



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2026 – 06:06 PM EDT

PDB ID : 9OZJ / pdb_00009ozj
Title : Structure of human Sec23a/Sec24a/Sec22b bound to ligand CPD1
Authors : Goldberg, J.
Deposited on : 2025-06-05
Resolution : 2.72 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

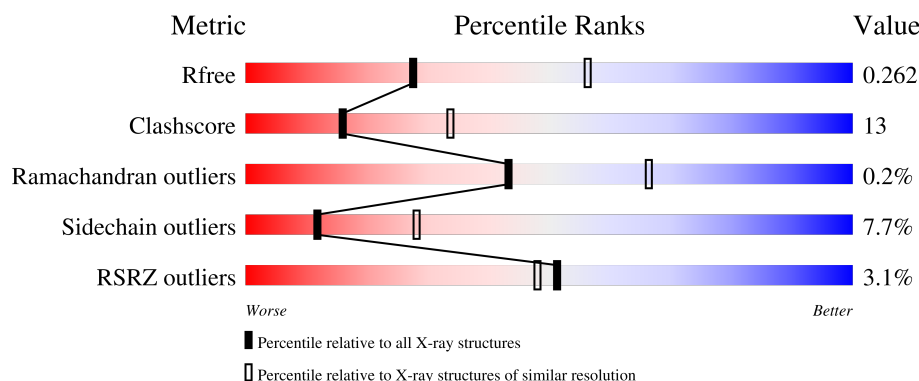
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	B	765	
2	C	748	
3	D	157	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12143 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	B	689	Total	C	N	O	S	0	0	0
			5394	3448	911	996	39			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	727	Total	C	N	O	S	0	0	0
			5649	3618	946	1052	33			

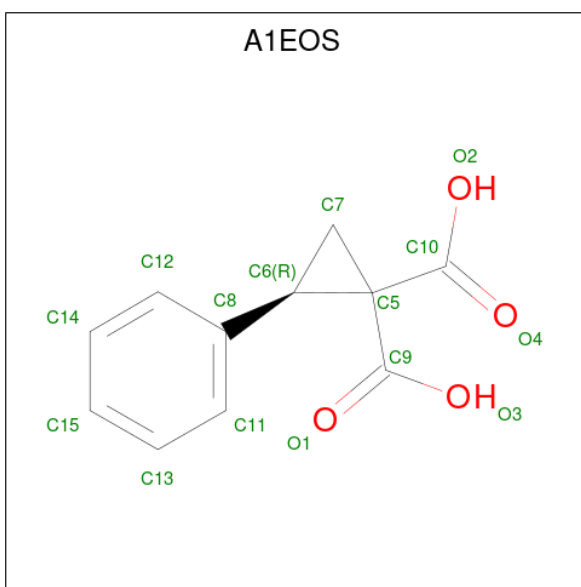
- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	132	Total	C	N	O	S	0	0	0
			1050	676	173	195	6			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is (2 {R})-2-phenylcyclopropane-1,1-dicarboxylic acid (CCD ID: A1EOS) (formula: C₁₁H₁₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			15	11	4		

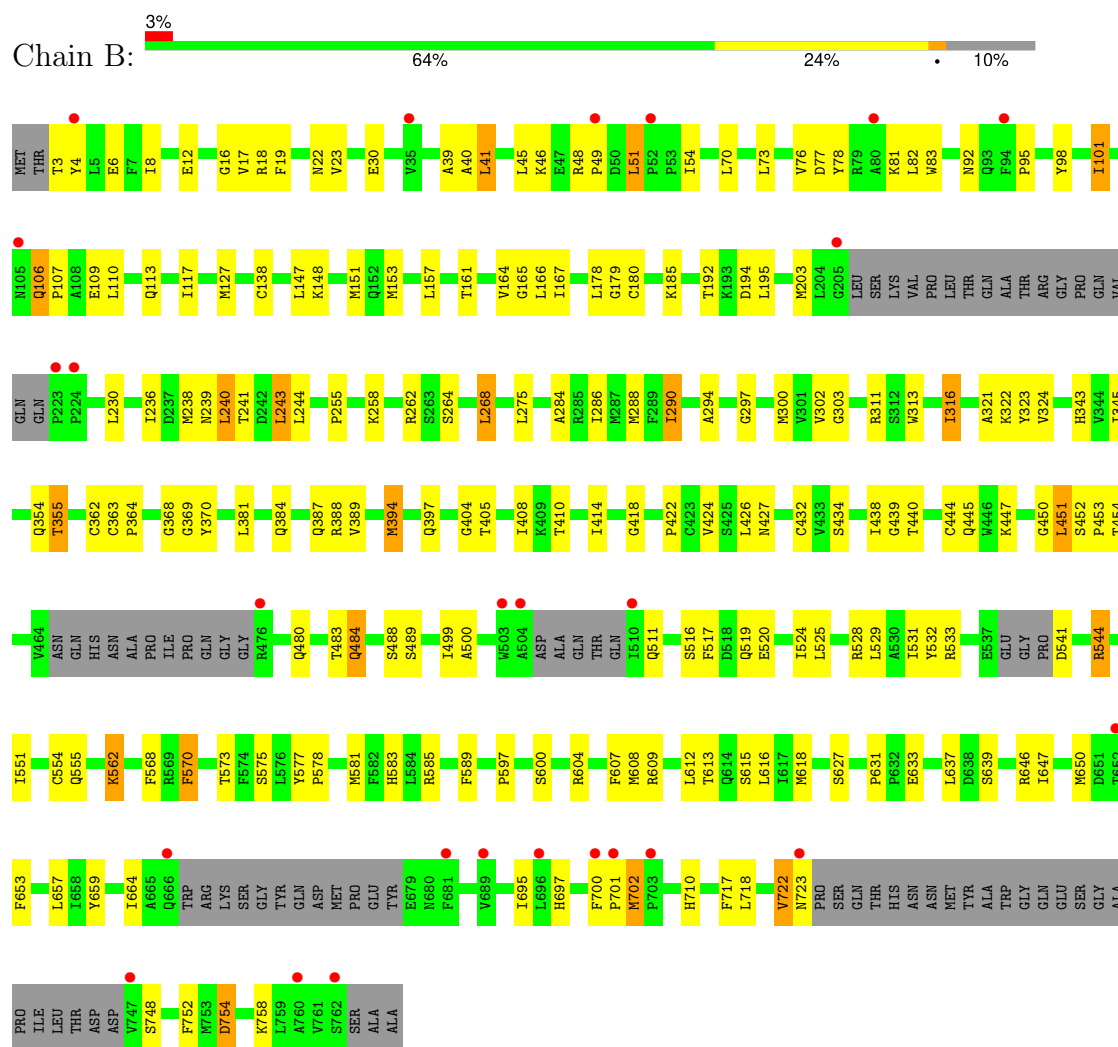
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	17	Total	O	0	0
			17	17		
6	C	14	Total	O	0	0
			14	14		
6	D	2	Total	O	0	0
			2	2		

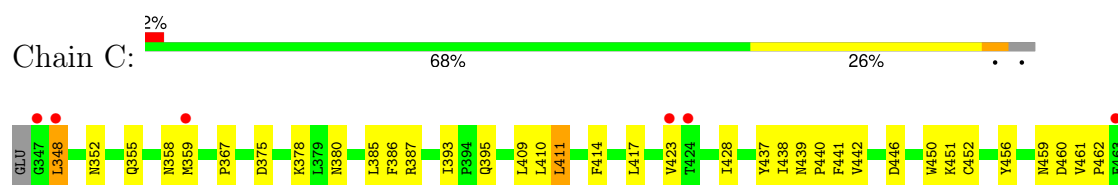
3 Residue-property plots

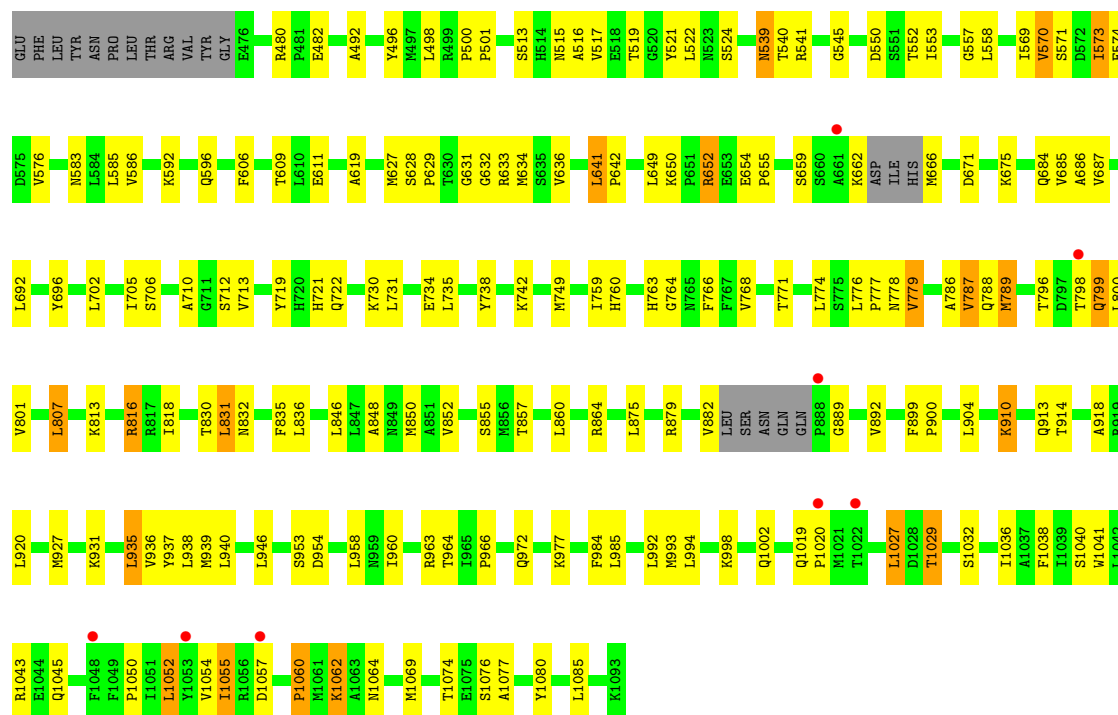
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

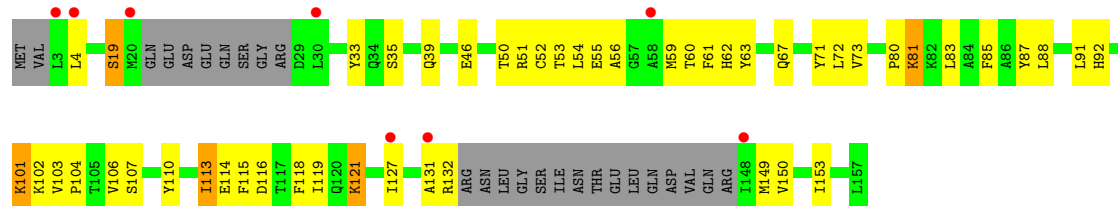


• Molecule 2: Protein transport protein Sec24A





• Molecule 3: Vesicle-trafficking protein SEC22b



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.64Å 96.48Å 130.68Å 90.00° 90.36° 90.00°	Depositor
Resolution (Å)	130.68 – 2.72 130.68 – 2.72	Depositor EDS
% Data completeness (in resolution range)	98.0 (130.68-2.72) 98.4 (130.68-2.72)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.210 , 0.260 0.213 , 0.262	Depositor DCC
R_{free} test set	2000 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12143	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: A1EOS, 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	B	0.26	0/5518	0.40	1/7480 (0.0%)
2	C	0.26	0/5771	0.43	1/7859 (0.0%)
3	D	0.25	0/1069	0.38	0/1441
All	All	0.26	0/12358	0.42	2/16780 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1060	PRO	N-CA-CB	6.71	110.30	103.25
1	B	444	CYS	N-CA-C	-5.48	105.81	112.88

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	B	5394	0	5306	146	0
2	C	5649	0	5639	135	0
3	D	1050	0	1043	39	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	C	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	17	0	0	1	0
6	C	14	0	0	0	0
6	D	2	0	0	0	0
All	All	12143	0	11988	318	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 13.

All (318) 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)
1:B:101:ILE:HD11	1:B:107:PRO:HD3	1.46	0.95
1:B:255:PRO:HG2	1:B:258:LYS:HG3	1.52	0.89
1:B:297:GLY:H	1:B:300:MET:HE2	1.41	0.84
1:B:153:MET:HE2	1:B:157:LEU:HD11	1.59	0.84
1:B:531:ILE:HD11	1:B:589:PHE:HB3	1.60	0.83
2:C:759:ILE:HG23	2:C:787:VAL:HG13	1.60	0.83
1:B:541:ASP:HB3	1:B:544:ARG:HD2	1.63	0.80
2:C:875:LEU:HD22	2:C:892:VAL:HG12	1.64	0.78
1:B:422:PRO:HG3	1:B:609:ARG:HG2	1.64	0.78
2:C:1074:THR:HG22	2:C:1077:ALA:HB3	1.64	0.78
1:B:54:ILE:HG13	1:B:117:ILE:HD11	1.66	0.77
2:C:1074:THR:HG23	2:C:1076:SER:H	1.48	0.77
2:C:721:HIS:CD2	2:C:722:GLN:HG3	2.20	0.76
2:C:395:GLN:HE21	2:C:796:THR:HA	1.50	0.75
3:D:81:LYS:H	3:D:81:LYS:HD3	1.51	0.75
1:B:264:SER:HB2	1:B:294:ALA:HB2	1.68	0.75
1:B:39:ALA:HB3	1:B:525:LEU:HD13	1.70	0.73
1:B:627:SER:HB3	1:B:646:ARG:HG3	1.70	0.73
3:D:110:TYR:HB3	3:D:113:ILE:CG2	2.18	0.73
1:B:288:MET:HE2	1:B:290:ILE:HD11	1.69	0.73
2:C:830:THR:HG22	2:C:832:ASN:H	1.53	0.72
2:C:702:LEU:O	2:C:705:ILE:HG22	1.90	0.72
2:C:759:ILE:HG12	2:C:789:MET:HE3	1.71	0.72
3:D:110:TYR:HB3	3:D:113:ILE:HG23	1.73	0.71
1:B:138:CYS:HB2	1:B:262:ARG:NH1	2.05	0.70
2:C:641:LEU:HD23	2:C:642:PRO:HD2	1.72	0.70
1:B:127:MET:HA	1:B:127:MET:HE2	1.72	0.69
3:D:113:ILE:HD13	3:D:113:ILE:H	1.56	0.69
1:B:45:LEU:HD11	1:B:451:LEU:HD13	1.74	0.69
1:B:3:THR:HG22	1:B:6:GLU:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:VAL:HG12	1:B:77:ASP:H	1.59	0.67
2:C:631:GLY:HA2	2:C:685:VAL:HG22	1.75	0.67
2:C:1043:ARG:HG3	2:C:1050:PRO:HG2	1.77	0.66
1:B:153:MET:CE	1:B:157:LEU:HD11	2.25	0.66
1:B:12:GLU:OE1	1:B:18:ARG:HD2	1.95	0.65
3:D:113:ILE:O	3:D:116:ASP:HB2	1.95	0.65
1:B:70:LEU:HD23	1:B:109:GLU:HG3	1.79	0.65
1:B:288:MET:HG2	1:B:290:ILE:HD13	1.79	0.65
2:C:634:MET:HE2	2:C:687:VAL:HG13	1.79	0.64
1:B:195:LEU:HD13	1:B:203:MET:HE1	1.78	0.64
2:C:831:LEU:HD22	2:C:835:PHE:CE2	2.32	0.64
1:B:394:MET:HE3	1:B:394:MET:H	1.62	0.64
2:C:395:GLN:NE2	2:C:796:THR:HA	2.12	0.64
1:B:76:VAL:HG21	1:B:110:LEU:HD13	1.80	0.64
2:C:450:TRP:HD1	2:C:461:VAL:HG22	1.62	0.64
1:B:650:MET:HE1	1:B:718:LEU:HA	1.80	0.64
2:C:496:TYR:HD2	2:C:818:ILE:HD11	1.63	0.63
2:C:480:ARG:HG3	2:C:482:GLU:OE1	1.99	0.63
2:C:641:LEU:HD21	2:C:649:LEU:HB2	1.81	0.63
2:C:766:PHE:HB3	2:C:776:LEU:CD2	2.28	0.63
2:C:515:ASN:O	2:C:519:THR:HG23	2.00	0.62
1:B:529:LEU:O	1:B:533:ARG:HG3	2.00	0.61
2:C:387:ARG:HD2	2:C:935:LEU:HD12	1.82	0.61
1:B:313:TRP:HA	1:B:316:ILE:HG22	1.82	0.61
2:C:1041:TRP:O	2:C:1045:GLN:HG2	2.00	0.61
2:C:641:LEU:CD2	2:C:649:LEU:HB2	2.31	0.61
2:C:831:LEU:HD22	2:C:835:PHE:HE2	1.65	0.61
1:B:95:PRO:HG2	1:B:98:TYR:CD1	2.36	0.61
3:D:52:CYS:HB3	3:D:63:TYR:CE2	2.35	0.60
1:B:83:TRP:NE1	1:B:92:ASN:HB2	2.16	0.60
1:B:48:ARG:HE	1:B:49:PRO:HD2	1.67	0.60
1:B:524:ILE:HD11	1:B:616:LEU:HD23	1.83	0.60
3:D:19:SER:HB3	3:D:119:ILE:HG21	1.84	0.60
1:B:73:LEU:HD11	1:B:500:ALA:HB2	1.84	0.59
1:B:528:ARG:HA	1:B:608:MET:HE1	1.84	0.59
1:B:554:CYS:HB3	1:B:568:PHE:CZ	2.37	0.59
1:B:368:GLY:HA3	1:B:450:GLY:O	2.02	0.59
2:C:666:MET:HE2	2:C:855:SER:HB3	1.85	0.59
1:B:554:CYS:HA	1:B:570:PHE:CZ	2.37	0.59
2:C:358:ASN:HA	2:C:972:GLN:OE1	2.03	0.59
1:B:76:VAL:HG12	1:B:77:ASP:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1019:GLN:CB	2:C:1020:PRO:HD3	2.31	0.59
2:C:633:ARG:HD2	2:C:738:TYR:OH	2.03	0.58
2:C:899:PHE:HB3	2:C:900:PRO:HD3	1.84	0.58
2:C:1043:ARG:HG2	2:C:1050:PRO:HD2	1.85	0.58
2:C:496:TYR:CD2	2:C:818:ILE:HD11	2.39	0.58
1:B:618:MET:HG2	1:B:653:PHE:HB3	1.86	0.58
1:B:439:GLY:HA2	1:B:532:TYR:CZ	2.38	0.58
2:C:409:LEU:C	2:C:410:LEU:HD12	2.29	0.58
2:C:410:LEU:CD2	2:C:935:LEU:HG	2.34	0.58
1:B:76:VAL:HG21	1:B:110:LEU:CD1	2.34	0.57
1:B:275:LEU:HD12	1:B:286:ILE:HD11	1.86	0.57
3:D:61:PHE:HD2	3:D:72:LEU:HD11	1.68	0.57
2:C:634:MET:HE2	2:C:687:VAL:CG1	2.34	0.57
2:C:766:PHE:HB3	2:C:776:LEU:HD21	1.87	0.57
1:B:531:ILE:CD1	1:B:589:PHE:HB3	2.33	0.57
2:C:438:ILE:HD12	2:C:442:VAL:HG11	1.86	0.57
2:C:558:LEU:HB2	2:C:586:VAL:HG11	1.86	0.56
3:D:87:TYR:CZ	3:D:91:LEU:HD11	2.40	0.56
1:B:81:LYS:O	1:B:82:LEU:HD23	2.06	0.56
2:C:1027:LEU:HB2	2:C:1029:THR:HG23	1.87	0.56
2:C:710:ALA:HB3	2:C:777:PRO:HD2	1.88	0.56
2:C:686:ALA:HB3	2:C:778:ASN:OD1	2.05	0.55
2:C:652:ARG:HB2	2:C:696:TYR:CE2	2.41	0.55
2:C:671:ASP:OD2	2:C:675:LYS:HE3	2.07	0.55
1:B:288:MET:HG2	1:B:290:ILE:CD1	2.36	0.55
1:B:418:GLY:HA3	1:B:438:ILE:O	2.07	0.55
2:C:642:PRO:HG2	2:C:702:LEU:HD21	1.88	0.55
1:B:45:LEU:O	1:B:453:PRO:HA	2.07	0.55
1:B:164:VAL:O	1:B:230:LEU:HA	2.07	0.55
1:B:451:LEU:HD12	1:B:451:LEU:H	1.71	0.55
2:C:807:LEU:O	2:C:818:ILE:HA	2.06	0.54
2:C:993:MET:HB3	2:C:1055:ILE:HD11	1.89	0.54
1:B:45:LEU:CD1	1:B:451:LEU:HD13	2.37	0.54
1:B:166:LEU:HD23	1:B:243:LEU:HD13	1.89	0.54
1:B:607:PHE:HD2	1:B:608:MET:HE3	1.72	0.54
2:C:1069:MET:HE2	2:C:1069:MET:HA	1.89	0.54
3:D:73:VAL:HG12	3:D:88:LEU:HD11	1.89	0.54
3:D:127:ILE:O	3:D:127:ILE:HG22	2.07	0.54
3:D:62:HIS:O	3:D:73:VAL:HG12	2.07	0.54
2:C:492:ALA:HB3	2:C:816:ARG:HB3	1.90	0.54
2:C:631:GLY:HA2	2:C:685:VAL:CG2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:846:LEU:O	2:C:850:MET:HG3	2.07	0.54
2:C:410:LEU:HD22	2:C:935:LEU:HG	1.90	0.54
2:C:452:CYS:O	2:C:456:TYR:HA	2.07	0.54
3:D:50:THR:C	3:D:51:ARG:HG2	2.32	0.54
2:C:879:ARG:HA	2:C:882:VAL:HG22	1.89	0.54
2:C:966:PRO:HG2	2:C:1038:PHE:HB2	1.90	0.54
2:C:375:ASP:O	2:C:378:LYS:HG2	2.09	0.53
1:B:322:LYS:HE3	1:B:323:TYR:CZ	2.44	0.53
1:B:345:ILE:O	1:B:369:GLY:HA3	2.09	0.53
1:B:647:ILE:HD11	1:B:664:ILE:HG21	1.91	0.53
1:B:554:CYS:HA	1:B:570:PHE:HZ	1.74	0.53
3:D:101:LYS:HE3	3:D:101:LYS:HA	1.91	0.53
2:C:393:ILE:HG13	2:C:801:VAL:HG21	1.90	0.53
2:C:411:LEU:N	2:C:411:LEU:HD23	2.23	0.53
1:B:562:LYS:NZ	1:B:562:LYS:HB3	2.25	0.52
3:D:54:LEU:O	3:D:60:THR:HG23	2.10	0.52
2:C:557:GLY:HA2	2:C:583:ASN:O	2.09	0.52
1:B:255:PRO:HG2	1:B:258:LYS:CG	2.32	0.52
3:D:71:TYR:CE2	3:D:92:HIS:HA	2.45	0.52
2:C:763:HIS:HB2	2:C:786:ALA:HB3	1.92	0.52
1:B:426:LEU:HD21	1:B:447:LYS:HB2	1.90	0.52
2:C:830:THR:HG22	2:C:832:ASN:N	2.23	0.52
2:C:428:ILE:HG21	2:C:437:TYR:HE2	1.76	0.51
2:C:768:VAL:HG22	2:C:774:LEU:CD2	2.40	0.51
3:D:73:VAL:HB	3:D:88:LEU:HD21	1.93	0.51
1:B:618:MET:HE2	1:B:653:PHE:CD2	2.46	0.51
2:C:913:GLN:HE21	2:C:918:ALA:HB2	1.75	0.51
3:D:121:LYS:NZ	3:D:121:LYS:HB3	2.25	0.51
1:B:101:ILE:HD11	1:B:107:PRO:CD	2.31	0.51
2:C:764:GLY:HA2	2:C:931:LYS:O	2.09	0.50
2:C:385:LEU:HD21	2:C:417:LEU:HD21	1.92	0.50
1:B:12:GLU:CD	1:B:18:ARG:HD2	2.36	0.50
2:C:936:VAL:O	2:C:940:LEU:HD23	2.11	0.50
2:C:1032:SER:O	2:C:1036:ILE:HG12	2.12	0.50
1:B:410:THR:HB	1:B:414:ILE:HB	1.94	0.50
2:C:553:ILE:HG12	2:C:619:ALA:HA	1.93	0.50
1:B:148:LYS:HE3	1:B:244:LEU:O	2.12	0.50
1:B:517:PHE:CE2	1:B:519:GLN:HA	2.47	0.49
3:D:118:PHE:HA	3:D:121:LYS:HE2	1.94	0.49
3:D:35:SER:O	3:D:39:GLN:HG2	2.12	0.49
1:B:138:CYS:HB2	1:B:262:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:MET:HE2	1:B:608:MET:HA	1.93	0.49
2:C:666:MET:HE1	2:C:927:MET:SD	2.53	0.49
1:B:397:GLN:OE1	1:B:489:SER:HB3	2.12	0.49
1:B:631:PRO:O	1:B:633:GLU:HG3	2.13	0.49
1:B:363:CYS:HB2	1:B:364:PRO:CD	2.43	0.49
1:B:524:ILE:HG12	1:B:615:SER:HB3	1.95	0.49
2:C:393:ILE:HG13	2:C:801:VAL:CG2	2.42	0.49
2:C:367:PRO:HB3	2:C:387:ARG:NH2	2.27	0.49
1:B:98:TYR:O	1:B:101:ILE:HB	2.13	0.49
1:B:754:ASP:O	1:B:758:LYS:HG3	2.13	0.49
3:D:103:VAL:N	3:D:104:PRO:HD2	2.27	0.49
1:B:354:GLN:OE1	1:B:597:PRO:HD2	2.13	0.49
2:C:498:LEU:HD12	2:C:498:LEU:N	2.28	0.49
2:C:749:MET:HE3	2:C:774:LEU:HD12	1.95	0.49
1:B:321:ALA:HB1	1:B:324:VAL:HG23	1.95	0.48
1:B:575:SER:O	1:B:578:PRO:HD2	2.12	0.48
1:B:600:SER:O	1:B:604:ARG:HG3	2.13	0.48
2:C:832:ASN:O	2:C:836:LEU:HG	2.13	0.48
1:B:388:ARG:NH2	1:B:697:HIS:HA	2.28	0.48
3:D:33:TYR:CZ	3:D:59:MET:HG3	2.48	0.48
1:B:12:GLU:HG2	1:B:46:LYS:NZ	2.28	0.48
2:C:414:PHE:CE2	2:C:742:LYS:HE2	2.48	0.48
2:C:848:ALA:O	2:C:852:VAL:HG23	2.13	0.48
2:C:692:LEU:HD21	2:C:731:LEU:HD22	1.94	0.48
1:B:268:LEU:HD22	1:B:268:LEU:O	2.14	0.48
3:D:110:TYR:O	3:D:113:ILE:HG23	2.14	0.47
2:C:386:PHE:CE1	2:C:409:LEU:HD13	2.49	0.47
2:C:450:TRP:CD1	2:C:461:VAL:HG22	2.45	0.47
1:B:153:MET:CE	1:B:387:GLN:HB3	2.45	0.47
1:B:452:SER:HB2	1:B:453:PRO:CD	2.44	0.47
2:C:541:ARG:HD3	3:D:114:GLU:HA	1.96	0.47
1:B:404:GLY:HA2	1:B:484:GLN:O	2.14	0.47
2:C:380:ASN:HA	2:C:441:PHE:HZ	1.78	0.47
1:B:363:CYS:HB2	1:B:364:PRO:HD3	1.96	0.47
2:C:438:ILE:HG23	2:C:438:ILE:O	2.13	0.47
3:D:80:PRO:HG2	3:D:83:LEU:HD12	1.95	0.47
1:B:381:LEU:HA	1:B:702:MET:HE2	1.96	0.47
2:C:860:LEU:O	2:C:864:ARG:HG3	2.15	0.47
3:D:56:ALA:HB2	3:D:153:ILE:HG21	1.97	0.47
3:D:61:PHE:CD2	3:D:72:LEU:HD11	2.48	0.47
1:B:612:LEU:HD23	1:B:613:THR:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:759:ILE:CG1	2:C:789:MET:HE3	2.43	0.46
1:B:524:ILE:CD1	1:B:616:LEU:HD23	2.44	0.46
2:C:552:THR:HA	2:C:573:ILE:HD11	1.97	0.46
2:C:730:LYS:O	2:C:734:GLU:HG3	2.15	0.46
2:C:992:LEU:HG	2:C:1050:PRO:HB2	1.97	0.46
3:D:81:LYS:HD3	3:D:81:LYS:N	2.26	0.46
1:B:22:ASN:HB2	1:B:516:SER:HB2	1.97	0.46
1:B:268:LEU:HG	1:B:288:MET:SD	2.54	0.46
1:B:517:PHE:HB3	1:B:573:THR:CG2	2.45	0.46
2:C:666:MET:HE1	2:C:927:MET:HE1	1.98	0.46
1:B:18:ARG:NH1	1:B:612:LEU:HD22	2.31	0.46
1:B:370:TYR:CE2	1:B:389:VAL:HG13	2.51	0.46
2:C:553:ILE:HB	2:C:570:VAL:HG13	1.97	0.46
2:C:1043:ARG:HG3	2:C:1050:PRO:CG	2.45	0.46
1:B:194:ASP:O	1:B:195:LEU:HD23	2.15	0.46
2:C:759:ILE:HD13	2:C:787:VAL:HG11	1.97	0.46
1:B:18:ARG:CZ	1:B:612:LEU:HD13	2.45	0.46
1:B:452:SER:HB2	1:B:453:PRO:HD2	1.98	0.46
2:C:641:LEU:HD23	2:C:642:PRO:CD	2.43	0.46
3:D:55:GLU:O	3:D:153:ILE:HG22	2.15	0.46
3:D:101:LYS:HE3	3:D:101:LYS:CA	2.46	0.46
2:C:992:LEU:O	2:C:1052:LEU:HA	2.15	0.46
1:B:238:MET:HE3	1:B:238:MET:HB3	1.82	0.45
1:B:701:PRO:O	1:B:702:MET:C	2.58	0.45
2:C:935:LEU:HD22	2:C:939:MET:HG2	1.98	0.45
1:B:101:ILE:HD11	1:B:106:GLN:HA	1.98	0.45
1:B:165:GLY:HA3	1:B:230:LEU:HD23	1.98	0.45
2:C:627:MET:HE1	2:C:632:GLY:C	2.42	0.45
2:C:799:GLN:H	2:C:799:GLN:HG2	1.68	0.45
1:B:240:LEU:HD22	1:B:244:LEU:HG	1.98	0.45
2:C:606:PHE:HB3	2:C:609:THR:OG1	2.16	0.45
3:D:149:MET:HG2	3:D:150:VAL:H	1.81	0.45
2:C:609:THR:HG22	2:C:611:GLU:H	1.82	0.45
2:C:348:LEU:H	2:C:348:LEU:HG	1.52	0.45
2:C:410:LEU:HD12	2:C:410:LEU:N	2.32	0.45
1:B:577:TYR:CZ	1:B:581:MET:HE3	2.51	0.44
1:B:664:ILE:O	1:B:664:ILE:HG22	2.17	0.44
2:C:985:LEU:C	2:C:985:LEU:HD23	2.42	0.44
3:D:131:ALA:C	3:D:132:ARG:HG2	2.43	0.44
1:B:17:VAL:HA	1:B:41:LEU:O	2.17	0.44
1:B:153:MET:HE1	1:B:387:GLN:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1074:THR:CG2	2:C:1077:ALA:HB3	2.42	0.44
3:D:115:PHE:CD2	3:D:119:ILE:HG13	2.53	0.44
1:B:19:PHE:CE2	1:B:40:ALA:HB2	2.52	0.44
1:B:19:PHE:CD2	1:B:40:ALA:HB2	2.53	0.44
1:B:384:GLN:O	1:B:388:ARG:HG2	2.18	0.44
2:C:684:GLN:OE1	2:C:684:GLN:HA	2.16	0.44
2:C:760:HIS:NE2	2:C:788:GLN:HG2	2.33	0.44
1:B:370:TYR:HE2	1:B:389:VAL:HG13	1.82	0.44
2:C:634:MET:HE3	2:C:636:VAL:CG2	2.48	0.44
2:C:692:LEU:N	2:C:692:LEU:HD12	2.33	0.44
1:B:637:LEU:HD23	1:B:637:LEU:HA	1.88	0.43
1:B:577:TYR:CE2	1:B:581:MET:HE3	2.52	0.43
2:C:592:LYS:O	2:C:596:GLN:HG3	2.19	0.43
3:D:106:VAL:HG23	3:D:107:SER:H	1.82	0.43
1:B:153:MET:HE1	1:B:387:GLN:CB	2.47	0.43
1:B:166:LEU:HD12	1:B:167:ILE:H	1.83	0.43
1:B:179:GLY:HA2	1:B:239:ASN:HD22	1.83	0.43
1:B:313:TRP:O	1:B:316:ILE:HG22	2.17	0.43
1:B:700:PHE:HB3	1:B:701:PRO:HD3	2.01	0.43
2:C:910:LYS:HA	2:C:913:GLN:CD	2.43	0.43
1:B:147:LEU:HG	1:B:151:MET:HE2	2.01	0.43
1:B:657:LEU:CD1	1:B:717:PHE:HB2	2.48	0.43
2:C:936:VAL:HG13	2:C:937:TYR:N	2.34	0.43
2:C:938:LEU:HD12	2:C:938:LEU:O	2.19	0.43
1:B:238:MET:O	1:B:241:THR:HG22	2.19	0.43
2:C:666:MET:HE1	2:C:927:MET:CE	2.48	0.43
2:C:1057:ASP:HA	2:C:1062:LYS:HD3	2.00	0.43
3:D:81:LYS:H	3:D:81:LYS:CD	2.17	0.43
2:C:875:LEU:CD2	2:C:892:VAL:HG12	2.42	0.43
1:B:284:ALA:HB3	1:B:343:HIS:CD2	2.54	0.43
1:B:405:THR:O	1:B:483:THR:HA	2.18	0.43
2:C:513:SER:O	2:C:517:VAL:HG23	2.18	0.43
1:B:520:GLU:HB3	1:B:616:LEU:HD11	2.00	0.42
2:C:450:TRP:CE2	2:C:459:ASN:HB2	2.53	0.42
1:B:51:LEU:HD22	1:B:51:LEU:HA	1.76	0.42
3:D:81:LYS:O	3:D:85:PHE:HD2	2.00	0.42
1:B:311:ARG:H	1:B:311:ARG:HD3	1.84	0.42
1:B:41:LEU:HD12	1:B:41:LEU:HA	1.89	0.42
1:B:311:ARG:HD3	1:B:311:ARG:N	2.34	0.42
1:B:585:ARG:HD3	1:B:752:PHE:CE1	2.55	0.42
1:B:524:ILE:HG12	1:B:615:SER:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:VAL:HG13	1:B:723:ASN:N	2.34	0.42
2:C:904:LEU:HD22	2:C:1080:TYR:HA	2.02	0.42
3:D:63:TYR:HA	3:D:71:TYR:O	2.20	0.42
1:B:426:LEU:O	1:B:427:ASN:C	2.62	0.42
2:C:352:ASN:ND2	2:C:355:GLN:HG2	2.35	0.42
3:D:50:THR:O	3:D:51:ARG:HG2	2.20	0.42
1:B:517:PHE:HB3	1:B:573:THR:HG22	2.02	0.42
1:B:650:MET:CE	1:B:718:LEU:HA	2.48	0.42
2:C:771:THR:HG22	2:C:771:THR:O	2.20	0.42
1:B:78:TYR:OH	1:B:106:GLN:HB3	2.19	0.42
1:B:583:HIS:HD2	6:B:907:HOH:O	2.02	0.42
2:C:414:PHE:CD2	2:C:779:VAL:HG22	2.55	0.42
2:C:799:GLN:O	2:C:800:LEU:HD23	2.20	0.42
1:B:23:VAL:HG23	1:B:516:SER:HB3	2.01	0.41
1:B:313:TRP:CA	1:B:316:ILE:HG22	2.49	0.41
2:C:439:ASN:HB2	2:C:440:PRO:CD	2.50	0.41
2:C:735:LEU:HD23	2:C:735:LEU:HA	1.83	0.41
2:C:1043:ARG:CG	2:C:1050:PRO:HD2	2.50	0.41
1:B:4:TYR:O	1:B:8:ILE:HG13	2.19	0.41
2:C:500:PRO:O	2:C:501:PRO:C	2.63	0.41
3:D:53:THR:O	3:D:150:VAL:HA	2.20	0.41
1:B:240:LEU:CD2	1:B:244:LEU:HG	2.51	0.41
1:B:551:ILE:O	1:B:555:GLN:HG3	2.20	0.41
2:C:516:ALA:HB1	2:C:521:TYR:HE2	1.84	0.41
2:C:539:ASN:HB2	2:C:540:THR:H	1.73	0.41
2:C:633:ARG:HD2	2:C:738:TYR:CZ	2.56	0.41
2:C:994:LEU:HD23	2:C:1054:VAL:HG22	2.02	0.41
1:B:313:TRP:HA	1:B:316:ILE:CG2	2.49	0.41
1:B:659:TYR:OH	1:B:710:HIS:HB2	2.20	0.41
2:C:692:LEU:HD23	2:C:719:TYR:CD2	2.56	0.41
1:B:185:LYS:HE3	2:C:569:ILE:CD1	2.51	0.41
1:B:302:VAL:HG22	1:B:303:GLY:N	2.36	0.41
1:B:408:ILE:HA	1:B:480:GLN:O	2.21	0.41
1:B:577:TYR:HB3	1:B:578:PRO:HD3	2.02	0.41
2:C:946:LEU:HD11	2:C:984:PHE:HB3	2.03	0.41
1:B:16:GLY:HA2	1:B:46:LYS:HD3	2.01	0.41
2:C:545:GLY:HA3	2:C:585:LEU:HD23	2.03	0.41
1:B:101:ILE:CD1	1:B:107:PRO:HD3	2.34	0.40
2:C:628:SER:HB3	2:C:629:PRO:HD3	2.03	0.40
2:C:904:LEU:CD2	2:C:1080:TYR:HA	2.50	0.40
1:B:290:ILE:HG21	1:B:355:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:654:GLU:HA	2:C:655:PRO:HD3	1.97	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	B	675/765 (88%)	639 (95%)	36 (5%)	0	100	100
2	C	719/748 (96%)	674 (94%)	42 (6%)	3 (0%)	30	52
3	D	126/157 (80%)	117 (93%)	9 (7%)	0	100	100
All	All	1520/1670 (91%)	1430 (94%)	87 (6%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	462	PRO
2	C	1060	PRO
2	C	889	GLY

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	B	590/666 (89%)	551 (93%)	39 (7%)	15	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	637/679 (94%)	582 (91%)	55 (9%)	10	23
3	D	112/138 (81%)	103 (92%)	9 (8%)	11	26
All	All	1339/1483 (90%)	1236 (92%)	103 (8%)	12	28

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	30	GLU
1	B	41	LEU
1	B	51	LEU
1	B	101	ILE
1	B	106	GLN
1	B	113	GLN
1	B	161	THR
1	B	178	LEU
1	B	180	CYS
1	B	192	THR
1	B	236	ILE
1	B	240	LEU
1	B	243	LEU
1	B	268	LEU
1	B	290	ILE
1	B	316	ILE
1	B	355	THR
1	B	362	CYS
1	B	394	MET
1	B	424	VAL
1	B	432	CYS
1	B	434	SER
1	B	440	THR
1	B	445	GLN
1	B	451	LEU
1	B	454	THR
1	B	484	GLN
1	B	488	SER
1	B	499	ILE
1	B	511	GLN
1	B	544	ARG
1	B	562	LYS
1	B	570	PHE
1	B	639	SER

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Mol	Chain	Res	Type
1	B	695	ILE
1	B	702	MET
1	B	722	VAL
1	B	748	SER
1	B	754	ASP
2	C	348	LEU
2	C	359	MET
2	C	411	LEU
2	C	423	VAL
2	C	446	ASP
2	C	451	LYS
2	C	460	ASP
2	C	522	LEU
2	C	524	SER
2	C	539	ASN
2	C	550	ASP
2	C	570	VAL
2	C	571	SER
2	C	573	ILE
2	C	574	GLU
2	C	576	VAL
2	C	641	LEU
2	C	650	LYS
2	C	652	ARG
2	C	659	SER
2	C	662	LYS
2	C	706	SER
2	C	712	SER
2	C	713	VAL
2	C	779	VAL
2	C	787	VAL
2	C	789	MET
2	C	798	THR
2	C	799	GLN
2	C	807	LEU
2	C	813	LYS
2	C	816	ARG
2	C	831	LEU
2	C	857	THR
2	C	910	LYS
2	C	914	THR
2	C	920	LEU

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Mol	Chain	Res	Type
2	C	935	LEU
2	C	953	SER
2	C	954	ASP
2	C	958	LEU
2	C	960	ILE
2	C	963	ARG
2	C	964	THR
2	C	977	LYS
2	C	998	LYS
2	C	1002	GLN
2	C	1027	LEU
2	C	1029	THR
2	C	1040	SER
2	C	1052	LEU
2	C	1055	ILE
2	C	1062	LYS
2	C	1064	ASN
2	C	1085	LEU
3	D	4	LEU
3	D	19	SER
3	D	46	GLU
3	D	67	GLN
3	D	81	LYS
3	D	101	LYS
3	D	102	LYS
3	D	113	ILE
3	D	121	LYS

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

Mol	Chain	Res	Type
1	B	22	ASN
1	B	145	GLN
1	B	239	ASN
1	B	387	GLN
1	B	583	HIS
1	B	620	GLN
1	B	755	HIS
2	C	352	ASN
2	C	515	ASN
2	C	587	ASN
2	C	596	GLN

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Mol	Chain	Res	Type
2	C	832	ASN
2	C	913	GLN
2	C	917	ASN
2	C	932	ASN
2	C	933	GLN
2	C	1090	GLN
3	D	36	GLN
3	D	99	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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$
5	A1EOS	C	1101	-	16,16,16	1.79	3 (18%)	22,24,24	2.74	7 (31%)

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
5	A1EOS	C	1101	-	-	9/16/24/24	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1101	A1EOS	O1-C9	4.50	1.36	1.22
5	C	1101	A1EOS	C5-C6	-3.36	1.49	1.54
5	C	1101	A1EOS	O3-C9	-2.20	1.22	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1101	A1EOS	O1-C9-C5	-7.67	111.20	122.93
5	C	1101	A1EOS	C7-C6-C8	-6.69	113.50	123.46
5	C	1101	A1EOS	O3-C9-C5	4.37	124.05	114.07
5	C	1101	A1EOS	C5-C6-C8	3.37	126.54	121.64
5	C	1101	A1EOS	C5-C7-C6	-3.00	59.67	61.92
5	C	1101	A1EOS	C7-C5-C6	2.75	59.98	58.09
5	C	1101	A1EOS	C7-C5-C9	2.02	119.79	115.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

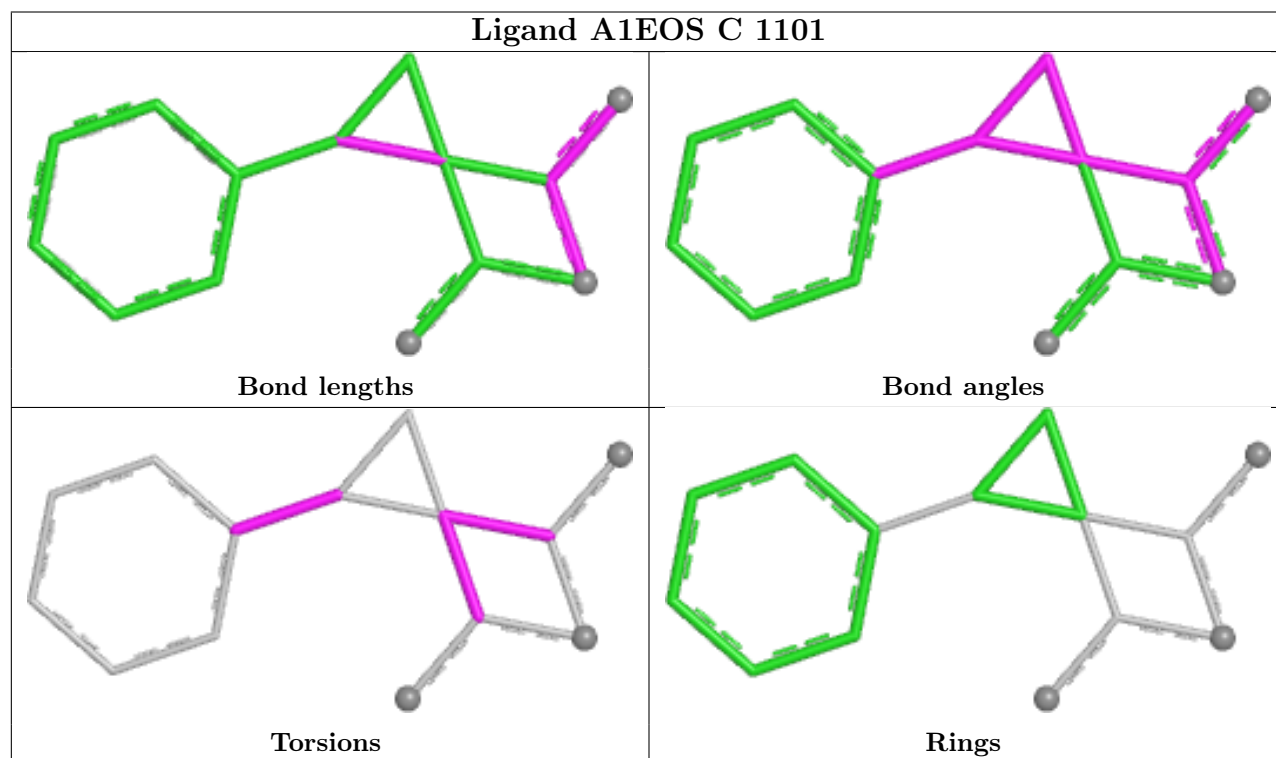
Mol	Chain	Res	Type	Atoms
5	C	1101	A1EOS	O2-C10-C5-C6
5	C	1101	A1EOS	O4-C10-C5-C6
5	C	1101	A1EOS	C10-C5-C9-O3
5	C	1101	A1EOS	C7-C5-C9-O3
5	C	1101	A1EOS	C7-C5-C9-O1
5	C	1101	A1EOS	O2-C10-C5-C9
5	C	1101	A1EOS	C5-C6-C8-C11
5	C	1101	A1EOS	C5-C6-C8-C12
5	C	1101	A1EOS	O2-C10-C5-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	B	689/765 (90%)	0.35	26 (3%)	44 40	49, 79, 118, 155	0
2	C	727/748 (97%)	0.18	14 (1%)	66 63	47, 71, 110, 148	0
3	D	132/157 (84%)	0.53	8 (6%)	27 24	59, 96, 144, 159	0
All	All	1548/1670 (92%)	0.28	48 (3%)	51 48	47, 76, 118, 159	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	463	GLU	5.8
2	C	347	GLY	4.9
1	B	476	ARG	4.1
2	C	1020	PRO	3.5
3	D	148	ILE	3.3
1	B	510	ILE	3.3
2	C	1057	ASP	3.2
1	B	35	VAL	3.2
3	D	3	LEU	3.1
1	B	762	SER	2.9
3	D	30	LEU	2.9
1	B	504	ALA	2.8
2	C	1022	THR	2.8
1	B	701	PRO	2.7
1	B	700	PHE	2.7
1	B	747	VAL	2.7
1	B	503	TRP	2.6
1	B	696	LEU	2.5
1	B	94	PHE	2.5
1	B	52	PRO	2.5
1	B	723	ASN	2.5
3	D	127	ILE	2.5
2	C	888	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	58	ALA	2.5
1	B	224	PRO	2.4
2	C	423	VAL	2.4
2	C	348	LEU	2.4
1	B	80	ALA	2.4
2	C	661	ALA	2.4
1	B	666	GLN	2.3
1	B	223	PRO	2.3
1	B	652	THR	2.3
3	D	20	MET	2.3
1	B	703	PRO	2.2
3	D	131	ALA	2.2
1	B	49	PRO	2.2
2	C	424	THR	2.2
1	B	4	TYR	2.2
1	B	681	PHE	2.2
2	C	1048	PHE	2.1
2	C	1053	TYR	2.1
1	B	760	ALA	2.1
1	B	205	GLY	2.1
2	C	798	THR	2.1
1	B	105	ASN	2.1
2	C	359	MET	2.0
3	D	4	LEU	2.0
1	B	689	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 ⓘ

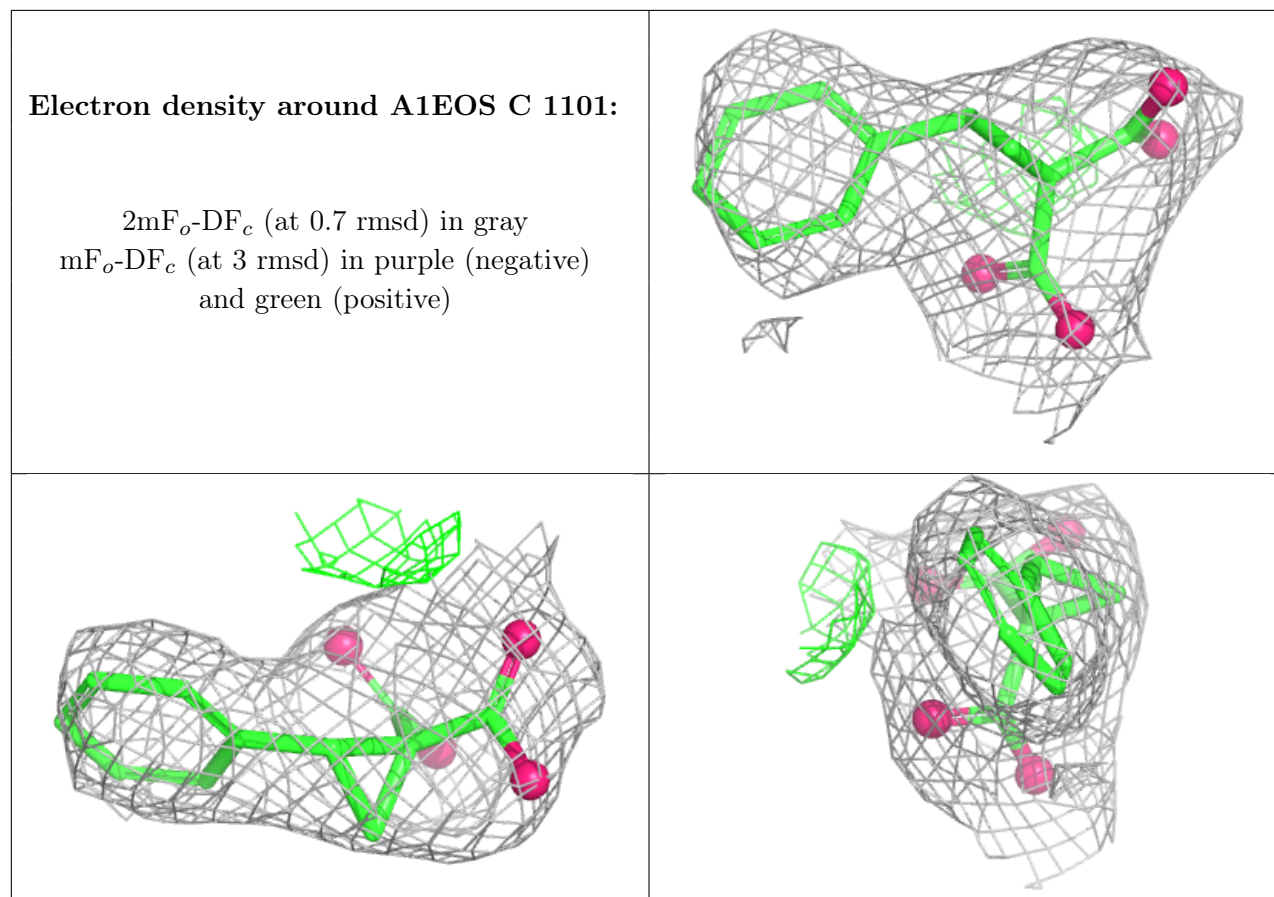
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	A1EOS	C	1101	15/15	0.89	0.11	69,92,110,110	0
4	ZN	C	1102	1/1	0.97	0.18	178,178,178,178	0
4	ZN	B	801	1/1	1.00	0.04	90,90,90,90	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.