



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:30 AM UTC

PDB ID : 4CZ9 / pdb_00004cz9
Title : Structure of the sodium proton antiporter PaNhaP from *Pyrococcus abyssi* at pH 4.
Authors : Woehlert, D.; Kuhlbrandt, W.; Yildiz, O.
Deposited on : 2014-04-16
Resolution : 3.50 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	:	4-5-2 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

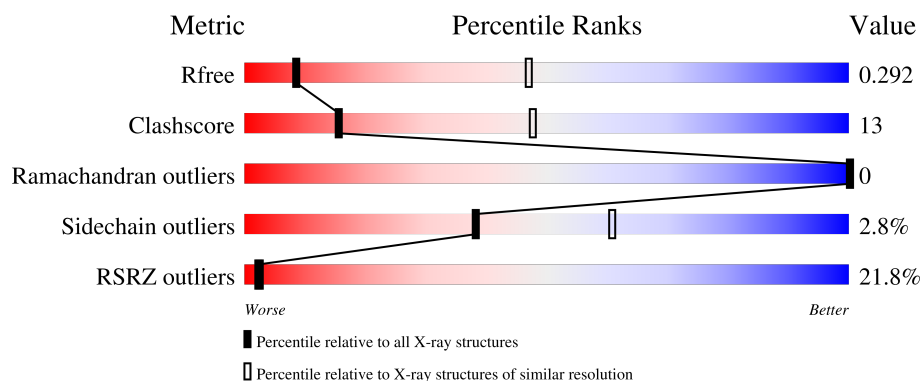
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	422	22% 68% 30% ..
1	B	422	22% 65% 33% .

2 Entry composition [i](#)

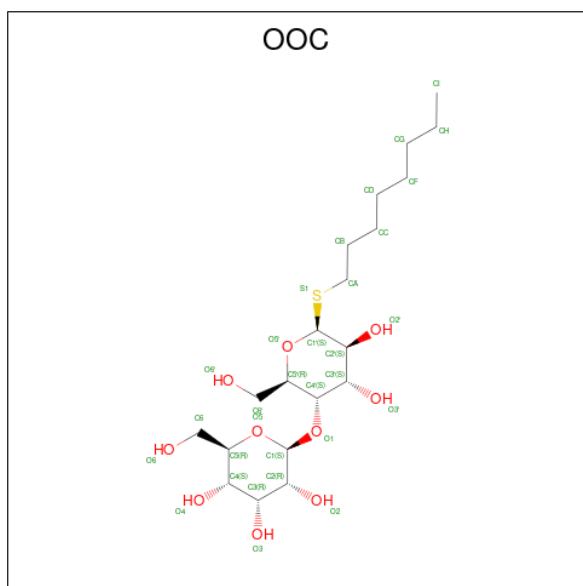
There are 3 unique types of molecules in this entry. The entry contains 6592 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NA⁺/H⁺ ANTIPORTER, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3276	2205	513	552	6			
1	B	420	Total	C	N	O	S	0	0	0
			3284	2210	514	553	7			

- Molecule 2 is octyl 4-O-beta-D-allopyranosyl-1-thio-beta-D-altropyranoside (CCD ID: OOC) (formula: C₂₀H₃₈O₁₀S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	S	0	0
			31	20	10	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total	0	0
			1		

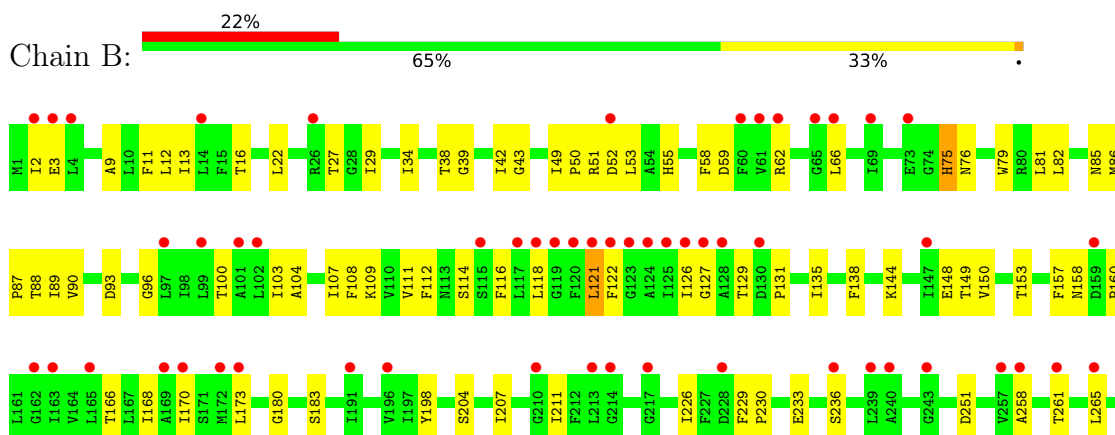
3 Residue-property plots

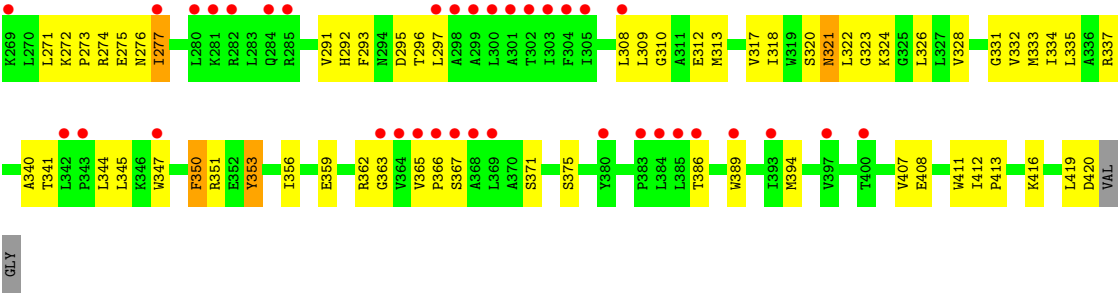
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NA⁺/H⁺ ANTIPTORTER, PUTATIVE



• Molecule 1: NA⁺/H⁺ ANTIPTORTER, PUTATIVE





4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	109.57Å 109.57Å 209.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-3.50) 98.7 (50.00-3.50)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.242 , 0.263 0.255 , 0.292	Depositor DCC
R_{free} test set	909 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	157.3	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 98.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.067 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6592	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
OOC

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	0.70	0/3349	0.88	3/4557 (0.1%)
1	B	0.66	0/3357	0.88	3/4567 (0.1%)
All	All	0.68	0/6706	0.88	6/9124 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	LEU	CA-C-N	-6.39	113.22	119.87
1	A	342	LEU	C-N-CA	-6.39	113.22	119.87
1	A	269	LYS	N-CA-C	-5.84	105.34	112.88
1	B	43	GLY	CA-C-N	5.74	127.02	119.84
1	B	43	GLY	C-N-CA	5.74	127.02	119.84
1	B	76	ASN	N-CA-C	5.47	117.25	111.28

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	3276	0	3510	86	0
1	B	3284	0	3522	100	0
2	B	31	0	38	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
All	All	6592	0	7070	183	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 13.

All (183) 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:323:GLY:HA2	1:B:326:LEU:HD12	1.64	0.80
1:A:233:GLU:OE1	1:A:236:SER:OG	2.00	0.79
1:B:109:LYS:NZ	1:B:114:SER:O	2.14	0.79
1:B:62:ARG:NH2	1:B:371:SER:OG	2.19	0.74
1:B:412:ILE:HG13	1:B:413:PRO:HD3	1.68	0.73
1:B:293:PHE:O	1:B:296:THR:OG1	2.05	0.71
1:B:75:HIS:HE1	1:B:265:LEU:HB2	1.56	0.70
1:A:50:PRO:HG2	1:A:53:LEU:HB3	1.73	0.69
1:A:173:LEU:HB3	1:A:385:LEU:HD11	1.76	0.68
1:A:293:PHE:O	1:A:296:THR:OG1	2.10	0.68
1:A:163:ILE:O	1:A:166:THR:OG1	2.10	0.68
1:B:127:GLY:O	1:B:362:ARG:NH1	2.27	0.66
1:A:383:PRO:HG2	1:A:384:LEU:HD12	1.78	0.65
1:A:3:GLU:HA	1:A:6:LEU:HD12	1.79	0.65
1:A:319:TRP:HA	1:A:322:LEU:HD23	1.79	0.64
1:A:227:PHE:CE2	1:A:283:LEU:HB3	2.33	0.63
1:A:339:LEU:HA	1:A:342:LEU:HD23	1.81	0.63
1:B:52:ASP:OD1	1:B:53:LEU:N	2.32	0.62
1:B:12:LEU:HB3	1:B:42:ILE:HD11	1.81	0.62
1:A:21:MET:HE1	1:B:230:PRO:HD2	1.81	0.62
1:A:386:THR:HG1	1:A:389:TRP:CD1	2.18	0.62
1:A:88:THR:HG23	1:A:344:LEU:HD11	1.82	0.61
1:A:416:LYS:NZ	1:A:420:ASP:OD2	2.33	0.61
1:A:220:PHE:O	1:A:224:THR:OG1	2.18	0.60
1:A:115:SER:HB3	1:A:118:LEU:HD13	1.84	0.59
1:A:75:HIS:CD2	1:A:291:VAL:HG22	2.38	0.59
1:B:2:ILE:HG13	1:B:3:GLU:H	1.68	0.59
1:B:111:VAL:HG21	1:B:328:VAL:HG22	1.84	0.59
1:B:198:TYR:OH	1:B:251:ASP:OD1	2.19	0.58
1:B:386:THR:HG1	1:B:389:TRP:CD1	2.20	0.58
1:B:271:LEU:HD11	1:B:275:GLU:HG2	1.85	0.58
1:B:310:GLY:HA2	1:B:313:MET:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:CE1	1:A:224:THR:HG21	2.39	0.57
1:A:12:LEU:HD13	1:A:42:ILE:HG21	1.85	0.57
1:B:408:GLU:OE1	1:B:411:TRP:NE1	2.35	0.57
1:A:72:THR:HG22	1:A:294:ASN:HB3	1.87	0.56
1:B:11:PHE:CD2	1:B:12:LEU:HD12	2.41	0.56
1:B:89:ILE:HG12	1:B:150:VAL:HG23	1.87	0.56
1:B:272:LYS:HD2	1:B:273:PRO:HD2	1.88	0.56
1:A:286:ALA:HA	1:A:289:LYS:HE2	1.87	0.55
1:B:309:LEU:HD22	1:B:367:SER:HB3	1.86	0.55
1:A:233:GLU:O	1:A:236:SER:OG	2.19	0.55
1:A:288:GLU:O	1:A:292:HIS:ND1	2.34	0.55
1:B:258:ALA:O	1:B:261:THR:OG1	2.22	0.55
1:B:112:PHE:CE1	1:B:324:LYS:HD3	2.41	0.55
1:B:16:THR:HG21	1:B:42:ILE:HD12	1.89	0.55
1:A:94:THR:OG1	1:A:95:ILE:N	2.40	0.54
1:B:180:GLY:O	1:B:183:SER:OG	2.21	0.54
1:A:77:LEU:HD23	1:A:263:ILE:HG23	1.88	0.54
1:B:233:GLU:O	1:B:236:SER:OG	2.14	0.54
1:A:126:ILE:O	1:A:362:ARG:NE	2.36	0.53
1:B:359:GLU:OE2	1:B:408:GLU:HB3	2.08	0.53
1:A:166:THR:HG21	1:A:369:LEU:HD13	1.90	0.53
1:B:81:LEU:HD21	1:B:149:THR:HB	1.91	0.53
1:B:144:LYS:HE3	1:B:416:LYS:HZ1	1.75	0.52
1:B:85:ASN:O	1:B:88:THR:OG1	2.27	0.52
1:B:51:ARG:HH21	1:B:394:MET:HE1	1.73	0.52
1:B:149:THR:OG1	1:B:150:VAL:N	2.41	0.52
1:A:129:THR:HG22	1:A:362:ARG:HD3	1.92	0.52
1:A:330:LEU:HA	1:A:333:MET:HE2	1.92	0.52
1:A:24:SER:OG	1:A:29:ILE:O	2.28	0.51
1:B:112:PHE:HE1	1:B:324:LYS:HD3	1.75	0.51
1:B:272:LYS:HG3	1:B:274:ARG:H	1.75	0.51
1:B:333:MET:HE1	1:B:407:VAL:HB	1.93	0.51
1:B:408:GLU:HA	1:B:411:TRP:NE1	2.24	0.51
1:B:12:LEU:HD23	1:B:42:ILE:HD11	1.93	0.51
1:A:38:THR:O	1:A:42:ILE:HG12	2.10	0.51
1:A:382:SER:HB2	1:A:385:LEU:HD13	1.93	0.51
1:A:242:LEU:HB2	1:B:11:PHE:CD1	2.46	0.51
1:B:9:ALA:O	1:B:13:ILE:HG12	2.12	0.50
1:B:51:ARG:NE	1:B:312:GLU:O	2.39	0.50
1:A:130:ASP:OD1	1:A:155:SER:OG	2.29	0.50
1:B:207:ILE:O	1:B:211:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ASN:OD1	1:B:277:ILE:N	2.45	0.50
1:A:183:SER:O	1:A:186:SER:OG	2.24	0.50
1:A:298:ALA:O	1:A:302:THR:OG1	2.29	0.49
1:B:86:MET:O	1:B:90:VAL:HG23	2.13	0.48
1:B:363:GLY:O	1:B:367:SER:OG	2.26	0.48
1:B:408:GLU:HA	1:B:411:TRP:CD1	2.47	0.48
1:B:345:LEU:HD11	1:B:350:PHE:HA	1.94	0.48
1:A:359:GLU:CD	1:A:408:GLU:HG3	2.39	0.48
1:A:151:ILE:O	1:A:154:GLU:HB3	2.13	0.48
1:A:198:TYR:OH	1:A:251:ASP:OD2	2.23	0.48
1:B:334:ILE:HG13	1:B:335:LEU:HD13	1.96	0.48
1:A:221:ILE:O	1:A:225:GLY:N	2.39	0.48
1:A:34:ILE:O	1:A:38:THR:OG1	2.24	0.47
1:A:77:LEU:O	1:A:267:ASN:ND2	2.44	0.47
1:A:333:MET:SD	1:A:404:SER:HA	2.54	0.47
1:A:129:THR:OG1	1:A:158:ASN:ND2	2.35	0.47
1:B:157:PHE:O	1:B:160:PRO:HD2	2.14	0.47
1:A:277:ILE:HA	1:A:280:LEU:HD12	1.96	0.47
1:B:55:HIS:CE1	1:B:375:SER:HB2	2.50	0.47
1:A:77:LEU:C	1:A:267:ASN:HD21	2.22	0.47
1:B:131:PRO:O	1:B:135:ILE:HG12	2.14	0.47
1:A:211:ILE:HA	1:A:264:VAL:HG21	1.96	0.47
1:A:242:LEU:HD13	1:B:11:PHE:CE2	2.50	0.47
1:B:313:MET:HB2	1:B:318:ILE:HD11	1.97	0.47
1:A:324:LYS:O	1:A:328:VAL:HG23	2.14	0.46
1:B:321:ASN:OD1	1:B:321:ASN:N	2.48	0.46
1:B:351:ARG:O	1:B:419:LEU:HD21	2.16	0.46
1:B:96:GLY:O	1:B:100:THR:OG1	2.24	0.46
1:B:328:VAL:O	1:B:332:VAL:HG23	2.15	0.46
1:B:104:ALA:HA	1:B:107:ILE:HB	1.97	0.46
1:A:23:ILE:HG23	1:A:34:ILE:HD13	1.97	0.46
1:B:129:THR:OG1	1:B:158:ASN:ND2	2.49	0.46
2:B:1001:OOC:H2	2:B:1001:OOC:H6'1	1.97	0.45
1:A:313:MET:HE3	1:A:318:ILE:HG21	1.97	0.45
1:B:118:LEU:HA	1:B:121:LEU:HD23	1.99	0.45
1:B:292:HIS:O	1:B:295:ASP:HB2	2.16	0.45
1:B:331:GLY:O	1:B:335:LEU:HB2	2.16	0.45
1:B:86:MET:N	1:B:87:PRO:HD2	2.31	0.45
1:A:155:SER:HA	1:A:158:ASN:ND2	2.32	0.45
1:B:93:ASP:N	1:B:93:ASP:OD1	2.48	0.45
1:A:145:GLN:O	1:A:149:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:O	1:B:111:VAL:HG23	2.16	0.45
1:A:32:VAL:O	1:A:35:PHE:HB2	2.17	0.45
1:B:58:PHE:HD2	1:B:308:LEU:HB3	1.82	0.45
1:B:104:ALA:O	1:B:108:PHE:N	2.44	0.45
1:A:62:ARG:HH22	1:A:371:SER:HB3	1.82	0.44
1:B:49:ILE:HA	1:B:50:PRO:HD3	1.77	0.44
1:B:59:ASP:HA	1:B:62:ARG:HH11	1.82	0.44
1:B:168:ILE:HD11	1:B:198:TYR:CD2	2.53	0.44
1:B:318:ILE:O	1:B:322:LEU:N	2.50	0.44
1:A:92:LEU:HD11	1:A:341:THR:HG22	2.00	0.44
1:A:75:HIS:CE1	1:A:265:LEU:HB2	2.53	0.43
1:A:75:HIS:O	1:A:77:LEU:N	2.51	0.43
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.84	0.43
1:A:102:LEU:HD12	1:A:120:PHE:HE1	1.83	0.43
1:A:121:LEU:HD21	1:A:373:PRO:HB3	2.00	0.43
1:A:123:GLY:O	1:A:126:ILE:HG13	2.18	0.43
1:B:317:VAL:O	1:B:320:SER:OG	2.37	0.43
1:A:164:VAL:O	1:A:168:ILE:HG12	2.19	0.43
1:A:404:SER:O	1:A:408:GLU:HB2	2.18	0.43
1:B:138:PHE:HD2	1:B:148:GLU:HG3	1.83	0.43
1:A:125:ILE:HG23	1:A:369:LEU:HB2	2.01	0.43
1:A:392:ILE:O	1:A:396:THR:OG1	2.36	0.43
1:B:55:HIS:NE2	1:B:375:SER:HB2	2.33	0.43
1:A:37:LEU:O	1:A:40:LEU:HB3	2.18	0.43
1:B:150:VAL:O	1:B:153:THR:OG1	2.33	0.43
1:B:324:LYS:O	1:B:328:VAL:HG23	2.19	0.43
1:A:12:LEU:HD21	1:A:49:ILE:HD11	2.00	0.43
1:A:363:GLY:O	1:A:366:PRO:HD2	2.18	0.43
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.76	0.42
1:B:416:LYS:NZ	1:B:420:ASP:OD2	2.40	0.42
1:A:280:LEU:O	1:A:283:LEU:HG	2.19	0.42
1:B:96:GLY:HA2	1:B:340:ALA:HB1	2.00	0.42
1:B:103:ILE:O	1:B:107:ILE:HG13	2.18	0.42
1:A:79:TRP:N	1:A:267:ASN:OD1	2.38	0.42
1:B:50:PRO:HB2	1:B:52:ASP:OD1	2.19	0.42
1:B:166:THR:O	1:B:170:ILE:HG12	2.19	0.42
1:B:204:SER:O	1:B:207:ILE:HG13	2.19	0.42
1:A:146:ASP:O	1:A:149:THR:OG1	2.27	0.42
1:B:39:GLY:HA2	1:B:42:ILE:HG22	2.01	0.42
1:B:386:THR:HG1	1:B:389:TRP:HD1	1.66	0.42
1:A:235:PHE:CE2	1:A:239:LEU:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASP:O	1:A:55:HIS:HB3	2.18	0.42
1:B:66:LEU:HD23	1:B:66:LEU:HA	1.79	0.42
1:B:79:TRP:O	1:B:82:LEU:HG	2.19	0.42
1:B:122:PHE:O	1:B:126:ILE:HG12	2.19	0.42
1:B:75:HIS:CD2	1:B:291:VAL:HG22	2.55	0.42
1:A:78:SER:OG	1:A:81:LEU:HB2	2.20	0.41
1:A:402:LEU:O	1:A:406:ILE:HG22	2.20	0.41
1:A:129:THR:O	1:A:155:SER:OG	2.24	0.41
1:A:354:LEU:HD12	1:A:354:LEU:HA	1.90	0.41
1:B:34:ILE:O	1:B:38:THR:OG1	2.24	0.41
1:A:226:ILE:HG12	1:B:22:LEU:HD21	2.01	0.41
1:A:158:ASN:OD1	1:A:159:ASP:N	2.54	0.41
1:B:27:THR:HG22	1:B:29:ILE:HG13	2.02	0.41
1:B:126:ILE:O	1:B:362:ARG:NH1	2.54	0.41
1:A:15:PHE:O	1:A:19:ILE:HG12	2.21	0.41
1:B:173:LEU:HA	1:B:173:LEU:HD23	1.82	0.41
1:B:121:LEU:HD13	1:B:170:ILE:HD11	2.03	0.41
1:B:337:ARG:O	1:B:341:THR:OG1	2.25	0.41
1:A:342:LEU:N	1:A:343:PRO:HD2	2.36	0.41
1:A:40:LEU:O	1:A:44:PRO:HD2	2.21	0.41
1:B:293:PHE:HE1	1:B:297:LEU:HD11	1.85	0.41
1:A:411:TRP:CE3	1:A:411:TRP:HA	2.55	0.40
1:B:39:GLY:O	1:B:42:ILE:HG22	2.21	0.40
1:B:365:VAL:HB	1:B:366:PRO:HD3	2.04	0.40
1:B:272:LYS:NZ	1:B:273:PRO:HG2	2.36	0.40
1:A:308:LEU:HA	1:A:308:LEU:HD23	1.89	0.40
1:B:272:LYS:NZ	1:B:274:ARG:HG3	2.37	0.40
1:B:344:LEU:HD11	1:B:353:TYR:HB2	2.02	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	417/422 (99%)	398 (95%)	19 (5%)	0	100	100
1	B	418/422 (99%)	396 (95%)	22 (5%)	0	100	100
All	All	835/844 (99%)	794 (95%)	41 (5%)	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	A	357/359 (99%)	348 (98%)	9 (2%)	42	63
1	B	358/359 (100%)	347 (97%)	11 (3%)	35	59
All	All	715/718 (100%)	695 (97%)	20 (3%)	38	61

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	16	THR
1	A	116	PHE
1	A	126	ILE
1	A	164	VAL
1	A	173	LEU
1	A	318	ILE
1	A	408	GLU
1	A	411	TRP
1	B	75	HIS
1	B	116	PHE
1	B	121	LEU
1	B	226	ILE
1	B	229	PHE
1	B	277	ILE
1	B	321	ASN
1	B	347	TRP
1	B	350	PHE

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Mol	Chain	Res	Type
1	B	353	TYR
1	B	356	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	B	75	HIS
1	B	267	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	OOC	B	1001	-	32,32,32	0.65	1 (3%)	42,43,43	1.19	3 (7%)

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	OOC	B	1001	-	-	10/17/57/57	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	OOC	CA-S1	-2.12	1.78	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	OOC	CA-S1-C1'	4.53	110.23	100.45
2	B	1001	OOC	C1'-O5'-C5'	-2.54	108.01	112.56
2	B	1001	OOC	C1-O1-C4'	-2.09	113.03	117.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	OOC	O5-C1-O1-C4'
2	B	1001	OOC	C2-C1-O1-C4'
2	B	1001	OOC	O5-C5-C6-O6
2	B	1001	OOC	C4-C5-C6-O6
2	B	1001	OOC	CD-CF-CG-CH
2	B	1001	OOC	O5'-C5'-C6'-O6'
2	B	1001	OOC	CB-CC-CD-CF
2	B	1001	OOC	C4'-C5'-C6'-O6'
2	B	1001	OOC	S1-CA-CB-CC
2	B	1001	OOC	CC-CD-CF-CG

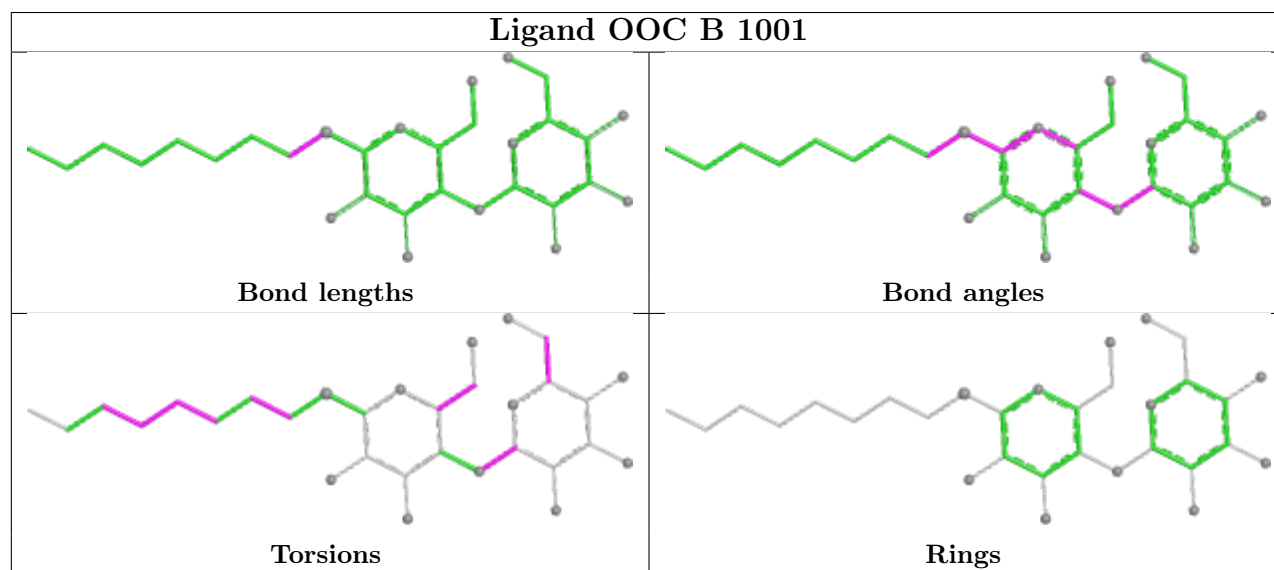
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	OOC	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	419/422 (99%)	1.33	92 (21%) 2 2	78, 137, 180, 244	0
1	B	420/422 (99%)	1.16	91 (21%) 2 3	92, 150, 205, 233	0
All	All	839/844 (99%)	1.24	183 (21%) 2 2	78, 143, 197, 244	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	LEU	16.4
1	A	47	LYS	14.9
1	A	142	ARG	13.3
1	A	46	LEU	13.1
1	A	106	PHE	12.4
1	A	51	ARG	10.5
1	B	384	LEU	10.1
1	A	44	PRO	10.0
1	B	117	LEU	9.6
1	A	102	LEU	9.3
1	A	48	LEU	8.3
1	B	383	PRO	7.9
1	A	316	GLU	7.9
1	B	173	LEU	7.5
1	A	315	LEU	6.9
1	B	301	ALA	6.8
1	B	115	SER	6.8
1	B	126	ILE	6.8
1	B	300	LEU	6.7
1	A	41	VAL	6.7
1	A	43	GLY	6.5
1	B	304	PHE	6.1
1	B	281	LYS	6.0
1	A	132	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	314	ASN	5.7
1	B	369	LEU	5.7
1	A	139	ARG	5.6
1	A	145	GLN	5.5
1	B	123	GLY	5.5
1	B	61	VAL	5.5
1	B	305	ILE	5.4
1	B	280	LEU	5.3
1	B	366	PRO	5.2
1	B	302	THR	5.2
1	B	284	GLN	5.2
1	B	121	LEU	5.1
1	B	128	ALA	5.1
1	A	230	PRO	5.0
1	A	110	VAL	5.0
1	B	118	LEU	4.9
1	B	261	THR	4.9
1	A	103	ILE	4.9
1	B	60	PHE	4.9
1	A	295	ASP	4.8
1	B	365	VAL	4.8
1	B	65	GLY	4.7
1	B	298	ALA	4.7
1	B	299	ALA	4.6
1	B	52	ASP	4.6
1	B	239	LEU	4.6
1	B	240	ALA	4.5
1	B	125	ILE	4.4
1	B	243	GLY	4.4
1	A	184	THR	4.3
1	B	172	MET	4.3
1	B	364	VAL	4.3
1	A	187	GLU	4.3
1	A	69	ILE	4.3
1	A	380	TYR	4.3
1	A	72	THR	4.2
1	B	343	PRO	4.2
1	B	127	GLY	4.2
1	A	325	GLY	4.1
1	A	209	LEU	4.1
1	A	192	TYR	4.1
1	B	368	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	42	ILE	4.1
1	A	298	ALA	4.1
1	A	40	LEU	4.0
1	B	265	LEU	4.0
1	A	99	LEU	4.0
1	B	285	ARG	3.9
1	A	379	LYS	3.9
1	B	66	LEU	3.9
1	A	382	SER	3.9
1	B	101	ALA	3.9
1	B	120	PHE	3.8
1	A	65	GLY	3.8
1	A	234	ALA	3.8
1	B	2	ILE	3.7
1	B	124	ALA	3.7
1	B	169	ALA	3.6
1	B	130	ASP	3.6
1	B	214	GLY	3.6
1	B	397	VAL	3.5
1	A	339	LEU	3.5
1	B	342	LEU	3.5
1	A	297	LEU	3.5
1	B	389	TRP	3.5
1	A	243	GLY	3.4
1	B	213	LEU	3.4
1	A	152	VAL	3.4
1	A	73	GLU	3.4
1	A	376	LEU	3.4
1	B	73	GLU	3.4
1	A	246	ILE	3.4
1	A	60	PHE	3.4
1	A	175	PRO	3.4
1	B	303	ILE	3.3
1	A	2	ILE	3.3
1	B	3	GLU	3.3
1	A	301	ALA	3.2
1	A	412	ILE	3.2
1	A	148	GLU	3.2
1	B	257	VAL	3.2
1	A	188	LYS	3.2
1	B	163	ILE	3.1
1	B	210	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	14	LEU	3.1
1	A	299	ALA	3.1
1	A	391	GLU	3.1
1	B	159	ASP	3.1
1	B	393	ILE	3.1
1	A	213	LEU	3.0
1	A	323	GLY	3.0
1	B	122	PHE	3.0
1	A	373	PRO	2.9
1	B	380	TYR	2.9
1	B	363	GLY	2.9
1	A	135	ILE	2.9
1	A	345	LEU	2.9
1	A	67	VAL	2.9
1	A	210	GLY	2.9
1	A	107	ILE	2.9
1	B	62	ARG	2.9
1	A	261	THR	2.9
1	B	258	ALA	2.8
1	B	386	THR	2.8
1	A	409	THR	2.8
1	A	68	ILE	2.8
1	A	70	LEU	2.8
1	B	269	LYS	2.7
1	B	165	LEU	2.7
1	A	359	GLU	2.7
1	A	335	LEU	2.7
1	B	170	ILE	2.7
1	B	277	ILE	2.6
1	B	282	ARG	2.6
1	A	165	LEU	2.6
1	B	367	SER	2.5
1	B	119	GLY	2.5
1	A	52	ASP	2.5
1	B	162	GLY	2.5
1	B	308	LEU	2.5
1	A	181	ILE	2.5
1	B	236	SER	2.5
1	A	241	PHE	2.5
1	A	247	GLY	2.5
1	A	383	PRO	2.4
1	B	99	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	64	PHE	2.4
1	B	69	ILE	2.4
1	A	270	LEU	2.4
1	B	102	LEU	2.4
1	A	350	PHE	2.3
1	A	361	PRO	2.3
1	A	257	VAL	2.3
1	A	233	GLU	2.3
1	A	400	THR	2.3
1	B	4	LEU	2.3
1	B	385	LEU	2.3
1	A	49	ILE	2.3
1	B	26	ARG	2.2
1	B	400	THR	2.2
1	A	385	LEU	2.2
1	B	97	LEU	2.2
1	B	297	LEU	2.2
1	B	196	VAL	2.2
1	A	396	THR	2.2
1	B	217	GLY	2.2
1	A	228	ASP	2.1
1	B	228	ASP	2.1
1	A	232	ILE	2.1
1	A	399	ILE	2.1
1	A	273	PRO	2.1
1	B	347	TRP	2.1
1	B	191	ILE	2.1
1	A	185	LEU	2.1
1	A	218	TYR	2.1
1	B	147	ILE	2.1
1	A	130	ASP	2.0
1	A	89	ILE	2.0
1	A	161	LEU	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](#)

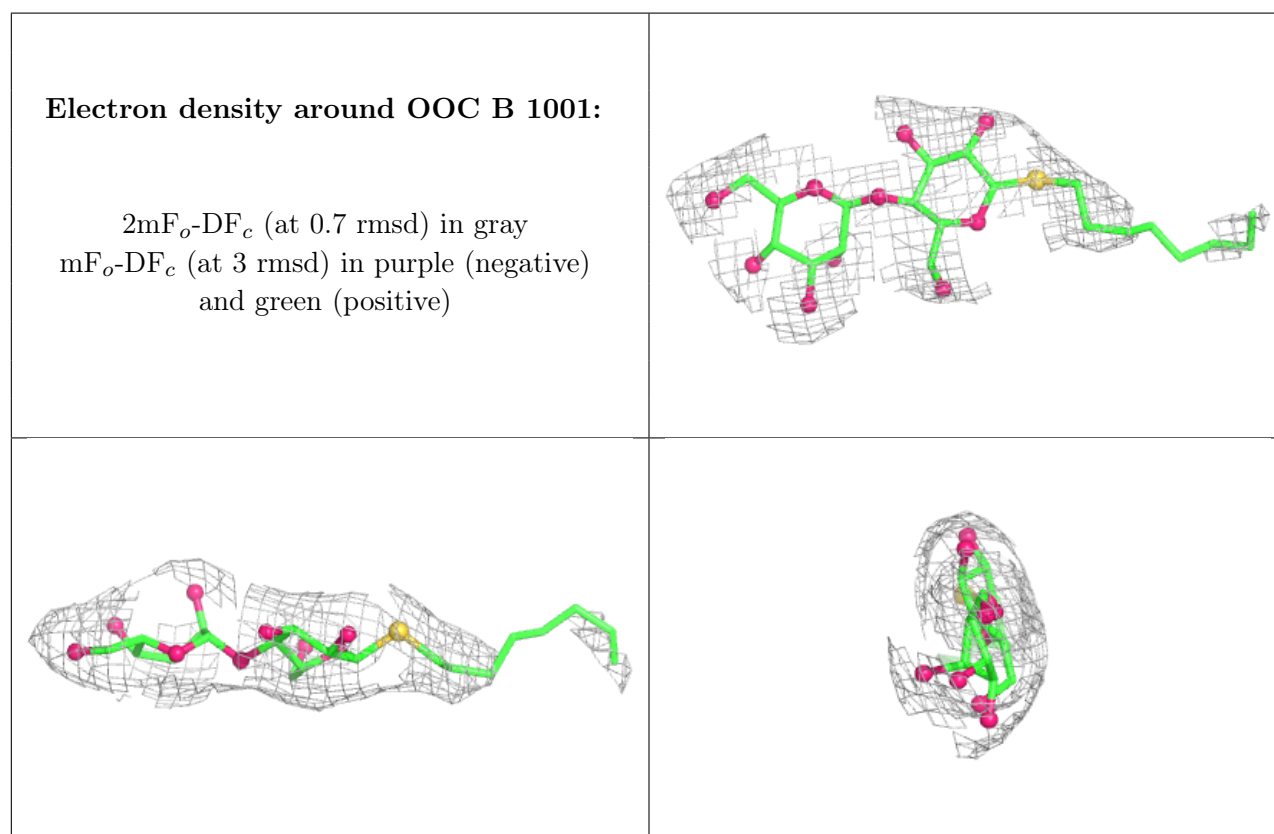
There are no oligosaccharides in this entry.

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	OOC	B	1001	31/31	0.86	0.14	97,157,183,196	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.