Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 12:13 PM EDT

PDB ID	:	6JTT
Title	:	MHETase in complex with BHET
Authors	:	Sagong, H.-Y.; Seo, H.; Kim, K.-J.
Deposited on	:	2019-04-12
Resolution	:	2.51 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

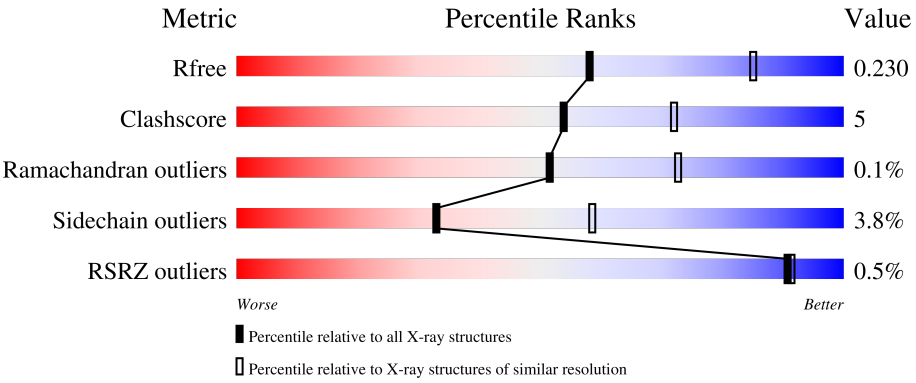
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	621	% 82% 8% • 10%
1	B	621	78% 10% • 10%
1	C	621	81% 8% • 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12951 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 Mono(2-hydroxyethyl) terephthalate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	1	0
			4143	2597	728	790	28			
1	B	558	Total	C	N	O	S	0	1	0
			4132	2592	725	787	28			
1	C	557	Total	C	N	O	S	0	1	0
			4127	2589	724	786	28			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP A0A0K8P8E7
A	-8	MET	-	expression tag	UNP A0A0K8P8E7
A	-7	ILE	-	expression tag	UNP A0A0K8P8E7
A	-6	THR	-	expression tag	UNP A0A0K8P8E7
A	-5	LEU	-	expression tag	UNP A0A0K8P8E7
A	-4	ARG	-	expression tag	UNP A0A0K8P8E7
A	-3	LYS	-	expression tag	UNP A0A0K8P8E7
A	-2	LEU	-	expression tag	UNP A0A0K8P8E7
A	-1	PRO	-	expression tag	UNP A0A0K8P8E7
A	0	LEU	-	expression tag	UNP A0A0K8P8E7
A	1	ALA	-	expression tag	UNP A0A0K8P8E7
A	2	VAL	-	expression tag	UNP A0A0K8P8E7
A	3	ALA	-	expression tag	UNP A0A0K8P8E7
A	4	VAL	-	expression tag	UNP A0A0K8P8E7
A	5	ALA	-	expression tag	UNP A0A0K8P8E7
A	6	ALA	-	expression tag	UNP A0A0K8P8E7
A	7	GLY	-	expression tag	UNP A0A0K8P8E7
A	8	VAL	-	expression tag	UNP A0A0K8P8E7
A	9	MET	-	expression tag	UNP A0A0K8P8E7
A	10	SER	-	expression tag	UNP A0A0K8P8E7
A	11	ALA	-	expression tag	UNP A0A0K8P8E7
A	12	GLN	-	expression tag	UNP A0A0K8P8E7
A	13	ALA	-	expression tag	UNP A0A0K8P8E7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	expression tag	UNP A0A0K8P8E7
A	15	ALA	-	expression tag	UNP A0A0K8P8E7
A	16	MET	-	expression tag	UNP A0A0K8P8E7
A	604	LEU	-	expression tag	UNP A0A0K8P8E7
A	605	GLU	-	expression tag	UNP A0A0K8P8E7
A	606	HIS	-	expression tag	UNP A0A0K8P8E7
A	607	HIS	-	expression tag	UNP A0A0K8P8E7
A	608	HIS	-	expression tag	UNP A0A0K8P8E7
A	609	HIS	-	expression tag	UNP A0A0K8P8E7
A	610	HIS	-	expression tag	UNP A0A0K8P8E7
A	611	HIS	-	expression tag	UNP A0A0K8P8E7
B	-9	MET	-	initiating methionine	UNP A0A0K8P8E7
B	-8	MET	-	expression tag	UNP A0A0K8P8E7
B	-7	ILE	-	expression tag	UNP A0A0K8P8E7
B	-6	THR	-	expression tag	UNP A0A0K8P8E7
B	-5	LEU	-	expression tag	UNP A0A0K8P8E7
B	-4	ARG	-	expression tag	UNP A0A0K8P8E7
B	-3	LYS	-	expression tag	UNP A0A0K8P8E7
B	-2	LEU	-	expression tag	UNP A0A0K8P8E7
B	-1	PRO	-	expression tag	UNP A0A0K8P8E7
B	0	LEU	-	expression tag	UNP A0A0K8P8E7
B	1	ALA	-	expression tag	UNP A0A0K8P8E7
B	2	VAL	-	expression tag	UNP A0A0K8P8E7
B	3	ALA	-	expression tag	UNP A0A0K8P8E7
B	4	VAL	-	expression tag	UNP A0A0K8P8E7
B	5	ALA	-	expression tag	UNP A0A0K8P8E7
B	6	ALA	-	expression tag	UNP A0A0K8P8E7
B	7	GLY	-	expression tag	UNP A0A0K8P8E7
B	8	VAL	-	expression tag	UNP A0A0K8P8E7
B	9	MET	-	expression tag	UNP A0A0K8P8E7
B	10	SER	-	expression tag	UNP A0A0K8P8E7
B	11	ALA	-	expression tag	UNP A0A0K8P8E7
B	12	GLN	-	expression tag	UNP A0A0K8P8E7
B	13	ALA	-	expression tag	UNP A0A0K8P8E7
B	14	MET	-	expression tag	UNP A0A0K8P8E7
B	15	ALA	-	expression tag	UNP A0A0K8P8E7
B	16	MET	-	expression tag	UNP A0A0K8P8E7
B	604	LEU	-	expression tag	UNP A0A0K8P8E7
B	605	GLU	-	expression tag	UNP A0A0K8P8E7
B	606	HIS	-	expression tag	UNP A0A0K8P8E7
B	607	HIS	-	expression tag	UNP A0A0K8P8E7
B	608	HIS	-	expression tag	UNP A0A0K8P8E7

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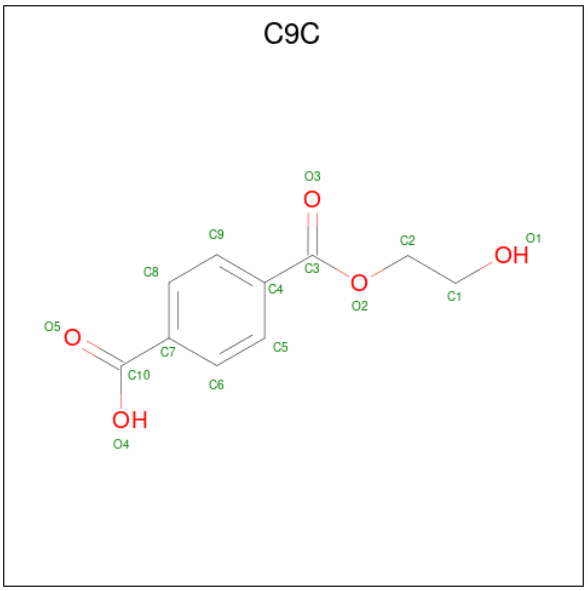
Chain	Residue	Modelled	Actual	Comment	Reference
B	609	HIS	-	expression tag	UNP A0A0K8P8E7
B	610	HIS	-	expression tag	UNP A0A0K8P8E7
B	611	HIS	-	expression tag	UNP A0A0K8P8E7
C	-9	MET	-	initiating methionine	UNP A0A0K8P8E7
C	-8	MET	-	expression tag	UNP A0A0K8P8E7
C	-7	ILE	-	expression tag	UNP A0A0K8P8E7
C	-6	THR	-	expression tag	UNP A0A0K8P8E7
C	-5	LEU	-	expression tag	UNP A0A0K8P8E7
C	-4	ARG	-	expression tag	UNP A0A0K8P8E7
C	-3	LYS	-	expression tag	UNP A0A0K8P8E7
C	-2	LEU	-	expression tag	UNP A0A0K8P8E7
C	-1	PRO	-	expression tag	UNP A0A0K8P8E7
C	0	LEU	-	expression tag	UNP A0A0K8P8E7
C	1	ALA	-	expression tag	UNP A0A0K8P8E7
C	2	VAL	-	expression tag	UNP A0A0K8P8E7
C	3	ALA	-	expression tag	UNP A0A0K8P8E7
C	4	VAL	-	expression tag	UNP A0A0K8P8E7
C	5	ALA	-	expression tag	UNP A0A0K8P8E7
C	6	ALA	-	expression tag	UNP A0A0K8P8E7
C	7	GLY	-	expression tag	UNP A0A0K8P8E7
C	8	VAL	-	expression tag	UNP A0A0K8P8E7
C	9	MET	-	expression tag	UNP A0A0K8P8E7
C	10	SER	-	expression tag	UNP A0A0K8P8E7
C	11	ALA	-	expression tag	UNP A0A0K8P8E7
C	12	GLN	-	expression tag	UNP A0A0K8P8E7
C	13	ALA	-	expression tag	UNP A0A0K8P8E7
C	14	MET	-	expression tag	UNP A0A0K8P8E7
C	15	ALA	-	expression tag	UNP A0A0K8P8E7
C	16	MET	-	expression tag	UNP A0A0K8P8E7
C	604	LEU	-	expression tag	UNP A0A0K8P8E7
C	605	GLU	-	expression tag	UNP A0A0K8P8E7
C	606	HIS	-	expression tag	UNP A0A0K8P8E7
C	607	HIS	-	expression tag	UNP A0A0K8P8E7
C	608	HIS	-	expression tag	UNP A0A0K8P8E7
C	609	HIS	-	expression tag	UNP A0A0K8P8E7
C	610	HIS	-	expression tag	UNP A0A0K8P8E7
C	611	HIS	-	expression tag	UNP A0A0K8P8E7

- Molecule 2 is 4-(2-hydroxyethyloxycarbonyl)benzoic acid (three-letter code: C9C) (formula: $C_{10}H_{10}O_5$).

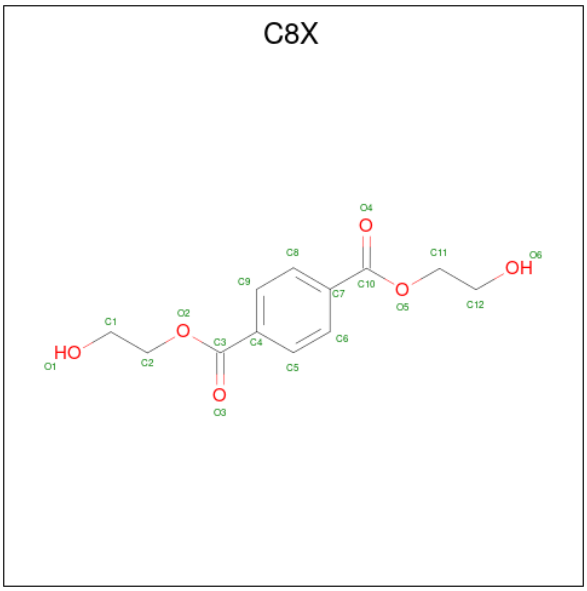


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 14 10 4	0	0
2	C	1	Total C O 14 10 4	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is bis(2-hydroxyethyl) benzene-1,4-dicarboxylate (three-letter code: C8X) (formula: $C_{12}H_{14}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 18 12 6	0	0

- Molecule 5 is water.

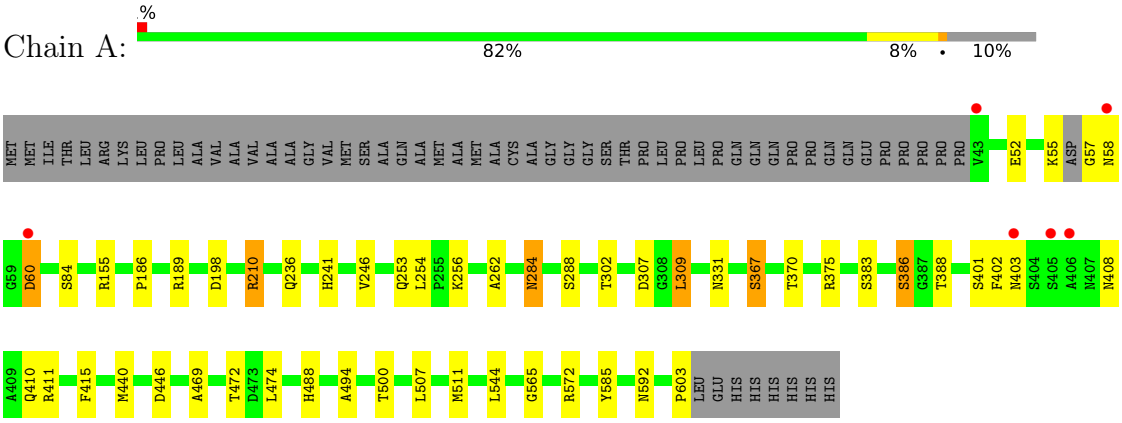
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	146	Total O 146 146	0	0
5	B	174	Total O 174 174	0	0
5	C	180	Total O 180 180	0	0

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.

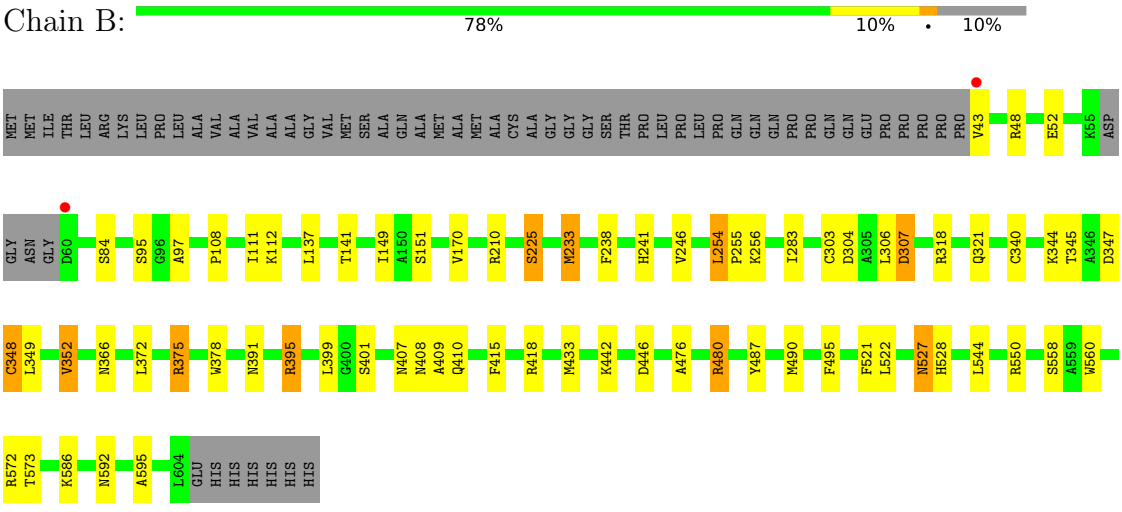
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain A:



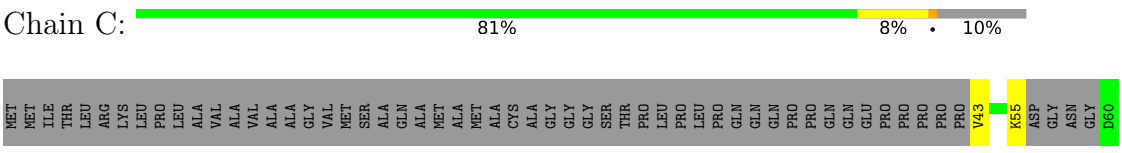
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

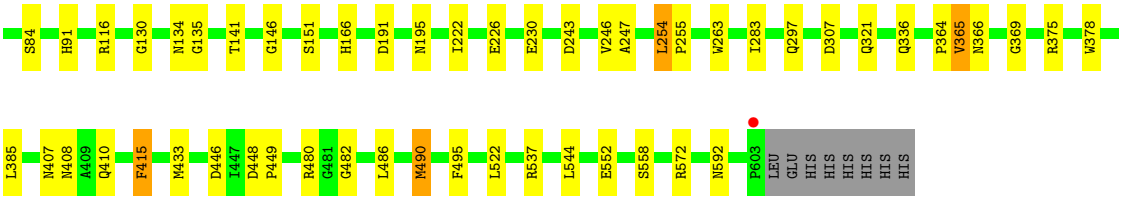
Chain B:



• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain C:




S84
H91
R116
G130
N134
G135
T141
G146
S151
H166
D191
N195
I222
E226
E230
D243
V246
A247
L254
P255
W263
I283
Q297
D307
Q321
Q336
P364
V365
N366
G369
R375
W378
L385
N407
M408
A409
Q410
F415
M433
D446
I447
D448
P449
R480
G481
G482
L486
M490
F495
L522
R537
L544
E552
S558
R572
N592
P603
LEU
GLU
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	215.26Å 173.80Å 106.67Å 90.00° 119.51° 90.00°	Depositor
Resolution (Å)	33.21 – 2.51 33.19 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.9 (33.21-2.51) 97.9 (33.19-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.93 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.190 , 0.226 0.196 , 0.230	Depositor DCC
R_{free} test set	5549 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 27.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12951	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C8X, CA, C9C

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	0.75	0/4251	0.91	1/5787 (0.0%)
1	B	0.76	0/4240	0.96	6/5773 (0.1%)
1	C	0.74	0/4235	0.92	2/5766 (0.0%)
All	All	0.75	0/12726	0.93	9/17326 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	307	ASP	CB-CA-C	-9.30	91.81	110.40
1	C	480	ARG	CB-CA-C	-8.11	94.18	110.40
1	B	550	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	480	ARG	CB-CA-C	-6.53	97.35	110.40
1	C	490	MET	CG-SD-CE	-6.22	90.24	100.20
1	B	550	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	318	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	395	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	155	ARG	NE-CZ-NH2	-5.13	117.74	120.30

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	4143	0	3931	38	0
1	B	4132	0	3922	58	0
1	C	4127	0	3919	36	0
2	A	14	0	0	1	0
2	C	14	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	B	18	0	0	3	0
5	A	146	0	0	0	0
5	B	174	0	0	3	0
5	C	180	0	0	1	0
All	All	12951	0	11772	129	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 (129) 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:284:ASN:H	1:A:284:ASN:HD22	1.07	0.96
1:B:401:SER:H	1:B:408:ASN:HD21	1.02	0.96
1:A:411:ARG:NH2	1:A:494:ALA:O	2.09	0.85
1:B:391:ASN:HD21	1:B:527:ASN:HD21	1.24	0.84
1:C:572:ARG:HH21	1:C:592:ASN:HD21	1.26	0.83
1:A:474:LEU:HB2	1:A:511:MET:HE3	1.62	0.82
1:C:572:ARG:HE	1:C:592:ASN:HD22	1.24	0.81
1:B:410:GLN:OE1	1:B:415[B]:PHE:CD2	2.35	0.80
1:B:283:ILE:H	1:B:407:ASN:HD21	1.32	0.77
1:B:572:ARG:HE	1:B:592:ASN:HD22	1.33	0.77
1:C:490:MET:HE3	1:C:522:LEU:HB3	1.66	0.76
1:C:321:GLN:HE22	1:C:378:TRP:H	1.30	0.76
1:C:91:HIS:HE1	1:C:116:ARG:HH11	1.33	0.76
1:A:401:SER:H	1:A:408:ASN:HD21	1.34	0.75
1:A:474:LEU:H	1:A:511:MET:HE1	1.52	0.74
1:B:490:MET:CE	1:B:522:LEU:HD13	2.17	0.74
1:B:401:SER:N	1:B:408:ASN:HD21	1.84	0.73
1:A:60:ASP:N	1:A:60:ASP:OD1	2.21	0.73
1:B:572:ARG:HH21	1:B:592:ASN:HD21	1.37	0.72
1:A:284:ASN:H	1:A:284:ASN:ND2	1.85	0.72
1:C:490:MET:HE1	1:C:522:LEU:HD22	1.71	0.72
1:A:507:LEU:HD11	1:A:511:MET:HE3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:MET:HE2	1:B:522:LEU:HD22	1.75	0.69
1:A:474:LEU:HB2	1:A:511:MET:CE	2.22	0.68
1:A:262:ALA:HB2	1:A:440:MET:HE3	1.76	0.68
1:B:210:ARG:HG2	1:B:210:ARG:HH11	1.59	0.67
1:B:307:ASP:OD1	5:B:801:HOH:O	2.13	0.67
1:B:321:GLN:HE22	1:B:378:TRP:H	1.43	0.67
1:C:572:ARG:HE	1:C:592:ASN:ND2	1.93	0.66
1:A:262:ALA:HB2	1:A:440:MET:CE	2.26	0.66
1:C:410:GLN:NE2	1:C:415[A]:PHE:CD2	2.59	0.65
1:A:284:ASN:HD22	1:A:284:ASN:N	1.87	0.65
1:B:345:THR:HG22	1:B:347:ASP:H	1.62	0.64
1:C:91:HIS:CE1	1:C:116:ARG:HH11	2.13	0.64
1:C:490:MET:CE	1:C:522:LEU:HB3	2.26	0.64
1:C:246:VAL:HG23	1:C:544:LEU:HD22	1.80	0.64
1:C:283:ILE:H	1:C:407:ASN:HD21	1.46	0.63
1:B:225:SER:HG	1:B:528:HIS:CE1	2.16	0.62
1:A:246:VAL:HG23	1:A:544:LEU:HD22	1.81	0.61
1:B:233:MET:HE3	1:B:238:PHE:CE2	2.35	0.61
1:C:572:ARG:HH21	1:C:592:ASN:ND2	1.99	0.61
1:B:572:ARG:HE	1:B:592:ASN:ND2	2.00	0.60
1:B:246:VAL:HG23	1:B:544:LEU:HD22	1.85	0.59
1:C:490:MET:CE	1:C:522:LEU:HD22	2.32	0.59
1:B:348:CYS:SG	1:B:349:LEU:N	2.75	0.57
1:B:233:MET:CE	1:B:238:PHE:CD2	2.89	0.56
1:C:247:ALA:HB3	1:C:486:LEU:HD23	1.87	0.55
1:B:254:LEU:HD13	1:B:495:PHE:CE1	2.42	0.54
1:B:344:LYS:H	1:C:297:GLN:HE22	1.55	0.54
1:A:262:ALA:CB	1:A:440:MET:HE3	2.37	0.54
1:B:141:THR:O	1:B:151:SER:HB2	2.07	0.54
1:B:225:SER:OG	1:B:528:HIS:NE2	2.28	0.54
1:B:233:MET:HE1	1:B:238:PHE:HD2	1.73	0.54
1:C:321:GLN:NE2	1:C:378:TRP:H	2.03	0.53
1:B:233:MET:HE3	1:B:238:PHE:CD2	2.43	0.53
1:A:309:LEU:HD12	1:A:585:TYR:HB2	1.91	0.53
1:A:572:ARG:HE	1:A:592:ASN:ND2	2.06	0.53
1:A:411:ARG:NH1	2:A:701:C9C:O3	2.42	0.53
1:A:288:SER:HA	1:A:402:PHE:CD2	2.44	0.52
1:B:586:LYS:HE3	1:B:595:ALA:O	2.08	0.52
1:A:415[B]:PHE:C	1:A:415[B]:PHE:CD1	2.83	0.52
1:B:410:GLN:OE1	1:B:415[B]:PHE:CE2	2.62	0.52
1:A:472:THR:O	1:A:511:MET:HE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:OD1	1:A:241:HIS:HE1	1.93	0.51
1:B:375:ARG:HD2	5:B:962:HOH:O	2.10	0.51
1:A:253:GLN:HE22	1:A:256:LYS:NZ	2.09	0.50
1:A:331:ASN:C	1:A:331:ASN:OD1	2.49	0.50
1:A:386:SER:OG	1:A:565:GLY:HA3	2.12	0.50
1:B:97:ALA:HA	1:B:111:ILE:O	2.12	0.50
1:B:352:VAL:CG2	1:C:385:LEU:HD23	2.42	0.50
1:B:366:ASN:HB2	1:B:446:ASP:OD1	2.13	0.49
1:C:254:LEU:HD13	1:C:495:PHE:HE1	1.77	0.49
1:B:283:ILE:H	1:B:407:ASN:ND2	2.08	0.48
1:B:225:SER:HB3	4:B:701:C8X:O3	2.13	0.48
1:B:112:LYS:HB3	1:B:137:LEU:HD22	1.94	0.48
1:A:262:ALA:CA	1:A:440:MET:HE3	2.43	0.48
1:B:233:MET:HE2	1:B:233:MET:C	2.35	0.48
1:B:233:MET:CE	1:B:238:PHE:HD2	2.27	0.47
1:B:490:MET:HE1	1:B:522:LEU:HD13	1.96	0.47
1:A:236:GLN:HE22	1:A:469:ALA:C	2.18	0.47
1:A:572:ARG:HE	1:A:592:ASN:HD22	1.62	0.47
1:B:352:VAL:HG21	1:C:385:LEU:HD23	1.97	0.46
1:B:528:HIS:HE1	4:B:701:C8X:O2	1.98	0.46
1:A:55:LYS:O	1:A:57:GLY:N	2.48	0.46
1:A:410:GLN:NE2	1:A:415[B]:PHE:CE2	2.83	0.46
1:B:233:MET:HE2	1:B:233:MET:O	2.15	0.46
1:A:367:SER:OG	1:A:446:ASP:OD2	2.33	0.46
1:C:408:ASN:HB3	5:C:844:HOH:O	2.15	0.46
1:A:186:PRO:O	1:A:189:ARG:HB2	2.16	0.46
1:C:243:ASP:O	1:C:482:GLY:HA2	2.16	0.46
1:B:572:ARG:HH21	1:B:592:ASN:ND2	2.08	0.46
1:B:418:ARG:NH1	1:B:433:MET:HE2	2.30	0.45
1:C:135:GLY:HA2	1:C:166:HIS:O	2.16	0.45
1:C:254:LEU:HD13	1:C:495:PHE:CE1	2.50	0.45
1:A:210:ARG:HA	1:A:210:ARG:HD3	1.86	0.45
1:B:254:LEU:N	1:B:255:PRO:CD	2.80	0.45
1:B:399:LEU:C	1:B:409:ALA:HB2	2.37	0.45
1:B:573:THR:HG23	5:B:887:HOH:O	2.15	0.45
1:B:304:ASP:C	1:B:304:ASP:OD1	2.56	0.44
1:B:256:LYS:HD3	1:B:372:LEU:O	2.18	0.44
1:B:48:ARG:HH11	1:B:48:ARG:HB2	1.83	0.43
1:B:487:TYR:HA	1:B:521:PHE:O	2.19	0.43
1:B:303:CYS:HA	1:B:306:LEU:HD12	2.01	0.43
1:C:222:ILE:HG12	1:C:246:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ALA:O	1:B:480:ARG:HG3	2.19	0.42
1:C:130:GLY:HA3	1:C:134:ASN:OD1	2.19	0.42
1:C:191:ASP:HA	1:C:195:ASN:HB3	2.01	0.42
1:B:254:LEU:HD13	1:B:495:PHE:HE1	1.82	0.42
1:A:507:LEU:HD11	1:A:511:MET:CE	2.44	0.42
1:C:226:GLU:OE2	1:C:230:GLU:OE2	2.37	0.42
1:C:366:ASN:HB2	1:C:446:ASP:OD1	2.19	0.42
1:B:225:SER:OG	4:B:701:C8X:C3	2.68	0.42
1:A:507:LEU:CD1	1:A:511:MET:CE	2.98	0.41
1:B:210:ARG:HH11	1:B:210:ARG:CG	2.31	0.41
1:A:488:HIS:HD2	1:A:500:THR:OG1	2.03	0.41
1:C:448:ASP:N	1:C:449:PRO:CD	2.84	0.41
1:C:263:TRP:CD2	1:C:364:PRO:HA	2.56	0.41
1:C:91:HIS:HE1	1:C:116:ARG:NH1	2.09	0.41
1:B:108:PRO:HG2	1:B:170:VAL:CG1	2.50	0.41
1:C:146:GLY:O	1:C:537:ARG:HA	2.20	0.41
1:B:108:PRO:HG2	1:B:170:VAL:HG11	2.02	0.41
1:C:365:VAL:HG13	1:C:369:GLY:HA2	2.03	0.41
1:A:572:ARG:NE	1:A:592:ASN:ND2	2.69	0.41
1:A:198:ASP:OD1	1:A:241:HIS:CE1	2.73	0.40
1:A:572:ARG:NE	1:A:592:ASN:HD22	2.19	0.40
1:B:560:TRP:HB3	1:B:573:THR:HG22	2.02	0.40
1:C:141:THR:O	1:C:151:SER:HB2	2.21	0.40
1:C:254:LEU:N	1:C:255:PRO:CD	2.84	0.40
1:B:391:ASN:ND2	1:B:527:ASN:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	557/621 (90%)	530 (95%)	27 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	555/621 (89%)	533 (96%)	21 (4%)	1 (0%)	47 68
1	C	554/621 (89%)	532 (96%)	22 (4%)	0	100 100
All	All	1666/1863 (89%)	1595 (96%)	70 (4%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	527	ASN

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	407/454 (90%)	389 (96%)	18 (4%)	28 52
1	B	406/454 (89%)	390 (96%)	16 (4%)	32 57
1	C	406/454 (89%)	393 (97%)	13 (3%)	39 65
All	All	1219/1362 (90%)	1172 (96%)	47 (4%)	33 57

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	58	ASN
1	A	60	ASP
1	A	84	SER
1	A	210	ARG
1	A	254	LEU
1	A	284	ASN
1	A	302	THR
1	A	307	ASP
1	A	309	LEU
1	A	367	SER
1	A	370	THR
1	A	375	ARG

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Mol	Chain	Res	Type
1	A	383	SER
1	A	386	SER
1	A	388	THR
1	A	403	ASN
1	A	603	PRO
1	B	43	VAL
1	B	52	GLU
1	B	84	SER
1	B	95	SER
1	B	149	ILE
1	B	225	SER
1	B	233	MET
1	B	241	HIS
1	B	254	LEU
1	B	340	CYS
1	B	348	CYS
1	B	352	VAL
1	B	375	ARG
1	B	395	ARG
1	B	442	LYS
1	B	558	SER
1	C	43	VAL
1	C	55	LYS
1	C	84	SER
1	C	254	LEU
1	C	307	ASP
1	C	336	GLN
1	C	365	VAL
1	C	375	ARG
1	C	415[A]	PHE
1	C	415[B]	PHE
1	C	433	MET
1	C	552	GLU
1	C	558	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	236	GLN
1	A	241	HIS
1	A	253	GLN

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Mol	Chain	Res	Type
1	A	284	ASN
1	A	336	GLN
1	A	339	GLN
1	A	408	ASN
1	A	435	GLN
1	A	488	HIS
1	A	592	ASN
1	B	148	GLN
1	B	187	GLN
1	B	253	GLN
1	B	321	GLN
1	B	407	ASN
1	B	408	ASN
1	B	527	ASN
1	B	581	GLN
1	B	592	ASN
1	C	91	HIS
1	C	253	GLN
1	C	297	GLN
1	C	321	GLN
1	C	407	ASN
1	C	592	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
2	C9C	C	701	-	14,14,15	2.55	5 (35%)	17,17,19	3.23	7 (41%)
2	C9C	A	701	-	14,14,15	2.20	4 (28%)	17,17,19	3.06	3 (17%)
4	C8X	B	701	-	18,18,18	2.35	3 (16%)	22,22,22	3.66	8 (36%)

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	C9C	C	701	-	-	1/10/10/12	0/1/1/1
2	C9C	A	701	-	-	5/10/10/12	0/1/1/1
4	C8X	B	701	-	-	9/16/16/16	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	C9C	O2-C3	7.16	1.51	1.33
4	B	701	C8X	O2-C3	6.56	1.50	1.33
2	A	701	C9C	O2-C3	6.30	1.49	1.33
4	B	701	C8X	O5-C10	6.25	1.49	1.33
2	C	701	C9C	O4-C10	-3.43	1.27	1.41
2	C	701	C9C	O2-C2	3.23	1.55	1.45
2	A	701	C9C	C7-C10	2.41	1.54	1.47
2	A	701	C9C	O1-C1	2.37	1.54	1.42
2	C	701	C9C	O1-C1	2.15	1.53	1.42
2	A	701	C9C	O5-C10	2.13	1.28	1.21
2	C	701	C9C	C2-C1	2.07	1.60	1.49
4	B	701	C8X	O6-C12	2.05	1.52	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	C9C	O2-C3-C4	9.48	128.64	112.14
2	A	701	C9C	O2-C3-C4	9.36	128.43	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	701	C8X	O5-C10-C7	8.43	126.81	112.14
4	B	701	C8X	C11-O5-C10	7.25	131.72	116.43
4	B	701	C8X	O2-C3-C4	7.15	124.60	112.14
2	A	701	C9C	O2-C2-C1	6.46	128.40	108.30
4	B	701	C8X	C2-O2-C3	6.45	130.02	116.43
4	B	701	C8X	O5-C11-C12	6.17	127.49	108.30
2	C	701	C9C	O2-C2-C1	6.07	127.18	108.30
2	A	701	C9C	O2-C3-O3	-3.83	115.89	123.67
4	B	701	C8X	O2-C3-O3	-3.31	116.96	123.67
2	C	701	C9C	O1-C1-C2	3.29	130.90	111.81
4	B	701	C8X	O5-C10-O4	-3.18	117.22	123.67
2	C	701	C9C	O3-C3-C4	-2.80	112.92	122.09
2	C	701	C9C	C2-O2-C3	2.73	122.19	116.43
2	C	701	C9C	C9-C4-C3	2.65	126.39	120.40
2	C	701	C9C	O2-C3-O3	-2.61	118.38	123.67
4	B	701	C8X	O2-C2-C1	2.22	115.21	108.30

There are no chirality outliers.

All (15) torsion outliers are listed below:

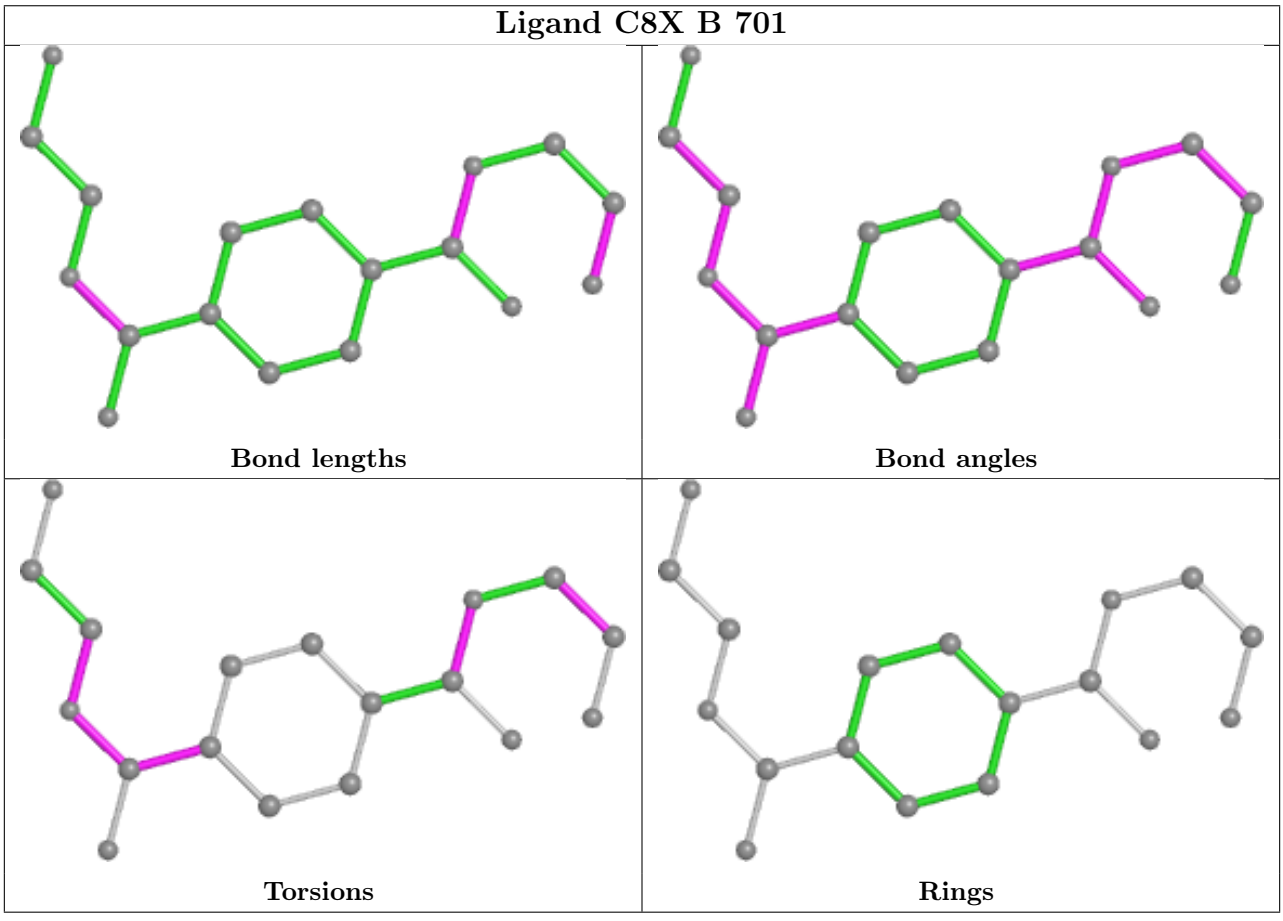
Mol	Chain	Res	Type	Atoms
2	A	701	C9C	O5-C10-C7-C8
4	B	701	C8X	C1-C2-O2-C3
4	B	701	C8X	C4-C3-O2-C2
4	B	701	C8X	O3-C3-O2-C2
2	A	701	C9C	C4-C3-O2-C2
4	B	701	C8X	C7-C10-O5-C11
2	A	701	C9C	O3-C3-O2-C2
4	B	701	C8X	O4-C10-O5-C11
2	A	701	C9C	O5-C10-C7-C6
2	C	701	C9C	O1-C1-C2-O2
4	B	701	C8X	O5-C11-C12-O6
4	B	701	C8X	O2-C3-C4-C5
4	B	701	C8X	O2-C3-C4-C9
2	A	701	C9C	O1-C1-C2-O2
4	B	701	C8X	O3-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	C9C	1	0
4	B	701	C8X	3	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.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	560/621 (90%)	-0.25	6 (1%)	80	82	17, 30, 54, 95	0
1	B	558/621 (89%)	-0.50	2 (0%)	92	93	14, 25, 42, 63	0
1	C	557/621 (89%)	-0.47	1 (0%)	95	95	14, 25, 43, 67	0
All	All	1675/1863 (89%)	-0.41	9 (0%)	91	91	14, 26, 48, 95	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	ASN	6.2
1	C	603	PRO	2.7
1	A	60	ASP	2.7
1	A	403	ASN	2.4
1	B	60	ASP	2.2
1	A	406	ALA	2.2
1	A	43	VAL	2.1
1	B	43	VAL	2.1
1	A	405	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

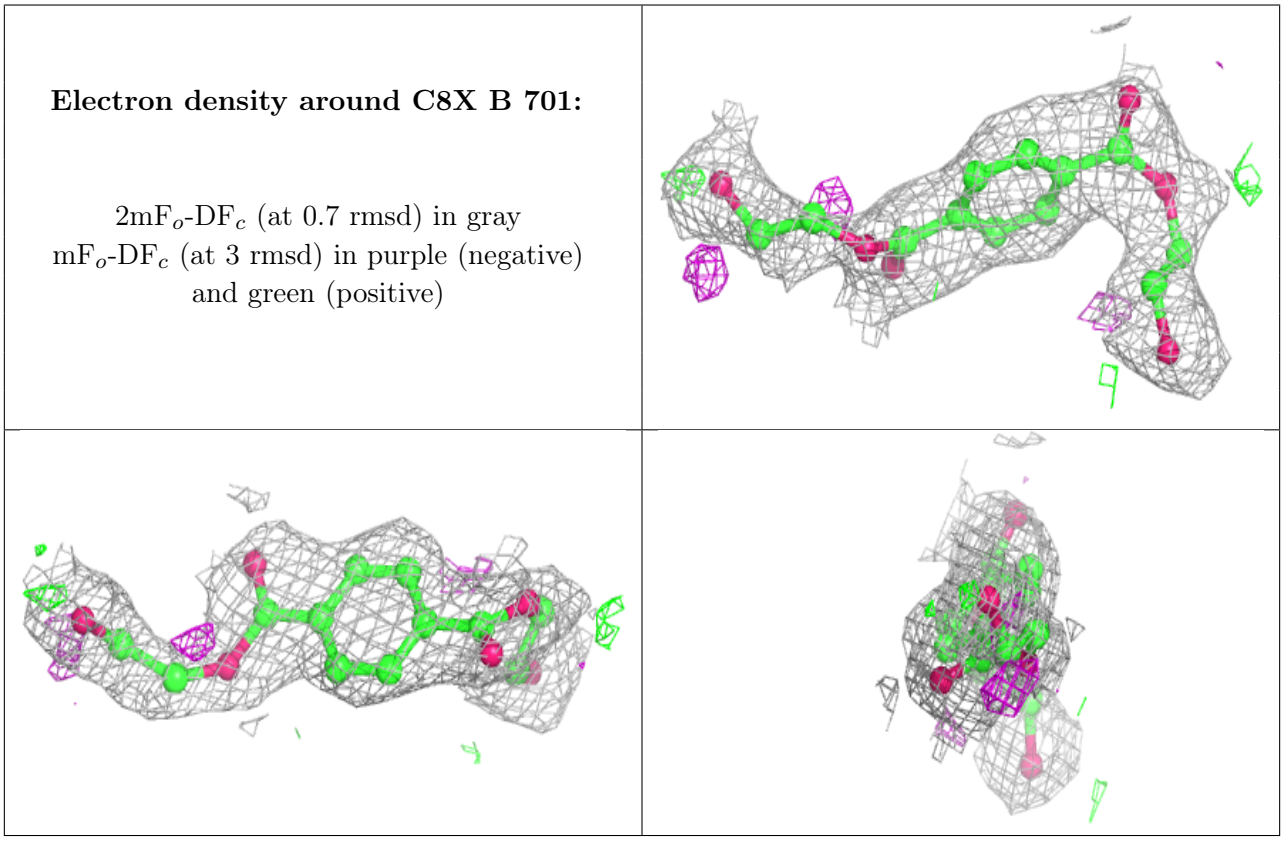
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	C9C	A	701	14/15	0.86	0.26	40,51,61,64	0
2	C9C	C	701	14/15	0.92	0.17	29,39,42,45	0
4	C8X	B	701	18/18	0.93	0.18	31,47,54,57	0
3	CA	B	702	1/1	0.96	0.05	33,33,33,33	0
3	CA	A	702	1/1	0.96	0.05	43,43,43,43	0
3	CA	C	702	1/1	0.99	0.05	25,25,25,25	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 C8X B 701:

$2mF_o$-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

There are no such residues in this entry.