



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 06:33 am GMT

PDB ID : 6HCL
Title : Crystal structure of a MFS transporter with Ligand at 2.69 Angstroem resolution
Authors : Kalbermatter, D.; Bosshart, P.; Bonetti, S.; Fotiadis, D.
Deposited on : 2018-08-15
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

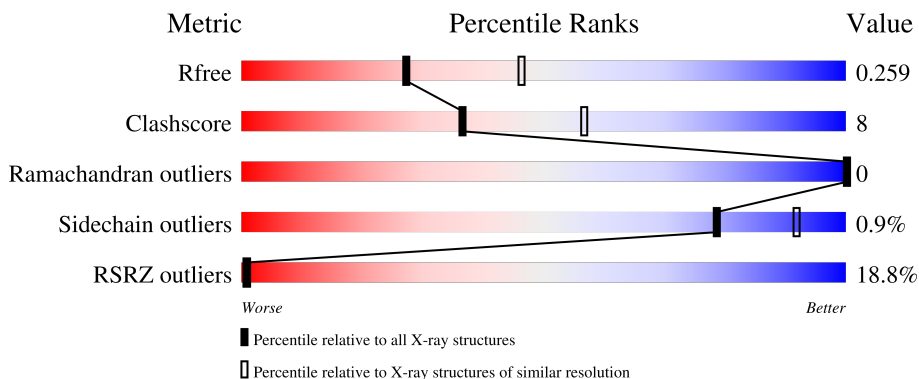
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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 $\leq 5\%$. 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	420	
1	B	420	

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
2	2OP	B	501	-	-	-	X
2	2OP	B	502	-	-	X	-

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5771 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.

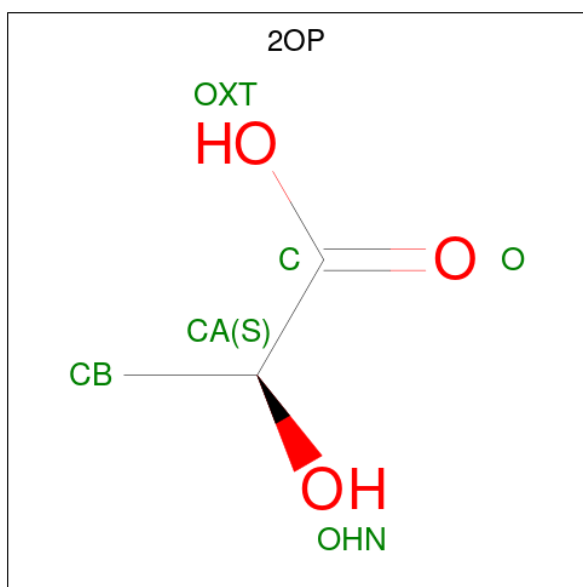
- Molecule 1 is a protein called Major facilitator superfamily MFS_1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	395	2980	1992	470	494	24	0	0	0
1	B	366	2752	1844	430	455	23	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

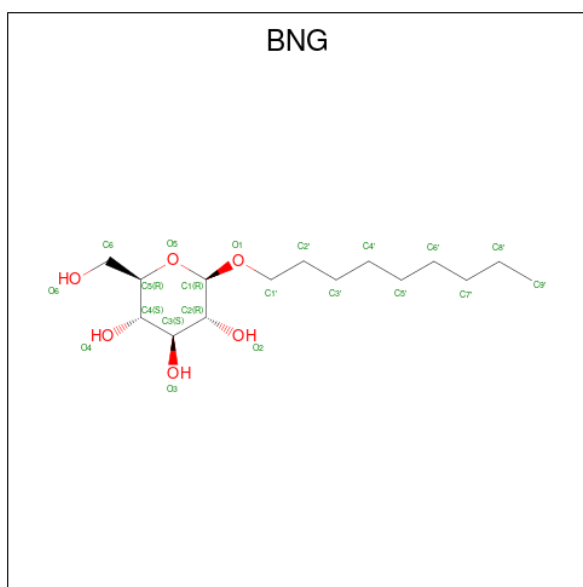
Chain	Residue	Modelled	Actual	Comment	Reference
A	413	LEU	-	expression tag	UNP A0LNN5
A	414	GLU	-	expression tag	UNP A0LNN5
A	415	LEU	-	expression tag	UNP A0LNN5
A	416	GLU	-	expression tag	UNP A0LNN5
A	417	VAL	-	expression tag	UNP A0LNN5
A	418	LEU	-	expression tag	UNP A0LNN5
A	419	PHE	-	expression tag	UNP A0LNN5
A	420	GLN	-	expression tag	UNP A0LNN5
B	413	LEU	-	expression tag	UNP A0LNN5
B	414	GLU	-	expression tag	UNP A0LNN5
B	415	LEU	-	expression tag	UNP A0LNN5
B	416	GLU	-	expression tag	UNP A0LNN5
B	417	VAL	-	expression tag	UNP A0LNN5
B	418	LEU	-	expression tag	UNP A0LNN5
B	419	PHE	-	expression tag	UNP A0LNN5
B	420	GLN	-	expression tag	UNP A0LNN5

- Molecule 2 is (2S)-2-HYDROXYPROPANOIC ACID (three-letter code: 2OP) (formula: C₃H₆O₃).



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

- Molecule 3 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: C₁₅H₃₀O₆).

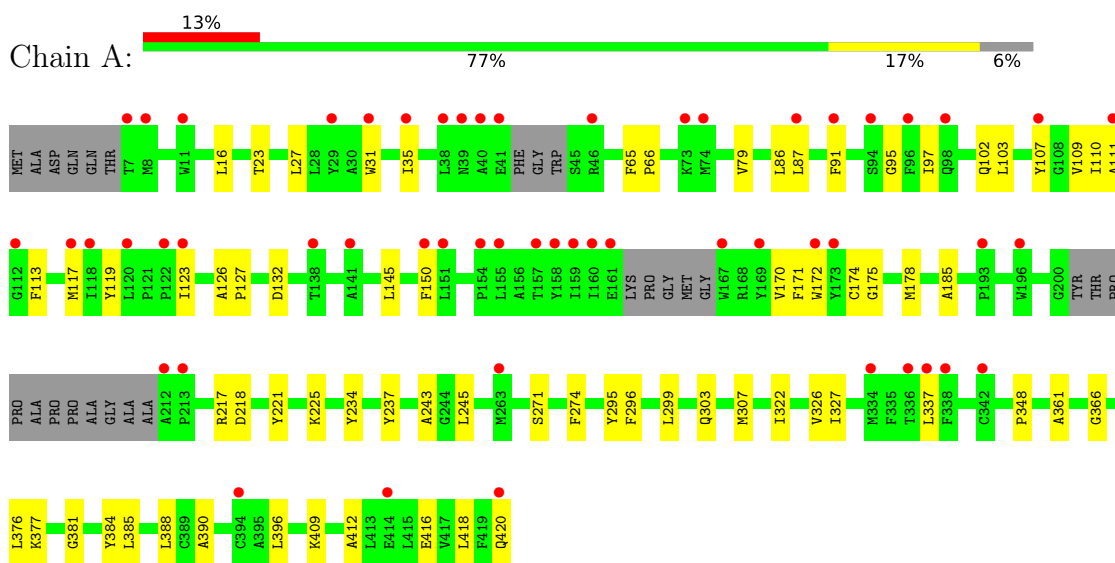


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	15	6		

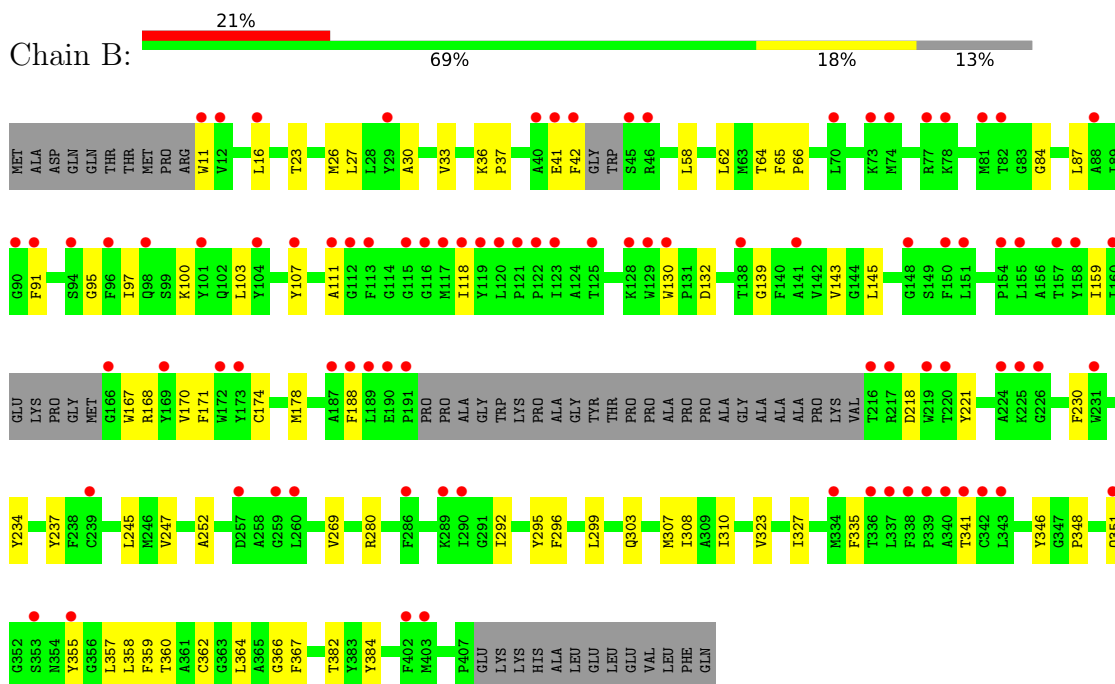
3 Residue-property plots [i](#)

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: Major facilitator superfamily MFS_1



- Molecule 1: Major facilitator superfamily MFS_1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.42Å 200.02Å 63.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.83 – 2.50 24.83 – 2.50	Depositor EDS
% Data completeness (in resolution range)	66.7 (24.83-2.50) 66.7 (24.83-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.50Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.239 , 0.259 0.239 , 0.259	Depositor DCC
R_{free} test set	1545 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	94.8	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 88.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5771	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: BNG, 2OP

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	0.39	0/3070	0.55	0/4177
1	B	0.35	0/2834	0.54	0/3855
All	All	0.37	0/5904	0.54	0/8032

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

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	2980	0	3023	46	0
1	B	2752	0	2784	47	0
2	A	6	0	5	1	0
2	B	12	0	10	4	0
3	A	21	0	30	0	0
All	All	5771	0	5852	92	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 8.

All (92) 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:27:LEU:HD22	1:B:87:LEU:HD11	1.62	0.81
1:B:145:LEU:HD22	2:B:502:2OP:HA	1.65	0.77
1:B:159:ILE:HB	1:B:170:VAL:HG22	1.76	0.68
1:A:97:ILE:HD13	1:A:103:LEU:HD13	1.77	0.65
1:A:174:CYS:HB3	1:A:178:MET:HE3	1.80	0.62
1:B:95:GLY:O	1:B:168:ARG:NH2	2.34	0.61
1:A:145:LEU:HD22	2:A:501:2OP:HA	1.82	0.61
1:B:97:ILE:HD13	1:B:103:LEU:HD13	1.82	0.60
1:B:335:PHE:HE2	1:B:362:CYS:HG	1.48	0.60
1:A:170:VAL:O	1:A:174:CYS:HB2	2.02	0.59
1:B:26:MET:HB3	1:B:178:MET:HE1	1.85	0.59
1:A:396:LEU:HD11	1:B:308:ILE:HD11	1.86	0.58
1:A:31:TRP:O	1:A:35:ILE:HG13	2.04	0.57
1:B:87:LEU:HG	1:B:91:PHE:CE2	2.40	0.57
1:B:84:GLY:HA2	1:B:118:ILE:HD11	1.87	0.56
1:B:348:PRO:HA	1:B:351:GLN:HB2	1.88	0.56
1:A:23:THR:HG23	1:A:178:MET:HB3	1.87	0.55
1:A:245:LEU:HD13	1:A:366:GLY:HA2	1.86	0.55
1:B:245:LEU:HD13	1:B:366:GLY:HA2	1.87	0.55
1:B:41:GLU:CD	1:B:167:TRP:HE1	2.12	0.54
1:B:16:LEU:HD21	1:B:188:PHE:HB2	1.91	0.53
1:A:174:CYS:HB3	1:A:178:MET:CE	2.38	0.52
1:A:97:ILE:HG22	1:A:102:GLN:HG2	1.91	0.52
1:B:382:THR:HG23	1:B:384:TYR:H	1.73	0.52
1:A:107:TYR:O	1:A:111:ALA:HB3	2.09	0.52
1:A:303:GLN:OE1	1:A:327:ILE:HA	2.11	0.51
1:B:139:GLY:O	1:B:143:VAL:HB	2.10	0.50
1:B:247:VAL:HG21	1:B:307:MET:SD	2.51	0.50
1:A:65:PHE:HB3	1:A:66:PRO:HD3	1.93	0.50
1:A:86:LEU:HD13	1:A:113:PHE:CD1	2.47	0.50
1:A:95:GLY:HA3	1:A:172:TRP:NE1	2.28	0.49
1:A:295:TYR:CE2	1:A:299:LEU:HD11	2.47	0.49
1:A:132:ASP:OD1	1:A:132:ASP:N	2.36	0.48
1:B:107:TYR:O	1:B:111:ALA:HB3	2.13	0.48
1:B:303:GLN:O	1:B:307:MET:HG2	2.14	0.47
1:B:335:PHE:CE2	2:B:502:2OP:HB3	2.50	0.47
1:B:132:ASP:N	1:B:132:ASP:OD1	2.39	0.47
1:B:355:TYR:CE1	1:B:358:LEU:HD23	2.50	0.47
1:A:91:PHE:CD1	1:A:171:PHE:HD1	2.32	0.47
1:A:243:ALA:HB1	1:A:390:ALA:HB1	1.95	0.47
1:A:303:GLN:O	1:A:307:MET:HG2	2.14	0.47
1:B:65:PHE:HZ	1:B:221:TYR:HH	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:TYR:CE1	1:A:123:ILE:HD11	2.50	0.47
1:B:36:LYS:HB3	1:B:37:PRO:HD3	1.97	0.47
1:B:23:THR:HG23	1:B:178:MET:HB3	1.97	0.46
1:A:16:LEU:HD22	1:A:185:ALA:HA	1.98	0.46
1:B:87:LEU:HG	1:B:91:PHE:CZ	2.49	0.46
1:A:409:LYS:HA	1:A:409:LYS:HD2	1.78	0.46
1:B:292:ILE:HG21	1:B:341:THR:OG1	2.15	0.46
1:B:310:ILE:HB	1:B:323:VAL:HG11	1.98	0.46
1:A:418:LEU:C	1:A:420:GLN:H	2.19	0.45
1:B:30:ALA:O	1:B:33:VAL:HG22	2.16	0.45
1:B:11:TRP:HB3	1:B:130:TRP:HZ2	1.79	0.45
1:B:295:TYR:CZ	1:B:299:LEU:HD11	2.51	0.45
1:B:335:PHE:HE2	1:B:362:CYS:SG	2.39	0.45
1:A:376:LEU:HD22	1:A:385:LEU:HD23	1.99	0.45
1:A:221:TYR:O	1:A:225:LYS:HB3	2.17	0.45
1:A:87:LEU:HA	1:A:111:ALA:HA	1.98	0.45
1:A:295:TYR:CZ	1:A:299:LEU:HD11	2.51	0.45
1:B:58:LEU:O	1:B:62:LEU:HG	2.17	0.45
1:A:86:LEU:O	1:A:110:ILE:HG22	2.17	0.44
1:A:113:PHE:O	1:A:117:MET:HG3	2.18	0.44
1:B:218:ASP:OD1	1:B:348:PRO:HD2	2.18	0.44
1:B:65:PHE:HB3	1:B:66:PRO:HD3	1.99	0.44
1:B:303:GLN:OE1	1:B:327:ILE:HA	2.18	0.44
1:A:217:ARG:O	1:A:409:LYS:HE3	2.18	0.44
1:B:360:THR:O	1:B:364:LEU:HG	2.18	0.43
1:A:27:LEU:HD22	1:A:87:LEU:HD13	2.00	0.43
1:A:218:ASP:OD2	1:A:348:PRO:HD2	2.18	0.43
1:B:174:CYS:HB3	1:B:178:MET:HE3	2.01	0.43
1:B:167:TRP:HA	1:B:170:VAL:HG23	2.00	0.43
1:A:91:PHE:HB3	1:A:175:GLY:HA3	2.01	0.43
1:A:271:SER:HA	1:A:274:PHE:HD2	1.83	0.43
1:A:150:PHE:HE2	1:A:274:PHE:CE1	2.37	0.43
1:B:42:PHE:HD2	1:B:100:LYS:NZ	2.17	0.43
1:B:58:LEU:HD22	1:B:367:PHE:CG	2.53	0.43
1:B:230:PHE:N	1:B:346:TYR:OH	2.52	0.42
1:A:322:ILE:O	1:A:326:VAL:HG23	2.19	0.42
1:B:280:ARG:NH1	2:B:502:2OP:OXT	2.51	0.42
1:A:109:VAL:O	1:A:113:PHE:HB2	2.19	0.42
1:A:174:CYS:O	1:A:178:MET:HG3	2.20	0.42
1:A:384:TYR:O	1:A:388:LEU:HG	2.20	0.42
1:A:234:TYR:CE1	1:A:361:ALA:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ALA:O	1:A:416:GLU:N	2.52	0.41
1:B:234:TYR:HE2	1:B:357:LEU:O	2.02	0.41
1:A:126:ALA:N	1:A:127:PRO:HD2	2.35	0.41
1:A:377:LYS:O	1:A:381:GLY:N	2.51	0.41
1:B:280:ARG:HH22	2:B:502:2OP:C	2.33	0.41
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.77	0.40
1:B:64:THR:HG21	1:B:359:PHE:CD2	2.56	0.40
1:B:252:ALA:HA	1:B:269:VAL:HG21	2.02	0.40
1:A:79:VAL:HG13	1:A:117:MET:HE3	2.04	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	387/420 (92%)	380 (98%)	7 (2%)	0	100	100
1	B	358/420 (85%)	354 (99%)	4 (1%)	0	100	100
All	All	745/840 (89%)	734 (98%)	11 (2%)	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	291/307 (95%)	289 (99%)	2 (1%)	84	94
1	B	267/307 (87%)	264 (99%)	3 (1%)	73	89
All	All	558/614 (91%)	553 (99%)	5 (1%)	78	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	TYR
1	A	296	PHE
1	B	171	PHE
1	B	237	TYR
1	B	296	PHE

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	2OP	B	502	-	5,5,5	1.00	0	4,6,6	0.94	0
3	BNG	A	502	-	21,21,21	1.09	1 (4%)	26,26,26	1.14	3 (11%)
2	2OP	A	501	-	5,5,5	0.98	0	4,6,6	1.12	0
2	2OP	B	501	-	5,5,5	1.00	0	4,6,6	1.13	1 (25%)

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	2OP	B	502	-	-	2/4/4/4	-
3	BNG	A	502	-	-	3/12/32/32	0/1/1/1
2	2OP	A	501	-	-	2/4/4/4	-
2	2OP	B	501	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	BNG	O5-C1	3.06	1.49	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	BNG	O1-C1-C2	2.52	112.23	108.30
3	A	502	BNG	C4-C3-C2	2.43	115.06	110.82
3	A	502	BNG	C3-C4-C5	2.23	114.22	110.24
2	B	501	2OP	OXT-C-O	-2.09	119.35	124.09

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	2OP	O-C-CA-CB
2	B	501	2OP	OXT-C-CA-CB
3	A	502	BNG	C2'-C1'-O1-C1
3	A	502	BNG	O5-C5-C6-O6
2	B	501	2OP	OXT-C-CA-OHN
3	A	502	BNG	C4-C5-C6-O6
2	A	501	2OP	O-C-CA-CB

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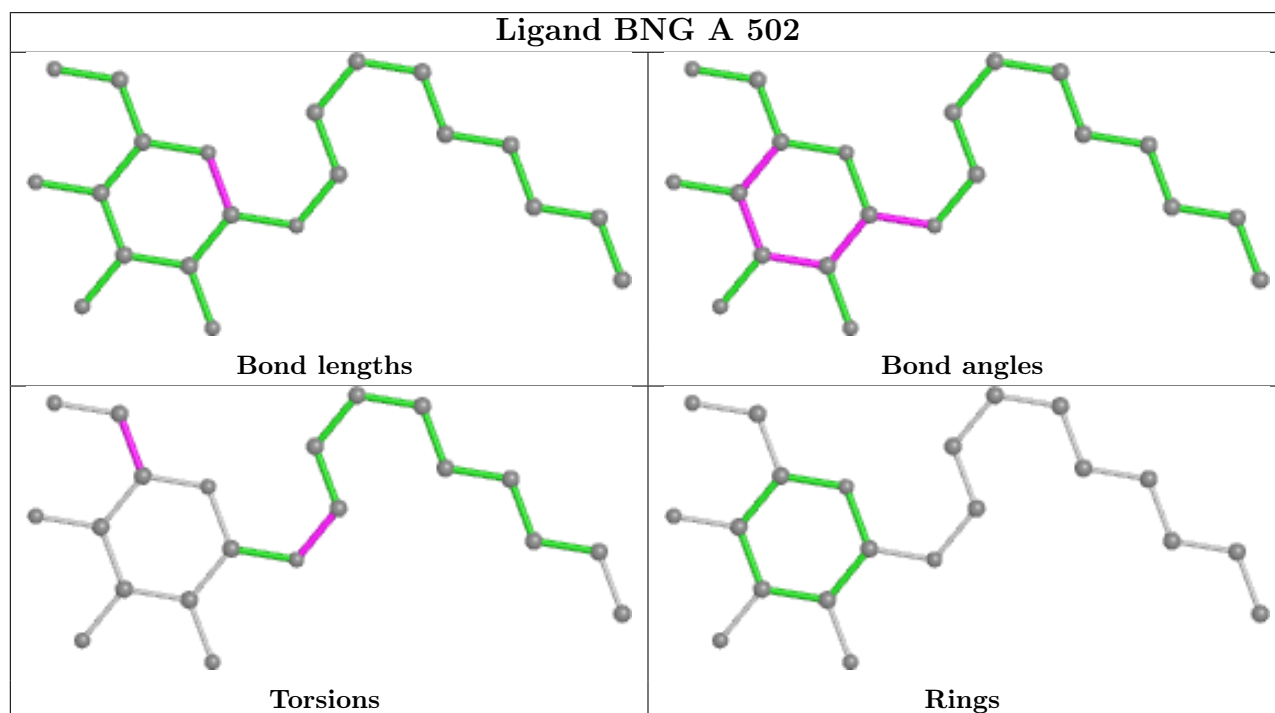
Mol	Chain	Res	Type	Atoms
2	A	501	2OP	OXT-C-CA-CB
2	B	502	2OP	O-C-CA-CB
2	B	502	2OP	OXT-C-CA-CB
2	B	501	2OP	O-C-CA-OHN

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	2OP	4	0
2	A	501	2OP	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.



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	A	395/420 (94%)	0.64	54 (13%) 3 2	54, 95, 165, 209	0
1	B	366/420 (87%)	1.05	89 (24%) 0 0	61, 127, 188, 217	0
All	All	761/840 (90%)	0.84	143 (18%) 1 1	54, 107, 180, 217	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	MET	8.8
1	A	169	TYR	8.5
1	A	151	LEU	8.4
1	B	158	TYR	8.2
1	B	191	PRO	7.8
1	B	129	TRP	7.4
1	A	73	LYS	7.4
1	A	107	TYR	7.1
1	A	173	TYR	6.7
1	B	216	THR	6.7
1	B	190	GLU	6.6
1	A	29	TYR	6.5
1	B	342	CYS	6.3
1	B	154	PRO	6.1
1	B	151	LEU	6.0
1	B	91	PHE	5.9
1	B	101	TYR	5.8
1	A	158	TYR	5.8
1	B	73	LYS	5.7
1	A	196	TRP	5.6
1	A	7	THR	5.5
1	B	111	ALA	5.4
1	B	98	GLN	5.4
1	A	212	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	125	THR	5.3
1	B	107	TYR	5.3
1	B	188	PHE	5.1
1	B	45	SER	5.1
1	B	70	LEU	4.9
1	B	157	THR	4.9
1	B	173	TYR	4.9
1	B	169	TYR	4.8
1	A	159	ILE	4.8
1	A	98	GLN	4.7
1	B	150	PHE	4.7
1	B	355	TYR	4.7
1	B	339	PRO	4.7
1	A	213	PRO	4.6
1	A	150	PHE	4.5
1	B	12	VAL	4.5
1	A	155	LEU	4.5
1	A	35	ILE	4.5
1	A	161	GLU	4.5
1	B	155	LEU	4.3
1	A	96	PHE	4.3
1	B	189	LEU	4.2
1	A	167	TRP	4.2
1	A	420	GLN	4.1
1	B	187	ALA	4.1
1	B	96	PHE	4.0
1	B	340	ALA	4.0
1	B	224	ALA	3.9
1	B	11	TRP	3.8
1	A	118	ILE	3.7
1	B	166	GLY	3.7
1	B	225	LYS	3.7
1	B	46	ARG	3.7
1	A	39	ASN	3.7
1	A	94	SER	3.7
1	A	91	PHE	3.7
1	B	40	ALA	3.7
1	B	259	GLY	3.6
1	B	343	LEU	3.5
1	B	138	THR	3.5
1	A	38	LEU	3.4
1	B	16	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	120	LEU	3.4
1	B	94	SER	3.4
1	A	160	ILE	3.4
1	B	336	THR	3.3
1	A	11	TRP	3.3
1	A	141	ALA	3.3
1	B	160	ILE	3.2
1	B	41	GLU	3.2
1	A	337	LEU	3.2
1	B	217	ARG	3.2
1	B	290	ILE	3.1
1	A	46	ARG	3.1
1	A	40	ALA	3.1
1	B	121	PRO	3.1
1	B	128	LYS	3.1
1	B	260	LEU	3.1
1	B	231	TRP	3.1
1	B	42	PHE	3.1
1	A	154	PRO	3.0
1	A	172	TRP	3.0
1	A	87	LEU	2.9
1	A	193	PRO	2.9
1	A	74	MET	2.8
1	A	112	GLY	2.8
1	B	341	THR	2.8
1	B	220	THR	2.8
1	A	342	CYS	2.8
1	B	337	LEU	2.8
1	B	29	TYR	2.7
1	B	119	TYR	2.7
1	B	118	ILE	2.7
1	B	286	PHE	2.7
1	A	31	TRP	2.7
1	A	394	CYS	2.6
1	A	334	MET	2.6
1	A	157	THR	2.6
1	B	112	GLY	2.6
1	B	219	TRP	2.5
1	A	123	ILE	2.5
1	B	351	GLN	2.4
1	B	104	TYR	2.4
1	B	115	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	82	THR	2.4
1	B	226	GLY	2.3
1	B	338	PHE	2.3
1	A	111	ALA	2.3
1	B	289	LYS	2.3
1	B	148	GLY	2.3
1	A	414	GLU	2.3
1	B	334	MET	2.3
1	B	122	PRO	2.3
1	B	402	PHE	2.3
1	A	41	GLU	2.3
1	A	122	PRO	2.2
1	B	78	LYS	2.2
1	B	403	MET	2.2
1	A	336	THR	2.2
1	B	172	TRP	2.2
1	B	353	SER	2.2
1	B	116	GLY	2.2
1	B	141	ALA	2.2
1	B	117	MET	2.2
1	B	90	GLY	2.1
1	B	77	ARG	2.1
1	B	239	CYS	2.1
1	B	113	PHE	2.1
1	B	88	ALA	2.1
1	A	8	MET	2.1
1	A	117	MET	2.1
1	A	138	THR	2.1
1	B	123	ILE	2.1
1	B	257	ASP	2.1
1	A	120	LEU	2.1
1	A	338	PHE	2.1
1	B	130	TRP	2.0
1	A	263	MET	2.0
1	B	81	MET	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](#)

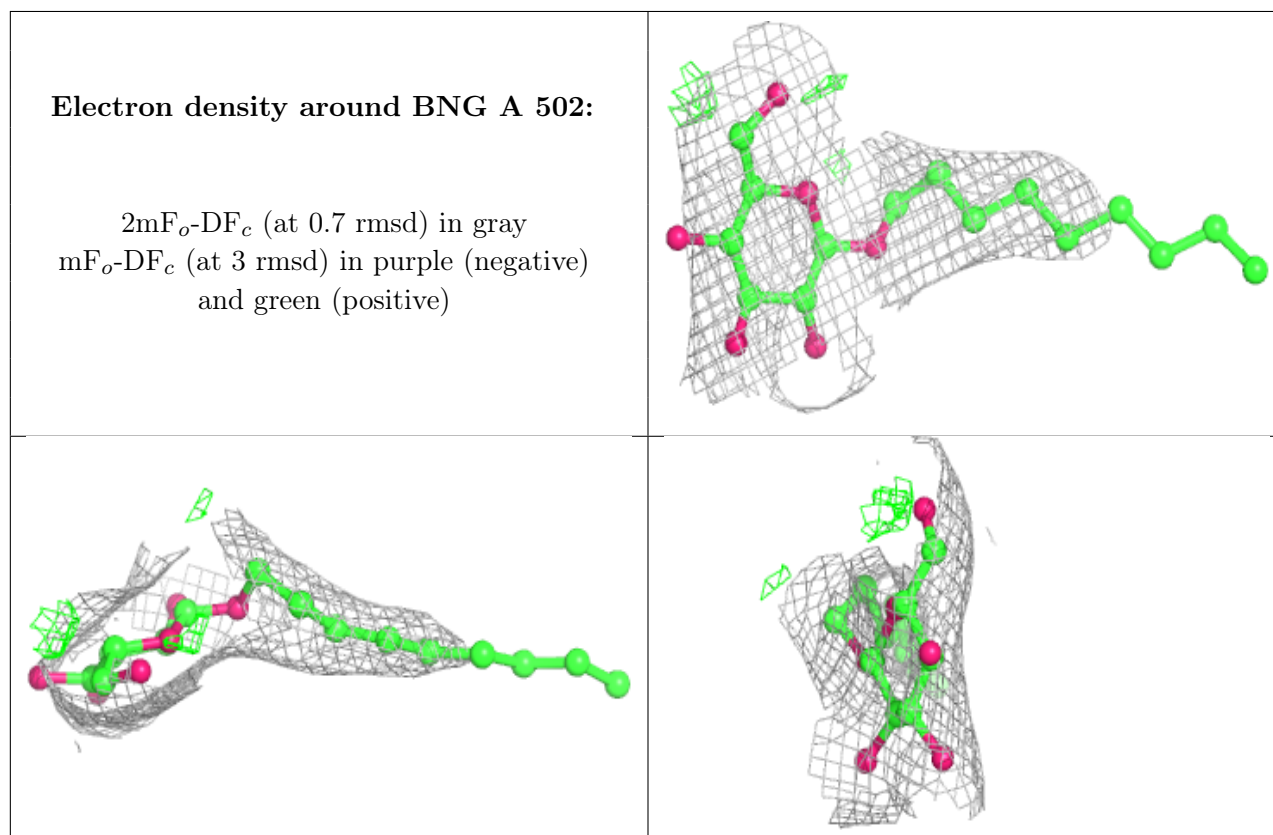
There are no monosaccharides in this entry.

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	2OP	B	501	6/6	0.44	0.55	106,123,128,128	0
3	BNG	A	502	21/21	0.76	0.27	101,125,151,164	0
2	2OP	B	502	6/6	0.83	0.28	106,115,119,121	0
2	2OP	A	501	6/6	0.93	0.29	81,110,110,119	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.