



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:20 AM UTC

PDB ID : 3TJO / pdb_00003tjo
Title : HtrA1 catalytic domain, mutationally inactivated
Authors : Eigenbrot, C.; Ultsch, M.
Deposited on : 2011-08-24
Resolution : 2.30 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

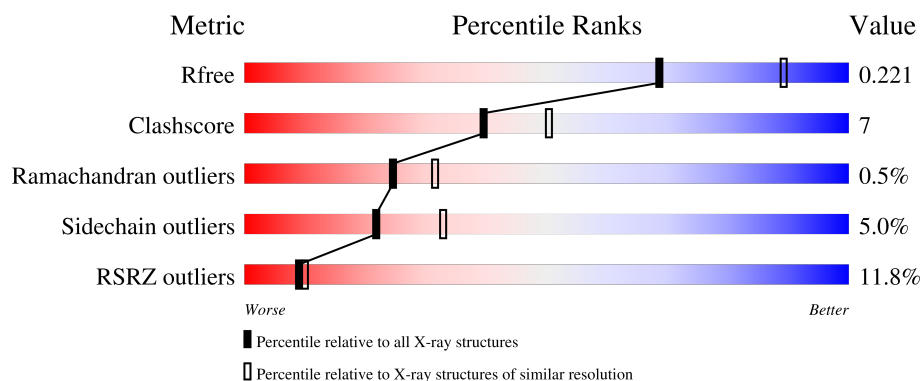
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	231	10% 74% 10% 14%
1	B	231	7% 72% 13% 14%
1	D	231	13% 68% 15% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	1	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4923 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 Serine protease HTRA1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	0	1	0
			1524	972	263	289			
1	B	198	Total	C	N	O	0	1	0
			1524	972	263	289			
1	D	197	Total	C	N	O	0	8	0
			1569	1001	273	295			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	MET	-	expression tag	UNP Q92743
A	141	GLY	-	expression tag	UNP Q92743
A	142	SER	-	expression tag	UNP Q92743
A	143	SER	-	expression tag	UNP Q92743
A	144	HIS	-	expression tag	UNP Q92743
A	145	HIS	-	expression tag	UNP Q92743
A	146	HIS	-	expression tag	UNP Q92743
A	147	HIS	-	expression tag	UNP Q92743
A	148	HIS	-	expression tag	UNP Q92743
A	149	HIS	-	expression tag	UNP Q92743
A	150	SER	-	expression tag	UNP Q92743
A	151	SER	-	expression tag	UNP Q92743
A	152	GLY	-	expression tag	UNP Q92743
A	153	LEU	-	expression tag	UNP Q92743
A	154	VAL	-	expression tag	UNP Q92743
A	155	PRO	-	expression tag	UNP Q92743
A	156	ARG	-	expression tag	UNP Q92743
A	157	GLY	-	expression tag	UNP Q92743
A	158	SER	-	expression tag	UNP Q92743
A	159	HIS	-	expression tag	UNP Q92743
A	160	MET	-	expression tag	UNP Q92743
A	328	ALA	SER	engineered mutation	UNP Q92743
B	140	MET	-	expression tag	UNP Q92743

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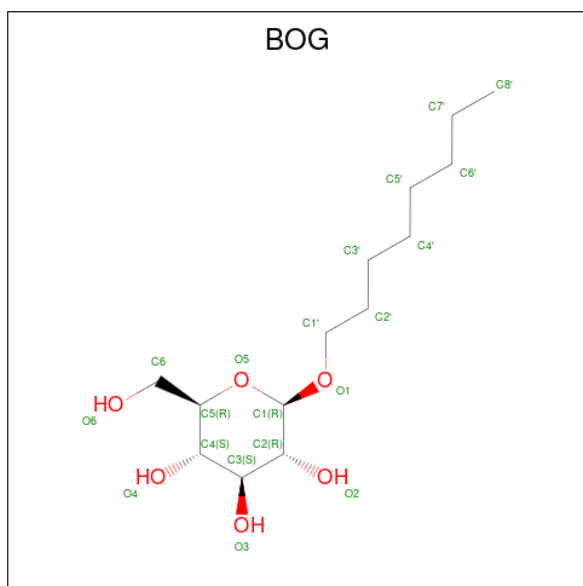
Chain	Residue	Modelled	Actual	Comment	Reference
B	141	GLY	-	expression tag	UNP Q92743
B	142	SER	-	expression tag	UNP Q92743
B	143	SER	-	expression tag	UNP Q92743
B	144	HIS	-	expression tag	UNP Q92743
B	145	HIS	-	expression tag	UNP Q92743
B	146	HIS	-	expression tag	UNP Q92743
B	147	HIS	-	expression tag	UNP Q92743
B	148	HIS	-	expression tag	UNP Q92743
B	149	HIS	-	expression tag	UNP Q92743
B	150	SER	-	expression tag	UNP Q92743
B	151	SER	-	expression tag	UNP Q92743
B	152	GLY	-	expression tag	UNP Q92743
B	153	LEU	-	expression tag	UNP Q92743
B	154	VAL	-	expression tag	UNP Q92743
B	155	PRO	-	expression tag	UNP Q92743
B	156	ARG	-	expression tag	UNP Q92743
B	157	GLY	-	expression tag	UNP Q92743
B	158	SER	-	expression tag	UNP Q92743
B	159	HIS	-	expression tag	UNP Q92743
B	160	MET	-	expression tag	UNP Q92743
B	328	ALA	SER	engineered mutation	UNP Q92743
D	140	MET	-	expression tag	UNP Q92743
D	141	GLY	-	expression tag	UNP Q92743
D	142	SER	-	expression tag	UNP Q92743
D	143	SER	-	expression tag	UNP Q92743
D	144	HIS	-	expression tag	UNP Q92743
D	145	HIS	-	expression tag	UNP Q92743
D	146	HIS	-	expression tag	UNP Q92743
D	147	HIS	-	expression tag	UNP Q92743
D	148	HIS	-	expression tag	UNP Q92743
D	149	HIS	-	expression tag	UNP Q92743
D	150	SER	-	expression tag	UNP Q92743
D	151	SER	-	expression tag	UNP Q92743
D	152	GLY	-	expression tag	UNP Q92743
D	153	LEU	-	expression tag	UNP Q92743
D	154	VAL	-	expression tag	UNP Q92743
D	155	PRO	-	expression tag	UNP Q92743
D	156	ARG	-	expression tag	UNP Q92743
D	157	GLY	-	expression tag	UNP Q92743
D	158	SER	-	expression tag	UNP Q92743
D	159	HIS	-	expression tag	UNP Q92743
D	160	MET	-	expression tag	UNP Q92743

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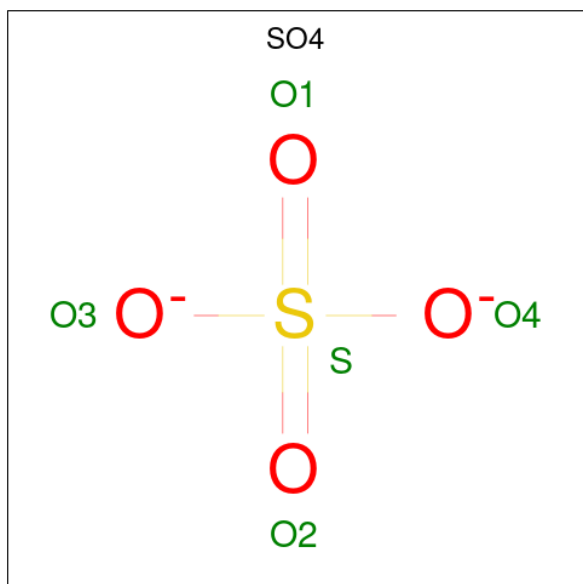
Chain	Residue	Modelled	Actual	Comment	Reference
D	328	ALA	SER	engineered mutation	UNP Q92743

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



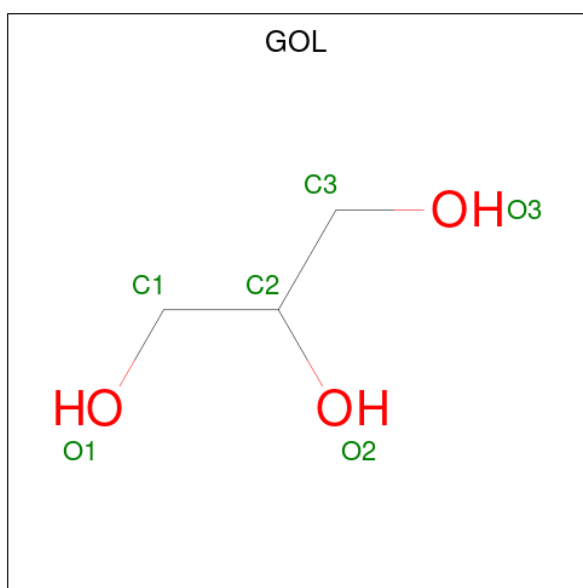
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	81	Total O 81 81	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	67	Total 67	O 67	0	0
5	D	68	Total 68	O 68	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.92Å 151.92Å 87.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.30) 99.8 (50.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.216 0.184 , 0.221	Depositor DCC
R_{free} test set	1052 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.0	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	4923	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, BOG

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	0.61	0/1549	0.80	2/2099 (0.1%)
1	B	0.58	0/1549	0.76	0/2099
1	D	0.57	0/1596	0.76	0/2164
All	All	0.58	0/4694	0.77	2/6362 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ASN	N-CA-C	5.42	122.34	110.80
1	A	287	SER	N-CA-C	5.33	117.78	111.33

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	1524	0	1563	15	0
1	B	1524	0	1563	25	0
1	D	1569	0	1610	31	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
3	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
4	A	6	0	8	2	0
4	B	18	0	24	9	0
4	D	6	0	8	1	0
5	A	81	0	0	0	0
5	B	67	0	0	1	0
5	D	68	0	0	3	0
All	All	4923	0	4796	64	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (64) 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:344:THR:HB	4:B:1:GOL:H11	1.50	0.94
1:A:300:THR:O	1:A:301:GLN:HB2	1.95	0.66
1:B:170:ASN:HD21	1:D:278:PHE:H	1.43	0.66
1:D:223[B]:THR:H	1:D:226[B]:HIS:HD2	1.43	0.66
1:A:220:HIS:HD2	1:A:250:ASP:OD2	1.79	0.64
1:D:214:LEU:HD13	1:D:255:LYS:HD3	1.81	0.61
1:D:220[B]:HIS:O	1:D:222[B]:VAL:HG22	2.01	0.59
1:B:342:ILE:HG13	1:B:360:ILE:HD11	1.85	0.58
1:B:223:THR:H	1:B:226:HIS:HD2	1.51	0.58
1:D:231:GLU:HG3	1:D:237:THR:HB	1.85	0.57
1:B:170:ASN:ND2	1:D:278:PHE:H	2.02	0.56
1:D:223[A]:THR:HG23	1:D:225[A]:LYS:HE2	1.86	0.56
1:D:237:THR:HG22	5:D:41:HOH:O	2.04	0.56
1:B:344:THR:HA	4:B:1:GOL:H32	1.87	0.56
1:B:345:LEU:H	4:B:1:GOL:H2	1.70	0.56
1:A:278:PHE:H	1:D:170:ASN:HD21	1.54	0.56
1:A:231:GLU:OE1	1:A:287:SER:HB3	2.07	0.55
1:B:223:THR:HG23	1:B:225:LYS:H	1.73	0.54
1:D:223[A]:THR:O	1:D:225[A]:LYS:N	2.40	0.54
1:B:191:LYS:HG3	1:B:198:GLU:HG2	1.90	0.53
1:A:170:ASN:HD21	1:B:278:PHE:H	1.55	0.53
1:D:341:GLY:HA2	1:D:355:ILE:O	2.08	0.53
1:A:191:LYS:HA	1:A:198:GLU:HG2	1.91	0.53
1:D:191:LYS:HD2	1:D:196:LYS:HG2	1.90	0.52
1:A:278:PHE:H	1:D:170:ASN:ND2	2.07	0.52
1:D:188:LEU:HD21	1:D:225[A]:LYS:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:LYS:NZ	5:D:391:HOH:O	2.32	0.51
1:A:299:THR:HG23	1:A:318:GLN:HB2	1.91	0.51
1:A:341:GLY:HA2	1:A:355:ILE:O	2.10	0.51
1:D:210:SER:OG	1:D:214:LEU:HB2	2.10	0.51
1:B:283:GLY:HA3	1:B:327:ASN:HA	1.92	0.51
1:D:223[B]:THR:H	1:D:226[B]:HIS:CD2	2.25	0.50
1:B:345:LEU:H	4:B:1:GOL:C2	2.24	0.50
1:D:237:THR:CG2	5:D:41:HOH:O	2.59	0.50
1:A:170:ASN:ND2	1:B:278:PHE:H	2.10	0.50
1:D:299:THR:HG23	1:D:318:GLN:HB2	1.93	0.50
1:B:348:THR:HG22	1:B:353:PHE:HE2	1.76	0.49
1:D:218:ASN:HB3	1:D:220[A]:HIS:H	1.77	0.49
1:B:273:LEU:HD11	1:B:340:ILE:HD13	1.94	0.48
1:B:223:THR:HG22	1:B:226:HIS:CD2	2.49	0.48
1:D:342:ILE:HG13	1:D:360:ILE:HD11	1.94	0.47
4:B:5:GOL:O2	1:D:348:THR:HG23	2.14	0.47
1:B:300:THR:O	1:B:301:GLN:HB2	2.15	0.47
1:A:273:LEU:HD11	1:A:340:ILE:HD13	1.97	0.46
4:B:5:GOL:O2	1:D:348:THR:CG2	2.65	0.45
4:A:2:GOL:H11	1:B:318:GLN:OE1	2.16	0.45
1:B:238:TYR:HE2	4:B:3:GOL:H32	1.80	0.45
1:D:181:PRO:HB3	4:D:4:GOL:H2	1.99	0.45
1:D:283:GLY:HA3	1:D:327:ASN:HA	1.98	0.45
1:D:225[A]:LYS:O	1:D:226[A]:HIS:C	2.61	0.44
1:D:273:LEU:HD11	1:D:340:ILE:HD13	2.00	0.44
1:B:341:GLY:HA2	1:B:355:ILE:O	2.17	0.43
1:D:161:ASP:HB3	1:D:162:PRO:HD3	2.01	0.43
1:A:289[B]:GLN:NE2	1:B:299:THR:HG21	2.35	0.42
1:D:348:THR:HG22	1:D:353:PHE:HE2	1.85	0.42
1:B:299:THR:CG2	5:B:129:HOH:O	2.67	0.41
1:D:211:GLU:OE2	1:D:261:LYS:HE3	2.21	0.41
1:A:342:ILE:HG13	1:A:360:ILE:HD11	2.03	0.41
1:D:323:ILE:HD12	1:D:352:SER:HB3	2.02	0.41
1:A:348:THR:HG22	1:A:353:PHE:HE2	1.85	0.41
1:B:345:LEU:H	4:B:1:GOL:C1	2.34	0.41
1:B:345:LEU:HB2	4:B:1:GOL:H2	2.03	0.41
1:A:289[B]:GLN:HE22	4:A:2:GOL:C1	2.34	0.40
1:B:231:GLU:HG2	1:B:237:THR:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/231 (84%)	191 (98%)	3 (2%)	1 (0%)	24	31
1	B	195/231 (84%)	193 (99%)	2 (1%)	0	100	100
1	D	201/231 (87%)	192 (96%)	7 (4%)	2 (1%)	12	15
All	All	591/693 (85%)	576 (98%)	12 (2%)	3 (0%)	24	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	198	GLU
1	D	163	ASN
1	A	224	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/196 (86%)	162 (96%)	7 (4%)	27	41
1	B	169/196 (86%)	161 (95%)	8 (5%)	23	35
1	D	174/196 (89%)	162 (93%)	12 (7%)	14	20
All	All	512/588 (87%)	485 (95%)	27 (5%)	22	30

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	HIS
1	A	222	VAL
1	A	225	LYS
1	A	253	LEU
1	A	287	SER
1	A	299	THR
1	A	333	VAL
1	B	188	LEU
1	B	191	LYS
1	B	222	VAL
1	B	224	ASN
1	B	253	LEU
1	B	299	THR
1	B	333	VAL
1	B	367	SER
1	D	188	LEU
1	D	214	LEU
1	D	222[A]	VAL
1	D	222[B]	VAL
1	D	225[A]	LYS
1	D	225[B]	LYS
1	D	231	GLU
1	D	237	THR
1	D	241	LYS
1	D	253	LEU
1	D	299	THR
1	D	333	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	220	HIS
1	A	259	GLN
1	B	170	ASN
1	B	218	ASN
1	B	224	ASN
1	B	226	HIS
1	B	289	GLN
1	B	290	ASN
1	D	170	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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	$\# Z > 2$
3	SO4	A	1	-	4,4,4	0.24	0	6,6,6	0.52	0
4	GOL	B	1	-	5,5,5	0.45	0	5,5,5	0.38	0
4	GOL	B	3	-	5,5,5	0.42	0	5,5,5	0.23	0
2	BOG	B	455	-	20,20,20	3.57	12 (60%)	25,25,25	1.70	3 (12%)
2	BOG	A	455	-	20,20,20	3.60	12 (60%)	25,25,25	1.88	5 (20%)
3	SO4	A	4	-	4,4,4	0.27	0	6,6,6	0.13	0
4	GOL	D	4	-	5,5,5	0.38	0	5,5,5	0.15	0
3	SO4	B	2	-	4,4,4	0.25	0	6,6,6	0.19	0
4	GOL	B	5	-	5,5,5	0.47	0	5,5,5	0.46	0
4	GOL	A	2	-	5,5,5	0.40	0	5,5,5	0.16	0
3	SO4	A	3	-	4,4,4	0.25	0	6,6,6	0.08	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
4	GOL	B	1	-	-	2/4/4/4	-
4	GOL	B	3	-	-	2/4/4/4	-
2	BOG	B	455	-	-	1/11/31/31	0/1/1/1
2	BOG	A	455	-	-	4/11/31/31	0/1/1/1
4	GOL	D	4	-	-	2/4/4/4	-
4	GOL	B	5	-	-	2/4/4/4	-
4	GOL	A	2	-	-	0/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	455	BOG	C2'-C1'	-6.85	1.22	1.51
2	B	455	BOG	C2'-C1'	-6.67	1.23	1.51
2	B	455	BOG	C6'-C5'	-6.05	1.21	1.51
2	A	455	BOG	C6'-C5'	-6.02	1.21	1.51
2	A	455	BOG	C4'-C3'	-5.96	1.22	1.51
2	B	455	BOG	C4-C5	-5.91	1.40	1.53
2	B	455	BOG	C4'-C3'	-5.80	1.22	1.51
2	A	455	BOG	C4-C5	-5.61	1.41	1.53
2	A	455	BOG	O6-C6	-4.96	1.21	1.42
2	B	455	BOG	O6-C6	-4.79	1.22	1.42
2	B	455	BOG	C4-C3	-4.71	1.40	1.52
2	A	455	BOG	C4-C3	-4.65	1.40	1.52
2	A	455	BOG	C8'-C7'	-3.82	1.23	1.50
2	B	455	BOG	C8'-C7'	-3.81	1.23	1.50
2	A	455	BOG	O2-C2	3.72	1.52	1.43
2	B	455	BOG	O2-C2	3.21	1.50	1.43
2	A	455	BOG	O5-C1	3.13	1.49	1.41
2	B	455	BOG	O1-C1	-3.11	1.35	1.40
2	B	455	BOG	O5-C1	3.08	1.49	1.41
2	A	455	BOG	C6-C5	-2.47	1.43	1.51
2	A	455	BOG	O1-C1	-2.44	1.36	1.40
2	B	455	BOG	C6-C5	-2.28	1.44	1.51
2	A	455	BOG	C3-C2	-2.26	1.46	1.52
2	B	455	BOG	C3-C2	-2.17	1.46	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	455	BOG	O1-C1-C2	5.38	116.44	108.27
2	A	455	BOG	O1-C1-C2	5.09	116.01	108.27
2	B	455	BOG	C1'-O1-C1	4.18	120.83	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	455	BOG	C1'-O1-C1	4.12	120.71	113.68
2	A	455	BOG	O5-C5-C4	3.50	116.01	109.70
2	A	455	BOG	C3-C4-C5	3.38	116.36	110.23
2	A	455	BOG	O2-C2-C1	2.50	116.02	110.08
2	B	455	BOG	O2-C2-C1	2.38	115.75	110.08

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	GOL	O1-C1-C2-C3
4	B	3	GOL	C1-C2-C3-O3
4	B	3	GOL	O2-C2-C3-O3
4	B	5	GOL	C1-C2-C3-O3
2	A	455	BOG	O1-C1'-C2'-C3'
4	D	4	GOL	C1-C2-C3-O3
2	A	455	BOG	C2'-C1'-O1-C1
4	B	5	GOL	O2-C2-C3-O3
2	A	455	BOG	C2'-C3'-C4'-C5'
2	B	455	BOG	C2'-C3'-C4'-C5'
2	A	455	BOG	C5'-C6'-C7'-C8'
4	B	1	GOL	O1-C1-C2-O2
4	D	4	GOL	O2-C2-C3-O3

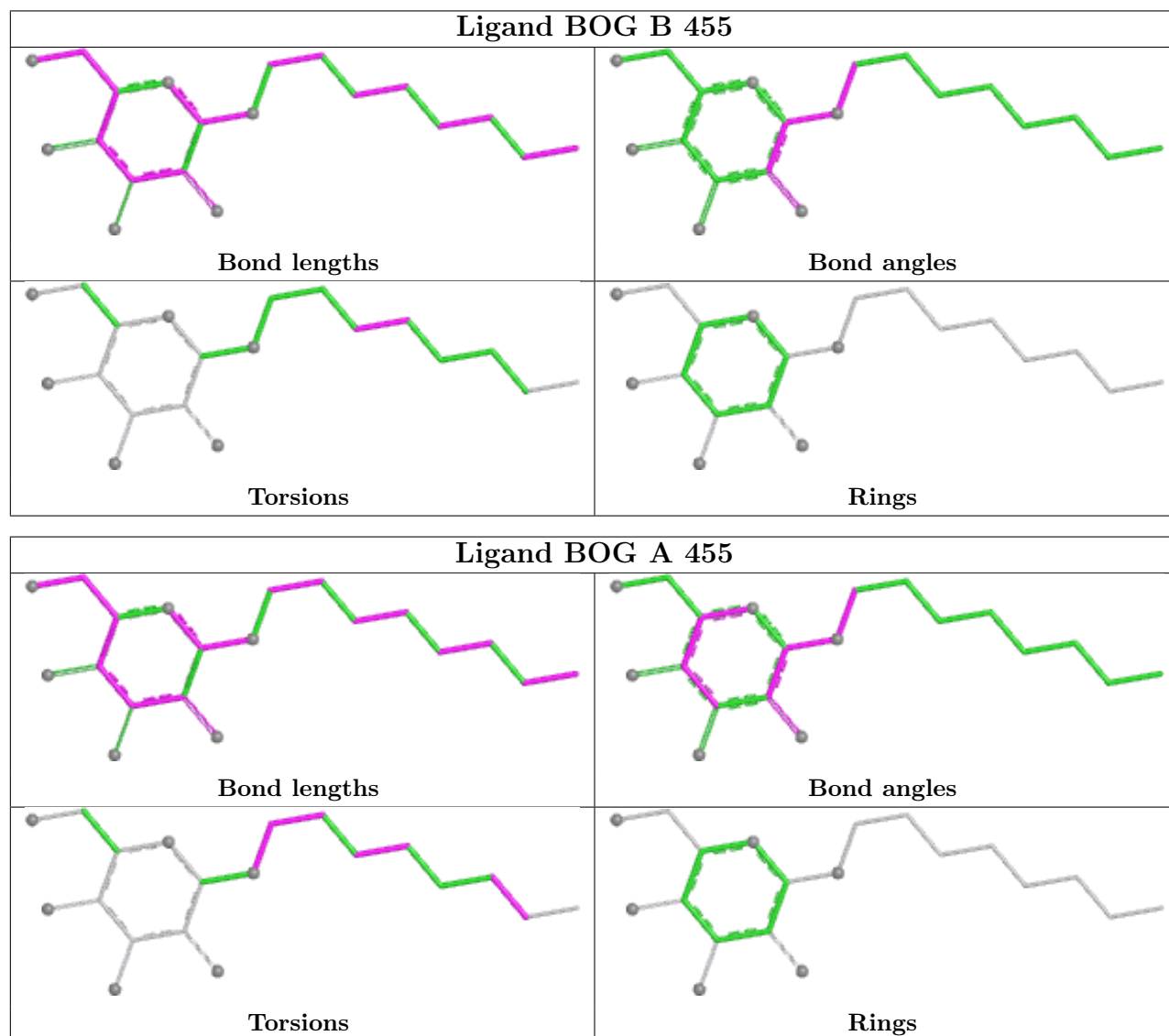
There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	GOL	6	0
4	B	3	GOL	1	0
4	D	4	GOL	1	0
4	B	5	GOL	2	0
4	A	2	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	198/231 (85%)	0.14	23 (11%) 9 10	17, 32, 89, 120	1 (0%)
1	B	198/231 (85%)	0.06	17 (8%) 16 17	18, 34, 73, 121	1 (0%)
1	D	197/231 (85%)	0.39	30 (15%) 5 6	18, 33, 108, 151	8 (4%)
All	All	593/693 (85%)	0.20	70 (11%) 9 10	17, 33, 93, 151	10 (1%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	160	MET	8.2
1	D	194	PHE	8.0
1	D	224[A]	ASN	7.8
1	D	222[A]	VAL	7.7
1	B	160	MET	7.6
1	A	160	MET	6.9
1	D	221[A]	VAL	6.9
1	D	192	LEU	6.8
1	D	225[A]	LYS	6.5
1	D	226[A]	HIS	5.9
1	D	193	PRO	5.6
1	D	220[A]	HIS	5.2
1	A	223	THR	5.1
1	A	370	ARG	4.7
1	A	225	LYS	4.3
1	A	301	GLN	4.3
1	D	197	ARG	4.2
1	D	162	PRO	4.2
1	D	196	LYS	4.0
1	B	370	ARG	3.9
1	D	191	LYS	3.9
1	A	162	PRO	3.9
1	D	370	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	161	ASP	3.6
1	A	224	ASN	3.6
1	D	190	ARG	3.6
1	B	301	GLN	3.5
1	A	221	VAL	3.4
1	A	226	HIS	3.3
1	D	161	ASP	3.2
1	A	194	PHE	3.2
1	B	162	PRO	3.2
1	A	167	HIS	3.1
1	A	287	SER	3.1
1	B	221	VAL	3.0
1	A	161	ASP	3.0
1	B	223	THR	2.9
1	A	196	LYS	2.9
1	D	167	HIS	2.9
1	D	195	SER	2.8
1	A	190	ARG	2.8
1	B	163	ASN	2.8
1	A	197	ARG	2.7
1	A	315	ASP	2.7
1	D	198	GLU	2.6
1	D	163	ASN	2.5
1	D	368	HIS	2.5
1	B	196	LYS	2.5
1	D	227	ARG	2.5
1	B	241	LYS	2.5
1	D	199	VAL	2.4
1	A	368	HIS	2.4
1	B	259[A]	GLN	2.4
1	B	315	ASP	2.4
1	B	287	SER	2.4
1	D	223[A]	THR	2.4
1	A	222	VAL	2.3
1	A	227	ARG	2.3
1	A	163	ASN	2.3
1	B	300	THR	2.3
1	D	315	ASP	2.3
1	D	299	THR	2.1
1	A	257	ASP	2.1
1	A	369	ASP	2.1
1	D	369	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	300	THR	2.1
1	B	194	PHE	2.1
1	B	195	SER	2.0
1	B	367	SER	2.0
1	D	287	SER	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 [i](#)

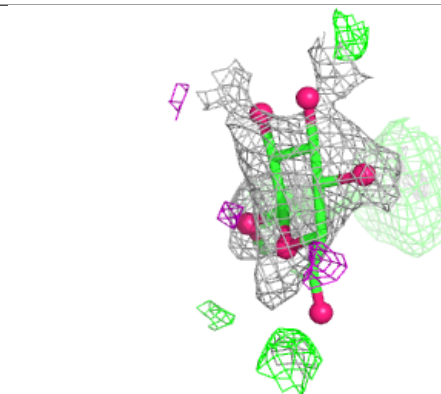
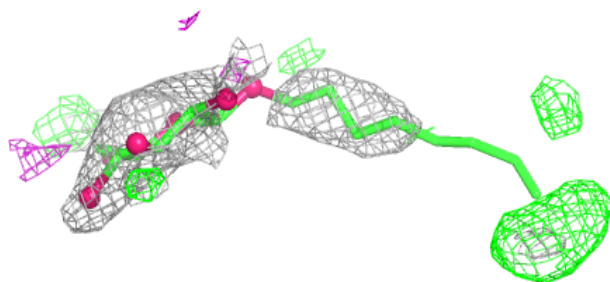
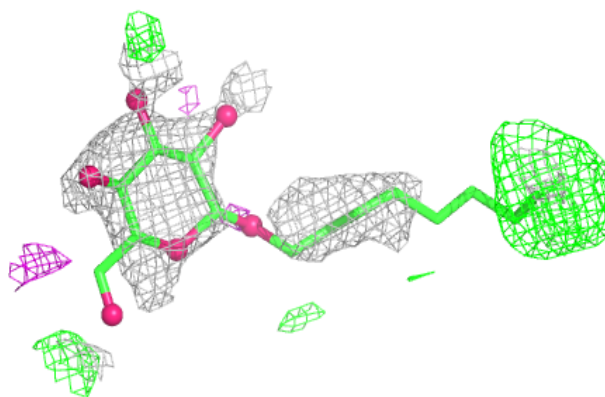
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BOG	A	455	20/20	0.59	0.39	128,131,135,135	0
3	SO4	A	4	5/5	0.75	0.30	50,55,58,62	5
3	SO4	B	2	5/5	0.75	0.15	99,102,103,103	0
4	GOL	B	3	6/6	0.76	0.22	58,76,81,83	0
3	SO4	A	3	5/5	0.78	0.13	94,96,97,98	0
4	GOL	B	1	6/6	0.82	0.26	22,39,54,59	0
4	GOL	B	5	6/6	0.82	0.57	58,61,70,72	6
4	GOL	D	4	6/6	0.84	0.20	66,71,74,81	0
4	GOL	A	2	6/6	0.85	0.28	66,81,85,88	0
2	BOG	B	455	20/20	0.90	0.12	40,45,54,58	0
3	SO4	A	1	5/5	0.95	0.08	41,42,49,54	0

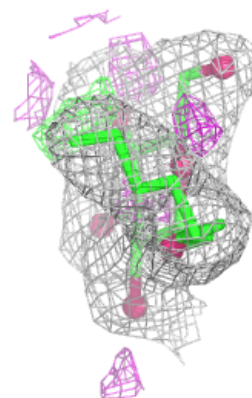
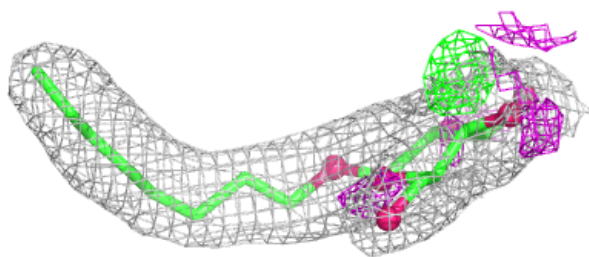
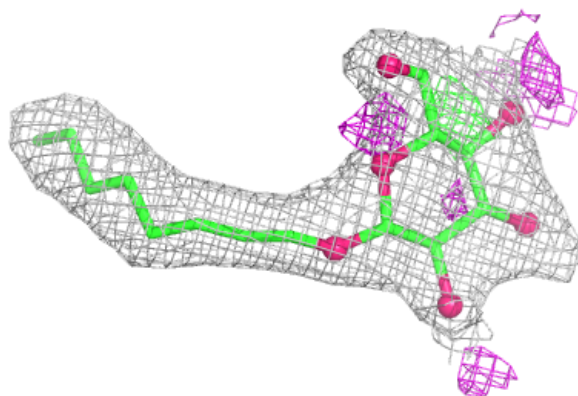
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG A 455:

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

**Electron density around BOG B 455:**

$2mF_o-DF_c$ (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.