



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:10 am BST

PDB ID : 4PA0  
Title : Omecamtiv Mercarbil binding site on the Human Beta-Cardiac Myosin Motor Domain  
Authors : Winkelmann, D.A.; Miller, M.T.; Stock, A.M.  
Deposited on : 2014-04-06  
Resolution : 2.25 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

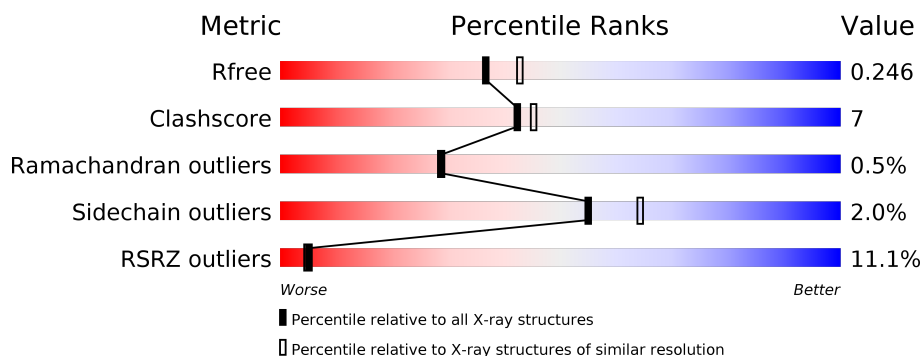
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	1024	<div> <div>5%</div> <div>80%</div> <div>15%</div> <div>• 5%</div> </div>
1	B	1024	<div> <div>16%</div> <div>76%</div> <div>13%</div> <div>• 10%</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
2	2OW	A	1101	-	-	X	-
2	2OW	B	1101	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14977 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 Myosin-7, Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	975	Total	C	N	O	S	0	0	0
			7601	4857	1291	1415	38			
1	B	921	Total	C	N	O	S	0	0	0
			6994	4449	1192	1316	37			

There are 34 discrepancies between the modelled and reference sequences:

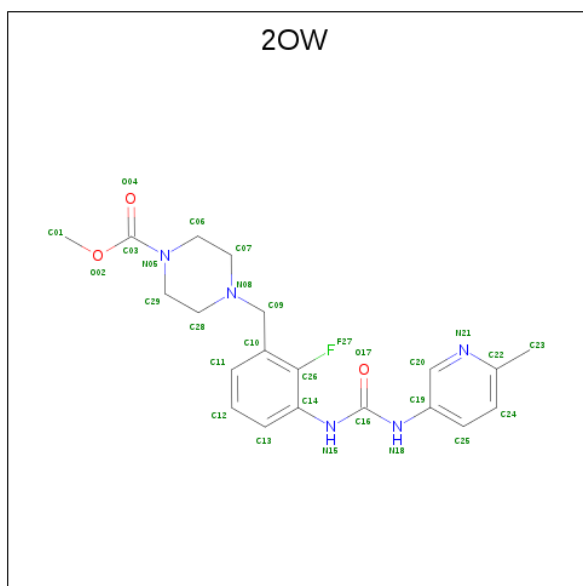
Chain	Residue	Modelled	Actual	Comment	Reference
A	788	THR	-	linker	UNP P12883
A	789	GLN	-	linker	UNP P12883
A	790	ALA	-	linker	UNP P12883
A	791	ALA	-	linker	UNP P12883
A	853	CRO	SER	chromophore	UNP P42212
A	853	CRO	TYR	chromophore	UNP P42212
A	853	CRO	GLY	chromophore	UNP P42212
A	867	ARG	GLN	engineered mutation	UNP P42212
A	950	ALA	VAL	engineered mutation	UNP P42212
A	954	THR	ILE	engineered mutation	UNP P42212
A	962	GLY	SER	engineered mutation	UNP P42212
A	977	ASN	ASP	engineered mutation	UNP P42212
A	1022	TYR	-	SEE REMARK 999	UNP P42212
A	1023	LYS	-	SEE REMARK 999	UNP P42212
A	1024	ASP	-	SEE REMARK 999	UNP P42212
A	1025	HIS	-	SEE REMARK 999	UNP P42212
A	1026	ASP	-	SEE REMARK 999	UNP P42212
B	788	THR	-	linker	UNP P12883
B	789	GLN	-	linker	UNP P12883
B	790	ALA	-	linker	UNP P12883
B	791	ALA	-	linker	UNP P12883
B	853	CRO	SER	chromophore	UNP P42212
B	853	CRO	TYR	chromophore	UNP P42212
B	853	CRO	GLY	chromophore	UNP P42212
B	867	ARG	GLN	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	950	ALA	VAL	engineered mutation	UNP P42212
B	954	THR	ILE	engineered mutation	UNP P42212
B	962	GLY	SER	engineered mutation	UNP P42212
B	977	ASN	ASP	engineered mutation	UNP P42212
B	1022	TYR	-	SEE REMARK 999	UNP P42212
B	1023	LYS	-	SEE REMARK 999	UNP P42212
B	1024	ASP	-	SEE REMARK 999	UNP P42212
B	1025	HIS	-	SEE REMARK 999	UNP P42212
B	1026	ASP	-	SEE REMARK 999	UNP P42212

- Molecule 2 is methyl 4-(2-fluoro-3-[(6-methylpyridin-3-yl)carbamoyl]amino}benzyl)piperazine-1-carboxylate (three-letter code: 2OW) (formula: C<sub>20</sub>H<sub>24</sub>FN<sub>5</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			29	20	1	5	3		
2	B	1	Total	C	F	N	O	0	0
			29	20	1	5	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	142	Total	O	0	0
			142	142		
4	B	164	Total	O	0	0
			164	164		

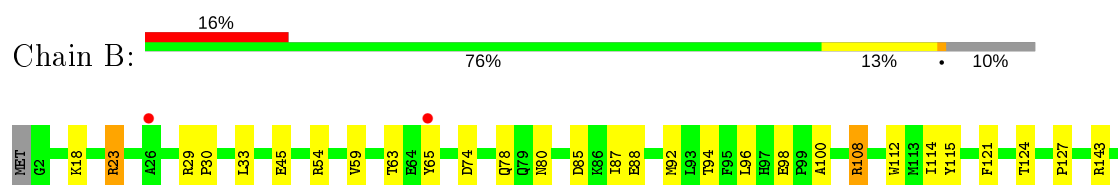
### 3 Residue-property plots [i](#)

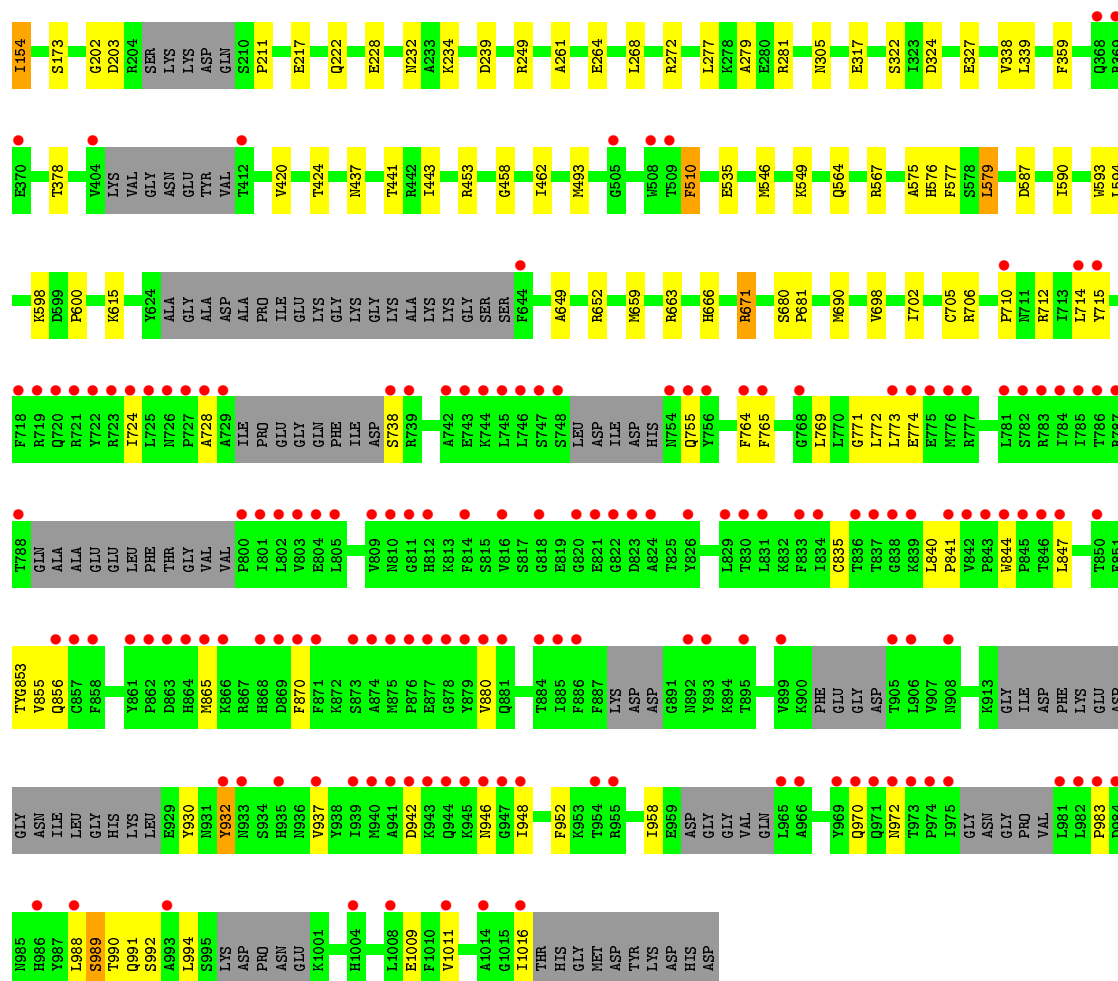
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Myosin-7, Green fluorescent protein



#### • Molecule 1: Myosin-7, Green fluorescent protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.17Å 88.92Å 137.79Å 90.00° 93.92° 90.00°	Depositor
Resolution (Å)	45.96 – 2.25 45.96 – 2.25	Depositor EDS
% Data completeness (in resolution range)	93.2 (45.96-2.25) 84.5 (45.96-2.25)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.82 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.201 , 0.246 0.204 , 0.246	Depositor DCC
$R_{free}$ test set	5386 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.30% 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: GOL, CRO, 2OW

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	0/7744	0.64	2/10478 (0.0%)
1	B	0.53	0/7119	0.65	3/9646 (0.0%)
All	All	0.53	0/14863	0.64	5/20124 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	B	108	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	671	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	202	GLY	N-CA-C	-5.79	98.62	113.10
1	A	202	GLY	N-CA-C	-5.04	100.49	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7601	0	7315	97	0
1	B	6994	0	6481	97	0
2	A	29	0	24	10	0
2	B	29	0	24	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	24	3	0
4	A	142	0	0	8	0
4	B	164	0	0	11	0
All	All	14977	0	13868	198	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (198) 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:705:CYS:HB2	2:B:1101:2OW:H5	1.46	0.94
1:B:63:THR:HG22	1:B:65:TYR:H	1.36	0.90
1:A:446:THR:O	4:A:1234:HOH:O	1.91	0.89
1:A:63:THR:HG22	1:A:65:TYR:H	1.42	0.84
1:B:702:ILE:HA	2:B:1101:2OW:H4	1.60	0.82
1:B:211:PRO:O	4:B:1322:HOH:O	2.00	0.79
1:A:203:ASP:O	1:A:451:GLN:NE2	2.16	0.78
1:B:143:ARG:NH1	4:B:1202:HOH:O	2.06	0.77
1:B:217:GLU:OE2	4:B:1201:HOH:O	2.02	0.75
1:B:268:LEU:H	3:B:1104:GOL:H2	1.52	0.75
1:B:564:GLN:OE1	4:B:1292:HOH:O	2.03	0.75
1:A:452:PRO:O	4:A:1238:HOH:O	2.05	0.74
1:B:712:ARG:O	2:B:1101:2OW:H23	1.88	0.74
1:A:711:ASN:HD22	2:A:1101:2OW:H20	1.53	0.73
1:A:192:ILE:HD11	1:A:248:ILE:HG21	1.70	0.72
1:B:45:GLU:OE1	4:B:1329:HOH:O	2.09	0.70
2:A:1101:2OW:H4	2:A:1101:2OW:C11	2.22	0.69
2:A:1101:2OW:H18	2:A:1101:2OW:H2	1.56	0.69
1:A:119:GLY:O	1:A:147:ARG:NH2	2.25	0.69
1:A:721:ARG:NH2	1:A:774:GLU:OE2	2.26	0.68
1:A:544:THR:HG23	1:A:547:THR:H	1.59	0.67
1:A:694:ARG:NE	4:A:1319:HOH:O	1.81	0.67
1:B:264:GLU:OE1	4:B:1361:HOH:O	2.12	0.67
1:B:714:LEU:N	4:B:1337:HOH:O	1.98	0.67
1:B:121:PHE:CD2	2:B:1101:2OW:H8	2.30	0.66
1:B:121:PHE:HD2	2:B:1101:2OW:H8	1.59	0.66
1:B:324:ASP:HB3	1:B:327:GLU:HG2	1.77	0.66
1:A:624:TYR:O	4:A:1301:HOH:O	2.13	0.66
1:A:437:ASN:O	1:A:441:THR:HG23	1.96	0.64
1:B:705:CYS:CB	2:B:1101:2OW:H5	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:PRO:O	4:A:1341:HOH:O	2.15	0.64
1:B:85:ASP:O	4:B:1300:HOH:O	2.14	0.63
1:A:448:GLU:OE1	1:A:453:ARG:NH2	2.32	0.63
1:B:649:ALA:HA	1:B:652:ARG:NH1	2.14	0.63
1:B:598:LYS:HG3	1:B:600:PRO:HD3	1.80	0.62
1:A:63:THR:HG22	1:A:65:TYR:N	2.15	0.61
1:A:784:ILE:O	1:A:788:THR:HG23	2.01	0.60
1:B:698:VAL:O	2:B:1101:2OW:H7	2.01	0.60
1:B:765:PHE:HD1	1:B:769:LEU:HD23	1.67	0.60
1:A:544:THR:HG22	1:A:547:THR:HG23	1.82	0.60
1:A:96:LEU:HD21	2:A:1101:2OW:H11	1.85	0.59
1:B:870:PHE:HB2	1:B:983:PRO:HD3	1.84	0.58
1:A:549:LYS:HB2	1:A:590:ILE:HD11	1.86	0.58
1:B:420:VAL:O	1:B:424:THR:HG23	2.04	0.57
1:A:143:ARG:NH1	4:A:1202:HOH:O	2.38	0.57
1:A:996:LYS:NZ	1:A:1004:HIS:O	2.37	0.57
1:A:849:THR:HG23	1:A:932:TYR:OH	2.05	0.57
1:B:98:GLU:HB3	1:B:690:MET:CE	2.34	0.57
1:B:339:LEU:HD13	1:B:443:ILE:HG12	1.86	0.56
1:A:358:HIS:ND1	1:A:380:GLU:OE1	2.35	0.56
2:A:1101:2OW:N15	2:A:1101:2OW:H2	2.20	0.56
1:B:549:LYS:HB2	1:B:590:ILE:HD11	1.88	0.55
1:B:143:ARG:NH2	4:B:1203:HOH:O	2.38	0.55
1:A:724:ILE:H	1:A:724:ILE:HD12	1.71	0.55
1:A:234:LYS:HD3	1:A:239:ASP:HA	1.89	0.55
1:B:114:ILE:HG21	1:B:127:PRO:HB3	1.89	0.54
1:B:856:GLN:OE1	1:B:970:GLN:NE2	2.34	0.54
1:B:840:LEU:HD22	1:B:844:TRP:CE2	2.43	0.54
1:A:242:SER:OG	4:A:1334:HOH:O	2.17	0.54
1:B:706:ARG:HA	1:B:710:PRO:HG3	1.89	0.54
1:A:598:LYS:HG3	1:A:600:PRO:HD3	1.90	0.53
2:A:1101:2OW:H18	2:A:1101:2OW:C20	2.21	0.53
1:B:990:THR:HG22	1:B:1011:VAL:HG22	1.91	0.53
1:A:216:LEU:HD21	1:A:260:SER:HA	1.91	0.53
1:A:743:GLU:HG2	1:A:758:PHE:CE2	2.44	0.53
1:B:724:ILE:H	1:B:724:ILE:HD12	1.73	0.53
1:B:698:VAL:HG13	2:B:1101:2OW:H6	1.90	0.52
1:B:115:TYR:CE1	1:B:124:THR:HG23	2.44	0.52
1:B:853:CRO:HA1	1:B:855:VAL:HG22	1.90	0.52
1:B:154:ILE:HD12	1:B:154:ILE:O	2.10	0.51
1:A:698:VAL:HG13	2:A:1101:2OW:H6	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:HIS:ND1	1:A:512:ASP:OD2	2.38	0.51
1:A:715:TYR:HB3	1:A:738:SER:HB3	1.94	0.50
1:B:774:GLU:OE1	4:B:1331:HOH:O	2.19	0.50
1:B:712:ARG:HG2	1:B:764:PHE:CD1	2.47	0.50
1:B:272:ARG:NH2	3:B:1103:GOL:H2	2.26	0.50
1:A:516:ASP:OD2	1:A:707:LYS:NZ	2.41	0.49
1:A:719:ARG:HG3	1:A:730:ILE:HG21	1.94	0.49
1:B:63:THR:HG22	1:B:65:TYR:N	2.17	0.49
1:A:553:PHE:CD2	1:A:557:LEU:HD22	2.47	0.49
1:A:849:THR:O	1:A:883:ARG:NH1	2.43	0.49
1:B:710:PRO:HB3	2:B:1101:2OW:H15	1.94	0.49
1:B:228:GLU:O	1:B:232:ASN:HB2	2.13	0.49
1:A:566:PRO:HB2	1:A:568:ASN:ND2	2.28	0.49
1:B:932:TYR:HB3	1:B:992:SER:HB2	1.95	0.49
1:A:225:PRO:HG2	1:A:335:ALA:HB2	1.95	0.49
1:A:192:ILE:HD13	1:A:248:ILE:HD13	1.95	0.49
1:A:705:CYS:HB3	2:A:1101:2OW:H16	1.95	0.49
1:B:88:GLU:HG2	1:B:108:ARG:NH2	2.26	0.49
1:A:228:GLU:O	1:A:232:ASN:HB2	2.12	0.48
1:A:858:PHE:CE2	1:A:906:LEU:HD13	2.47	0.48
1:A:24:LEU:O	1:A:28:THR:HG23	2.13	0.48
1:A:544:THR:CG2	1:A:547:THR:H	2.27	0.48
1:B:281:ARG:HG2	1:B:317:GLU:O	2.13	0.48
1:B:54:ARG:HG3	1:B:59:VAL:HG22	1.96	0.48
1:B:112:TRP:HA	1:B:112:TRP:CE3	2.49	0.48
1:B:865:MET:HE1	1:B:1016:ILE:H	1.79	0.48
1:B:29:ARG:HB2	1:B:30:PRO:HD2	1.95	0.48
1:B:510:PHE:CD2	1:B:510:PHE:N	2.81	0.48
1:A:114:ILE:HG21	1:A:127:PRO:HB3	1.96	0.47
1:A:719:ARG:O	1:A:723:ARG:HB2	2.13	0.47
1:B:305:ASN:N	1:B:305:ASN:OD1	2.46	0.47
1:B:493:MET:CE	4:B:1340:HOH:O	2.62	0.47
1:A:120:LEU:HD11	1:A:496:LEU:HD12	1.95	0.47
1:B:94:THR:HG21	1:B:771:GLY:CA	2.44	0.47
1:A:743:GLU:HG2	1:A:758:PHE:CZ	2.49	0.47
1:B:659:MET:O	1:B:663:ARG:HG3	2.15	0.47
1:A:193:GLN:O	1:A:197:VAL:HG23	2.15	0.47
1:A:546:MET:SD	1:B:74:ASP:HB2	2.54	0.47
1:A:935:HIS:NE2	1:A:954:THR:HA	2.30	0.47
2:B:1101:2OW:C11	2:B:1101:2OW:H25	2.44	0.47
1:B:98:GLU:HB3	1:B:690:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLU:OE2	1:A:694:ARG:NH1	2.48	0.46
1:B:989:SER:O	1:B:1011:VAL:HA	2.16	0.46
1:A:372:GLN:NE2	1:A:373:ALA:O	2.36	0.46
1:A:568:ASN:HD22	1:A:568:ASN:H	1.63	0.46
1:B:615:LYS:HE3	1:B:615:LYS:HB2	1.80	0.46
1:A:932:TYR:HB2	1:A:994:LEU:CD1	2.46	0.46
1:B:772:LEU:HD12	1:B:773:LEU:N	2.31	0.46
1:A:579:LEU:HA	1:A:579:LEU:HD12	1.69	0.46
1:A:484:LYS:NZ	1:A:525:GLU:OE2	2.44	0.46
1:B:948:ILE:HG12	1:B:972:ASN:HB2	1.97	0.46
1:B:932:TYR:HB2	1:B:994:LEU:HD21	1.98	0.45
1:A:671:ARG:HD2	1:A:671:ARG:HA	1.75	0.45
1:B:930:TYR:CZ	1:B:994:LEU:HB3	2.51	0.45
1:A:553:PHE:HD2	1:A:557:LEU:HD22	1.78	0.45
1:B:234:LYS:NZ	1:B:279:ALA:O	2.40	0.45
1:A:912:LEU:HD23	1:A:913:LYS:N	2.31	0.45
1:A:941:ALA:HA	1:A:948:ILE:HA	1.97	0.45
1:B:510:PHE:HD2	1:B:510:PHE:N	2.14	0.45
1:B:249:ARG:O	1:B:261:ALA:HA	2.17	0.45
1:B:87:ILE:CD1	1:B:92:MET:HB2	2.47	0.45
1:A:194:TYR:O	1:A:198:ILE:HG12	2.17	0.44
1:B:535:GLU:OE2	1:B:652:ARG:NH1	2.50	0.44
1:B:437:ASN:O	1:B:441:THR:HG23	2.16	0.44
1:B:546:MET:CE	1:B:549:LYS:HD3	2.48	0.44
1:B:575:ALA:CB	1:B:587:ASP:HB3	2.48	0.44
1:A:391:ASN:HB3	1:A:394:ASP:HB2	1.99	0.44
1:B:239:ASP:OD2	1:B:322:SER:OG	2.29	0.44
1:B:33:LEU:HD11	1:B:78:GLN:HG2	1.99	0.44
1:B:277:LEU:HG	3:B:1103:GOL:H32	2.00	0.43
1:B:222:GLN:HG3	1:B:338:VAL:HG11	1.99	0.43
1:B:577:PHE:CE1	1:B:579:LEU:HD13	2.53	0.43
1:A:807:GLY:HA3	1:A:814:PHE:CZ	2.53	0.43
1:B:579:LEU:HA	1:B:579:LEU:HD12	1.62	0.43
1:A:347:ASN:O	1:A:351:LYS:HG3	2.18	0.43
1:A:339:LEU:HD13	1:A:443:ILE:HG12	2.00	0.43
1:A:893:TYR:CD1	1:A:912:LEU:HD21	2.53	0.43
1:B:92:MET:HA	2:B:1101:2OW:N21	2.34	0.43
1:A:184:LYS:HB3	1:A:461:ASP:OD1	2.18	0.43
1:B:755:GLN:CB	1:B:769:LEU:HD22	2.49	0.43
1:A:655:LEU:O	1:A:659:MET:HG2	2.19	0.43
1:B:840:LEU:HA	1:B:841:PRO:HD3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:THR:HG21	1:B:771:GLY:N	2.33	0.42
1:A:540:PHE:HA	1:A:541:PRO:HD2	1.91	0.42
1:A:694:ARG:CD	4:A:1319:HOH:O	2.51	0.42
1:A:143:ARG:HD2	1:A:159:ASP:OD2	2.18	0.42
1:A:121:PHE:CD2	2:A:1101:2OW:H7	2.54	0.42
1:A:956:HIS:N	1:A:963:VAL:HG13	2.34	0.42
1:B:835:CYS:HB2	1:B:840:LEU:HD13	2.02	0.42
1:B:937:VAL:CG1	1:B:988:LEU:HB2	2.50	0.42
1:A:939:ILE:HD12	1:A:986:HIS:CE1	2.55	0.42
1:A:996:LYS:O	1:A:998:PRO:HD3	2.20	0.42
2:B:1101:2OW:H25	2:B:1101:2OW:H16	2.01	0.42
1:B:18:LYS:O	1:B:23:ARG:NH1	2.52	0.42
1:A:420:VAL:O	1:A:424:THR:HG23	2.20	0.42
1:A:50:LYS:HE3	1:A:50:LYS:HB2	1.97	0.42
1:A:590:ILE:HA	1:A:593:TRP:CE2	2.55	0.42
1:A:840:LEU:HD22	1:A:844:TRP:CE2	2.55	0.42
1:B:937:VAL:HG23	1:B:952:PHE:CD2	2.54	0.42
1:A:851:PHE:O	1:A:908:ASN:ND2	2.53	0.41
1:B:590:ILE:HA	1:B:593:TRP:NE1	2.35	0.41
1:B:991:GLN:O	1:B:1009:GLU:HA	2.21	0.41
1:B:96:LEU:HA	1:B:96:LEU:HD23	1.87	0.41
1:A:880:VAL:O	1:A:972:ASN:HA	2.20	0.41
1:B:715:TYR:HB3	1:B:738:SER:HB3	2.01	0.41
1:A:352:LEU:HA	1:A:352:LEU:HD23	1.80	0.41
1:A:98:GLU:CD	1:A:694:ARG:HH12	2.23	0.41
1:B:847:LEU:HD13	1:B:847:LEU:HA	1.90	0.41
1:A:937:VAL:HG13	1:A:952:PHE:CD2	2.56	0.41
1:B:680:SER:HA	1:B:681:PRO:HD3	1.79	0.41
1:B:880:VAL:O	1:B:972:ASN:HA	2.20	0.41
1:A:590:ILE:HA	1:A:593:TRP:NE1	2.36	0.41
1:A:63:THR:CG2	1:A:65:TYR:H	2.23	0.41
1:A:729:ALA:HB1	1:A:744:LYS:HB3	2.02	0.41
1:A:705:CYS:HB2	2:A:1101:2OW:H15	2.02	0.41
1:A:756:TYR:HA	1:A:764:PHE:O	2.21	0.41
1:A:74:ASP:OD2	1:B:576:HIS:NE2	2.46	0.40
1:B:80:ASN:ND2	1:B:100:ALA:HB1	2.36	0.40
1:B:173:SER:HA	1:B:458:GLY:O	2.22	0.40
1:A:306:ASN:OD1	1:A:308:TYR:HB2	2.21	0.40
1:A:566:PRO:HB2	1:A:568:ASN:HD22	1.85	0.40
1:A:59:VAL:O	1:A:70:THR:HA	2.21	0.40
1:A:990:THR:HG22	1:A:1011:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLY:N	1:A:184:LYS:HD3	2.37	0.40
1:A:211:PRO:HG2	1:A:446:THR:HA	2.03	0.40
1:B:54:ARG:HH11	1:B:54:ARG:HD3	1.78	0.40
1:B:590:ILE:HA	1:B:593:TRP:CE2	2.57	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	960/1024 (94%)	907 (94%)	48 (5%)	5 (0%)	29	29
1	B	892/1024 (87%)	858 (96%)	29 (3%)	5 (1%)	25	25
All	All	1852/2048 (90%)	1765 (95%)	77 (4%)	10 (0%)	29	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	568	ASN
1	A	999	ASN
1	B	203	ASP
1	B	728	ALA
1	B	946	ASN
1	A	413	LYS
1	A	890	ASP
1	A	942	ASP
1	B	942	ASP
1	B	958	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	785/882 (89%)	770 (98%)	15 (2%)	57	66
1	B	690/882 (78%)	676 (98%)	14 (2%)	55	64
All	All	1475/1764 (84%)	1446 (98%)	29 (2%)	55	64

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	105	LEU
1	A	177	THR
1	A	359	PHE
1	A	418	GLN
1	A	462	ILE
1	A	671	ARG
1	A	683	VAL
1	A	750	ASP
1	A	825	THR
1	A	884	THR
1	A	932	TYR
1	A	989	SER
1	A	996	LYS
1	A	1012	THR
1	B	23	ARG
1	B	154	ILE
1	B	359	PHE
1	B	378	THR
1	B	453	ARG
1	B	462	ILE
1	B	510	PHE
1	B	567	ARG
1	B	579	LEU
1	B	594	LEU
1	B	666	HIS
1	B	671	ARG

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Mol	Chain	Res	Type
1	B	932	TYR
1	B	989	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	568	ASN
1	A	711	ASN
1	A	810	ASN
1	B	44	GLN
1	B	564	GLN
1	B	711	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CRO	B	853	1	22,22,24	4.90	6 (27%)	27,30,34	3.81	8 (29%)
1	CRO	A	853	1	22,22,24	4.91	6 (27%)	27,30,34	3.54	6 (22%)

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
1	CRO	B	853	1	-	5/9/29/32	0/2/2/2
1	CRO	A	853	1	-	2/9/29/32	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	853	CRO	CB2-CA2	17.73	1.49	1.35
1	A	853	CRO	CB2-CA2	17.01	1.49	1.35
1	A	853	CRO	CA2-C2	-11.58	1.37	1.48
1	B	853	CRO	CA2-C2	-10.52	1.38	1.48
1	A	853	CRO	O2-C2	7.40	1.38	1.23
1	B	853	CRO	O2-C2	7.22	1.38	1.23
1	A	853	CRO	OG1-CB1	-4.86	1.21	1.42
1	B	853	CRO	OG1-CB1	-4.69	1.22	1.42
1	B	853	CRO	C1-N2	3.28	1.37	1.32
1	A	853	CRO	C1-N2	3.08	1.36	1.32
1	A	853	CRO	C2-N3	-2.50	1.34	1.39
1	B	853	CRO	C2-N3	-2.27	1.34	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	853	CRO	CG2-CB2-CA2	-11.40	115.97	129.94
1	B	853	CRO	CA2-C2-N3	10.87	108.51	103.37
1	A	853	CRO	O2-C2-CA2	-10.61	125.00	130.96
1	A	853	CRO	CG2-CB2-CA2	-9.36	118.47	129.94
1	A	853	CRO	CA2-C2-N3	9.35	107.79	103.37
1	B	853	CRO	O2-C2-CA2	-7.88	126.53	130.96
1	B	853	CRO	N3-C1-N2	-5.06	107.95	111.45
1	A	853	CRO	N3-C1-N2	-4.56	108.30	111.45
1	B	853	CRO	OG1-CB1-CA1	3.47	120.03	110.85
1	B	853	CRO	CB2-CA2-C2	3.44	126.38	122.28
1	B	853	CRO	CA2-N2-C1	3.40	108.28	105.77
1	A	853	CRO	OG1-CB1-CA1	2.42	117.25	110.85
1	B	853	CRO	C2-CA2-N2	-2.29	107.33	108.93
1	A	853	CRO	O3-C3-CA3	-2.20	119.75	126.39

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	853	CRO	N2-CA2-CB2-CG2

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Mol	Chain	Res	Type	Atoms
1	B	853	CRO	C2-CA2-CB2-CG2
1	A	853	CRO	N2-CA2-CB2-CG2
1	A	853	CRO	C2-CA2-CB2-CG2
1	B	853	CRO	CA2-CB2-CG2-CD1
1	B	853	CRO	CA2-CB2-CG2-CD2
1	B	853	CRO	C3-CA3-N3-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	853	CRO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	B	1102	-	5,5,5	0.29	0	5,5,5	0.59	0
2	2OW	B	1101	-	31,31,31	2.83	15 (48%)	41,42,42	2.42	16 (39%)
2	2OW	A	1101	-	31,31,31	2.78	12 (38%)	41,42,42	2.48	12 (29%)
3	GOL	B	1103	-	5,5,5	0.45	0	5,5,5	0.76	0
3	GOL	B	1104	-	5,5,5	0.22	0	5,5,5	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	1102	-	-	3/4/4/4	-
2	2OW	B	1101	-	-	6/18/28/28	0/3/3/3
2	2OW	A	1101	-	-	8/18/28/28	1/3/3/3
3	GOL	B	1103	-	-	2/4/4/4	-
3	GOL	B	1104	-	-	0/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	2OW	C16-N15	6.70	1.51	1.37
2	A	1101	2OW	C16-N15	6.32	1.50	1.37
2	B	1101	2OW	C03-N05	5.41	1.44	1.35
2	A	1101	2OW	C03-N05	5.37	1.44	1.35
2	A	1101	2OW	O04-C03	5.27	1.29	1.21
2	B	1101	2OW	O04-C03	4.86	1.28	1.21
2	A	1101	2OW	C25-C24	4.73	1.47	1.38
2	B	1101	2OW	C25-C24	4.70	1.47	1.38
2	B	1101	2OW	O02-C01	-4.60	1.34	1.45
2	A	1101	2OW	O02-C01	-4.40	1.35	1.45
2	B	1101	2OW	C29-N05	-4.22	1.39	1.47
2	A	1101	2OW	C16-N18	3.74	1.45	1.37
2	A	1101	2OW	C29-N05	-3.60	1.40	1.47
2	A	1101	2OW	C20-N21	3.56	1.41	1.34
2	B	1101	2OW	C16-N18	3.47	1.44	1.37
2	A	1101	2OW	C11-C10	3.40	1.45	1.39
2	B	1101	2OW	C20-N21	3.34	1.41	1.34
2	B	1101	2OW	C11-C10	3.25	1.45	1.39
2	A	1101	2OW	O02-C03	2.81	1.39	1.34
2	A	1101	2OW	C19-N18	2.71	1.47	1.41
2	B	1101	2OW	C13-C14	2.58	1.44	1.39
2	B	1101	2OW	C10-C26	2.56	1.41	1.38
2	B	1101	2OW	O02-C03	2.55	1.38	1.34
2	A	1101	2OW	C25-C19	2.49	1.43	1.39
2	B	1101	2OW	C19-N18	2.45	1.46	1.41
2	B	1101	2OW	C09-C10	2.30	1.55	1.51
2	B	1101	2OW	C25-C19	2.22	1.43	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	2OW	C01-O02-C03	6.64	123.01	115.34
2	B	1101	2OW	C01-O02-C03	6.29	122.60	115.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	2OW	C11-C10-C26	5.54	120.46	116.43
2	B	1101	2OW	N18-C16-N15	5.05	121.31	112.49
2	A	1101	2OW	C09-N08-C28	4.94	122.06	111.06
2	A	1101	2OW	C06-N05-C03	-4.68	108.39	121.77
2	B	1101	2OW	O04-C03-N05	-4.60	116.63	124.32
2	A	1101	2OW	C10-C09-N08	-4.47	104.92	112.75
2	B	1101	2OW	C20-N21-C22	4.26	122.38	117.45
2	A	1101	2OW	O04-C03-N05	-4.01	117.62	124.32
2	B	1101	2OW	C11-C10-C26	3.92	119.28	116.43
2	B	1101	2OW	C19-C20-N21	-3.88	120.64	124.13
2	A	1101	2OW	C09-N08-C07	3.59	119.06	111.06
2	B	1101	2OW	C09-N08-C07	3.57	119.01	111.06
2	B	1101	2OW	O17-C16-N18	-3.47	117.75	123.62
2	A	1101	2OW	C19-C20-N21	-3.29	121.17	124.13
2	B	1101	2OW	C06-C07-N08	3.19	117.19	110.64
2	A	1101	2OW	O17-C16-N18	-3.13	118.32	123.62
2	A	1101	2OW	C20-N21-C22	3.11	121.06	117.45
2	A	1101	2OW	C09-C10-C26	-2.96	116.86	121.48
2	B	1101	2OW	O17-C16-N15	-2.94	118.64	123.62
2	B	1101	2OW	C14-N15-C16	-2.92	118.90	125.39
2	B	1101	2OW	C09-N08-C28	2.92	117.56	111.06
2	B	1101	2OW	C06-N05-C03	-2.64	114.23	121.77
2	B	1101	2OW	C09-C10-C26	-2.37	117.78	121.48
2	B	1101	2OW	C10-C09-N08	2.31	116.79	112.75
2	B	1101	2OW	C07-C06-N05	2.30	115.36	110.44
2	A	1101	2OW	F27-C26-C14	2.06	121.72	118.32

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1102	GOL	O1-C1-C2-C3
2	B	1101	2OW	C26-C14-N15-C16
2	B	1101	2OW	N15-C16-N18-C19
2	B	1101	2OW	O17-C16-N18-C19
2	A	1101	2OW	N05-C03-O02-C01
2	A	1101	2OW	O04-C03-N05-C06
2	A	1101	2OW	C10-C09-N08-C07
3	B	1103	GOL	O1-C1-C2-C3
2	A	1101	2OW	N15-C16-N18-C19
2	A	1101	2OW	C10-C09-N08-C28
2	A	1101	2OW	O17-C16-N18-C19

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Mol	Chain	Res	Type	Atoms
3	B	1103	GOL	O1-C1-C2-O2
3	B	1102	GOL	O1-C1-C2-O2
2	B	1101	2OW	C13-C14-N15-C16
2	A	1101	2OW	N18-C16-N15-C14
2	B	1101	2OW	O02-C03-N05-C29
2	B	1101	2OW	O04-C03-N05-C29
2	A	1101	2OW	O04-C03-O02-C01
3	B	1102	GOL	O2-C2-C3-O3

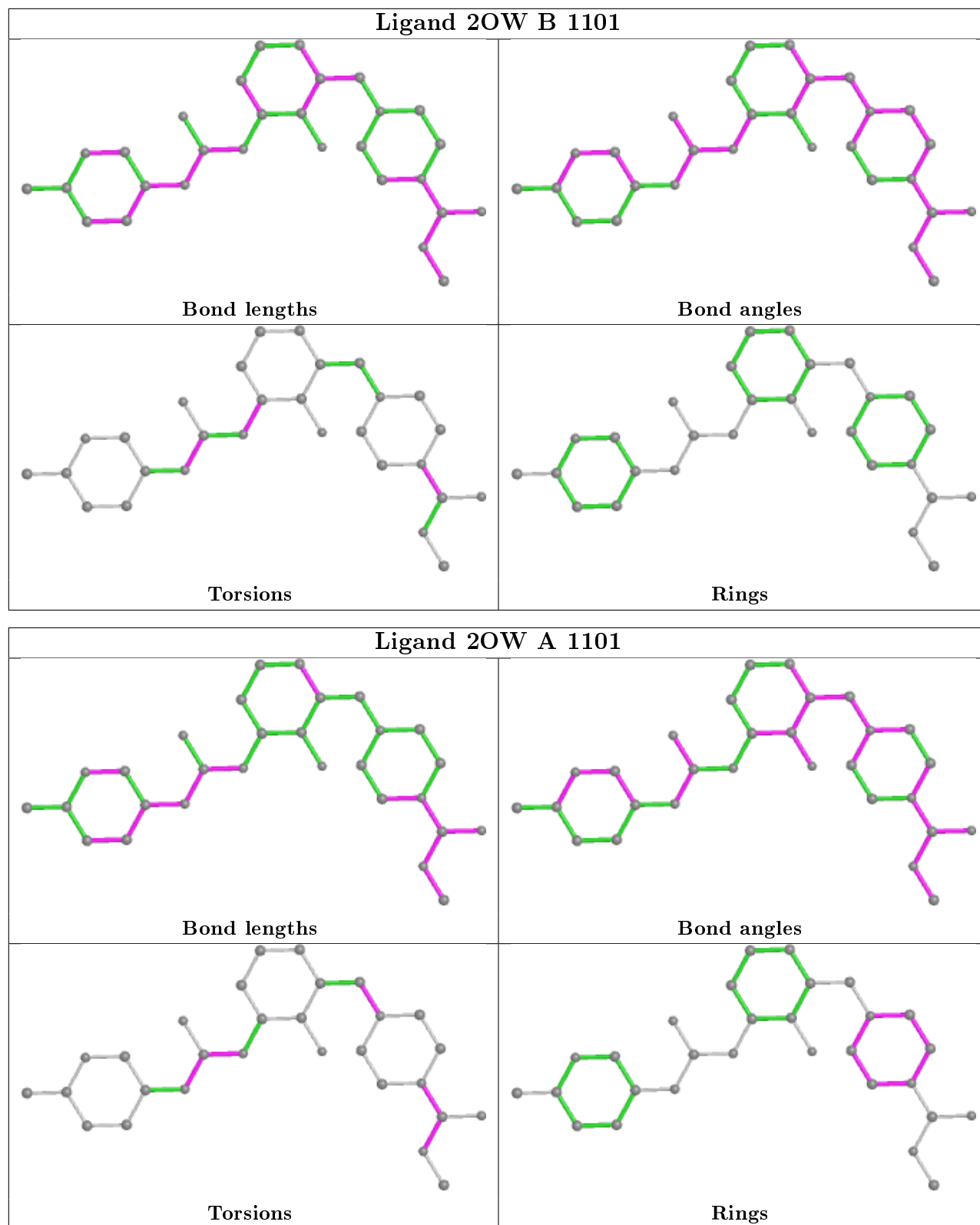
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	2OW	C06-C07-C28-C29-N05-N08

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	2OW	12	0
2	A	1101	2OW	10	0
3	B	1103	GOL	2	0
3	B	1104	GOL	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.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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	974/1024 (95%)	0.26	51 (5%)	27 30	15, 40, 79, 100	0
1	B	920/1024 (89%)	0.76	159 (17%)	1 1	17, 35, 104, 130	0
All	All	1894/2048 (92%)	0.50	210 (11%)	5 5	15, 38, 99, 130	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	803	VAL	11.9
1	B	875	MET	8.9
1	B	725	LEU	8.3
1	B	871	PHE	8.1
1	B	874	ALA	7.6
1	B	820	GLY	7.5
1	B	822	GLY	7.5
1	B	941	ALA	7.4
1	B	966	ALA	7.4
1	B	942	ASP	7.2
1	B	842	VAL	7.2
1	B	834	ILE	7.2
1	B	947	GLY	6.9
1	B	746	LEU	6.9
1	B	838	GLY	6.6
1	B	944	GLN	6.6
1	B	843	PRO	6.4
1	B	718	PHE	6.3
1	B	811	GLY	6.3
1	B	870	PHE	6.1
1	B	877	GLU	6.1
1	B	876	PRO	6.1
1	B	729	ALA	6.0
1	B	893	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	788	THR	5.5
1	B	802	LEU	5.5
1	B	786	THR	5.4
1	B	805	LEU	5.3
1	B	857	CYS	5.2
1	B	738	SER	5.1
1	B	765	PHE	5.1
1	B	965	LEU	5.1
1	B	908	ASN	5.1
1	B	939	ILE	5.1
1	B	812	HIS	5.0
1	B	818	GLY	5.0
1	A	975	ILE	4.9
1	B	850	THR	4.8
1	B	844	TRP	4.8
1	B	784	ILE	4.8
1	B	726	ASN	4.7
1	A	977	ASN	4.7
1	A	923	ILE	4.7
1	B	847	LEU	4.7
1	B	982	LEU	4.7
1	B	895	THR	4.7
1	A	921	GLY	4.6
1	B	722	TYR	4.6
1	B	829	LEU	4.5
1	B	723	ARG	4.5
1	B	831	LEU	4.4
1	B	814	PHE	4.4
1	B	885	ILE	4.4
1	B	981	LEU	4.4
1	A	978	GLY	4.4
1	B	742	ALA	4.4
1	B	973	THR	4.4
1	B	727	PRO	4.3
1	B	787	ARG	4.3
1	B	892	ASN	4.3
1	B	945	LYS	4.3
1	B	954	THR	4.2
1	B	801	ILE	4.2
1	B	810	ASN	4.1
1	B	862	PRO	4.1
1	B	823	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	508	TRP	4.0
1	B	816	VAL	4.0
1	B	858	PHE	4.0
1	A	733	GLY	4.0
1	B	899	VAL	3.9
1	B	861	TYR	3.9
1	B	739	ARG	3.9
1	A	946	ASN	3.8
1	B	720	GLN	3.8
1	B	856	GLN	3.8
1	B	946	ASN	3.8
1	B	880	VAL	3.7
1	B	878	GLY	3.7
1	A	28	THR	3.7
1	A	976	GLY	3.7
1	A	937	VAL	3.7
1	B	845	PRO	3.6
1	A	956	HIS	3.6
1	B	721	ARG	3.6
1	A	886	PHE	3.6
1	A	940	MET	3.6
1	B	879	TYR	3.6
1	A	979	PRO	3.6
1	B	1016	ILE	3.5
1	A	862	PRO	3.5
1	B	983	PRO	3.5
1	B	714	LEU	3.5
1	B	932	TYR	3.5
1	B	943	LYS	3.5
1	B	744	LYS	3.5
1	B	863	ASP	3.5
1	B	948	ILE	3.5
1	B	368	GLN	3.5
1	B	830	THR	3.4
1	B	369	ARG	3.4
1	B	764	PHE	3.4
1	B	777	ARG	3.4
1	B	864	HIS	3.4
1	B	869	ASP	3.4
1	B	715	TYR	3.4
1	B	800	PRO	3.4
1	B	940	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	905	THR	3.3
1	B	776	MET	3.3
1	B	728	ALA	3.3
1	B	745	LEU	3.3
1	B	783	ARG	3.3
1	A	797	GLY	3.2
1	B	826	TYR	3.2
1	B	986	HIS	3.2
1	A	932	TYR	3.2
1	A	371	GLU	3.1
1	B	873	SER	3.1
1	A	420	VAL	3.1
1	B	865	MET	3.1
1	B	906	LEU	3.1
1	A	889	ASP	3.1
1	B	773	LEU	3.0
1	B	837	THR	3.0
1	B	886	PHE	3.0
1	B	781	LEU	3.0
1	A	890	ASP	3.0
1	A	998	PRO	3.0
1	B	821	GLU	2.9
1	A	920	ASP	2.9
1	A	369	ARG	2.9
1	A	644	PHE	2.9
1	B	719	ARG	2.9
1	A	948	ILE	2.9
1	B	975	ILE	2.9
1	B	755	GLN	2.9
1	B	65	TYR	2.9
1	B	1004	HIS	2.9
1	A	539	MET	2.9
1	B	804	GLU	2.9
1	B	724	ILE	2.8
1	B	833	PHE	2.8
1	A	842	VAL	2.7
1	B	937	VAL	2.7
1	B	866	LYS	2.7
1	B	935	HIS	2.7
1	B	412	THR	2.7
1	B	370	GLU	2.6
1	A	404	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	403	ARG	2.6
1	B	748	SER	2.6
1	B	839	LYS	2.6
1	B	756	TYR	2.5
1	B	775	GLU	2.5
1	A	917	PHE	2.5
1	A	790	ALA	2.5
1	A	887	PHE	2.5
1	B	955	ARG	2.5
1	A	938	TYR	2.5
1	B	754	ASN	2.5
1	B	505	GLY	2.5
1	B	404	VAL	2.4
1	B	710	PRO	2.4
1	B	933	ASN	2.4
1	B	743	GLU	2.4
1	B	836	THR	2.4
1	B	785	ILE	2.4
1	B	970	GLN	2.4
1	A	864	HIS	2.4
1	B	988	LEU	2.4
1	B	993	ALA	2.3
1	B	782	SER	2.3
1	A	730	ILE	2.3
1	A	982	LEU	2.3
1	A	935	HIS	2.3
1	B	971	GLN	2.3
1	A	366	LEU	2.3
1	A	793	GLU	2.3
1	B	774	GLU	2.3
1	A	971	GLN	2.3
1	B	974	PRO	2.3
1	A	24	LEU	2.3
1	A	993	ALA	2.3
1	B	972	ASN	2.2
1	B	846	THR	2.2
1	A	370	GLU	2.2
1	B	884	THR	2.2
1	A	985	ASN	2.2
1	B	969	TYR	2.2
1	A	2	GLY	2.2
1	A	919	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	747	SER	2.2
1	A	994	LEU	2.2
1	A	571	GLY	2.2
1	B	868	HIS	2.1
1	B	26	ALA	2.1
1	B	509	THR	2.1
1	B	644	PHE	2.1
1	B	824	ALA	2.1
1	B	809	VAL	2.1
1	B	1011	VAL	2.1
1	B	881	GLN	2.1
1	B	841	PRO	2.1
1	B	1008	LEU	2.1
1	B	768	GLY	2.1
1	B	984	ASP	2.0
1	A	393	ALA	2.0
1	B	1014	ALA	2.0
1	A	373	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CRO	B	853	21/23	0.63	0.37	92,98,105,109	0
1	CRO	A	853	21/23	0.94	0.14	49,56,73,81	0

## 6.3 Carbohydrates [i](#)

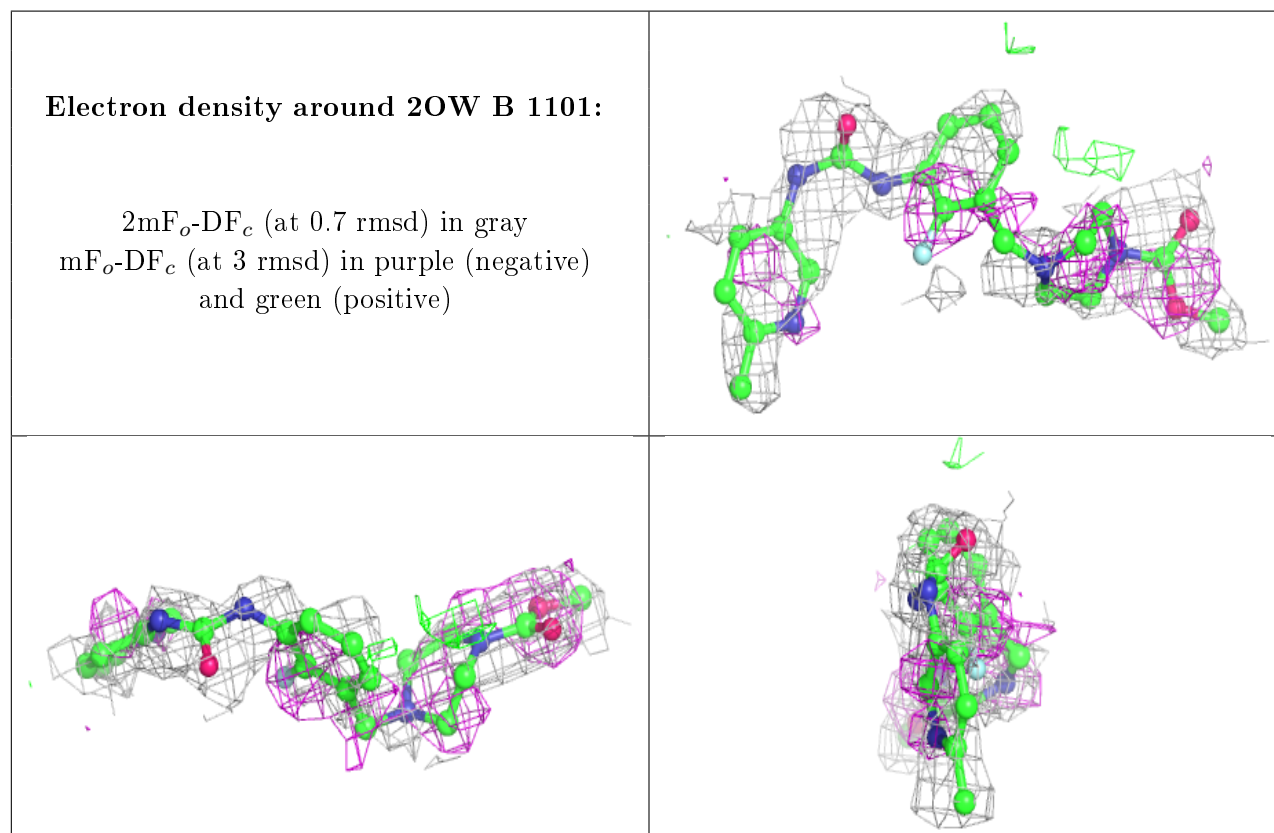
There are no carbohydrates in this entry.

## 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
2	2OW	B	1101	29/29	0.74	0.44	26,70,78,79	0
2	2OW	A	1101	29/29	0.82	0.32	25,48,59,65	0
3	GOL	B	1104	6/6	0.84	0.20	36,41,43,47	0
3	GOL	B	1102	6/6	0.88	0.13	39,42,44,50	0
3	GOL	B	1103	6/6	0.92	0.17	28,34,39,41	0

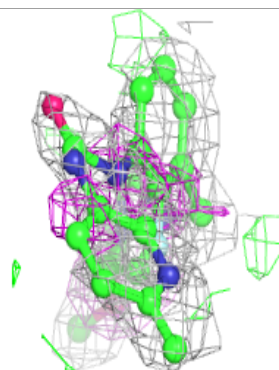
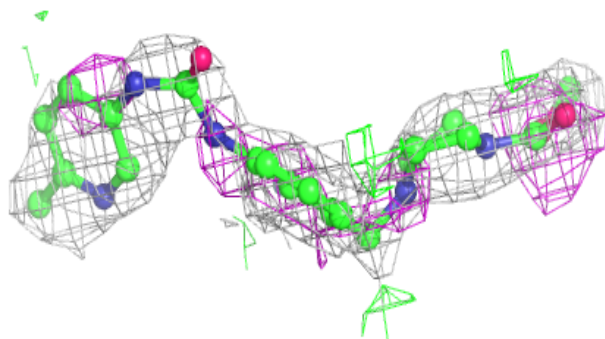
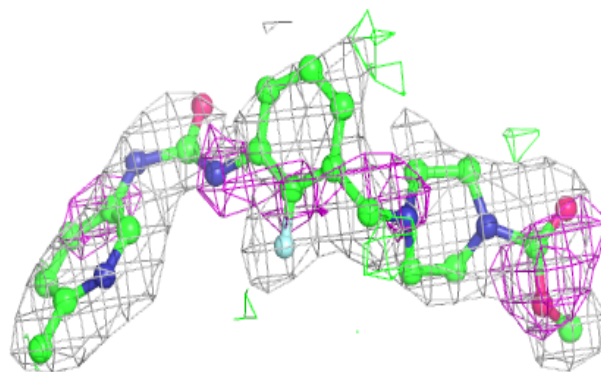
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





**Electron density around 2OW A 1101:**

$2mF_o-DF_c$  (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.