



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 12:41 PM JST

PDB ID : 9UVD / pdb_00009uvd
Title : Crystal structure of Sec23a/24a/22b bound to STING pSGME motif
Authors : Ma, W.F.
Deposited on : 2025-05-10
Resolution : 2.98 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

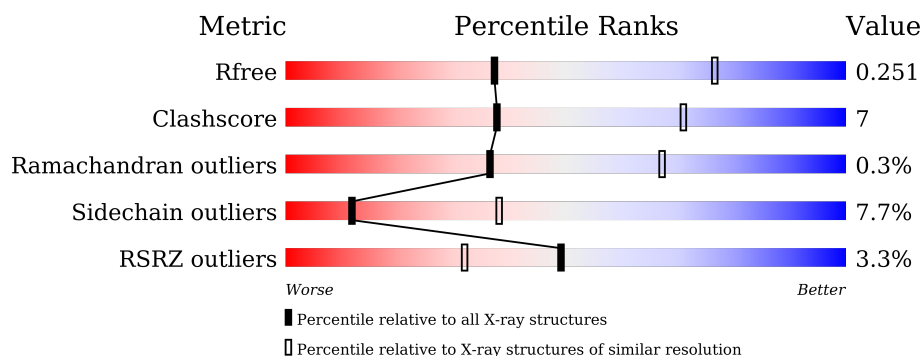
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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>2%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>•</div> <div>8%</div> </div> </div>
2	B	748	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>• •</div> </div> </div>
3	C	157	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>19%</div> <div>•</div> <div>15%</div> </div> </div>
4	D	5	<div> <div></div> <div> <div>20%</div> <div>60%</div> <div>20%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12340 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	704	Total	C	N	O	S	0	0	0
			5551	3545	940	1026	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
			5705	3643	965	1063	34			

- 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
			1046	676	165	197	8			

- Molecule 4 is a protein called ALA-SEP-GLY-MET-GLU.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	5	Total	C	N	O	P	S	0	0	0
			36	18	5	11	1	1			

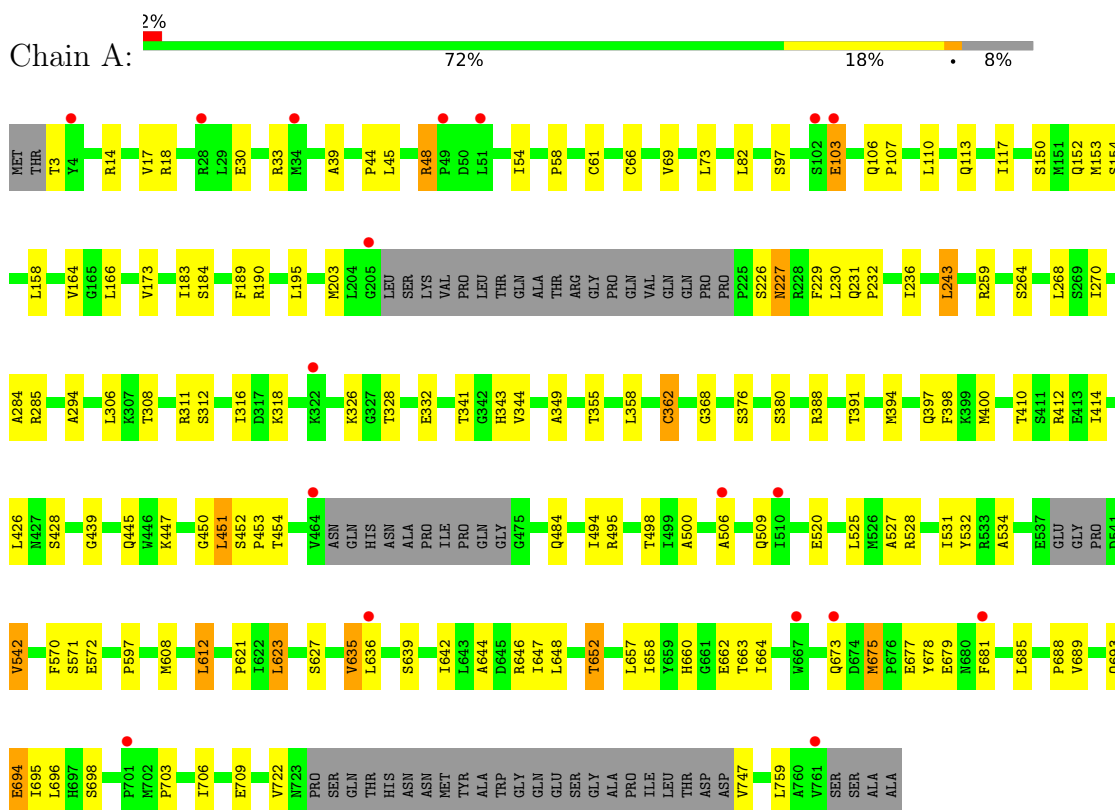
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

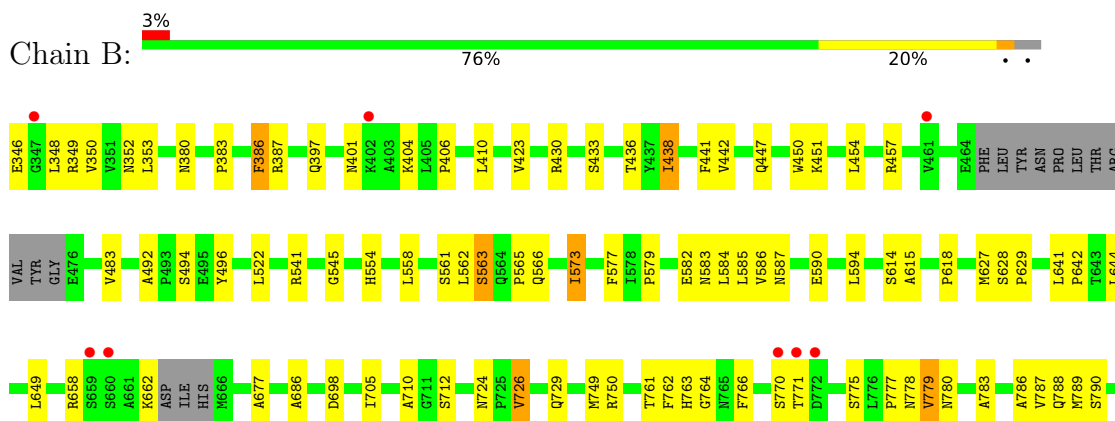
3 Residue-property plots

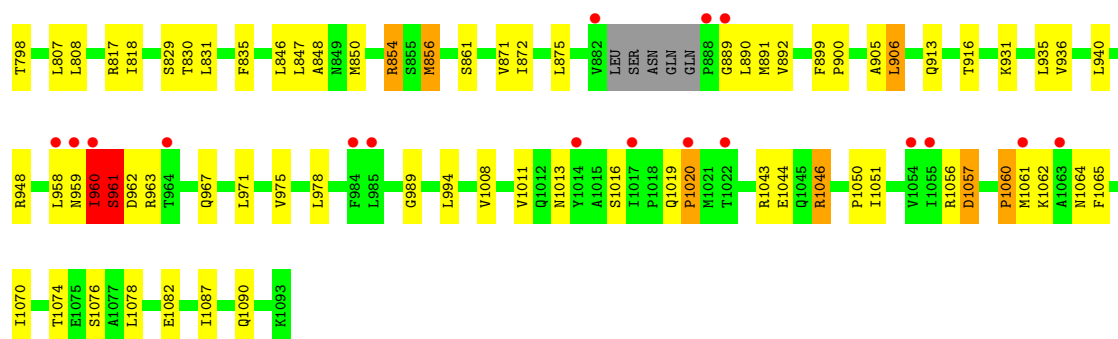
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

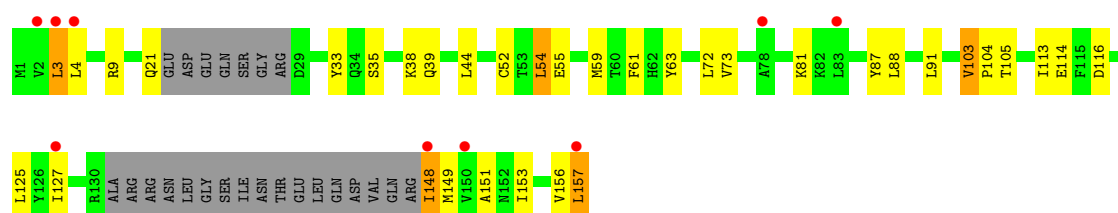


• Molecule 2: Protein transport protein Sec24A

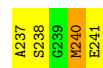




• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: ALA-SEP-GLY-MET-GLU



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.21Å 96.02Å 131.07Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	64.71 – 2.98 64.71 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.6 (64.71-2.98) 99.6 (64.71-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.216 , 0.249 0.217 , 0.251	Depositor DCC
R_{free} test set	1996 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12340	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 4.10% 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: SEP, 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	0.17	0/5682	0.37	1/7701 (0.0%)
2	B	0.25	0/5827	0.47	5/7927 (0.1%)
3	C	0.22	0/1065	0.41	0/1438
4	D	0.72	0/24	1.30	0/28
All	All	0.22	0/12598	0.42	6/17094 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	635	VAL	CB-CA-C	-7.28	101.16	111.34
2	B	386	PHE	CB-CA-C	6.22	119.73	109.72
2	B	1064	ASN	N-CA-C	-5.94	105.89	113.02
2	B	447	GLN	N-CA-C	-5.39	105.73	114.09
2	B	1060	PRO	N-CA-C	-5.24	107.36	114.80
2	B	1065	PHE	N-CA-CB	-5.02	102.58	110.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5551	0	5458	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5705	0	5719	86	0
3	C	1046	0	1030	18	0
4	D	36	0	25	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	12340	0	12232	172	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 (172) 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:960:ILE:O	2:B:961:SER:HB2	1.76	0.86
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.61	0.82
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.66	0.77
2:B:960:ILE:O	2:B:961:SER:CB	2.32	0.73
1:A:621:PRO:HG3	1:A:652:THR:HG23	1.75	0.69
1:A:410:THR:HB	1:A:414:ILE:HB	1.74	0.67
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.33	0.64
1:A:173:VAL:HG21	1:A:270:ILE:HD12	1.78	0.64
2:B:410:LEU:HD12	2:B:935:LEU:HD22	1.80	0.64
2:B:749:MET:HB2	2:B:807:LEU:HD13	1.80	0.63
1:A:195:LEU:HD13	1:A:203:MET:HE1	1.80	0.63
1:A:639:SER:O	1:A:642:ILE:CG1	2.47	0.63
1:A:623:LEU:HD11	1:A:648:LEU:HD13	1.81	0.62
2:B:779:VAL:HG21	2:B:807:LEU:HD21	1.80	0.62
2:B:872:ILE:HD12	2:B:1090:GLN:HB2	1.82	0.62
1:A:190:ARG:HH11	2:B:577:PHE:HB3	1.63	0.62
2:B:1074:THR:HG22	2:B:1076:SER:H	1.65	0.61
1:A:528:ARG:HA	1:A:608:MET:HE1	1.82	0.61
3:C:39:GLN:HB3	3:C:157:LEU:HD11	1.82	0.60
1:A:195:LEU:HD12	1:A:270:ILE:HD11	1.83	0.59
1:A:412:ARG:H	1:A:412:ARG:HD3	1.68	0.59
2:B:558:LEU:HD12	2:B:594:LEU:HG	1.84	0.59
1:A:166:LEU:HD23	1:A:243:LEU:HD13	1.84	0.58
2:B:780:ASN:HD21	2:B:783:ALA:HB2	1.68	0.58
2:B:686:ALA:HB2	2:B:777:PRO:HB2	1.86	0.58
1:A:639:SER:O	1:A:642:ILE:HG12	2.04	0.58
2:B:848:ALA:HB2	2:B:906:LEU:HD21	1.84	0.58
2:B:960:ILE:HG12	2:B:963:ARG:CB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:948:ARG:HG3	2:B:971:LEU:HD11	1.85	0.58
2:B:729:GLN:HG3	2:B:1051:ILE:HD12	1.87	0.57
1:A:30:GLU:HA	1:A:33:ARG:HB2	1.87	0.57
2:B:545:GLY:HA3	2:B:585:LEU:HD23	1.87	0.56
2:B:579:PRO:HD2	2:B:584:LEU:HD11	1.86	0.56
1:A:452:SER:HB2	1:A:453:PRO:HD2	1.87	0.56
2:B:562:LEU:HD12	2:B:563:SER:H	1.71	0.56
1:A:388:ARG:HA	1:A:391:THR:HG23	1.88	0.56
2:B:975:VAL:HG23	2:B:978:LEU:HD12	1.88	0.55
2:B:587:ASN:HB3	2:B:590:GLU:HG2	1.88	0.54
2:B:750:ARG:HH22	4:D:241:GLU:HG2	1.73	0.54
2:B:847:LEU:HA	2:B:850:MET:HE3	1.90	0.54
3:C:81:LYS:HE3	3:C:148:ILE:HG21	1.89	0.54
2:B:959:ASN:O	2:B:960:ILE:C	2.51	0.54
2:B:541:ARG:HD3	3:C:114:GLU:HA	1.88	0.54
3:C:33:TYR:CE1	3:C:59:MET:HG3	2.43	0.54
2:B:1056:ARG:O	2:B:1057:ASP:C	2.51	0.53
1:A:358:LEU:HD22	1:A:597:PRO:HB3	1.89	0.53
1:A:284:ALA:HB3	1:A:343:HIS:ND1	2.24	0.53
2:B:1056:ARG:H	2:B:1060:PRO:HB3	1.74	0.53
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.91	0.53
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.90	0.52
2:B:352:ASN:HD21	2:B:889:GLY:HA3	1.74	0.52
1:A:14:ARG:HG3	1:A:48:ARG:NH2	2.25	0.51
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.93	0.51
2:B:1060:PRO:C	2:B:1062:LYS:N	2.68	0.51
1:A:285:ARG:HE	1:A:344:VAL:HG11	1.75	0.51
2:B:442:VAL:HG21	2:B:450:TRP:HE3	1.75	0.51
1:A:73:LEU:HD11	1:A:500:ALA:HB2	1.93	0.51
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.92	0.51
1:A:639:SER:O	1:A:642:ILE:HG13	2.09	0.51
2:B:940:LEU:HD13	2:B:989:GLY:HA2	1.92	0.51
2:B:383:PRO:HA	2:B:386:PHE:O	2.11	0.50
1:A:527:ALA:O	1:A:531:ILE:HG12	2.12	0.50
2:B:831:LEU:HD22	2:B:835:PHE:HE2	1.75	0.50
1:A:398:PHE:HB3	1:A:400:MET:HG2	1.94	0.49
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.94	0.49
2:B:905:ALA:HB2	2:B:1070:ILE:HD13	1.94	0.49
3:C:73:VAL:HB	3:C:88:LEU:HD21	1.93	0.49
3:C:54:LEU:HD21	3:C:156:VAL:HG21	1.93	0.49
1:A:107:PRO:HD2	1:A:110:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:PRO:HB2	2:B:846:LEU:HD23	1.94	0.49
1:A:506:ALA:HA	1:A:509:GLN:HG3	1.94	0.49
1:A:426:LEU:HD21	1:A:447:LYS:HB2	1.93	0.49
2:B:1043:ARG:HG2	2:B:1050:PRO:HD2	1.95	0.49
2:B:677:ALA:HB2	2:B:705:ILE:HA	1.95	0.48
2:B:764:GLY:HA2	2:B:931:LYS:O	2.13	0.48
1:A:226:SER:HB2	1:A:232:PRO:HD3	1.95	0.48
1:A:696:LEU:HD12	1:A:703:PRO:HD2	1.95	0.48
1:A:520:GLU:HB3	1:A:612:LEU:HD11	1.95	0.48
1:A:58:PRO:HB3	1:A:69:VAL:HG13	1.96	0.47
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.96	0.47
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.48	0.47
2:B:582:GLU:HG2	2:B:583:ASN:H	1.80	0.47
3:C:61:PHE:HD2	3:C:72:LEU:HD11	1.79	0.47
1:A:328:THR:O	1:A:332:GLU:HG2	2.16	0.46
2:B:1046:ARG:HE	2:B:1050:PRO:HG3	1.80	0.46
1:A:259:ARG:HG2	1:A:306:LEU:HD12	1.97	0.46
1:A:484:GLN:HG2	1:A:494:ILE:HG23	1.96	0.46
2:B:875:LEU:HD22	2:B:892:VAL:HG12	1.98	0.46
2:B:856:MET:HE2	2:B:856:MET:HB2	1.81	0.46
2:B:353:LEU:HB2	2:B:890:LEU:HD23	1.98	0.46
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.97	0.46
1:A:153:MET:HE3	1:A:153:MET:HB3	1.76	0.46
1:A:428:SER:OG	1:A:445:GLN:HB2	2.16	0.46
1:A:164:VAL:HG23	1:A:236:ILE:HD11	1.98	0.45
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.31	0.45
2:B:442:VAL:HG21	2:B:450:TRP:CE3	2.51	0.45
2:B:401:ASN:O	2:B:404:LYS:HD3	2.17	0.45
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.96	0.45
1:A:231:GLN:HB2	1:A:236:ILE:HD13	1.99	0.45
1:A:678:TYR:HD2	1:A:681:PHE:HB2	1.80	0.45
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.99	0.45
2:B:959:ASN:O	2:B:961:SER:N	2.50	0.45
1:A:190:ARG:HD3	2:B:577:PHE:CD1	2.52	0.45
2:B:808:LEU:HD13	2:B:818:ILE:HG12	1.99	0.45
2:B:872:ILE:HD13	2:B:1087:ILE:HG23	1.98	0.45
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.98	0.45
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.51	0.45
1:A:657:LEU:HD12	1:A:706:ILE:HD13	1.99	0.45
1:A:675:MET:H	1:A:675:MET:HG2	1.61	0.45
2:B:724:ASN:OD1	2:B:726:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASN:HB3	1:A:229:PHE:H	1.81	0.44
2:B:871:VAL:HG11	2:B:1087:ILE:HD13	1.98	0.44
3:C:54:LEU:HG	3:C:153:ILE:HA	1.98	0.44
2:B:1060:PRO:O	2:B:1061:MET:C	2.58	0.44
2:B:710:ALA:HB3	2:B:777:PRO:HD2	1.98	0.44
2:B:1078:LEU:HD22	2:B:1082:GLU:HB3	1.99	0.44
3:C:87:TYR:CZ	3:C:91:LEU:HD11	2.52	0.44
3:C:52:CYS:SG	3:C:149:MET:HE2	2.57	0.44
1:A:284:ALA:O	1:A:344:VAL:HG12	2.17	0.44
2:B:380:ASN:HA	2:B:441:PHE:HZ	1.81	0.44
2:B:762:PHE:HB3	2:B:766:PHE:CZ	2.52	0.44
1:A:341:THR:HB	1:A:343:HIS:HD2	1.83	0.43
1:A:644:ALA:HB1	1:A:663:THR:HG22	2.00	0.43
1:A:368:GLY:HA3	1:A:450:GLY:O	2.18	0.43
1:A:184:SER:HB2	2:B:566:GLN:HG3	2.00	0.43
2:B:940:LEU:HA	2:B:940:LEU:HD23	1.83	0.43
1:A:694:GLU:HG2	1:A:695:ILE:N	2.32	0.43
2:B:658:ARG:HH11	2:B:658:ARG:HB3	1.82	0.43
2:B:615:ALA:HB2	2:B:644:LEU:HD23	2.01	0.43
3:C:103:VAL:HG23	3:C:104:PRO:HD3	2.00	0.43
1:A:154:SER:O	1:A:158:LEU:HG	2.19	0.43
2:B:854:ARG:HE	2:B:854:ARG:HB2	1.57	0.43
2:B:686:ALA:HB3	2:B:778:ASN:OD1	2.18	0.43
2:B:397:GLN:OE1	2:B:790:SER:HB2	2.19	0.42
1:A:312:SER:O	1:A:316:ILE:HG13	2.19	0.42
1:A:44:PRO:O	1:A:495:ARG:HD3	2.18	0.42
1:A:173:VAL:HG22	1:A:189:PHE:HB2	2.01	0.42
2:B:350:VAL:HG12	2:B:891:MET:HE3	2.01	0.42
2:B:383:PRO:O	2:B:387:ARG:HD2	2.18	0.42
1:A:103:GLU:H	1:A:103:GLU:HG3	1.54	0.42
4:D:237:ALA:HB3	4:D:240:MET:SD	2.59	0.42
2:B:846:LEU:HG	2:B:850:MET:HE2	2.01	0.42
3:C:55:GLU:HG2	3:C:151:ALA:O	2.19	0.42
1:A:689:VAL:O	1:A:693:GLN:HG2	2.20	0.42
2:B:436:THR:HG21	2:B:454:LEU:HD13	2.01	0.42
2:B:438:ILE:HD12	2:B:450:TRP:CD2	2.55	0.41
1:A:311:ARG:NH2	1:A:358:LEU:HB3	2.35	0.41
3:C:113:ILE:O	3:C:116:ASP:HB2	2.19	0.41
1:A:164:VAL:O	1:A:230:LEU:HA	2.20	0.41
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.90	0.41
2:B:761:THR:HB	2:B:788:GLN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:913:GLN:HG3	2:B:916:THR:HG21	2.01	0.41
1:A:332:GLU:HB3	1:A:362:CYS:SG	2.61	0.41
1:A:183:ILE:HD12	2:B:565:PRO:HG2	2.01	0.41
1:A:534:ALA:HB2	1:A:542:VAL:HG21	2.02	0.41
2:B:430:ARG:HH12	4:D:238:SEP:HB3	1.86	0.41
2:B:492:ALA:HB1	2:B:496:TYR:HB2	2.02	0.41
2:B:962:ASP:OD1	2:B:962:ASP:N	2.54	0.41
2:B:975:VAL:HA	2:B:978:LEU:HG	2.03	0.41
3:C:38:LYS:HB2	3:C:38:LYS:HE2	1.91	0.41
2:B:442:VAL:CG2	2:B:450:TRP:HE3	2.34	0.41
2:B:628:SER:N	2:B:629:PRO:HD2	2.36	0.41
2:B:1011:VAL:HG12	2:B:1013:ASN:H	1.85	0.41
2:B:641:LEU:HD12	2:B:642:PRO:HD2	2.04	0.40
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	2.03	0.40
3:C:61:PHE:CD2	3:C:72:LEU:HD11	2.55	0.40
2:B:831:LEU:HD22	2:B:835:PHE:CE2	2.54	0.40
2:B:906:LEU:HD12	2:B:906:LEU:HA	1.96	0.40
3:C:54:LEU:HD12	3:C:54:LEU:HA	1.80	0.40
1:A:658:ILE:HD13	1:A:688:PRO:HB2	2.03	0.40
1:A:660:HIS:HB2	1:A:709:GLU:HB3	2.04	0.40
3:C:3:LEU:HD22	3:C:3:LEU:HA	1.95	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%)	664 (96%)	30 (4%)	0	100	100
2	B	721/748 (96%)	684 (95%)	33 (5%)	4 (1%)	21	53
3	C	127/157 (81%)	118 (93%)	9 (7%)	0	100	100
4	D	2/5 (40%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1544/1675 (92%)	1468 (95%)	72 (5%)	4 (0%)	36 67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	961	SER
2	B	1057	ASP
2	B	960	ILE
2	B	1020	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	607/666 (91%)	560 (92%)	47 (8%)	12 38
2	B	648/679 (95%)	604 (93%)	44 (7%)	14 43
3	C	112/138 (81%)	99 (88%)	13 (12%)	5 21
4	D	2/2 (100%)	1 (50%)	1 (50%)	0 0
All	All	1369/1485 (92%)	1264 (92%)	105 (8%)	12 38

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	17	VAL
1	A	48	ARG
1	A	61	CYS
1	A	66	CYS
1	A	82	LEU
1	A	97	SER
1	A	103	GLU
1	A	106	GLN
1	A	113	GLN
1	A	150	SER

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Mol	Chain	Res	Type
1	A	152	GLN
1	A	227	ASN
1	A	243	LEU
1	A	268	LEU
1	A	308	THR
1	A	318	LYS
1	A	326	LYS
1	A	362	CYS
1	A	376	SER
1	A	380	SER
1	A	394	MET
1	A	397	GLN
1	A	451	LEU
1	A	454	THR
1	A	498	THR
1	A	542	VAL
1	A	570	PHE
1	A	571	SER
1	A	572	GLU
1	A	612	LEU
1	A	623	LEU
1	A	635	VAL
1	A	636	LEU
1	A	647	ILE
1	A	652	THR
1	A	662	GLU
1	A	664	ILE
1	A	673	GLN
1	A	675	MET
1	A	677	GLU
1	A	679	GLU
1	A	694	GLU
1	A	698	SER
1	A	722	VAL
1	A	747	VAL
1	A	759	LEU
2	B	346	GLU
2	B	348	LEU
2	B	349	ARG
2	B	423	VAL
2	B	433	SER
2	B	438	ILE

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Mol	Chain	Res	Type
2	B	451	LYS
2	B	457	ARG
2	B	483	VAL
2	B	494	SER
2	B	522	LEU
2	B	554	HIS
2	B	561	SER
2	B	563	SER
2	B	573	ILE
2	B	614	SER
2	B	627	MET
2	B	662	LYS
2	B	712	SER
2	B	726	VAL
2	B	770	SER
2	B	771	THR
2	B	775	SER
2	B	779	VAL
2	B	787	VAL
2	B	789	MET
2	B	798	THR
2	B	817	ARG
2	B	829	SER
2	B	830	THR
2	B	854	ARG
2	B	856	MET
2	B	861	SER
2	B	906	LEU
2	B	936	VAL
2	B	958	LEU
2	B	960	ILE
2	B	961	SER
2	B	967	GLN
2	B	994	LEU
2	B	1008	VAL
2	B	1016	SER
2	B	1044	GLU
2	B	1046	ARG
3	C	3	LEU
3	C	4	LEU
3	C	9	ARG
3	C	21	GLN

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Mol	Chain	Res	Type
3	C	35	SER
3	C	44	LEU
3	C	54	LEU
3	C	103	VAL
3	C	105	THR
3	C	125	LEU
3	C	127	ILE
3	C	148	ILE
3	C	157	LEU
4	D	240	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	152	GLN
1	A	174	GLN
1	A	227	ASN
1	A	395	HIS
1	A	484	GLN
1	A	549	GLN
1	A	620	GLN
1	A	655	GLN
2	B	527	GLN
2	B	532	ASN
2	B	566	GLN
2	B	583	ASN
2	B	587	ASN
2	B	736	GLN
2	B	780	ASN
2	B	1064	ASN
3	C	47	GLN
3	C	67	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SEP	D	238	4	8,9,10	0.61	0	8,12,14	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SEP	D	238	4	-	5/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	238	SEP	N-CA-CB-OG
4	D	238	SEP	CB-OG-P-O2P
4	D	238	SEP	CB-OG-P-O3P
4	D	238	SEP	CB-OG-P-O1P
4	D	238	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	238	SEP	1	0

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	704/765 (92%)	0.29	18 (2%) 57 38	43, 66, 117, 196	0
2	B	729/748 (97%)	0.23	25 (3%) 48 31	41, 63, 101, 128	0
3	C	133/157 (84%)	0.63	9 (6%) 23 14	48, 86, 121, 135	0
4	D	4/5 (80%)	0.79	0 100 100	81, 81, 86, 97	0
All	All	1570/1675 (93%)	0.29	52 (3%) 49 32	41, 66, 110, 196	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	888	PRO	3.5
2	B	1055	ILE	3.4
2	B	960	ILE	3.2
1	A	4	TYR	3.1
3	C	150	VAL	3.0
2	B	347	GLY	2.9
3	C	4	LEU	2.9
3	C	127	ILE	2.9
1	A	34	MET	2.8
3	C	148	ILE	2.8
1	A	103	GLU	2.7
2	B	660	SER	2.7
2	B	1054	VAL	2.7
3	C	3	LEU	2.7
2	B	770	SER	2.7
1	A	322	LYS	2.6
2	B	772	ASP	2.6
1	A	205	GLY	2.6
3	C	78	ALA	2.5
2	B	1020	PRO	2.5
2	B	958	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	1061	MET	2.5
2	B	1063	ALA	2.4
2	B	1022	THR	2.4
3	C	83	LEU	2.4
1	A	510	ILE	2.4
1	A	49	PRO	2.4
2	B	964	THR	2.3
1	A	28	ARG	2.3
1	A	636	LEU	2.3
3	C	2	VAL	2.3
1	A	673	GLN	2.3
2	B	771	THR	2.3
2	B	1014	TYR	2.3
1	A	506	ALA	2.2
2	B	889	GLY	2.2
2	B	985	LEU	2.2
1	A	701	PRO	2.2
1	A	761	VAL	2.2
1	A	51	LEU	2.2
1	A	667	TRP	2.2
3	C	157	LEU	2.2
2	B	959	ASN	2.1
2	B	882	VAL	2.1
1	A	681	PHE	2.1
2	B	984	PHE	2.1
2	B	1017	ILE	2.1
1	A	102	SER	2.0
2	B	461	VAL	2.0
2	B	659	SER	2.0
2	B	402	LYS	2.0
1	A	464	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
4	SEP	D	238	10/11	0.74	0.20	73,85,90,101	0

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	0.98	0.05	85,85,85,85	0
5	ZN	B	1101	1/1	1.00	0.02	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.