



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:01 am BST

PDB ID : 3FGO  
Title : Crystal Structure of the E2 magnesium fluoride complex of the (SR) Ca<sup>2+</sup>-ATPase with bound CPA and AMPPCP  
Authors : Laursen, M.; Bublitz, M.; Moncoq, K.; Olesen, C.; Moller, J.V.; Young, H.S.; Nissen, P.; Morth, J.P.  
Deposited on : 2008-12-08  
Resolution : 2.50 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

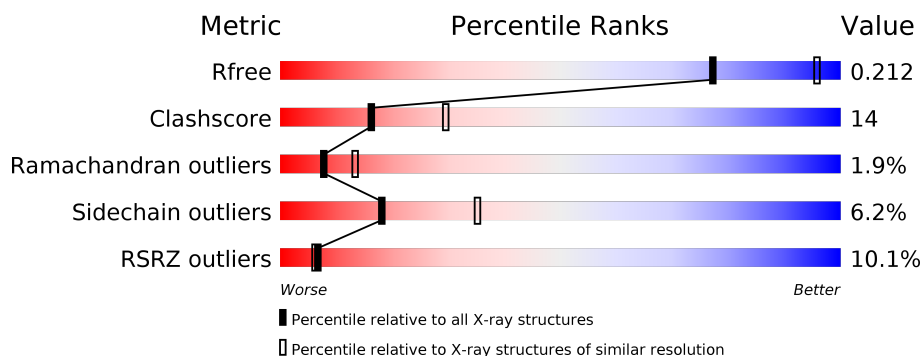
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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	994	<div> <div>13%</div> <div>68%</div> <div>27%</div> <div>.</div> </div>
1	B	994	<div> <div>7%</div> <div>71%</div> <div>26%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ACT	A	3002	-	-	X	-
8	ACT	B	3002	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15950 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 Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7670	4876	1287	1450	57			
1	B	994	Total	C	N	O	S	0	0	0
			7670	4876	1287	1450	57			

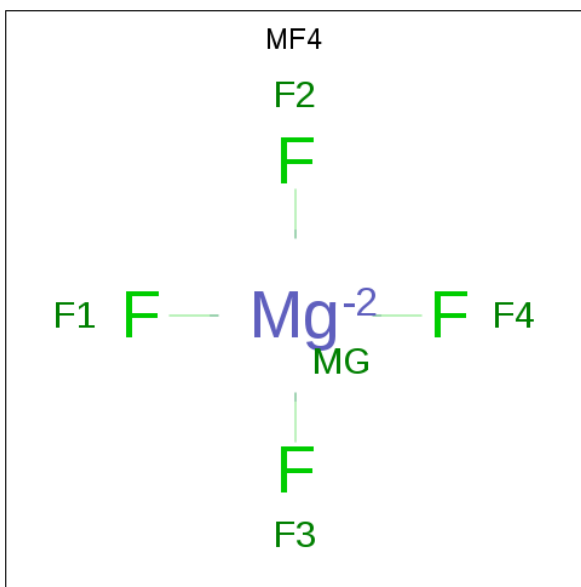
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	ASP	SEE REMARK 999	UNP P04191
B	994	GLY	ASP	SEE REMARK 999	UNP P04191

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F<sub>4</sub>Mg).

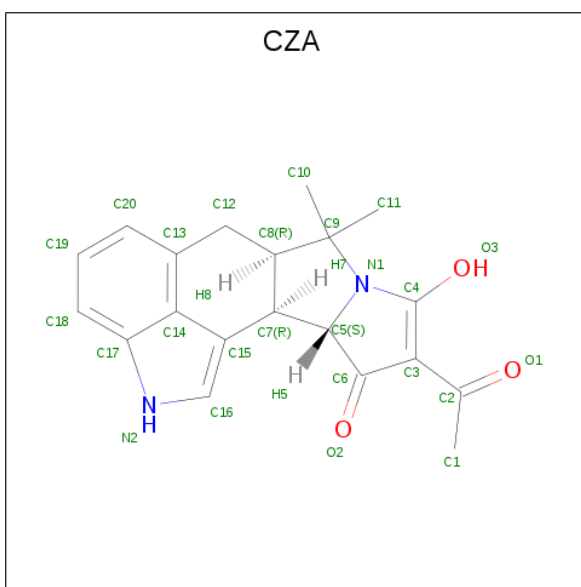


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	F	Mg	0	0
			5	4	1		
3	B	1	Total	F	Mg	0	0
			5	4	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is (6AR,11AS,11BR)-10-ACETYL-9-HYDROXY-7,7-DIMETHYL-2,6,6A,7,11A,11B-HEXAHYDRO-11H-PYRROLO[1',2':2,3]ISOINDOLO[4,5,6-CD]INDOL-11-ONE (three-letter code: CZA) (formula: C<sub>20</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>).

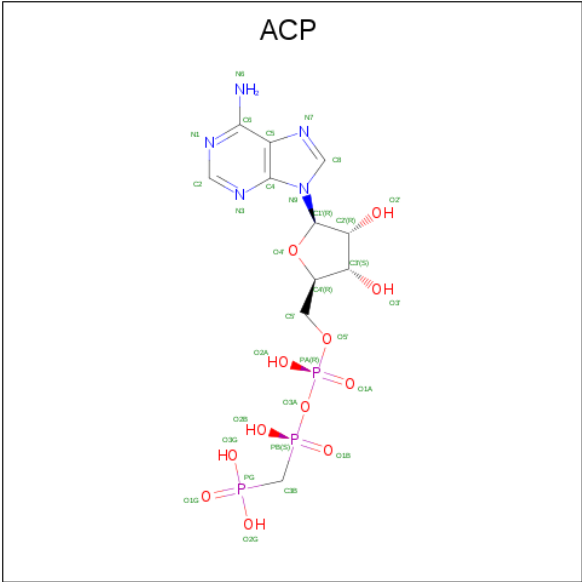


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			25	20	2	3		
5	B	1	Total	C	N	O	0	0
			25	20	2	3		

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

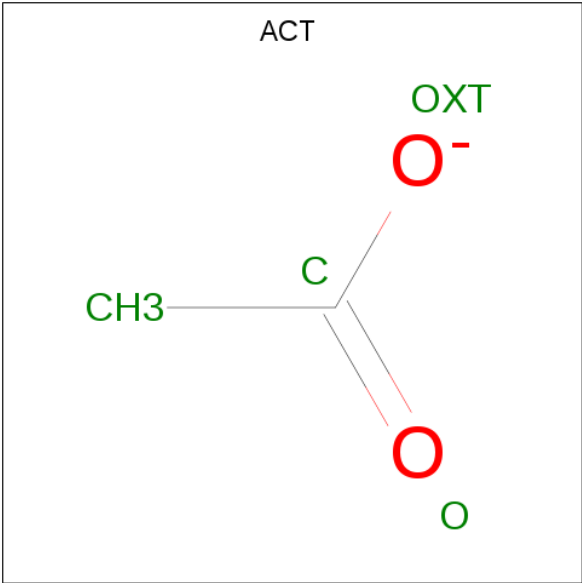
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mn	0	0
			1	1		
6	A	2	Total	Mn	0	0
			2	2		

- Molecule 7 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
7	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is water.

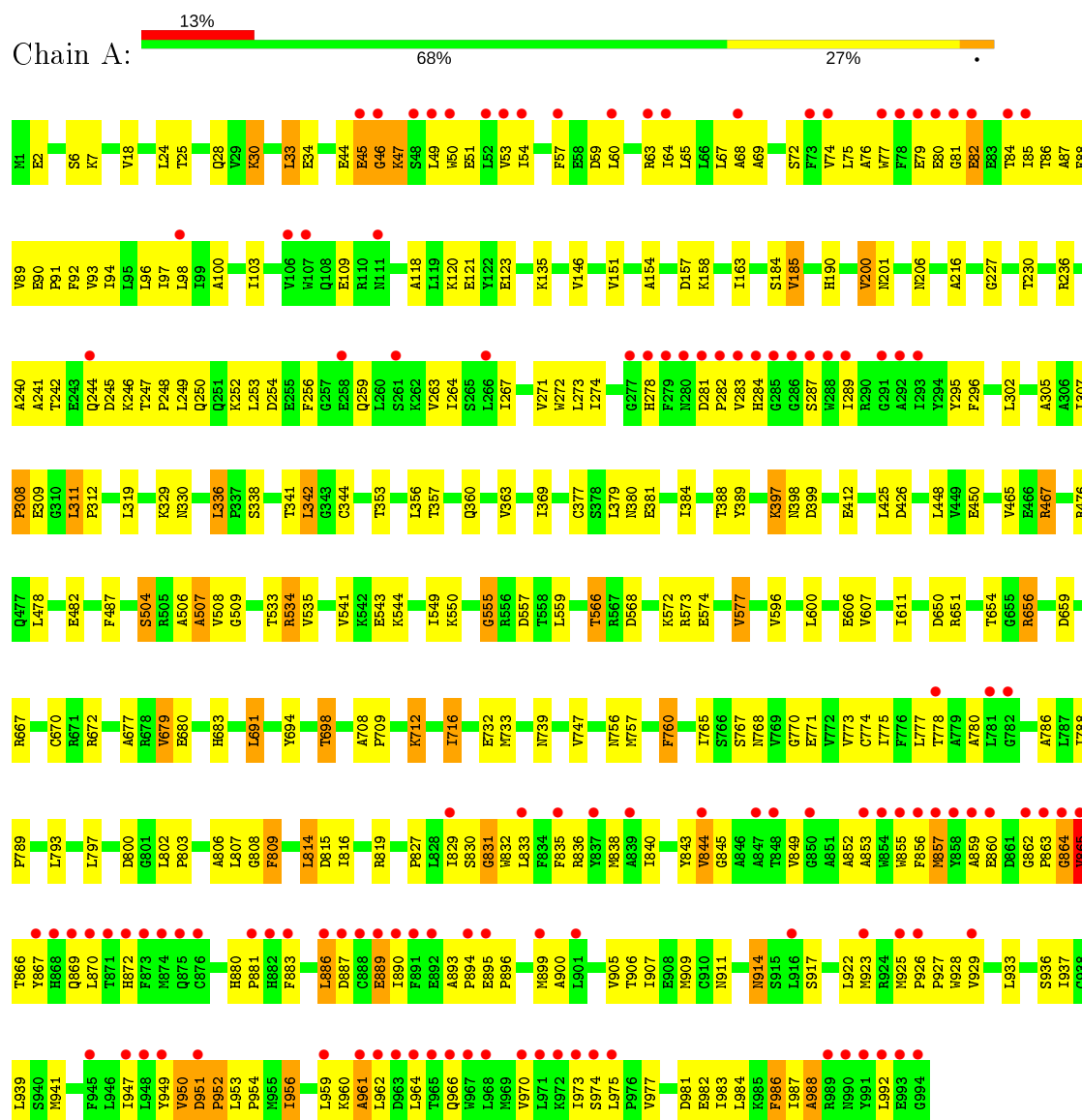
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	263	Total	O	0	0
			263	263		
9	B	202	Total	O	0	0
			202	202		



### 3 Residue-property plots

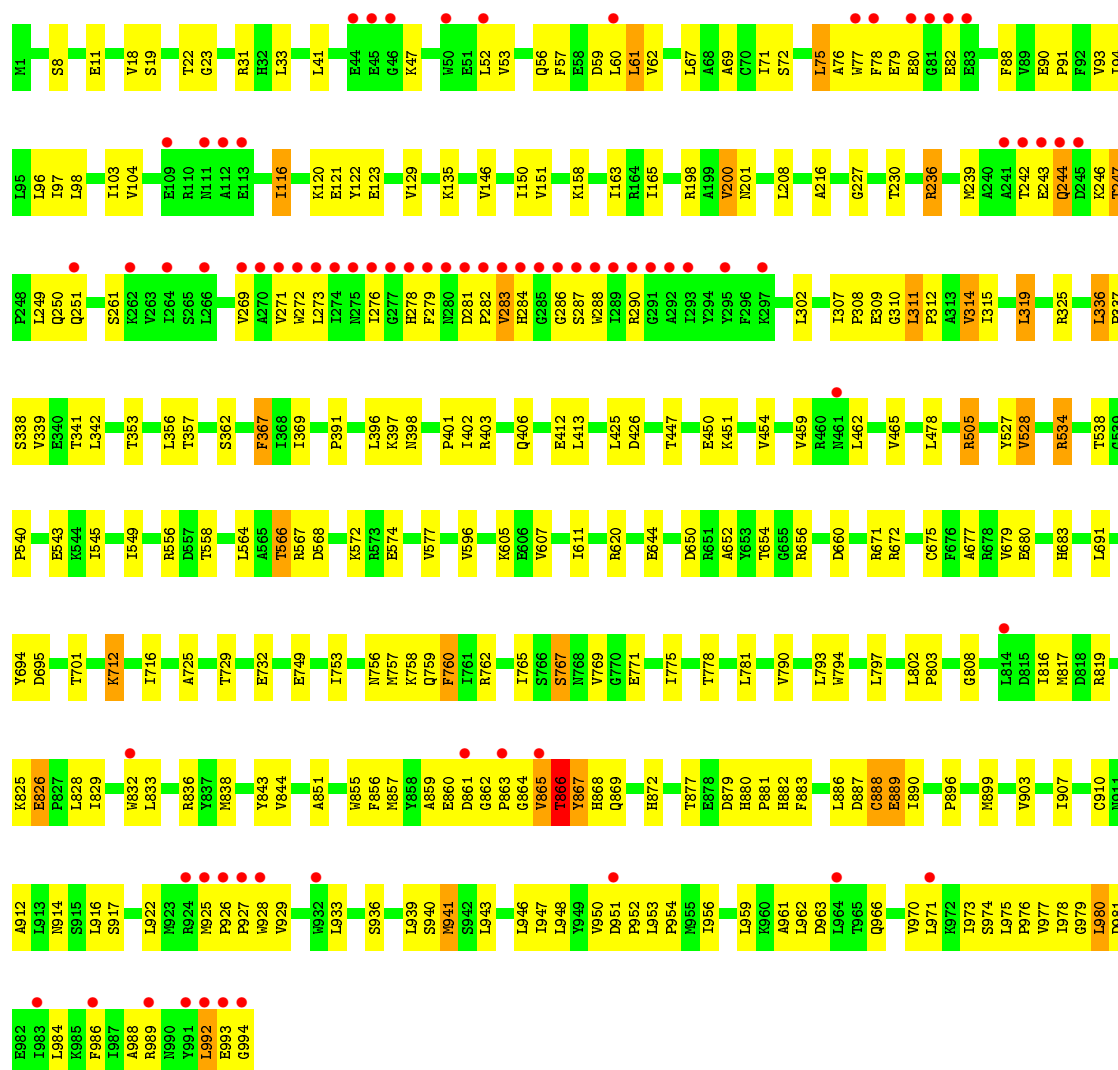
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.43Å 108.87Å 274.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.93 – 2.50 45.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (24.93-2.50) 97.6 (45.97-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.174 , 0.217 0.169 , 0.212	Depositor DCC
$R_{free}$ test set	3075 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.0	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 66.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15950	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, MN, ACP, MF4, ACT, CZA

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	0.50	0/7811	0.64	3/10592 (0.0%)
1	B	0.49	0/7811	0.64	1/10592 (0.0%)
All	All	0.50	0/15622	0.64	4/21184 (0.0%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	567	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	467	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	A	476	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	476	ARG	CG-CD-NE	-5.32	100.62	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	555	GLY	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	7670	0	7764	233	0
1	B	7670	0	7764	214	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	25	0	20	3	0
5	B	25	0	20	2	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
7	A	31	0	14	2	0
7	B	31	0	14	0	0
8	A	8	0	6	3	0
8	B	8	0	6	4	0
9	A	263	0	0	6	0
9	B	202	0	0	4	0
All	All	15950	0	15608	447	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 14.

All (447) 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:963:ASP:H	1:B:966:GLN:HG3	1.33	0.90
1:A:246:LYS:HB2	1:A:250:GLN:HG3	1.54	0.89
1:A:894:PRO:HB2	1:A:960:LYS:HB2	1.56	0.86
1:A:185:VAL:HG12	9:A:1218:HOH:O	1.75	0.86
1:B:216:ALA:HB1	8:B:3001:ACT:H2	1.56	0.84
1:A:216:ALA:HB1	8:A:3001:ACT:H2	1.58	0.83
1:A:247:THR:HG22	1:A:250:GLN:H	1.42	0.83
1:A:863:PRO:HB2	1:A:864:GLY:HA2	1.61	0.82
1:B:61:LEU:HD12	5:B:1005:CZA:H8	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:993:GLU:HA	1:B:994:GLY:C	2.00	0.81
1:B:865:VAL:O	1:B:866:THR:HG23	1.81	0.81
1:A:865:VAL:HG12	1:A:867:TYR:CE2	2.16	0.80
1:A:862:GLY:H	1:A:863:PRO:HD3	1.46	0.78
1:A:814:LEU:HD12	1:A:814:LEU:H	1.49	0.77
1:B:756:ASN:HB3	1:B:808:GLY:HA2	1.67	0.76
1:A:951:ASP:HB2	1:A:952:PRO:HD3	1.66	0.76
1:B:116:ILE:HD13	1:B:236:ARG:HG2	1.68	0.75
1:A:905:VAL:O	1:A:909:MET:HG2	1.86	0.74
1:A:85:ILE:HG12	1:A:86:THR:HG23	1.69	0.74
1:B:856:PHE:HA	1:B:863:PRO:HG2	1.69	0.74
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.70	0.73
1:A:248:PRO:O	1:A:252:LYS:HG2	1.89	0.73
1:A:840:ILE:O	1:A:844:VAL:HG12	1.88	0.72
1:A:75:LEU:HD21	1:A:296:PHE:HB2	1.71	0.72
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.72	0.72
1:A:242:THR:HG22	1:A:244:GLN:HG3	1.70	0.71
1:B:122:TYR:HA	1:B:158:LYS:HE3	1.72	0.71
1:A:249:LEU:HD13	1:A:757:MET:HE2	1.71	0.71
1:A:773:VAL:HB	1:A:845:GLY:HA3	1.72	0.70
1:B:926:PRO:O	1:B:929:VAL:HG23	1.92	0.70
1:A:92:PHE:O	1:A:96:LEU:HB2	1.92	0.69
1:A:227:GLY:O	8:A:3002:ACT:H3	1.92	0.69
1:A:947:ILE:HG12	1:A:953:LEU:HD13	1.75	0.69
1:A:329:LYS:O	1:A:330:ASN:HB2	1.94	0.68
1:B:863:PRO:CD	1:B:864:GLY:HA2	2.23	0.68
1:A:983:ILE:O	1:A:987:ILE:HG22	1.94	0.67
1:B:857:MET:HA	1:B:865:VAL:HA	1.76	0.67
1:A:774:CYS:O	1:A:778:THR:HG22	1.95	0.67
1:A:256:PHE:HA	1:A:259:GLN:HB2	1.76	0.67
1:B:887:ASP:O	1:B:890:ILE:HG13	1.94	0.67
1:A:555:GLY:HA3	1:A:557:ASP:H	1.60	0.67
1:B:863:PRO:CB	1:B:864:GLY:HA2	2.24	0.66
1:A:79:GLU:HB3	1:A:84:THR:HG22	1.76	0.66
1:A:949:TYR:O	1:A:950:VAL:HG23	1.94	0.66
1:B:816:ILE:HG23	1:B:817:MET:HG2	1.79	0.65
1:B:151:VAL:HG21	1:B:163:ILE:HD13	1.79	0.65
1:B:680:GLU:HG3	1:B:683:HIS:CE1	2.32	0.64
1:A:151:VAL:HG21	1:A:163:ILE:HD13	1.81	0.63
1:A:756:ASN:HB3	1:A:808:GLY:HA2	1.80	0.63
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:THR:HG22	1:B:23:GLY:O	1.99	0.63
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.80	0.63
1:A:381:GLU:O	1:A:397:LYS:HE2	1.99	0.62
1:A:412:GLU:OE2	1:A:566:THR:HG21	1.98	0.62
1:A:72:SER:OG	1:A:90:GLU:HG2	2.00	0.62
1:A:200:VAL:HG22	1:A:680:GLU:CG	2.30	0.62
1:A:281:ASP:N	1:A:282:PRO:HD3	2.14	0.61
1:B:855:TRP:CZ3	1:B:863:PRO:HG3	2.35	0.61
1:A:504:SER:C	1:A:506:ALA:H	2.02	0.61
1:A:988:ALA:HA	1:A:992:LEU:CB	2.29	0.61
1:A:893:ALA:HB1	1:A:895:GLU:OE1	2.00	0.61
1:B:286:GLY:O	1:B:290:ARG:HB2	2.00	0.61
1:B:767:SER:O	1:B:771:GLU:HG3	2.00	0.61
1:B:863:PRO:HB2	1:B:864:GLY:HA2	1.82	0.61
1:B:933:LEU:O	1:B:936:SER:HB3	2.00	0.61
1:B:8:SER:OG	1:B:11:GLU:HG3	2.01	0.60
1:B:916:LEU:HD12	1:B:927:PRO:HA	1.83	0.60
1:B:922:LEU:O	1:B:927:PRO:HD3	2.01	0.60
1:B:988:ALA:HA	1:B:992:LEU:CB	2.31	0.60
1:B:988:ALA:HA	1:B:992:LEU:HB2	1.84	0.60
1:B:247:THR:HG21	1:B:337:PRO:HB2	1.84	0.60
1:B:338:SER:HA	1:B:341:THR:HG23	1.83	0.60
1:A:962:LEU:HB3	1:A:966:GLN:HB2	1.82	0.60
1:A:923:MET:HE1	1:A:986:PHE:HE2	1.67	0.60
1:B:869:GLN:NE2	1:B:882:HIS:O	2.34	0.60
1:B:369:ILE:HG13	1:B:528:VAL:HG13	1.84	0.59
1:A:607:VAL:O	1:A:611:ILE:HG12	2.01	0.59
1:B:863:PRO:HD2	1:B:864:GLY:HA2	1.85	0.59
1:A:274:ILE:HG21	1:A:780:ALA:HB1	1.83	0.59
1:A:832:TRP:HZ2	1:A:984:LEU:O	1.86	0.59
1:B:794:TRP:CE2	1:B:947:ILE:HD11	2.37	0.59
1:B:844:VAL:HG22	1:B:907:ILE:HG21	1.84	0.59
1:A:981:ASP:HA	1:A:984:LEU:HD12	1.85	0.59
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.84	0.59
1:A:380:ASN:OD1	1:A:397:LYS:HE3	2.03	0.58
1:A:988:ALA:HA	1:A:992:LEU:HB2	1.83	0.58
1:A:398:ASN:O	1:A:399:ASP:HB2	2.03	0.58
1:A:953:LEU:HB2	1:A:954:PRO:HD3	1.84	0.58
1:B:910:CYS:HB3	1:B:978:ILE:HG13	1.85	0.58
1:A:815:ASP:OD2	1:A:819:ARG:HD3	2.02	0.58
1:A:863:PRO:CB	1:A:864:GLY:HA2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:VAL:HG22	1:B:680:GLU:CG	2.33	0.58
1:B:505:ARG:HG3	1:B:505:ARG:HH21	1.68	0.58
1:A:151:VAL:HG21	1:A:163:ILE:CD1	2.33	0.58
1:A:263:VAL:O	1:A:267:ILE:HG13	2.04	0.58
1:A:895:GLU:N	1:A:896:PRO:HD2	2.18	0.58
1:A:60:LEU:HA	1:A:63:ARG:HD2	1.85	0.58
1:B:120:LYS:HG2	1:B:123:GLU:OE2	2.04	0.58
1:A:305:ALA:HB1	1:A:771:GLU:HB3	1.84	0.58
1:A:450:GLU:OE2	1:A:467:ARG:NH1	2.37	0.57
1:A:506:ALA:O	1:A:507:ALA:HB2	2.04	0.57
1:A:650:ASP:O	1:A:672:ARG:HD2	2.04	0.57
1:A:308:PRO:HB3	1:A:768:ASN:ND2	2.19	0.57
1:A:659:ASP:HA	9:A:1188:HOH:O	2.04	0.57
1:A:865:VAL:HG12	1:A:867:TYR:HE2	1.68	0.57
1:B:922:LEU:HB3	1:B:927:PRO:HG3	1.86	0.57
1:A:800:ASP:C	1:A:803:PRO:HD2	2.24	0.57
1:B:574:GLU:N	1:B:574:GLU:OE2	2.34	0.57
1:B:971:LEU:O	1:B:975:LEU:HD23	2.04	0.57
1:B:974:SER:O	1:B:977:VAL:HG12	2.04	0.57
1:A:271:VAL:HG21	1:A:302:LEU:HD11	1.87	0.57
1:A:65:LEU:HB2	1:A:307:ILE:HD13	1.86	0.57
1:B:962:LEU:HB3	1:B:966:GLN:HB2	1.85	0.56
1:B:868:HIS:O	1:B:872:HIS:HD2	1.88	0.56
1:A:914:ASN:HD22	1:A:914:ASN:N	2.04	0.56
1:A:832:TRP:CH2	1:A:987:ILE:HG23	2.40	0.56
1:B:198:ARG:HH12	1:B:660:ASP:HA	1.71	0.56
1:B:855:TRP:HA	1:B:859:ALA:CB	2.35	0.56
1:B:856:PHE:CA	1:B:863:PRO:HG2	2.36	0.56
1:A:247:THR:HB	1:A:250:GLN:HB3	1.88	0.55
1:B:679:VAL:HB	1:B:683:HIS:HB2	1.88	0.55
1:B:200:VAL:HG22	1:B:680:GLU:HG2	1.88	0.55
1:B:866:THR:O	1:B:867:TYR:HB2	2.06	0.55
1:A:201:ASN:HB2	9:A:1276:HOH:O	2.07	0.55
1:A:862:GLY:N	1:A:863:PRO:HD3	2.20	0.55
1:B:963:ASP:HB3	1:B:966:GLN:HG2	1.89	0.55
1:A:118:ALA:O	1:A:121:GLU:HB2	2.07	0.55
1:A:65:LEU:HB2	1:A:307:ILE:CD1	2.37	0.55
1:A:246:LYS:HB2	1:A:250:GLN:CG	2.33	0.54
1:B:201:ASN:HB2	9:B:1022:HOH:O	2.06	0.54
1:B:116:ILE:HG12	1:B:239:MET:HE2	1.90	0.54
1:A:93:VAL:O	1:A:97:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ARG:NH1	1:B:568:ASP:HB2	2.23	0.54
1:A:555:GLY:CA	1:A:557:ASP:H	2.20	0.54
1:A:909:MET:SD	1:A:937:ILE:HG23	2.47	0.54
1:B:538:THR:OG1	1:B:540:PRO:HD2	2.07	0.54
1:A:872:HIS:O	1:A:883:PHE:HZ	1.91	0.54
1:B:856:PHE:O	1:B:863:PRO:HG2	2.08	0.54
1:B:88:PHE:C	1:B:91:PRO:HD2	2.28	0.54
1:B:948:LEU:CD2	1:B:959:LEU:HD13	2.38	0.54
1:A:249:LEU:HA	1:A:252:LYS:CG	2.38	0.54
1:B:855:TRP:HA	1:B:859:ALA:HB3	1.89	0.54
1:B:534:ARG:HH11	1:B:568:ASP:HB2	1.73	0.53
1:B:76:ALA:O	1:B:79:GLU:HB3	2.07	0.53
1:B:413:LEU:HG	1:B:564:LEU:HD12	1.90	0.53
1:A:259:GLN:O	1:A:263:VAL:HG23	2.09	0.53
1:A:670:CYS:HB3	1:A:691:LEU:HD13	1.89	0.53
1:B:67:LEU:O	1:B:71:ILE:HG13	2.09	0.53
1:B:151:VAL:HG21	1:B:163:ILE:CD1	2.39	0.53
1:A:94:ILE:HG12	1:A:793:LEU:HD11	1.91	0.53
1:A:832:TRP:HH2	1:A:987:ILE:HG23	1.72	0.53
1:A:72:SER:O	1:A:91:PRO:HG3	2.09	0.53
1:B:851:ALA:HB1	1:B:899:MET:HB3	1.91	0.53
1:A:788:ILE:HB	1:A:789:PRO:HD2	1.92	0.52
1:A:866:THR:HB	1:A:869:GLN:HB2	1.90	0.52
1:A:248:PRO:HB2	9:A:1142:HOH:O	2.07	0.52
1:B:281:ASP:N	1:B:282:PRO:HD3	2.23	0.52
1:B:863:PRO:HB2	1:B:864:GLY:CA	2.39	0.52
1:B:832:TRP:NE1	1:B:836:ARG:HD3	2.24	0.52
1:B:883:PHE:CD2	1:B:883:PHE:N	2.78	0.52
1:B:981:ASP:HA	1:B:984:LEU:HD12	1.91	0.52
1:B:948:LEU:O	1:B:961:ALA:HB2	2.10	0.52
1:A:33:LEU:HD13	1:A:146:VAL:CG1	2.40	0.52
1:A:950:VAL:CG1	1:A:952:PRO:HD2	2.39	0.52
1:B:412:GLU:OE2	1:B:566:THR:HG21	2.10	0.52
1:B:917:SER:HB2	1:B:925:MET:SD	2.49	0.52
1:B:362:SER:HB3	9:B:1190:HOH:O	2.10	0.52
1:B:308:PRO:O	1:B:311:LEU:HB2	2.10	0.51
1:B:93:VAL:HG12	1:B:793:LEU:HD13	1.91	0.51
1:B:793:LEU:O	1:B:797:LEU:HB2	2.10	0.51
1:B:828:LEU:O	1:B:829:ILE:HG23	2.10	0.51
1:B:757:MET:HG2	1:B:760:PHE:CZ	2.46	0.51
1:B:860:GLU:O	1:B:862:GLY:HA3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ILE:HD11	1:B:596:VAL:HG21	1.92	0.51
1:B:90:GLU:O	1:B:94:ILE:HG13	2.11	0.51
1:B:650:ASP:O	1:B:672:ARG:HD2	2.11	0.51
1:B:833:LEU:HD12	1:B:836:ARG:HE	1.75	0.51
1:A:573:ARG:HB2	1:A:574:GLU:OE2	2.11	0.51
1:B:338:SER:OG	1:B:732:GLU:HG2	2.11	0.51
1:B:856:PHE:HA	1:B:863:PRO:CG	2.41	0.51
1:A:914:ASN:OD1	1:A:981:ASP:HB3	2.11	0.51
1:B:953:LEU:HB2	1:B:954:PRO:HD3	1.93	0.51
1:A:338:SER:OG	1:A:732:GLU:HG2	2.11	0.51
1:B:459:VAL:HA	1:B:462:LEU:HG	1.92	0.50
1:A:240:ALA:O	1:A:242:THR:N	2.44	0.50
1:A:950:VAL:O	1:A:954:PRO:HD3	2.11	0.50
1:B:230:THR:OG1	8:B:3002:ACT:H2	2.11	0.50
1:B:868:HIS:O	1:B:872:HIS:CD2	2.64	0.50
1:A:830:SER:O	1:A:831:GLY:C	2.50	0.50
1:B:336:LEU:O	1:B:339:VAL:HG12	2.11	0.50
1:A:667:ARG:HG2	1:A:694:TYR:CE1	2.46	0.50
1:A:923:MET:CE	1:A:986:PHE:HE2	2.24	0.50
1:B:56:GLN:OE1	5:B:1005:CZA:O1	2.29	0.50
1:A:504:SER:C	1:A:506:ALA:N	2.65	0.50
1:A:50:TRP:O	1:A:54:ILE:HD13	2.12	0.50
1:A:757:MET:HA	1:A:760:PHE:CE2	2.46	0.50
1:A:883:PHE:CD1	1:A:886:LEU:HD11	2.47	0.50
1:A:947:ILE:O	1:A:947:ILE:HG22	2.11	0.50
1:A:307:ILE:HG21	5:A:1005:CZA:H102	1.94	0.49
1:A:534:ARG:HH11	1:A:568:ASP:HB2	1.76	0.49
1:A:716:ILE:HD11	1:A:733:MET:HE3	1.92	0.49
1:A:80:GLU:HG3	1:A:81:GLY:N	2.27	0.49
1:B:279:PHE:HE1	1:B:288:TRP:CZ3	2.30	0.49
1:A:853:ALA:HA	1:A:856:PHE:HD1	1.77	0.49
1:B:319:LEU:HB3	1:B:336:LEU:HG	1.94	0.49
1:B:72:SER:OG	1:B:90:GLU:HG2	2.12	0.49
1:B:963:ASP:HB3	1:B:966:GLN:CG	2.42	0.49
1:A:25:THR:OG1	1:A:28:GLN:HG3	2.11	0.49
1:B:33:LEU:HD13	1:B:146:VAL:CG1	2.42	0.49
1:B:310:GLY:O	1:B:314:VAL:HG12	2.13	0.49
1:B:843:TYR:OH	1:B:976:PRO:HB2	2.12	0.49
1:A:80:GLU:HG3	1:A:81:GLY:H	1.78	0.49
1:A:829:ILE:O	1:A:829:ILE:HD12	2.12	0.49
1:B:454:VAL:HG22	9:B:1011:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:794:TRP:CZ2	1:B:947:ILE:HD11	2.48	0.49
1:B:916:LEU:CD1	1:B:927:PRO:HA	2.43	0.49
1:A:230:THR:OG1	8:A:3002:ACT:H2	2.13	0.49
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.94	0.49
1:B:940:SER:HA	1:B:943:LEU:HD12	1.95	0.49
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.94	0.49
1:A:803:PRO:HA	1:A:936:SER:OG	2.13	0.48
1:B:694:TYR:O	1:B:695:ASP:HB2	2.12	0.48
1:A:869:GLN:HB3	1:A:883:PHE:CE1	2.48	0.48
1:B:725:ALA:O	1:B:729:THR:HG23	2.14	0.48
1:A:777:LEU:HB2	1:A:849:VAL:HG21	1.94	0.48
1:A:771:GLU:O	1:A:775:ILE:HG12	2.13	0.48
1:B:758:LYS:O	1:B:762:ARG:HG3	2.13	0.48
1:B:950:VAL:HG12	1:B:952:PRO:HD2	1.95	0.48
1:B:986:PHE:CD2	1:B:989:ARG:NH1	2.81	0.48
1:A:384:ILE:HD12	1:A:384:ILE:N	2.28	0.48
1:A:577:VAL:HG22	1:A:577:VAL:O	2.13	0.48
1:A:656:ARG:HB3	1:A:656:ARG:HH11	1.77	0.48
1:A:950:VAL:HG12	1:A:950:VAL:O	2.14	0.48
1:A:988:ALA:HA	1:A:992:LEU:HB3	1.95	0.48
1:B:829:ILE:O	1:B:829:ILE:HD12	2.12	0.48
1:A:773:VAL:O	1:A:777:LEU:HG	2.12	0.48
1:A:855:TRP:HA	1:A:859:ALA:CB	2.43	0.48
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.96	0.48
1:B:760:PHE:CD1	1:B:760:PHE:C	2.87	0.48
1:B:856:PHE:C	1:B:863:PRO:HG2	2.34	0.48
1:B:863:PRO:N	1:B:864:GLY:HA2	2.28	0.48
1:A:606:GLU:CD	1:A:606:GLU:H	2.17	0.48
1:A:883:PHE:HD1	1:A:886:LEU:HD11	1.79	0.48
1:A:922:LEU:HD13	1:A:982:GLU:OE1	2.13	0.48
1:B:353:THR:HA	1:B:357:THR:OG1	2.14	0.48
1:B:397:LYS:HB2	1:B:402:ILE:HG21	1.95	0.48
1:A:272:TRP:HB2	1:A:295:TYR:OH	2.13	0.47
1:A:30:LYS:O	1:A:34:GLU:HG3	2.14	0.47
1:B:271:VAL:HG21	1:B:302:LEU:HD11	1.96	0.47
1:B:765:ILE:O	1:B:769:VAL:HG23	2.14	0.47
1:A:77:TRP:C	1:A:79:GLU:H	2.18	0.47
1:A:89:VAL:O	1:A:93:VAL:HG23	2.15	0.47
1:B:939:LEU:O	1:B:943:LEU:HG	2.14	0.47
1:A:691:LEU:HB3	1:A:698:THR:HG21	1.95	0.47
1:B:77:TRP:HD1	1:B:78:PHE:CE1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:832:TRP:O	1:B:836:ARG:N	2.46	0.47
1:B:77:TRP:HE3	1:B:88:PHE:HZ	1.62	0.47
1:B:941:MET:HA	1:B:941:MET:CE	2.45	0.47
1:A:770:GLY:HA3	1:A:844:VAL:HG13	1.96	0.47
1:A:80:GLU:C	1:A:82:GLU:H	2.17	0.47
1:B:269:VAL:O	1:B:273:LEU:HG	2.13	0.47
1:A:857:MET:HA	1:A:865:VAL:HA	1.95	0.47
1:A:64:ILE:HG21	1:A:264:ILE:HD13	1.96	0.47
1:A:377:CYS:HB2	1:A:541:VAL:HG22	1.97	0.47
1:A:947:ILE:HG22	1:A:959:LEU:HD12	1.96	0.47
1:A:120:LYS:HG2	1:A:123:GLU:OE2	2.15	0.47
1:B:556:ARG:HD2	1:B:644:GLU:HB3	1.97	0.47
1:B:896:PRO:O	1:B:899:MET:HB2	2.14	0.47
1:A:190:HIS:O	1:A:206:ASN:HA	2.14	0.46
1:A:573:ARG:HE	1:A:573:ARG:HB3	1.58	0.46
1:B:77:TRP:HA	1:B:88:PHE:CZ	2.51	0.46
1:A:76:ALA:HB1	1:A:87:ALA:O	2.16	0.46
1:A:835:PHE:HA	1:A:838:MET:HB2	1.97	0.46
1:A:887:ASP:HB3	1:A:890:ILE:HG13	1.97	0.46
1:B:325:ARG:NH1	1:B:749:GLU:OE1	2.49	0.46
1:B:527:TYR:CD1	1:B:534:ARG:HD3	2.51	0.46
1:B:866:THR:HB	1:B:869:GLN:HB2	1.96	0.46
1:A:154:ALA:N	1:A:157:ASP:OD1	2.40	0.46
1:A:249:LEU:O	1:A:253:LEU:HG	2.15	0.46
1:A:487:PHE:CE2	7:A:1007:ACP:C4	2.98	0.46
1:B:129:VAL:HG12	1:B:151:VAL:HG12	1.98	0.46
1:A:890:ILE:HG22	1:A:890:ILE:O	2.16	0.46
1:A:833:LEU:HD12	1:A:836:ARG:HD3	1.98	0.46
1:B:41:LEU:HD21	8:B:3002:ACT:H1	1.98	0.46
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.80	0.46
1:A:806:ALA:HB1	1:A:933:LEU:HA	1.98	0.46
1:A:853:ALA:O	1:A:856:PHE:HB2	2.16	0.46
1:B:391:PRO:HB3	1:B:450:GLU:HB3	1.97	0.46
1:B:975:LEU:N	1:B:976:PRO:CD	2.78	0.46
1:A:987:ILE:O	1:A:987:ILE:HG12	2.15	0.45
1:A:651:ARG:NH1	9:A:1209:HOH:O	2.49	0.45
1:B:977:VAL:HG13	1:B:978:ILE:N	2.30	0.45
1:B:311:LEU:HB3	1:B:312:PRO:HD3	1.98	0.45
1:A:74:VAL:C	1:A:76:ALA:H	2.19	0.45
1:A:775:ILE:O	1:A:775:ILE:HG22	2.17	0.45
1:A:800:ASP:O	1:A:803:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LYS:O	1:B:247:THR:O	2.34	0.45
1:B:926:PRO:HB3	1:B:928:TRP:CE2	2.51	0.45
1:A:559:LEU:HD23	1:A:600:LEU:HB3	1.98	0.45
1:A:760:PHE:C	1:A:760:PHE:CD1	2.89	0.45
1:A:833:LEU:O	1:A:836:ARG:HB3	2.17	0.45
1:A:860:GLU:C	1:A:862:GLY:HA3	2.36	0.45
1:A:880:HIS:N	1:A:881:PRO:CD	2.80	0.45
1:A:960:LYS:O	1:A:961:ALA:O	2.35	0.45
1:A:843:TYR:HE2	1:A:977:VAL:HB	1.82	0.45
1:A:984:LEU:HA	1:A:987:ILE:HG22	1.98	0.45
1:B:970:VAL:O	1:B:973:ILE:HG22	2.16	0.45
1:A:549:ILE:CD1	1:A:596:VAL:HG21	2.47	0.45
1:A:860:GLU:H	1:A:860:GLU:HG2	1.57	0.45
1:A:887:ASP:OD2	1:A:889:GLU:HB3	2.17	0.45
1:A:970:VAL:O	1:A:973:ILE:HG22	2.17	0.45
1:B:864:GLY:O	1:B:865:VAL:O	2.36	0.44
1:A:311:LEU:HD12	5:A:1005:CZA:H20	1.99	0.44
1:A:555:GLY:C	1:A:557:ASP:N	2.70	0.44
1:A:807:LEU:C	1:A:809:PHE:H	2.19	0.44
1:A:926:PRO:O	1:A:929:VAL:HG23	2.17	0.44
1:A:100:ALA:O	1:A:103:ILE:HG12	2.18	0.44
1:A:67:LEU:C	1:A:69:ALA:H	2.21	0.44
1:B:912:ALA:O	1:B:933:LEU:HD21	2.17	0.44
1:B:90:GLU:HB3	1:B:91:PRO:HD3	2.00	0.44
1:A:907:ILE:O	1:A:911:ASN:HB2	2.16	0.44
1:B:273:LEU:O	1:B:276:ILE:HG22	2.17	0.44
1:B:865:VAL:HG12	1:B:866:THR:N	2.32	0.44
1:B:802:LEU:HB2	1:B:803:PRO:HD3	1.99	0.44
1:B:946:LEU:O	1:B:953:LEU:HD12	2.18	0.44
1:A:353:THR:HA	1:A:357:THR:OG1	2.18	0.44
1:A:864:GLY:O	1:A:866:THR:HG23	2.18	0.44
1:A:896:PRO:O	1:A:899:MET:HB2	2.18	0.44
1:B:425:LEU:HD12	1:B:425:LEU:HA	1.82	0.44
1:B:391:PRO:HB3	1:B:450:GLU:CB	2.48	0.44
1:A:906:THR:HG22	1:A:974:SER:HB3	2.00	0.44
1:A:889:GLU:HG2	1:A:889:GLU:O	2.17	0.44
1:A:88:PHE:C	1:A:91:PRO:HD2	2.38	0.44
1:B:986:PHE:HD2	1:B:989:ARG:HH12	1.65	0.44
1:B:793:LEU:HD23	1:B:793:LEU:HA	1.85	0.43
1:B:69:ALA:HB2	1:B:94:ILE:CG2	2.48	0.43
1:B:863:PRO:CB	1:B:864:GLY:CA	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:TRP:CE3	1:A:273:LEU:HD23	2.54	0.43
1:B:403:ARG:O	1:B:406:GLN:CG	2.67	0.43
1:A:2:GLU:O	1:A:7:LYS:NZ	2.51	0.43
1:B:556:ARG:CZ	1:B:556:ARG:HB3	2.49	0.43
1:B:558:THR:O	1:B:558:THR:HG22	2.19	0.43
1:B:712:LYS:HE2	1:B:712:LYS:HB3	1.60	0.43
1:B:757:MET:HA	1:B:760:PHE:CE2	2.53	0.43
1:B:879:ASP:OD2	1:B:882:HIS:ND1	2.52	0.43
1:B:103:ILE:CG1	1:B:104:VAL:N	2.82	0.43
1:B:23:GLY:HA2	1:B:150:ILE:HG12	2.01	0.43
1:B:412:GLU:OE2	1:B:566:THR:CG2	2.67	0.43
1:B:60:LEU:HD23	1:B:261:SER:OG	2.19	0.43
1:B:61:LEU:HD11	1:B:307:ILE:HG12	2.00	0.43
1:B:650:ASP:N	1:B:650:ASP:OD1	2.51	0.43
1:A:135:LYS:HD2	1:A:135:LYS:HA	1.63	0.43
1:A:802:LEU:HG	1:A:939:LEU:HD23	2.00	0.43
1:B:249:LEU:C	1:B:251:GLN:N	2.72	0.43
1:B:272:TRP:CE3	1:B:273:LEU:HD23	2.54	0.43
1:B:607:VAL:O	1:B:611:ILE:HG12	2.18	0.43
1:B:652:ALA:HA	1:B:675:CYS:O	2.19	0.43
1:B:71:ILE:O	1:B:75:LEU:HD13	2.18	0.43
1:B:903:VAL:O	1:B:907:ILE:HG13	2.19	0.43
1:A:482:GLU:HG2	1:A:573:ARG:NH1	2.33	0.43
1:A:667:ARG:HG2	1:A:694:TYR:CZ	2.54	0.43
1:A:853:ALA:HA	1:A:856:PHE:CD1	2.54	0.43
1:A:880:HIS:N	1:A:881:PRO:HD2	2.32	0.43
1:B:311:LEU:HD22	1:B:315:ILE:HG13	2.00	0.43
1:A:926:PRO:HB3	1:A:928:TRP:CE2	2.54	0.43
1:B:279:PHE:CG	1:B:279:PHE:O	2.71	0.43
1:B:447:THR:HG22	1:B:451:LYS:HE3	2.01	0.43
1:B:880:HIS:N	1:B:881:PRO:CD	2.82	0.43
1:A:249:LEU:HA	1:A:252:LYS:HG3	2.01	0.43
1:B:771:GLU:O	1:B:775:ILE:HG12	2.19	0.43
1:B:948:LEU:HD23	1:B:959:LEU:HD13	2.01	0.43
1:A:287:SER:OG	1:A:289:ILE:HG22	2.19	0.42
1:A:49:LEU:HD12	1:A:50:TRP:N	2.34	0.42
1:B:947:ILE:HG22	1:B:959:LEU:HD12	2.00	0.42
1:B:914:ASN:HB3	1:B:981:ASP:OD2	2.19	0.42
1:A:97:ILE:HD11	1:A:797:LEU:CD2	2.50	0.42
1:A:949:TYR:CZ	1:A:961:ALA:HB1	2.55	0.42
1:A:962:LEU:HB3	1:A:966:GLN:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:ARG:NH2	1:B:671:ARG:HA	2.34	0.42
1:B:242:THR:O	1:B:244:GLN:N	2.52	0.42
1:B:283:VAL:O	1:B:283:VAL:HG12	2.20	0.42
1:B:302:LEU:HA	1:B:302:LEU:HD23	1.81	0.42
1:B:311:LEU:N	1:B:312:PRO:CD	2.82	0.42
1:B:654:THR:HA	1:B:677:ALA:O	2.19	0.42
1:B:947:ILE:HG12	1:B:953:LEU:HD13	2.02	0.42
1:B:97:ILE:N	1:B:97:ILE:HD13	2.34	0.42
1:A:158:LYS:HD3	9:A:1197:HOH:O	2.19	0.42
1:B:80:GLU:O	1:B:82:GLU:N	2.47	0.42
1:A:852:ALA:HB2	1:A:900:ALA:HB2	2.02	0.42
1:A:870:LEU:C	1:A:872:HIS:H	2.22	0.42
1:B:860:GLU:C	1:B:862:GLY:HA3	2.40	0.42
1:A:250:GLN:HA	1:A:253:LEU:HG	2.01	0.42
1:A:369:ILE:CD1	1:A:379:LEU:HD22	2.49	0.42
1:A:606:GLU:HG3	1:A:739:ASN:OD1	2.19	0.42
1:A:777:LEU:HD12	1:A:845:GLY:O	2.20	0.42
1:B:80:GLU:HB3	1:B:82:GLU:HG3	2.01	0.42
1:B:61:LEU:HD22	1:B:61:LEU:HA	1.89	0.42
1:B:342:LEU:HG	1:B:716:ILE:HD13	2.01	0.41
1:B:825:LYS:O	1:B:826:GLU:C	2.58	0.41
1:A:308:PRO:O	1:A:311:LEU:HB2	2.21	0.41
1:A:46:GLY:O	1:A:47:LYS:O	2.38	0.41
1:B:53:VAL:O	1:B:56:GLN:HB2	2.20	0.41
1:A:363:VAL:HG11	1:A:448:LEU:HD22	2.02	0.41
1:A:712:LYS:HB3	1:A:712:LYS:HE2	1.31	0.41
1:A:342:LEU:HD22	1:A:747:VAL:HG22	2.02	0.41
1:B:396:LEU:HD23	1:B:401:PRO:HA	2.02	0.41
1:B:398:ASN:HA	9:B:1166:HOH:O	2.20	0.41
1:B:397:LYS:HB2	1:B:402:ILE:CG2	2.50	0.41
1:A:508:VAL:HG22	1:A:509:GLY:N	2.35	0.41
1:B:19:SER:HB3	1:B:22:THR:HB	2.02	0.41
1:B:310:GLY:HA3	1:B:797:LEU:HD12	2.01	0.41
1:A:482:GLU:HG2	1:A:573:ARG:HH12	1.85	0.41
1:A:506:ALA:O	1:A:507:ALA:CB	2.68	0.41
1:A:654:THR:HA	1:A:677:ALA:O	2.20	0.41
1:A:870:LEU:O	1:A:870:LEU:HD12	2.21	0.41
1:A:926:PRO:HA	1:A:927:PRO:HD3	1.90	0.41
1:A:534:ARG:NH1	1:A:568:ASP:HB2	2.35	0.41
1:A:77:TRP:C	1:A:77:TRP:CD1	2.94	0.41
1:A:57:PHE:HE1	1:A:98:LEU:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ILE:HD11	1:B:208:LEU:HG	2.03	0.41
1:B:880:HIS:HD2	1:B:888:CYS:SG	2.43	0.41
1:B:988:ALA:O	1:B:992:LEU:HB3	2.20	0.41
1:A:778:THR:HG21	1:A:786:ALA:H	1.85	0.41
1:A:200:VAL:HG22	1:A:680:GLU:CD	2.41	0.41
1:A:953:LEU:HA	1:A:956:ILE:HD11	2.01	0.41
1:B:887:ASP:C	1:B:889:GLU:H	2.24	0.41
1:B:227:GLY:O	8:B:3002:ACT:H3	2.21	0.41
1:B:369:ILE:HD11	1:B:545:ILE:HD11	2.02	0.41
1:B:749:GLU:O	1:B:753:ILE:HG12	2.21	0.41
1:B:979:GLY:O	1:B:980:LEU:C	2.59	0.41
1:A:49:LEU:O	1:A:53:VAL:HG23	2.21	0.41
1:B:57:PHE:HD1	1:B:62:VAL:CG1	2.34	0.41
1:B:883:PHE:HB3	1:B:886:LEU:HD12	2.03	0.41
1:B:249:LEU:O	1:B:251:GLN:N	2.54	0.40
1:A:336:LEU:HA	1:A:336:LEU:HD12	1.72	0.40
1:B:367:PHE:C	1:B:367:PHE:CD2	2.93	0.40
1:A:18:VAL:HG11	1:A:24:LEU:HD23	2.02	0.40
1:A:247:THR:HG22	1:A:249:LEU:N	2.36	0.40
1:A:360:GLN:OE1	1:A:388:THR:HB	2.21	0.40
1:A:765:ILE:HA	1:A:765:ILE:HD12	1.83	0.40
1:B:88:PHE:O	1:B:91:PRO:HD2	2.20	0.40
1:A:917:SER:HB2	1:A:925:MET:SD	2.61	0.40
1:B:574:GLU:CD	1:B:574:GLU:H	2.23	0.40
1:B:880:HIS:C	1:B:882:HIS:H	2.25	0.40
1:A:59:ASP:OD1	5:A:1005:CZA:H161	2.22	0.40
1:A:487:PHE:CD2	7:A:1007:ACP:C5	3.05	0.40
1:B:135:LYS:HA	1:B:135:LYS:HD2	1.73	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	992/994 (100%)	892 (90%)	77 (8%)	23 (2%)	6	10
1	B	992/994 (100%)	898 (90%)	80 (8%)	14 (1%)	11	20
All	All	1984/1988 (100%)	1790 (90%)	157 (8%)	37 (2%)	8	13

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	82	GLU
1	A	504	SER
1	A	507	ALA
1	A	961	ALA
1	B	243	GLU
1	B	283	VAL
1	B	865	VAL
1	A	47	LYS
1	A	241	ALA
1	A	245	ASP
1	A	309	GLU
1	A	831	GLY
1	A	865	VAL
1	A	988	ALA
1	B	866	THR
1	A	46	GLY
1	A	827	PRO
1	A	889	GLU
1	A	951	ASP
1	B	47	LYS
1	B	284	HIS
1	B	826	GLU
1	B	867	TYR
1	A	864	GLY
1	B	244	GLN
1	B	250	GLN
1	B	287	SER
1	A	68	ALA
1	A	284	HIS
1	A	857	MET
1	B	247	THR
1	B	888	CYS
1	B	951	ASP
1	A	952	PRO

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Mol	Chain	Res	Type
1	A	283	VAL
1	A	950	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	840/840 (100%)	786 (94%)	54 (6%)	17	33
1	B	840/840 (100%)	790 (94%)	50 (6%)	19	37
All	All	1680/1680 (100%)	1576 (94%)	104 (6%)	18	35

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	30	LYS
1	A	33	LEU
1	A	44	GLU
1	A	45	GLU
1	A	51	GLU
1	A	109	GLU
1	A	184	SER
1	A	185	VAL
1	A	200	VAL
1	A	236	ARG
1	A	254	ASP
1	A	278	HIS
1	A	308	PRO
1	A	311	LEU
1	A	319	LEU
1	A	336	LEU
1	A	341	THR
1	A	342	LEU
1	A	344	CYS
1	A	356	LEU

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Mol	Chain	Res	Type
1	A	397	LYS
1	A	426	ASP
1	A	465	VAL
1	A	478	LEU
1	A	533	THR
1	A	534	ARG
1	A	535	VAL
1	A	543	GLU
1	A	544	LYS
1	A	550	LYS
1	A	566	THR
1	A	572	LYS
1	A	577	VAL
1	A	656	ARG
1	A	679	VAL
1	A	691	LEU
1	A	698	THR
1	A	712	LYS
1	A	716	ILE
1	A	760	PHE
1	A	767	SER
1	A	809	PHE
1	A	814	LEU
1	A	816	ILE
1	A	844	VAL
1	A	865	VAL
1	A	886	LEU
1	A	914	ASN
1	A	941	MET
1	A	956	ILE
1	A	964	LEU
1	A	975	LEU
1	A	986	PHE
1	B	18	VAL
1	B	31	ARG
1	B	59	ASP
1	B	61	LEU
1	B	75	LEU
1	B	96	LEU
1	B	98	LEU
1	B	116	ILE
1	B	121	GLU

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Mol	Chain	Res	Type
1	B	200	VAL
1	B	236	ARG
1	B	278	HIS
1	B	309	GLU
1	B	311	LEU
1	B	314	VAL
1	B	319	LEU
1	B	336	LEU
1	B	356	LEU
1	B	367	PHE
1	B	426	ASP
1	B	465	VAL
1	B	478	LEU
1	B	505	ARG
1	B	528	VAL
1	B	534	ARG
1	B	543	GLU
1	B	566	THR
1	B	572	LYS
1	B	577	VAL
1	B	605	LYS
1	B	656	ARG
1	B	691	LEU
1	B	701	THR
1	B	712	LYS
1	B	759	GLN
1	B	760	PHE
1	B	767	SER
1	B	778	THR
1	B	781	LEU
1	B	790	VAL
1	B	819	ARG
1	B	838	MET
1	B	861	ASP
1	B	866	THR
1	B	877	THR
1	B	889	GLU
1	B	941	MET
1	B	956	ILE
1	B	980	LEU
1	B	992	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	759	GLN
1	A	810	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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
8	ACT	B	3002	-	1,3,3	2.15	1 (100%)	0,3,3	0.00	-
7	ACP	B	1007	-	27,33,33	1.77	6 (22%)	32,52,52	2.02	8 (25%)
5	CZA	A	1005	6	27,29,29	1.64	6 (22%)	24,48,48	1.51	3 (12%)
3	MF4	A	1003	1	0,4,4	0.00	-	-	-	-
5	CZA	B	1005	6	27,29,29	1.74	10 (37%)	24,48,48	1.55	5 (20%)
7	ACP	A	1007	-	27,33,33	1.66	4 (14%)	32,52,52	2.17	7 (21%)
3	MF4	B	1003	1	0,4,4	0.00	-	-	-	-
8	ACT	A	3001	-	1,3,3	3.53	1 (100%)	0,3,3	0.00	-
8	ACT	A	3002	-	1,3,3	1.93	0	0,3,3	0.00	-
8	ACT	B	3001	-	1,3,3	3.12	1 (100%)	0,3,3	0.00	-

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
7	ACP	A	1007	-	-	4/15/38/38	0/3/3/3
7	ACP	B	1007	-	-	7/15/38/38	0/3/3/3
5	CZA	A	1005	6	-	0/4/52/52	0/5/5/5
5	CZA	B	1005	6	-	0/4/52/52	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1005	CZA	C4-N1	-4.59	1.34	1.39
7	A	1007	ACP	PG-O1G	4.02	1.58	1.50
7	B	1007	ACP	PG-O1G	3.98	1.58	1.50
5	A	1005	CZA	C4-N1	-3.72	1.35	1.39
7	B	1007	ACP	PB-O2B	-3.70	1.47	1.56
8	A	3001	ACT	CH3-C	3.53	1.53	1.48
7	A	1007	ACP	PB-O2B	-3.43	1.48	1.56
5	A	1005	CZA	C12-C8	3.41	1.58	1.53
8	B	3001	ACT	CH3-C	3.12	1.52	1.48
7	B	1007	ACP	PG-O3G	-2.92	1.48	1.54
5	B	1005	CZA	C12-C8	2.91	1.57	1.53
7	A	1007	ACP	PB-O1B	2.88	1.58	1.51
7	A	1007	ACP	PG-O3G	-2.80	1.48	1.54
7	B	1007	ACP	PB-O1B	2.74	1.58	1.51
5	B	1005	CZA	C3-C4	-2.62	1.35	1.40
7	B	1007	ACP	PG-O2G	2.56	1.60	1.54
5	A	1005	CZA	C3-C4	-2.34	1.36	1.40
5	A	1005	CZA	C19-C18	2.32	1.42	1.36
5	B	1005	CZA	C19-C18	2.30	1.41	1.36
5	A	1005	CZA	O3-C4	2.30	1.37	1.30
7	B	1007	ACP	C2-N3	2.24	1.35	1.32
5	B	1005	CZA	C9-N1	-2.21	1.46	1.49
5	B	1005	CZA	O3-C4	2.16	1.37	1.30
8	B	3002	ACT	CH3-C	2.15	1.51	1.48
5	B	1005	CZA	C7-C5	-2.06	1.52	1.55
5	B	1005	CZA	C5-C6	-2.06	1.51	1.53
5	A	1005	CZA	C20-C13	2.04	1.41	1.37
5	B	1005	CZA	C13-C14	-2.03	1.39	1.43
5	B	1005	CZA	C20-C13	2.00	1.41	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1007	ACP	PA-O3A-PB	7.26	155.60	132.56
7	A	1007	ACP	PA-O3A-PB	6.81	154.17	132.56
7	A	1007	ACP	O2G-PG-O1G	-5.66	97.42	112.39
5	A	1005	CZA	C8-C7-C5	-4.32	95.92	103.37
7	B	1007	ACP	O2G-PG-O1G	-4.14	101.43	112.39
5	B	1005	CZA	C13-C14-C15	4.12	127.94	123.48
5	A	1005	CZA	C13-C14-C15	3.94	127.74	123.48
7	A	1007	ACP	C1'-N9-C4	-3.72	120.10	126.64
5	B	1005	CZA	C8-C7-C5	-3.12	97.99	103.37
7	B	1007	ACP	O5'-PA-O1A	-3.05	97.14	109.07
7	B	1007	ACP	C1'-N9-C4	-3.05	121.29	126.64
7	A	1007	ACP	O5'-PA-O1A	-2.99	97.37	109.07
7	A	1007	ACP	O2A-PA-O5'	2.95	121.43	107.75
7	A	1007	ACP	O2B-PB-C3B	2.90	118.44	106.58
7	B	1007	ACP	O3G-PG-C3B	2.83	113.25	106.40
5	B	1005	CZA	O1-C2-C3	2.64	125.30	120.41
7	A	1007	ACP	O3G-PG-C3B	2.46	112.36	106.40
7	B	1007	ACP	O2A-PA-O5'	2.33	118.58	107.75
5	B	1005	CZA	C18-C17-N2	2.33	137.25	130.80
5	A	1005	CZA	C18-C17-N2	2.32	137.23	130.80
5	B	1005	CZA	O2-C6-C5	-2.22	122.41	124.60
7	B	1007	ACP	C3'-C2'-C1'	2.08	104.11	100.98
7	B	1007	ACP	O2G-PG-C3B	2.03	111.33	106.40

There are no chirality outliers.

All (11) torsion outliers are listed below:

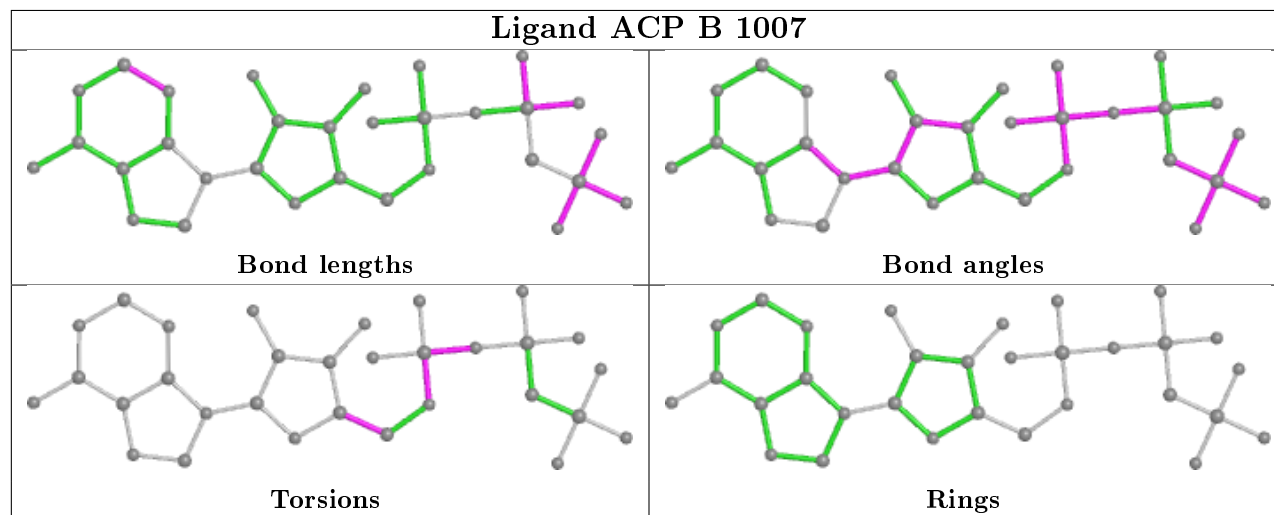
Mol	Chain	Res	Type	Atoms
7	B	1007	ACP	C5'-O5'-PA-O2A
7	B	1007	ACP	O4'-C4'-C5'-O5'
7	A	1007	ACP	C5'-O5'-PA-O3A
7	A	1007	ACP	O4'-C4'-C5'-O5'
7	B	1007	ACP	C3'-C4'-C5'-O5'
7	A	1007	ACP	C3'-C4'-C5'-O5'
7	B	1007	ACP	PB-O3A-PA-O1A
7	B	1007	ACP	C5'-O5'-PA-O1A
7	A	1007	ACP	C5'-O5'-PA-O2A
7	B	1007	ACP	PB-O3A-PA-O2A
7	B	1007	ACP	C5'-O5'-PA-O3A

There are no ring outliers.

7 monomers are involved in 14 short contacts:

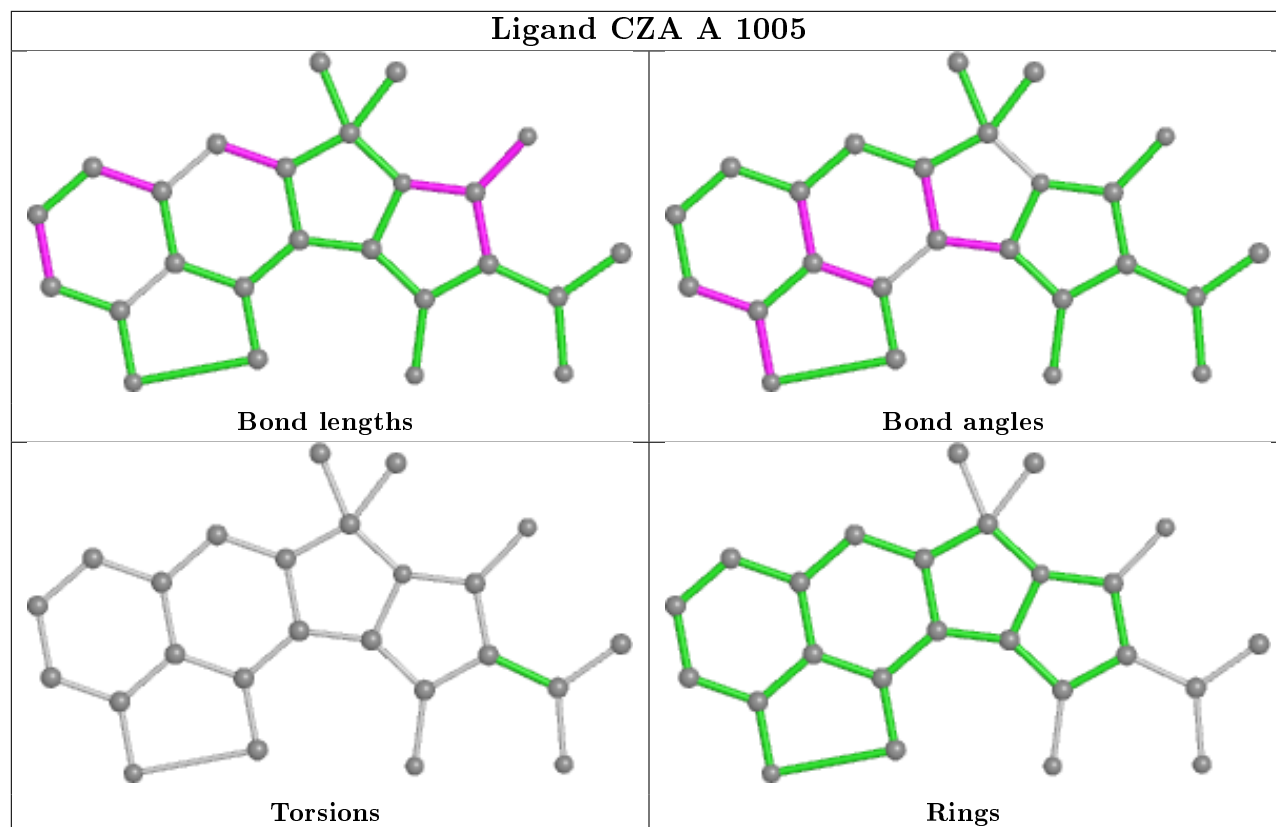
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	3002	ACT	3	0
5	A	1005	CZA	3	0
5	B	1005	CZA	2	0
7	A	1007	ACP	2	0
8	A	3001	ACT	1	0
8	A	3002	ACT	2	0
8	B	3001	ACT	1	0

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.

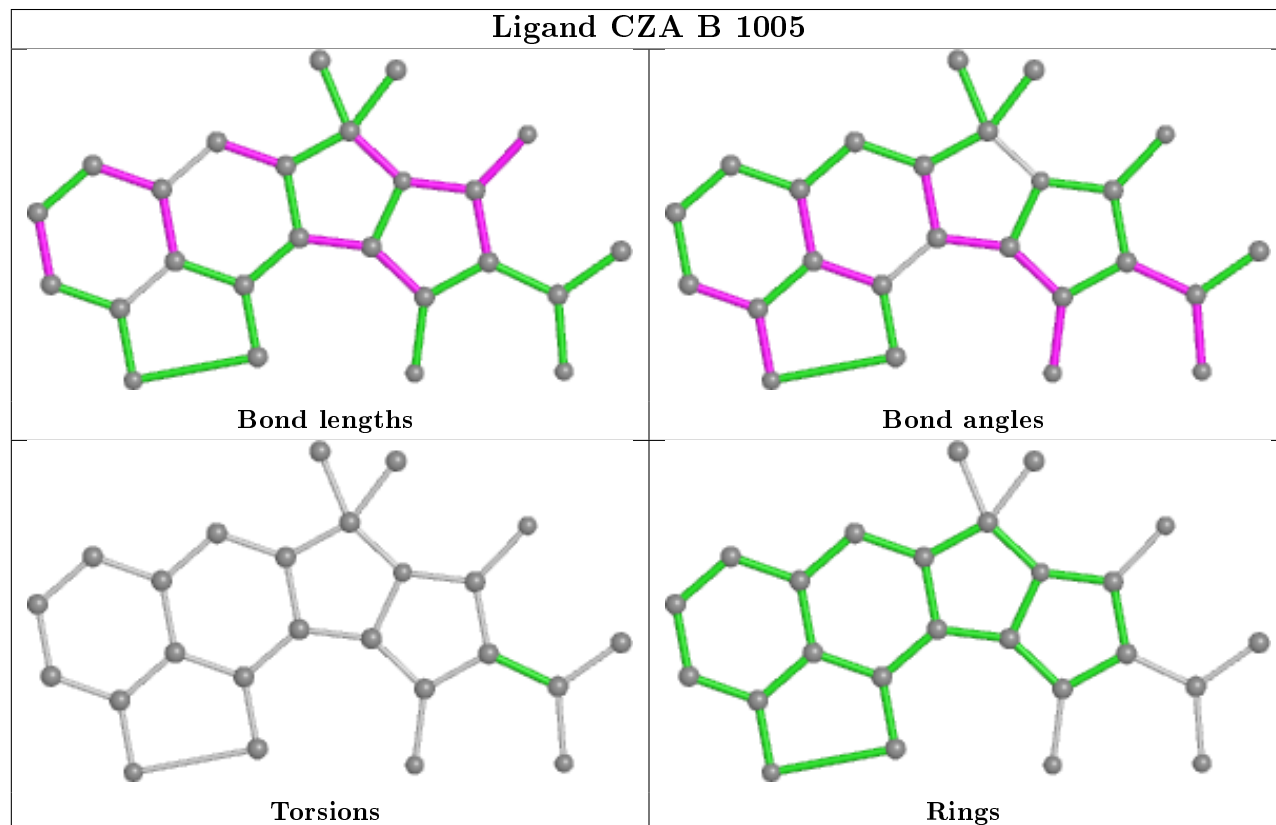


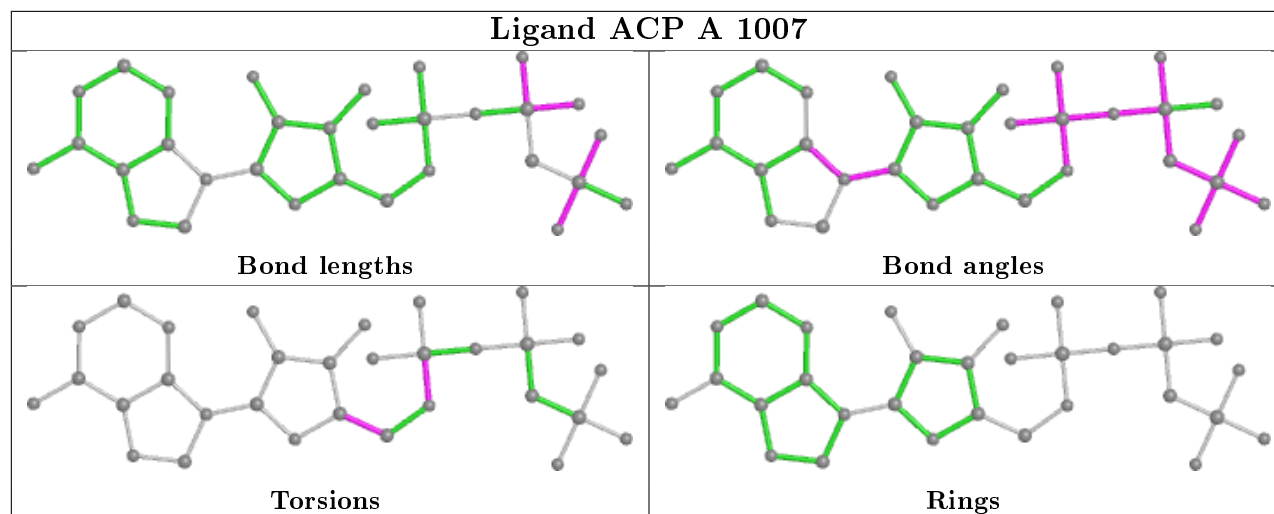


## Ligand CZA A 1005



## Ligand CZA B 1005





## 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	994/994 (100%)	0.44	126 (12%) 3 3	27, 62, 204, 387	0
1	B	994/994 (100%)	0.17	74 (7%) 14 15	31, 66, 161, 261	0
All	All	1988/1988 (100%)	0.30	200 (10%) 7 6	27, 64, 186, 387	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	VAL	16.7
1	A	284	HIS	13.1
1	B	288	TRP	10.3
1	A	281	ASP	10.1
1	A	285	GLY	10.0
1	A	280	ASN	9.8
1	A	282	PRO	9.4
1	A	891	PHE	9.0
1	A	78	PHE	8.3
1	A	874	MET	8.1
1	A	875	GLN	8.1
1	A	82	GLU	8.0
1	A	948	LEU	7.4
1	A	81	GLY	7.4
1	A	288	TRP	7.2
1	B	245	ASP	7.1
1	A	890	ILE	7.0
1	B	112	ALA	6.8
1	A	80	GLU	6.6
1	A	77	TRP	6.5
1	B	275	ASN	6.5
1	B	287	SER	6.4
1	A	868	HIS	6.4
1	B	283	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	276	ILE	6.3
1	B	282	PRO	6.3
1	B	271	VAL	6.3
1	B	992	LEU	6.2
1	B	280	ASN	6.1
1	A	994	GLY	6.1
1	B	284	HIS	6.0
1	A	111	ASN	6.0
1	B	81	GLY	6.0
1	A	970	VAL	5.9
1	A	856	PHE	5.9
1	B	285	GLY	5.8
1	A	287	SER	5.8
1	A	863	PRO	5.8
1	B	289	ILE	5.6
1	B	77	TRP	5.4
1	B	243	GLU	5.4
1	A	286	GLY	5.4
1	A	853	ALA	5.2
1	A	50	TRP	5.1
1	A	873	PHE	5.1
1	B	279	PHE	5.1
1	A	949	TYR	5.1
1	A	292	ALA	5.0
1	A	991	TYR	5.0
1	A	962	LEU	4.9
1	A	858	TYR	4.9
1	B	281	ASP	4.8
1	A	782	GLY	4.8
1	B	991	TYR	4.8
1	A	857	MET	4.7
1	B	295	TYR	4.7
1	B	286	GLY	4.7
1	B	111	ASN	4.7
1	A	860	GLU	4.6
1	B	927	PRO	4.6
1	B	928	TRP	4.5
1	A	279	PHE	4.5
1	B	272	TRP	4.5
1	A	865	VAL	4.5
1	A	60	LEU	4.4
1	A	266	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	883	PHE	4.4
1	A	289	ILE	4.3
1	A	52	LEU	4.3
1	B	78	PHE	4.2
1	B	244	GLN	4.2
1	A	967	TRP	4.1
1	A	291	GLY	4.1
1	A	781	LEU	4.0
1	B	293	ILE	4.0
1	A	886	LEU	4.0
1	B	274	ILE	4.0
1	B	964	LEU	4.0
1	A	46	GLY	3.9
1	A	278	HIS	3.9
1	B	924	ARG	3.9
1	B	986	PHE	3.9
1	A	961	ALA	3.9
1	A	951	ASP	3.8
1	B	994	GLY	3.8
1	A	57	PHE	3.8
1	A	925	MET	3.8
1	B	60	LEU	3.8
1	A	64	ILE	3.7
1	B	292	ALA	3.7
1	B	46	GLY	3.7
1	B	50	TRP	3.7
1	A	870	LEU	3.6
1	A	881	PRO	3.6
1	A	84	THR	3.6
1	A	48	SER	3.5
1	B	290	ARG	3.5
1	A	973	ILE	3.4
1	A	916	LEU	3.4
1	A	945	PHE	3.4
1	B	278	HIS	3.3
1	A	899	MET	3.3
1	B	925	MET	3.3
1	A	74	VAL	3.3
1	A	844	VAL	3.3
1	A	974	SER	3.3
1	A	965	THR	3.2
1	B	45	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	85	ILE	3.2
1	A	850	GLY	3.2
1	A	968	LEU	3.2
1	A	876	CYS	3.1
1	A	49	LEU	3.1
1	A	835	PHE	3.0
1	A	63	ARG	3.0
1	A	45	GLU	3.0
1	B	44	GLU	3.0
1	A	867	TYR	2.9
1	A	894	PRO	2.9
1	A	106	VAL	2.9
1	A	892	GLU	2.9
1	A	864	GLY	2.9
1	B	993	GLU	2.9
1	A	871	THR	2.8
1	A	261	SER	2.8
1	A	990	ASN	2.8
1	B	269	VAL	2.8
1	B	865	VAL	2.8
1	A	966	GLN	2.8
1	B	242	THR	2.8
1	A	854	TRP	2.8
1	A	79	GLU	2.8
1	A	53	VAL	2.8
1	B	291	GLY	2.8
1	A	888	CYS	2.8
1	A	972	LYS	2.7
1	B	82	GLU	2.7
1	A	993	GLU	2.7
1	B	814	LEU	2.7
1	B	297	LYS	2.7
1	A	837	TYR	2.6
1	B	273	LEU	2.6
1	A	73	PHE	2.6
1	A	829	ILE	2.6
1	A	889	GLU	2.6
1	A	992	LEU	2.6
1	A	778	THR	2.6
1	A	872	HIS	2.6
1	A	882	HIS	2.6
1	A	107	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	277	GLY	2.5
1	A	963	ASP	2.5
1	B	989	ARG	2.5
1	B	251	GLN	2.5
1	A	887	ASP	2.5
1	B	951	ASP	2.5
1	A	847	ALA	2.5
1	B	262	LYS	2.4
1	A	971	LEU	2.4
1	A	869	GLN	2.4
1	A	98	LEU	2.4
1	A	293	ILE	2.4
1	B	270	ALA	2.4
1	A	833	LEU	2.4
1	A	989	ARG	2.4
1	A	895	GLU	2.4
1	B	113	GLU	2.4
1	B	241	ALA	2.4
1	B	971	LEU	2.4
1	A	862	GLY	2.4
1	A	947	ILE	2.4
1	A	859	ALA	2.3
1	B	832	TRP	2.3
1	A	68	ALA	2.3
1	A	839	ALA	2.3
1	A	54	ILE	2.3
1	A	964	LEU	2.3
1	A	258	GLU	2.3
1	A	244	GLN	2.3
1	B	861	ASP	2.3
1	A	926	PRO	2.2
1	A	975	LEU	2.2
1	B	52	LEU	2.2
1	B	266	LEU	2.2
1	B	80	GLU	2.2
1	A	923	MET	2.2
1	B	109	GLU	2.2
1	B	926	PRO	2.2
1	B	932	TRP	2.1
1	B	264	ILE	2.1
1	B	461	ASN	2.1
1	A	848	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	277	GLY	2.1
1	B	863	PRO	2.1
1	A	901	LEU	2.1
1	A	855	TRP	2.1
1	B	83	GLU	2.1
1	A	929	VAL	2.0
1	A	959	LEU	2.0
1	B	983	ILE	2.0

## 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 carbohydrates 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
7	ACP	B	1007	31/31	0.82	0.24	33,75,151,385	31
6	MN	A	1008	1/1	0.84	0.29	149,149,149,149	1
4	K	B	1004	1/1	0.84	0.21	95,95,95,95	0
7	ACP	A	1007	31/31	0.89	0.19	38,59,118,420	31
8	ACT	B	3002	4/4	0.92	0.20	55,57,60,61	0
4	K	A	1004	1/1	0.93	0.23	87,87,87,87	0
8	ACT	A	3002	4/4	0.94	0.18	38,52,53,58	0
8	ACT	B	3001	4/4	0.94	0.27	50,68,69,75	0
5	CZA	A	1005	25/25	0.95	0.16	110,122,127,177	0
8	ACT	A	3001	4/4	0.96	0.17	52,64,64,71	0
6	MN	B	1006	1/1	0.97	0.11	96,96,96,96	0
5	CZA	B	1005	25/25	0.97	0.13	74,86,99,101	0
6	MN	A	1006	1/1	0.98	0.07	103,103,103,103	0
3	MF4	B	1003	5/5	0.99	0.21	33,33,36,52	0
2	MG	B	1002	1/1	0.99	0.25	36,36,36,36	0

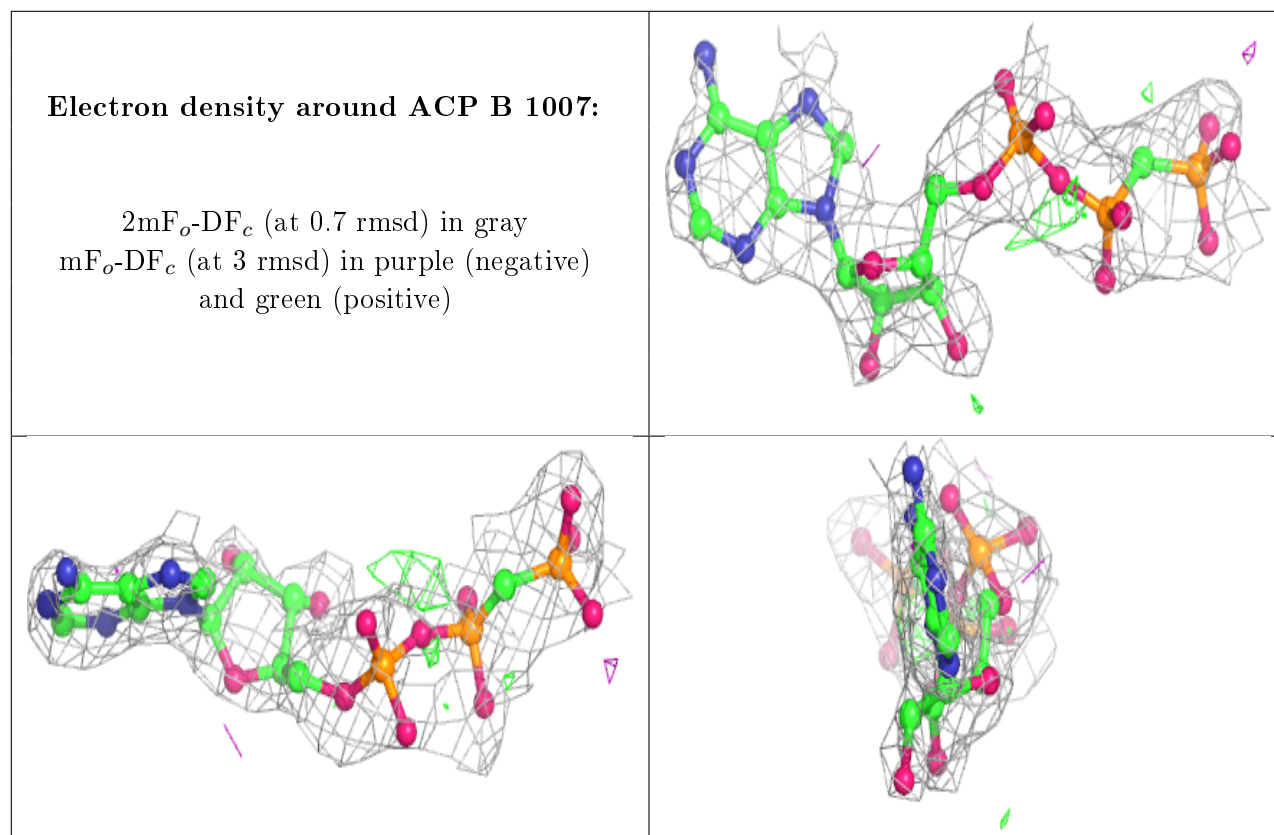
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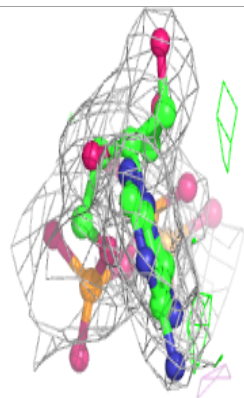
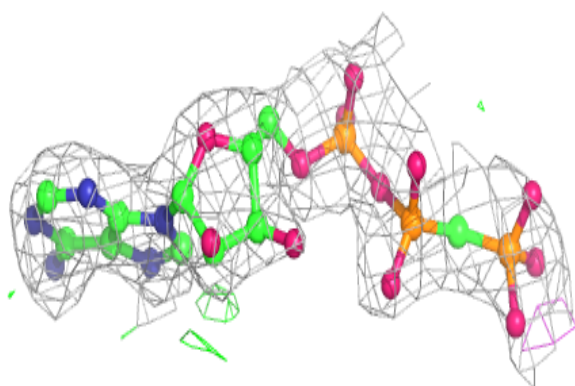
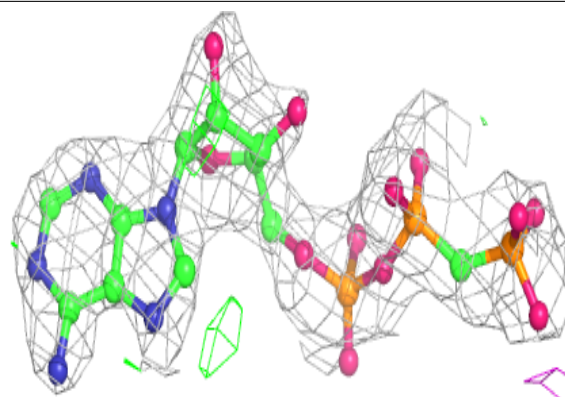
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	1002	1/1	0.99	0.21	36,36,36,36	0
3	MF4	A	1003	5/5	0.99	0.24	33,40,42,47	0

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.

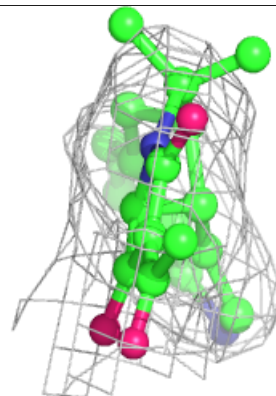
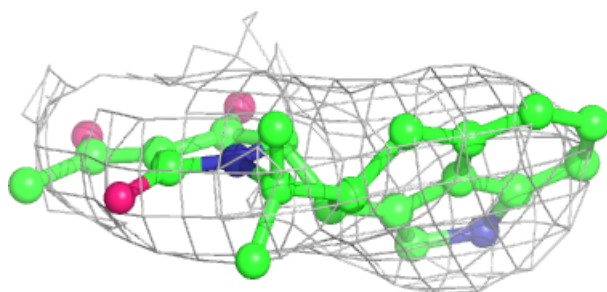
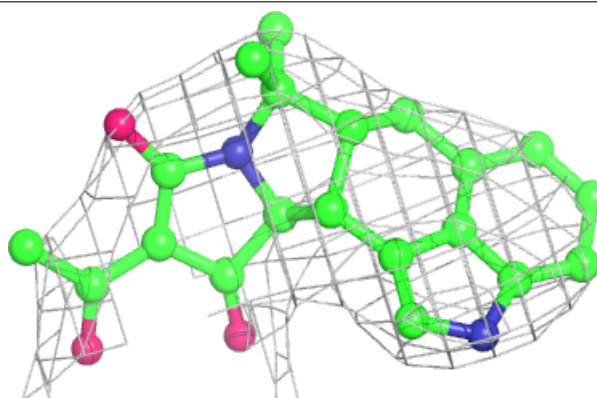


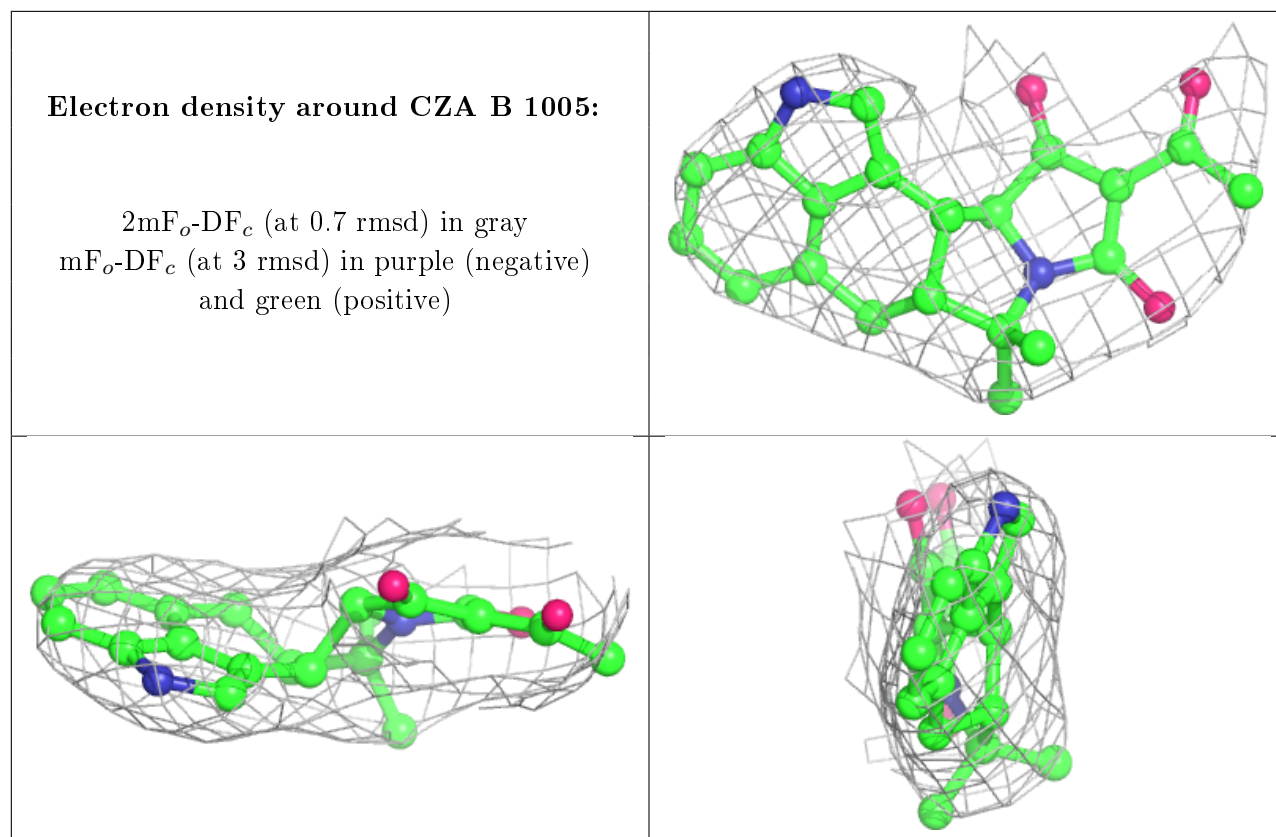
**Electron density around ACP A 1007:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CZA A 1005:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.