



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:45 AM UTC

PDB ID : 7PR6 / pdb_00007pr6
Title : Crystal structure of E. coli beta-glucuronidase in complex with covalent inhibitor ME727
Authors : Wu, L.; Armstrong, Z.; Davies, G.J.
Deposited on : 2021-09-20
Resolution : 1.99 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

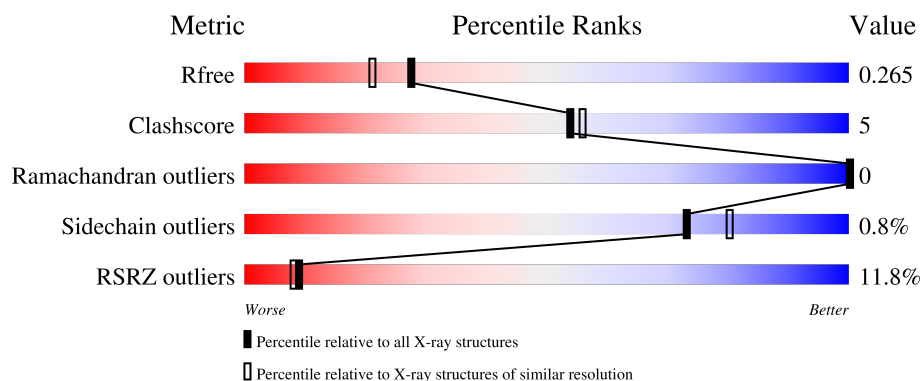
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	AAA	601	4% 84% 15% .
1	BBB	601	20% 87% 11% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 19287 atoms, of which 9218 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 Beta-glucuronidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	599	Total	C	H	N	O	S	134	1	0
			9440	3059	4625	831	902	23			
1	BBB	592	Total	C	H	N	O	S	134	0	0
			9332	3024	4573	821	892	22			

There are 38 discrepancies between the modelled and reference sequences:

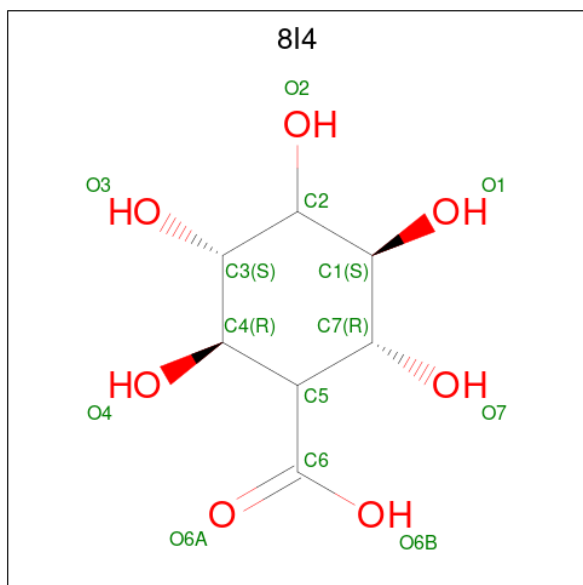
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	SER	-	expression tag	UNP P05804
AAA	0	HIS	-	expression tag	UNP P05804
AAA	1	MET	-	expression tag	UNP P05804
AAA	2	LEU	-	expression tag	UNP P05804
AAA	3	ARG	-	expression tag	UNP P05804
AAA	4	PRO	-	expression tag	UNP P05804
AAA	5	VAL	-	expression tag	UNP P05804
AAA	6	GLU	-	expression tag	UNP P05804
AAA	7	THR	-	expression tag	UNP P05804
AAA	8	PRO	-	expression tag	UNP P05804
AAA	9	THR	-	expression tag	UNP P05804
AAA	10	ARG	-	expression tag	UNP P05804
AAA	11	GLU	-	expression tag	UNP P05804
AAA	12	ILE	-	expression tag	UNP P05804
AAA	13	LYS	-	expression tag	UNP P05804
AAA	14	LYS	-	expression tag	UNP P05804
AAA	15	LEU	-	expression tag	UNP P05804
AAA	16	ASP	-	expression tag	UNP P05804
AAA	17	GLY	-	expression tag	UNP P05804
BBB	-1	SER	-	expression tag	UNP P05804
BBB	0	HIS	-	expression tag	UNP P05804
BBB	1	MET	-	expression tag	UNP P05804
BBB	2	LEU	-	expression tag	UNP P05804
BBB	3	ARG	-	expression tag	UNP P05804
BBB	4	PRO	-	expression tag	UNP P05804

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	5	VAL	-	expression tag	UNP P05804
BBB	6	GLU	-	expression tag	UNP P05804
BBB	7	THR	-	expression tag	UNP P05804
BBB	8	PRO	-	expression tag	UNP P05804
BBB	9	THR	-	expression tag	UNP P05804
BBB	10	ARG	-	expression tag	UNP P05804
BBB	11	GLU	-	expression tag	UNP P05804
BBB	12	ILE	-	expression tag	UNP P05804
BBB	13	LYS	-	expression tag	UNP P05804
BBB	14	LYS	-	expression tag	UNP P05804
BBB	15	LEU	-	expression tag	UNP P05804
BBB	16	ASP	-	expression tag	UNP P05804
BBB	17	GLY	-	expression tag	UNP P05804

- Molecule 2 is (2R,3S,5R,6R)-2,3,4,5,6-pentakis(oxidanyl)cyclohexane-1-carboxylic acid (CCD ID: 8I4) (formula: C₇H₁₂O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	4	0
			23	7	10	6		
2	BBB	1	Total	C	H	O	4	0
			23	7	10	6		

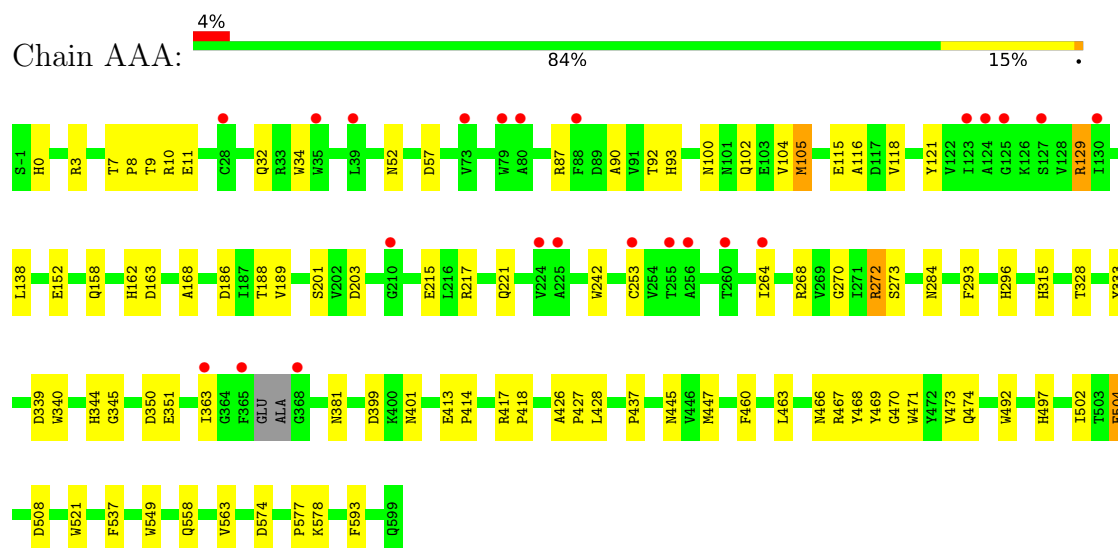
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	321	Total 321	O 321	0	0
3	BBB	148	Total 148	O 148	0	0

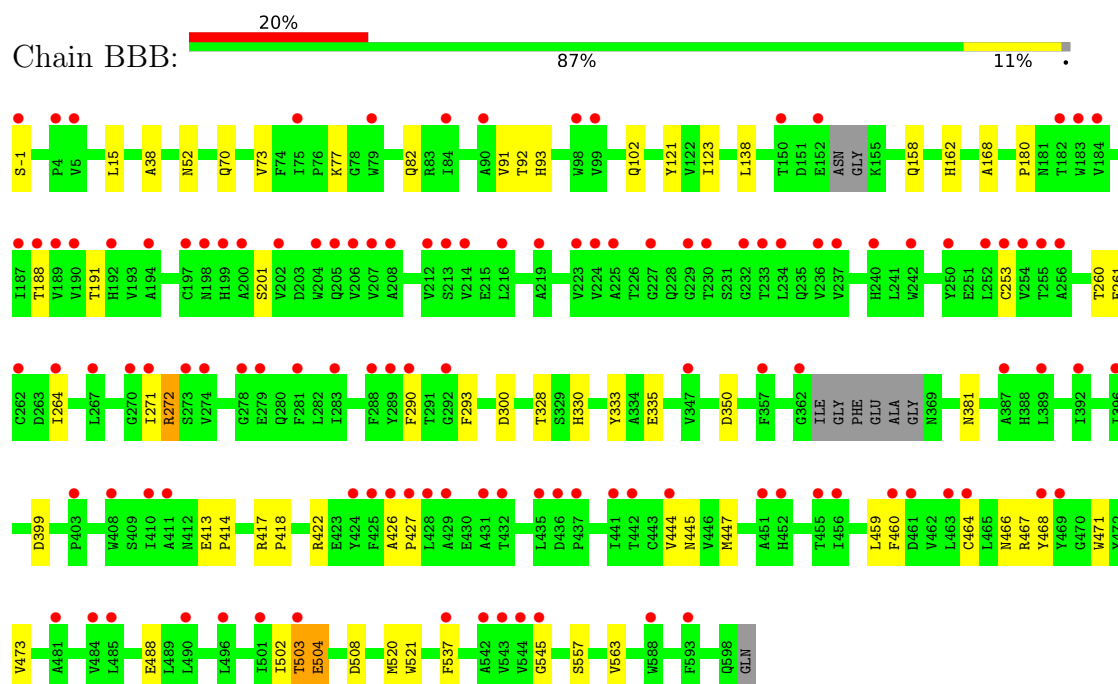
3 Residue-property plots

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: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.80Å 76.58Å 125.74Å 90.00° 125.01° 90.00°	Depositor
Resolution (Å)	47.80 – 1.99 47.80 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.80-1.99) 92.9 (47.80-1.99)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.221 , 0.263 0.226 , 0.265	Depositor DCC
R_{free} test set	4333 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19287	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: 8I4

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	AAA	1.16	10/4944 (0.2%)	1.39	19/6725 (0.3%)
1	BBB	1.11	4/4886 (0.1%)	1.36	9/6647 (0.1%)
All	All	1.13	14/9830 (0.1%)	1.38	28/13372 (0.2%)

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	AAA	0	2
1	BBB	0	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	504	GLU	CD-OE2	10.43	1.45	1.25
1	AAA	504	GLU	CD-OE2	7.16	1.39	1.25
1	AAA	437	PRO	C-O	-6.91	1.15	1.24
1	AAA	296	HIS	CE1-NE2	6.38	1.39	1.32
1	AAA	351	GLU	C-O	6.37	1.31	1.23
1	AAA	152	GLU	C-O	6.33	1.32	1.24
1	AAA	162	HIS	CE1-NE2	6.08	1.38	1.32
1	BBB	91	VAL	C-O	5.70	1.30	1.24
1	AAA	428	LEU	C-O	5.64	1.30	1.24
1	AAA	577	PRO	C-O	-5.49	1.17	1.23
1	AAA	90	ALA	C-O	5.37	1.30	1.24
1	BBB	123	ILE	C-O	5.13	1.29	1.24
1	BBB	300	ASP	C-O	5.11	1.29	1.23
1	AAA	203	ASP	C-O	5.00	1.30	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	503	THR	CB-CA-C	7.27	123.10	110.01
1	BBB	563	VAL	CA-C-O	-6.48	116.99	122.63
1	AAA	129	ARG	NE-CZ-NH2	6.25	124.82	119.20
1	AAA	563	VAL	CA-C-O	-6.25	117.20	122.63
1	BBB	188	THR	CA-CB-OG1	-6.01	100.58	109.60
1	AAA	381	ASN	CA-C-N	5.83	126.41	119.94
1	AAA	381	ASN	C-N-CA	5.83	126.41	119.94
1	AAA	188	THR	CA-CB-OG1	-5.77	100.94	109.60
1	AAA	563	VAL	O-C-N	5.75	126.79	121.96
1	AAA	129	ARG	NE-CZ-NH1	-5.71	115.79	121.50
1	AAA	574	ASP	CA-CB-CG	5.67	118.27	112.60
1	AAA	593	PHE	CA-CB-CG	-5.66	108.14	113.80
1	BBB	460	PHE	CA-C-O	-5.65	115.02	121.68
1	BBB	473	VAL	CA-C-O	-5.58	116.10	121.63
1	AAA	57	ASP	CA-C-N	5.56	127.73	120.28
1	AAA	57	ASP	C-N-CA	5.56	127.73	120.28
1	BBB	381	ASN	CA-C-N	5.37	126.06	119.99
1	BBB	381	ASN	C-N-CA	5.37	126.06	119.99
1	AAA	460	PHE	CA-C-O	-5.28	115.21	121.60
1	AAA	268	ARG	CB-CA-C	5.25	118.41	109.53
1	BBB	563	VAL	O-C-N	5.21	126.34	121.96
1	BBB	335	GLU	CB-CG-CD	5.20	121.43	112.60
1	AAA	473	VAL	CA-C-O	-5.12	116.56	121.63
1	AAA	549	TRP	CA-C-N	5.04	130.78	121.70
1	AAA	549	TRP	C-N-CA	5.04	130.78	121.70
1	AAA	578	LYS	CA-C-O	-5.04	115.86	121.81
1	AAA	270	GLY	CA-C-O	-5.03	116.49	120.81
1	AAA	497	HIS	CA-C-O	-5.01	115.72	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	105	MET	Mainchain
1	AAA	293	PHE	Peptide
1	BBB	293	PHE	Peptide

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	AAA	4815	4625	4603	49	0
1	BBB	4759	4573	4551	43	0
2	AAA	13	10	0	0	0
2	BBB	13	10	0	1	0
3	AAA	321	0	0	3	0
3	BBB	148	0	0	2	1
All	All	10069	9218	9154	91	1

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 (91) 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:AAA:7:THR:HG21	1:AAA:264:ILE:O	1.55	1.05
1:AAA:272:ARG:HA	1:AAA:284:ASN:HD21	1.43	0.81
1:AAA:104:VAL:HG21	1:AAA:118:VAL:HG12	1.63	0.80
1:BBB:467:ARG:NH2	1:BBB:488:GLU:OE1	2.22	0.73
1:AAA:426:ALA:HB3	1:AAA:427:PRO:HD3	1.72	0.71
1:BBB:253:CYS:SG	1:BBB:264:ILE:HG23	2.30	0.71
1:BBB:191:THR:HG21	1:BBB:272:ARG:H	1.55	0.71
1:AAA:253:CYS:SG	1:AAA:264:ILE:HG23	2.33	0.69
1:AAA:7:THR:HG22	1:AAA:9:THR:H	1.59	0.68
1:AAA:32:GLN:HE21	1:AAA:34:TRP:HE1	1.41	0.67
1:BBB:466:ASN:OD1	1:BBB:503:THR:HG23	1.96	0.64
1:BBB:191:THR:CG2	1:BBB:271:ILE:HA	2.27	0.64
1:BBB:426:ALA:HB3	1:BBB:427:PRO:HD3	1.79	0.64
1:BBB:191:THR:CG2	1:BBB:272:ARG:H	2.12	0.63
1:AAA:447[A]:MET:HE2	1:AAA:469:TYR:CZ	2.34	0.63
1:BBB:464:CYS:HB3	1:BBB:503:THR:HG21	1.80	0.62
1:BBB:422:ARG:NH1	1:BBB:459:LEU:HD11	2.16	0.60
1:AAA:502:ILE:HG13	1:AAA:537:PHE:CE1	2.37	0.59
1:BBB:502:ILE:HG13	1:BBB:537:PHE:CE1	2.38	0.58
1:AAA:7:THR:HG23	1:AAA:8:PRO:HD2	1.86	0.58
1:AAA:32:GLN:NE2	1:AAA:34:TRP:HE1	2.01	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:191:THR:HG21	1:BBB:271:ILE:HA	1.85	0.57
1:AAA:445:ASN:HD21	1:AAA:467:ARG:HH22	1.53	0.56
1:BBB:138:LEU:H	1:BBB:158:GLN:HE22	1.54	0.56
1:BBB:330:HIS:HE1	2:BBB:601:8I4:O3	1.89	0.55
1:AAA:52:ASN:HD21	1:AAA:168:ALA:H	1.54	0.54
1:BBB:52:ASN:HD21	1:BBB:168:ALA:H	1.56	0.54
1:AAA:189:VAL:H	1:AAA:401:ASN:ND2	2.05	0.53
1:AAA:189:VAL:H	1:AAA:401:ASN:HD21	1.56	0.53
1:AAA:215:GLU:OE2	1:AAA:217:ARG:NH2	2.42	0.53
1:AAA:340:TRP:O	1:AAA:344:HIS:HD2	1.92	0.52
1:BBB:138:LEU:H	1:BBB:158:GLN:NE2	2.07	0.52
1:AAA:344:HIS:HE1	3:BBB:759:HOH:O	1.94	0.51
1:BBB:444:VAL:HG13	1:BBB:503:THR:HG21	1.93	0.51
1:BBB:191:THR:HG23	1:BBB:271:ILE:HA	1.93	0.50
1:AAA:7:THR:HB	1:AAA:10:ARG:HB2	1.94	0.50
1:AAA:100:ASN:HA	1:AAA:129:ARG:NH2	2.27	0.50
1:AAA:7:THR:CG2	1:AAA:264:ILE:O	2.45	0.49
1:BBB:350:ASP:OD2	1:BBB:399:ASP:OD2	2.31	0.49
1:BBB:508:ASP:HB3	1:BBB:521:TRP:CZ3	2.48	0.49
1:AAA:447[A]:MET:HG2	3:AAA:996:HOH:O	2.11	0.49
1:BBB:426:ALA:HA	1:BBB:459:LEU:CD2	2.43	0.49
1:AAA:273:SER:H	1:AAA:284:ASN:ND2	2.11	0.49
1:BBB:444:VAL:HG13	1:BBB:503:THR:CG2	2.43	0.48
1:BBB:38:ALA:HA	1:BBB:70:GLN:HE22	1.78	0.48
1:BBB:445:ASN:ND2	1:BBB:467:ARG:HH12	2.11	0.48
1:BBB:290:PHE:HB2	1:BBB:545:GLY:HA3	1.95	0.48
1:AAA:87:ARG:HD2	1:AAA:115:GLU:OE1	2.14	0.47
1:AAA:508:ASP:HB3	1:AAA:521:TRP:CZ3	2.50	0.47
1:BBB:445:ASN:HD22	1:BBB:467:ARG:HH12	1.62	0.47
1:AAA:3:ARG:CZ	1:AAA:339:ASP:OD2	2.63	0.47
1:AAA:445:ASN:ND2	1:AAA:467:ARG:HH22	2.12	0.47
1:AAA:463:LEU:HD21	1:AAA:492:TRP:CD2	2.50	0.47
1:AAA:471:TRP:CZ2	1:AAA:508:ASP:HB2	2.50	0.46
1:BBB:260:THR:HG23	1:BBB:261:GLU:HG3	1.97	0.46
1:BBB:162:HIS:HD2	3:BBB:705:HOH:O	1.98	0.45
1:AAA:350:ASP:OD2	1:AAA:399:ASP:OD2	2.35	0.45
1:BBB:328:THR:HA	1:BBB:333:TYR:CZ	2.51	0.45
1:BBB:426:ALA:HA	1:BBB:459:LEU:HD23	1.99	0.45
1:BBB:466:ASN:HB3	1:BBB:504:GLU:OE1	2.16	0.45
1:BBB:471:TRP:CZ2	1:BBB:508:ASP:HB2	2.52	0.45
1:BBB:92:THR:HA	1:BBB:93:HIS:HA	1.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:191:THR:CG2	1:BBB:272:ARG:N	2.78	0.44
1:AAA:11:GLU:OE2	1:BBB:77:LYS:HE2	2.17	0.44
1:AAA:558:GLN:HA	3:AAA:860:HOH:O	2.17	0.44
1:AAA:466:ASN:HB3	1:AAA:504:GLU:OE1	2.17	0.44
1:AAA:138:LEU:HB2	1:AAA:158:GLN:NE2	2.33	0.43
1:AAA:221:GLN:HE21	1:AAA:221:GLN:HB3	1.67	0.43
1:AAA:163:ASP:HB2	1:AAA:363:ILE:HD12	2.00	0.43
1:AAA:92:THR:HA	1:AAA:93:HIS:HA	1.82	0.43
1:BBB:191:THR:HG21	1:BBB:272:ARG:N	2.29	0.43
1:AAA:447[A]:MET:HE3	1:AAA:467:ARG:HA	1.98	0.43
1:AAA:315:HIS:HE1	3:AAA:729:HOH:O	2.01	0.43
1:BBB:15:LEU:CD2	1:BBB:73:VAL:HG21	2.50	0.42
1:BBB:413:GLU:N	1:BBB:414:PRO:CD	2.82	0.42
1:AAA:163:ASP:HB2	1:AAA:363:ILE:HB	2.01	0.42
1:BBB:102:GLN:HG2	1:BBB:121:TYR:CD1	2.55	0.42
1:AAA:105:MET:HG3	1:AAA:116:ALA:HB2	2.02	0.42
1:AAA:413:GLU:N	1:AAA:414:PRO:CD	2.81	0.42
1:AAA:417:ARG:N	1:AAA:418:PRO:CD	2.82	0.42
1:BBB:471:TRP:CE3	1:BBB:520:MET:HE3	2.55	0.42
1:AAA:242:TRP:CZ2	1:AAA:345:GLY:HA2	2.55	0.41
1:AAA:0:HIS:CG	1:AAA:186:ASP:HB2	2.55	0.41
1:BBB:466:ASN:HA	1:BBB:504:GLU:HB3	2.02	0.41
1:AAA:102:GLN:HG2	1:AAA:121:TYR:CD1	2.56	0.41
1:AAA:328:THR:HA	1:AAA:333:TYR:CZ	2.56	0.41
1:BBB:82:GLN:HE22	1:BBB:180:PRO:HA	1.85	0.41
1:AAA:100:ASN:HA	1:AAA:129:ARG:HH21	1.85	0.40
1:BBB:417:ARG:N	1:BBB:418:PRO:CD	2.84	0.40
1:AAA:470:GLY:HA2	1:AAA:474:GLN:O	2.21	0.40
1:BBB:447:MET:HA	1:BBB:467:ARG:NH1	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BBB:838:HOH:O	3:BBB:838:HOH:O[2_556]	1.30	0.90

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	AAA	596/601 (99%)	570 (96%)	26 (4%)	0	100	100
1	BBB	586/601 (98%)	561 (96%)	25 (4%)	0	100	100
All	All	1182/1202 (98%)	1131 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	511/511 (100%)	508 (99%)	3 (1%)	78	85
1	BBB	506/511 (99%)	501 (99%)	5 (1%)	68	75
All	All	1017/1022 (100%)	1009 (99%)	8 (1%)	73	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	201	SER
1	AAA	272	ARG
1	AAA	468	TYR
1	BBB	-1	SER
1	BBB	201	SER
1	BBB	272	ARG
1	BBB	468	TYR
1	BBB	557	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	8I4	BBB	601	-	13,13,14	0.97	1 (7%)	18,19,21	2.02	5 (27%)
2	8I4	AAA	601	-	13,13,14	1.41	3 (23%)	18,19,21	1.16	1 (5%)

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	8I4	BBB	601	-	-	2/4/24/28	0/1/1/1
2	8I4	AAA	601	-	-	2/4/24/28	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	601	8I4	O4-C4	2.70	1.49	1.43
2	AAA	601	8I4	O6B-C6	-2.38	1.23	1.30
2	AAA	601	8I4	C2-C3	2.28	1.56	1.52
2	AAA	601	8I4	O6A-C6	2.14	1.28	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	601	8I4	C7-C1-C2	4.74	117.00	111.50
2	BBB	601	8I4	O6A-C6-C5	-3.59	113.68	122.84
2	BBB	601	8I4	C2-C3-C4	3.24	116.56	110.86
2	BBB	601	8I4	C5-C4-C3	-3.05	106.07	110.58
2	BBB	601	8I4	O6B-C6-C5	2.57	121.31	113.91
2	AAA	601	8I4	O7-C7-C5	2.25	114.91	110.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	601	8I4	C4-C5-C6-O6B
2	AAA	601	8I4	C4-C5-C6-O6A
2	BBB	601	8I4	C4-C5-C6-O6B
2	BBB	601	8I4	C4-C5-C6-O6A

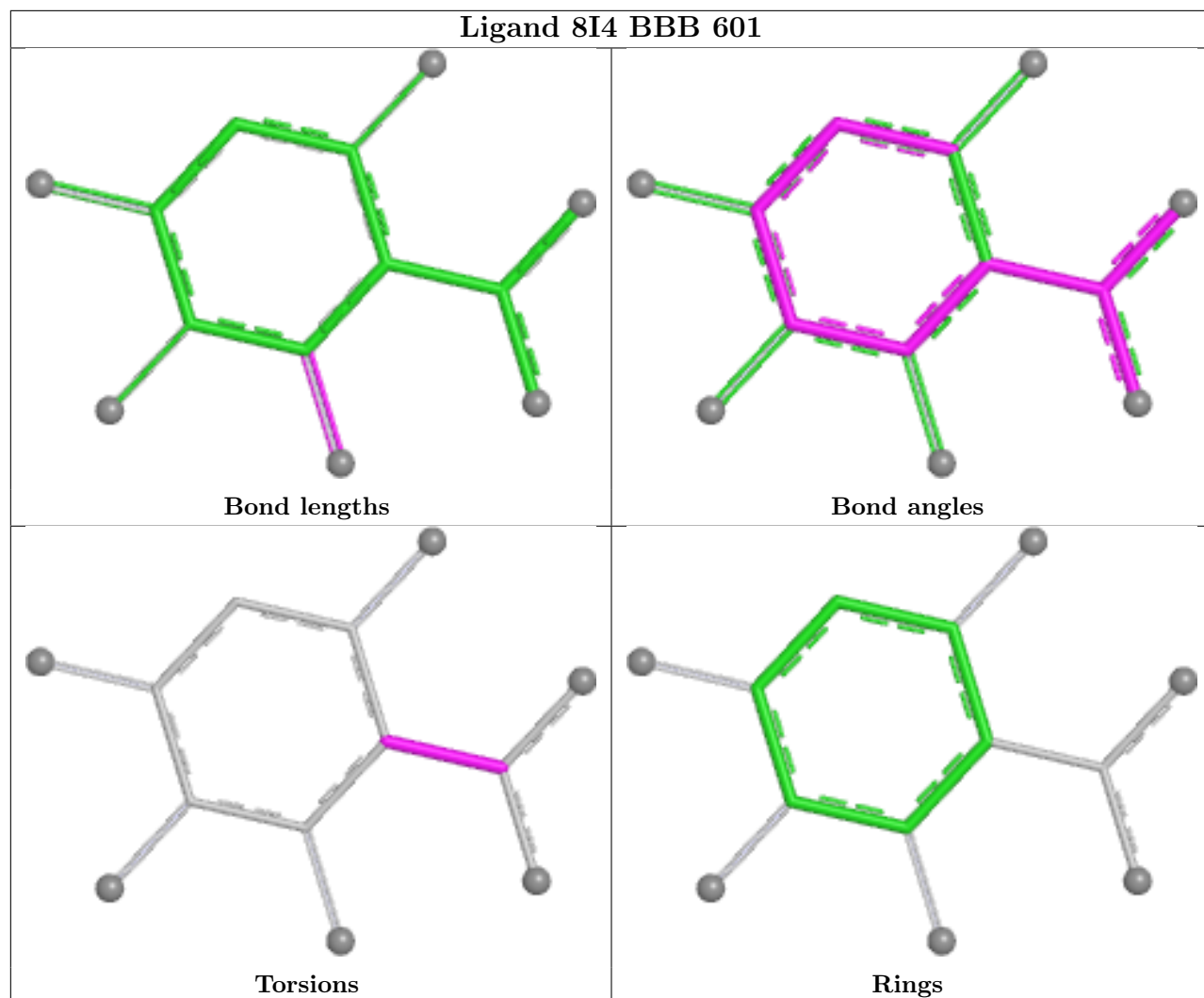
There are no ring outliers.

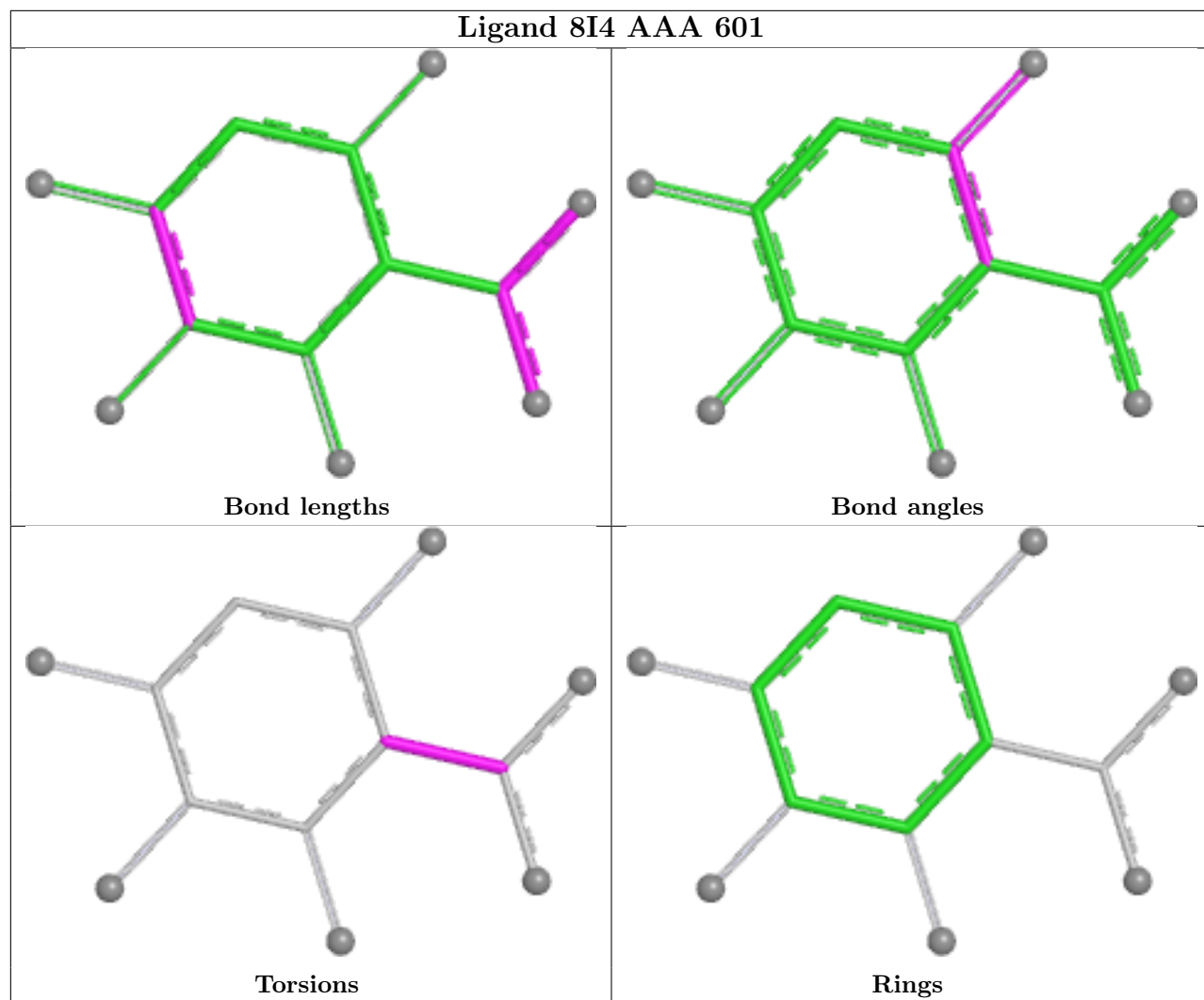
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	601	8I4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 8I4 BBB 601





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 ⓘ

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	AAA	599/601 (99%)	0.42	23 (3%) 44 43	20, 40, 68, 95	1 (0%)
1	BBB	592/601 (98%)	1.18	118 (19%) 3 2	33, 58, 85, 118	0
All	All	1191/1202 (99%)	0.80	141 (11%) 9 8	20, 49, 81, 118	1 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	365	PHE	5.4
1	BBB	435	LEU	4.8
1	BBB	428	LEU	4.3
1	BBB	227	GLY	4.1
1	BBB	256	ALA	4.0
1	BBB	214	VAL	4.0
1	BBB	496	LEU	3.7
1	BBB	460	PHE	3.7
1	BBB	200	ALA	3.5
1	BBB	442	THR	3.5
1	BBB	206	VAL	3.5
1	BBB	207	VAL	3.5
1	BBB	252	LEU	3.5
1	BBB	188	THR	3.4
1	BBB	396	ILE	3.4
1	BBB	225	ALA	3.3
1	BBB	431	ALA	3.3
1	AAA	264	ILE	3.3
1	BBB	234	LEU	3.3
1	BBB	270	GLY	3.2
1	BBB	267	LEU	3.2
1	BBB	424	TYR	3.1
1	AAA	368	GLY	3.1
1	AAA	363	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BBB	202	VAL	3.1
1	BBB	204	TRP	3.1
1	BBB	197	CYS	3.1
1	BBB	250	TYR	3.0
1	BBB	389	LEU	3.0
1	BBB	5	VAL	3.0
1	BBB	544	VAL	3.0
1	AAA	253	CYS	2.9
1	BBB	456	ILE	2.9
1	BBB	190	VAL	2.9
1	BBB	240	HIS	2.9
1	BBB	347	VAL	2.8
1	BBB	199	HIS	2.8
1	BBB	216	LEU	2.8
1	BBB	223	VAL	2.8
1	BBB	237	VAL	2.8
1	BBB	408	TRP	2.8
1	BBB	184	VAL	2.8
1	BBB	254	VAL	2.8
1	BBB	362	GLY	2.7
1	BBB	271	ILE	2.7
1	BBB	441	ILE	2.7
1	AAA	224	VAL	2.7
1	BBB	387	ALA	2.7
1	AAA	123	ILE	2.7
1	AAA	124	ALA	2.7
1	AAA	256	ALA	2.7
1	BBB	183	TRP	2.7
1	AAA	79	TRP	2.6
1	BBB	283	ILE	2.6
1	BBB	392	ILE	2.6
1	BBB	501	ILE	2.6
1	BBB	292	GLY	2.6
1	BBB	542	ALA	2.6
1	BBB	432	THR	2.6
1	BBB	242	TRP	2.6
1	AAA	130	ILE	2.6
1	BBB	224	VAL	2.6
1	BBB	230	THR	2.6
1	AAA	35	TRP	2.6
1	BBB	212	VAL	2.6
1	BBB	79	TRP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BBB	274	VAL	2.5
1	BBB	233	THR	2.5
1	BBB	545	GLY	2.5
1	BBB	187	ILE	2.5
1	AAA	225	ALA	2.5
1	BBB	262	CYS	2.5
1	BBB	229	GLY	2.5
1	BBB	264	ILE	2.5
1	BBB	236	VAL	2.5
1	BBB	427	PRO	2.5
1	BBB	437	PRO	2.5
1	BBB	289	TYR	2.4
1	BBB	150	THR	2.4
1	BBB	182	THR	2.4
1	BBB	194	ALA	2.4
1	AAA	125	GLY	2.4
1	BBB	273	SER	2.4
1	BBB	537	PHE	2.4
1	BBB	503	THR	2.4
1	BBB	451	ALA	2.4
1	BBB	219	ALA	2.4
1	BBB	279	GLU	2.4
1	BBB	192	HIS	2.4
1	BBB	189	VAL	2.4
1	AAA	39	LEU	2.3
1	BBB	485	LEU	2.3
1	BBB	288	PHE	2.3
1	BBB	255	THR	2.3
1	BBB	425	PHE	2.3
1	BBB	198	ASN	2.3
1	BBB	208	ALA	2.3
1	BBB	410	ILE	2.3
1	BBB	205	GLN	2.3
1	BBB	429	ALA	2.3
1	AAA	73	VAL	2.3
1	BBB	543	VAL	2.3
1	AAA	28	CYS	2.3
1	BBB	452	HIS	2.3
1	AAA	255	THR	2.3
1	BBB	281	PHE	2.2
1	BBB	357	PHE	2.2
1	BBB	99	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BBB	232	GLY	2.2
1	BBB	278	GLY	2.2
1	BBB	90	ALA	2.2
1	BBB	426	ALA	2.2
1	AAA	88	PHE	2.2
1	BBB	588	TRP	2.2
1	BBB	455	THR	2.2
1	BBB	411	ALA	2.2
1	BBB	75	ILE	2.2
1	BBB	84	ILE	2.2
1	BBB	444	VAL	2.2
1	BBB	464	CYS	2.2
1	BBB	403	PRO	2.2
1	AAA	80	ALA	2.2
1	BBB	481	ALA	2.2
1	BBB	469	TYR	2.1
1	BBB	98	TRP	2.1
1	BBB	461	ASP	2.1
1	AAA	260	THR	2.1
1	BBB	213	SER	2.1
1	BBB	152	GLU	2.1
1	BBB	463	LEU	2.1
1	BBB	290	PHE	2.0
1	BBB	4	PRO	2.0
1	BBB	253	CYS	2.0
1	BBB	490	LEU	2.0
1	BBB	436	ASP	2.0
1	AAA	127	SER	2.0
1	BBB	-1	SER	2.0
1	BBB	593	PHE	2.0
1	AAA	210	GLY	2.0
1	BBB	468	TYR	2.0
1	BBB	484	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

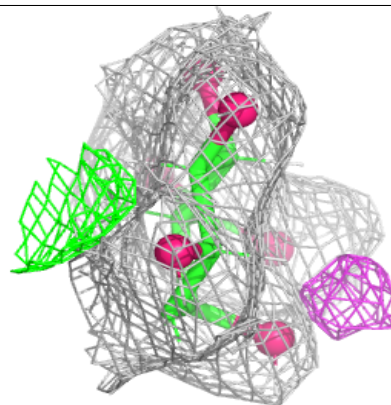
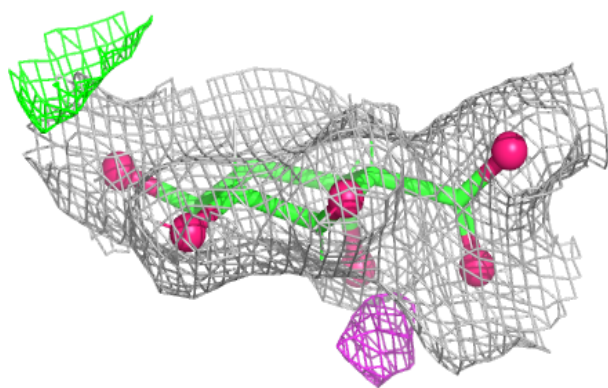
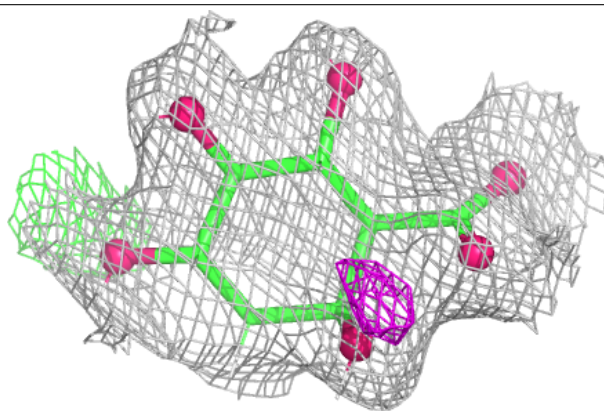
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	8I4	BBB	601	13/14	0.90	0.07	40,42,44,46	4
2	8I4	AAA	601	13/14	0.97	0.04	25,28,29,32	4

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.

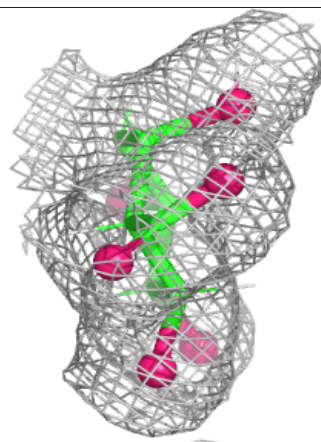
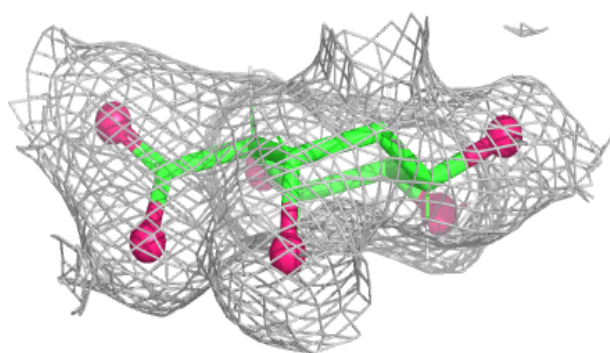
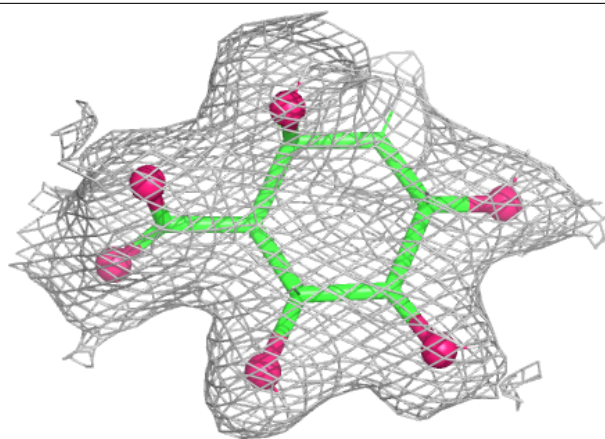
Electron density around 8I4 BBB 601:

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 8I4 AAA 601:

$2mF_o-DF_c$ (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.