



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2026 – 06:06 PM EDT

PDB ID : 9P06 / pdb\_00009p06  
Title : Structure of human Sec23a/Sec24a/Sec22b bound to ligand CPD12  
Authors : Goldberg, J.  
Deposited on : 2025-06-06  
Resolution : 2.65 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

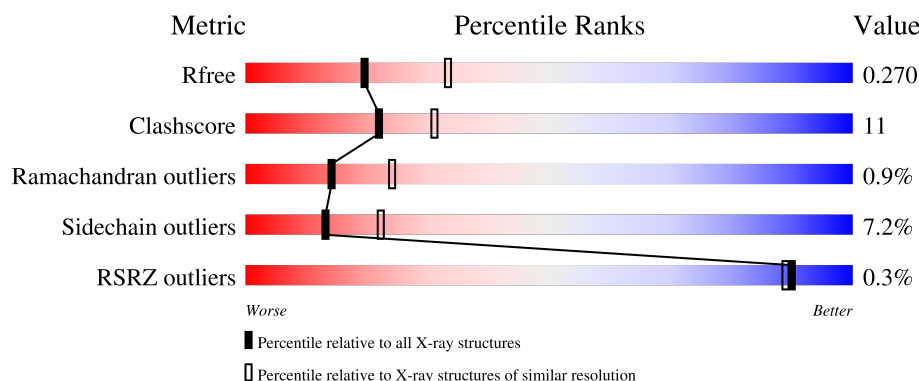
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	 66% 21% 9%
2	B	748	 69% 25%
3	C	157	 59% 23% 15%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12346 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
			5473	3495	934	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			

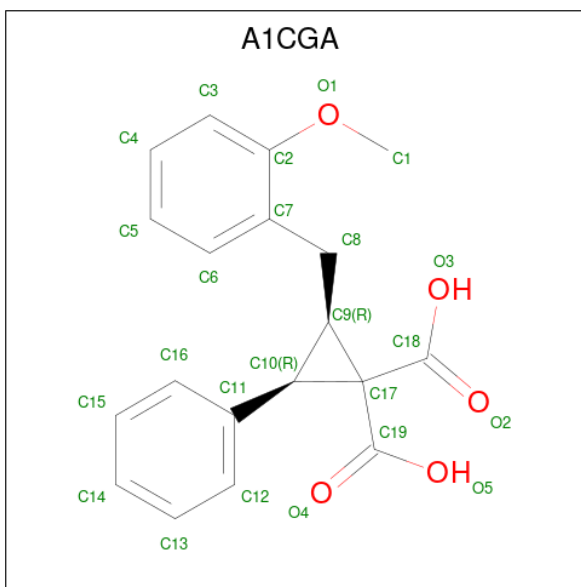
- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	133	Total	C	N	O	S	0	0	0
			1063	686	174	196	7			

- 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-[(2-methoxyphenyl)methyl]-3-phenylcyclopropane-1,1-dicarboxylic acid (CCD ID: A1CGA) (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		

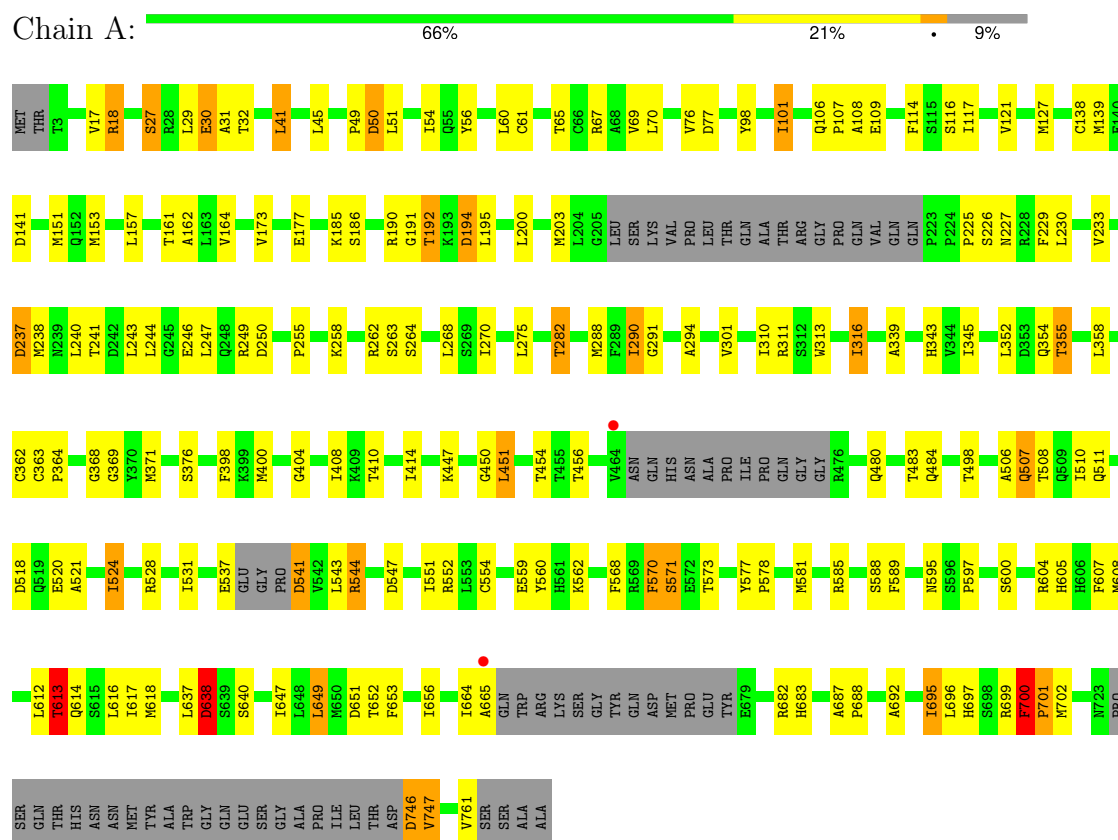
- Molecule 6 is water.

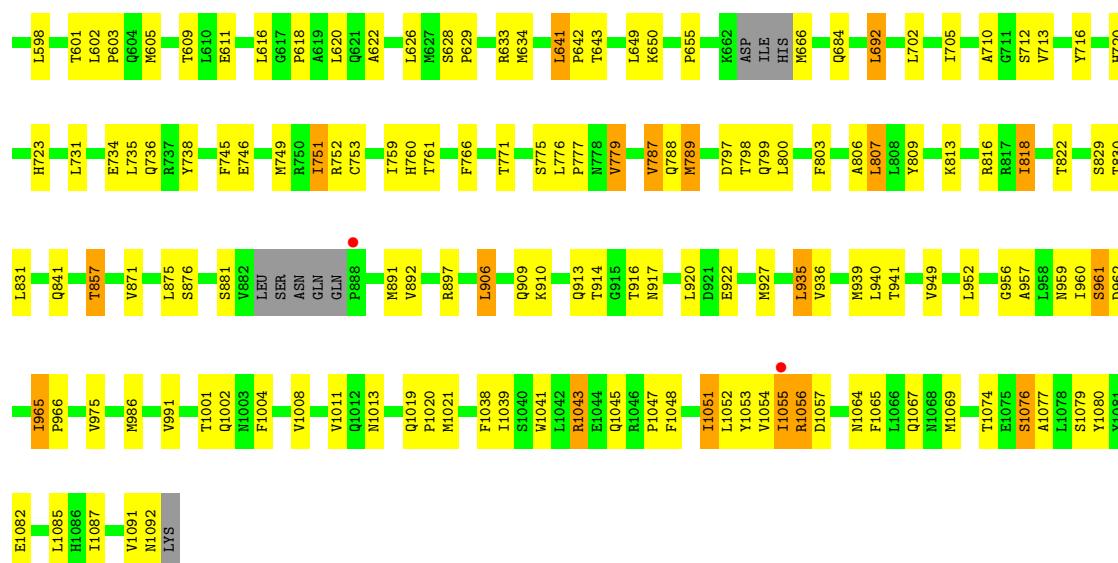
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total	O	0	0
			27	27		
6	B	32	Total	O	0	0
			32	32		
6	C	4	Total	O	0	0
			4	4		

### 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.

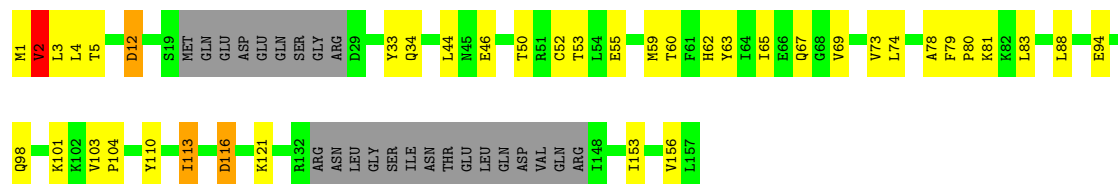
#### • Molecule 1: Protein transport protein Sec23A





• Molecule 3: Vesicle-trafficking protein SEC22b

Chain C: 59% 23% 15%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.78Å 95.94Å 129.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.00 – 2.65 74.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (74.00-2.65) 99.2 (74.00-2.65)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.206 , 0.275 0.209 , 0.270	Depositor DCC
$R_{free}$ test set	1990 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	88.2	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 63.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12346	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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, A1CGA

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	0.54	1/5600 (0.0%)	1.02	16/7587 (0.2%)
2	B	0.54	0/5845	1.04	6/7952 (0.1%)
3	C	0.52	0/1082	1.04	1/1458 (0.1%)
All	All	0.54	1/12527 (0.0%)	1.03	23/16997 (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	1
3	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	665	ALA	C-O	10.33	1.44	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	THR	CA-CB-OG1	-7.17	98.85	109.60
2	B	1048	PHE	N-CA-CB	6.64	119.74	109.85
1	A	192	THR	CA-CB-OG1	-6.07	100.50	109.60
1	A	652	THR	CA-CB-OG1	-6.06	100.51	109.60
2	B	857	THR	CA-CB-OG1	-6.00	100.60	109.60
1	A	700	PHE	N-CA-CB	5.69	120.50	110.37
2	B	416	ASP	CA-CB-CG	5.67	118.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	THR	CA-CB-OG1	-5.57	101.24	109.60
3	C	5	THR	CA-CB-OG1	-5.55	101.28	109.60
1	A	613	THR	CA-CB-OG1	-5.52	101.32	109.60
2	B	830	THR	CA-CB-OG1	-5.47	101.39	109.60
1	A	701	PRO	N-CA-C	-5.35	101.45	112.47
1	A	18	ARG	CB-CA-C	-5.33	104.82	111.43
2	B	941	THR	CA-CB-OG1	-5.33	101.60	109.60
1	A	638	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	747	VAL	N-CA-CB	5.30	118.15	110.52
1	A	454	THR	CA-CB-OG1	-5.23	101.76	109.60
1	A	194	ASP	CA-CB-CG	5.12	117.72	112.60
2	B	1065	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	250	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	541	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	237	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	746	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	651	ASP	Peptide
3	C	2	VAL	Peptide

## 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	5473	0	5416	109	0
2	B	5721	0	5729	134	0
3	C	1063	0	1071	21	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	24	0	0	0	0
6	A	27	0	0	3	0
6	B	32	0	0	0	0
6	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12346	0	12216	262	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 (262) 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:528:ARG:HA	1:A:608:MET:HE1	1.53	0.89
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.60	0.84
2:B:417:LEU:HD12	2:B:420:LEU:HD13	1.67	0.76
2:B:875:LEU:HD22	2:B:892:VAL:HG12	1.67	0.76
1:A:101:ILE:HD11	1:A:107:PRO:HD3	1.69	0.74
2:B:436:THR:HG21	2:B:454:LEU:HD13	1.71	0.73
1:A:138:CYS:HB2	1:A:262:ARG:NH1	2.04	0.72
2:B:1074:THR:HG22	2:B:1077:ALA:HB3	1.70	0.71
1:A:313:TRP:HA	1:A:316:ILE:HG22	1.72	0.71
1:A:138:CYS:HB2	1:A:262:ARG:HH11	1.55	0.70
2:B:841:GLN:HG2	2:B:939:MET:HG3	1.74	0.70
1:A:456:THR:O	1:A:528:ARG:NH2	2.26	0.69
1:A:531:ILE:HD11	1:A:589:PHE:HB3	1.76	0.68
3:C:113:ILE:O	3:C:116:ASP:HB2	1.94	0.67
2:B:576:VAL:HG11	2:B:622:ALA:HB2	1.77	0.67
1:A:195:LEU:HD13	1:A:203:MET:HE1	1.77	0.67
1:A:577:TYR:CE2	1:A:581:MET:HE3	2.29	0.67
2:B:986:MET:HE1	2:B:1069:MET:HE3	1.78	0.66
2:B:1055:ILE:O	2:B:1057:ASP:N	2.28	0.66
2:B:609:THR:HG22	2:B:611:GLU:H	1.61	0.66
2:B:716:TYR:OH	2:B:734:GLU:OE1	2.07	0.66
2:B:578:ILE:HD11	2:B:626:LEU:CA	2.26	0.65
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.79	0.65
1:A:410:THR:HB	1:A:414:ILE:HB	1.79	0.65
2:B:429:VAL:HG21	2:B:465:PHE:CE1	2.31	0.65
1:A:537:GLU:N	1:A:537:GLU:OE1	2.29	0.65
2:B:759:ILE:HG23	2:B:787:VAL:HG13	1.80	0.64
2:B:578:ILE:HD11	2:B:626:LEU:HA	1.79	0.64
2:B:578:ILE:CD1	2:B:626:LEU:HA	2.28	0.63
1:A:127:MET:HE1	1:A:225:PRO:HG3	1.79	0.63
1:A:108:ALA:HB1	1:A:114:PHE:CD2	2.34	0.63
2:B:350:VAL:CG1	2:B:891:MET:HE3	2.29	0.62
1:A:618:MET:HG2	1:A:653:PHE:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:567:MET:HE2	2:B:569:ILE:HD11	1.81	0.62
1:A:451:LEU:H	1:A:451:LEU:HD12	1.65	0.62
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	1.81	0.62
2:B:913:GLN:NE2	2:B:916:THR:HG21	2.14	0.61
2:B:909:GLN:HG2	2:B:910:LYS:N	2.14	0.61
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.84	0.60
1:A:275:LEU:HB3	1:A:343:HIS:CE1	2.37	0.60
2:B:710:ALA:HB3	2:B:777:PRO:HD2	1.86	0.58
1:A:70:LEU:HD23	1:A:109:GLU:HG3	1.86	0.58
1:A:313:TRP:HA	1:A:316:ILE:CG2	2.35	0.57
1:A:290:ILE:HG21	1:A:355:THR:HG21	1.86	0.57
2:B:601:THR:CG2	2:B:605:MET:HE3	2.34	0.57
2:B:414:PHE:CD2	2:B:779:VAL:HG22	2.39	0.56
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.87	0.56
3:C:53:THR:HG23	3:C:62:HIS:CE1	2.41	0.56
2:B:633:ARG:HD2	2:B:738:TYR:OH	2.05	0.56
2:B:655:PRO:HD3	2:B:920:LEU:HD13	1.87	0.56
1:A:288:MET:HG2	1:A:290:ILE:HD13	1.86	0.56
2:B:1069:MET:HE2	2:B:1069:MET:HA	1.88	0.56
2:B:620:LEU:HD22	2:B:634:MET:CE	2.35	0.56
2:B:684:GLN:OE1	2:B:746:GLU:HA	2.05	0.56
1:A:700:PHE:CB	1:A:701:PRO:HD3	2.34	0.55
2:B:601:THR:HG22	2:B:605:MET:HE3	1.88	0.55
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.87	0.55
1:A:560:TYR:CD2	1:A:761:VAL:HG12	2.41	0.55
1:A:339:ALA:O	1:A:447:LYS:HE3	2.07	0.55
2:B:807:LEU:O	2:B:818:ILE:HA	2.07	0.55
2:B:1054:VAL:O	2:B:1056:ARG:N	2.39	0.55
1:A:173:VAL:HG11	1:A:270:ILE:HD12	1.89	0.55
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.88	0.54
2:B:497:MET:HE2	2:B:816:ARG:HG3	1.88	0.54
1:A:290:ILE:HG21	1:A:355:THR:CG2	2.37	0.54
2:B:749:MET:HE3	2:B:751:ILE:HD11	1.90	0.54
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.91	0.53
2:B:759:ILE:HG12	2:B:789:MET:HE3	1.91	0.53
2:B:359:MET:HE2	2:B:1080:TYR:CE2	2.43	0.53
1:A:153:MET:CE	1:A:157:LEU:HD11	2.38	0.53
1:A:607:PHE:HD2	1:A:608:MET:HE3	1.74	0.53
2:B:409:LEU:C	2:B:410:LEU:HD12	2.34	0.53
2:B:480:ARG:HG3	2:B:482:GLU:OE1	2.09	0.53
2:B:760:HIS:NE2	2:B:788:GLN:HG2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ILE:CD1	1:A:589:PHE:HB3	2.39	0.53
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.89	0.53
2:B:482:GLU:OE1	2:B:482:GLU:N	2.37	0.52
2:B:965:ILE:N	2:B:965:ILE:HD12	2.23	0.52
2:B:1039:ILE:O	2:B:1043:ARG:HG3	2.08	0.52
2:B:410:LEU:CD2	2:B:935:LEU:HG	2.38	0.52
3:C:33:TYR:CZ	3:C:59:MET:HG3	2.44	0.52
3:C:103:VAL:N	3:C:104:PRO:HD2	2.25	0.52
1:A:121:VAL:HG11	6:A:907:HOH:O	2.09	0.52
2:B:428:ILE:HG21	2:B:437:TYR:HE2	1.75	0.52
2:B:871:VAL:HG11	2:B:1087:ILE:HD13	1.90	0.52
1:A:177:GLU:CD	1:A:185:LYS:HE2	2.35	0.52
2:B:463:GLU:O	2:B:465:PHE:N	2.43	0.52
2:B:641:LEU:HD23	2:B:642:PRO:HD2	1.93	0.52
2:B:1054:VAL:O	2:B:1055:ILE:C	2.52	0.51
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.92	0.51
1:A:588:SER:OG	1:A:595:ASN:OD1	2.24	0.51
2:B:411:LEU:N	2:B:411:LEU:HD23	2.24	0.51
2:B:956:GLY:HA3	2:B:965:ILE:O	2.10	0.51
1:A:30:GLU:CD	1:A:510:ILE:HD11	2.35	0.51
1:A:141:ASP:OD1	1:A:249:ARG:HD3	2.10	0.51
2:B:936:VAL:O	2:B:940:LEU:HD23	2.10	0.51
3:C:1:MET:HA	3:C:79:PHE:HD2	1.75	0.51
2:B:578:ILE:HD11	2:B:626:LEU:N	2.26	0.51
1:A:98:TYR:O	1:A:101:ILE:HB	2.11	0.51
2:B:959:ASN:O	2:B:961:SER:N	2.44	0.51
2:B:433:SER:OG	2:B:457:ARG:HD3	2.11	0.50
2:B:766:PHE:HB3	2:B:776:LEU:HD21	1.92	0.50
1:A:398:PHE:HB3	1:A:400:MET:HG2	1.92	0.50
1:A:577:TYR:CZ	1:A:581:MET:HE3	2.46	0.50
1:A:194:ASP:O	1:A:195:LEU:HD23	2.11	0.50
1:A:521:ALA:HA	1:A:612:LEU:HD12	1.91	0.50
2:B:598:LEU:HD11	2:B:602:LEU:HG	1.93	0.50
1:A:200:LEU:HD21	1:A:270:ILE:HG23	1.94	0.50
2:B:655:PRO:CD	2:B:920:LEU:HD13	2.42	0.50
2:B:966:PRO:HG2	2:B:1038:PHE:HB2	1.93	0.50
1:A:139:MET:HE2	1:A:291:GLY:HA3	1.94	0.50
2:B:489:GLU:OE2	2:B:809:TYR:OH	2.17	0.50
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.93	0.50
2:B:633:ARG:HD2	2:B:738:TYR:HH	1.77	0.50
3:C:1:MET:SD	3:C:1:MET:N	2.81	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:THR:HG22	3:C:62:HIS:NE2	2.27	0.49
3:C:110:TYR:HB3	3:C:113:ILE:HG23	1.92	0.49
1:A:700:PHE:O	1:A:702:MET:N	2.44	0.49
1:A:153:MET:HE2	1:A:157:LEU:HD11	1.93	0.49
1:A:27:SER:O	1:A:31:ALA:HB2	2.13	0.49
3:C:12:ASP:OD1	3:C:12:ASP:N	2.44	0.49
1:A:101:ILE:HD11	1:A:106:GLN:HA	1.94	0.49
2:B:548:THR:OG1	2:B:554:HIS:HB2	2.12	0.49
2:B:513:SER:O	2:B:517:VAL:HG23	2.12	0.49
2:B:598:LEU:CD1	2:B:602:LEU:HG	2.43	0.49
2:B:598:LEU:HD12	2:B:598:LEU:O	2.13	0.49
1:A:190:ARG:NH1	2:B:575:ASP:OD1	2.46	0.49
1:A:76:VAL:HG12	1:A:77:ASP:N	2.28	0.48
1:A:696:LEU:O	1:A:697:HIS:ND1	2.46	0.48
2:B:876:SER:HA	2:B:1091:VAL:HG13	1.94	0.48
2:B:628:SER:N	2:B:629:PRO:HD3	2.29	0.48
2:B:910:LYS:HD3	2:B:922:GLU:HB3	1.95	0.48
1:A:371:MET:HB3	1:A:605:HIS:CD2	2.49	0.48
2:B:799:GLN:O	2:B:800:LEU:HD23	2.13	0.48
2:B:429:VAL:HG12	2:B:438:ILE:HB	1.96	0.48
2:B:1079:SER:OG	2:B:1082:GLU:HG3	2.13	0.48
1:A:368:GLY:HA3	1:A:450:GLY:O	2.13	0.48
1:A:577:TYR:HB3	1:A:578:PRO:HD3	1.96	0.48
1:A:547:ASP:OD2	1:A:585:ARG:NH2	2.47	0.48
1:A:408:ILE:HA	1:A:480:GLN:O	2.14	0.47
1:A:520:GLU:HB3	1:A:616:LEU:HD11	1.96	0.47
2:B:457:ARG:HG3	2:B:458:VAL:N	2.28	0.47
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.79	0.47
2:B:1004:PHE:CE1	2:B:1008:VAL:HG11	2.50	0.47
1:A:18:ARG:HH21	1:A:518:ASP:CG	2.21	0.47
1:A:164:VAL:O	1:A:230:LEU:HA	2.15	0.47
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.45	0.47
2:B:1064:ASN:HA	2:B:1067:GLN:HG3	1.97	0.47
3:C:73:VAL:HB	3:C:88:LEU:HD21	1.96	0.47
2:B:410:LEU:HD22	2:B:935:LEU:HG	1.96	0.47
1:A:354:GLN:OE1	1:A:597:PRO:HD2	2.14	0.47
1:A:541:ASP:HB3	1:A:544:ARG:HD2	1.97	0.46
1:A:700:PHE:C	1:A:700:PHE:CD1	2.92	0.46
2:B:424:THR:HG22	2:B:491:MET:HG3	1.98	0.46
1:A:246:GLU:O	1:A:247:LEU:C	2.58	0.46
1:A:506:ALA:O	1:A:507:GLN:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:553:ILE:HB	2:B:570:VAL:HG13	1.98	0.46
2:B:585:LEU:HG	2:B:626:LEU:HD11	1.97	0.46
3:C:69:VAL:HG22	3:C:103:VAL:HG11	1.97	0.46
2:B:500:PRO:O	2:B:501:PRO:C	2.58	0.46
2:B:1074:THR:HG23	2:B:1076:SER:H	1.81	0.46
1:A:521:ALA:HA	1:A:612:LEU:CD1	2.46	0.46
1:A:451:LEU:HD12	1:A:451:LEU:N	2.30	0.46
1:A:695:ILE:HD11	1:A:699:ARG:NH1	2.31	0.45
2:B:551:SER:OG	2:B:611:GLU:OE1	2.32	0.45
2:B:957:ALA:C	2:B:959:ASN:H	2.24	0.45
2:B:350:VAL:HG11	2:B:891:MET:HE3	1.96	0.45
2:B:641:LEU:CD2	2:B:649:LEU:HB2	2.45	0.45
2:B:766:PHE:HB3	2:B:776:LEU:CD2	2.46	0.45
1:A:41:LEU:HD21	1:A:524:ILE:HG21	1.99	0.45
1:A:649:LEU:HD11	1:A:656:ILE:HG23	1.97	0.45
2:B:521:TYR:CD1	2:B:521:TYR:C	2.94	0.45
2:B:875:LEU:HD22	2:B:892:VAL:CG1	2.42	0.45
1:A:151:MET:HE3	1:A:244:LEU:HD22	1.98	0.45
2:B:545:GLY:HA3	2:B:585:LEU:HD23	1.98	0.45
2:B:916:THR:HG22	2:B:917:ASN:N	2.32	0.45
1:A:682:ARG:NH1	6:A:904:HOH:O	2.48	0.44
2:B:1041:TRP:O	2:B:1045:GLN:HG2	2.17	0.44
3:C:44:LEU:HD13	3:C:65:ILE:HD11	1.98	0.44
3:C:94:GLU:OE2	3:C:98:GLN:NE2	2.40	0.44
1:A:687:ALA:N	1:A:688:PRO:HD2	2.32	0.44
2:B:909:GLN:HG2	2:B:910:LYS:H	1.82	0.44
1:A:649:LEU:HD12	1:A:649:LEU:C	2.42	0.44
2:B:387:ARG:HD2	2:B:935:LEU:HD12	2.00	0.44
2:B:602:LEU:N	2:B:603:PRO:CD	2.80	0.44
2:B:753:CYS:HB2	2:B:803:PHE:CD1	2.53	0.44
2:B:1053:TYR:HD1	2:B:1055:ILE:HB	1.82	0.44
3:C:63:TYR:CD1	3:C:63:TYR:C	2.96	0.44
3:C:80:PRO:HB2	3:C:83:LEU:HG	2.00	0.44
1:A:692:ALA:O	1:A:696:LEU:HB2	2.18	0.44
1:A:345:ILE:O	1:A:369:GLY:HA3	2.18	0.44
2:B:381:CYS:HB2	2:B:822:THR:O	2.18	0.44
2:B:499:ARG:HA	3:C:34:GLN:HE22	1.83	0.43
2:B:655:PRO:CD	2:B:920:LEU:CD1	2.96	0.43
1:A:311:ARG:NH2	1:A:358:LEU:HB3	2.33	0.43
2:B:1074:THR:CG2	2:B:1077:ALA:HB3	2.43	0.43
1:A:49:PRO:O	1:A:50:ASP:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASP:O	1:A:241:THR:HG22	2.19	0.43
1:A:54:ILE:HG23	1:A:56:TYR:CE2	2.54	0.43
1:A:310:ILE:HD11	6:A:909:HOH:O	2.18	0.43
2:B:437:TYR:O	2:B:438:ILE:C	2.61	0.43
3:C:2:VAL:HB	3:C:3:LEU:H	1.80	0.43
2:B:666:MET:HE1	2:B:927:MET:SD	2.59	0.43
1:A:191:GLY:HA3	1:A:263:SER:OG	2.19	0.43
1:A:683:HIS:O	1:A:687:ALA:N	2.51	0.43
2:B:454:LEU:CD2	2:B:752:ARG:HB3	2.49	0.43
1:A:194:ASP:OD1	1:A:195:LEU:N	2.51	0.42
1:A:404:GLY:HA2	1:A:484:GLN:O	2.19	0.42
1:A:614:GLN:HA	1:A:617:ILE:HD12	2.00	0.42
2:B:1011:VAL:HG12	2:B:1013:ASN:H	1.83	0.42
1:A:600:SER:O	1:A:604:ARG:HG3	2.19	0.42
2:B:616:LEU:O	2:B:620:LEU:HG	2.19	0.42
1:A:162:ALA:O	1:A:233:VAL:HG23	2.18	0.42
2:B:535:LEU:O	2:B:536:LEU:C	2.62	0.42
2:B:735:LEU:O	2:B:736:GLN:C	2.62	0.42
2:B:369:VAL:O	2:B:370:PRO:C	2.63	0.42
1:A:227:ASN:HB3	1:A:229:PHE:H	1.84	0.42
2:B:949:VAL:O	2:B:952:LEU:HG	2.19	0.42
1:A:695:ILE:C	1:A:697:HIS:H	2.27	0.42
1:A:61:CYS:O	1:A:67:ARG:HA	2.20	0.42
1:A:106:GLN:HB2	1:A:107:PRO:HD2	2.01	0.42
2:B:357:ARG:C	2:B:359:MET:HE3	2.45	0.42
2:B:462:PRO:O	2:B:463:GLU:C	2.63	0.42
2:B:628:SER:N	2:B:629:PRO:CD	2.82	0.42
2:B:702:LEU:O	2:B:705:ILE:HG22	2.20	0.42
2:B:906:LEU:HD12	2:B:906:LEU:HA	1.94	0.41
1:A:41:LEU:HD21	1:A:524:ILE:CG2	2.51	0.41
2:B:720:HIS:HB3	2:B:723:HIS:HB2	2.02	0.41
2:B:745:PHE:O	2:B:746:GLU:C	2.64	0.41
1:A:682:ARG:O	1:A:683:HIS:C	2.64	0.41
2:B:705:ILE:HD12	2:B:705:ILE:HA	1.95	0.41
3:C:1:MET:CE	3:C:78:ALA:HB1	2.50	0.41
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.89	0.41
1:A:571:SER:C	1:A:573:THR:N	2.77	0.41
2:B:576:VAL:CG1	2:B:622:ALA:HB2	2.48	0.41
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.56	0.41
1:A:559:GLU:O	1:A:568:PHE:HA	2.21	0.41
2:B:692:LEU:HD21	2:B:731:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1055:ILE:O	2:B:1056:ARG:C	2.63	0.41
1:A:608:MET:HE2	1:A:608:MET:HA	2.03	0.41
1:A:638:ASP:HB3	1:A:640:SER:OG	2.20	0.41
2:B:509:VAL:HA	2:B:547:ILE:O	2.20	0.41
2:B:766:PHE:CD1	2:B:766:PHE:C	2.98	0.41
3:C:33:TYR:HB3	3:C:74:LEU:CD2	2.51	0.41
1:A:69:VAL:HB	1:A:480:GLN:NE2	2.36	0.41
1:A:311:ARG:H	1:A:311:ARG:HD3	1.86	0.41
2:B:991:VAL:HG12	2:B:1051:ILE:CD1	2.51	0.41
1:A:577:TYR:CD2	1:A:581:MET:HE3	2.56	0.41
2:B:509:VAL:HG22	2:B:547:ILE:HB	2.02	0.41
3:C:55:GLU:O	3:C:153:ILE:HG22	2.21	0.41
1:A:363:CYS:HB2	1:A:364:PRO:CD	2.52	0.40
1:A:613:THR:OG1	1:A:614:GLN:N	2.54	0.40
1:A:551:ILE:O	1:A:552:ARG:C	2.63	0.40
2:B:749:MET:HA	2:B:806:ALA:O	2.21	0.40
2:B:991:VAL:HG12	2:B:1051:ILE:HD13	2.04	0.40
1:A:60:LEU:CD2	1:A:69:VAL:HG22	2.52	0.40
1:A:101:ILE:CD1	1:A:106:GLN:HA	2.52	0.40
2:B:359:MET:N	2:B:359:MET:SD	2.95	0.40
2:B:554:HIS:CD2	2:B:554:HIS:N	2.89	0.40
2:B:480:ARG:HA	2:B:481:PRO:HD3	1.93	0.40
2:B:960:ILE:O	2:B:962:ASP:N	2.54	0.40
3:C:52:CYS:SG	3:C:53:THR:N	2.94	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	681/765 (89%)	623 (92%)	54 (8%)	4 (1%)	21 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	721/748 (96%)	665 (92%)	49 (7%)	7 (1%)	12	20
3	C	127/157 (81%)	116 (91%)	8 (6%)	3 (2%)	4	7
All	All	1529/1670 (92%)	1404 (92%)	111 (7%)	14 (1%)	14	24

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	464	GLU
2	B	1056	ARG
3	C	4	LEU
3	C	116	ASP
2	B	961	SER
2	B	1047	PRO
2	B	1055	ILE
2	B	1076	SER
1	A	507	GLN
1	A	511	GLN
1	A	637	LEU
1	A	700	PHE
2	B	456	TYR
3	C	2	VAL

### 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	601/666 (90%)	560 (93%)	41 (7%)	14	25
2	B	652/679 (96%)	605 (93%)	47 (7%)	13	22
3	C	115/138 (83%)	105 (91%)	10 (9%)	9	16
All	All	1368/1483 (92%)	1270 (93%)	98 (7%)	13	22

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	27	SER
1	A	29	LEU
1	A	30	GLU
1	A	41	LEU
1	A	50	ASP
1	A	51	LEU
1	A	65	THR
1	A	101	ILE
1	A	116	SER
1	A	161	THR
1	A	186	SER
1	A	192	THR
1	A	226	SER
1	A	238	MET
1	A	240	LEU
1	A	243	LEU
1	A	268	LEU
1	A	282	THR
1	A	290	ILE
1	A	301	VAL
1	A	316	ILE
1	A	355	THR
1	A	362	CYS
1	A	376	SER
1	A	451	LEU
1	A	483	THR
1	A	498	THR
1	A	508	THR
1	A	524	ILE
1	A	543	LEU
1	A	544	ARG
1	A	562	LYS
1	A	570	PHE
1	A	571	SER
1	A	613	THR
1	A	638	ASP
1	A	649	LEU
1	A	695	ILE
1	A	746	ASP
1	A	747	VAL
2	B	350	VAL
2	B	356	GLU

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Mol	Chain	Res	Type
2	B	359	MET
2	B	363	THR
2	B	386	PHE
2	B	396	THR
2	B	411	LEU
2	B	423	VAL
2	B	431	CYS
2	B	454	LEU
2	B	570	VAL
2	B	573	ILE
2	B	641	LEU
2	B	643	THR
2	B	650	LYS
2	B	692	LEU
2	B	712	SER
2	B	713	VAL
2	B	751	ILE
2	B	761	THR
2	B	771	THR
2	B	775	SER
2	B	779	VAL
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	818	ILE
2	B	829	SER
2	B	831	LEU
2	B	857	THR
2	B	881	SER
2	B	897	ARG
2	B	906	LEU
2	B	914	THR
2	B	935	LEU
2	B	965	ILE
2	B	975	VAL
2	B	1001	THR
2	B	1002	GLN
2	B	1043	ARG
2	B	1051	ILE

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Mol	Chain	Res	Type
2	B	1052	LEU
2	B	1085	LEU
2	B	1092	ASN
3	C	2	VAL
3	C	12	ASP
3	C	46	GLU
3	C	50	THR
3	C	67	GLN
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	248	GLN
1	A	296	GLN
1	A	660	HIS
2	B	395	GLN
2	B	596	GLN
2	B	683	GLN
2	B	732	GLN
2	B	999	ASN
2	B	1064	ASN
2	B	1092	ASN
3	C	34	GLN
3	C	36	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	A1CGA	B	1201	-	24,26,26	0.88	1 (4%)	29,38,38	1.29	4 (13%)

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	A1CGA	B	1201	-	-	12/22/35/35	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1201	A1CGA	O2-C18	2.01	1.28	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1201	A1CGA	C17-C10-C11	3.41	127.95	121.65
5	B	1201	A1CGA	C8-C7-C2	2.81	123.92	120.88
5	B	1201	A1CGA	O1-C2-C3	-2.66	119.82	124.30
5	B	1201	A1CGA	O1-C2-C7	2.22	119.27	115.96

There are no chirality outliers.

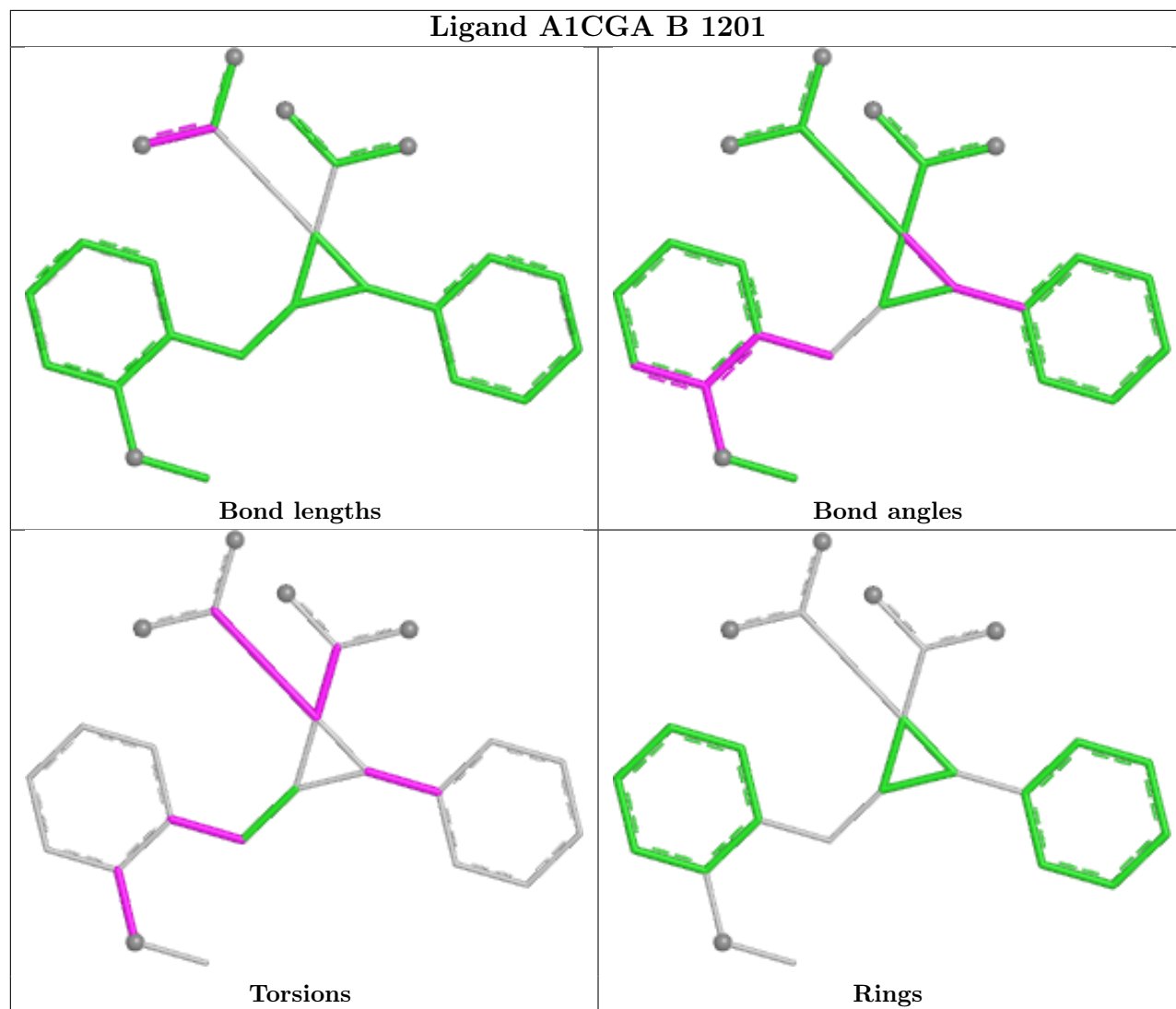
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1201	A1CGA	C6-C7-C8-C9
5	B	1201	A1CGA	C2-C7-C8-C9
5	B	1201	A1CGA	C19-C17-C18-O3
5	B	1201	A1CGA	C9-C17-C19-O4
5	B	1201	A1CGA	C9-C17-C19-O5
5	B	1201	A1CGA	C18-C17-C19-O4
5	B	1201	A1CGA	C18-C17-C19-O5
5	B	1201	A1CGA	C3-C2-O1-C1
5	B	1201	A1CGA	C7-C2-O1-C1
5	B	1201	A1CGA	C9-C17-C18-O3
5	B	1201	A1CGA	C19-C17-C18-O2
5	B	1201	A1CGA	C17-C10-C11-C12

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.19	2 (0%) 90 89	57, 93, 137, 194	0
2	B	729/748 (97%)	-0.34	2 (0%) 90 89	58, 82, 126, 186	0
3	C	133/157 (84%)	-0.15	0 100 100	68, 107, 160, 174	0
All	All	1555/1670 (93%)	-0.26	4 (0%) 90 89	57, 88, 137, 194	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	665	ALA	3.9
2	B	1055	ILE	3.2
1	A	464	VAL	2.2
2	B	888	PRO	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

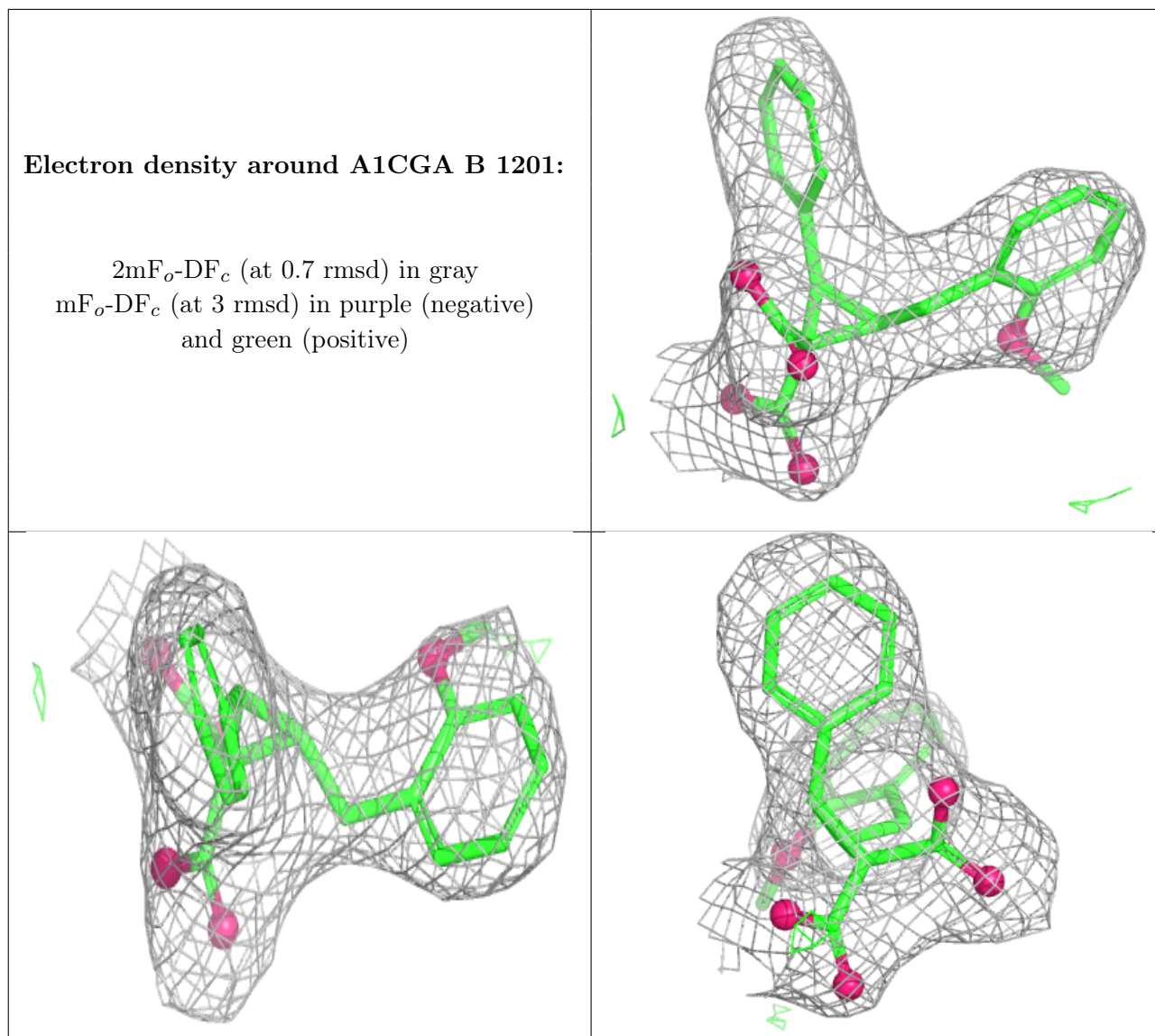
### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	A1CGA	B	1201	24/24	0.91	0.10	58,78,100,109	0
4	ZN	A	800	1/1	0.99	0.02	95,95,95,95	0
4	ZN	B	1202	1/1	1.00	0.01	80,80,80,80	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 [\(i\)](#)

There are no such residues in this entry.