Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 12:33 pm BST

PDB ID	:	5ABF
Title	:	Structure of GH84 with ligand
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Deposited on	:	2015-08-05
Resolution	:	2.10 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 (i) symbol.

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

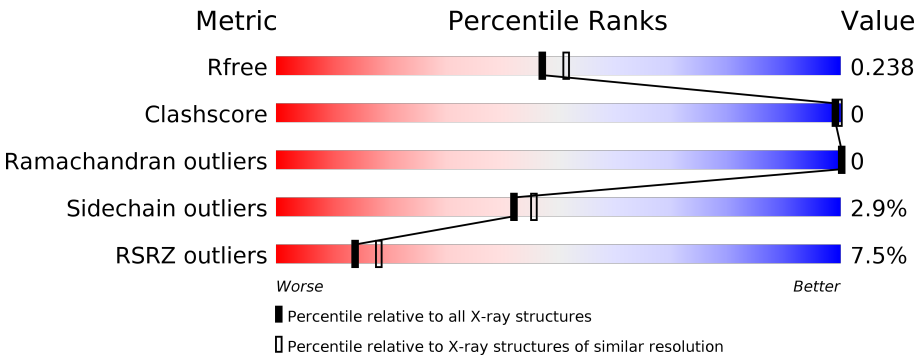
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 >=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 <=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	726	5% 88% • 9%
2	B	726	8% 87% • 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21754 atoms, of which 10664 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-GLCNACASE BT_4395.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	663	10762	3464	5351	915	1012	20	0	7	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP Q89ZI2
A	-8	GLY	-	expression tag	UNP Q89ZI2
A	-7	SER	-	expression tag	UNP Q89ZI2
A	-6	SER	-	expression tag	UNP Q89ZI2
A	-5	HIS	-	expression tag	UNP Q89ZI2
A	-4	HIS	-	expression tag	UNP Q89ZI2
A	-3	HIS	-	expression tag	UNP Q89ZI2
A	-2	HIS	-	expression tag	UNP Q89ZI2
A	-1	HIS	-	expression tag	UNP Q89ZI2
A	0	HIS	-	expression tag	UNP Q89ZI2

- Molecule 2 is a protein called O-GLCNACASE BT_4395.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	651	10563	3406	5249	897	992	19	0	6	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	expression tag	UNP Q89ZI2
B	-8	GLY	-	expression tag	UNP Q89ZI2
B	-7	SER	-	expression tag	UNP Q89ZI2
B	-6	SER	-	expression tag	UNP Q89ZI2
B	-5	HIS	-	expression tag	UNP Q89ZI2
B	-4	HIS	-	expression tag	UNP Q89ZI2

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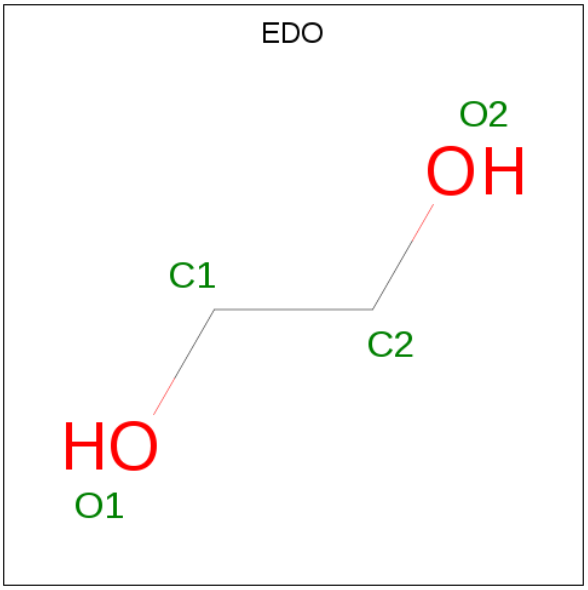
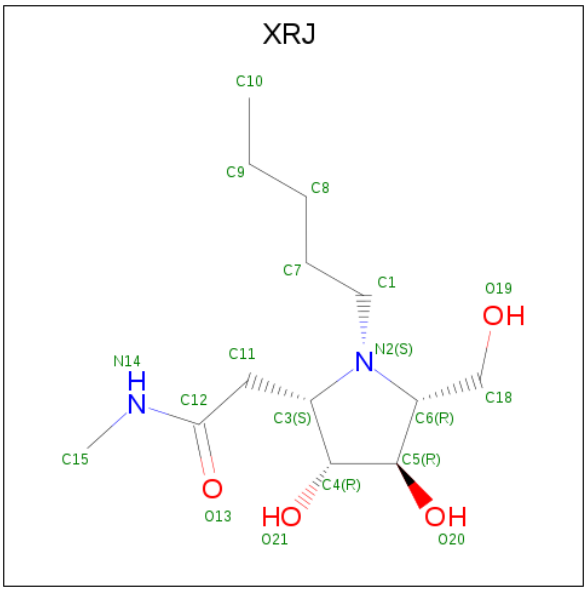
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP Q89ZI2
B	-2	HIS	-	expression tag	UNP Q89ZI2
B	-1	HIS	-	expression tag	UNP Q89ZI2
B	0	HIS	-	expression tag	UNP Q89ZI2
B	2	GLN	ASN	conflict	UNP Q89ZI2

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	10	2	6	2	0	0
			Total	C	H	O		
3	B	1	10	2	6	2	0	0

- Molecule 4 is 2-[(2S,3R,4R,5R)-5-(hydroxymethyl)-3,4-bis(oxidanyl)-1-pentyl-pyrrolidin-2-yl]-N-methyl-ethanamide (three-letter code: XRJ) (formula: $C_{13}H_{26}N_2O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	A	1	45	13	26	2	4	0	0
			Total	C	H	N	O		
4	B	1	45	13	26	2	4	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	B	1	1	1	0	0

- Molecule 6 is water.

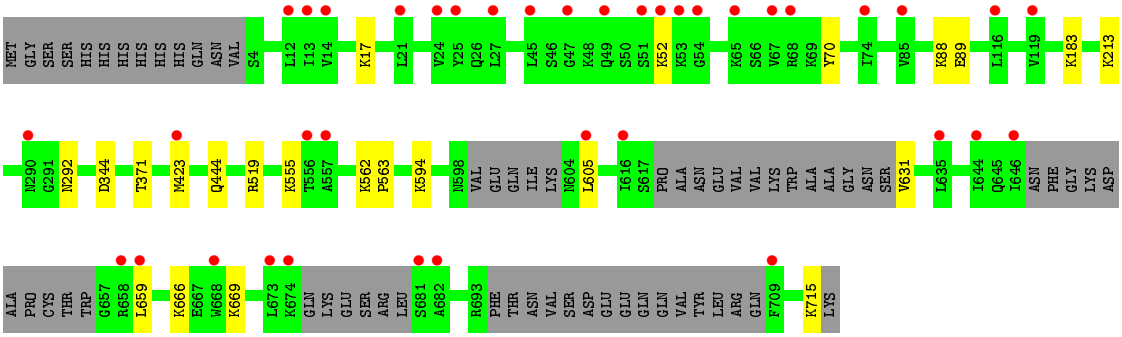
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	169	169	169	0	0
			Total	O		
6	B	149	149	149	0	0

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.

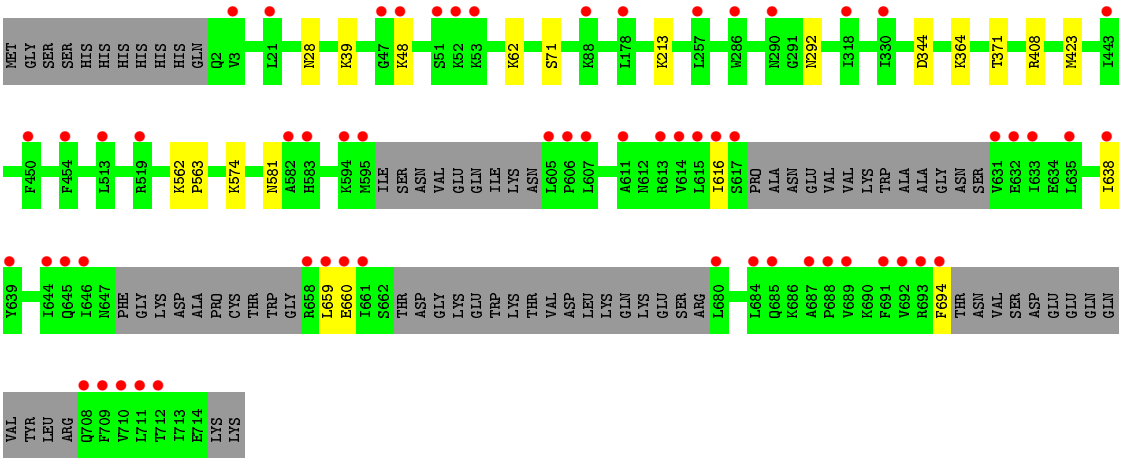
- Molecule 1: O-GLCNACASE BT_4395

Chain A:



- Molecule 2: O-GLCNACASE BT_4395

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.59Å 160.99Å 223.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.73 – 2.10 75.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (54.73-2.10) 99.9 (75.75-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.206 , 0.234 0.210 , 0.238	Depositor DCC
R_{free} test set	5457 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.783	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21754	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1025e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, EDO, XRJ

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	0.23	0/5569	0.40	0/7538
2	B	0.24	0/5462	0.40	0/7394
All	All	0.24	0/11031	0.40	0/14932

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	5411	5351	5337	4	0
2	B	5314	5249	5237	3	0
3	A	4	6	6	0	0
3	B	4	6	6	0	0
4	A	19	26	26	1	0
4	B	19	26	26	1	0
5	B	1	0	0	0	0
6	A	169	0	0	1	0
6	B	149	0	0	0	0
All	All	11090	10664	10638	7	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 0.

All (7) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ASP:OD1	4:A:1717:XRJ:O19	2.08	0.69
2:B:344:ASP:OD1	4:B:1717:XRJ:O19	2.22	0.58
1:A:70:TYR:OH	1:A:89:GLU:OE1	2.27	0.52
1:A:555:LYS:NZ	6:A:2158:HOH:O	2.36	0.52
2:B:62[A]:LYS:NZ	2:B:71:SER:O	2.39	0.50
2:B:562:LYS:HB3	2:B:563:PRO:HD3	1.99	0.44
1:A:562[A]:LYS:HB3	1:A:563:PRO:HD3	2.03	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	658/726 (91%)	640 (97%)	18 (3%)	0	100	100
2	B	645/726 (89%)	622 (96%)	23 (4%)	0	100	100
All	All	1303/1452 (90%)	1262 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	590/639 (92%)	572 (97%)	18 (3%)	40	43
2	B	578/639 (90%)	561 (97%)	17 (3%)	42	46
All	All	1168/1278 (91%)	1133 (97%)	35 (3%)	42	44

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	52	LYS
1	A	88	LYS
1	A	183	LYS
1	A	213	LYS
1	A	292	ASN
1	A	371	THR
1	A	423[A]	MET
1	A	423[B]	MET
1	A	444	GLN
1	A	519	ARG
1	A	594	LYS
1	A	605	LEU
1	A	631	VAL
1	A	659	LEU
1	A	666	LYS
1	A	669	LYS
1	A	715	LYS
2	B	28	ASN
2	B	39	LYS
2	B	48	LYS
2	B	213	LYS
2	B	292	ASN
2	B	364	LYS
2	B	371	THR
2	B	408	ARG
2	B	423[A]	MET
2	B	423[B]	MET
2	B	574	LYS
2	B	581	ASN
2	B	616	ILE
2	B	638	ILE
2	B	659	LEU
2	B	660	GLU
2	B	694	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	645	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	EDO	A	1716	-	3,3,3	0.44	0	2,2,2	0.16	0
3	EDO	B	1716	-	3,3,3	0.46	0	2,2,2	0.11	0
4	XRJ	A	1717	-	19,19,19	0.39	0	23,25,25	1.47	3 (13%)
4	XRJ	B	1717	-	19,19,19	0.69	0	23,25,25	1.75	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	1716	-	-	0/1/1/1	-
3	EDO	B	1716	-	-	0/1/1/1	-
4	XRJ	A	1717	-	-	9/13/33/33	0/1/1/1
4	XRJ	B	1717	-	-	3/13/33/33	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1717	XRJ	C3-C11-C12	-6.39	103.63	112.51
4	A	1717	XRJ	C3-C11-C12	-5.29	105.16	112.51
4	B	1717	XRJ	C4-C5-C6	2.84	107.02	102.45
4	A	1717	XRJ	C18-C6-C5	2.28	117.25	113.44
4	A	1717	XRJ	C1-N2-C6	-2.09	109.76	114.05
4	B	1717	XRJ	C1-N2-C3	2.03	118.22	114.05

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1717	XRJ	C12-C11-C3-C4
4	A	1717	XRJ	C12-C11-C3-N2
4	A	1717	XRJ	O19-C18-C6-C5
4	A	1717	XRJ	O19-C18-C6-N2
4	A	1717	XRJ	C7-C1-N2-C3
4	A	1717	XRJ	C7-C1-N2-C6
4	B	1717	XRJ	N2-C1-C7-C8
4	B	1717	XRJ	C1-C7-C8-C9
4	A	1717	XRJ	C1-C7-C8-C9
4	B	1717	XRJ	C12-C11-C3-C4
4	A	1717	XRJ	C7-C8-C9-C10
4	A	1717	XRJ	N2-C1-C7-C8

There are no ring outliers.

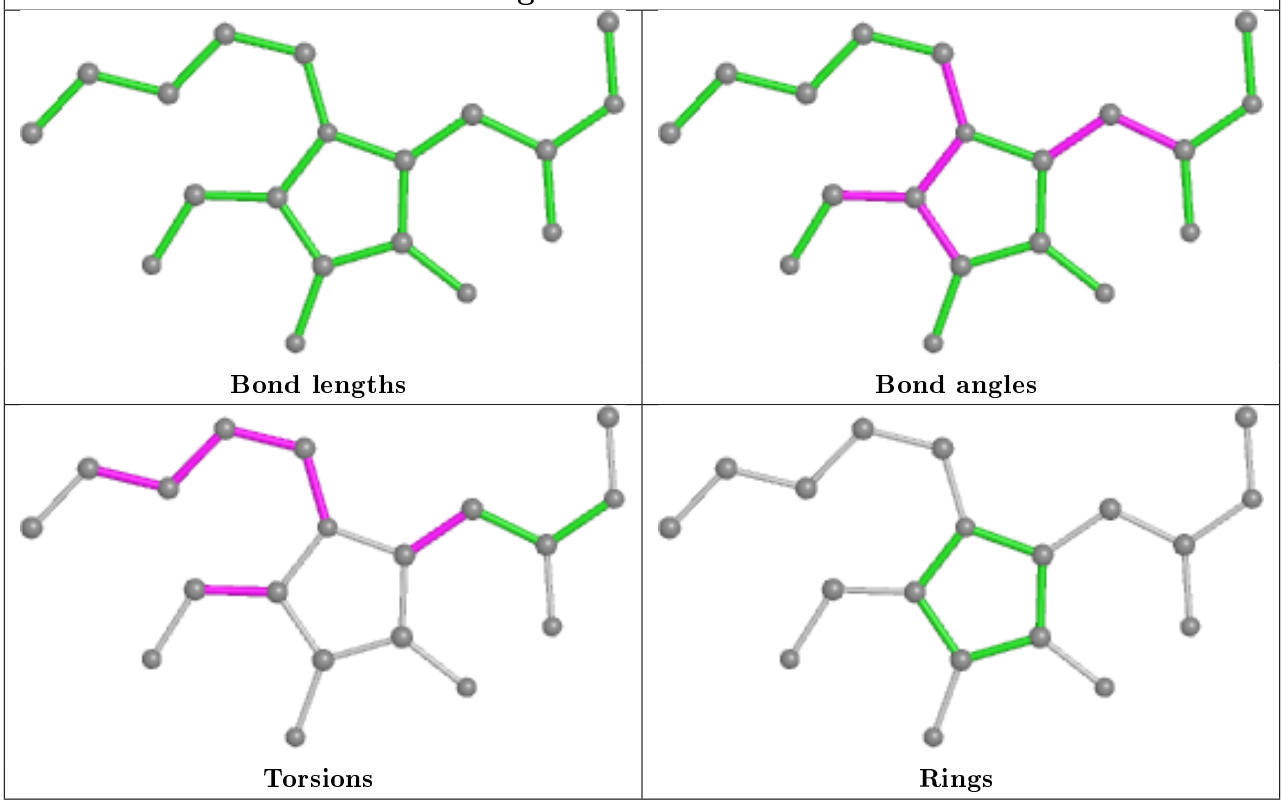
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1717	XRJ	1	0
4	B	1717	XRJ	1	0

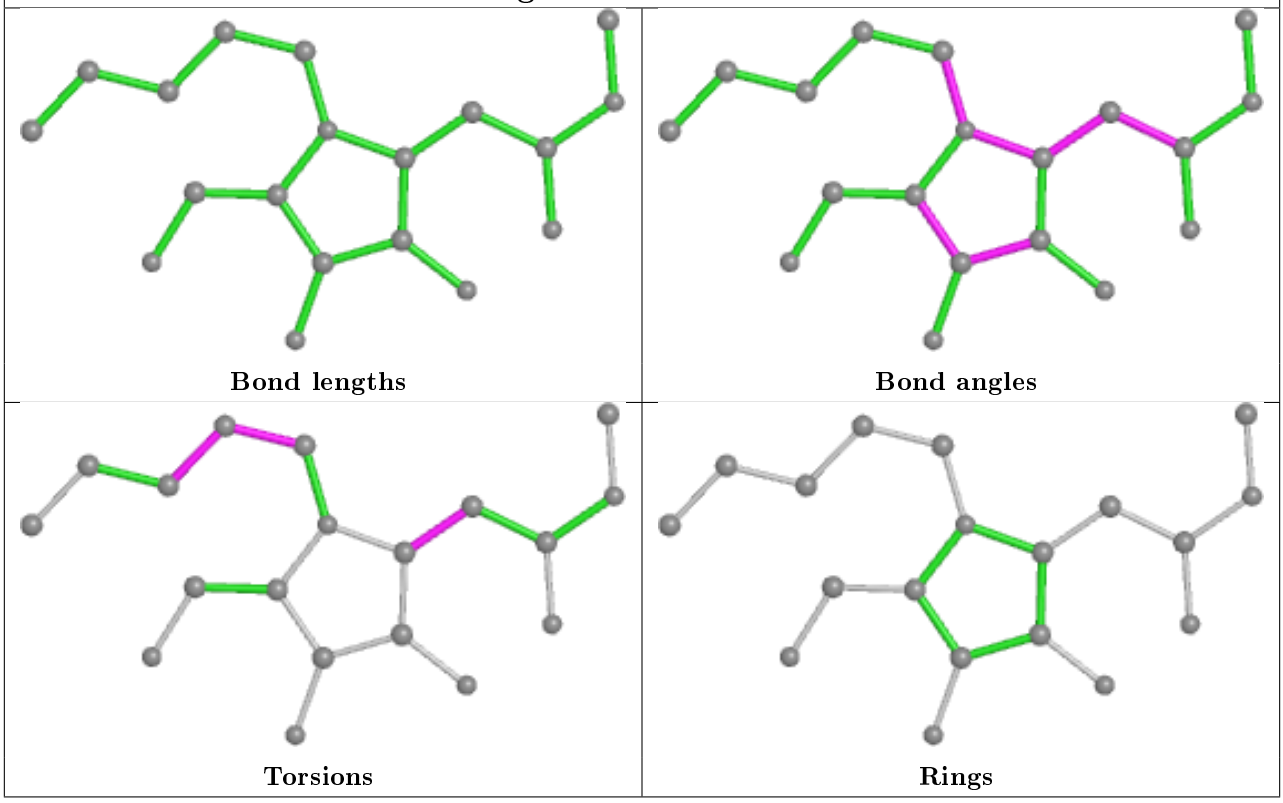
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand XRJ A 1717



Ligand XRJ B 1717



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	663/726 (91%)	0.75	38 (5%)	23	29	40, 59, 117, 150	0
2	B	651/726 (89%)	0.71	60 (9%)	9	11	38, 59, 115, 154	0
All	All	1314/1452 (90%)	0.73	98 (7%)	14	18	38, 59, 117, 154	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	673	LEU	8.5
2	B	659	LEU	8.5
2	B	692	VAL	8.2
2	B	631	VAL	7.5
2	B	646	ILE	7.2
2	B	694	PHE	6.9
2	B	633	ILE	6.3
2	B	688	PRO	6.1
2	B	709	PHE	6.0
1	A	709	PHE	5.9
2	B	605	LEU	5.7
2	B	644	ILE	5.6
2	B	290	ASN	5.5
2	B	680	LEU	5.5
2	B	693	ARG	5.4
2	B	689	VAL	5.3
2	B	632	GLU	5.3
2	B	48	LYS	5.2
2	B	684	LEU	5.1
1	A	21	LEU	4.3
2	B	595	MET	4.3
2	B	53	LYS	4.3
1	A	54	GLY	4.2
2	B	616	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	635	LEU	4.2
1	A	24	VAL	4.0
2	B	519	ARG	4.0
2	B	454	PHE	3.9
1	A	27	LEU	3.9
2	B	661	ILE	3.9
2	B	691	PHE	3.9
1	A	674	LYS	3.8
2	B	685	GLN	3.8
1	A	53	LYS	3.8
1	A	646	ILE	3.8
2	B	606	PRO	3.7
2	B	658	ARG	3.7
1	A	616	ILE	3.7
2	B	638	ILE	3.5
1	A	45	LEU	3.5
1	A	682	ALA	3.5
1	A	658	ARG	3.4
2	B	21	LEU	3.3
2	B	687	ALA	3.3
2	B	286	TRP	3.2
2	B	617	SER	3.2
1	A	49	GLN	3.1
2	B	450	PHE	3.1
1	A	644	ILE	3.1
2	B	614	VAL	3.0
2	B	639	TYR	3.0
1	A	52	LYS	2.9
1	A	65	LYS	2.9
1	A	12	LEU	2.9
1	A	605	LEU	2.9
2	B	443	ILE	2.8
2	B	708	GLN	2.7
1	A	116	LEU	2.7
1	A	423[A]	MET	2.7
2	B	583	HIS	2.7
2	B	712	THR	2.7
1	A	659	LEU	2.7
1	A	25	TYR	2.6
1	A	290	ASN	2.6
1	A	119	VAL	2.6
2	B	711	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	51	SER	2.5
2	B	613	ARG	2.5
2	B	615	LEU	2.5
1	A	51	SER	2.4
2	B	710	VAL	2.4
1	A	668	TRP	2.4
2	B	257	LEU	2.4
2	B	318	ILE	2.4
1	A	74	ILE	2.4
2	B	582	ALA	2.3
1	A	14	VAL	2.3
2	B	611	ALA	2.3
2	B	3	VAL	2.3
2	B	52	LYS	2.2
2	B	645	GLN	2.2
2	B	594	LYS	2.2
1	A	557	ALA	2.2
2	B	88	LYS	2.2
1	A	13	ILE	2.2
2	B	178	LEU	2.2
2	B	607	LEU	2.2
1	A	68	ARG	2.2
1	A	635	LEU	2.1
2	B	47	GLY	2.1
1	A	67	VAL	2.1
1	A	47	GLY	2.1
2	B	513	LEU	2.1
1	A	681	SER	2.0
2	B	330	ILE	2.0
2	B	660	GLU	2.0
1	A	556	THR	2.0
1	A	85	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

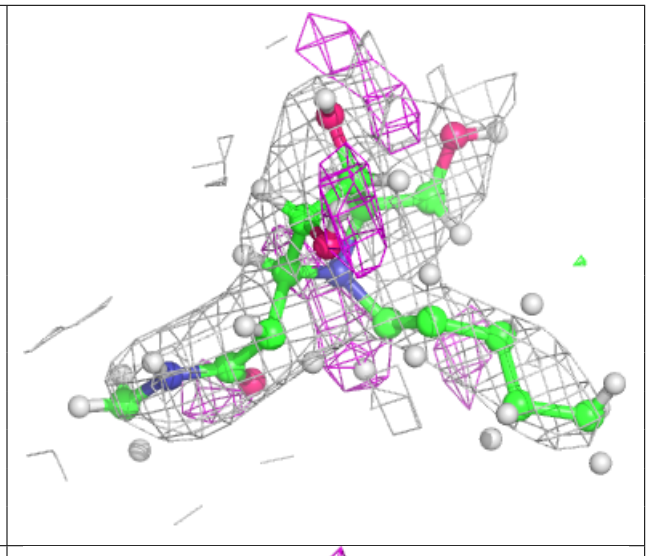
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

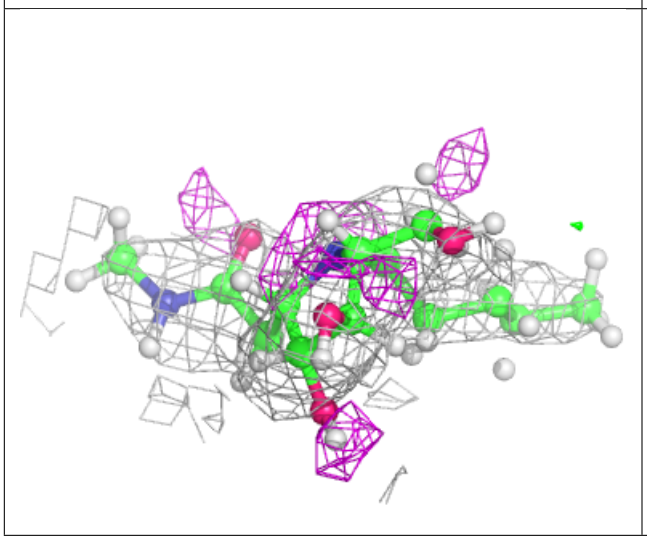
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	XRJ	B	1717	19/19	0.87	0.35	68,81,89,95	0
3	EDO	B	1716	4/4	0.88	0.27	53,64,68,68	0
4	XRJ	A	1717	19/19	0.91	0.27	60,79,92,101	0
3	EDO	A	1716	4/4	0.95	0.15	48,58,62,62	0
5	CA	B	1715	1/1	0.99	0.16	49,49,49,49	0

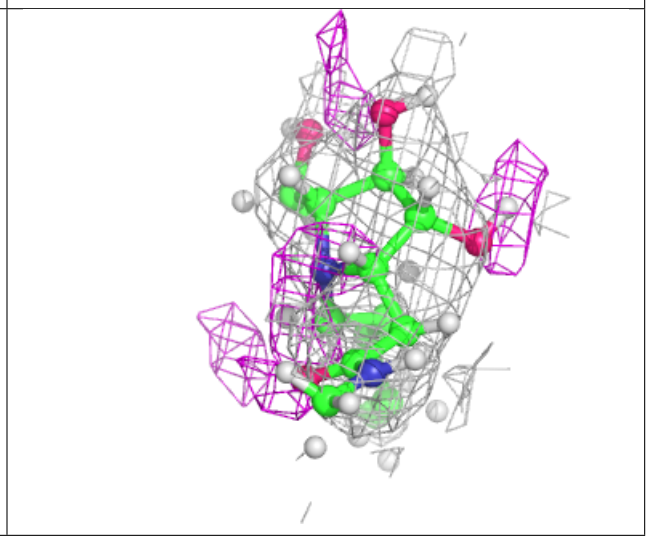
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XRJ B 1717:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

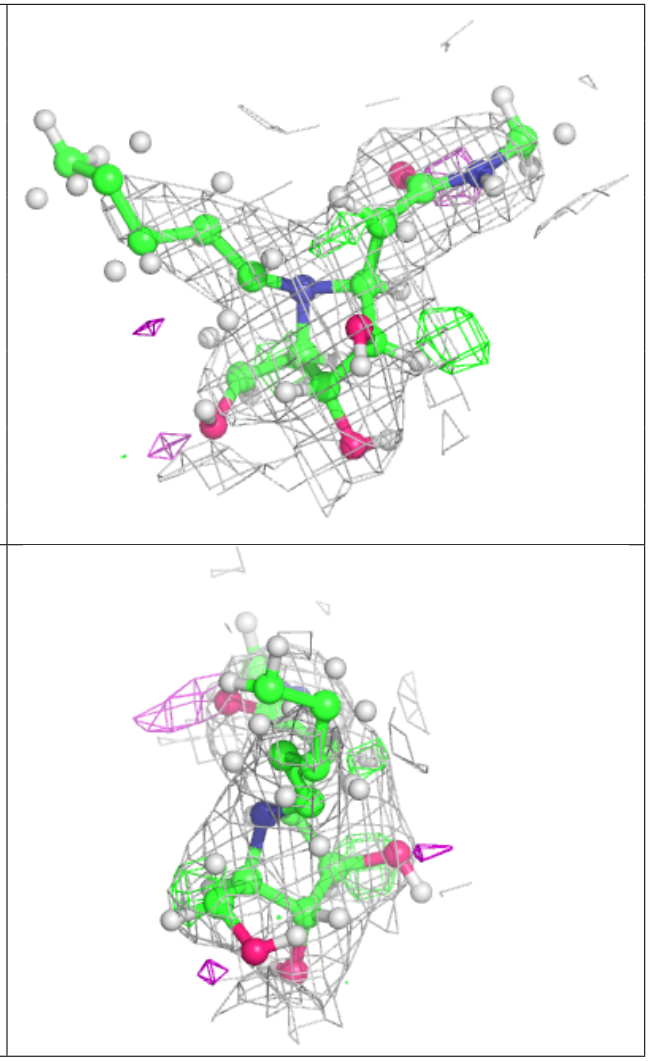






Electron density around XRJ A 1717:

$2mF_o$-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.