



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 12:44 PM JST

PDB ID : 9UVG / pdb\_00009uvg  
Title : Crystal structure of Sec23a/24a/22b bound to mouse STING pSGMD motif  
Authors : Ma, W.F.  
Deposited on : 2025-05-10  
Resolution : 2.54 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](mailto: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>.

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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

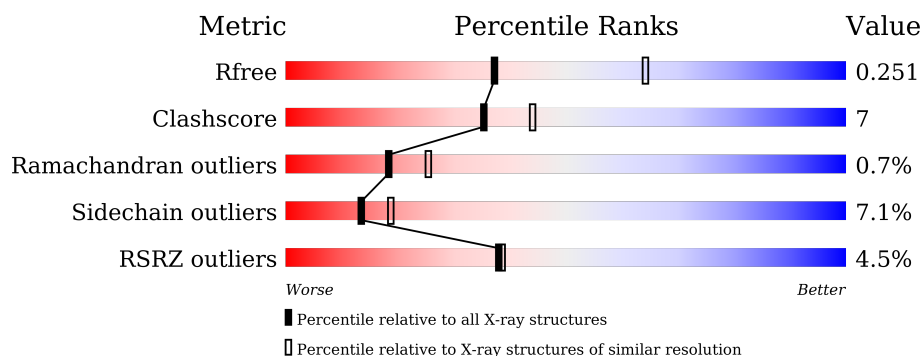
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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  $\geq 3$ , 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>4%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>•</div> <div>7%</div> </div> </div>
2	B	748	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>
3	C	157	<div> <div>10%</div> <div> <div></div> <div>62%</div> <div>20%</div> <div>•</div> <div>14%</div> </div> </div>
4	D	4	<div> <div></div> <div> <div>25%</div> <div>75%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12559 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	708	Total	C	N	O	S	0	0	0
			5593	3563	958	1032	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
			5725	3652	970	1069	34			

- 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
			1071	690	170	203	8			

- Molecule 4 is a protein called SEP-GLY-MET-ASP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	P	S	0	0
			30	14	4	10	1	1		

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

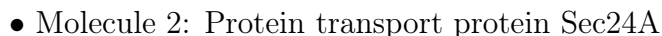
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total 54	O 54	0	0
6	B	72	Total 72	O 72	0	0
6	C	11	Total 11	O 11	0	0
6	D	1	Total 1	O 1	0	0



- Molecule 1: Protein transport protein Sec23A





• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: SEP-GLY-MET-ASP



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.00Å 96.91Å 129.60Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	21.43 – 2.54 21.43 – 2.54	Depositor EDS
% Data completeness (in resolution range)	86.5 (21.43-2.54) 87.8 (21.43-2.54)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.53Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.225 , 0.253 0.226 , 0.251	Depositor DCC
$R_{free}$ test set	1996 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12559	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.20	0/5722	0.39	0/7749
2	B	0.36	0/5847	0.57	3/7952 (0.0%)
3	C	0.33	0/1090	0.56	0/1471
4	D	0.71	0/19	1.29	0/23
All	All	0.30	0/12678	0.50	3/17195 (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	1064	ASN	N-CA-C	-6.60	105.23	113.28
2	B	1054	VAL	N-CA-C	-5.30	105.86	113.07
2	B	1065	PHE	CA-CB-CG	5.01	118.81	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	5593	0	5520	69	0
2	B	5725	0	5746	81	0
3	C	1071	0	1058	34	0
4	D	30	0	21	2	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
6	A	54	0	0	3	0
6	B	72	0	0	0	0
6	C	11	0	0	1	0
6	D	1	0	0	0	0
All	All	12559	0	12345	184	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 (184) 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)
3:C:79:PHE:CZ	3:C:126:TYR:HE2	2.00	0.79
2:B:446:ASP:C	2:B:448:ARG:H	1.92	0.75
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.71	0.73
1:A:722:VAL:O	1:A:723:ASN:HB2	1.94	0.67
1:A:410:THR:HB	1:A:414:ILE:HB	1.75	0.67
1:A:195:LEU:HD13	1:A:203:MET:HE1	1.78	0.66
3:C:4:LEU:HB3	3:C:74:LEU:HB3	1.77	0.65
1:A:528:ARG:HA	1:A:608:MET:HE1	1.79	0.65
1:A:678:TYR:HB3	1:A:681:PHE:HB2	1.79	0.65
3:C:4:LEU:HD23	3:C:74:LEU:HD23	1.78	0.64
1:A:164:VAL:HG23	1:A:236:ILE:HD11	1.79	0.64
1:A:415:LYS:HD2	1:A:464:VAL:HG21	1.79	0.64
1:A:647:ILE:HG21	1:A:688:PRO:HG3	1.80	0.63
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.81	0.62
1:A:672:TYR:HB3	1:A:681:PHE:HE2	1.65	0.62
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.81	0.62
2:B:779:VAL:HG21	2:B:807:LEU:HD21	1.82	0.61
2:B:959:ASN:O	2:B:961:SER:N	2.30	0.61
2:B:562:LEU:HD12	2:B:563:SER:H	1.66	0.61
1:A:46:LYS:HD2	6:A:929:HOH:O	2.01	0.61
1:A:548:ARG:HE	1:A:552:ARG:HE	1.49	0.61
2:B:994:LEU:HB3	2:B:1054:VAL:HG13	1.83	0.60
3:C:75:CYS:HB2	3:C:79:PHE:HD2	1.64	0.60
3:C:79:PHE:CZ	3:C:126:TYR:CE2	2.87	0.59
3:C:1:MET:HA	3:C:127:ILE:HG23	1.83	0.58
1:A:618:MET:HA	6:A:923:HOH:O	2.02	0.58
2:B:442:VAL:HG21	2:B:450:TRP:HE3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:VAL:HG21	1:A:270:ILE:HD12	1.86	0.58
2:B:847:LEU:HA	2:B:850:MET:HE3	1.85	0.57
3:C:83:LEU:HB3	3:C:126:TYR:HE1	1.70	0.56
2:B:1004:PHE:HA	2:B:1008:VAL:HG13	1.87	0.56
2:B:410:LEU:HD12	2:B:935:LEU:HD22	1.87	0.56
1:A:3:THR:N	6:A:901:HOH:O	2.39	0.55
2:B:876:SER:HA	2:B:1091:VAL:HG13	1.87	0.55
2:B:841:GLN:HG2	2:B:939:MET:HE2	1.89	0.55
2:B:986:MET:HE1	2:B:1065:PHE:HA	1.88	0.54
3:C:79:PHE:HD1	3:C:80:PRO:HD2	1.72	0.54
1:A:183:ILE:HD12	2:B:565:PRO:HG2	1.88	0.53
2:B:446:ASP:C	2:B:448:ARG:N	2.62	0.53
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.43	0.53
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.90	0.53
3:C:75:CYS:HB2	3:C:79:PHE:CD2	2.42	0.53
2:B:872:ILE:HD12	2:B:1090:GLN:HB2	1.90	0.53
2:B:446:ASP:O	2:B:448:ARG:N	2.42	0.52
2:B:958:LEU:O	2:B:960:ILE:N	2.41	0.52
3:C:1:MET:N	3:C:79:PHE:CZ	2.77	0.52
1:A:166:LEU:HD23	1:A:243:LEU:HD13	1.91	0.52
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.91	0.52
2:B:948:ARG:HG3	2:B:971:LEU:HD11	1.91	0.52
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.91	0.51
3:C:79:PHE:O	3:C:80:PRO:C	2.53	0.51
2:B:956:GLY:HA3	2:B:966:PRO:HA	1.92	0.51
4:D:236:MET:SD	4:D:236:MET:N	2.84	0.51
2:B:959:ASN:C	2:B:961:SER:H	2.19	0.51
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.26	0.50
1:A:154:SER:O	1:A:158:LEU:HG	2.11	0.50
2:B:1043:ARG:HG2	2:B:1050:PRO:HG2	1.92	0.50
1:A:506:ALA:HA	1:A:509:GLN:HG3	1.93	0.50
2:B:504:PRO:HG2	2:B:542:THR:HA	1.92	0.50
2:B:406:PRO:HB2	2:B:846:LEU:HD23	1.94	0.50
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.94	0.50
3:C:62:HIS:HE1	3:C:81:LYS:HG3	1.77	0.50
1:A:388:ARG:HA	1:A:391:THR:HG23	1.94	0.50
1:A:484:GLN:HG2	1:A:494:ILE:HG12	1.93	0.50
2:B:380:ASN:HA	2:B:441:PHE:HZ	1.77	0.49
2:B:846:LEU:HG	2:B:850:MET:HE2	1.93	0.49
1:A:699:ARG:HD2	1:A:703:PRO:HG3	1.94	0.49
2:B:422:VAL:HG11	2:B:817:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:478:HIS:CE1	2:B:479:ARG:HH11	2.30	0.49
1:A:287:MET:HE1	1:A:390:PHE:HZ	1.77	0.49
1:A:312:SER:O	1:A:316:ILE:HG12	2.13	0.49
2:B:587:ASN:HB3	2:B:590:GLU:HG2	1.95	0.49
1:A:368:GLY:HA3	1:A:450:GLY:O	2.12	0.49
1:A:626:TYR:HB2	1:A:647:ILE:HB	1.94	0.49
1:A:358:LEU:HD22	1:A:597:PRO:HB3	1.96	0.48
2:B:1009:LEU:HD21	2:B:1054:VAL:HG11	1.96	0.48
3:C:62:HIS:CE1	3:C:81:LYS:HG3	2.49	0.48
2:B:353:LEU:HD22	2:B:359:MET:HE2	1.96	0.48
2:B:952:LEU:HD12	2:B:952:LEU:H	1.79	0.48
2:B:958:LEU:O	2:B:959:ASN:C	2.57	0.48
2:B:995:TRP:HA	2:B:1056:ARG:O	2.13	0.48
3:C:3:LEU:HB3	6:C:203:HOH:O	2.14	0.48
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.49	0.47
2:B:660:SER:O	2:B:662:LYS:N	2.47	0.47
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.96	0.47
2:B:555:PHE:HZ	2:B:622:ALA:HB1	1.79	0.47
2:B:582:GLU:HG2	2:B:583:ASN:H	1.79	0.47
1:A:233:VAL:HG22	1:A:237:ASP:HB3	1.96	0.47
2:B:1060:PRO:O	2:B:1061:MET:C	2.57	0.47
1:A:155:LEU:HD21	1:A:240:LEU:HD23	1.95	0.47
2:B:710:ALA:HB3	2:B:777:PRO:HD2	1.97	0.47
3:C:74:LEU:HD12	3:C:75:CYS:H	1.79	0.47
3:C:106:VAL:HG11	3:C:112:PHE:CZ	2.50	0.47
1:A:4:TYR:O	1:A:8:ILE:HG12	2.16	0.46
2:B:686:ALA:HB2	2:B:777:PRO:HB2	1.96	0.46
2:B:965:ILE:HG12	2:B:1041:TRP:HB2	1.98	0.46
3:C:35:SER:O	3:C:39:GLN:HG3	2.15	0.46
1:A:660:HIS:HB3	1:A:664:ILE:HG22	1.98	0.46
1:A:665:ALA:O	1:A:666:GLN:C	2.59	0.46
2:B:430:ARG:HH21	2:B:435:ARG:HB3	1.80	0.45
2:B:978:LEU:HA	2:B:984:PHE:CE2	2.51	0.45
3:C:59:MET:HA	3:C:76:GLU:HA	1.97	0.45
1:A:284:ALA:HB3	1:A:343:HIS:ND1	2.32	0.45
2:B:764:GLY:HA2	2:B:931:LYS:O	2.16	0.45
2:B:830:THR:HG23	2:B:833:ASP:HB2	1.98	0.45
1:A:415:LYS:HB3	1:A:434:SER:HB2	1.99	0.45
3:C:103:VAL:HG23	3:C:104:PRO:HD3	1.99	0.44
1:A:694:GLU:HG2	1:A:695:ILE:N	2.31	0.44
2:B:978:LEU:HA	2:B:984:PHE:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ALA:O	1:A:531:ILE:HG12	2.17	0.44
2:B:749:MET:HB2	2:B:807:LEU:HD13	2.00	0.44
2:B:957:ALA:N	2:B:965:ILE:O	2.50	0.44
1:A:412:ARG:H	1:A:412:ARG:HD3	1.82	0.44
1:A:520:GLU:HB3	1:A:616:LEU:HD11	1.99	0.44
2:B:724:ASN:OD1	2:B:726:VAL:HG13	2.17	0.44
3:C:83:LEU:HB3	3:C:126:TYR:CE1	2.52	0.44
2:B:541:ARG:HD3	3:C:114:GLU:HA	1.99	0.44
2:B:642:PRO:HG3	2:B:702:LEU:HD21	2.00	0.44
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.99	0.44
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.52	0.44
3:C:73:VAL:HB	3:C:88:LEU:HD21	2.00	0.44
1:A:73:LEU:HD11	1:A:500:ALA:HB2	2.00	0.44
1:A:195:LEU:HD12	1:A:270:ILE:HD11	1.99	0.44
2:B:442:VAL:HG21	2:B:450:TRP:CE3	2.51	0.44
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.99	0.44
1:A:637:LEU:HD23	1:A:637:LEU:HA	1.89	0.43
1:A:159:PRO:HG2	1:A:162:ALA:HB2	2.00	0.43
2:B:411:LEU:HD12	2:B:413:PRO:HG3	2.00	0.43
1:A:398:PHE:HB3	1:A:400:MET:HG2	2.00	0.43
1:A:660:HIS:HB2	1:A:709:GLU:HB3	2.00	0.43
4:D:235:GLY:C	4:D:237:ASP:H	2.27	0.43
1:A:667:TRP:O	1:A:668:ARG:C	2.61	0.43
2:B:1009:LEU:HD13	2:B:1017:ILE:HD11	2.00	0.43
1:A:181:GLU:C	1:A:183:ILE:H	2.26	0.43
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.87	0.43
2:B:573:ILE:HD12	2:B:573:ILE:HA	1.80	0.43
2:B:958:LEU:HG	2:B:964:THR:HG22	2.00	0.43
2:B:1059:SER:N	2:B:1060:PRO:HD3	2.34	0.43
3:C:6:MET:HE2	3:C:6:MET:HB3	1.93	0.43
1:A:345:ILE:O	1:A:369:GLY:HA3	2.19	0.43
3:C:79:PHE:CE1	3:C:126:TYR:HE2	2.36	0.42
1:A:153:MET:SD	1:A:387:GLN:HB3	2.60	0.42
1:A:284:ALA:O	1:A:344:VAL:HG12	2.19	0.42
1:A:618:MET:HE2	1:A:653:PHE:CD2	2.55	0.42
2:B:687:VAL:O	2:B:711:GLY:HA3	2.20	0.42
3:C:36:GLN:OE1	3:C:153:ILE:HG12	2.20	0.42
1:A:452:SER:HB2	1:A:453:PRO:HD2	2.02	0.42
2:B:421:PRO:HG2	2:B:488:ILE:HD12	2.01	0.42
2:B:909:GLN:HG2	2:B:910:LYS:N	2.34	0.42
2:B:950:ASP:HB3	2:B:983:ALA:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:545:GLY:HA3	2:B:585:LEU:HD23	2.02	0.42
3:C:21:GLN:H	3:C:21:GLN:HG2	1.55	0.42
1:A:310:ILE:H	1:A:310:ILE:HD12	1.85	0.42
2:B:975:VAL:HG23	2:B:978:LEU:HD12	2.02	0.42
3:C:157:LEU:HD13	3:C:157:LEU:HA	1.85	0.42
2:B:455:CYS:SG	2:B:457:ARG:HB3	2.60	0.41
3:C:75:CYS:CB	3:C:79:PHE:HD2	2.31	0.41
1:A:190:ARG:H	1:A:190:ARG:HG2	1.62	0.41
2:B:906:LEU:HD12	2:B:906:LEU:HA	1.95	0.41
2:B:924:ILE:HD13	2:B:927:MET:HE2	2.03	0.41
3:C:33:TYR:CE2	3:C:59:MET:HG3	2.56	0.41
2:B:515:ASN:O	2:B:519:THR:HG23	2.20	0.41
2:B:578:ILE:HA	2:B:579:PRO:HD3	1.94	0.41
1:A:264:SER:HB2	1:A:294:ALA:HB2	2.02	0.41
1:A:394:MET:H	1:A:394:MET:HG2	1.66	0.41
2:B:1057:ASP:O	2:B:1060:PRO:HG3	2.19	0.41
1:A:108:ALA:HB1	1:A:114:PHE:CD2	2.55	0.41
3:C:33:TYR:CD2	3:C:74:LEU:HD21	2.56	0.41
1:A:570:PHE:HD1	1:A:570:PHE:HA	1.79	0.41
1:A:689:VAL:O	1:A:693:GLN:HG2	2.21	0.41
3:C:3:LEU:HG	3:C:127:ILE:HD11	2.03	0.41
1:A:169:PHE:HB2	1:A:173:VAL:HG12	2.02	0.41
3:C:33:TYR:HD2	3:C:74:LEU:HD21	1.86	0.41
2:B:422:VAL:HG22	2:B:489:GLU:HB3	2.03	0.40
2:B:430:ARG:NH2	2:B:435:ARG:HB3	2.35	0.40
2:B:508:PHE:CZ	2:B:529:LEU:HD21	2.56	0.40
2:B:1005:LEU:HA	2:B:1009:LEU:HB2	2.03	0.40
1:A:285:ARG:HG2	1:A:402:PHE:HE2	1.87	0.40
2:B:795:LEU:HD13	2:B:801:VAL:HG11	2.04	0.40
2:B:948:ARG:HA	2:B:984:PHE:CD1	2.56	0.40
1:A:103:GLU:H	1:A:103:GLU:HG3	1.65	0.40
2:B:681:SER:HA	2:B:777:PRO:HG3	2.02	0.40
2:B:445:LEU:C	2:B:447:GLN:H	2.29	0.40
3:C:95:PHE:CE1	3:C:99:HIS:HB2	2.56	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	698/765 (91%)	667 (96%)	31 (4%)	0	100	100
2	B	721/748 (96%)	677 (94%)	35 (5%)	9 (1%)	10	13
3	C	129/157 (82%)	120 (93%)	7 (5%)	2 (2%)	7	9
4	D	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
All	All	1550/1674 (93%)	1465 (94%)	74 (5%)	11 (1%)	18	25

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	960	ILE
2	B	954	ASP
2	B	959	ASN
2	B	1056	ARG
3	C	80	PRO
2	B	447	GLN
2	B	1047	PRO
2	B	951	ASN
2	B	1060	PRO
3	C	4	LEU
2	B	661	ALA

### 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	613/666 (92%)	579 (94%)	34 (6%)	19	29
2	B	653/679 (96%)	599 (92%)	54 (8%)	10	14
3	C	116/138 (84%)	106 (91%)	10 (9%)	10	13
4	D	2/2 (100%)	2 (100%)	0	100	100
All	All	1384/1485 (93%)	1286 (93%)	98 (7%)	13	19

All (98) 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	65	THR
1	A	82	LEU
1	A	103	GLU
1	A	106	GLN
1	A	109	GLU
1	A	164	VAL
1	A	183	ILE
1	A	184	SER
1	A	190	ARG
1	A	236	ILE
1	A	243	LEU
1	A	268	LEU
1	A	308	THR
1	A	326	LYS
1	A	355	THR
1	A	362	CYS
1	A	376	SER
1	A	435	GLU
1	A	451	LEU
1	A	570	PHE
1	A	612	LEU
1	A	635	VAL
1	A	647	ILE
1	A	664	ILE
1	A	673	GLN
1	A	675	MET
1	A	677	GLU
1	A	681	PHE
1	A	694	GLU
1	A	722	VAL

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Mol	Chain	Res	Type
1	A	748	SER
2	B	354	LEU
2	B	411	LEU
2	B	423	VAL
2	B	433	SER
2	B	443	SER
2	B	445	LEU
2	B	448	ARG
2	B	451	LYS
2	B	457	ARG
2	B	461	VAL
2	B	483	VAL
2	B	522	LEU
2	B	554	HIS
2	B	563	SER
2	B	573	ILE
2	B	580	MET
2	B	627	MET
2	B	659	SER
2	B	660	SER
2	B	662	LYS
2	B	726	VAL
2	B	748	VAL
2	B	750	ARG
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	830	THR
2	B	856	MET
2	B	954	ASP
2	B	958	LEU
2	B	960	ILE
2	B	961	SER
2	B	966	PRO
2	B	967	GLN
2	B	985	LEU
2	B	992	LEU
2	B	993	MET
2	B	994	LEU

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Mol	Chain	Res	Type
2	B	1000	CYS
2	B	1002	GLN
2	B	1008	VAL
2	B	1011	VAL
2	B	1029	THR
2	B	1051	ILE
2	B	1052	LEU
2	B	1054	VAL
2	B	1059	SER
2	B	1061	MET
2	B	1064	ASN
2	B	1067	GLN
2	B	1075	GLU
3	C	1	MET
3	C	20	MET
3	C	21	GLN
3	C	38	LYS
3	C	44	LEU
3	C	54	LEU
3	C	81	LYS
3	C	103	VAL
3	C	105	THR
3	C	157	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	296	GLN
1	A	549	GLN
1	A	583	HIS
1	A	591	GLN
1	A	614	GLN
1	A	620	GLN
2	B	604	GLN
2	B	832	ASN
2	B	1012	GLN
2	B	1067	GLN
2	B	1068	ASN
3	C	21	GLN
3	C	32	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	234	4	8,9,10	0.65	0	8,12,14	0.65	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	234	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	234	SEP	N-CA-CB-OG
4	D	234	SEP	CB-OG-P-O2P
4	D	234	SEP	CB-OG-P-O3P
4	D	234	SEP	CB-OG-P-O1P
4	D	234	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	708/765 (92%)	0.25	34 (4%) 35 35	37, 61, 104, 157	0
2	B	729/748 (97%)	0.07	21 (2%) 53 55	33, 53, 91, 144	0
3	C	135/157 (85%)	0.68	16 (11%) 9 8	43, 77, 125, 143	0
4	D	3/4 (75%)	1.27	0 100 100	104, 104, 109, 113	0
All	All	1575/1674 (94%)	0.21	71 (4%) 38 38	33, 59, 104, 157	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1055	ILE	5.9
2	B	959	ASN	4.3
2	B	960	ILE	4.0
1	A	681	PHE	4.0
3	C	150	VAL	4.0
3	C	126	TYR	3.7
3	C	1	MET	3.3
2	B	958	LEU	3.3
1	A	700	PHE	3.2
3	C	55	GLU	3.1
1	A	764	ALA	2.9
2	B	1058	GLU	2.9
1	A	49	PRO	2.8
3	C	157	LEU	2.8
1	A	124	GLY	2.8
1	A	322	LYS	2.8
2	B	888	PRO	2.8
2	B	964	THR	2.8
3	C	127	ILE	2.7
1	A	673	GLN	2.7
1	A	82	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	562	LEU	2.7
1	A	13	GLU	2.7
1	A	678	TYR	2.7
1	A	123	ARG	2.6
2	B	428	ILE	2.6
3	C	148	ILE	2.6
1	A	235	LYS	2.6
3	C	78	ALA	2.6
3	C	23	ASP	2.5
1	A	504	ALA	2.5
1	A	746	ASP	2.5
1	A	94	PHE	2.5
2	B	1002	GLN	2.5
1	A	435	GLU	2.4
1	A	672	TYR	2.4
3	C	2	VAL	2.4
2	B	446	ASP	2.4
2	B	1054	VAL	2.4
1	A	125	PRO	2.4
1	A	711	GLY	2.4
1	A	50	ASP	2.4
1	A	31	ALA	2.3
3	C	58	ALA	2.3
2	B	1014	TYR	2.3
1	A	506	ALA	2.3
3	C	87	TYR	2.3
1	A	431	PRO	2.3
1	A	89	TYR	2.3
1	A	641	SER	2.2
3	C	3	LEU	2.2
3	C	128	ASP	2.2
2	B	984	PHE	2.2
3	C	79	PHE	2.2
1	A	152	GLN	2.2
2	B	478	HIS	2.2
2	B	1057	ASP	2.2
1	A	464	VAL	2.2
1	A	103	GLU	2.2
1	A	747	VAL	2.1
3	C	130	ARG	2.1
1	A	122	LEU	2.1
2	B	889	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	953	SER	2.1
1	A	695	ILE	2.1
2	B	461	VAL	2.1
1	A	692	ALA	2.1
2	B	948	ARG	2.0
2	B	1063	ALA	2.0
1	A	205	GLY	2.0
1	A	676	PRO	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	SEP	D	234	10/11	0.76	0.17	86,95,103,114	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	ZN	B	1101	1/1	0.99	0.03	53,53,53,53	0
5	ZN	A	801	1/1	1.00	0.01	72,72,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.