



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:12 PM UTC

PDB ID : 8RSK / pdb_00008rsk
Title : Crystal structure of Methanobrevibacter oralis macrodomain in complex with Asn-ADPr
Authors : Ariza, A.
Deposited on : 2024-01-24
Resolution : 2.36 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

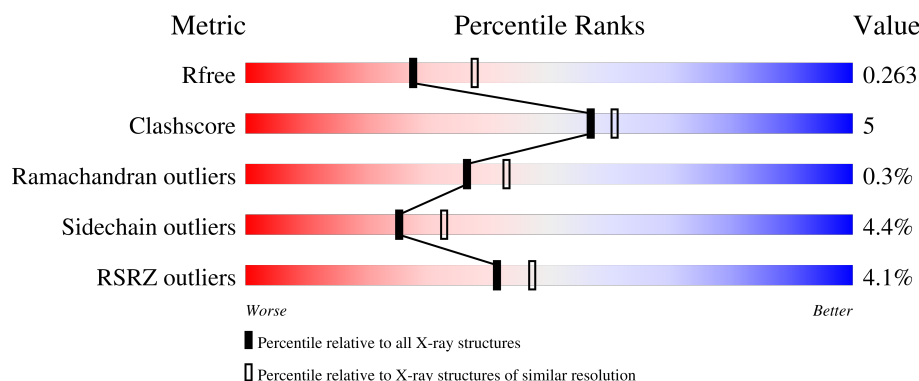
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	262	4% 81% 16% .
1	B	262	6% 82% 15% .
1	C	262	2% 84% 14% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6647 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 O-acetyl-ADP-ribose deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	4	0
			2096	1315	356	410	15			
1	B	262	Total	C	N	O	S	0	4	0
			2096	1313	356	412	15			
1	C	262	Total	C	N	O	S	0	4	0
			2096	1315	356	410	15			

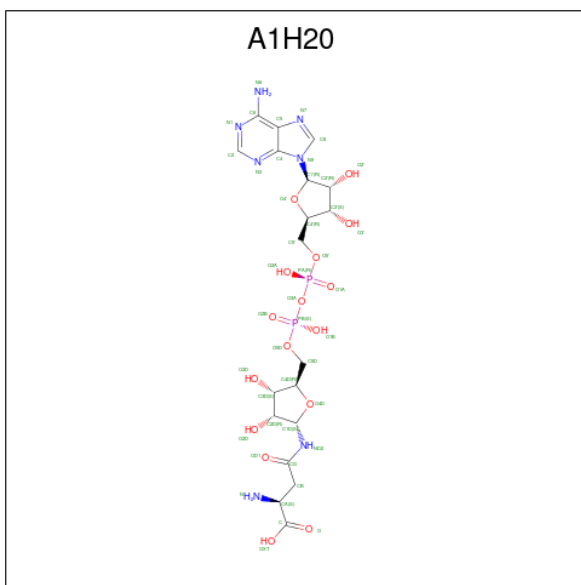
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A166ACJ5
A	0	PRO	-	expression tag	UNP A0A166ACJ5
B	-1	GLY	-	expression tag	UNP A0A166ACJ5
B	0	PRO	-	expression tag	UNP A0A166ACJ5
C	-1	GLY	-	expression tag	UNP A0A166ACJ5
C	0	PRO	-	expression tag	UNP A0A166ACJ5

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

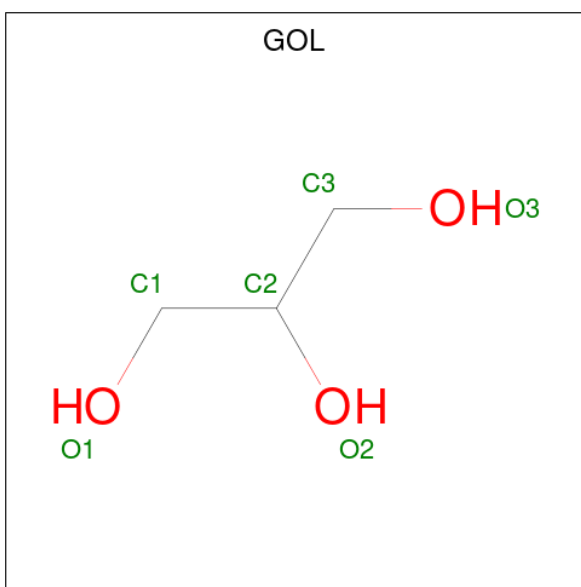
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	4	Total	Zn	0	0
			4	4		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is (2 {S})-4-[[[(2 {S}),3 {R}),4 {S}),5 {R}))-5-[[[(2 {R}),3 {S}),4 {R}),5 {R}))-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxymethyl]-3,4-bis(oxidanyl)oxolan-2-yl]amino]-2-azanyl-4-oxidanylidene-butanoic acid (CCD ID: A1H20) (formula: C₁₉H₂₉N₇O₁₆P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 19	N 7	O 16	P 2	0	0
3	B	1	Total 44	C 19	N 7	O 16	P 2	0	0
3	C	1	Total 44	C 19	N 7	O 16	P 2	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



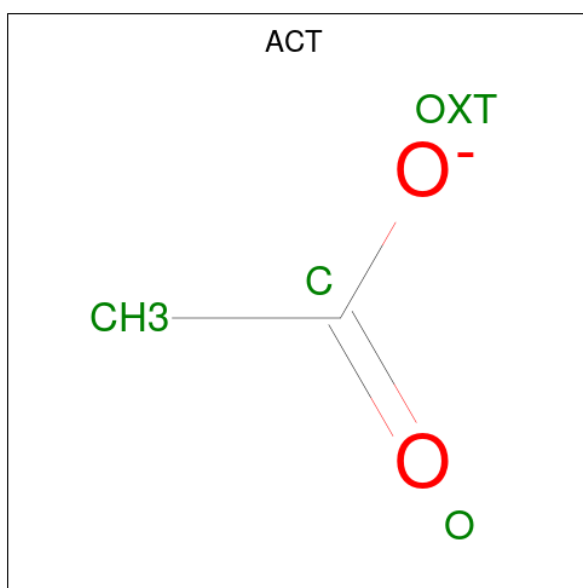
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	63	Total	O	0	0
			63	63		
6	B	55	Total	O	0	0
			55	55		

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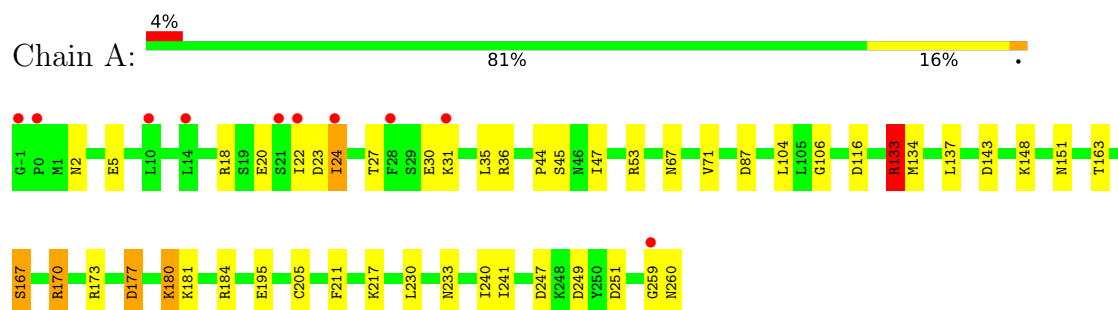
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	56	Total	O	0	0
			56	56		

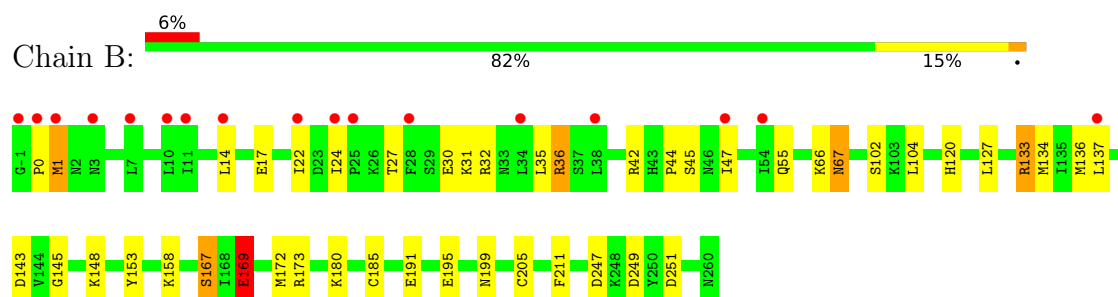
3 Residue-property plots [i](#)

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.

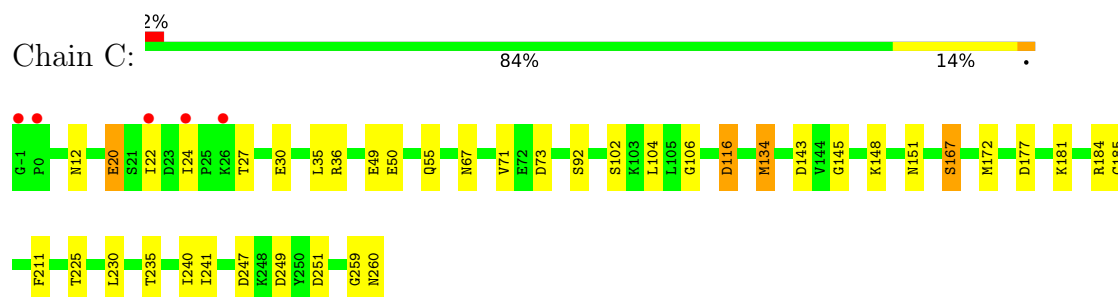
- Molecule 1: O-acetyl-ADP-ribose deacetylase



- Molecule 1: O-acetyl-ADP-ribose deacetylase



- Molecule 1: O-acetyl-ADP-ribose deacetylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.15Å 110.44Å 104.61Å 90.00° 119.56° 90.00°	Depositor
Resolution (Å)	69.95 – 2.36 69.95 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.2 (69.95-2.36) 99.1 (69.95-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.213 , 0.261 0.220 , 0.263	Depositor DCC
R_{free} test set	1960 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6647	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: ACT, GOL, ZN, A1H2O

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	0.85	0/2140	1.32	11/2884 (0.4%)
1	B	0.88	0/2140	1.34	13/2883 (0.5%)
1	C	0.89	1/2140 (0.0%)	1.34	10/2883 (0.3%)
All	All	0.87	1/6420 (0.0%)	1.33	34/8650 (0.4%)

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	3
1	B	0	3
1	C	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	102	SER	CA-CB	-5.48	1.44	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	ASP	CA-CB-CG	8.31	120.91	112.60
1	B	249	ASP	CA-CB-CG	7.84	120.44	112.60
1	C	247	ASP	CA-CB-CG	7.53	120.12	112.60
1	A	247	ASP	CA-CB-CG	7.28	119.88	112.60
1	C	143	ASP	CA-CB-CG	7.25	119.85	112.60
1	B	143	ASP	CA-CB-CG	7.01	119.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ASP	CA-CB-CG	6.81	119.41	112.60
1	C	116	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	195	GLU	CB-CG-CD	6.47	123.59	112.60
1	B	169	GLU	CB-CA-C	6.27	120.38	109.65
1	A	87	ASP	CA-CB-CG	6.16	118.75	112.60
1	C	251	ASP	CA-CB-CG	6.15	118.75	112.60
1	C	73	ASP	CA-CB-CG	6.07	118.67	112.60
1	C	249	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	143	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	247	ASP	CA-CB-CG	5.84	118.44	112.60
1	C	67	ASN	CA-CB-CG	-5.84	106.76	112.60
1	B	143	ASP	CA-C-N	5.80	128.28	120.50
1	B	143	ASP	C-N-CA	5.80	128.28	120.50
1	B	199	ASN	CA-CB-CG	-5.79	106.81	112.60
1	B	67[A]	ASN	CB-CA-C	5.72	121.03	111.30
1	B	67[B]	ASN	CB-CA-C	5.72	121.03	111.30
1	C	50	GLU	CB-CG-CD	5.66	122.22	112.60
1	C	20	GLU	CB-CA-C	5.45	120.44	109.38
1	B	153	TYR	CB-CA-C	5.42	121.20	110.42
1	B	205	CYS	CA-C-N	5.37	128.53	120.69
1	B	205	CYS	C-N-CA	5.37	128.53	120.69
1	A	205	CYS	CA-C-N	5.35	127.87	120.49
1	A	205	CYS	C-N-CA	5.35	127.87	120.49
1	A	163	THR	CA-CB-OG1	5.31	117.57	109.60
1	C	49	GLU	CB-CG-CD	5.12	121.30	112.60
1	A	177	ASP	CA-CB-CG	-5.04	107.56	112.60
1	A	251	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	67	ASN	CB-CA-C	5.00	119.80	111.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	ARG	Sidechain
1	A	170	ARG	Sidechain
1	A	53	ARG	Sidechain
1	B	133	ARG	Sidechain
1	B	32	ARG	Sidechain
1	B	36	ARG	Sidechain
1	C	184	ARG	Sidechain

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	2096	0	2092	24	0
1	B	2096	0	2085	20	0
1	C	2096	0	2092	16	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
2	C	2	0	0	0	0
3	A	44	0	0	0	0
3	B	44	0	0	0	0
3	C	44	0	0	0	0
4	A	12	0	16	5	0
4	B	6	0	8	1	0
4	C	18	0	24	3	0
5	A	4	0	3	0	0
5	C	4	0	3	0	0
6	A	63	0	0	2	0
6	B	55	0	0	4	0
6	C	56	0	0	0	0
All	All	6647	0	6323	59	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 5.

All (59) 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:24:ILE:HB	6:B:451:HOH:O	1.73	0.88
1:A:134:MET:HE3	1:A:148:LYS:HD3	1.70	0.73
1:B:27:THR:HG23	1:B:30:GLU:OE2	1.89	0.72
1:C:27:THR:HG23	1:C:30:GLU:OE2	1.91	0.70
1:A:151[A]:ASN:ND2	4:A:305:GOL:H31	2.07	0.70
1:A:27:THR:HG23	1:A:30:GLU:OE2	1.91	0.70
1:B:66:LYS:HB3	6:B:406:HOH:O	1.93	0.67
1:C:134:MET:HE3	1:C:148:LYS:HD2	1.79	0.64
1:A:134:MET:CE	1:A:148:LYS:HD3	2.27	0.63
4:A:306:GOL:H31	1:B:191:GLU:OE2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:GLY:O	1:C:260:ASN:HB2	2.04	0.57
1:B:134:MET:HE3	1:B:148:LYS:HD2	1.87	0.57
1:C:12:ASN:OD1	1:C:24:ILE:HD11	2.06	0.55
1:C:134:MET:HE3	1:C:148:LYS:CD	2.36	0.54
1:A:180:LYS:NZ	1:C:172:MET:HE2	2.23	0.54
1:C:230:LEU:HD11	1:C:240:ILE:HD12	1.91	0.51
1:A:170:ARG:N	4:A:306:GOL:O1	2.44	0.51
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.76	0.50
1:B:14:LEU:HD22	1:B:42:ARG:HD2	1.93	0.50
1:A:151[A]:ASN:HD21	4:A:305:GOL:H31	1.77	0.49
1:B:167:SER:HB2	1:B:211:PHE:CD1	2.47	0.49
1:A:259:GLY:O	1:A:260:ASN:HB2	2.12	0.49
1:A:71:VAL:HG13	1:A:241:ILE:HD11	1.95	0.49
1:C:167:SER:HB2	1:C:211:PHE:CD1	2.48	0.49
1:A:233:ASN:HA	6:A:423:HOH:O	2.13	0.47
1:B:120:HIS:HD2	6:B:424:HOH:O	1.97	0.46
1:C:225:THR:HA	4:C:304:GOL:H32	1.97	0.46
1:C:151[A]:ASN:ND2	4:C:306:GOL:H11	2.31	0.46
1:A:35:LEU:O	1:A:36:ARG:C	2.59	0.46
1:A:106:GLY:HA2	1:A:116:ASP:CG	2.41	0.45
1:B:134:MET:HE3	1:B:148:LYS:CD	2.46	0.45
1:A:151[A]:ASN:HD21	4:A:305:GOL:C3	2.29	0.45
1:A:2:ASN:OD1	1:A:5:GLU:OE1	2.35	0.44
1:B:169:GLU:HG2	1:B:172:MET:HE2	1.99	0.44
1:A:230:LEU:HD11	1:A:240:ILE:HD12	1.99	0.44
1:A:133:ARG:O	1:A:137:LEU:HG	2.18	0.44
1:B:134:MET:CE	1:B:148:LYS:HD2	2.46	0.44
1:B:145:GLY:HA2	1:B:185:CYS:SG	2.58	0.43
1:B:191:GLU:O	1:B:195:GLU:HG3	2.18	0.43
1:A:180:LYS:HE3	1:A:184:ARG:HH22	1.83	0.43
1:B:191:GLU:OE1	6:B:401:HOH:O	2.21	0.43
1:C:145:GLY:HA2	1:C:185:CYS:SG	2.58	0.43
1:C:177:ASP:O	1:C:181:LYS:HG2	2.19	0.43
1:A:24[A]:ILE:HD11	1:A:31:LYS:HD3	2.00	0.43
1:B:24:ILE:HD11	1:B:31:LYS:CD	2.48	0.43
1:B:133:ARG:O	1:B:137:LEU:HG	2.19	0.43
1:A:217:LYS:HE3	6:A:418:HOH:O	2.19	0.43
1:B:35:LEU:O	1:B:36:ARG:C	2.60	0.43
1:C:106:GLY:HA2	1:C:116:ASP:CG	2.43	0.43
1:A:106:GLY:HA2	1:A:116:ASP:OD1	2.19	0.42
1:B:120:HIS:CD2	1:B:127:LEU:HD23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:O	1:C:36:ARG:C	2.62	0.42
1:A:167:SER:HB2	1:A:211:PHE:CD1	2.55	0.42
1:A:177:ASP:O	1:A:181:LYS:HG2	2.19	0.42
1:A:44:PRO:O	1:A:45:SER:HB3	2.20	0.42
1:B:102:SER:HB3	4:B:306:GOL:H12	2.01	0.42
1:C:225:THR:HG23	4:C:304:GOL:H32	2.02	0.41
1:B:44:PRO:O	1:B:45:SER:HB3	2.20	0.41
1:C:71:VAL:HG13	1:C:241[A]:ILE:HD11	2.02	0.41

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	264/262 (101%)	253 (96%)	11 (4%)	0	100	100
1	B	264/262 (101%)	251 (95%)	11 (4%)	2 (1%)	16	17
1	C	264/262 (101%)	257 (97%)	7 (3%)	0	100	100
All	All	792/786 (101%)	761 (96%)	29 (4%)	2 (0%)	36	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	0	PRO
1	B	1	MET

5.3.2 Protein sidechains [i](#)

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	241/237 (102%)	230 (95%)	11 (5%)	24	31
1	B	241/237 (102%)	227 (94%)	14 (6%)	18	22
1	C	241/237 (102%)	233 (97%)	8 (3%)	33	44
All	All	723/711 (102%)	690 (95%)	33 (5%)	25	31

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	22	ILE
1	A	23	ASP
1	A	24[A]	ILE
1	A	24[B]	ILE
1	A	47	ILE
1	A	104	LEU
1	A	133	ARG
1	A	167	SER
1	A	173	ARG
1	A	180	LYS
1	B	1	MET
1	B	17	GLU
1	B	22	ILE
1	B	47	ILE
1	B	55	GLN
1	B	67[A]	ASN
1	B	67[B]	ASN
1	B	104	LEU
1	B	136	MET
1	B	158	LYS
1	B	167	SER
1	B	169	GLU
1	B	173	ARG
1	B	180	LYS
1	C	20	GLU
1	C	22	ILE
1	C	55	GLN
1	C	92	SER
1	C	104	LEU
1	C	134	MET

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Mol	Chain	Res	Type
1	C	167	SER
1	C	235	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	154	ASN
1	A	162	HIS
1	A	231	ASN
1	B	43	HIS
1	B	120	HIS
1	B	132	ASN
1	B	151	ASN
1	B	154	ASN
1	B	162	HIS
1	C	162	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 9 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ACT	C	307	-	3,3,3	1.83	1 (33%)	3,3,3	0.75	0
3	A1H20	B	305	2	46,47,47	2.26	18 (39%)	64,71,71	2.62	23 (35%)
4	GOL	A	305	-	5,5,5	0.16	0	5,5,5	0.47	0
4	GOL	C	305	-	5,5,5	0.24	0	5,5,5	0.52	0
3	A1H20	C	303	2	46,47,47	1.48	9 (19%)	64,71,71	2.69	25 (39%)
3	A1H20	A	303	2	46,47,47	1.85	9 (19%)	64,71,71	2.61	30 (46%)
4	GOL	C	304	-	5,5,5	0.34	0	5,5,5	0.57	0
4	GOL	B	306	-	5,5,5	0.63	0	5,5,5	1.15	0
5	ACT	A	307	-	3,3,3	1.18	0	3,3,3	1.49	1 (33%)
4	GOL	C	306	-	5,5,5	0.08	0	5,5,5	0.36	0
4	GOL	A	306	-	5,5,5	0.15	0	5,5,5	0.48	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	A1H20	B	305	2	-	7/34/66/66	0/4/4/4
4	GOL	A	305	-	-	4/4/4/4	-
4	GOL	C	305	-	-	2/4/4/4	-
3	A1H20	C	303	2	-	8/34/66/66	0/4/4/4
3	A1H20	A	303	2	-	6/34/66/66	0/4/4/4
4	GOL	C	304	-	-	4/4/4/4	-
4	GOL	B	306	-	-	1/4/4/4	-
4	GOL	C	306	-	-	2/4/4/4	-
4	GOL	A	306	-	-	2/4/4/4	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	A1H20	PA-O3A	-6.16	1.52	1.59
3	B	305	A1H20	PA-O3A	5.34	1.65	1.59
3	B	305	A1H20	OD1-CG	5.18	1.33	1.23
3	A	303	A1H20	C8-N7	5.17	1.41	1.31
3	B	305	A1H20	CB-CG	4.41	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	305	A1H20	C2-N1	4.35	1.41	1.33
3	B	305	A1H20	C5-C4	4.01	1.46	1.39
3	C	303	A1H20	C2'-C1'	-3.98	1.41	1.53
3	B	305	A1H20	C2'-C1'	-3.93	1.41	1.53
3	B	305	A1H20	PB-O3A	3.87	1.63	1.59
3	A	303	A1H20	C5-C4	3.44	1.45	1.39
3	B	305	A1H20	O4D-C1D	3.32	1.48	1.43
3	A	303	A1H20	C2D-C3D	-3.28	1.44	1.53
3	B	305	A1H20	C2-N3	3.17	1.39	1.33
3	C	303	A1H20	C5-C4	3.13	1.44	1.39
3	B	305	A1H20	PB-O2B	2.88	1.60	1.50
3	C	303	A1H20	C5-C6	2.86	1.49	1.41
5	C	307	ACT	CH3-C	2.84	1.60	1.49
3	B	305	A1H20	C4-N3	2.79	1.39	1.34
3	C	303	A1H20	C8-N7	2.69	1.36	1.31
3	A	303	A1H20	O3D-C3D	2.64	1.49	1.43
3	B	305	A1H20	C8-N7	2.57	1.36	1.31
3	A	303	A1H20	C8-N9	-2.47	1.33	1.37
3	C	303	A1H20	C2D-C3D	-2.46	1.46	1.53
3	B	305	A1H20	C8-N9	-2.38	1.33	1.37
3	A	303	A1H20	O4'-C1'	2.36	1.47	1.42
3	B	305	A1H20	C5'-C4'	2.26	1.58	1.51
3	C	303	A1H20	O4'-C4'	-2.23	1.40	1.45
3	B	305	A1H20	O4'-C1'	2.19	1.47	1.42
3	B	305	A1H20	C6-N6	2.16	1.39	1.34
3	C	303	A1H20	C6-N1	-2.15	1.29	1.35
3	C	303	A1H20	PB-O3A	2.09	1.61	1.59
3	A	303	A1H20	PB-O2B	2.08	1.58	1.50
3	B	305	A1H20	PA-O2A	-2.06	1.45	1.55
3	C	303	A1H20	O4'-C1'	-2.04	1.37	1.42
3	B	305	A1H20	C1D-ND2	-2.02	1.40	1.43
3	A	303	A1H20	C2'-C1'	-2.01	1.47	1.53

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	A1H20	O4D-C1D-ND2	-8.26	100.87	110.22
3	B	305	A1H20	C4-N9-C8	8.17	114.32	105.74
3	B	305	A1H20	O1B-PB-O3A	7.28	126.96	107.27
3	A	303	A1H20	O4D-C1D-C2D	-6.59	99.44	106.29
3	C	303	A1H20	C2D-C1D-ND2	6.20	119.80	112.02
3	C	303	A1H20	O1B-PB-O3A	6.15	123.91	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	A1H20	O1B-PB-O3A	5.66	122.56	107.27
3	B	305	A1H20	N6-C6-N1	5.40	130.41	118.38
3	A	303	A1H20	OD1-CG-CB	5.38	129.40	121.54
3	B	305	A1H20	C5-C4-N9	-5.25	100.09	105.81
3	B	305	A1H20	C4-N9-C1'	-5.24	114.37	126.63
3	B	305	A1H20	C2'-C3'-C4'	5.03	112.32	102.61
3	C	303	A1H20	C4-N9-C1'	-4.89	115.20	126.63
3	C	303	A1H20	C4-C5-N7	-4.65	105.27	110.58
3	C	303	A1H20	C4-N9-C8	4.61	110.58	105.74
3	C	303	A1H20	O4D-C4D-C5D	4.36	123.30	109.33
3	B	305	A1H20	C3'-C2'-C1'	-4.32	93.28	101.46
3	C	303	A1H20	N9-C8-N7	-4.22	107.95	113.94
3	A	303	A1H20	C5-C4-N3	-4.16	120.99	126.72
3	A	303	A1H20	C4-C5-N7	-4.14	105.85	110.58
3	A	303	A1H20	O4D-C4D-C5D	4.13	122.58	109.33
3	A	303	A1H20	N9-C8-N7	-4.13	108.08	113.94
3	B	305	A1H20	C5-C6-N6	-4.08	113.18	123.29
3	C	303	A1H20	O4D-C1D-C2D	-4.05	102.08	106.29
3	A	303	A1H20	C5-N7-C8	4.02	109.77	103.45
3	A	303	A1H20	C4-N9-C1'	-4.00	117.28	126.63
3	C	303	A1H20	C2'-C3'-C4'	3.88	110.11	102.61
3	C	303	A1H20	C5-C4-N3	-3.87	121.38	126.72
3	C	303	A1H20	C5-N7-C8	3.87	109.54	103.45
3	C	303	A1H20	O5D-C5D-C4D	3.83	122.03	108.99
3	A	303	A1H20	C2'-C3'-C4'	3.78	109.92	102.61
3	B	305	A1H20	O3A-PB-O2B	-3.78	99.34	110.70
3	B	305	A1H20	N9-C8-N7	-3.76	108.60	113.94
3	C	303	A1H20	C6-C5-N7	3.72	139.26	132.09
3	A	303	A1H20	C4-N9-C8	3.70	109.63	105.74
3	A	303	A1H20	C3D-C2D-C1D	3.70	108.45	101.46
3	B	305	A1H20	N3-C4-N9	3.63	133.35	127.17
3	A	303	A1H20	O2D-C2D-C3D	-3.49	100.64	111.82
3	C	303	A1H20	O4'-C4'-C3'	-3.49	98.23	105.15
3	A	303	A1H20	O4'-C1'-C2'	3.44	113.98	106.62
3	A	303	A1H20	C4D-O4D-C1D	3.43	115.75	108.63
3	C	303	A1H20	O4D-C4D-C3D	-3.34	98.51	105.15
3	B	305	A1H20	CB-CG-ND2	-3.27	111.79	116.25
3	B	305	A1H20	O2D-C2D-C1D	3.24	121.25	110.10
3	A	303	A1H20	C1D-ND2-CG	3.24	128.28	122.54
3	A	303	A1H20	O3D-C3D-C2D	-3.21	101.52	111.82
3	C	303	A1H20	C1'-N9-C8	3.21	134.22	127.09
3	B	305	A1H20	C2D-C1D-ND2	3.19	116.03	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	A1H20	O1B-PB-O5D	3.12	121.70	107.57
3	A	303	A1H20	N3-C4-N9	3.00	132.27	127.17
3	A	303	A1H20	CB-CG-ND2	-2.95	112.23	116.25
3	B	305	A1H20	O4'-C4'-C3'	-2.89	99.42	105.15
3	C	303	A1H20	C4D-O4D-C1D	2.86	114.56	108.63
3	C	303	A1H20	N3-C4-N9	2.81	131.95	127.17
3	A	303	A1H20	C3'-C2'-C1'	-2.79	96.18	101.46
3	A	303	A1H20	OD1-CG-ND2	-2.73	118.33	122.95
3	A	303	A1H20	O2D-C2D-C1D	2.72	119.43	110.10
3	A	303	A1H20	C1'-N9-C8	2.70	133.09	127.09
3	C	303	A1H20	C1D-ND2-CG	-2.67	117.80	122.54
3	C	303	A1H20	C3'-C2'-C1'	-2.52	96.69	101.46
3	A	303	A1H20	CA-CB-CG	2.51	121.27	113.72
3	A	303	A1H20	O3A-PA-O1A	-2.51	103.16	110.70
3	B	305	A1H20	C1D-ND2-CG	2.49	126.95	122.54
3	C	303	A1H20	O2A-PA-O3A	-2.44	100.68	107.27
3	A	303	A1H20	O3A-PB-O2B	-2.43	103.39	110.70
3	A	303	A1H20	O4D-C4D-C3D	-2.40	100.39	105.15
3	A	303	A1H20	C4'-O4'-C1'	-2.39	104.19	109.47
3	B	305	A1H20	O4'-C1'-N9	-2.36	103.56	108.09
3	B	305	A1H20	C2'-C1'-N9	2.34	119.13	113.30
3	C	303	A1H20	CB-CG-ND2	-2.29	113.13	116.25
3	A	303	A1H20	O5D-PB-O2B	-2.27	99.92	108.94
3	C	303	A1H20	CB-CA-N	2.22	122.13	112.42
3	B	305	A1H20	O2A-PA-O3A	-2.13	101.50	107.27
3	B	305	A1H20	O4D-C4D-C5D	2.10	116.06	109.33
3	B	305	A1H20	CB-CA-N	2.05	121.38	112.42
3	B	305	A1H20	N3-C2-N1	2.04	131.68	128.58
3	B	305	A1H20	C2-N3-C4	-2.04	106.86	111.83
3	C	303	A1H20	C2D-C3D-C4D	2.02	106.51	102.61
5	A	307	ACT	O-C-CH3	-2.01	114.30	122.53

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	305	GOL	O1-C1-C2-C3
4	A	305	GOL	C1-C2-C3-O3
4	A	306	GOL	C1-C2-C3-O3
4	C	305	GOL	C1-C2-C3-O3
4	C	306	GOL	C1-C2-C3-O3
3	C	303	A1H20	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	A	303	A1H20	C3'-C4'-C5'-O5'
4	C	304	GOL	O1-C1-C2-C3
4	C	304	GOL	C1-C2-C3-O3
4	A	305	GOL	O1-C1-C2-O2
4	C	304	GOL	O1-C1-C2-O2
4	C	304	GOL	O2-C2-C3-O3
4	C	306	GOL	O2-C2-C3-O3
3	A	303	A1H20	O4'-C4'-C5'-O5'
3	C	303	A1H20	O4'-C4'-C5'-O5'
4	A	305	GOL	O2-C2-C3-O3
4	A	306	GOL	O2-C2-C3-O3
3	B	305	A1H20	OXT-C-CA-CB
3	B	305	A1H20	O-C-CA-CB
3	B	305	A1H20	PA-O3A-PB-O2B
3	C	303	A1H20	O-C-CA-CB
3	C	303	A1H20	OXT-C-CA-CB
4	B	306	GOL	O2-C2-C3-O3
3	A	303	A1H20	O-C-CA-CB
3	B	305	A1H20	C2'-C1'-N9-C8
3	C	303	A1H20	C2'-C1'-N9-C8
4	C	305	GOL	O2-C2-C3-O3
3	A	303	A1H20	OXT-C-CA-CB
3	C	303	A1H20	PA-O3A-PB-O1B
3	B	305	A1H20	C2'-C1'-N9-C4
3	C	303	A1H20	C2'-C1'-N9-C4
3	A	303	A1H20	O4'-C1'-N9-C8
3	A	303	A1H20	C2'-C1'-N9-C8
3	B	305	A1H20	O4'-C1'-N9-C8
3	C	303	A1H20	O4'-C1'-N9-C8
3	B	305	A1H20	C3'-C4'-C5'-O5'

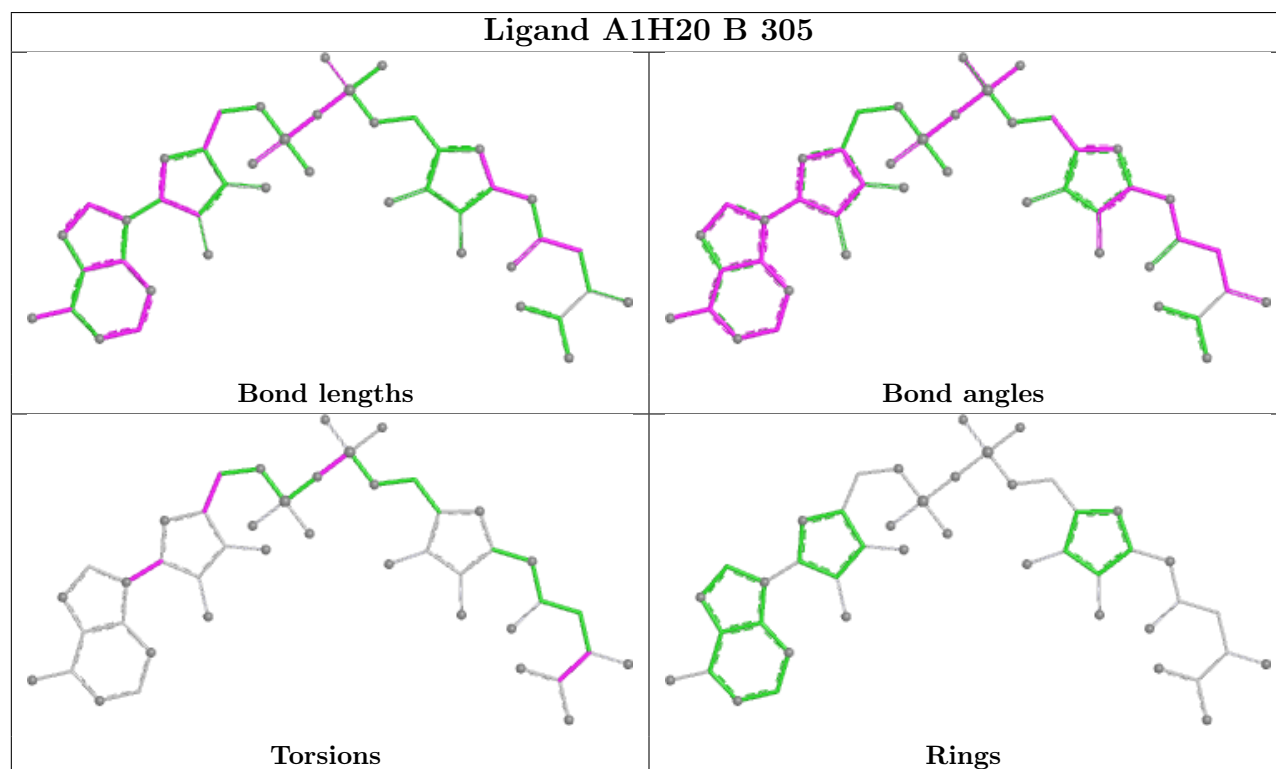
There are no ring outliers.

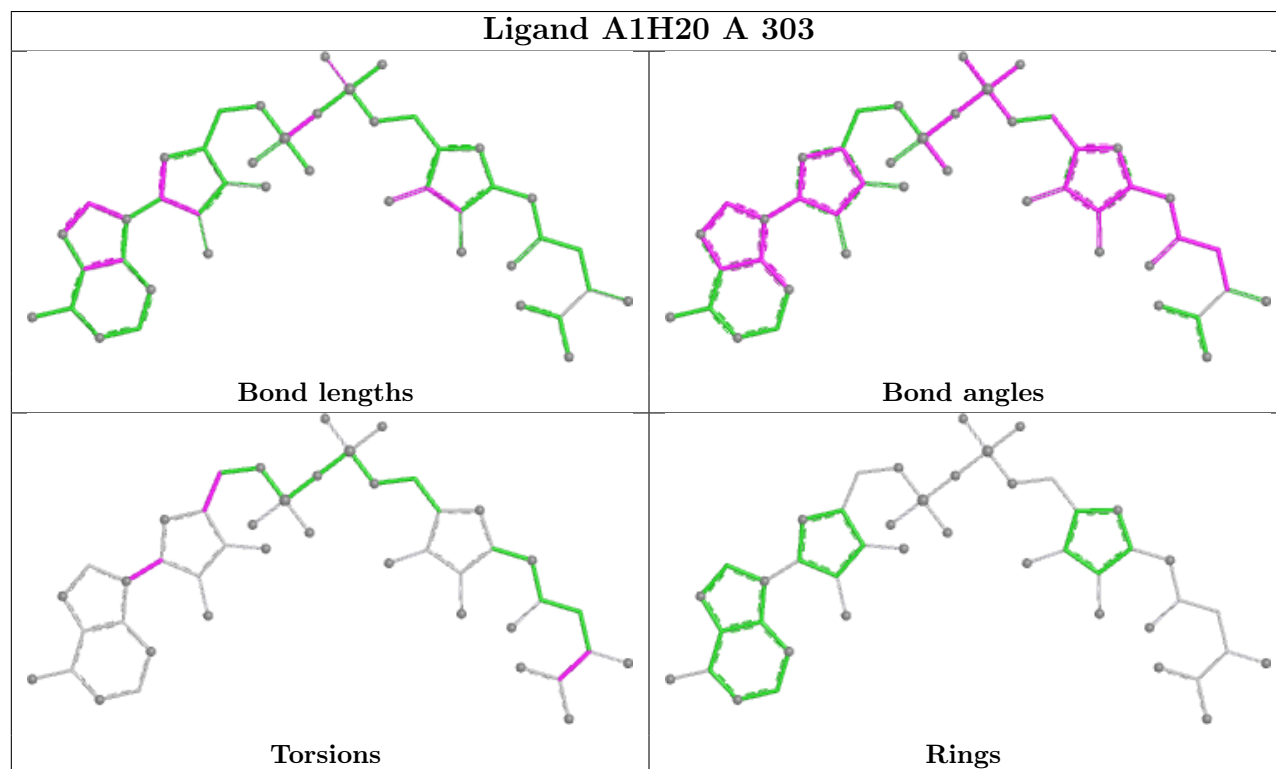
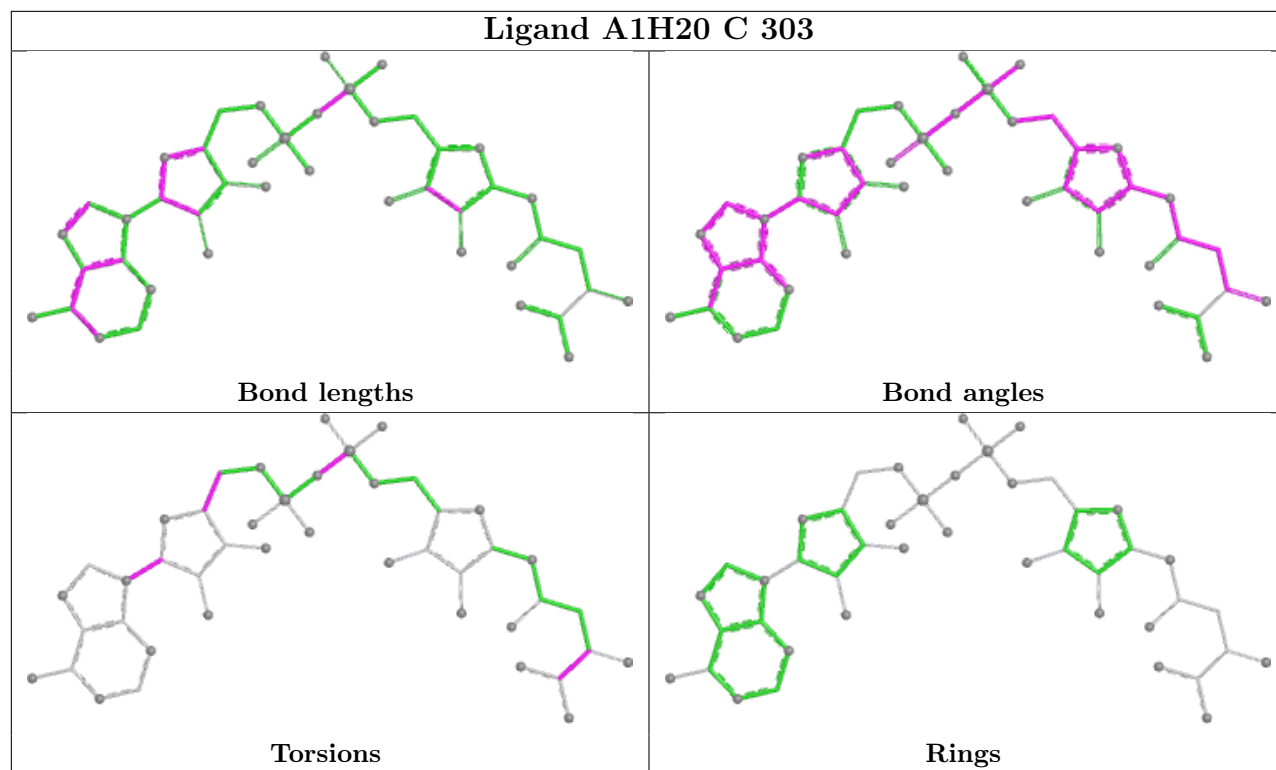
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	305	GOL	3	0
4	C	304	GOL	2	0
4	B	306	GOL	1	0
4	C	306	GOL	1	0
4	A	306	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 [i](#)

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	262/262 (100%)	0.28	10 (3%) 44 50	22, 53, 117, 162	4 (1%)
1	B	262/262 (100%)	0.35	17 (6%) 25 28	25, 51, 132, 172	4 (1%)
1	C	262/262 (100%)	0.15	5 (1%) 66 71	19, 49, 102, 154	4 (1%)
All	All	786/786 (100%)	0.26	32 (4%) 41 47	19, 51, 121, 172	12 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-1	GLY	4.0
1	A	22	ILE	3.8
1	B	-1	GLY	3.6
1	C	0	PRO	3.6
1	B	1	MET	3.4
1	A	0	PRO	3.4
1	A	24[A]	ILE	3.4
1	B	24	ILE	3.3
1	B	34	LEU	3.2
1	B	22	ILE	3.2
1	C	24	ILE	3.2
1	A	-1	GLY	3.1
1	C	22	ILE	3.1
1	B	25	PRO	3.1
1	B	0	PRO	3.0
1	B	10	LEU	2.8
1	B	54	ILE	2.7
1	A	28	PHE	2.7
1	B	14	LEU	2.5
1	A	10	LEU	2.4
1	B	7	LEU	2.3
1	A	21	SER	2.3
1	B	28	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	47	ILE	2.3
1	B	3[A]	ASN	2.2
1	A	31	LYS	2.2
1	C	26	LYS	2.2
1	B	11	ILE	2.1
1	B	137	LEU	2.1
1	A	14	LEU	2.1
1	B	38	LEU	2.1
1	A	259	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

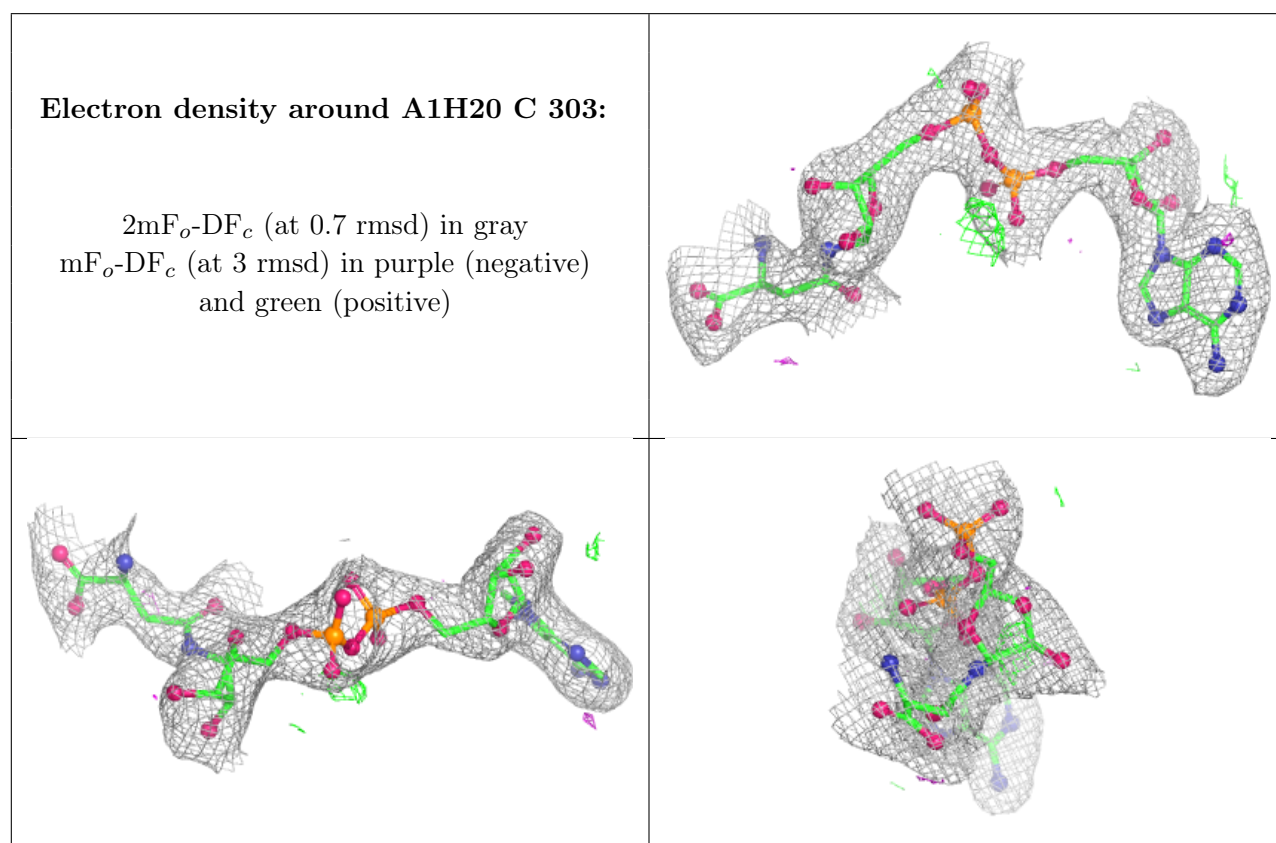
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	C	304	6/6	0.63	0.26	74,104,109,111	0
5	ACT	C	307	4/4	0.79	0.16	57,61,62,75	0
4	GOL	C	306	6/6	0.83	0.15	49,73,77,80	0
4	GOL	A	306	6/6	0.85	0.18	62,72,94,117	0
4	GOL	B	306	6/6	0.87	0.21	48,53,63,65	0
4	GOL	A	305	6/6	0.87	0.14	53,83,101,113	0
4	GOL	C	305	6/6	0.88	0.18	64,86,89,104	0
5	ACT	A	307	4/4	0.89	0.29	58,61,83,101	0
3	A1H20	C	303	44/44	0.98	0.05	32,37,44,46	0
3	A1H20	A	303	44/44	0.98	0.05	28,33,38,43	0
3	A1H20	B	305	44/44	0.98	0.05	26,32,35,39	0
2	ZN	A	302	1/1	0.99	0.02	35,35,35,35	1
2	ZN	B	302	1/1	1.00	0.01	35,35,35,35	0
2	ZN	B	303	1/1	1.00	0.04	40,40,40,40	0

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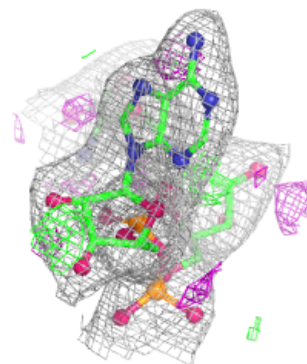
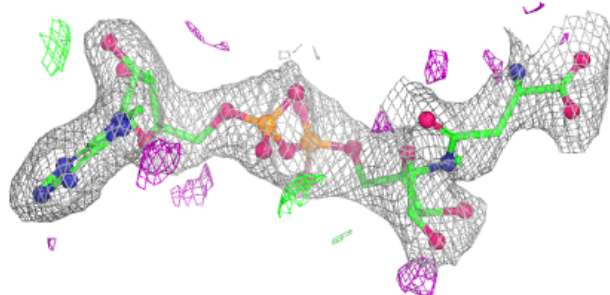
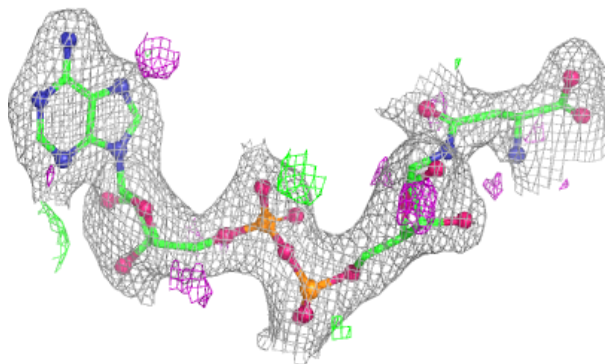
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	304	1/1	1.00	0.02	36,36,36,36	1
2	ZN	C	301	1/1	1.00	0.03	36,36,36,36	0
2	ZN	C	302	1/1	1.00	0.02	33,33,33,33	1
2	ZN	A	301	1/1	1.00	0.03	32,32,32,32	0
2	ZN	A	304	1/1	1.00	0.01	51,51,51,51	0
2	ZN	B	301	1/1	1.00	0.04	42,42,42,42	0

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.

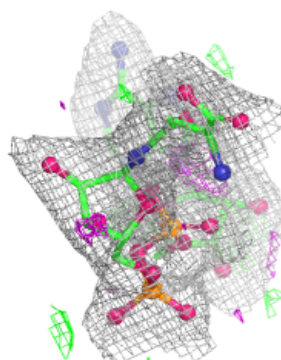
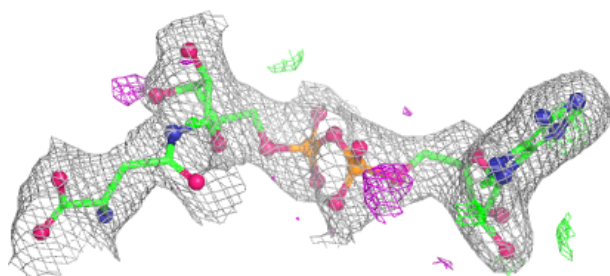
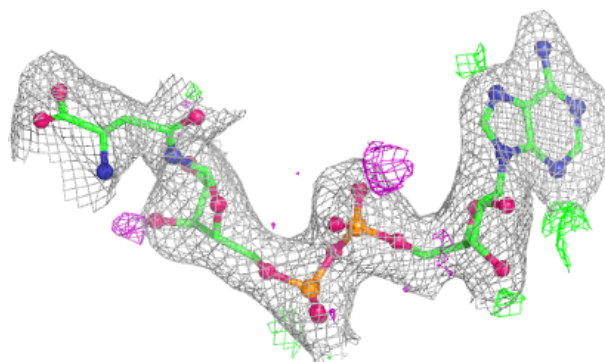


Electron density around A1H20 A 303:

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

**Electron density around A1H20 B 305:**

$2mF_o-DF_c$ (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.