



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2026 – 06:06 PM EDT

PDB ID : 9P09 / pdb\_00009p09  
Title : Structure of human Sec23a/Sec24a/Sec22b bound to ligand CPD14  
Authors : Goldberg, J.  
Deposited on : 2025-06-06  
Resolution : 2.49 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 : 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

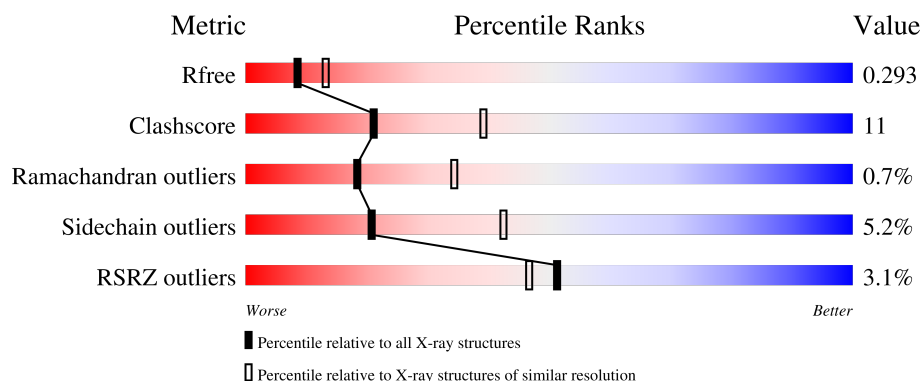
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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>3%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>•</div> <div>9%</div> </div> </div>
2	B	748	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
3	C	157	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>24%</div> <div>•</div> <div>17%</div> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12296 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	693	Total	C	N	O	S	0	0	0
			5467	3492	931	1005	39			

- 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
			5721	3656	961	1070	34			

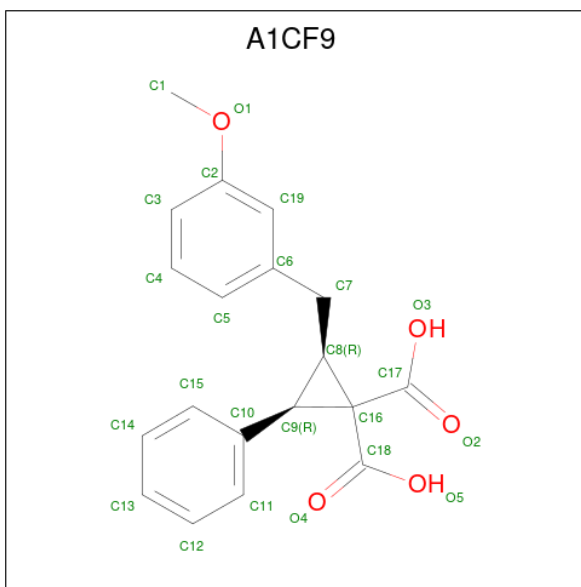
- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	131	Total	C	N	O	S	0	0	0
			1042	673	169	194	6			

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

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

- Molecule 5 is (2R,3R)-2-[(3-methoxyphenyl)methyl]-3-phenylcyclopropane-1,1-dicarboxylic acid (CCD ID: A1CF9) (formula: C<sub>19</sub>H<sub>18</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			24	19	5		

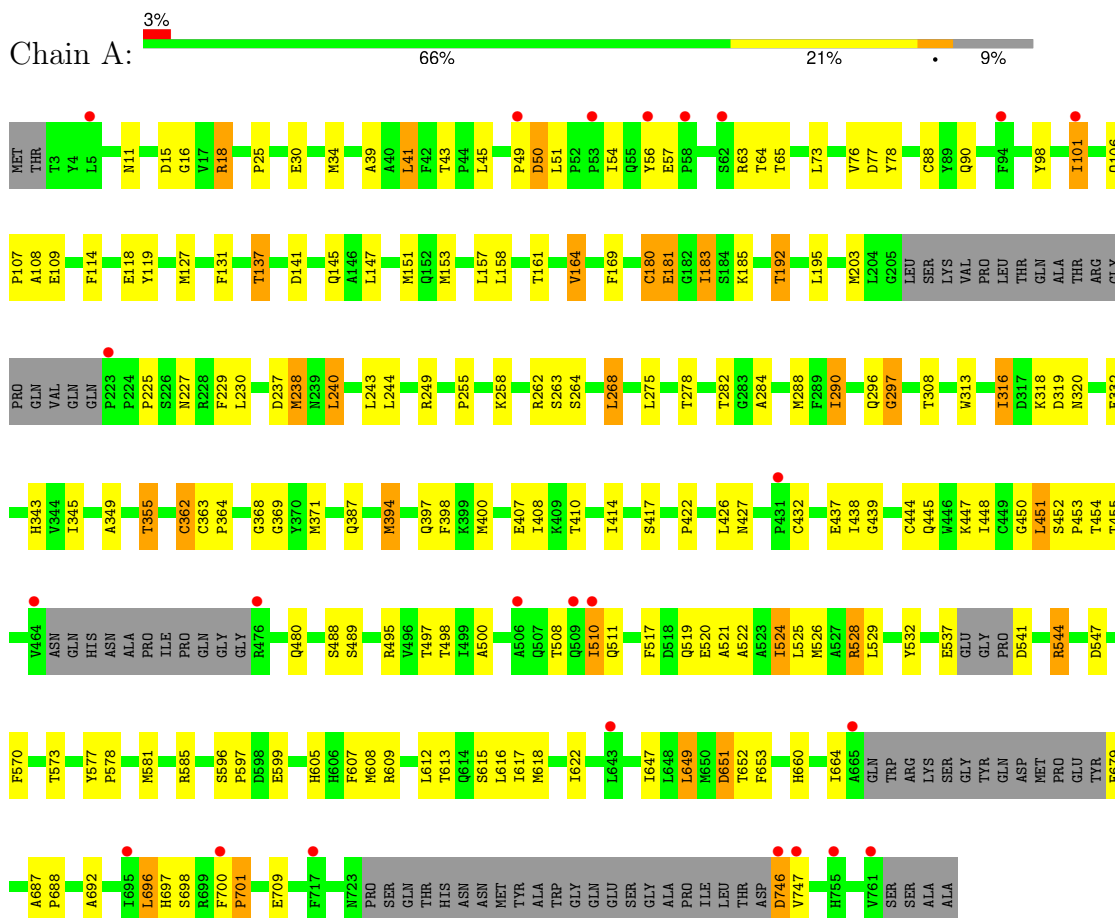
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	15	Total	O	0	0
			15	15		
6	B	23	Total	O	0	0
			23	23		
6	C	2	Total	O	0	0
			2	2		

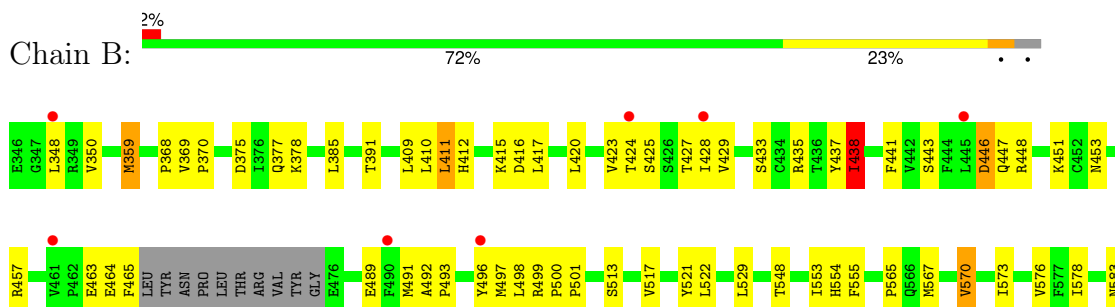
### 3 Residue-property plots

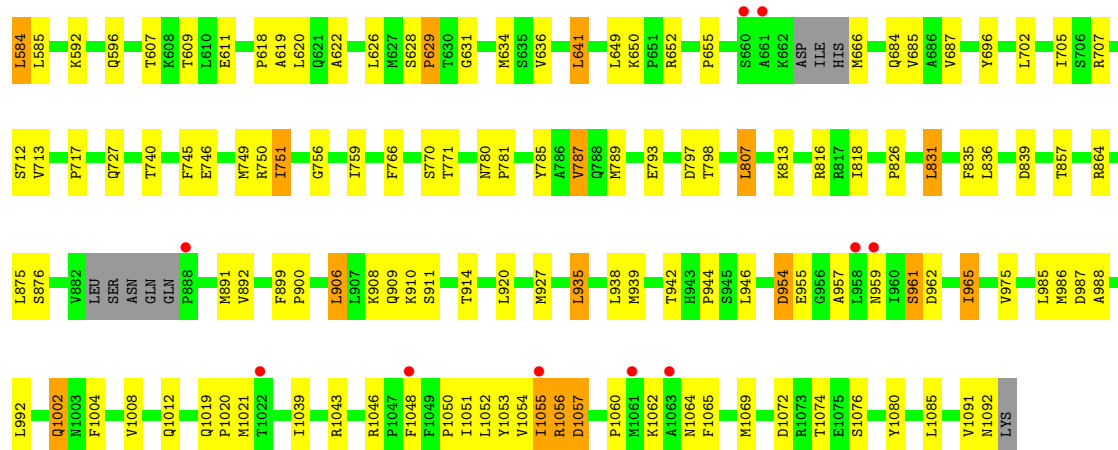
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

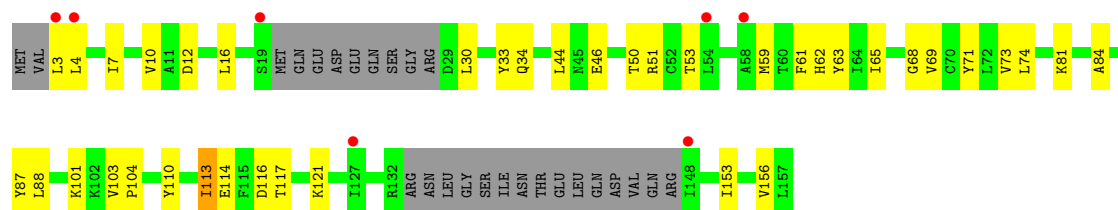


#### • Molecule 2: Protein transport protein Sec24A





• 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, $\alpha$ , $\beta$ , $\gamma$	147.45Å 96.80Å 128.69Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	81.05 – 2.49 81.05 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.0 (81.05-2.49) 99.2 (81.05-2.49)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.232 , 0.292 0.242 , 0.293	Depositor DCC
$R_{free}$ test set	1999 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.8	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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: ZN, A1CF9

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	0.53	0/5594	1.05	12/7580 (0.2%)
2	B	0.56	0/5845	1.07	11/7952 (0.1%)
3	C	0.53	0/1061	1.05	2/1431 (0.1%)
All	All	0.55	0/12500	1.06	25/16963 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
All	All	0	3

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	THR	CA-CB-OG1	-7.91	97.74	109.60
1	A	701	PRO	N-CA-C	-7.83	96.34	112.47
2	B	954	ASP	CB-CA-C	-7.50	101.72	111.40
1	A	43	THR	CA-CB-OG1	-7.00	99.10	109.60
1	A	573	THR	CA-CB-OG1	-6.77	99.45	109.60
1	A	192	THR	CA-CB-OG1	-6.29	100.17	109.60
2	B	707	ARG	N-CA-CB	6.29	119.13	110.01
1	A	746	ASP	CA-CB-CG	6.01	118.61	112.60
2	B	416	ASP	CA-CB-CG	5.98	118.58	112.60
2	B	629	PRO	N-CA-C	5.97	121.60	113.84
1	A	308	THR	CA-CB-OG1	-5.96	100.65	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	740	THR	CA-CB-OG1	-5.85	100.83	109.60
3	C	12	ASP	CA-CB-CG	5.59	118.19	112.60
2	B	1048	PHE	CA-CB-CG	5.51	119.31	113.80
1	A	137	THR	CA-CB-OG1	-5.49	101.36	109.60
1	A	497	THR	CA-CB-OG1	-5.44	101.44	109.60
2	B	1057	ASP	CA-CB-CG	5.40	118.00	112.60
3	C	117	THR	CA-CB-OG1	-5.21	101.79	109.60
1	A	237	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	651	ASP	CA-CB-CG	5.13	117.73	112.60
2	B	446	ASP	CA-CB-CG	5.12	117.72	112.60
2	B	1065	PHE	N-CA-CB	-5.09	102.43	110.06
2	B	962	ASP	CA-CB-CG	5.07	117.67	112.60
2	B	839	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	180	CYS	CB-CA-C	5.02	118.52	110.29

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	ARG	Sidechain
1	A	262	ARG	Sidechain
2	B	864	ARG	Sidechain

## 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	5467	0	5405	118	0
2	B	5721	0	5729	127	0
3	C	1042	0	1039	25	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	24	0	0	4	0
6	A	15	0	0	1	0
6	B	23	0	0	1	0
6	C	2	0	0	1	0
All	All	12296	0	12173	269	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 11.

All (269) 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:A:101:ILE:HD11	1:A:107:PRO:HD3	1.46	0.94
1:A:528:ARG:HA	1:A:608:MET:HE1	1.60	0.83
1:A:137:THR:OG1	1:A:169:PHE:O	1.96	0.81
1:A:153:MET:HE2	1:A:157:LEU:HD11	1.62	0.79
1:A:313:TRP:HA	1:A:316:ILE:HG22	1.69	0.75
1:A:127:MET:HE1	1:A:225:PRO:HG3	1.67	0.75
2:B:620:LEU:HD22	2:B:634:MET:CE	2.18	0.74
1:A:432:CYS:HB2	1:A:444:CYS:SG	2.27	0.73
2:B:955:GLU:OE1	2:B:955:GLU:N	2.23	0.71
1:A:410:THR:HB	1:A:414:ILE:HB	1.70	0.71
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.72	0.71
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.72	0.71
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.73	0.69
2:B:583:ASN:O	2:B:584:LEU:HG	1.92	0.68
1:A:195:LEU:HD13	1:A:203:MET:HE1	1.75	0.67
2:B:609:THR:HG22	2:B:611:GLU:H	1.58	0.67
1:A:651:ASP:OD1	1:A:652:THR:O	2.13	0.67
1:A:541:ASP:HB3	1:A:544:ARG:HD2	1.75	0.67
2:B:1057:ASP:O	2:B:1060:PRO:HD3	1.96	0.66
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	1.78	0.66
2:B:875:LEU:HD22	2:B:892:VAL:HG12	1.77	0.65
2:B:620:LEU:HD22	2:B:634:MET:HE1	1.79	0.65
2:B:1054:VAL:O	2:B:1056:ARG:N	2.30	0.64
1:A:30:GLU:CD	1:A:510:ILE:HD11	2.22	0.64
2:B:410:LEU:CD2	2:B:935:LEU:HG	2.28	0.64
2:B:576:VAL:HG11	2:B:622:ALA:HB2	1.78	0.64
3:C:113:ILE:O	3:C:116:ASP:HB2	1.98	0.64
2:B:684:GLN:OE1	2:B:746:GLU:HA	1.99	0.63
2:B:831:LEU:HD22	2:B:835:PHE:CE2	2.34	0.62
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.81	0.62
2:B:975:VAL:HG23	2:B:1072:ASP:OD2	1.99	0.62
2:B:578:ILE:HD11	2:B:626:LEU:HA	1.81	0.61
1:A:56:TYR:CE1	1:A:98:TYR:OH	2.53	0.61
2:B:513:SER:O	2:B:517:VAL:HG23	2.01	0.61
1:A:127:MET:HE2	1:A:127:MET:HA	1.83	0.61
2:B:411:LEU:N	2:B:411:LEU:HD23	2.16	0.61
1:A:696:LEU:O	1:A:697:HIS:ND1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.37	0.60
2:B:985:LEU:C	2:B:985:LEU:HD23	2.26	0.60
1:A:284:ALA:HB3	1:A:343:HIS:CD2	2.36	0.59
2:B:420:LEU:HD21	2:B:489:GLU:HB2	1.85	0.59
2:B:1069:MET:HE2	2:B:1069:MET:HA	1.84	0.59
2:B:944:PRO:HB3	2:B:988:ALA:HA	1.86	0.58
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.84	0.58
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.86	0.58
2:B:750:ARG:NH1	2:B:771:THR:O	2.31	0.58
2:B:702:LEU:O	2:B:705:ILE:HG22	2.03	0.58
3:C:7:ILE:O	3:C:16:LEU:HB2	2.04	0.57
2:B:359:MET:HE2	2:B:1080:TYR:OH	2.04	0.57
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.40	0.56
1:A:649:LEU:HD12	1:A:649:LEU:C	2.30	0.56
2:B:954:ASP:C	2:B:955:GLU:OE1	2.49	0.56
2:B:548:THR:OG1	2:B:554:HIS:HB2	2.05	0.56
1:A:108:ALA:HB1	1:A:114:PHE:CD2	2.41	0.55
2:B:578:ILE:CD1	2:B:626:LEU:HA	2.36	0.55
2:B:759:ILE:HG23	2:B:787:VAL:HG13	1.88	0.55
2:B:409:LEU:C	2:B:410:LEU:HD12	2.32	0.55
1:A:577:TYR:CE2	1:A:581:MET:HE3	2.42	0.55
1:A:596:SER:HG	1:A:599:GLU:HG3	1.70	0.55
1:A:56:TYR:OH	1:A:109:GLU:OE1	2.20	0.55
2:B:385:LEU:HD21	2:B:417:LEU:HD21	1.89	0.55
2:B:909:GLN:HG2	2:B:910:LYS:N	2.22	0.54
5:B:1201:A1CF9:C7	5:B:1201:A1CF9:O5	2.54	0.54
1:A:692:ALA:O	1:A:696:LEU:HB2	2.07	0.54
2:B:429:VAL:HG21	2:B:465:PHE:CE1	2.43	0.54
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.72	0.54
2:B:446:ASP:C	2:B:448:ARG:H	2.15	0.54
1:A:153:MET:CE	1:A:157:LEU:HD11	2.36	0.54
2:B:441:PHE:O	2:B:453:ASN:HB3	2.08	0.54
1:A:290:ILE:HG21	1:A:355:THR:HG23	1.90	0.54
1:A:537:GLU:N	1:A:537:GLU:OE1	2.39	0.54
2:B:770:SER:O	2:B:771:THR:OG1	2.23	0.54
3:C:44:LEU:HD13	3:C:65:ILE:HD11	1.89	0.54
1:A:426:LEU:O	1:A:427:ASN:C	2.50	0.54
1:A:517:PHE:CE2	1:A:519:GLN:HA	2.43	0.54
1:A:368:GLY:HA3	1:A:450:GLY:O	2.08	0.54
1:A:596:SER:OG	1:A:599:GLU:HG3	2.08	0.53
2:B:412:HIS:CE1	2:B:415:LYS:HB2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.90	0.53
2:B:987:ASP:OD2	2:B:1046:ARG:NH2	2.39	0.53
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.38	0.53
3:C:50:THR:O	3:C:51:ARG:HG2	2.08	0.53
2:B:578:ILE:HD11	2:B:626:LEU:CA	2.38	0.53
1:A:417:SER:O	1:A:437:GLU:HA	2.10	0.52
2:B:435:ARG:NH2	5:B:1201:A1CF9:O4	2.43	0.52
2:B:992:LEU:O	2:B:1052:LEU:HA	2.10	0.52
2:B:359:MET:SD	2:B:359:MET:N	2.82	0.52
2:B:1055:ILE:O	2:B:1057:ASP:N	2.43	0.52
2:B:1004:PHE:CE1	2:B:1008:VAL:HG11	2.45	0.52
2:B:634:MET:HE3	2:B:636:VAL:CG2	2.39	0.51
2:B:655:PRO:HD3	2:B:920:LEU:HD13	1.91	0.51
3:C:10:VAL:HG23	3:C:68:GLY:O	2.09	0.51
3:C:113:ILE:HD13	3:C:113:ILE:H	1.74	0.51
1:A:11:ASN:ND2	6:A:901:HOH:O	2.32	0.51
2:B:493:PRO:HD2	2:B:496:TYR:CD2	2.46	0.51
2:B:634:MET:HE2	2:B:687:VAL:HG13	1.92	0.51
2:B:433:SER:OG	2:B:457:ARG:HD3	2.10	0.51
3:C:63:TYR:CD1	3:C:63:TYR:C	2.89	0.51
2:B:987:ASP:CG	2:B:1046:ARG:HH22	2.17	0.51
2:B:965:ILE:N	2:B:965:ILE:HD12	2.26	0.51
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.91	0.51
1:A:313:TRP:HA	1:A:316:ILE:CG2	2.39	0.51
1:A:180:CYS:O	1:A:181:GLU:C	2.54	0.50
1:A:185:LYS:HB2	2:B:567:MET:HB3	1.94	0.50
2:B:1002:GLN:OE1	2:B:1012:GLN:O	2.29	0.50
2:B:576:VAL:CG1	2:B:622:ALA:HB2	2.41	0.50
2:B:410:LEU:HD22	2:B:935:LEU:HG	1.92	0.50
1:A:183:ILE:O	1:A:183:ILE:HG23	2.11	0.50
1:A:371:MET:HB3	1:A:605:HIS:CD2	2.46	0.49
1:A:687:ALA:N	1:A:688:PRO:HD2	2.27	0.49
1:A:607:PHE:HD2	1:A:608:MET:HE3	1.76	0.49
2:B:592:LYS:O	2:B:596:GLN:HG3	2.12	0.49
1:A:547:ASP:OD2	1:A:585:ARG:NH2	2.43	0.49
3:C:33:TYR:CZ	3:C:59:MET:HG3	2.47	0.49
1:A:521:ALA:HA	1:A:612:LEU:HD12	1.95	0.49
2:B:906:LEU:HD13	2:B:942:THR:HG21	1.94	0.49
1:A:313:TRP:CE3	1:A:316:ILE:HG21	2.48	0.49
1:A:422:PRO:O	1:A:448:ILE:HG23	2.13	0.49
1:A:88:CYS:C	1:A:90:GLN:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:MET:HE2	1:A:290:ILE:HD11	1.94	0.49
2:B:437:TYR:O	2:B:438:ILE:C	2.56	0.49
2:B:368:PRO:HB2	2:B:391:THR:HG21	1.93	0.49
2:B:780:ASN:HB2	2:B:781:PRO:HD2	1.95	0.48
1:A:240:LEU:HD22	1:A:244:LEU:HG	1.94	0.48
2:B:1053:TYR:HD2	2:B:1055:ILE:HB	1.78	0.48
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.95	0.48
1:A:438:ILE:HG21	1:A:529:LEU:HD21	1.94	0.48
1:A:164:VAL:O	1:A:230:LEU:HA	2.13	0.48
2:B:496:TYR:CD2	2:B:818:ILE:HD11	2.49	0.48
3:C:103:VAL:N	3:C:104:PRO:HD2	2.29	0.48
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.48	0.48
2:B:641:LEU:CD2	2:B:649:LEU:HB2	2.44	0.48
1:A:524:ILE:HG13	1:A:615:SER:HB3	1.95	0.47
1:A:25:PRO:HD3	1:A:34:MET:HE3	1.96	0.47
2:B:500:PRO:O	2:B:501:PRO:C	2.57	0.47
1:A:41:LEU:HD21	1:A:524:ILE:HG21	1.95	0.47
1:A:296:GLN:O	1:A:297:GLY:O	2.32	0.47
2:B:785:TYR:OH	6:B:1301:HOH:O	2.20	0.47
1:A:238:MET:HE2	1:A:238:MET:HB3	1.73	0.47
2:B:553:ILE:HG12	2:B:619:ALA:HA	1.96	0.47
2:B:666:MET:HE2	2:B:927:MET:HE1	1.95	0.47
1:A:452:SER:HB2	1:A:453:PRO:CD	2.45	0.46
2:B:620:LEU:HD22	2:B:634:MET:HE3	1.95	0.46
2:B:424:THR:HG22	2:B:491:MET:HG3	1.97	0.46
3:C:53:THR:HG23	3:C:62:HIS:CE1	2.50	0.46
1:A:41:LEU:HD13	1:A:525:LEU:HG	1.98	0.46
1:A:63:ARG:O	1:A:64:THR:C	2.59	0.46
1:A:313:TRP:CA	1:A:316:ILE:HG22	2.41	0.46
2:B:620:LEU:CD2	2:B:636:VAL:HG21	2.44	0.46
1:A:101:ILE:CD1	1:A:107:PRO:HD3	2.33	0.46
1:A:700:PHE:C	1:A:700:PHE:CD1	2.93	0.46
2:B:1054:VAL:O	2:B:1055:ILE:C	2.59	0.46
3:C:110:TYR:HB3	3:C:113:ILE:CG2	2.46	0.46
2:B:957:ALA:C	2:B:959:ASN:H	2.22	0.46
3:C:10:VAL:HG23	3:C:68:GLY:C	2.41	0.46
3:C:61:PHE:CE1	3:C:153:ILE:HD12	2.51	0.46
2:B:959:ASN:O	2:B:961:SER:N	2.49	0.46
1:A:618:MET:HG2	1:A:653:PHE:HB3	1.98	0.45
2:B:499:ARG:HA	3:C:34:GLN:HE22	1.81	0.45
2:B:909:GLN:HG2	2:B:911:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:TYR:O	1:A:57:GLU:C	2.57	0.45
1:A:147:LEU:HG	1:A:151:MET:HE2	1.98	0.45
1:A:153:MET:CE	1:A:387:GLN:HB3	2.46	0.45
2:B:377:GLN:OE1	2:B:377:GLN:HA	2.17	0.45
3:C:73:VAL:HB	3:C:88:LEU:HD21	1.98	0.45
1:A:183:ILE:HD12	2:B:565:PRO:HG2	1.97	0.45
2:B:985:LEU:HD23	2:B:986:MET:N	2.31	0.45
3:C:63:TYR:HA	3:C:71:TYR:O	2.16	0.45
1:A:49:PRO:C	1:A:50:ASP:CG	2.85	0.45
1:A:577:TYR:CZ	1:A:581:MET:HE3	2.52	0.45
1:A:227:ASN:HB3	1:A:229:PHE:H	1.82	0.45
1:A:700:PHE:CB	1:A:701:PRO:HD3	2.47	0.45
1:A:153:MET:HE2	1:A:157:LEU:CD1	2.40	0.45
1:A:454:THR:O	1:A:455:THR:C	2.60	0.45
2:B:628:SER:HB3	2:B:629:PRO:HD3	1.98	0.45
1:A:398:PHE:HB3	1:A:400:MET:HG2	1.98	0.45
2:B:463:GLU:O	2:B:465:PHE:N	2.50	0.45
2:B:766:PHE:CD1	2:B:766:PHE:C	2.95	0.45
2:B:1046:ARG:HD2	2:B:1050:PRO:HG3	1.98	0.45
2:B:521:TYR:CD1	2:B:521:TYR:C	2.94	0.45
2:B:631:GLY:HA2	2:B:685:VAL:HG22	1.98	0.45
1:A:15:ASP:O	1:A:16:GLY:C	2.60	0.44
1:A:54:ILE:HG23	1:A:56:TYR:CE2	2.52	0.44
1:A:679:GLU:HA	1:A:679:GLU:OE1	2.17	0.44
3:C:110:TYR:HB3	3:C:113:ILE:HG23	1.99	0.44
1:A:397:GLN:OE1	1:A:489:SER:HB3	2.16	0.44
3:C:103:VAL:N	3:C:104:PRO:CD	2.81	0.44
1:A:345:ILE:O	1:A:369:GLY:HA3	2.17	0.44
1:A:577:TYR:HB3	1:A:578:PRO:HD3	1.98	0.44
1:A:617:ILE:HG12	1:A:622:ILE:CD1	2.47	0.44
2:B:375:ASP:O	2:B:378:LYS:HG2	2.16	0.44
3:C:69:VAL:HG22	3:C:103:VAL:HG11	2.00	0.44
1:A:268:LEU:HG	1:A:288:MET:SD	2.57	0.44
1:A:407:GLU:HG3	1:A:445:GLN:HG3	1.99	0.44
2:B:438:ILE:O	2:B:438:ILE:HG23	2.17	0.44
2:B:369:VAL:O	2:B:370:PRO:C	2.61	0.44
2:B:831:LEU:HD22	2:B:835:PHE:HE2	1.82	0.44
1:A:56:TYR:HD1	1:A:57:GLU:O	2.01	0.44
2:B:350:VAL:HG12	2:B:891:MET:HE3	2.00	0.44
2:B:749:MET:HE3	2:B:751:ILE:HD11	2.00	0.43
3:C:33:TYR:HB3	3:C:74:LEU:CD2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:CE2	1:A:158:LEU:HD22	2.54	0.43
1:A:255:PRO:O	1:A:258:LYS:HB2	2.19	0.43
1:A:408:ILE:HA	1:A:480:GLN:O	2.19	0.43
1:A:605:HIS:O	1:A:609:ARG:HD3	2.19	0.43
2:B:425:SER:HB3	2:B:427:THR:O	2.19	0.43
2:B:938:LEU:O	2:B:938:LEU:HD12	2.19	0.43
1:A:195:LEU:HD13	1:A:203:MET:CE	2.46	0.43
2:B:497:MET:HE2	2:B:816:ARG:HG3	2.01	0.43
2:B:428:ILE:HG21	2:B:437:TYR:HE2	1.84	0.43
2:B:727:GLN:OE1	2:B:727:GLN:HA	2.19	0.43
2:B:875:LEU:HD22	2:B:892:VAL:CG1	2.46	0.43
5:B:1201:A1CF9:O5	5:B:1201:A1CF9:C15	2.67	0.43
2:B:553:ILE:HD12	2:B:573:ILE:CD1	2.48	0.42
2:B:583:ASN:O	2:B:584:LEU:CG	2.65	0.42
2:B:807:LEU:O	2:B:818:ILE:HA	2.19	0.42
1:A:73:LEU:HD11	1:A:500:ALA:HB2	2.01	0.42
2:B:489:GLU:HA	2:B:818:ILE:O	2.19	0.42
3:C:84:ALA:O	3:C:87:TYR:HB3	2.20	0.42
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.33	0.42
1:A:76:VAL:HG11	1:A:78:TYR:CE1	2.55	0.42
1:A:541:ASP:CB	1:A:544:ARG:HD2	2.46	0.42
2:B:1039:ILE:O	2:B:1043:ARG:HG2	2.20	0.42
2:B:443:SER:HB2	2:B:451:LYS:HB3	2.02	0.42
2:B:1074:THR:C	2:B:1076:SER:H	2.27	0.42
2:B:655:PRO:CD	2:B:920:LEU:HD13	2.49	0.42
2:B:756:GLY:HA2	2:B:793:GLU:HB2	2.00	0.42
1:A:320:ASN:O	1:A:320:ASN:CG	2.63	0.42
1:A:522:ALA:O	1:A:526:MET:HG2	2.20	0.42
1:A:660:HIS:HB2	1:A:709:GLU:HB3	2.01	0.42
2:B:348:LEU:HD12	2:B:836:LEU:HD21	2.01	0.42
2:B:529:LEU:HD23	2:B:529:LEU:HA	1.81	0.42
2:B:745:PHE:O	2:B:746:GLU:C	2.62	0.42
2:B:1060:PRO:O	2:B:1062:LYS:HG3	2.20	0.42
1:A:108:ALA:O	1:A:109:GLU:C	2.63	0.42
1:A:39:ALA:HB3	1:A:525:LEU:HD13	2.01	0.42
1:A:101:ILE:HD11	1:A:106:GLN:HA	2.00	0.42
2:B:585:LEU:HG	2:B:626:LEU:HD11	2.02	0.42
1:A:30:GLU:OE1	1:A:510:ILE:HD11	2.20	0.42
1:A:118:GLU:HB2	1:A:495:ARG:HD2	2.02	0.42
1:A:263:SER:O	1:A:264:SER:C	2.63	0.42
1:A:426:LEU:HD21	1:A:447:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:GLU:HB3	1:A:616:LEU:HD11	2.02	0.41
2:B:555:PHE:HE1	2:B:570:VAL:CG1	2.33	0.41
3:C:114:GLU:HB2	6:C:202:HOH:O	2.20	0.41
1:A:290:ILE:HG21	1:A:355:THR:CG2	2.50	0.41
1:A:332:GLU:HG3	1:A:362:CYS:SG	2.60	0.41
2:B:985:LEU:C	2:B:985:LEU:CD2	2.92	0.41
3:C:53:THR:CG2	3:C:62:HIS:CE1	3.04	0.41
1:A:394:MET:H	1:A:394:MET:HE3	1.86	0.41
2:B:908:LYS:NZ	2:B:1072:ASP:O	2.54	0.41
2:B:946:LEU:HD22	2:B:1069:MET:HE1	2.02	0.41
2:B:1020:PRO:HA	2:B:1055:ILE:CG1	2.47	0.41
3:C:113:ILE:HD13	3:C:113:ILE:N	2.35	0.41
1:A:313:TRP:NE1	1:A:597:PRO:HA	2.36	0.41
1:A:76:VAL:HG12	1:A:77:ASP:N	2.36	0.41
1:A:363:CYS:HB2	1:A:364:PRO:CD	2.51	0.41
1:A:101:ILE:HA	1:A:101:ILE:HD13	1.60	0.40
1:A:275:LEU:HA	1:A:278:THR:OG1	2.21	0.40
2:B:410:LEU:HD23	2:B:935:LEU:HG	2.02	0.40
1:A:318:LYS:O	1:A:319:ASP:C	2.65	0.40
2:B:498:LEU:CD1	5:B:1201:A1CF9:C3	2.99	0.40
2:B:717:PRO:HD2	2:B:727:GLN:NE2	2.35	0.40
2:B:876:SER:HA	2:B:1091:VAL:HG13	2.02	0.40
2:B:935:LEU:HD22	2:B:939:MET:HG2	2.04	0.40
1:A:54:ILE:O	1:A:119:TYR:HA	2.21	0.40
1:A:141:ASP:OD1	1:A:249:ARG:HD3	2.21	0.40
2:B:1054:VAL:C	2:B:1056:ARG:N	2.79	0.40
3:C:4:LEU:HD13	3:C:30:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	681/765 (89%)	627 (92%)	51 (8%)	3 (0%)	30	49
2	B	721/748 (96%)	659 (91%)	55 (8%)	7 (1%)	12	24
3	C	125/157 (80%)	117 (94%)	8 (6%)	0	100	100
All	All	1527/1670 (91%)	1403 (92%)	114 (8%)	10 (1%)	18	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	464	GLU
2	B	584	LEU
2	B	1056	ARG
1	A	297	GLY
2	B	438	ILE
2	B	1055	ILE
1	A	181	GLU
2	B	961	SER
2	B	447	GLN
1	A	183	ILE

### 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	600/666 (90%)	566 (94%)	34 (6%)	18	39
2	B	652/679 (96%)	622 (95%)	30 (5%)	24	48
3	C	112/138 (81%)	105 (94%)	7 (6%)	16	34
All	All	1364/1483 (92%)	1293 (95%)	71 (5%)	21	42

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	50	ASP
1	A	51	LEU

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Mol	Chain	Res	Type
1	A	65	THR
1	A	101	ILE
1	A	145	GLN
1	A	161	THR
1	A	164	VAL
1	A	192	THR
1	A	238	MET
1	A	240	LEU
1	A	243	LEU
1	A	268	LEU
1	A	290	ILE
1	A	316	ILE
1	A	355	THR
1	A	362	CYS
1	A	394	MET
1	A	451	LEU
1	A	488	SER
1	A	498	THR
1	A	508	THR
1	A	510	ILE
1	A	511	GLN
1	A	524	ILE
1	A	528	ARG
1	A	544	ARG
1	A	570	PHE
1	A	613	THR
1	A	649	LEU
1	A	696	LEU
1	A	698	SER
1	A	746	ASP
1	A	747	VAL
2	B	359	MET
2	B	411	LEU
2	B	423	VAL
2	B	438	ILE
2	B	522	LEU
2	B	570	VAL
2	B	607	THR
2	B	641	LEU
2	B	650	LYS
2	B	712	SER
2	B	713	VAL

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Mol	Chain	Res	Type
2	B	751	ILE
2	B	787	VAL
2	B	789	MET
2	B	797	ASP
2	B	798	THR
2	B	807	LEU
2	B	813	LYS
2	B	826	PRO
2	B	831	LEU
2	B	857	THR
2	B	906	LEU
2	B	914	THR
2	B	935	LEU
2	B	965	ILE
2	B	1002	GLN
2	B	1051	ILE
2	B	1064	ASN
2	B	1085	LEU
2	B	1092	ASN
3	C	3	LEU
3	C	46	GLU
3	C	81	LYS
3	C	101	LYS
3	C	113	ILE
3	C	121	LYS
3	C	156	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	343	HIS
1	A	512	ASN
1	A	660	HIS
2	B	395	GLN
2	B	514	HIS
2	B	596	GLN
2	B	604	GLN
2	B	832	ASN
2	B	1007	GLN
2	B	1092	ASN
3	C	34	GLN

### 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	A1CF9	B	1201	-	24,26,26	1.37	3 (12%)	30,38,38	1.61	6 (20%)

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	A1CF9	B	1201	-	-	11/22/35/35	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1201	A1CF9	O2-C17	3.10	1.31	1.22
5	B	1201	A1CF9	C11-C10	3.00	1.43	1.39
5	B	1201	A1CF9	C16-C8	-2.89	1.49	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1201	A1CF9	C9-C16-C18	4.60	130.65	117.33
5	B	1201	A1CF9	C10-C9-C8	4.49	129.77	123.07
5	B	1201	A1CF9	C15-C10-C9	2.52	126.64	120.99
5	B	1201	A1CF9	C17-C16-C18	-2.28	111.50	115.36
5	B	1201	A1CF9	C11-C10-C9	-2.27	115.90	120.99
5	B	1201	A1CF9	C8-C16-C18	-2.20	110.64	118.58

There are no chirality outliers.

All (11) torsion outliers are listed below:

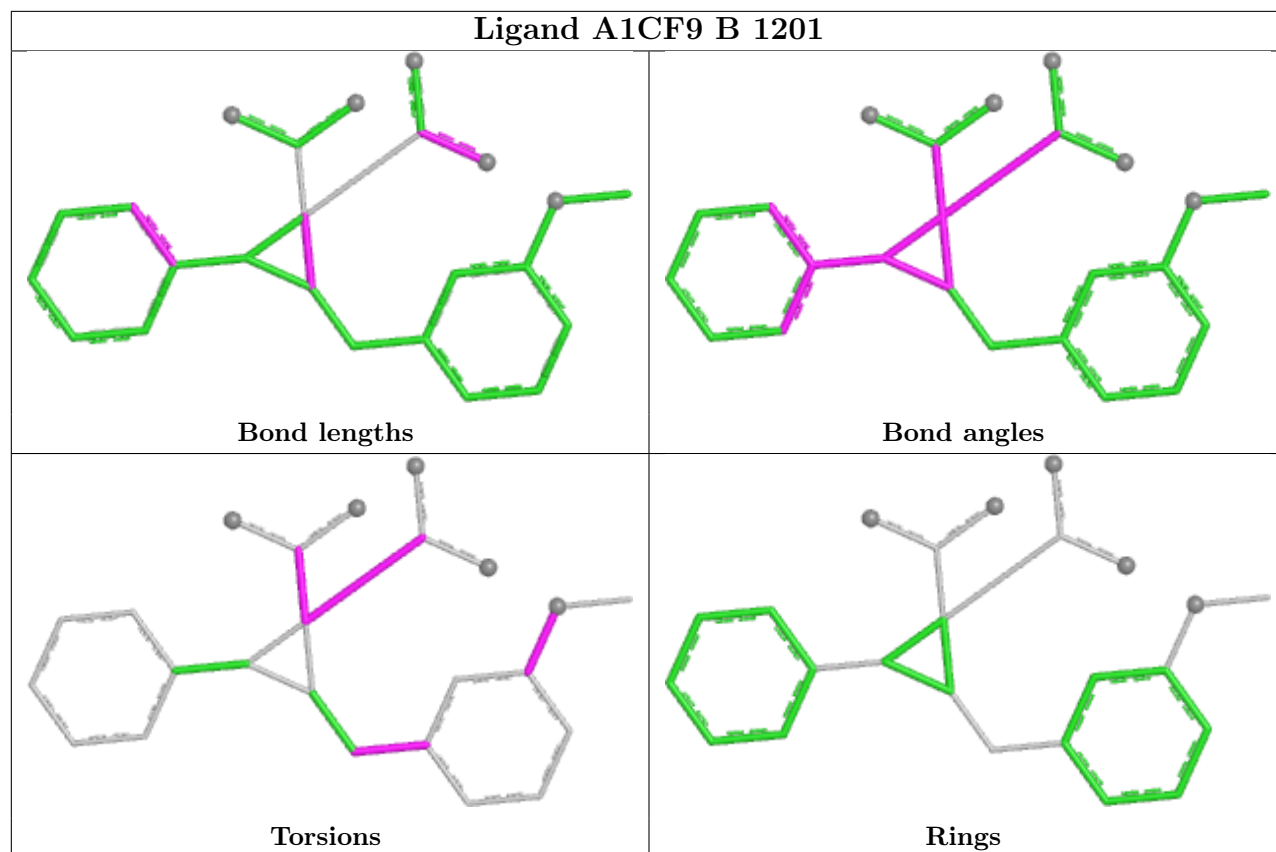
Mol	Chain	Res	Type	Atoms
5	B	1201	A1CF9	C9-C16-C17-O2
5	B	1201	A1CF9	C9-C16-C17-O3
5	B	1201	A1CF9	C18-C16-C17-O3
5	B	1201	A1CF9	C19-C2-O1-C1
5	B	1201	A1CF9	C3-C2-O1-C1
5	B	1201	A1CF9	C19-C6-C7-C8
5	B	1201	A1CF9	C5-C6-C7-C8
5	B	1201	A1CF9	C9-C16-C18-O4
5	B	1201	A1CF9	C9-C16-C18-O5
5	B	1201	A1CF9	C17-C16-C18-O4
5	B	1201	A1CF9	C8-C16-C18-O4

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1201	A1CF9	4	0

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, 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	693/765 (90%)	0.29	24 (3%) 47 42	47, 75, 117, 153	0
2	B	729/748 (97%)	0.08	17 (2%) 61 57	43, 65, 107, 148	0
3	C	131/157 (83%)	0.49	7 (5%) 32 28	51, 90, 129, 150	0
All	All	1553/1670 (92%)	0.21	48 (3%) 51 47	43, 71, 117, 153	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	665	ALA	3.9
2	B	1055	ILE	3.9
3	C	127	ILE	3.9
2	B	348	LEU	3.4
3	C	148	ILE	3.3
3	C	3	LEU	3.2
2	B	424	THR	3.1
2	B	496	TYR	3.1
2	B	959	ASN	3.1
1	A	49	PRO	3.0
2	B	888	PRO	3.0
2	B	445	LEU	2.9
1	A	506	ALA	2.9
2	B	661	ALA	2.8
2	B	1048	PHE	2.8
2	B	1063	ALA	2.7
1	A	223	PRO	2.7
1	A	464	VAL	2.6
2	B	1022	THR	2.6
1	A	700	PHE	2.6
1	A	62	SER	2.6
1	A	747	VAL	2.4
1	A	755	HIS	2.4

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	A	643	LEU	2.3
2	B	428	ILE	2.3
1	A	509	GLN	2.3
3	C	54	LEU	2.3
1	A	101	ILE	2.2
1	A	431	PRO	2.2
3	C	58	ALA	2.2
1	A	53	PRO	2.2
1	A	58	PRO	2.2
1	A	761	VAL	2.1
2	B	1061	MET	2.1
3	C	19	SER	2.1
2	B	461	VAL	2.1
2	B	958	LEU	2.1
1	A	510	ILE	2.1
1	A	695	ILE	2.1
1	A	476	ARG	2.1
2	B	660	SER	2.1
1	A	94	PHE	2.0
3	C	4	LEU	2.0
1	A	717	PHE	2.0
2	B	490	PHE	2.0
1	A	5	LEU	2.0
1	A	746	ASP	2.0
1	A	56	TYR	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, 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.

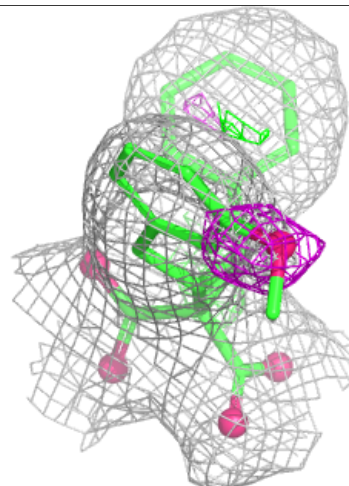
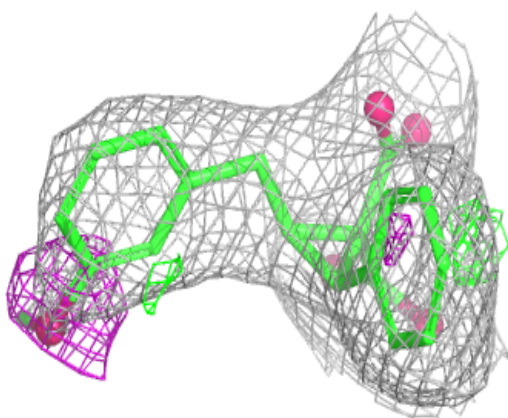
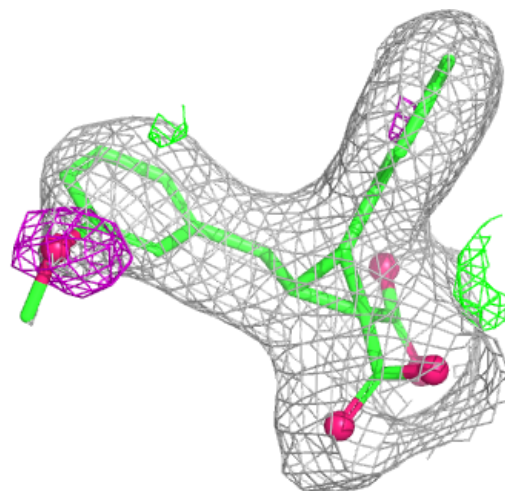


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	A1CF9	B	1201	24/24	0.90	0.10	35,49,64,70	0
4	ZN	B	1202	1/1	0.99	0.02	71,71,71,71	0
4	ZN	A	800	1/1	1.00	0.02	86,86,86,86	0

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.

**Electron density around A1CF9 B 1201:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.