O	-5.49	1.17	1.23
2	B	965	ILE	C-O	-5.40	1.18	1.24
2	B	965	ILE	N-CA	-5.38	1.41	1.46
2	B	968	PRO	CA-C	-5.35	1.48	1.52
2	B	968	PRO	CA-CB	-5.33	1.49	1.54
2	B	859	SER	C-O	-5.15	1.18	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1046	ARG	CA-C-N	9.26	131.42	119.84
2	B	1046	ARG	C-N-CA	9.26	131.42	119.84
2	B	1017	ILE	CA-C-N	8.25	128.27	119.78
2	B	1017	ILE	C-N-CA	8.25	128.27	119.78
2	B	1056	ALA	N-CA-C	-7.93	98.15	109.96
2	B	967	GLN	CA-C-N	7.19	124.83	119.66
2	B	967	GLN	C-N-CA	7.19	124.83	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1046	ARG	N-CA-C	7.17	117.36	108.11
2	B	1019	GLN	CA-C-N	-6.55	111.65	119.84
2	B	1019	GLN	C-N-CA	-6.55	111.65	119.84
1	A	478	ALA	N-CA-C	6.08	118.87	109.07
1	A	116	SER	N-CA-C	-5.74	99.16	108.52
2	B	961	SER	CB-CA-C	-5.55	110.19	116.63
2	B	1020	PRO	N-CA-C	-5.27	101.61	112.47
1	A	184	SER	N-CA-C	5.15	116.93	110.91
2	B	961	SER	N-CA-C	5.09	116.68	108.08
1	A	49	PRO	N-CA-C	-5.02	102.13	112.47

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	85	0
2	B	5728	0	5760	118	0
3	C	1084	0	1082	25	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
6	D	2	0	0	0	0
All	All	12409	0	12330	225	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 9.

All (225) 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:1069:MET:HE2	2:B:1069:MET:HA	1.51	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:1057:ASP:C	2:B:1060:PRO:HD3	2.11	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:497:MET:HE2	2:B:816:ARG:HB2	1.70	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
2:B:666:MET:HB3	2:B:856:MET:HE1	1.72	0.70
1:A:30:GLU:HB3	1:A:33:ARG:HE	1.56	0.70
2:B:1052:LEU:C	2:B:1052:LEU:HD23	2.17	0.69
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:OD1	2:B:1064:ASN:N	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:759:LEU:C	1:A:762:SER:OG	2.44	0.60
2:B:1054:VAL:HG12	2:B:1054:VAL:O	2.01	0.60
2:B:841:GLN:HG2	2:B:939:MET:HE2	1.83	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:1069:MET:HE2	2:B:1069:MET:CA	2.30	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:1057:ASP:C	2:B:1060:PRO:CD	2.73	0.59
1:A:528:ARG:HA	1:A:608:MET:HE1	1.86	0.58
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
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:39:ALA:HB3	1:A:525:LEU:HD13	1.88	0.55
2:B:416:ASP:OD1	2:B:742:LYS:NZ	2.40	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:1074:THR:HG23	2:B:1076:SER:H	1.72	0.54
1:A:30:GLU:HB3	1:A:33:ARG:NE	2.22	0.54
1:A:381:LEU:HA	1:A:702:MET:HE2	1.89	0.54
2:B:1059:SER:N	2:B:1060:PRO:CD	2.70	0.54
2:B:1014:TYR:CD1	2:B:1014:TYR:C	2.85	0.53
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PRO:HD3	1:A:34:MET:HE3	1.91	0.51
2:B:991:VAL:HG21	2:B:1053:TYR:CE2	2.46	0.51
2:B:447:GLN:O	2:B:447:GLN:HG2	2.09	0.51
2:B:550:ASP:CG	2:B:551:SER:H	2.16	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
3:C:99:HIS:HA	3:C:102:LYS:HZ3	1.76	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:607:PHE:HD2	1:A:608:MET:HE2	1.78	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:957:ALA:C	2:B:959:ASN:H	2.22	0.48
1:A:107:PRO:HG2	1:A:110:LEU:HD12	1.95	0.48
2:B:1049:PHE:CD1	2:B:1049:PHE:C	2.91	0.48
2:B:1052:LEU:C	2:B:1052:LEU:CD2	2.86	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
2:B:434:CYS:SG	2:B:436:THR:OG1	2.68	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)
1:A:368:GLY:HA3	1:A:450:GLY:O	2.15	0.46
2:B:1069:MET:HA	2:B:1069:MET:CE	2.36	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
1:A:193:LYS:NZ	2:B:572:ASP:OD2	2.33	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
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.98	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
2:B:446:ASP:C	2:B:448:ARG:H	2.25	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:350:VAL:HG12	2:B:891:MET:HE3	2.00	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:443:SER:HB2	2:B:451:LYS:HB3	2.00	0.43
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
3:C:4:LEU:HD11	3:C:20:MET:HE2	2.01	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:682:ARG:HA	1:A:682:ARG:HD3	1.81	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
1:A:759:LEU:C	1:A:762:SER:HG	2.16	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:973:LEU:HB3	2:B:1069:MET:HE2	2.01	0.41
2:B:359:MET:HE2	2:B:359:MET:HB3	1.93	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:177:GLU:CD	1:A:185:LYS:HE2	2.46	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:1069:MET:CA	2:B:1069:MET:CE	2.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.55	0.41
2:B:634:MET:HE2	2:B:687:VAL:HG22	2.03	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:666:MET:HB3	2:B:856:MET:CE	2.45	0.40
2:B:958:LEU:HD23	2:B:964:THR:HG23	2.04	0.40
1:A:139:MET:HE2	1:A:291:GLY:HA3	2.03	0.40
1:A:435:GLU:CD	1:A:435:GLU:H	2.28	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
1:A:542:VAL:C	1:A:544:ARG:H	2.30	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%)	30	51
2	B	720/748 (96%)	688 (96%)	28 (4%)	4 (1%)	21	42
3	C	129/157 (82%)	122 (95%)	6 (5%)	1 (1%)	16	34
4	D	2/6 (33%)	2 (100%)	0	0	100	100
All	All	1535/1675 (92%)	1453 (95%)	74 (5%)	8 (0%)	24	46

All (8) Ramachandran outliers are listed below:

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

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%)	584 (96%)	22 (4%)	31	58
2	B	653/678 (96%)	625 (96%)	28 (4%)	26	51
3	C	118/138 (86%)	111 (94%)	7 (6%)	18	38
4	D	3/6 (50%)	3 (100%)	0	100	100
All	All	1380/1488 (93%)	1323 (96%)	57 (4%)	27	54

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	65	THR
1	A	76	VAL
1	A	113	GLN
1	A	116	SER
1	A	123	ARG
1	A	181	GLU
1	A	192	THR
1	A	236	ILE
1	A	249	ARG
1	A	305	GLU
1	A	311	ARG

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Mol	Chain	Res	Type
1	A	435	GLU
1	A	451	LEU
1	A	543	LEU
1	A	544	ARG
1	A	562	LYS
1	A	569	ARG
1	A	570	PHE
1	A	637	LEU
1	A	713	SER
1	A	714	GLN
2	B	348	LEU
2	B	349	ARG
2	B	411	LEU
2	B	423	VAL
2	B	445	LEU
2	B	483	VAL
2	B	602	LEU
2	B	652	ARG
2	B	662	LYS
2	B	713	VAL
2	B	771	THR
2	B	787	VAL
2	B	798	THR
2	B	857	THR
2	B	882	VAL
2	B	910	LYS
2	B	940	LEU
2	B	955	GLU
2	B	958	LEU
2	B	964	THR
2	B	1018	PRO
2	B	1022	THR
2	B	1023	ASP
2	B	1043	ARG
2	B	1051	ILE
2	B	1057	ASP
2	B	1064	ASN
2	B	1069	MET
3	C	2	VAL
3	C	50	THR
3	C	76	GLU
3	C	113	ILE

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Mol	Chain	Res	Type
3	C	127	ILE
3	C	155	GLU
3	C	156	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	579	GLN
1	A	614	GLN
1	A	620	GLN
1	A	710	HIS
2	B	523	ASN
2	B	638	GLN
2	B	765	ASN
2	B	778	ASN
2	B	967	GLN
2	B	1007	GLN
2	B	1045	GLN
2	B	1090	GLN
3	C	21	GLN
3	C	34	GLN
3	C	67	GLN
3	C	152	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	696/764 (91%)	0.13	14 (2%) 65 60	49, 85, 135, 197	0
2	B	728/748 (97%)	-0.07	17 (2%) 61 55	43, 72, 118, 167	0
3	C	135/157 (85%)	0.17	4 (2%) 52 47	64, 109, 166, 222	0
4	D	4/6 (66%)	0.61	0 100 100	104, 106, 108, 110	0
All	All	1563/1675 (93%)	0.04	35 (2%) 62 57	43, 80, 138, 222	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1053	TYR	4.6
1	A	478	ALA	4.2
2	B	1019	GLN	4.1
1	A	700	PHE	4.0
1	A	681	PHE	3.7
1	A	506	ALA	3.3
1	A	58	PRO	3.2
1	A	165	GLY	3.2
2	B	960	ILE	3.2
1	A	34	MET	3.2
1	A	764	ALA	2.9
1	A	31	ALA	2.7
1	A	464	VAL	2.7
2	B	959	ASN	2.6
2	B	455	CYS	2.5
2	B	1063	ALA	2.5
1	A	33	ARG	2.4
2	B	347	GLY	2.4
2	B	1020	PRO	2.4
2	B	957	ALA	2.4
2	B	1056	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	148	ILE	2.3
3	C	23	ASP	2.3
2	B	1055	ILE	2.3
2	B	888	PRO	2.3
2	B	423	VAL	2.3
2	B	882	VAL	2.2
1	A	283	GLY	2.2
1	A	652	THR	2.2
2	B	1047	PRO	2.2
2	B	424	THR	2.2
1	A	226	SER	2.2
3	C	2	VAL	2.1
3	C	156	VAL	2.1
2	B	1054	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	B	1101	1/1	0.83	0.20	201,201,201,201	0
5	ZN	A	801	1/1	0.97	0.09	119,119,119,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.