



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 06:02 PM EDT

PDB ID : 2Y4E
Title : X-ray crystallographic structure of E. coli ppix-EfeB
Authors : Bamford, V.A.; Andrews, S.C.; Watson, K.A.
Deposited on : 2011-01-05
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

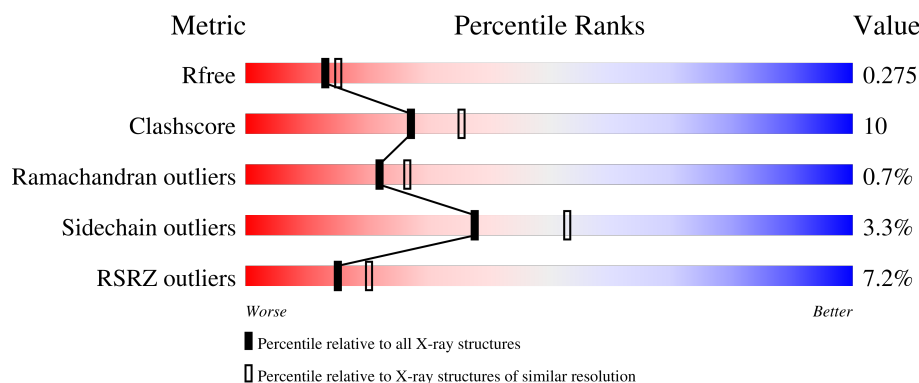
1 Overall quality at a glance

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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	403	<div> <div>6%</div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div>
1	B	403	<div> <div>8%</div> <div>78%</div> <div>17%</div> <div>5%</div> </div>

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	PP9	B	1389	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6409 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 PEROXIDASE YCDB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	5	0
			3033	1918	530	574	11			
1	B	384	Total	C	N	O	S	0	0	0
			2998	1898	525	564	11			

There are 30 discrepancies between the modelled and reference sequences:

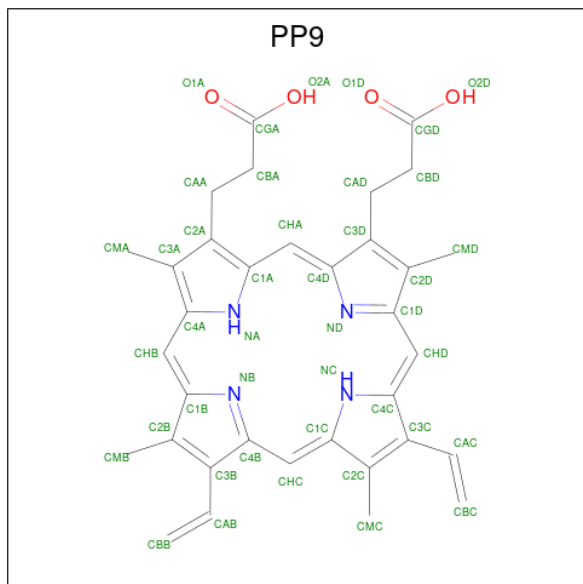
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	expression tag	UNP P31545
A	-13	ALA	-	expression tag	UNP P31545
A	-12	HIS	-	expression tag	UNP P31545
A	-11	HIS	-	expression tag	UNP P31545
A	-10	HIS	-	expression tag	UNP P31545
A	-9	HIS	-	expression tag	UNP P31545
A	-8	HIS	-	expression tag	UNP P31545
A	-7	HIS	-	expression tag	UNP P31545
A	-6	VAL	-	expression tag	UNP P31545
A	-5	ASP	-	expression tag	UNP P31545
A	-4	ASP	-	expression tag	UNP P31545
A	-3	ASP	-	expression tag	UNP P31545
A	-2	ASP	-	expression tag	UNP P31545
A	-1	LYS	-	expression tag	UNP P31545
A	0	ILE	-	expression tag	UNP P31545
B	-14	MET	-	expression tag	UNP P31545
B	-13	ALA	-	expression tag	UNP P31545
B	-12	HIS	-	expression tag	UNP P31545
B	-11	HIS	-	expression tag	UNP P31545
B	-10	HIS	-	expression tag	UNP P31545
B	-9	HIS	-	expression tag	UNP P31545
B	-8	HIS	-	expression tag	UNP P31545
B	-7	HIS	-	expression tag	UNP P31545
B	-6	VAL	-	expression tag	UNP P31545
B	-5	ASP	-	expression tag	UNP P31545

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ASP	-	expression tag	UNP P31545
B	-3	ASP	-	expression tag	UNP P31545
B	-2	ASP	-	expression tag	UNP P31545
B	-1	LYS	-	expression tag	UNP P31545
B	0	ILE	-	expression tag	UNP P31545

- Molecule 2 is PROTOPORPHYRIN IX (three-letter code: PP9) (formula: $C_{34}H_{34}N_4O_4$).



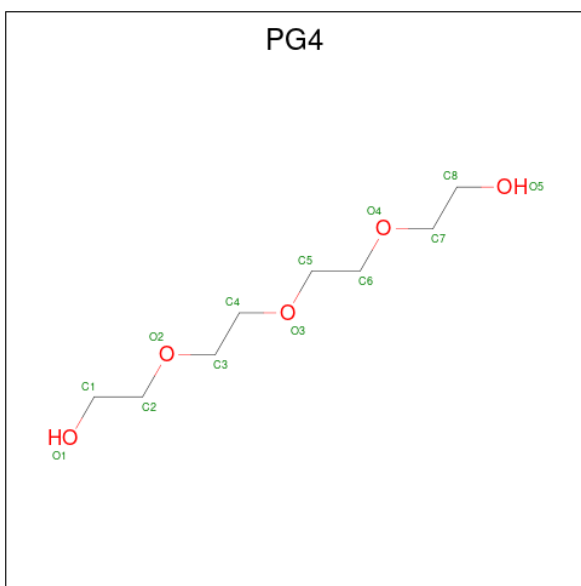
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			42	34	4	4		
2	B	1	Total	C	N	O	0	0
			42	34	4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			13	8	5		

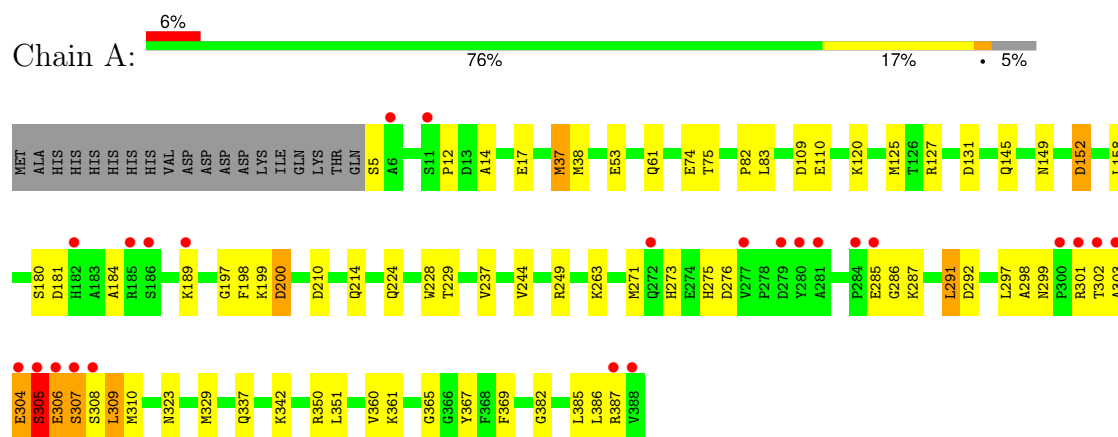
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	166	Total 166	O 166	0	0
5	B	92	Total 92	O 92	0	0

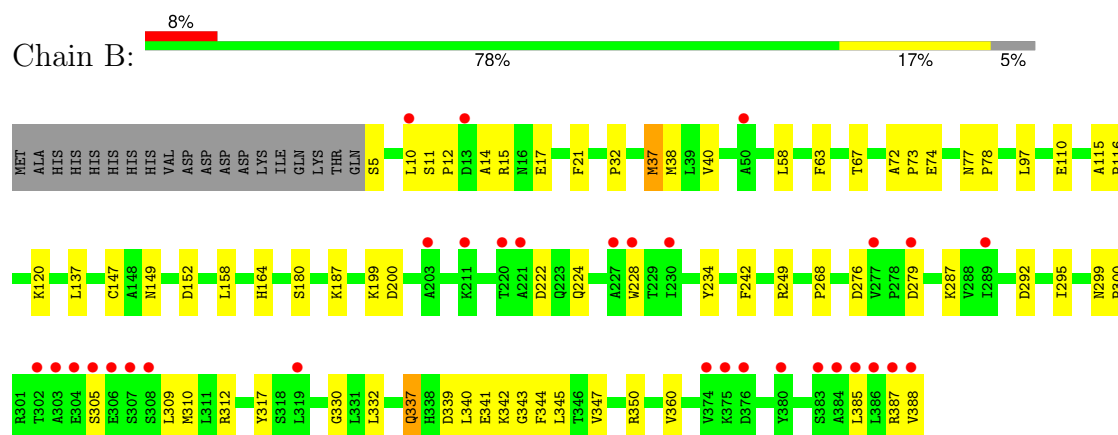
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PEROXIDASE YCDB



• Molecule 1: PEROXIDASE YCDB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.95Å 86.62Å 120.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.30 48.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.6 (48.80-2.30) 93.6 (48.79-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.208 , 0.283 0.204 , 0.275	Depositor DCC
R_{free} test set	1840 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6409	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: PP9, PG4, SO4

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	0/3102	0.69	2/4204 (0.0%)
1	B	0.54	0/3067	0.65	0/4157
All	All	0.58	0/6169	0.67	2/8361 (0.0%)

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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	109	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	329	MET	CG-SD-CE	-5.16	91.95	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	GLU	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	A	3033	0	2993	74	0
1	B	2998	0	2962	49	0
2	A	42	0	32	13	0
2	B	42	0	32	8	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	26	0	36	0	0
5	A	166	0	0	9	0
5	B	92	0	0	4	0
All	All	6409	0	6055	123	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 10.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305[B]:SER:OG	1:A:309[B]:LEU:HD21	1.37	1.18
1:A:307[B]:SER:OG	2:A:1389:PP9:HMD1	1.51	1.07
1:A:299:ASN:HD22	2:A:1389:PP9:HBD1	1.32	0.94
1:A:306[A]:GLU:O	1:A:309[A]:LEU:HD11	1.68	0.94
1:B:295:ILE:HD11	2:B:1389:PP9:HAA1	1.51	0.91
1:A:75:THR:HG21	1:A:82:PRO:HA	1.53	0.91
1:A:75:THR:CG2	1:A:83:LEU:H	1.83	0.91
1:A:306[B]:GLU:O	1:A:309[B]:LEU:HG	1.74	0.87
1:A:249:ARG:HG3	5:A:2123:HOH:O	1.74	0.86
1:A:305[B]:SER:OG	1:A:309[B]:LEU:CD2	2.23	0.85
1:A:305[B]:SER:HG	1:A:309[B]:LEU:HD21	1.41	0.85
1:B:21:PHE:HB2	1:B:67:THR:HG21	1.59	0.84
1:A:306[A]:GLU:O	1:A:306[A]:GLU:HG3	1.76	0.83
1:A:304:GLU:O	1:A:305[B]:SER:HB2	1.76	0.83
1:A:351:LEU:HD12	2:A:1389:PP9:HBC1	1.61	0.81
1:A:306[B]:GLU:HG2	1:A:308[B]:SER:H	1.48	0.77
1:A:286:GLY:HA3	1:A:291:LEU:HD13	1.64	0.77
1:B:360:VAL:HG21	2:B:1389:PP9:HBB2	1.69	0.75
1:A:305[B]:SER:CB	1:A:309[B]:LEU:HD21	2.17	0.74
1:B:37:MET:HE1	1:B:332:LEU:CD1	2.21	0.70
1:B:63:PHE:O	1:B:67:THR:HG22	1.93	0.69
1:B:120:LYS:HG3	1:B:224:GLN:O	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:GLN:HG2	1:B:343:GLY:HA3	1.75	0.69
1:A:12:PRO:HA	1:A:149:ASN:HB3	1.74	0.68
1:B:110:GLU:H	1:B:110:GLU:CD	1.95	0.68
1:A:198:PHE:CE1	1:A:263:LYS:HG3	2.29	0.68
1:B:309:LEU:HD12	5:B:2022:HOH:O	1.94	0.67
1:A:298:ALA:HB2	1:A:351:LEU:HD21	1.78	0.66
1:A:304:GLU:HG3	5:A:2136:HOH:O	1.96	0.65
1:B:37:MET:HE1	1:B:332:LEU:HD13	1.79	0.64
1:A:38:MET:SD	1:A:158:LEU:HD22	2.37	0.64
1:A:75:THR:HG21	1:A:83:LEU:H	1.61	0.63
1:A:307[B]:SER:CB	2:A:1389:PP9:HMD1	2.28	0.62
1:B:199:LYS:O	2:B:1389:PP9:HMA2	1.99	0.62
1:A:302:THR:HG22	1:A:303:ALA:H	1.65	0.61
1:A:152:ASP:OD2	1:B:180:SER:HA	2.02	0.60
1:A:125:MET:HG3	1:A:367:TYR:CZ	2.37	0.59
1:A:299:ASN:ND2	1:A:307[B]:SER:HB3	2.18	0.59
1:A:307[B]:SER:OG	2:A:1389:PP9:CMD	2.41	0.58
1:B:5:SER:HA	5:B:2041:HOH:O	2.04	0.57
1:B:310:MET:HE1	1:B:344:PHE:HA	1.85	0.57
1:A:307[B]:SER:C	1:A:309[B]:LEU:H	2.08	0.57
1:A:75:THR:HG22	1:A:83:LEU:H	1.65	0.56
1:A:301:ARG:HA	1:A:306[B]:GLU:HB2	1.88	0.56
1:B:341:GLU:HA	1:B:345:LEU:HB2	1.88	0.56
1:A:199:LYS:O	2:A:1389:PP9:HMA2	2.07	0.55
1:B:37:MET:HE1	1:B:332:LEU:HD12	1.88	0.55
2:B:1389:PP9:HHA	2:B:1389:PP9:CGA	2.36	0.55
1:B:14:ALA:HB1	1:B:17:GLU:HB2	1.88	0.54
1:B:310:MET:HE3	1:B:347:VAL:HG21	1.90	0.54
1:B:40:VAL:HG11	1:B:158:LEU:HD13	1.90	0.53
1:A:299:ASN:OD1	1:A:306[B]:GLU:HG3	2.09	0.53
1:A:228:TRP:CE2	1:A:385:LEU:HD13	2.44	0.53
1:B:300:PRO:HD3	1:B:350:ARG:HD3	1.91	0.52
1:B:337:GLN:HE21	1:B:337:GLN:N	2.08	0.52
1:B:10:LEU:HG	1:B:32:PRO:HB2	1.92	0.52
1:A:181:ASP:O	1:A:184:ALA:HB3	2.10	0.52
1:B:137:LEU:HD21	3:B:1390:SO4:O1	2.08	0.51
1:A:249:ARG:CG	5:A:2123:HOH:O	2.45	0.51
1:A:110:GLU:H	1:A:110:GLU:CD	2.14	0.51
1:A:360:VAL:HG21	2:A:1389:PP9:HBB2	1.93	0.50
1:A:323:ASN:ND2	5:A:2148:HOH:O	2.44	0.49
1:B:11:SER:HB2	1:B:187:LYS:HE3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LYS:HD2	1:A:224:GLN:O	2.13	0.48
1:A:200:ASP:OD2	2:A:1389:PP9:HHB	2.14	0.48
2:A:1389:PP9:HMC3	5:A:2116:HOH:O	2.12	0.48
1:A:214:GLN:O	5:A:2109:HOH:O	2.20	0.47
1:B:37:MET:HG2	1:B:38:MET:N	2.29	0.47
1:B:110:GLU:N	1:B:110:GLU:OE1	2.44	0.47
1:A:302:THR:HG22	1:A:303:ALA:N	2.30	0.46
1:A:307[B]:SER:C	1:A:309[B]:LEU:N	2.68	0.46
1:B:228:TRP:CE2	1:B:385:LEU:HD13	2.51	0.46
1:A:74:GLU:O	1:A:83:LEU:HD12	2.16	0.46
1:A:299:ASN:ND2	2:A:1389:PP9:HBD1	2.14	0.46
1:B:234:TYR:CD2	1:B:340:LEU:HB2	2.49	0.46
1:B:268:PRO:HG2	1:B:276:ASP:O	2.16	0.46
1:A:75:THR:HG21	1:A:83:LEU:N	2.29	0.46
1:A:304:GLU:O	1:A:305[B]:SER:CB	2.56	0.46
1:A:37:MET:HG3	1:A:38:MET:N	2.29	0.46
1:A:198:PHE:CZ	1:A:263:LYS:HG3	2.50	0.46
1:A:199:LYS:O	2:A:1389:PP9:HBA2	2.15	0.45
1:A:382:GLY:HA2	5:A:2162:HOH:O	2.16	0.45
1:A:37:MET:HE1	1:A:145:GLN:HG3	1.98	0.45
1:B:242:PHE:CD2	1:B:330:GLY:HA2	2.51	0.45
1:B:200:ASP:OD2	2:B:1389:PP9:HHB	2.16	0.45
1:A:5:SER:HB3	1:A:275:HIS:NE2	2.31	0.45
1:A:361:LYS:HG3	5:A:2067:HOH:O	2.17	0.45
1:B:312:ARG:NH2	2:B:1389:PP9:HAD1	2.32	0.45
1:A:237:VAL:O	1:A:365:GLY:HA3	2.16	0.45
1:A:180:SER:HA	1:B:152:ASP:OD2	2.17	0.44
1:A:271:MET:CE	1:A:276:ASP:HB3	2.47	0.44
1:B:287:LYS:HG3	5:B:2066:HOH:O	2.16	0.44
1:B:317:TYR:CD1	1:B:317:TYR:C	2.91	0.44
1:B:37:MET:CE	1:B:332:LEU:HD12	2.46	0.44
1:A:197:GLY:HA3	1:A:263:LYS:HE2	1.98	0.44
1:A:298:ALA:O	1:A:350:ARG:NH1	2.51	0.44
1:B:249:ARG:NH2	5:B:2057:HOH:O	2.47	0.43
1:A:306[B]:GLU:O	1:A:308[B]:SER:N	2.51	0.43
1:A:351:LEU:CD1	2:A:1389:PP9:HBC1	2.42	0.43
1:A:308[A]:SER:HA	1:A:342:LYS:O	2.19	0.43
1:B:312:ARG:HH21	2:B:1389:PP9:HAD1	1.82	0.43
1:A:310:MET:CE	2:A:1389:PP9:HMD2	2.48	0.43
1:A:229:THR:HB	1:A:369:PHE:CZ	2.54	0.43
1:A:75:THR:HG21	1:A:82:PRO:CA	2.36	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:PRO:HA	1:B:149:ASN:HB3	2.00	0.42
1:B:97:LEU:HA	1:B:147:CYS:O	2.19	0.42
1:B:115:ALA:N	1:B:116:PRO:HD2	2.34	0.42
1:A:292:ASP:HA	1:A:297:LEU:HD11	2.00	0.42
1:B:37:MET:HG3	1:B:147:CYS:SG	2.60	0.42
1:B:339:ASP:HB3	1:B:342:LYS:HB2	2.01	0.42
1:A:299:ASN:OD1	1:A:301:ARG:HG3	2.20	0.41
1:B:120:LYS:CG	1:B:224:GLN:O	2.64	0.41
1:B:77:ASN:HA	1:B:78:PRO:HD2	1.90	0.41
1:A:285:GLU:HB2	1:A:287:LYS:HG3	2.02	0.41
1:A:14:ALA:CB	1:A:17:GLU:OE1	2.69	0.41
1:A:53:GLU:HB2	1:A:386:LEU:HD13	2.03	0.41
1:A:127:ARG:HB2	1:A:131:ASP:HB2	2.02	0.41
1:A:273:HIS:CD2	5:A:2129:HOH:O	2.74	0.41
1:B:310:MET:CE	1:B:344:PHE:HA	2.48	0.41
1:B:72:ALA:HA	1:B:73:PRO:HD3	1.99	0.40
1:B:344:PHE:HE2	2:B:1389:PP9:HMC1	1.86	0.40
1:A:37:MET:HE3	1:A:37:MET:HB2	1.97	0.40
1:B:58:LEU:HD21	1:B:164:HIS:O	2.22	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	387/403 (96%)	364 (94%)	16 (4%)	7 (2%)	8	7
1	B	382/403 (95%)	361 (94%)	20 (5%)	1 (0%)	41	50
All	All	769/806 (95%)	725 (94%)	36 (5%)	8 (1%)	22	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305[A]	SER
1	A	305[B]	SER
1	A	387	ARG
1	A	306[A]	GLU
1	A	306[B]	GLU
1	A	307[A]	SER
1	A	307[B]	SER
1	B	387	ARG

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	325/338 (96%)	312 (96%)	13 (4%)	31	44
1	B	320/338 (95%)	310 (97%)	10 (3%)	40	55
All	All	645/676 (95%)	622 (96%)	23 (4%)	38	49

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	MET
1	A	61	GLN
1	A	152	ASP
1	A	189	LYS
1	A	200	ASP
1	A	210	ASP
1	A	244	VAL
1	A	291	LEU
1	A	305[A]	SER
1	A	305[B]	SER
1	A	309[A]	LEU
1	A	309[B]	LEU
1	A	337	GLN
1	B	15	ARG
1	B	37	MET
1	B	74	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	222	ASP
1	B	279	ASP
1	B	292	ASP
1	B	299	ASN
1	B	305	SER
1	B	337	GLN
1	B	388	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	1390	-	4,4,4	0.28	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PG4	A	1392	-	12,12,12	0.53	0	11,11,11	0.27	0
2	PP9	B	1389	-	32,46,46	1.79	4 (12%)	24,68,68	1.15	1 (4%)
2	PP9	A	1389	-	32,46,46	1.78	3 (9%)	24,68,68	1.16	3 (12%)
3	SO4	B	1390	-	4,4,4	0.26	0	6,6,6	0.29	0
4	PG4	A	1391	-	12,12,12	0.49	0	11,11,11	0.39	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
2	PP9	A	1389	-	-	6/12/62/62	0/4/5/5
4	PG4	A	1391	-	-	1/10/10/10	-
2	PP9	B	1389	-	-	3/12/62/62	0/4/5/5
4	PG4	A	1392	-	-	5/10/10/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1389	PP9	CAB-C3B	-6.60	1.39	1.47
2	A	1389	PP9	CAB-C3B	-6.26	1.40	1.47
2	B	1389	PP9	C4B-C3B	-2.82	1.38	1.46
2	A	1389	PP9	C4B-C3B	-2.79	1.38	1.46
2	A	1389	PP9	C3C-C2C	-2.25	1.37	1.40
2	B	1389	PP9	CMD-C2D	2.21	1.54	1.50
2	B	1389	PP9	CAD-C3D	2.00	1.54	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1389	PP9	CBB-CAB-C3B	-2.33	121.30	125.93
2	A	1389	PP9	CBA-CAA-C2A	2.30	116.35	112.55
2	A	1389	PP9	O1D-CGD-CBD	-2.27	115.90	123.09
2	B	1389	PP9	CBB-CAB-C3B	-2.16	121.64	125.93

There are no chirality outliers.

All (15) torsion outliers are listed below:

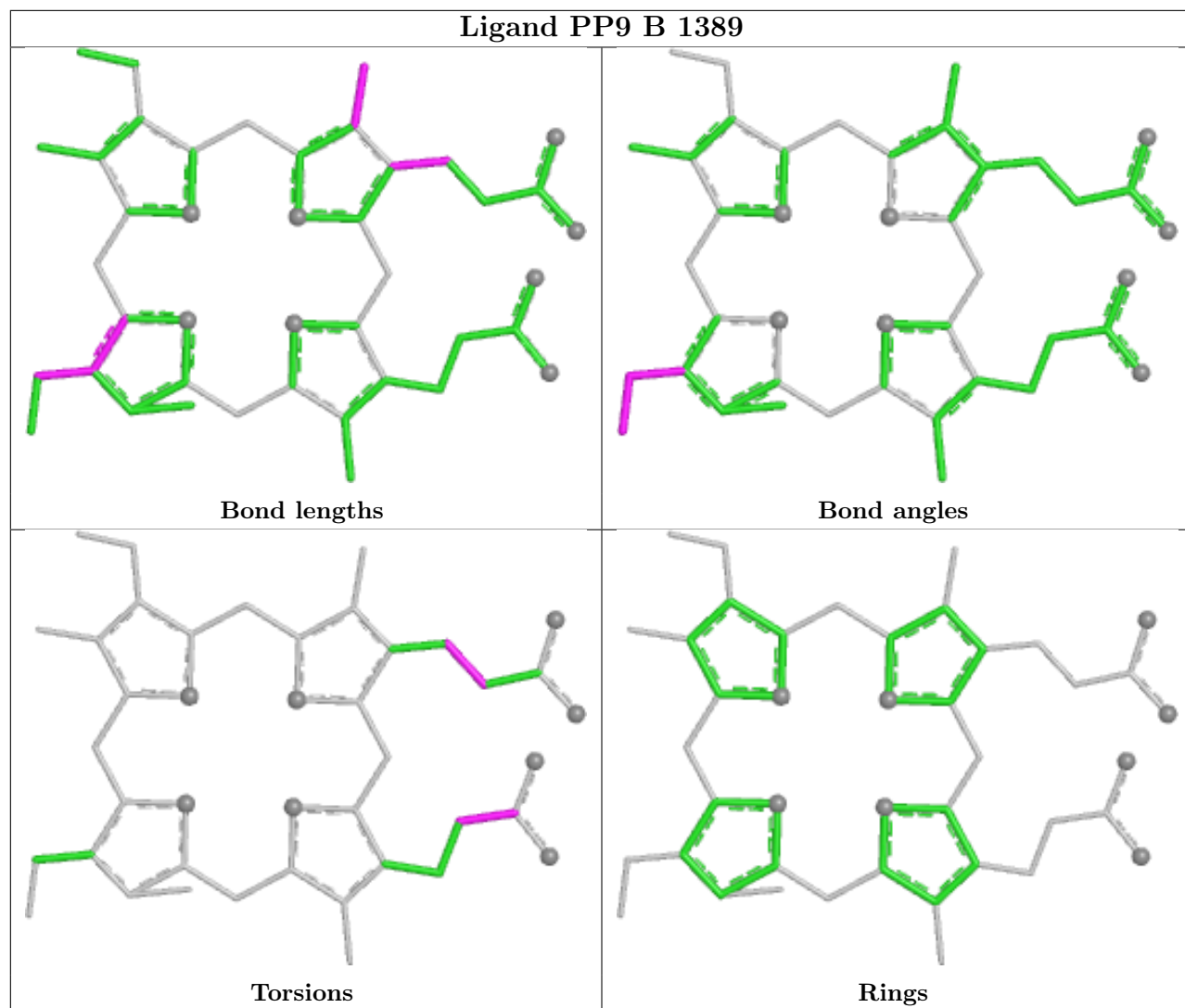
Mol	Chain	Res	Type	Atoms
2	B	1389	PP9	C3D-CAD-CBD-CGD
2	A	1389	PP9	C3D-CAD-CBD-CGD
4	A	1392	PG4	C6-C5-O3-C4
4	A	1392	PG4	C1-C2-O2-C3
4	A	1392	PG4	C3-C4-O3-C5
4	A	1392	PG4	C4-C3-O2-C2
2	A	1389	PP9	CAD-CBD-CGD-O2D
2	A	1389	PP9	CAD-CBD-CGD-O1D
2	A	1389	PP9	CAA-CBA-CGA-O1A
2	A	1389	PP9	CAA-CBA-CGA-O2A
4	A	1392	PG4	C8-C7-O4-C6
2	B	1389	PP9	CAA-CBA-CGA-O2A
2	B	1389	PP9	CAA-CBA-CGA-O1A
2	A	1389	PP9	C2B-C3B-CAB-CBB
4	A	1391	PG4	O2-C3-C4-O3

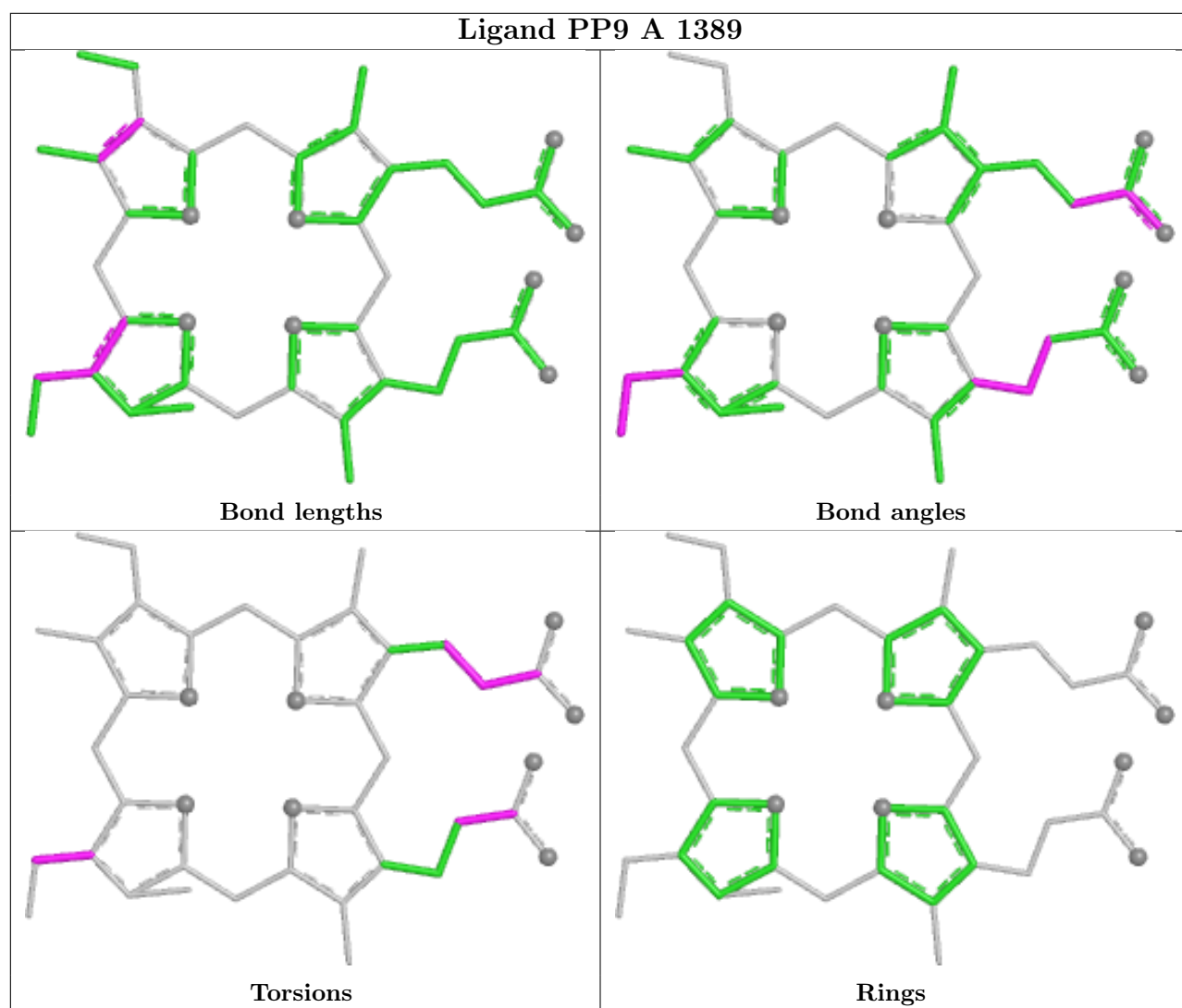
There are no ring outliers.

3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1389	PP9	8	0
2	A	1389	PP9	13	0
3	B	1390	SO4	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	384/403 (95%)	0.32	24 (6%)	20 25	15, 27, 54, 63	0
1	B	384/403 (95%)	0.47	31 (8%)	12 16	20, 38, 61, 77	0
All	All	768/806 (95%)	0.39	55 (7%)	15 20	15, 33, 59, 77	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	VAL	7.9
1	A	303	ALA	6.7
1	A	284	PRO	6.4
1	B	303	ALA	6.2
1	B	306	GLU	5.9
1	B	307	SER	5.3
1	B	304	GLU	4.7
1	A	277	VAL	4.3
1	A	304	GLU	4.2
1	B	230	ILE	4.0
1	B	386	LEU	3.9
1	B	228	TRP	3.8
1	A	281	ALA	3.7
1	B	305	SER	3.7
1	B	308	SER	3.5
1	A	280	TYR	3.5
1	A	307[A]	SER	3.4
1	B	387	ARG	3.4
1	A	6	ALA	3.2
1	B	302	THR	3.2
1	A	11	SER	3.1
1	A	279	ASP	3.1
1	B	374	VAL	3.1
1	A	302	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	227	ALA	3.0
1	A	189	LYS	3.0
1	B	13	ASP	2.9
1	B	380	TYR	2.9
1	B	220	THR	2.9
1	B	277	VAL	2.8
1	B	10	LEU	2.8
1	B	384	ALA	2.8
1	A	301	ARG	2.8
1	A	182	HIS	2.6
1	B	279	ASP	2.5
1	A	186	SER	2.5
1	B	211	LYS	2.5
1	A	308[A]	SER	2.4
1	A	185	ARG	2.4
1	B	375	LYS	2.4
1	B	383	SER	2.4
1	B	221	ALA	2.3
1	B	385	LEU	2.3
1	A	285	GLU	2.3
1	B	289	ILE	2.3
1	A	306[A]	GLU	2.2
1	A	272	GLN	2.2
1	A	388	VAL	2.1
1	A	300	PRO	2.1
1	B	376	ASP	2.1
1	B	50	ALA	2.1
1	A	305[A]	SER	2.1
1	A	387	ARG	2.0
1	B	319	LEU	2.0
1	B	203	ALA	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 ⓘ

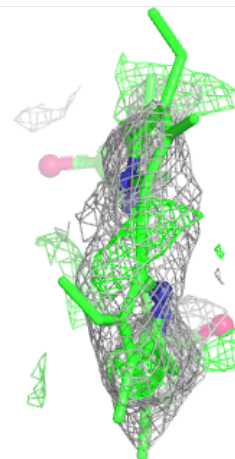
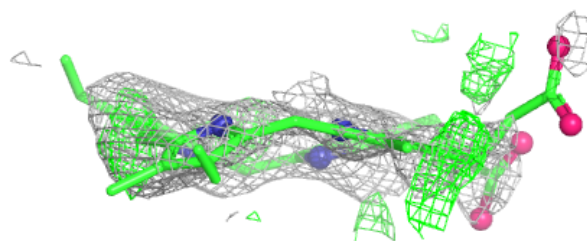
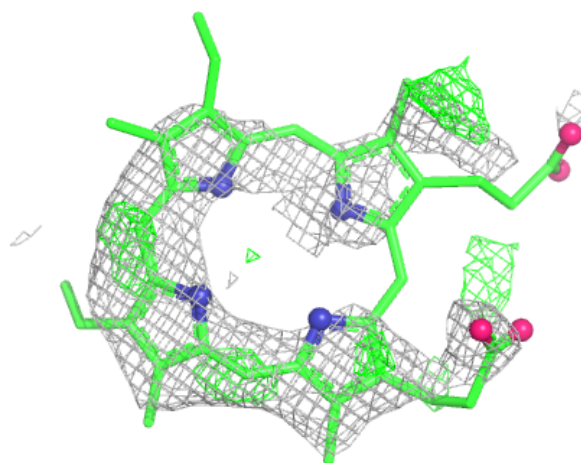
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PG4	A	1392	13/13	0.65	0.30	77,79,82,82	0
2	PP9	B	1389	42/42	0.71	0.44	63,65,70,72	42
2	PP9	A	1389	42/42	0.80	0.35	57,60,62,63	42
3	SO4	B	1390	5/5	0.86	0.29	78,79,80,80	0
4	PG4	A	1391	13/13	0.93	0.14	32,36,47,48	0
3	SO4	A	1390	5/5	0.95	0.16	64,64,65,66	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.

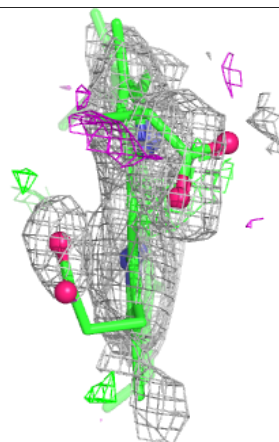
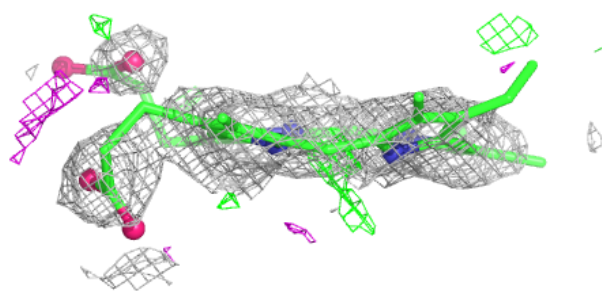
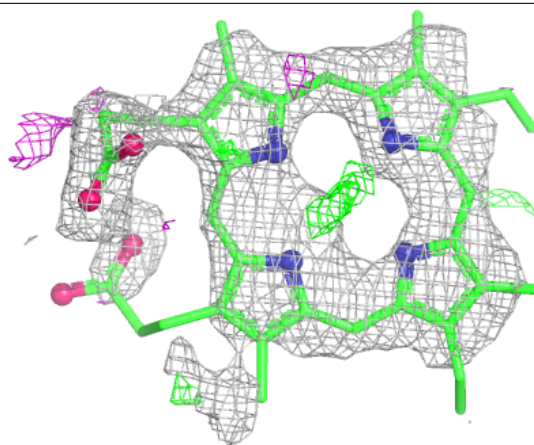
Electron density around PP9 B 1389:

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 PP9 A 1389:

$2mF_o-DF_c$ (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.