



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:48 AM UTC

PDB ID : 4PA0 / pdb_00004pa0
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

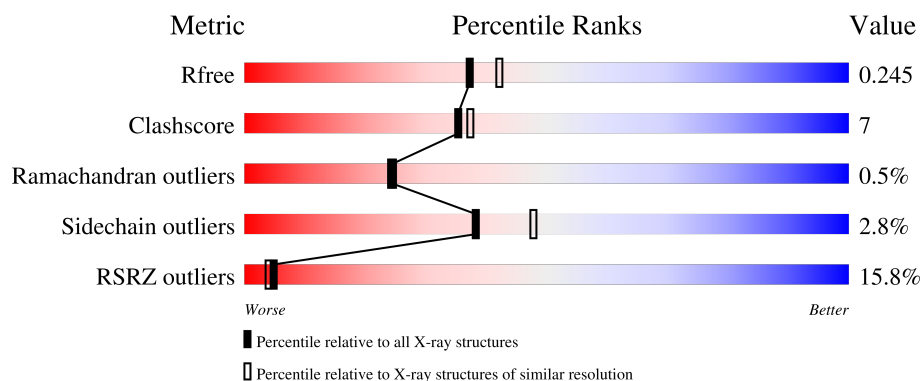
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1024	
1	B	1024	

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	-

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:

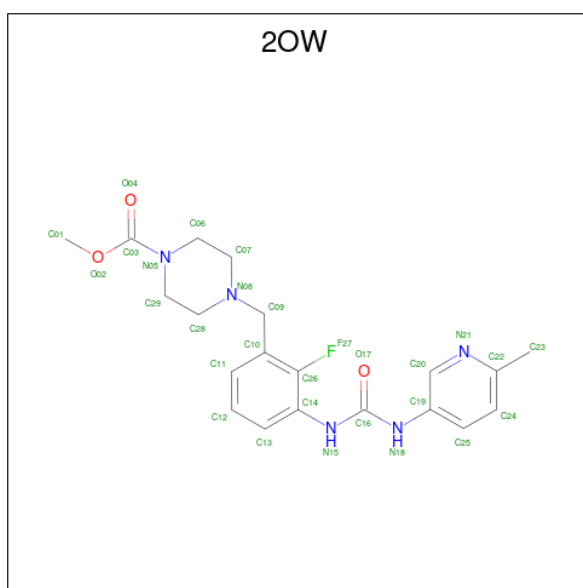
Chain	Residue	Modelled	Actual	Comment	Reference
A	788	THR	-	linker	UNP P12883
A	789	GLN	-	linker	UNP P12883
A	790	ALA	-	linker	UNP P12883
A	791	ALA	-	linker	UNP P12883
A	853	CRO	SER	chromophore	UNP P42212
A	853	CRO	TYR	chromophore	UNP P42212
A	853	CRO	GLY	chromophore	UNP P42212
A	867	ARG	GLN	engineered 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 (CCD ID: 2OW) (formula: $C_{20}H_{24}FN_5O_3$).



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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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		

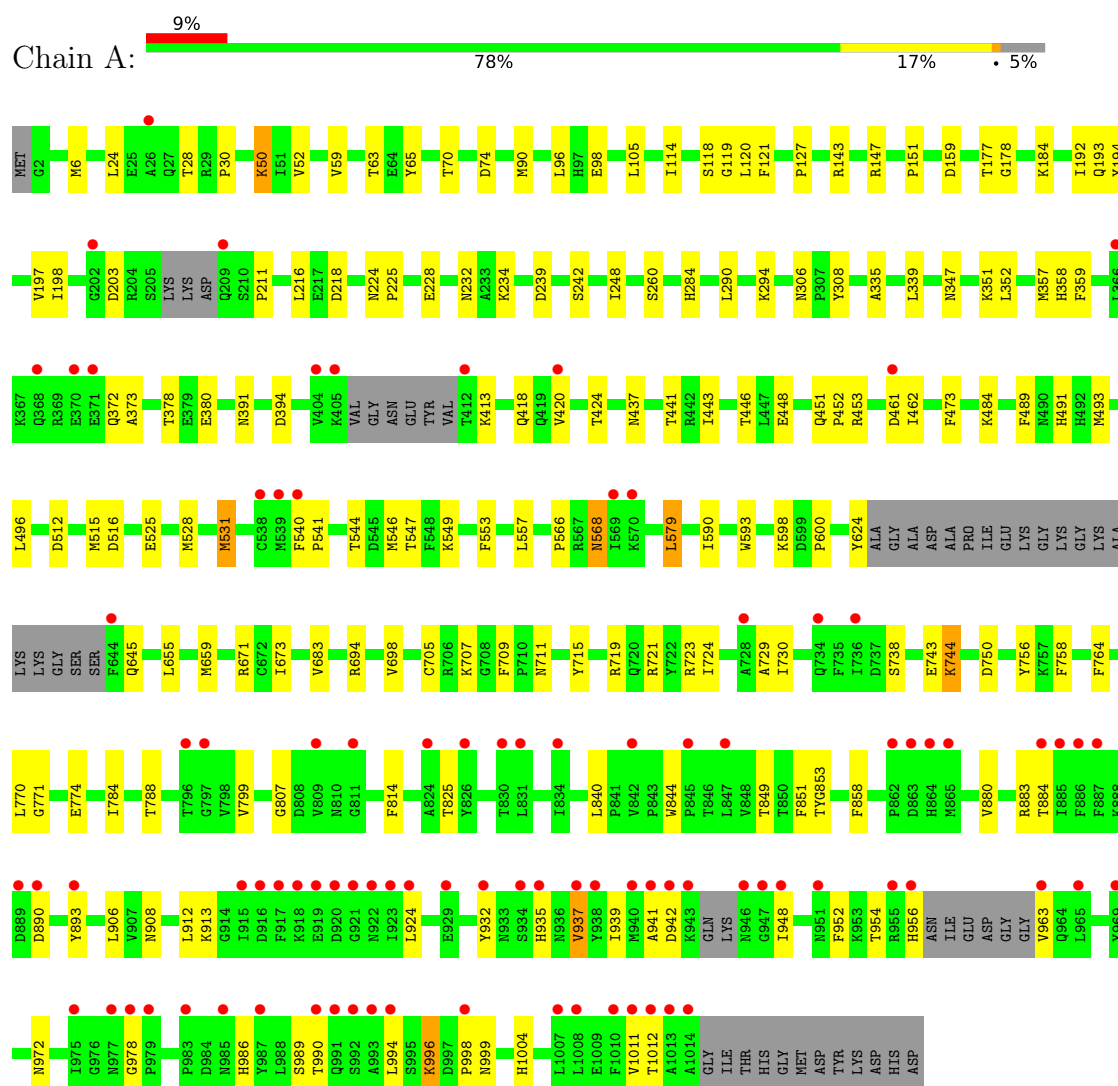
- Molecule 4 is water.

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

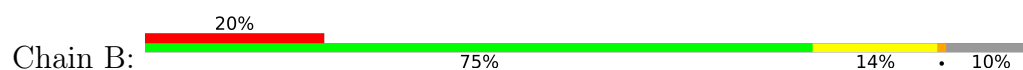
3 Residue-property plots

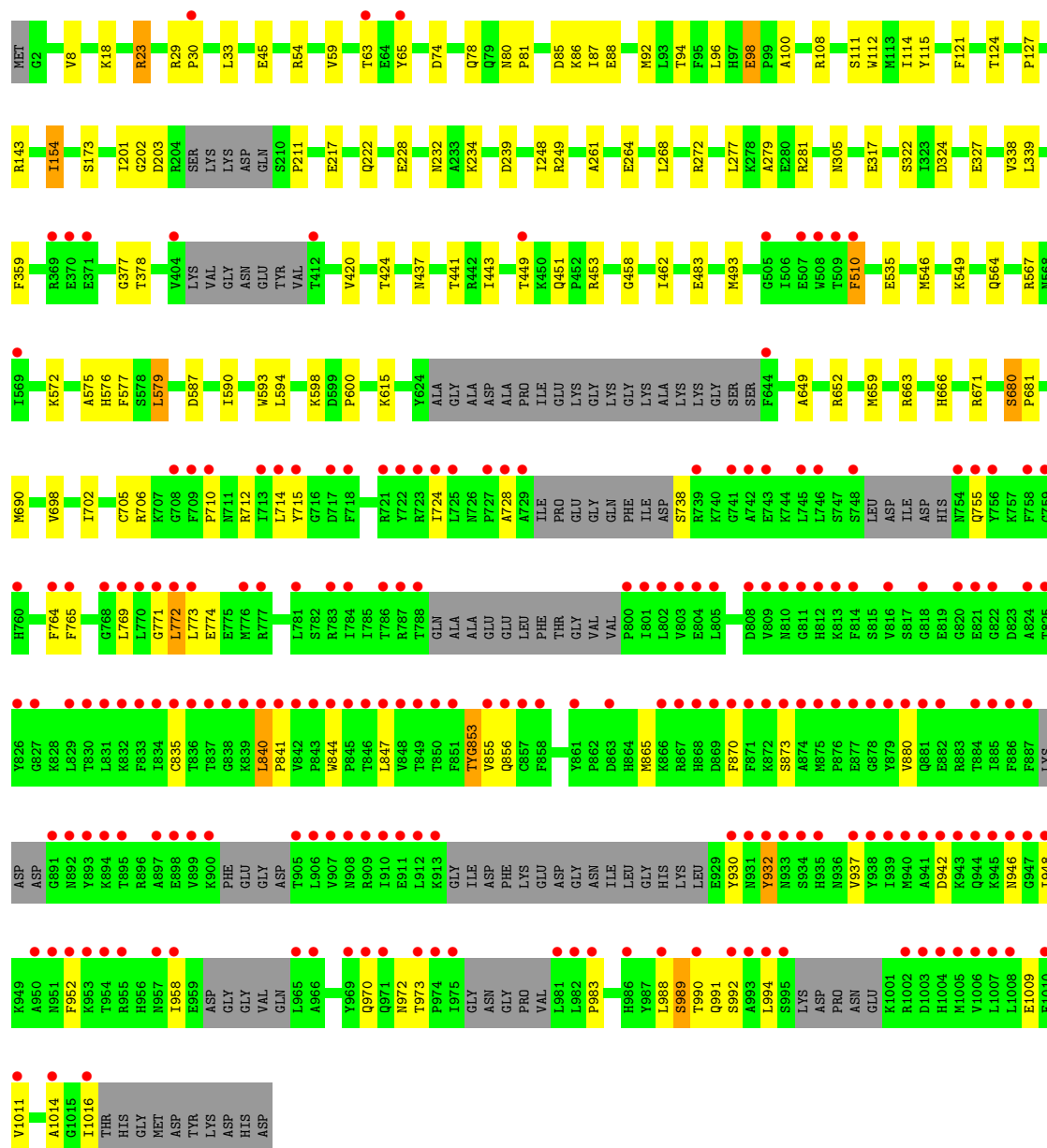
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	0.82 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.201 , 0.246 0.205 , 0.245	Depositor DCC
R_{free} test set	5386 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.67	0/7744	0.94	13/10478 (0.1%)
1	B	0.68	0/7119	0.95	13/9646 (0.1%)
All	All	0.67	0/14863	0.94	26/20124 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	709	PHE	CA-C-N	5.89	125.27	118.85
1	A	709	PHE	C-N-CA	5.89	125.27	118.85
1	B	377	GLY	N-CA-C	-5.74	105.03	111.63
1	B	81	PRO	CA-C-N	5.74	126.12	119.47
1	B	81	PRO	C-N-CA	5.74	126.12	119.47
1	A	294	LYS	CA-C-N	5.68	125.52	119.28
1	A	294	LYS	C-N-CA	5.68	125.52	119.28
1	B	98	GLU	CA-C-N	-5.57	113.28	119.19
1	B	98	GLU	C-N-CA	-5.57	113.28	119.19
1	B	840	LEU	CA-C-N	5.57	125.24	119.56
1	B	840	LEU	C-N-CA	5.57	125.24	119.56
1	A	224	ASN	CA-C-N	-5.49	113.38	119.19
1	A	224	ASN	C-N-CA	-5.49	113.38	119.19
1	A	218	ASP	N-CA-C	-5.26	105.54	111.28
1	A	978	GLY	CA-C-N	5.21	125.37	119.90
1	A	978	GLY	C-N-CA	5.21	125.37	119.90
1	B	973	THR	CA-C-N	5.20	125.20	120.21
1	B	973	THR	C-N-CA	5.20	125.20	120.21
1	B	572	LYS	N-CA-C	-5.17	102.51	110.32
1	B	680	SER	CA-C-N	5.10	124.86	119.76
1	B	680	SER	C-N-CA	5.10	124.86	119.76
1	B	202	GLY	N-CA-C	-5.06	98.62	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	284	HIS	N-CA-C	5.05	117.44	111.33
1	A	771	GLY	N-CA-C	-5.02	106.64	113.37
1	A	673	ILE	CA-C-N	-5.01	118.98	122.59
1	A	673	ILE	C-N-CA	-5.01	118.98	122.59

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	105	0
1	B	6994	0	6481	103	0
2	A	29	0	24	11	0
2	B	29	0	24	12	0
3	B	18	0	24	3	0
4	A	142	0	0	8	0
4	B	164	0	0	12	0
All	All	14977	0	13868	212	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 (212) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:119:GLY:O	1:A:147:ARG:NH2	2.25	0.69
2:A:1101:2OW:C11	2:A:1101:2OW:H4	2.22	0.69
2:A:1101:2OW:H18	2:A:1101:2OW:H2	1.56	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:HD2	2:B:1101:2OW:H8	1.59	0.66
1:B:121:PHE:CD2	2:B:1101:2OW:H8	2.30	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
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:B:98:GLU:HB3	1:B:690:MET:HE2	1.81	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: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:H2	2:A:1101:2OW:N15	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:865:MET:HE2	1:B:1016:ILE:HB	1.88	0.56
1:B:98:GLU:HB3	1:B:690:MET:CE	2.34	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:HD12	1:A:724:ILE:H	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:516:ASP:OD2	1:A:707:LYS:NZ	2.41	0.53
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:546:MET:HE1	1:B:549:LYS:HD3	1.90	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:HD12	1:B:724:ILE:H	1.73	0.53
1:B:698:VAL:HG13	2:B:1101:2OW:H6	1.90	0.52
1:A:512:ASP:HB3	1:A:515:MET:HE2	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:A:711:ASN:HD22	2:A:1101:2OW:H22	1.74	0.51
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
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: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:192:ILE:HD13	1:A:248:ILE:HD13	1.95	0.49
1:A:225:PRO:HG2	1:A:335:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:54:ARG:HG3	1:B:59:VAL:HG22	1.96	0.48
1:B:281:ARG:HG2	1:B:317:GLU:O	2.13	0.48
1:B:112:TRP:HA	1:B:112:TRP:CE3	2.49	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:528:MET:HA	1:A:528:MET:HE2	1.96	0.47
1:A:719:ARG:O	1:A:723:ARG:HB2	2.13	0.47
1:B:305:ASN:OD1	1:B:305:ASN:N	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:290:LEU:HD21	1:A:357:MET:HE1	1.97	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:H25	2:B:1101:2OW:C11	2.44	0.47
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:98:GLU:CD	1:A:694:ARG:HH12	2.23	0.46
1:A:579:LEU:HD12	1:A:579:LEU:HA	1.69	0.46
1:A:484:LYS:NZ	1:A:525:GLU:OE2	2.44	0.46
1:A:489:PHE:CZ	1:A:493:MET:HE2	2.51	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:HA	1:A:671:ARG:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:510:PHE:HD2	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: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:A:90:MET:HE3	1:A:118:SER:HB2	2.00	0.44
1:B:546:MET:CE	1:B:549:LYS:HD3	2.48	0.44
1:B:870:PHE:O	1:B:873:SER:OG	2.29	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:HD12	1:B:579:LEU:HA	1.62	0.43
1:A:339:LEU:HD13	1:A:443:ILE:HG12	2.00	0.43
1:A:347:ASN:O	1:A:351:LYS:HG3	2.18	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:85:ASP:OD2	1:B:86:LYS:NZ	2.49	0.43
1:B:840:LEU:HA	1:B:841:PRO:HD3	1.86	0.43
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:6:MET:HE1	1:A:151:PRO:HD3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1101:2OW:H25	2:B:1101:2OW:H16	2.01	0.42
1:A:473:PHE:HE1	1:A:531:MET:HE1	1.85	0.42
1:B:18:LYS:O	1:B:23:ARG:NH1	2.52	0.42
1:A:50:LYS:HE3	1:A:50:LYS:HB2	1.97	0.42
1:A:420:VAL:O	1:A:424:THR:HG23	2.20	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:865:MET:HE1	1:B:1014:ALA:C	2.45	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:HD23	1:B:96:LEU:HA	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:HD23	1:A:352:LEU:HA	1.80	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:770:LEU:HD21	2:A:1101:2OW:H21	2.03	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:B:449:THR:C	1:B:451:GLN:H	2.29	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
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:493:MET:HE3	4:B:1340:HOH:O	2.19	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

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	960/1024 (94%)	907 (94%)	48 (5%)	5 (0%)	24	24
1	B	892/1024 (87%)	858 (96%)	29 (3%)	5 (1%)	21	21
All	All	1852/2048 (90%)	1765 (95%)	77 (4%)	10 (0%)	24	24

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%)	763 (97%)	22 (3%)	38	48
1	B	690/882 (78%)	670 (97%)	20 (3%)	37	47
All	All	1475/1764 (84%)	1433 (97%)	42 (3%)	38	48

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	52	VAL
1	A	105	LEU
1	A	177	THR
1	A	359	PHE
1	A	378	THR
1	A	418	GLN
1	A	462	ILE
1	A	531	MET
1	A	579	LEU
1	A	645	GLN
1	A	683	VAL
1	A	744	LYS
1	A	750	ASP
1	A	799	VAL
1	A	825	THR
1	A	884	THR
1	A	924	LEU
1	A	937	VAL
1	A	989	SER
1	A	996	LYS
1	A	1012	THR
1	B	8	VAL
1	B	23	ARG
1	B	111	SER
1	B	154	ILE
1	B	201	ILE
1	B	248	ILE
1	B	359	PHE
1	B	378	THR
1	B	453	ARG
1	B	462	ILE
1	B	483	GLU
1	B	510	PHE
1	B	567	ARG
1	B	579	LEU
1	B	594	LEU
1	B	666	HIS
1	B	671	ARG
1	B	772	LEU
1	B	932	TYR
1	B	989	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	163	GLN
1	A	288	GLN
1	A	487	GLN
1	A	518	GLN
1	A	568	ASN
1	A	711	ASN
1	A	810	ASN
1	B	163	GLN
1	B	401	HIS
1	B	454	GLN
1	B	487	GLN
1	B	562	ASN
1	B	564	GLN
1	B	661	ASN
1	B	711	ASN
1	B	881	GLN
1	B	985	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	20,22,24	4.65	6 (30%)	25,30,34	3.37	7 (28%)
1	CRO	A	853	1	20,22,24	4.67	6 (30%)	25,30,34	3.17	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRO	B	853	1	-	5/10/29/32	0/2/2/2
1	CRO	A	853	1	-	2/10/29/32	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	15.36	1.49	1.35
1	A	853	CRO	CB2-CA2	14.74	1.49	1.35
1	A	853	CRO	CA2-C2	-10.49	1.37	1.48
1	B	853	CRO	CA2-C2	-9.52	1.38	1.48
1	A	853	CRO	O2-C2	7.67	1.38	1.23
1	B	853	CRO	O2-C2	7.49	1.38	1.23
1	A	853	CRO	OG1-CB1	-4.89	1.21	1.42
1	B	853	CRO	OG1-CB1	-4.71	1.22	1.42
1	B	853	CRO	C1-N2	3.29	1.37	1.32
1	A	853	CRO	C1-N2	3.10	1.36	1.32
1	A	853	CRO	C2-N3	-2.62	1.34	1.40
1	B	853	CRO	C2-N3	-2.38	1.34	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	853	CRO	CG2-CB2-CA2	-11.69	115.97	129.87
1	A	853	CRO	CG2-CB2-CA2	-9.59	118.47	129.87
1	A	853	CRO	O2-C2-CA2	-9.43	125.00	131.02
1	B	853	CRO	O2-C2-CA2	-7.03	126.53	131.02
1	B	853	CRO	CA2-C2-N3	5.97	108.51	103.50
1	A	853	CRO	CA2-C2-N3	5.11	107.79	103.50
1	B	853	CRO	N3-C1-N2	-4.48	107.95	111.48
1	A	853	CRO	N3-C1-N2	-4.04	108.30	111.48
1	B	853	CRO	CB2-CA2-C2	3.32	126.38	122.36
1	B	853	CRO	CA2-N2-C1	3.17	108.28	105.80
1	A	853	CRO	C3-CA3-N3	2.90	119.03	112.43
1	B	853	CRO	C2-CA2-N2	-2.26	107.33	108.95

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	853	CRO	N2-CA2-CB2-CG2
1	A	853	CRO	C2-CA2-CB2-CG2
1	B	853	CRO	N2-CA2-CB2-CG2
1	B	853	CRO	C2-CA2-CB2-CG2
1	B	853	CRO	CA2-CB2-CG2-CD2
1	B	853	CRO	CA2-CB2-CG2-CD1
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 oligosaccharides 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	$\# Z > 2$
2	2OW	A	1101	-	31,31,31	2.79	12 (38%)	41,42,42	2.59	13 (31%)
3	GOL	B	1102	-	5,5,5	0.30	0	5,5,5	0.62	0
2	2OW	B	1101	-	31,31,31	2.82	15 (48%)	41,42,42	2.76	17 (41%)
3	GOL	B	1104	-	5,5,5	0.22	0	5,5,5	0.49	0
3	GOL	B	1103	-	5,5,5	0.47	0	5,5,5	0.80	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
2	2OW	A	1101	-	-	8/18/28/28	1/3/3/3
3	GOL	B	1102	-	-	3/4/4/4	-
2	2OW	B	1101	-	-	7/18/28/28	0/3/3/3
3	GOL	B	1104	-	-	0/4/4/4	-
3	GOL	B	1103	-	-	2/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	2OW	C16-N15	6.34	1.51	1.37
2	A	1101	2OW	C16-N15	5.98	1.50	1.37
2	A	1101	2OW	C25-C24	5.29	1.47	1.38
2	A	1101	2OW	O04-C03	5.27	1.29	1.21
2	B	1101	2OW	C25-C24	5.26	1.47	1.38
2	B	1101	2OW	C03-N05	5.06	1.44	1.35
2	A	1101	2OW	C03-N05	5.01	1.44	1.35
2	B	1101	2OW	O04-C03	4.86	1.28	1.21
2	B	1101	2OW	O02-C01	-4.85	1.34	1.45
2	A	1101	2OW	O02-C01	-4.63	1.35	1.45
2	B	1101	2OW	C29-N05	-4.20	1.39	1.47
2	A	1101	2OW	C20-N21	3.69	1.41	1.34
2	A	1101	2OW	C29-N05	-3.58	1.40	1.47
2	A	1101	2OW	C11-C10	3.54	1.45	1.39
2	A	1101	2OW	C16-N18	3.54	1.45	1.37
2	B	1101	2OW	C20-N21	3.46	1.41	1.34
2	B	1101	2OW	C11-C10	3.39	1.45	1.39
2	B	1101	2OW	C16-N18	3.29	1.44	1.37
2	A	1101	2OW	O02-C03	2.89	1.39	1.34
2	A	1101	2OW	C19-N18	2.72	1.47	1.41
2	B	1101	2OW	C13-C14	2.68	1.44	1.39
2	B	1101	2OW	O02-C03	2.61	1.38	1.34
2	A	1101	2OW	C25-C19	2.48	1.43	1.39
2	B	1101	2OW	C19-N18	2.46	1.46	1.41
2	B	1101	2OW	C25-C19	2.21	1.43	1.39
2	B	1101	2OW	C09-C10	2.19	1.55	1.51
2	B	1101	2OW	C12-C13	2.04	1.42	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	2OW	O02-C03-N05	8.87	118.75	111.61
2	A	1101	2OW	C01-O02-C03	6.88	123.01	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	2OW	C01-O02-C03	6.51	122.60	115.29
2	A	1101	2OW	C11-C10-C26	5.44	120.46	116.46
2	A	1101	2OW	C09-N08-C28	5.11	122.06	111.07
2	A	1101	2OW	O02-C03-N05	5.11	115.72	111.61
2	A	1101	2OW	C06-N05-C03	-4.59	108.39	121.75
2	B	1101	2OW	N18-C16-N15	4.58	121.31	112.44
2	A	1101	2OW	C10-C09-N08	-4.41	104.92	112.75
2	B	1101	2OW	O04-C03-N05	-4.14	116.63	124.30
2	B	1101	2OW	C19-C20-N21	-4.14	120.64	124.07
2	B	1101	2OW	C20-N21-C22	4.12	122.38	117.53
2	B	1101	2OW	C11-C10-C26	3.84	119.28	116.46
2	A	1101	2OW	C09-N08-C07	3.72	119.06	111.07
2	B	1101	2OW	C09-N08-C07	3.69	119.01	111.07
2	A	1101	2OW	O04-C03-N05	-3.61	117.62	124.30
2	A	1101	2OW	C19-C20-N21	-3.50	121.17	124.07
2	B	1101	2OW	O17-C16-N18	-3.31	117.75	123.64
2	B	1101	2OW	C06-C07-N08	3.24	117.19	110.65
2	B	1101	2OW	C09-N08-C28	3.02	117.56	111.07
2	A	1101	2OW	C20-N21-C22	2.99	121.06	117.53
2	A	1101	2OW	O17-C16-N18	-2.99	118.32	123.64
2	A	1101	2OW	C09-C10-C26	-2.99	116.86	121.47
2	B	1101	2OW	O17-C16-N15	-2.81	118.64	123.64
2	B	1101	2OW	C14-N15-C16	-2.77	118.90	125.34
2	B	1101	2OW	C06-N05-C03	-2.58	114.23	121.75
2	B	1101	2OW	C07-C06-N05	2.49	115.36	110.42
2	B	1101	2OW	C09-C10-C26	-2.39	117.78	121.47
2	B	1101	2OW	C10-C09-N08	2.28	116.79	112.75
2	A	1101	2OW	F27-C26-C14	2.16	121.72	118.28

There are no chirality outliers.

All (20) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	A	1101	2OW	O17-C16-N18-C19
3	B	1102	GOL	O1-C1-C2-C3
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	A	1101	2OW	O04-C03-O02-C01
2	B	1101	2OW	O04-C03-N05-C29
3	B	1102	GOL	O2-C2-C3-O3
2	B	1101	2OW	N08-C09-C10-C11

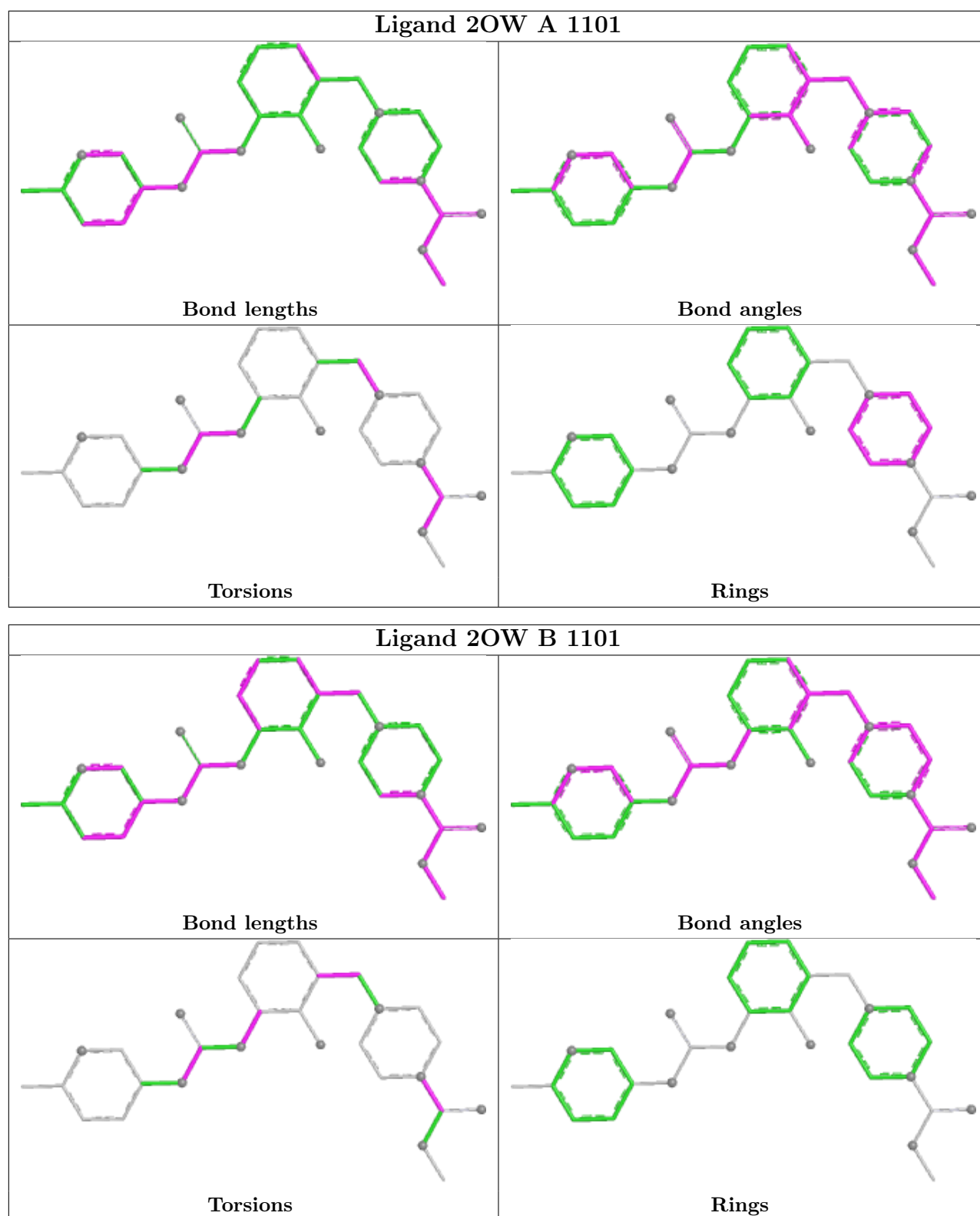
All (1) ring outliers are listed below:

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

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	2OW	11	0
2	B	1101	2OW	12	0
3	B	1104	GOL	1	0
3	B	1103	GOL	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	974/1024 (95%)	0.51	93 (9%) 14 13	15, 40, 79, 100	0
1	B	920/1024 (89%)	0.74	206 (22%) 2 1	17, 35, 104, 130	0
All	All	1894/2048 (92%)	0.62	299 (15%) 5 4	15, 38, 99, 130	0

All (299) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	803	VAL	7.4
1	B	966	ALA	6.7
1	B	965	LEU	6.1
1	B	834	ILE	6.0
1	B	755	GLN	5.4
1	A	938	TYR	5.1
1	B	802	LEU	4.8
1	B	831	LEU	4.8
1	B	855	VAL	4.8
1	B	746	LEU	4.8
1	B	975	ILE	4.7
1	B	908	ASN	4.7
1	B	800	PRO	4.7
1	A	923	ILE	4.6
1	B	850	THR	4.6
1	A	937	VAL	4.6
1	B	844	TRP	4.6
1	B	825	THR	4.6
1	B	874	ALA	4.5
1	B	906	LEU	4.5
1	B	508	TRP	4.5
1	B	724	ILE	4.5
1	A	922	ASN	4.4
1	B	871	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	843	PRO	4.3
1	B	954	THR	4.2
1	B	938	TYR	4.2
1	B	644	PHE	4.1
1	B	810	ASN	4.1
1	B	842	VAL	4.1
1	B	729	ALA	4.1
1	B	833	PHE	4.1
1	B	847	LEU	4.0
1	A	956	HIS	4.0
1	B	805	LEU	4.0
1	B	718	PHE	4.0
1	B	942	ASP	4.0
1	B	981	LEU	3.9
1	B	404	VAL	3.9
1	B	809	VAL	3.9
1	B	907	VAL	3.9
1	B	818	GLY	3.9
1	B	876	PRO	3.8
1	B	848	VAL	3.8
1	B	939	ILE	3.7
1	B	756	TYR	3.7
1	B	846	THR	3.7
1	A	932	TYR	3.7
1	B	932	TYR	3.7
1	B	725	LEU	3.7
1	B	992	SER	3.7
1	B	866	LYS	3.7
1	B	801	ILE	3.6
1	B	948	ILE	3.6
1	B	829	LEU	3.6
1	B	880	VAL	3.6
1	B	784	ILE	3.6
1	B	1008	LEU	3.6
1	B	892	ASN	3.6
1	B	930	TYR	3.6
1	B	742	ALA	3.6
1	B	1006	VAL	3.6
1	B	937	VAL	3.5
1	A	993	ALA	3.5
1	A	887	PHE	3.5
1	A	890	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	816	VAL	3.5
1	B	893	TYR	3.5
1	A	977	ASN	3.5
1	B	971	GLN	3.5
1	B	722	TYR	3.5
1	B	974	PRO	3.4
1	B	838	GLY	3.4
1	B	745	LEU	3.4
1	B	951	ASN	3.4
1	B	958	ILE	3.4
1	B	900	LYS	3.4
1	B	509	THR	3.4
1	B	899	VAL	3.4
1	B	713	ILE	3.4
1	B	895	THR	3.4
1	A	842	VAL	3.4
1	B	1011	VAL	3.4
1	B	728	ALA	3.4
1	B	824	ALA	3.3
1	B	993	ALA	3.3
1	B	727	PRO	3.3
1	B	955	ARG	3.3
1	A	405	LYS	3.3
1	A	963	VAL	3.3
1	B	505	GLY	3.3
1	B	764	PHE	3.3
1	B	835	CYS	3.3
1	B	887	PHE	3.3
1	A	992	SER	3.3
1	B	933	ASN	3.2
1	B	788	THR	3.2
1	A	26	ALA	3.2
1	B	758	PHE	3.2
1	B	765	PHE	3.2
1	B	783	ARG	3.2
1	B	743	GLU	3.2
1	B	845	PRO	3.2
1	B	945	LYS	3.1
1	B	994	LEU	3.1
1	B	875	MET	3.1
1	B	709	PHE	3.1
1	A	969	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	714	LEU	3.1
1	A	796	THR	3.1
1	B	723	ARG	3.1
1	A	797	GLY	3.0
1	B	886	PHE	3.0
1	A	1011	VAL	3.0
1	B	773	LEU	3.0
1	B	982	LEU	3.0
1	B	760	HIS	3.0
1	A	1014	ALA	3.0
1	B	1007	LEU	3.0
1	B	885	ILE	3.0
1	B	808	ASP	3.0
1	B	820	GLY	3.0
1	B	822	GLY	3.0
1	A	371	GLU	3.0
1	B	870	PHE	2.9
1	B	840	LEU	2.9
1	B	787	ARG	2.9
1	B	836	THR	2.9
1	B	969	TYR	2.9
1	A	920	ASP	2.9
1	B	912	LEU	2.9
1	B	935	HIS	2.9
1	B	1002	ARG	2.9
1	B	905	THR	2.9
1	A	863	ASP	2.9
1	A	921	GLY	2.9
1	A	924	LEU	2.9
1	B	877	GLU	2.9
1	A	994	LEU	2.9
1	B	1010	PHE	2.9
1	A	990	THR	2.9
1	B	894	LYS	2.8
1	B	856	GLN	2.8
1	B	941	ALA	2.8
1	B	931	ASN	2.8
1	B	811	GLY	2.8
1	A	1008	LEU	2.8
1	B	988	LEU	2.8
1	A	809	VAL	2.8
1	B	804	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	814	PHE	2.8
1	B	839	LYS	2.8
1	A	420	VAL	2.8
1	B	739	ARG	2.8
1	A	942	ASP	2.8
1	A	826	TYR	2.8
1	B	826	TYR	2.8
1	B	940	MET	2.8
1	B	858	PHE	2.8
1	B	973	THR	2.7
1	A	845	PRO	2.7
1	A	1010	PHE	2.7
1	B	813	LYS	2.7
1	A	965	LEU	2.7
1	A	728	ALA	2.7
1	B	950	ALA	2.7
1	A	946	ASN	2.7
1	B	830	THR	2.7
1	A	811	GLY	2.7
1	B	891	GLY	2.7
1	A	935	HIS	2.7
1	A	1013	ALA	2.7
1	B	879	TYR	2.7
1	B	881	GLN	2.7
1	B	851	PHE	2.7
1	A	412	THR	2.7
1	B	768	GLY	2.7
1	A	979	PRO	2.7
1	B	944	GLN	2.6
1	A	893	TYR	2.6
1	A	917	PHE	2.6
1	A	951	ASN	2.6
1	B	754	ASN	2.6
1	B	867	ARG	2.6
1	B	510	PHE	2.6
1	B	715	TYR	2.6
1	A	847	LEU	2.6
1	B	759	GLY	2.6
1	B	990	THR	2.6
1	A	885	ILE	2.6
1	B	769	LEU	2.6
1	B	898	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1005	MET	2.6
1	A	998	PRO	2.6
1	B	708	GLY	2.6
1	B	884	THR	2.6
1	B	569	ILE	2.6
1	B	861	TYR	2.6
1	A	918	LYS	2.6
1	B	943	LYS	2.6
1	A	366	LEU	2.5
1	B	821	GLU	2.5
1	A	889	ASP	2.5
1	A	916	ASP	2.5
1	A	940	MET	2.5
1	A	886	PHE	2.5
1	A	569	ILE	2.5
1	B	812	HIS	2.5
1	B	995	SER	2.5
1	A	539	MET	2.5
1	A	824	ALA	2.5
1	B	832	LYS	2.5
1	B	878	GLY	2.5
1	A	736	ILE	2.5
1	A	915	ILE	2.5
1	B	770	LEU	2.5
1	B	913	LYS	2.5
1	B	1016	ILE	2.5
1	A	538	CYS	2.4
1	B	412	THR	2.4
1	B	837	THR	2.4
1	B	65	TYR	2.4
1	B	1004	HIS	2.4
1	B	946	ASN	2.4
1	B	882	GLU	2.4
1	B	986	HIS	2.4
1	A	978	GLY	2.4
1	B	849	THR	2.4
1	A	404	VAL	2.4
1	B	863	ASP	2.3
1	A	862	PRO	2.3
1	B	30	PRO	2.3
1	A	202	GLY	2.3
1	A	934	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	748	SER	2.3
1	B	873	SER	2.3
1	A	644	PHE	2.3
1	B	857	CYS	2.3
1	A	864	HIS	2.3
1	B	370	GLU	2.3
1	A	985	ASN	2.3
1	B	710	PRO	2.3
1	A	830	THR	2.3
1	B	63	THR	2.3
1	B	776	MET	2.3
1	A	919	GLU	2.3
1	A	991	GLN	2.3
1	B	1014	ALA	2.3
1	B	909	ARG	2.3
1	A	834	ILE	2.3
1	B	872	LYS	2.3
1	B	717	ASP	2.3
1	A	1012	THR	2.3
1	B	911	GLU	2.3
1	A	1007	LEU	2.2
1	B	983	PRO	2.2
1	B	771	GLY	2.2
1	B	970	GLN	2.2
1	A	570	LYS	2.2
1	A	975	ILE	2.2
1	B	772	LEU	2.2
1	B	952	PHE	2.2
1	B	897	ALA	2.2
1	B	741	GLY	2.2
1	B	827	GLY	2.2
1	B	869	ASP	2.2
1	B	1003	ASP	2.2
1	B	507	GLU	2.2
1	B	953	LYS	2.2
1	B	934	SER	2.2
1	A	987	TYR	2.1
1	A	865	MET	2.1
1	B	786	THR	2.1
1	A	955	ARG	2.1
1	B	369	ARG	2.1
1	B	721	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	948	ILE	2.1
1	A	209	GLN	2.1
1	A	983	PRO	2.1
1	A	884	THR	2.1
1	B	371	GLU	2.1
1	B	781	LEU	2.1
1	A	461	ASP	2.1
1	B	910	ILE	2.1
1	A	368	GLN	2.1
1	A	540	PHE	2.1
1	A	947	GLY	2.1
1	B	947	GLY	2.1
1	A	941	ALA	2.1
1	A	943	LYS	2.1
1	A	734	GLN	2.1
1	A	831	LEU	2.1
1	B	449	THR	2.0
1	B	841	PRO	2.0
1	B	777	ARG	2.0
1	A	370	GLU	2.0
1	A	929	GLU	2.0
1	B	868	HIS	2.0
1	B	957	ASN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CRO	B	853	21/23	0.59	0.24	92,98,105,109	0
1	CRO	A	853	21/23	0.91	0.11	49,56,73,81	0

6.3 Carbohydrates [i](#)

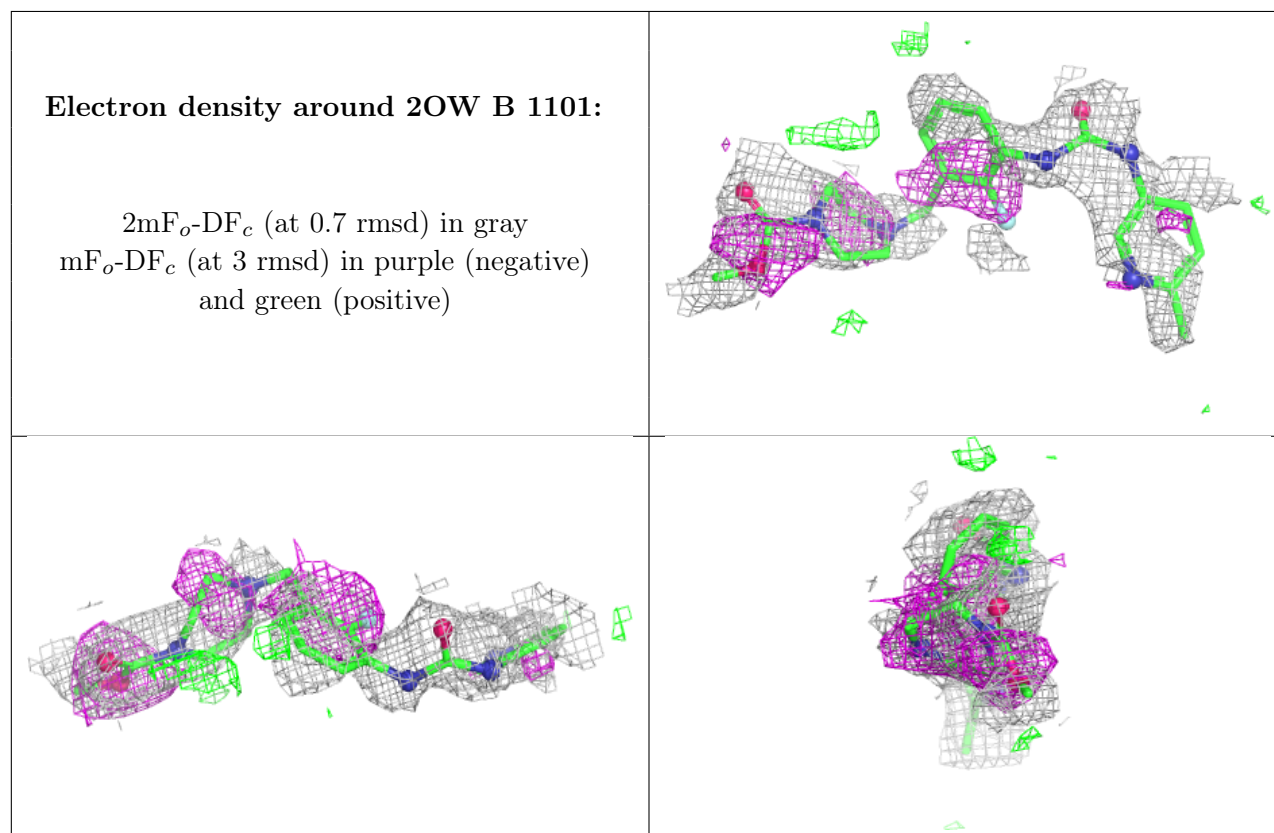
There are no oligosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

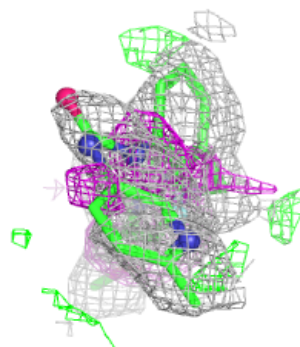
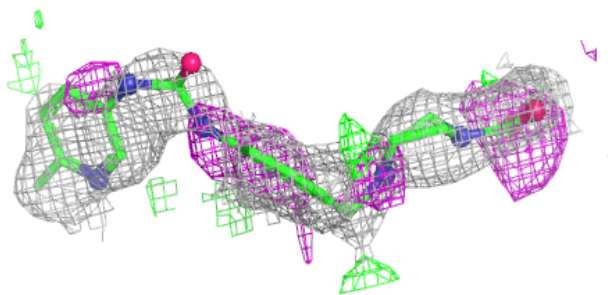
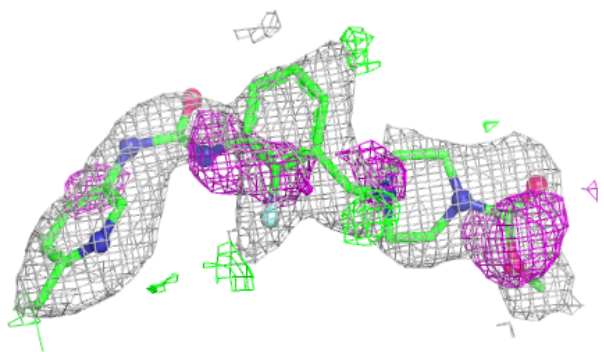
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2OW	B	1101	29/29	0.68	0.22	26,70,78,79	0
2	2OW	A	1101	29/29	0.79	0.16	25,48,59,65	0
3	GOL	B	1104	6/6	0.86	0.17	36,41,43,47	0
3	GOL	B	1102	6/6	0.90	0.11	39,42,44,50	0
3	GOL	B	1103	6/6	0.93	0.16	28,34,39,41	0

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.