



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 12:37 PM JST

PDB ID : 9UVF / pdb_00009uvf
Title : Crystal structure of Sec23a/24a/22b bound to mouse STING LI motif
Authors : Ma, W.F.
Deposited on : 2025-05-10
Resolution : 3.15 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

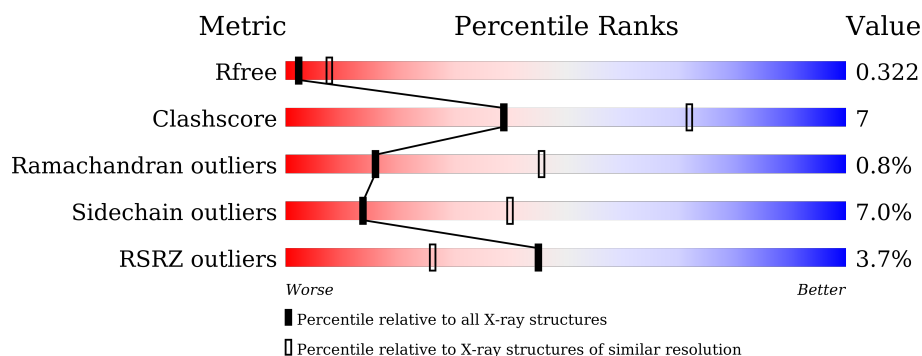
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	765	<div> <div>0%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 8%</div> </div> </div>
2	B	748	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• •</div> </div> </div>
3	C	157	<div> <div>15%</div> <div> <div></div> <div>62%</div> <div>21%</div> <div>• 15%</div> </div> </div>
4	E	5	<div> <div></div> <div> <div></div> <div>80%</div> <div>20%</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12401 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	706	Total	C	N	O	S	0	0	0
			5591	3565	958	1028	40			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	732	Total	C	N	O	S	0	0	0
			5703	3643	957	1071	32			

- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	133	Total	C	N	O	S	0	0	0
			1062	683	171	201	7			

- Molecule 4 is a protein called ARG-THR-ASP-LEU-ILE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total	C	N	O	0	0	0
			43	26	8	9			

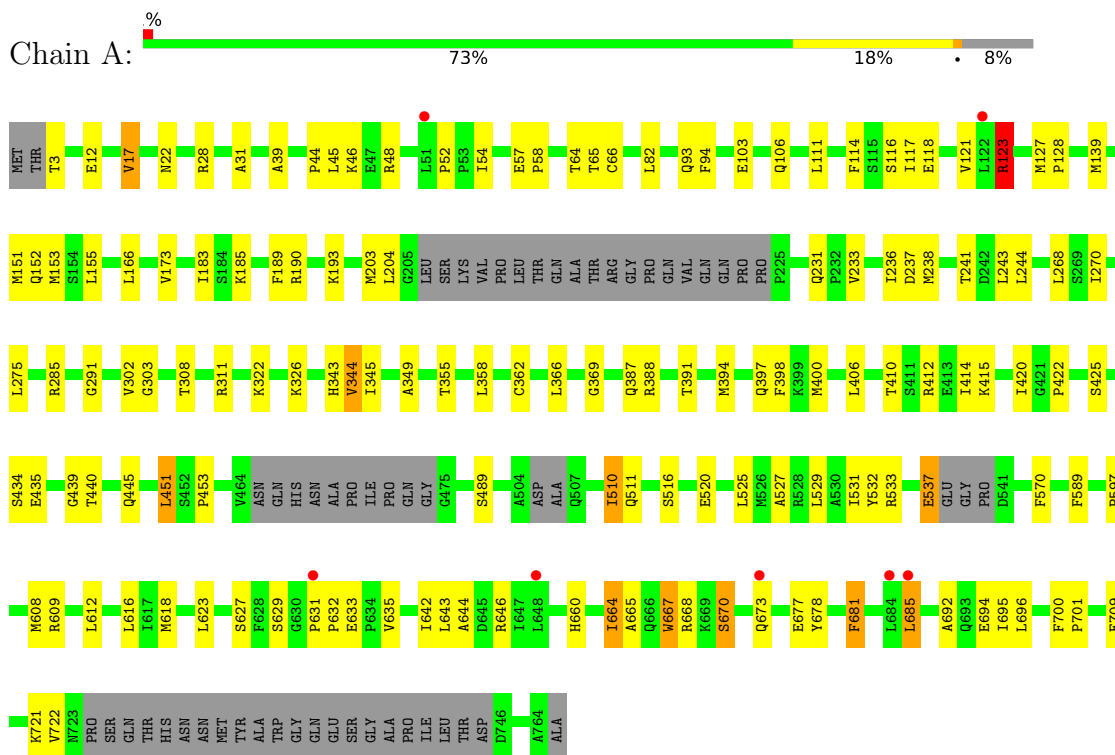
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

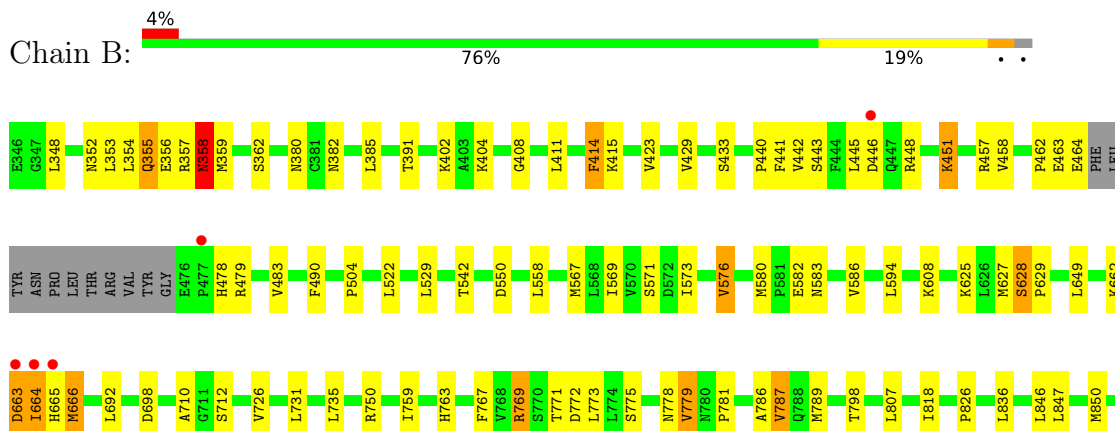
3 Residue-property plots

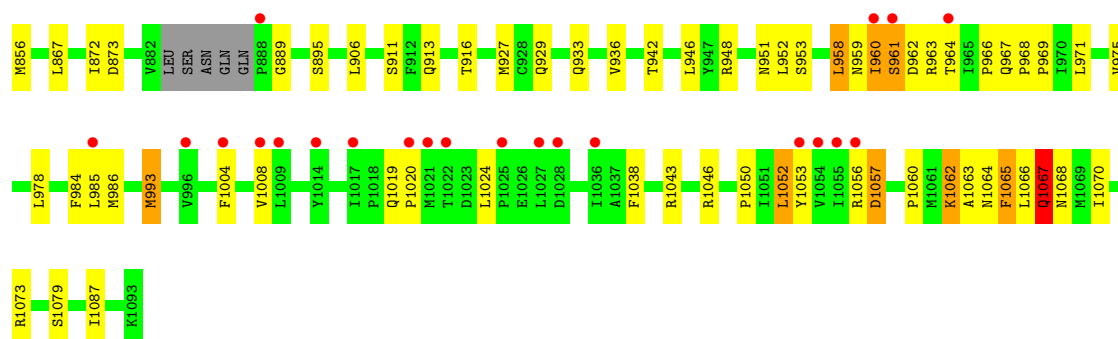
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

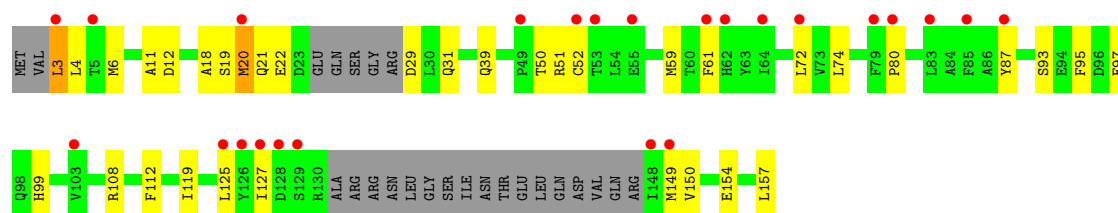


• Molecule 2: Protein transport protein Sec24A

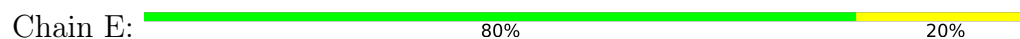




• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: ARG-THR-ASP-LEU-ILE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.29Å 95.50Å 130.78Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	48.99 – 3.15 48.99 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.99-3.15) 98.6 (48.99-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.265 , 0.320 0.266 , 0.322	Depositor DCC
R_{free} test set	2002 reflections (6.31%)	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12401	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 4.20% 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

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	0.13	0/5721	0.33	0/7746
2	B	0.23	0/5826	0.43	3/7934 (0.0%)
3	C	0.11	0/1081	0.32	0/1458
4	E	0.15	0/42	0.45	0/54
All	All	0.18	0/12670	0.38	3/17192 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1065	PHE	N-CA-CB	-5.36	101.49	110.39
2	B	958	LEU	N-CA-C	-5.15	107.65	114.04
2	B	1065	PHE	CA-CB-CG	5.10	118.90	113.80

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	5591	0	5521	75	0
2	B	5703	0	5687	77	0
3	C	1062	0	1048	17	0
4	E	43	0	45	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	12401	0	12301	167	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 (167) 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:1056:ARG:H	2:B:1060:PRO:HB3	1.50	0.75
1:A:48:ARG:HH21	1:A:116:SER:HB2	1.51	0.74
1:A:668:ARG:HD2	1:A:685:LEU:HD11	1.71	0.72
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.70	0.72
2:B:906:LEU:HD12	2:B:942:THR:HG21	1.73	0.68
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.77	0.66
1:A:410:THR:HB	1:A:414:ILE:HB	1.78	0.66
2:B:958:LEU:HG	2:B:964:THR:HG22	1.78	0.65
2:B:1024:LEU:HG	2:B:1052:LEU:HD21	1.80	0.64
3:C:50:THR:HG23	3:C:51:ARG:HG2	1.80	0.64
2:B:348:LEU:HD13	2:B:836:LEU:HD21	1.80	0.63
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.80	0.63
1:A:412:ARG:H	1:A:412:ARG:HD3	1.63	0.62
2:B:948:ARG:HG3	2:B:971:LEU:HD11	1.82	0.62
1:A:203:MET:HB3	2:B:571:SER:HB2	1.80	0.61
1:A:631:PRO:HB2	1:A:632:PRO:HD3	1.81	0.61
2:B:952:LEU:HD21	2:B:968:PRO:HB3	1.83	0.59
1:A:22:ASN:HB2	1:A:516:SER:HB2	1.84	0.59
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.83	0.59
2:B:847:LEU:HA	2:B:850:MET:HE3	1.85	0.59
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.85	0.59
1:A:153:MET:HE1	1:A:387:GLN:HB3	1.86	0.58
1:A:28:ARG:H	1:A:28:ARG:HD3	1.69	0.58
2:B:978:LEU:HD23	2:B:984:PHE:HD2	1.68	0.58
1:A:152:GLN:HE22	1:A:241:THR:HB	1.68	0.57
2:B:779:VAL:HG21	2:B:807:LEU:HD21	1.86	0.57
1:A:397:GLN:HG2	1:A:489:SER:HB3	1.86	0.57
2:B:664:ILE:O	2:B:665:HIS:C	2.48	0.56
2:B:961:SER:C	2:B:963:ARG:H	2.14	0.56
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.88	0.55
2:B:352:ASN:HD21	2:B:889:GLY:HA3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:440:PRO:HA	2:B:483:VAL:HG13	1.89	0.55
2:B:567:MET:HE2	2:B:569:ILE:HD11	1.88	0.54
1:A:520:GLU:HB3	1:A:616:LEU:HD11	1.87	0.54
2:B:504:PRO:HG2	2:B:542:THR:HA	1.89	0.54
1:A:665:ALA:HB2	1:A:709:GLU:HB2	1.89	0.54
2:B:993:MET:HG2	2:B:1053:TYR:CZ	2.42	0.54
1:A:127:MET:HG3	1:A:128:PRO:HD2	1.91	0.53
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.91	0.53
1:A:388:ARG:HA	1:A:391:THR:HG23	1.89	0.53
1:A:527:ALA:O	1:A:531:ILE:HG12	2.08	0.53
1:A:667:TRP:HA	1:A:670:SER:HB3	1.91	0.53
1:A:358:LEU:HD22	1:A:597:PRO:HB3	1.89	0.53
2:B:769:ARG:HG3	2:B:773:LEU:O	2.09	0.53
2:B:929:GLN:O	2:B:933:GLN:HB2	2.08	0.53
1:A:660:HIS:HB2	1:A:709:GLU:HB3	1.91	0.53
3:C:39:GLN:HB2	3:C:157:LEU:HD11	1.90	0.53
2:B:382:ASN:HB2	2:B:385:LEU:HD12	1.90	0.52
1:A:660:HIS:HB3	1:A:664:ILE:HG22	1.92	0.52
1:A:173:VAL:HG21	1:A:270:ILE:HD12	1.91	0.52
3:C:18:ALA:HB1	3:C:20:MET:HE3	1.92	0.51
1:A:231:GLN:HB2	1:A:236:ILE:HG12	1.93	0.51
3:C:93:SER:O	3:C:97:GLU:HB2	2.09	0.51
1:A:692:ALA:O	1:A:696:LEU:HB2	2.10	0.51
1:A:233:VAL:O	1:A:237:ASP:HB3	2.10	0.51
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.92	0.51
1:A:151:MET:HE3	1:A:244:LEU:HD22	1.93	0.51
2:B:1060:PRO:HG2	2:B:1063:ALA:H	1.76	0.50
2:B:946:LEU:HD23	2:B:971:LEU:HB2	1.93	0.50
2:B:362:SER:HB2	2:B:969:PRO:HB3	1.91	0.50
2:B:1060:PRO:O	2:B:1062:LYS:N	2.44	0.50
2:B:966:PRO:HD2	2:B:1038:PHE:HB2	1.93	0.50
2:B:446:ASP:C	2:B:448:ARG:H	2.19	0.50
2:B:665:HIS:O	2:B:666:MET:C	2.54	0.50
3:C:31:GLN:H	3:C:31:GLN:CD	2.20	0.49
3:C:61:PHE:HB3	3:C:72:LEU:HD11	1.93	0.49
3:C:61:PHE:HD2	3:C:72:LEU:HD11	1.78	0.48
1:A:644:ALA:O	1:A:664:ILE:HD13	2.14	0.48
2:B:978:LEU:HA	2:B:984:PHE:HE2	1.78	0.48
1:A:45:LEU:HB2	1:A:453:PRO:HA	1.96	0.48
1:A:152:GLN:HA	1:A:155:LEU:HD12	1.96	0.48
1:A:52:PRO:HD2	1:A:114:PHE:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:TYR:OH	3:C:119:ILE:HG23	2.14	0.48
2:B:1066:LEU:O	2:B:1068:ASN:N	2.46	0.48
1:A:678:TYR:HB3	1:A:681:PHE:HB2	1.96	0.48
2:B:1066:LEU:O	2:B:1067:GLN:C	2.56	0.47
1:A:398:PHE:HB3	1:A:400:MET:HG2	1.95	0.47
2:B:710:ALA:HB3	2:B:778:ASN:H	1.79	0.47
2:B:380:ASN:HA	2:B:441:PHE:HZ	1.79	0.47
2:B:414:PHE:HB3	2:B:781:PRO:HA	1.96	0.47
2:B:490:PHE:HB2	2:B:818:ILE:HB	1.95	0.47
2:B:1060:PRO:HG2	2:B:1063:ALA:N	2.29	0.47
1:A:415:LYS:HB3	1:A:434:SER:HB2	1.96	0.47
2:B:354:LEU:HB2	2:B:355:GLN:HE21	1.80	0.47
2:B:911:SER:HB2	2:B:927:MET:HG2	1.97	0.47
3:C:4:LEU:HG	3:C:74:LEU:HB3	1.95	0.47
2:B:750:ARG:HG3	2:B:772:ASP:O	2.15	0.47
1:A:121:VAL:HG12	1:A:123:ARG:HD2	1.97	0.46
2:B:961:SER:C	2:B:963:ARG:N	2.73	0.46
1:A:422:PRO:HG3	1:A:609:ARG:HG2	1.98	0.46
2:B:356:GLU:O	2:B:358:ASN:N	2.48	0.46
1:A:190:ARG:HG3	1:A:193:LYS:HE2	1.97	0.46
2:B:443:SER:HB2	2:B:451:LYS:HB3	1.98	0.46
2:B:913:GLN:HG3	2:B:916:THR:HG21	1.98	0.46
1:A:189:PHE:HZ	1:A:204:LEU:HD21	1.81	0.46
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.51	0.46
1:A:311:ARG:NH2	1:A:358:LEU:HB3	2.31	0.45
2:B:576:VAL:HG23	2:B:625:LYS:NZ	2.31	0.45
3:C:3:LEU:HB3	3:C:4:LEU:H	1.57	0.45
2:B:769:ARG:O	2:B:773:LEU:HB3	2.16	0.45
2:B:959:ASN:C	2:B:961:SER:N	2.74	0.45
1:A:322:LYS:HE2	1:A:322:LYS:HB2	1.75	0.45
1:A:510:ILE:H	1:A:510:ILE:HG12	1.52	0.45
1:A:285:ARG:HA	1:A:344:VAL:HG12	1.99	0.45
2:B:961:SER:O	2:B:963:ARG:N	2.43	0.45
2:B:582:GLU:HG2	2:B:583:ASN:N	2.32	0.45
3:C:19:SER:HB3	3:C:119:ILE:HG21	1.99	0.45
1:A:139:MET:HE2	1:A:291:GLY:HA3	1.99	0.44
3:C:29:ASP:HB2	3:C:31:GLN:OE1	2.18	0.44
3:C:95:PHE:CE1	3:C:99:HIS:HB2	2.52	0.44
1:A:589:PHE:HZ	1:A:618:MET:HB3	1.83	0.44
2:B:872:ILE:HD13	2:B:1087:ILE:HG23	2.00	0.44
2:B:558:LEU:HD12	2:B:594:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:608:LYS:HB3	2:B:608:LYS:HE3	1.85	0.43
1:A:39:ALA:HB3	1:A:525:LEU:HD13	2.00	0.43
1:A:529:LEU:O	1:A:533:ARG:HG2	2.18	0.43
3:C:59:MET:HB3	3:C:74:LEU:HD11	2.00	0.43
2:B:353:LEU:HD22	2:B:359:MET:HE2	2.01	0.43
2:B:1043:ARG:HG2	2:B:1050:PRO:HD2	2.00	0.43
2:B:959:ASN:O	2:B:961:SER:N	2.52	0.43
1:A:166:LEU:HD23	1:A:243:LEU:HD13	2.01	0.43
1:A:394:MET:H	1:A:394:MET:HG3	1.51	0.43
1:A:694:GLU:OE2	1:A:695:ILE:HG13	2.18	0.43
3:C:6:MET:HE2	3:C:6:MET:HB3	1.83	0.43
1:A:302:VAL:HG22	1:A:303:GLY:H	1.83	0.43
1:A:435:GLU:CD	1:A:435:GLU:H	2.26	0.43
2:B:628:SER:N	2:B:629:PRO:HD2	2.33	0.43
3:C:99:HIS:HB3	3:C:112:PHE:CE1	2.54	0.43
3:C:52:CYS:SG	3:C:149:MET:HE2	2.59	0.43
1:A:57:GLU:HG3	1:A:58:PRO:HD2	2.00	0.42
1:A:700:PHE:HB3	1:A:701:PRO:HD3	2.01	0.42
2:B:985:LEU:HD23	2:B:986:MET:N	2.35	0.42
1:A:12:GLU:O	1:A:46:LYS:HD3	2.20	0.42
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	2.02	0.42
1:A:667:TRP:C	1:A:667:TRP:HE3	2.28	0.42
2:B:404:LYS:HG3	2:B:873:ASP:HB3	2.01	0.42
2:B:759:ILE:HG23	2:B:787:VAL:HG13	2.01	0.42
1:A:345:ILE:O	1:A:369:GLY:HA3	2.19	0.42
1:A:533:ARG:O	1:A:537:GLU:HG2	2.19	0.42
2:B:408:GLY:HA3	2:B:846:LEU:HD22	2.01	0.42
2:B:975:VAL:HG23	2:B:978:LEU:HD12	2.00	0.42
1:A:12:GLU:HA	1:A:17:VAL:H	1.85	0.41
1:A:106:GLN:HB2	1:A:111:LEU:HD21	2.02	0.41
2:B:767:PHE:HB3	2:B:775:SER:HB3	2.01	0.41
2:B:1062:LYS:C	2:B:1064:ASN:N	2.77	0.41
1:A:425:SER:HB2	1:A:440:THR:HG22	2.02	0.41
1:A:93:GLN:HG2	1:A:94:PHE:N	2.34	0.41
2:B:959:ASN:O	2:B:960:ILE:C	2.62	0.41
1:A:406:LEU:O	1:A:445:GLN:HA	2.20	0.41
2:B:1004:PHE:O	2:B:1008:VAL:HG22	2.21	0.41
1:A:28:ARG:HA	1:A:31:ALA:HB3	2.02	0.41
2:B:580:MET:HE3	2:B:583:ASN:HB2	2.02	0.41
2:B:731:LEU:O	2:B:735:LEU:HB2	2.21	0.41
1:A:643:LEU:HD23	1:A:643:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.79	0.41
2:B:663:ASP:O	2:B:666:MET:N	2.54	0.41
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.56	0.41
1:A:275:LEU:HB3	1:A:343:HIS:CE1	2.56	0.40
2:B:867:LEU:HD23	2:B:867:LEU:HA	1.87	0.40
1:A:44:PRO:O	1:A:45:LEU:HD23	2.20	0.40
1:A:185:LYS:HA	2:B:567:MET:HB3	2.03	0.40
1:A:589:PHE:CZ	1:A:618:MET:HB3	2.57	0.40
2:B:958:LEU:O	2:B:959:ASN:C	2.64	0.40
2:B:429:VAL:HG22	2:B:462:PRO:HG2	2.04	0.40
1:A:123:ARG:HE	1:A:123:ARG:HB3	1.34	0.40
2:B:391:THR:O	2:B:826:PRO:HD2	2.21	0.40
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.94	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	694/765 (91%)	650 (94%)	42 (6%)	2 (0%)	36	64
2	B	726/748 (97%)	664 (92%)	53 (7%)	9 (1%)	10	37
3	C	127/157 (81%)	118 (93%)	7 (6%)	2 (2%)	7	32
4	E	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
All	All	1550/1675 (92%)	1434 (92%)	103 (7%)	13 (1%)	16	46

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	357	ARG
2	B	433	SER

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Mol	Chain	Res	Type
2	B	1057	ASP
2	B	358	ASN
2	B	666	MET
2	B	771	THR
2	B	1062	LYS
2	B	1067	GLN
3	C	11	ALA
1	A	629	SER
1	A	123	ARG
2	B	961	SER
3	C	80	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	613/666 (92%)	576 (94%)	37 (6%)	17	45
2	B	646/679 (95%)	597 (92%)	49 (8%)	12	37
3	C	115/138 (83%)	105 (91%)	10 (9%)	9	32
4	E	5/5 (100%)	4 (80%)	1 (20%)	1	6
All	All	1379/1488 (93%)	1282 (93%)	97 (7%)	14	40

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	17	VAL
1	A	64	THR
1	A	65	THR
1	A	66	CYS
1	A	82	LEU
1	A	103	GLU
1	A	118	GLU
1	A	123	ARG
1	A	183	ILE

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Mol	Chain	Res	Type
1	A	238	MET
1	A	268	LEU
1	A	308	THR
1	A	326	LYS
1	A	344	VAL
1	A	362	CYS
1	A	420	ILE
1	A	451	LEU
1	A	510	ILE
1	A	511	GLN
1	A	537	GLU
1	A	570	PHE
1	A	608	MET
1	A	612	LEU
1	A	623	LEU
1	A	633	GLU
1	A	635	VAL
1	A	642	ILE
1	A	664	ILE
1	A	667	TRP
1	A	670	SER
1	A	673	GLN
1	A	677	GLU
1	A	681	PHE
1	A	685	LEU
1	A	721	LYS
1	A	722	VAL
2	B	355	GLN
2	B	358	ASN
2	B	402	LYS
2	B	411	LEU
2	B	414	PHE
2	B	415	LYS
2	B	423	VAL
2	B	442	VAL
2	B	445	LEU
2	B	451	LYS
2	B	457	ARG
2	B	458	VAL
2	B	463	GLU
2	B	464	GLU
2	B	478	HIS

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Mol	Chain	Res	Type
2	B	479	ARG
2	B	522	LEU
2	B	529	LEU
2	B	550	ASP
2	B	573	ILE
2	B	576	VAL
2	B	627	MET
2	B	628	SER
2	B	662	LYS
2	B	663	ASP
2	B	664	ILE
2	B	692	LEU
2	B	712	SER
2	B	726	VAL
2	B	769	ARG
2	B	779	VAL
2	B	787	VAL
2	B	789	MET
2	B	798	THR
2	B	856	MET
2	B	895	SER
2	B	936	VAL
2	B	951	ASN
2	B	953	SER
2	B	960	ILE
2	B	962	ASP
2	B	967	GLN
2	B	993	MET
2	B	1046	ARG
2	B	1052	LEU
2	B	1057	ASP
2	B	1065	PHE
2	B	1067	GLN
2	B	1070	ILE
3	C	3	LEU
3	C	12	ASP
3	C	20	MET
3	C	21	GLN
3	C	22	GLU
3	C	108	ARG
3	C	125	LEU
3	C	127	ILE

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Mol	Chain	Res	Type
3	C	150	VAL
3	C	154	GLU
4	E	203	ILE

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	152	GLN
1	A	227	ASN
1	A	248	GLN
1	A	502	ASN
1	A	555	GLN
1	A	614	GLN
1	A	710	HIS
2	B	352	ASN
2	B	355	GLN
2	B	358	ASN
2	B	515	ASN
2	B	559	GLN
2	B	587	ASN
2	B	778	ASN
2	B	951	ASN
3	C	92	HIS

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	706/765 (92%)	0.21	7 (0%) 79 62	52, 72, 154, 224	0
2	B	732/748 (97%)	0.28	27 (3%) 45 26	30, 71, 167, 224	0
3	C	133/157 (84%)	1.15	24 (18%) 3 2	85, 127, 183, 218	0
4	E	5/5 (100%)	0.56	0 100 100	108, 116, 126, 136	0
All	All	1576/1675 (94%)	0.32	58 (3%) 45 26	30, 73, 168, 224	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	64	ILE	4.3
2	B	663	ASP	3.9
2	B	960	ILE	3.7
3	C	55	GLU	3.6
2	B	1055	ILE	3.6
1	A	648	LEU	3.3
3	C	80	PRO	3.0
3	C	128	ASP	3.0
3	C	129	SER	2.9
2	B	665	HIS	2.8
2	B	1020	PRO	2.8
2	B	1009	LEU	2.8
3	C	126	TYR	2.8
3	C	127	ILE	2.8
2	B	1022	THR	2.8
1	A	122	LEU	2.7
2	B	1027	LEU	2.6
3	C	61	PHE	2.6
2	B	1017	ILE	2.6
2	B	664	ILE	2.6
2	B	1028	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	996	VAL	2.6
3	C	148	ILE	2.5
3	C	87	TYR	2.5
3	C	5	THR	2.5
3	C	52	CYS	2.5
2	B	1053	TYR	2.5
1	A	673	GLN	2.5
2	B	888	PRO	2.4
1	A	685	LEU	2.4
2	B	961	SER	2.4
3	C	53	THR	2.3
3	C	85	PHE	2.3
2	B	1056	ARG	2.3
2	B	1025	PRO	2.3
2	B	1036	ILE	2.3
2	B	985	LEU	2.3
2	B	446	ASP	2.3
3	C	20	MET	2.2
2	B	1004	PHE	2.2
3	C	79	PHE	2.2
1	A	684	LEU	2.2
3	C	125	LEU	2.2
2	B	1014	TYR	2.2
2	B	1054	VAL	2.2
1	A	51	LEU	2.2
3	C	83	LEU	2.2
2	B	1021	MET	2.2
3	C	49	PRO	2.1
3	C	149	MET	2.1
1	A	631	PRO	2.1
2	B	477	PRO	2.1
3	C	3	LEU	2.1
3	C	72	LEU	2.0
3	C	62	HIS	2.0
2	B	964	THR	2.0
2	B	1008	VAL	2.0
3	C	103	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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(\AA^2)	Q<0.9
5	ZN	A	801	1/1	0.95	0.05	87,87,87,87	0
5	ZN	B	1101	1/1	1.00	0.03	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.