



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2025 – 02:06 PM JST

PDB ID : 9J25 / pdb_00009j25
Title : Structural basis of the bifunctionality of *M. salinexigens* ZYF650T glucosyl-glycerol phosphorylase in glucosylglycerol catabolism
Authors : Lu, D.; Ma, H.L.
Deposited on : 2024-08-06
Resolution : 2.74 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 Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

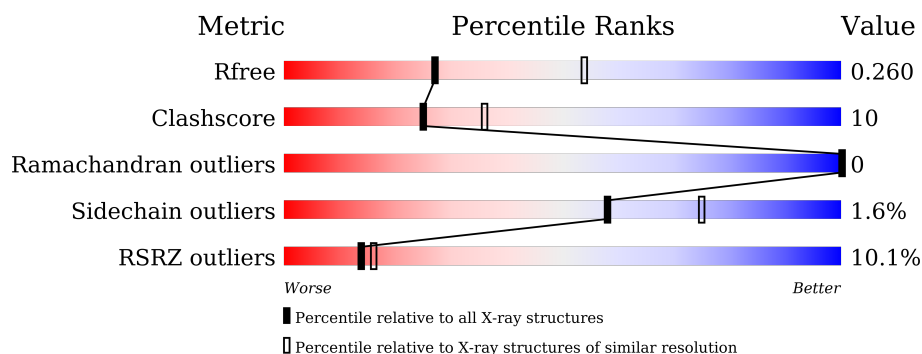
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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}	164625	1649 (2.76-2.72)
Clashscore	180529	1744 (2.76-2.72)
Ramachandran outliers	177936	1710 (2.76-2.72)
Sidechain outliers	177891	1711 (2.76-2.72)
RSRZ outliers	164620	1649 (2.76-2.72)

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	480	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 9%</div> </div> </div>
1	B	480	<div> <div>12%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>• 8%</div> </div> </div>
1	C	480	<div> <div>11%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>• 9%</div> </div> </div>

2 Entry composition [i](#)

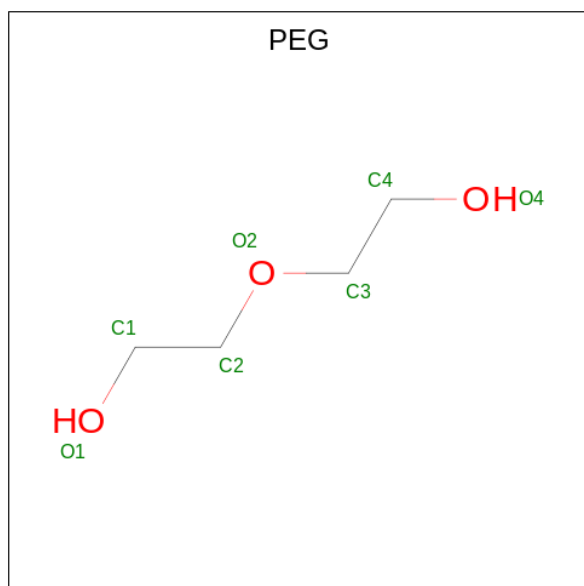
There are 6 unique types of molecules in this entry. The entry contains 10814 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sucrose phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3544	2270	586	667	21			
1	B	441	Total	C	N	O	S	0	0	0
			3553	2277	584	671	21			
1	C	435	Total	C	N	O	S	0	0	0
			3515	2255	578	662	20			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



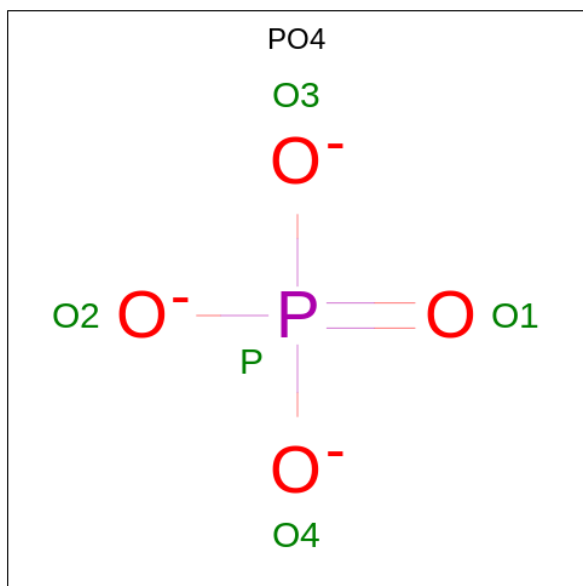
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



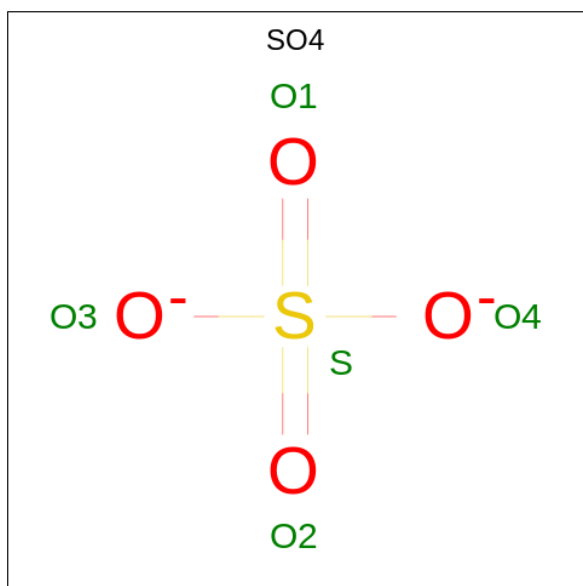
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

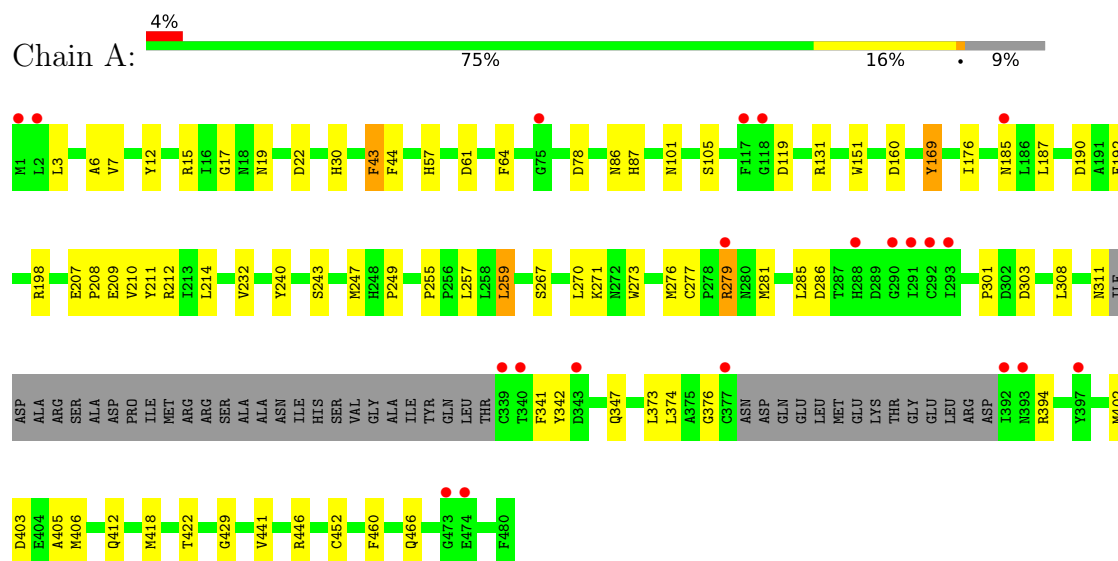
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total	O	0	0
			54	54		
6	B	55	Total	O	0	0
			55	55		
6	C	53	Total	O	0	0
			53	53		

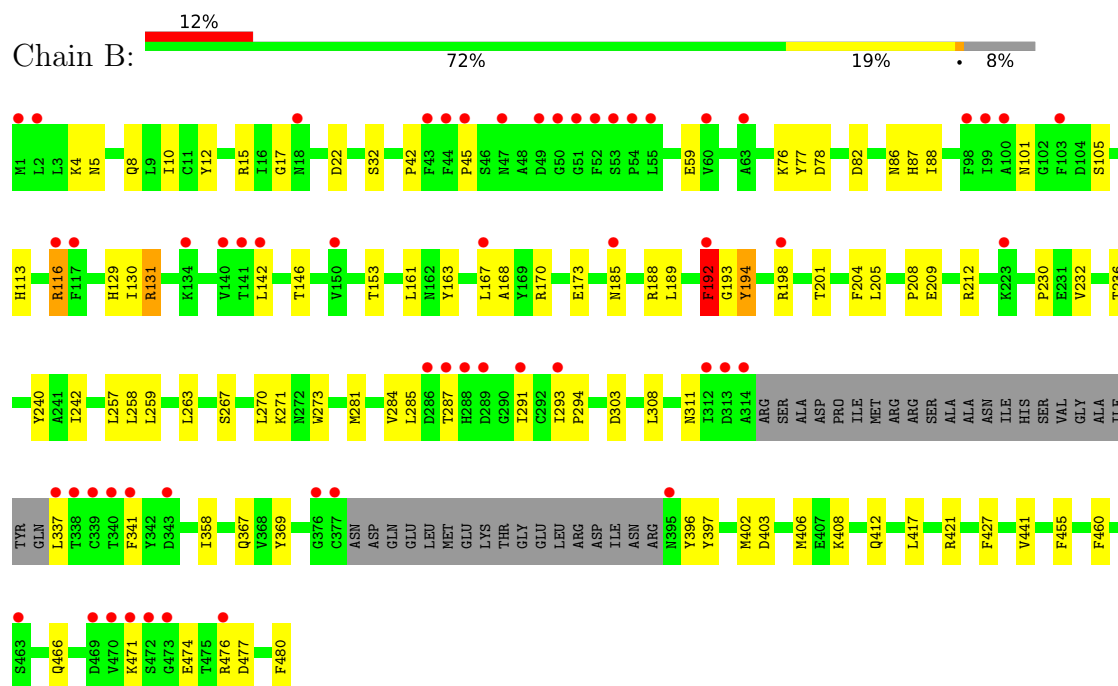
3 Residue-property plots

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.

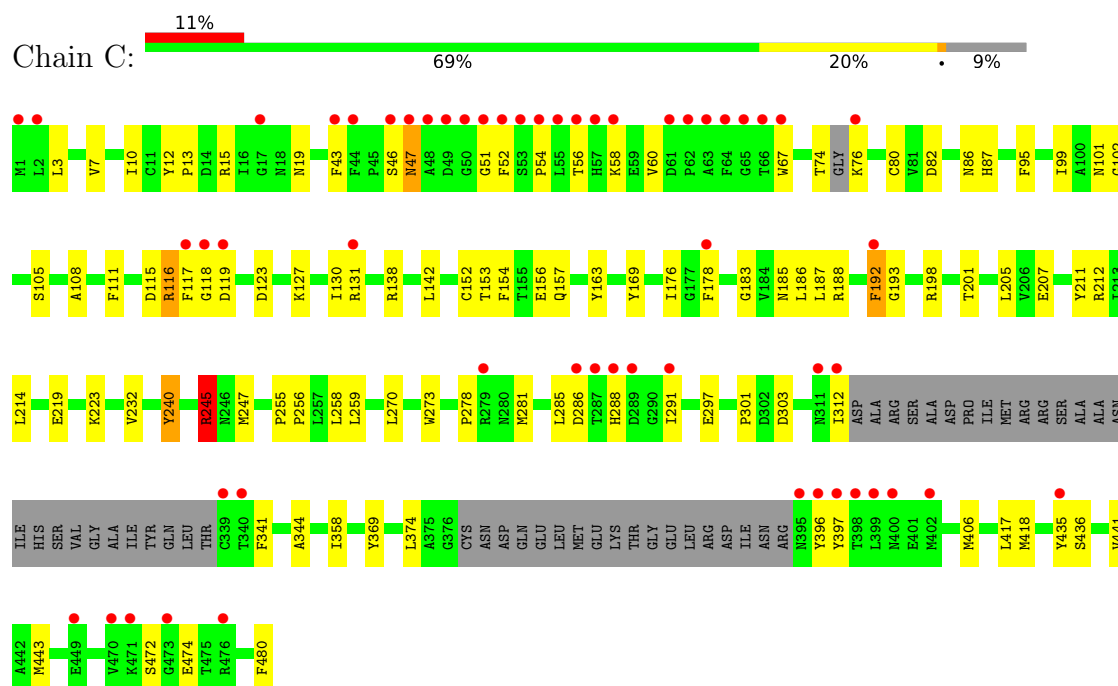
• Molecule 1: Sucrose phosphorylase



• Molecule 1: Sucrose phosphorylase



● Molecule 1: Sucrose phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.24Å 176.12Å 177.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.74 49.09 – 2.74	Depositor EDS
% Data completeness (in resolution range)	90.5 (49.09-2.74) 90.5 (49.09-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.222 , 0.260 0.226 , 0.260	Depositor DCC
R_{free} test set	1917 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10814	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: PEG, SO4, PO4, TRS

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	0.32	0/3636	0.60	1/4939 (0.0%)
1	B	0.30	0/3645	0.58	1/4953 (0.0%)
1	C	0.34	0/3606	0.64	1/4898 (0.0%)
All	All	0.32	0/10887	0.60	3/14790 (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	C	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	PHE	CA-CB-CG	6.36	120.16	113.80
1	C	118	GLY	CA-C-O	-5.80	116.97	122.13
1	A	279	ARG	CG-CD-NE	-5.11	100.77	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	116	ARG	Sidechain
1	C	245	ARG	Sidechain

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	3544	0	3402	56	0
1	B	3553	0	3410	69	0
1	C	3515	0	3374	78	1
2	A	7	0	10	0	0
3	A	8	0	12	0	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
6	A	54	0	0	5	0
6	B	55	0	0	9	0
6	C	53	0	0	13	0
All	All	10814	0	10208	201	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (201) 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:208:PRO:HG2	1:B:212:ARG:HH12	1.34	0.90
1:C:297:GLU:OE1	6:C:601:HOH:O	1.90	0.89
1:C:214:LEU:HB3	1:C:247:MET:HE1	1.56	0.86
1:C:74:THR:O	1:C:76:LYS:N	2.10	0.85
1:A:190:ASP:O	6:A:601:HOH:O	1.94	0.84
1:A:342:TYR:CE2	1:A:347:GLN:HG2	2.13	0.83
1:C:142:LEU:HA	6:C:604:HOH:O	1.81	0.79
1:B:455:PHE:O	6:B:601:HOH:O	2.02	0.77
1:B:403:ASP:OD1	6:B:602:HOH:O	2.02	0.77
1:C:102:GLY:O	6:C:603:HOH:O	2.03	0.77
1:C:397:TYR:O	6:C:602:HOH:O	2.03	0.75
4:A:503:PO4:O2	6:A:602:HOH:O	2.04	0.74
1:C:192:PHE:HE2	1:C:214:LEU:HD21	1.51	0.74
1:C:192:PHE:CD2	1:C:214:LEU:HD11	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ILE:O	6:C:604:HOH:O	2.08	0.72
1:C:192:PHE:CE1	1:C:232:VAL:HB	2.26	0.71
1:A:311:ASN:OD1	6:A:604:HOH:O	2.09	0.69
1:B:131:ARG:NH1	6:B:609:HOH:O	2.26	0.69
1:B:406:MET:O	1:B:412:GLN:NE2	2.22	0.68
1:B:205:LEU:O	6:B:603:HOH:O	2.12	0.68
1:C:286:ASP:OD1	6:C:605:HOH:O	2.12	0.67
1:A:402:MET:HE3	1:A:406:MET:HE3	1.76	0.67
1:B:208:PRO:HG2	1:B:212:ARG:NH1	2.10	0.64
1:B:113:HIS:O	1:B:116:ARG:HG2	1.98	0.64
1:B:259:LEU:HG	1:B:341:PHE:HE1	1.61	0.64
1:C:157:GLN:NE2	6:C:611:HOH:O	2.30	0.63
1:A:208:PRO:HG2	1:A:212:ARG:HH12	1.65	0.61
1:C:60:VAL:HG23	1:C:67:TRP:CE2	2.34	0.61
1:A:30:HIS:NE2	1:A:403:ASP:OD1	2.25	0.61
1:A:86:ASN:HB3	1:A:87:HIS:ND1	2.16	0.61
1:A:374:LEU:HD21	1:A:406:MET:HE2	1.83	0.61
1:C:47:ASN:HD22	1:C:157:GLN:HB3	1.66	0.61
1:C:192:PHE:CE2	1:C:214:LEU:HD21	2.34	0.61
1:A:460:PHE:HE1	1:B:130:ILE:HG21	1.66	0.61
1:B:192:PHE:CE1	1:B:232:VAL:HB	2.36	0.60
1:C:46:SER:HB3	1:C:51:GLY:HA2	1.84	0.59
1:B:8:GLN:HB2	1:B:367:GLN:HG2	1.84	0.59
1:B:192:PHE:CD2	1:B:230:PRO:HB3	2.38	0.59
1:A:243:SER:HB2	1:A:249:PRO:HG3	1.85	0.58
1:C:3:LEU:HD11	1:C:186:LEU:HD13	1.84	0.58
1:C:205:LEU:HD11	1:C:232:VAL:HG21	1.85	0.58
1:A:6:ALA:HB1	1:A:422:THR:HG23	1.84	0.58
1:A:303:ASP:OD1	1:A:303:ASP:N	2.35	0.58
1:B:259:LEU:HB3	1:B:308:LEU:HD11	1.84	0.58
1:C:240:TYR:CE1	1:C:278:PRO:HG3	2.38	0.57
1:C:245:ARG:HB2	1:C:247:MET:HE2	1.86	0.57
1:C:105:SER:HB3	6:C:603:HOH:O	2.04	0.57
1:A:273:TRP:CH2	1:A:281:MET:HE1	2.40	0.57
1:B:192:PHE:HD1	1:B:193:GLY:N	2.03	0.57
1:B:460:PHE:HE1	1:C:130:ILE:HG21	1.69	0.56
1:C:15:ARG:CZ	1:C:396:TYR:HE1	2.19	0.56
1:B:281:MET:HG2	6:B:620:HOH:O	2.06	0.56
1:C:130:ILE:HD11	1:C:153:THR:HG23	1.88	0.56
1:B:198:ARG:HE	1:B:201:THR:HG21	1.72	0.55
1:B:303:ASP:OD1	1:B:303:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLU:HG3	1:C:223:LYS:HE2	1.88	0.55
1:B:88:ILE:HG12	1:B:161:LEU:HD21	1.88	0.54
1:B:284:VAL:HG21	1:B:287:THR:HG22	1.89	0.54
1:C:10:ILE:HB	1:C:369:TYR:HA	1.90	0.54
1:B:291:ILE:O	1:B:337:LEU:N	2.40	0.54
1:B:105:SER:O	6:B:604:HOH:O	2.18	0.54
1:C:374:LEU:HD21	1:C:406:MET:HE2	1.89	0.53
1:B:270:LEU:HD23	1:B:441:VAL:HG21	1.89	0.53
1:B:192:PHE:C	1:B:192:PHE:CD1	2.86	0.53
1:B:258:LEU:HD21	1:B:358:ILE:HG21	1.89	0.53
1:B:163:TYR:CE1	1:B:168:ALA:HB1	2.43	0.53
1:C:119:ASP:N	1:C:119:ASP:OD1	2.40	0.53
1:A:30:HIS:CD2	1:A:402:MET:HE2	2.44	0.53
1:C:270:LEU:HD23	1:C:441:VAL:HG21	1.91	0.53
1:C:256:PRO:HB3	1:C:291:ILE:HG23	1.91	0.53
1:C:131:ARG:HH22	1:C:154:PHE:HE1	1.55	0.52
1:A:286:ASP:HB3	1:A:341:PHE:HB2	1.91	0.52
1:A:214:LEU:HG	1:A:247:MET:HE1	1.92	0.51
1:B:5:ASN:OD1	1:B:421:ARG:NH2	2.30	0.51
1:A:19:ASN:HB2	1:A:64:PHE:O	2.11	0.51
1:B:285:LEU:HD13	1:B:341:PHE:CE2	2.46	0.51
1:C:99:ILE:HA	6:C:604:HOH:O	2.10	0.51
1:B:101:ASN:HB2	1:B:105:SER:HB2	1.93	0.51
1:C:108:ALA:HB2	6:C:603:HOH:O	2.10	0.51
1:B:402:MET:HE3	1:B:406:MET:HE2	1.93	0.51
1:A:270:LEU:HD23	1:A:441:VAL:HG21	1.93	0.51
1:C:58:LYS:HA	1:C:178:PHE:CE2	2.46	0.51
1:C:258:LEU:HD21	1:C:358:ILE:HG21	1.92	0.50
1:A:43:PHE:HE1	1:A:44:PHE:CZ	2.30	0.50
1:B:192:PHE:HE1	1:B:205:LEU:HD21	1.76	0.50
1:C:15:ARG:HG2	1:C:396:TYR:CE1	2.46	0.50
1:C:19:ASN:ND2	6:C:615:HOH:O	2.45	0.50
1:C:435:TYR:CD1	1:C:436:SER:N	2.79	0.50
1:C:417:LEU:HD21	1:C:480:PHE:CE2	2.47	0.50
1:B:82:ASP:OD1	1:B:188:ARG:HD3	2.12	0.49
1:B:263:LEU:HD13	1:B:311:ASN:ND2	2.27	0.49
1:C:116:ARG:O	1:C:117:PHE:C	2.55	0.49
1:A:207:GLU:HG2	1:A:211:TYR:CE2	2.47	0.49
1:B:142:LEU:HD12	1:B:146:THR:OG1	2.12	0.49
1:B:259:LEU:HG	1:B:341:PHE:CE1	2.45	0.49
1:A:406:MET:O	1:A:412:GLN:NE2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASP:HA	1:B:185:ASN:OD1	2.13	0.49
1:B:198:ARG:NH1	1:B:209:GLU:OE2	2.46	0.49
1:C:240:TYR:CD1	1:C:278:PRO:HG3	2.48	0.48
1:A:12:TYR:CD2	1:A:15:ARG:HD2	2.49	0.48
1:A:169:TYR:N	1:A:169:TYR:HD1	2.10	0.48
1:B:173:GLU:OE1	6:B:605:HOH:O	2.20	0.48
1:A:208:PRO:HG2	1:A:212:ARG:NH1	2.28	0.48
1:C:52:PHE:C	1:C:54:PRO:HD3	2.39	0.48
1:C:214:LEU:HD23	1:C:247:MET:HE1	1.95	0.48
1:A:17:GLY:HA3	1:A:22:ASP:HB3	1.95	0.47
1:A:169:TYR:N	1:A:169:TYR:CD1	2.81	0.47
1:B:273:TRP:CH2	1:B:281:MET:HE1	2.49	0.47
1:C:12:TYR:CD2	1:C:15:ARG:HD2	2.49	0.47
1:C:101:ASN:HB2	1:C:105:SER:HB2	1.97	0.47
1:A:402:MET:HE3	1:A:406:MET:CE	2.43	0.47
1:C:82:ASP:OD1	1:C:188:ARG:HD3	2.15	0.47
1:A:452:CYS:HA	1:A:466:GLN:O	2.14	0.46
1:A:119:ASP:OD1	1:A:119:ASP:N	2.49	0.46
1:A:376:GLY:HA2	6:A:634:HOH:O	2.16	0.46
1:C:74:THR:HG21	1:C:183:GLY:HA3	1.98	0.46
1:B:130:ILE:CD1	1:B:153:THR:HG23	2.45	0.46
1:C:130:ILE:CD1	1:C:153:THR:HG23	2.44	0.46
1:A:192:PHE:CE2	1:A:232:VAL:HB	2.51	0.46
1:B:192:PHE:CZ	1:B:242:ILE:HD11	2.51	0.46
1:A:101:ASN:HB2	1:A:105:SER:HB2	1.98	0.46
1:C:15:ARG:HG2	1:C:396:TYR:CD1	2.51	0.46
1:C:102:GLY:HA2	1:C:142:LEU:HD22	1.98	0.46
1:C:207:GLU:HG2	1:C:211:TYR:CE2	2.50	0.46
1:B:421:ARG:HA	1:B:427:PHE:CE2	2.52	0.46
1:A:279:ARG:NH1	6:A:603:HOH:O	2.06	0.45
1:A:43:PHE:H	1:A:43:PHE:HD1	1.63	0.45
1:B:192:PHE:CD1	1:B:193:GLY:N	2.83	0.45
1:C:80:CYS:HB2	1:C:186:LEU:HD23	1.98	0.45
1:C:192:PHE:HE1	1:C:232:VAL:HB	1.77	0.45
1:A:61:ASP:HB3	1:A:64:PHE:CD2	2.52	0.45
1:C:435:TYR:HD1	1:C:436:SER:N	2.14	0.45
1:B:194:TYR:N	1:B:194:TYR:CD1	2.84	0.45
1:B:10:ILE:HB	1:B:369:TYR:HA	1.99	0.45
1:C:56:THR:HG23	1:C:58:LYS:H	1.82	0.45
1:C:142:LEU:HD23	6:C:604:HOH:O	2.17	0.44
1:A:267:SER:O	1:A:271:LYS:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:VAL:HG12	1:C:443:MET:HG3	1.99	0.44
1:B:130:ILE:HD11	1:B:153:THR:HG23	2.00	0.44
1:C:285:LEU:HA	1:C:285:LEU:HD12	1.77	0.44
1:C:192:PHE:CD1	1:C:193:GLY:N	2.84	0.44
1:C:273:TRP:CH2	1:C:281:MET:HE1	2.53	0.44
1:C:7:VAL:HG11	1:C:418:MET:HE3	1.98	0.44
1:C:198:ARG:HE	1:C:201:THR:HG21	1.82	0.44
1:C:259:LEU:HG	1:C:341:PHE:CE1	2.53	0.44
1:B:267:SER:OG	1:B:271:LYS:HE2	2.18	0.44
1:C:212:ARG:NE	6:C:618:HOH:O	2.50	0.44
1:A:259:LEU:HB3	1:A:308:LEU:HD11	2.00	0.43
1:A:44:PHE:CD1	1:A:57:HIS:HA	2.53	0.43
1:B:466:GLN:HG2	1:B:477:ASP:OD1	2.18	0.43
1:B:167:LEU:HD23	1:B:170:ARG:HH11	1.83	0.43
1:B:293:ILE:N	1:B:294:PRO:HD2	2.33	0.43
1:B:129:HIS:HB3	1:B:204:PHE:HB3	2.00	0.43
1:B:474:GLU:OE2	1:B:476:ARG:HD2	2.18	0.43
1:C:312:ILE:HD12	1:C:344:ALA:HB1	2.01	0.43
1:C:176:ILE:HG23	1:C:187:LEU:HD11	2.01	0.43
1:A:15:ARG:NH1	1:A:394:ARG:HB3	2.34	0.43
1:A:273:TRP:O	1:A:277:CYS:N	2.52	0.43
1:B:192:PHE:HD2	1:B:230:PRO:HB3	1.82	0.43
1:A:78:ASP:HA	1:A:185:ASN:OD1	2.19	0.43
1:A:460:PHE:CE1	1:B:130:ILE:HG21	2.50	0.43
1:B:189:LEU:HB2	1:B:230:PRO:HA	2.01	0.43
1:A:301:PRO:HB2	1:A:303:ASP:OD1	2.19	0.43
1:A:429:GLY:HA3	1:A:446:ARG:O	2.19	0.43
1:B:257:LEU:HD21	1:B:270:LEU:HA	2.01	0.43
1:A:210:VAL:O	1:A:214:LEU:HB2	2.19	0.42
1:A:257:LEU:HD21	1:A:270:LEU:HA	1.99	0.42
1:C:472:SER:OG	1:C:474:GLU:HG2	2.19	0.42
1:C:3:LEU:HD21	1:C:185:ASN:HB3	2.00	0.42
1:A:198:ARG:HH12	1:A:209:GLU:CD	2.28	0.42
1:A:7:VAL:HG11	1:A:418:MET:HE3	2.02	0.42
1:A:3:LEU:HD21	1:A:185:ASN:HB3	2.02	0.42
1:A:249:PRO:HG2	1:A:281:MET:HB3	2.01	0.42
1:B:12:TYR:CD2	1:B:15:ARG:HD2	2.54	0.42
1:A:255:PRO:HG3	1:A:285:LEU:HA	2.02	0.42
1:B:45:PRO:HD3	1:B:59:GLU:O	2.20	0.41
1:B:153:THR:HG21	1:B:194:TYR:CD2	2.55	0.41
1:B:4:LYS:NZ	1:B:76:LYS:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:PRO:HD3	1:B:82:ASP:OD2	2.21	0.41
1:B:236:THR:HG23	6:B:627:HOH:O	2.20	0.41
1:C:138:ARG:NH1	1:C:156:GLU:O	2.53	0.41
1:A:176:ILE:HG23	1:A:187:LEU:HD11	2.02	0.41
1:C:86:ASN:HB3	1:C:87:HIS:ND1	2.35	0.41
1:B:32:SER:HA	1:B:77:TYR:OH	2.21	0.41
1:C:43:PHE:CE2	1:C:60:VAL:HG22	2.55	0.41
1:C:46:SER:CB	1:C:51:GLY:HA2	2.50	0.41
1:C:152:CYS:SG	1:C:156:GLU:HA	2.61	0.41
1:B:86:ASN:HB3	1:B:87:HIS:ND1	2.35	0.41
1:A:374:LEU:HD22	1:A:405:ALA:HB3	2.03	0.41
1:B:17:GLY:HA3	1:B:22:ASP:HB3	2.03	0.41
1:B:471:LYS:HE3	1:B:471:LYS:HB3	1.85	0.41
1:C:13:PRO:HG3	1:C:43:PHE:HB3	2.03	0.41
1:C:301:PRO:HB2	1:C:303:ASP:OD1	2.21	0.41
1:B:417:LEU:HD21	1:B:480:PHE:CZ	2.56	0.41
1:A:373:LEU:HD21	1:A:406:MET:HE1	2.02	0.40
1:C:255:PRO:HG2	1:C:256:PRO:HD3	2.03	0.40
1:C:163:TYR:HD1	1:C:169:TYR:CZ	2.39	0.40
1:B:408:LYS:HD3	6:B:649:HOH:O	2.20	0.40
1:A:151:TRP:HD1	1:A:160:ASP:OD2	2.03	0.40
1:C:95:PHE:HD1	1:C:111:PHE:CZ	2.39	0.40
1:A:276:MET:HE2	1:A:276:MET:HB3	1.91	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASP:OD2	1:C:127:LYS:NZ[3_554]	2.17	0.03

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	433/480 (90%)	423 (98%)	10 (2%)	0	100	100
1	B	435/480 (91%)	423 (97%)	12 (3%)	0	100	100
1	C	427/480 (89%)	416 (97%)	11 (3%)	0	100	100
All	All	1295/1440 (90%)	1262 (98%)	33 (2%)	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	387/421 (92%)	382 (99%)	5 (1%)	65	80
1	B	388/421 (92%)	381 (98%)	7 (2%)	54	72
1	C	384/421 (91%)	378 (98%)	6 (2%)	58	75
All	All	1159/1263 (92%)	1141 (98%)	18 (2%)	58	75

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	PHE
1	A	131	ARG
1	A	169	TYR
1	A	240	TYR
1	A	259	LEU
1	B	116	ARG
1	B	131	ARG
1	B	192	PHE
1	B	194	TYR
1	B	240	TYR
1	B	396	TYR
1	B	397	TYR
1	C	47	ASN
1	C	115	ASP
1	C	192	PHE

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Mol	Chain	Res	Type
1	C	240	TYR
1	C	245	ARG
1	C	288	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	GLN
1	A	395	ASN
1	A	430	HIS
1	A	453	HIS
1	B	101	ASN
1	B	430	HIS
1	B	434	ASN
1	B	447	HIS
1	C	19	ASN
1	C	47	ASN
1	C	447	HIS

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](#)

7 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	$\# Z > 2$
5	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.10	0
2	PEG	A	501	-	6,6,6	0.51	0	5,5,5	0.31	0
4	PO4	C	501	-	4,4,4	0.75	0	6,6,6	0.42	0
4	PO4	A	503	-	4,4,4	0.97	0	6,6,6	0.47	0
3	TRS	A	502	-	7,7,7	0.48	0	9,9,9	0.52	0
4	PO4	B	501	-	4,4,4	0.72	0	6,6,6	0.42	0
5	SO4	C	502	-	4,4,4	0.13	0	6,6,6	0.10	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	PEG	A	501	-	-	2/4/4/4	-
3	TRS	A	502	-	-	4/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

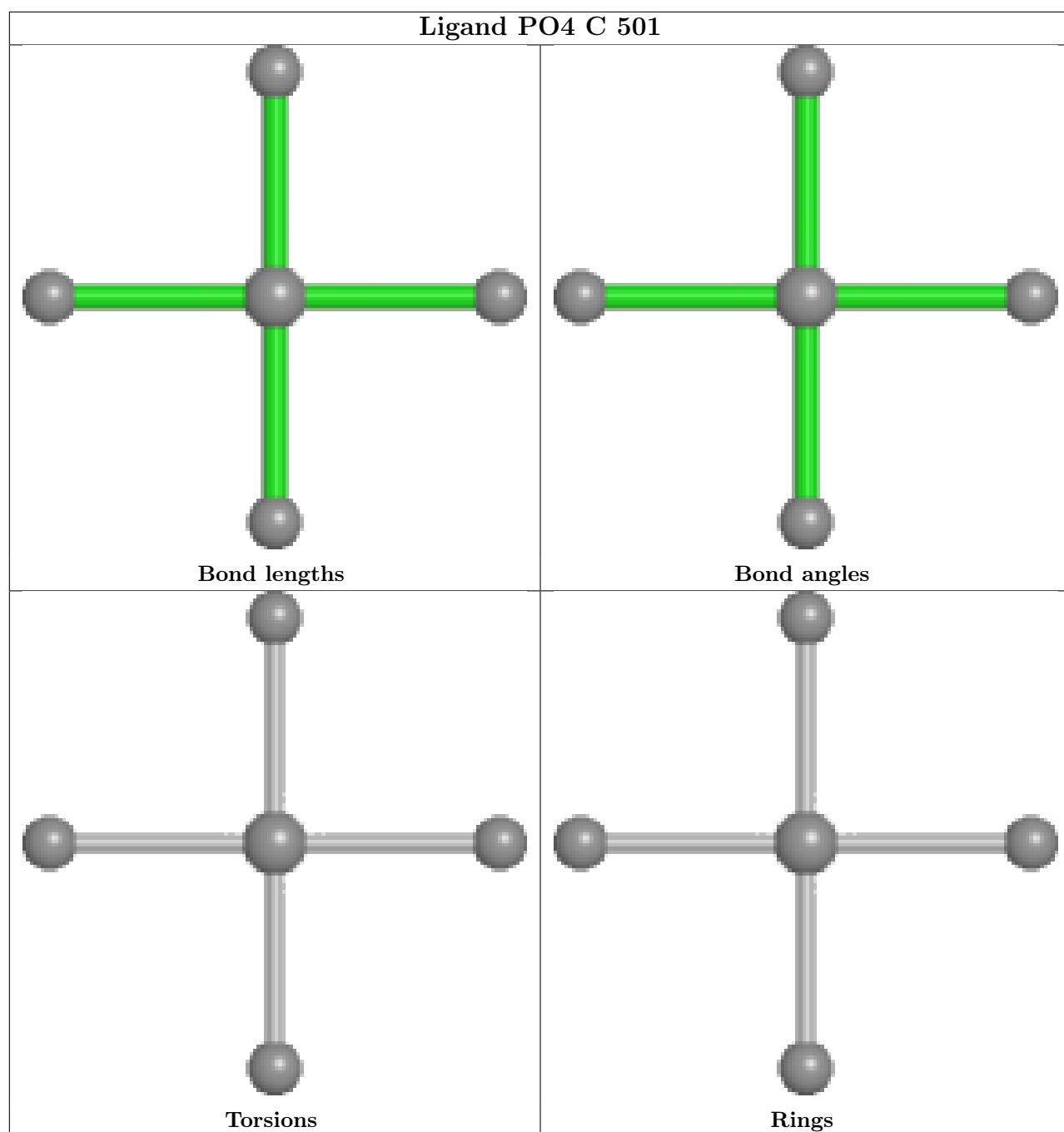
Mol	Chain	Res	Type	Atoms
3	A	502	TRS	C3-C-C2-O2
2	A	501	PEG	C4-C3-O2-C2
2	A	501	PEG	O2-C3-C4-O4
3	A	502	TRS	N-C-C2-O2
3	A	502	TRS	C1-C-C2-O2
3	A	502	TRS	C3-C-C1-O1

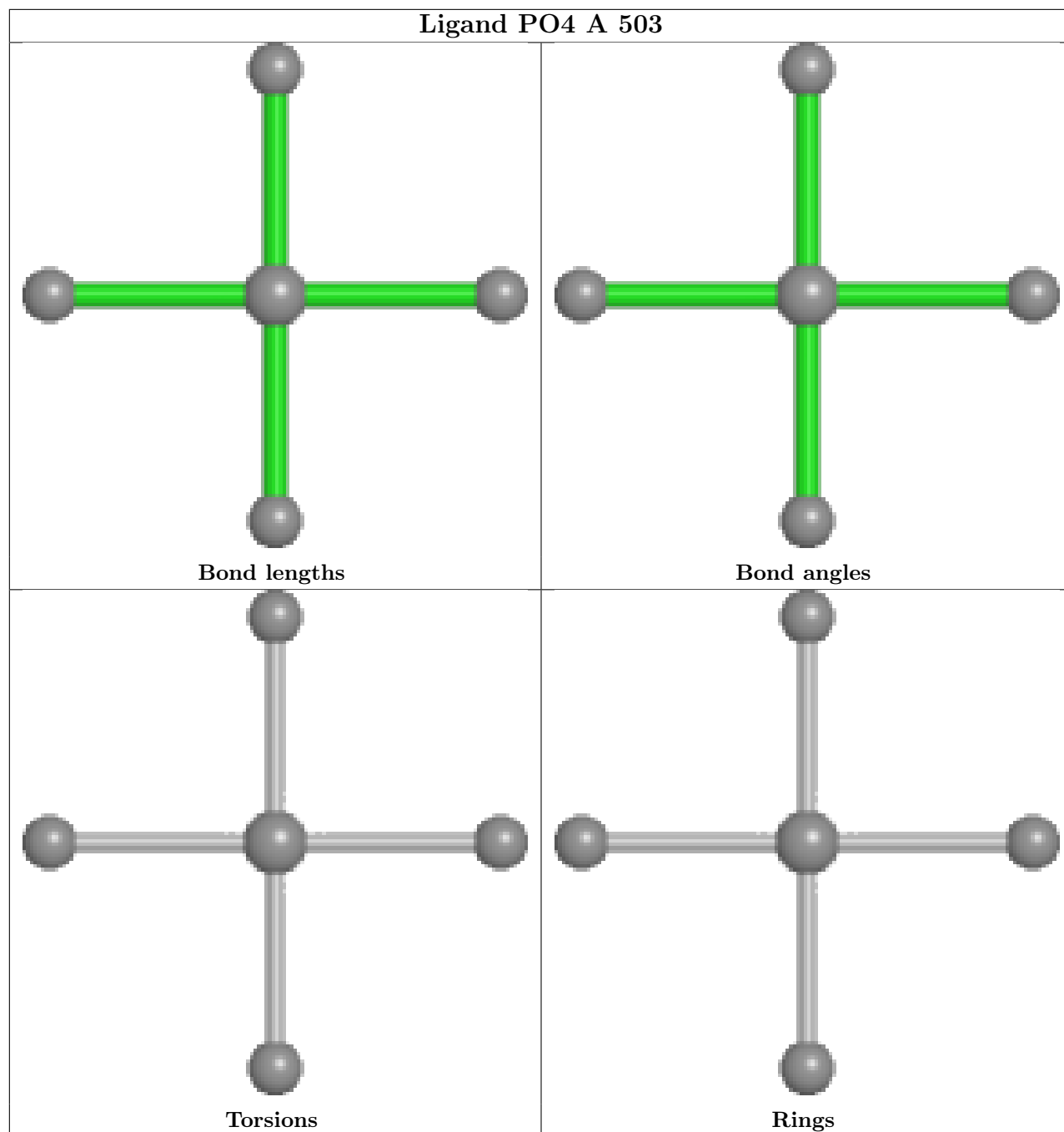
There are no ring outliers.

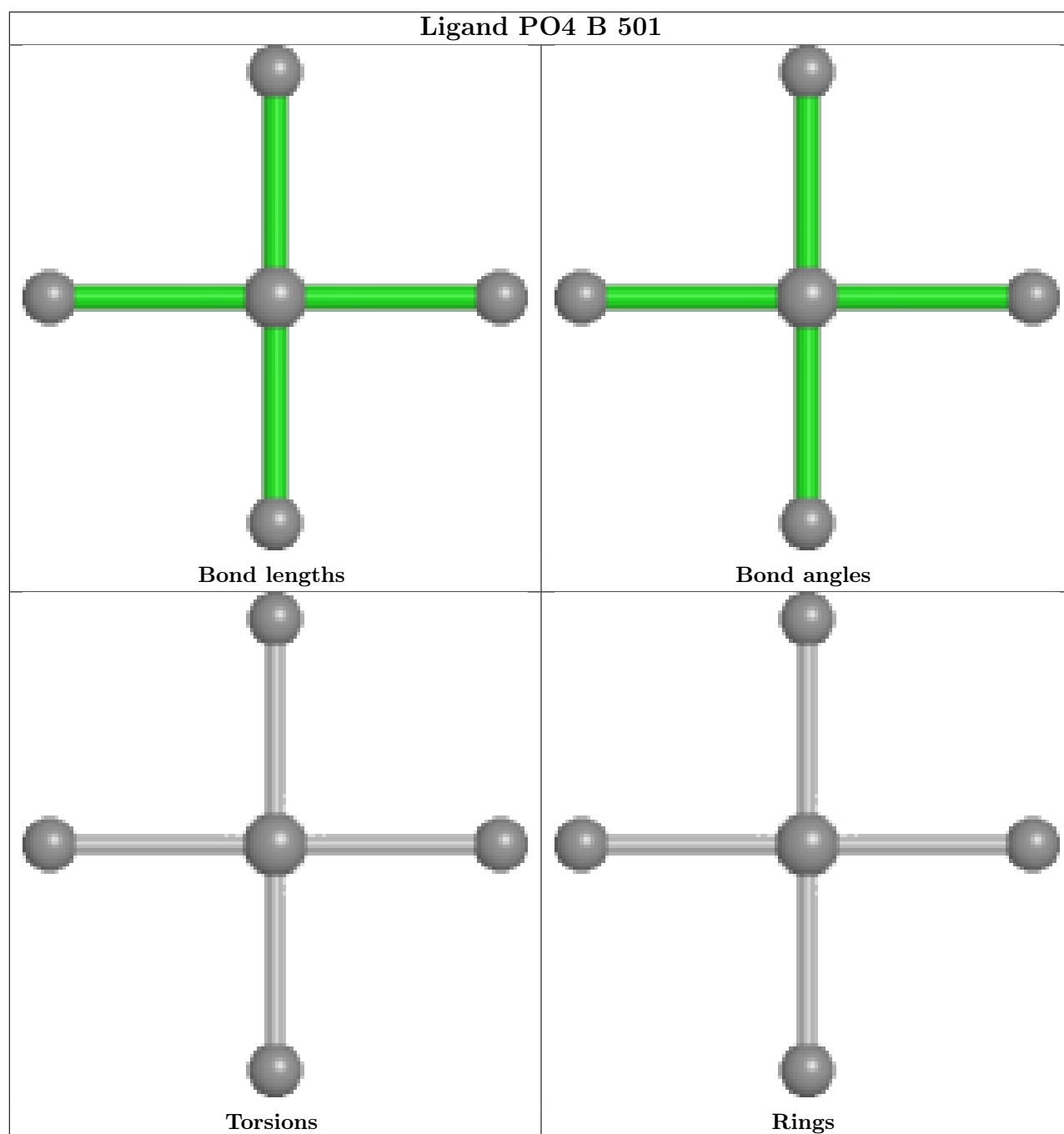
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	PO4	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	439/480 (91%)	0.29	21 (4%)	36 38	23, 45, 80, 115	0
1	B	441/480 (91%)	0.59	57 (12%)	9 11	25, 51, 105, 145	0
1	C	435/480 (90%)	0.72	55 (12%)	9 11	25, 55, 111, 182	0
All	All	1315/1440 (91%)	0.53	133 (10%)	14 16	23, 50, 100, 182	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	6.2
1	C	400	ASN	5.7
1	C	55	LEU	5.6
1	B	470	VAL	5.3
1	B	471	LYS	5.2
1	B	314	ALA	5.2
1	B	337	LEU	5.2
1	A	291	ILE	4.9
1	C	48	ALA	4.9
1	C	47	ASN	4.8
1	C	52	PHE	4.5
1	B	288	HIS	4.4
1	C	54	PRO	4.4
1	B	142	LEU	4.2
1	C	1	MET	4.2
1	C	279	ARG	4.0
1	C	43	PHE	3.9
1	C	44	PHE	3.9
1	A	392	ILE	3.8
1	C	291	ILE	3.8
1	C	50	GLY	3.8
1	C	51	GLY	3.7
1	C	57	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	288	HIS	3.7
1	B	341	PHE	3.7
1	B	2	LEU	3.6
1	B	54	PRO	3.6
1	A	118	GLY	3.6
1	B	116	ARG	3.5
1	C	470	VAL	3.5
1	C	289	ASP	3.4
1	C	53	SER	3.4
1	A	393	ASN	3.3
1	C	58	LYS	3.3
1	B	49	ASP	3.3
1	B	141	THR	3.3
1	C	396	TYR	3.3
1	C	63	ALA	3.2
1	C	49	ASP	3.2
1	C	62	PRO	3.2
1	A	1	MET	3.2
1	C	2	LEU	3.2
1	B	376	GLY	3.2
1	B	340	THR	3.2
1	B	55	LEU	3.2
1	B	473	GLY	3.1
1	A	293	ILE	3.1
1	C	46	SER	3.1
1	C	56	THR	3.1
1	B	293	ILE	3.1
1	A	290	GLY	3.1
1	B	339	CYS	3.1
1	C	340	THR	3.1
1	A	377	CYS	3.0
1	B	52	PHE	3.0
1	A	185	ASN	3.0
1	A	117	PHE	3.0
1	B	117	PHE	3.0
1	B	223	LYS	3.0
1	B	44	PHE	3.0
1	C	118	GLY	2.9
1	B	99	ILE	2.9
1	B	395	ASN	2.9
1	C	64	PHE	2.9
1	C	473	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	288	HIS	2.8
1	C	449	GLU	2.8
1	B	185	ASN	2.8
1	A	279	ARG	2.8
1	B	338	THR	2.8
1	C	339	CYS	2.7
1	B	377	CYS	2.7
1	A	339	CYS	2.7
1	B	103	PHE	2.7
1	B	45	PRO	2.7
1	B	192	PHE	2.7
1	B	100	ALA	2.6
1	B	53	SER	2.6
1	B	43	PHE	2.6
1	C	286	ASP	2.6
1	C	399	LEU	2.6
1	C	287	THR	2.6
1	C	471	LYS	2.6
1	B	289	ASP	2.6
1	C	395	ASN	2.6
1	B	312	ILE	2.6
1	C	67	TRP	2.5
1	C	435	TYR	2.5
1	C	61	ASP	2.5
1	B	291	ILE	2.4
1	A	397	TYR	2.4
1	B	343	ASP	2.4
1	C	476	ARG	2.4
1	C	76	LYS	2.3
1	B	140	VAL	2.3
1	B	98	PHE	2.3
1	B	63	ALA	2.3
1	B	51	GLY	2.3
1	A	343	ASP	2.3
1	B	150	VAL	2.3
1	B	313	ASP	2.3
1	B	50	GLY	2.3
1	B	198	ARG	2.3
1	C	65	GLY	2.3
1	B	18	ASN	2.2
1	B	134	LYS	2.2
1	C	17	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	119	ASP	2.2
1	A	2	LEU	2.2
1	C	66	THR	2.2
1	C	311	ASN	2.2
1	B	476	ARG	2.2
1	A	474	GLU	2.2
1	B	286	ASP	2.2
1	B	287	THR	2.1
1	C	397	TYR	2.1
1	A	292	CYS	2.1
1	A	75	GLY	2.1
1	A	340	THR	2.1
1	B	469	ASP	2.1
1	B	60	VAL	2.1
1	C	117	PHE	2.1
1	C	192	PHE	2.1
1	A	473	GLY	2.1
1	C	131	ARG	2.1
1	C	402	MET	2.0
1	B	463	SER	2.0
1	C	178	PHE	2.0
1	B	167	LEU	2.0
1	C	312	ILE	2.0
1	C	398	THR	2.0
1	B	472	SER	2.0
1	B	47	ASN	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](#)

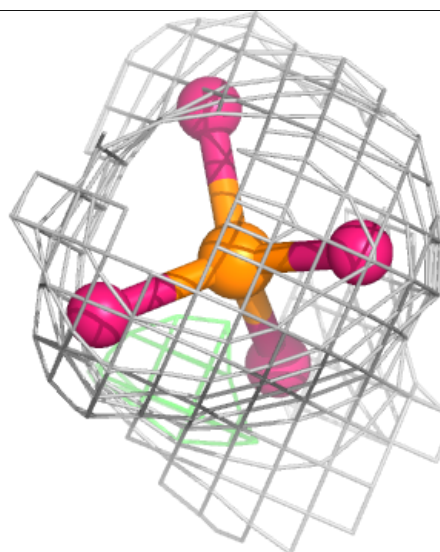
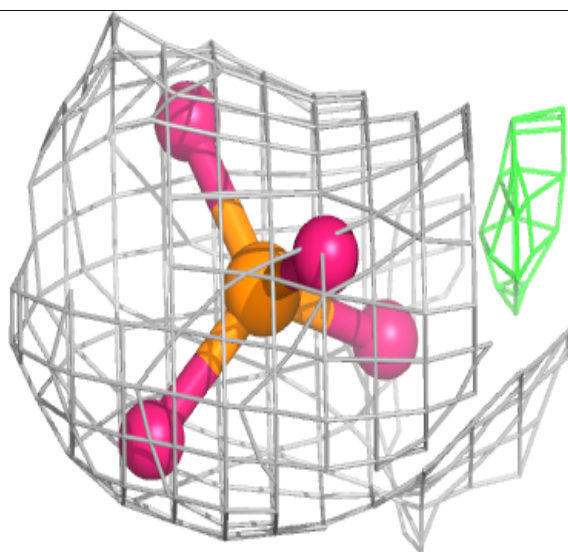
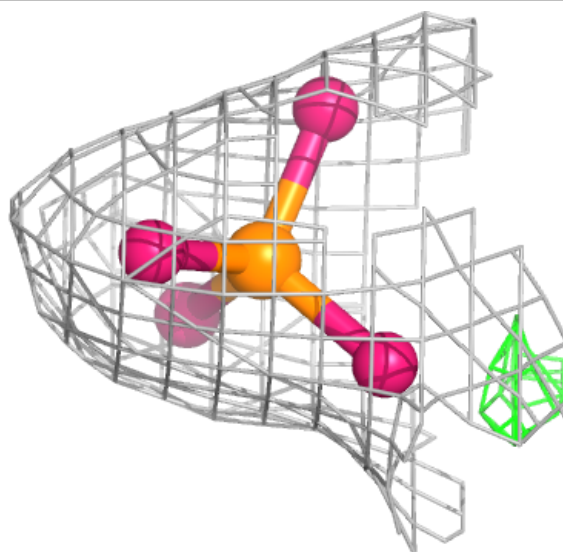
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PEG	A	501	7/7	0.68	0.24	74,76,81,83	0
4	PO4	C	501	5/5	0.71	0.19	109,109,109,109	0
5	SO4	A	504	5/5	0.71	0.17	108,109,109,109	0
5	SO4	C	502	5/5	0.71	0.21	121,121,122,122	0
3	TRS	A	502	8/8	0.81	0.15	47,51,53,53	0
4	PO4	B	501	5/5	0.83	0.14	109,109,110,110	0
4	PO4	A	503	5/5	0.88	0.13	84,84,85,85	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.

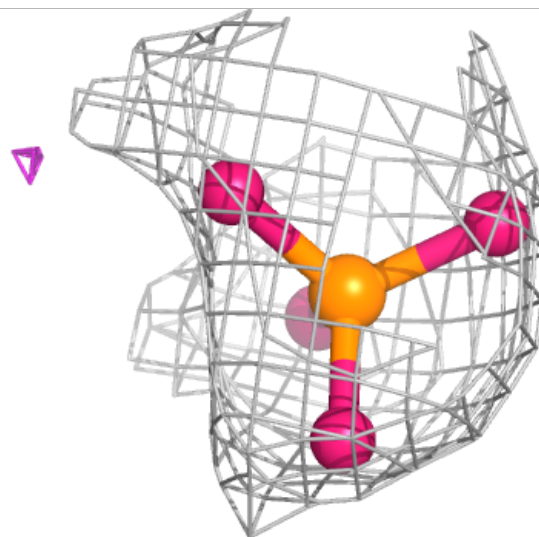
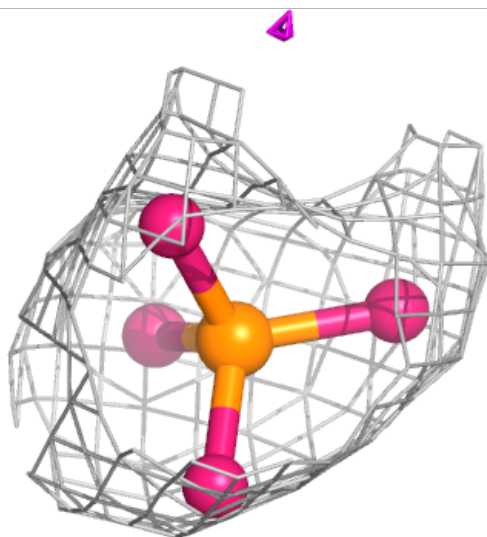
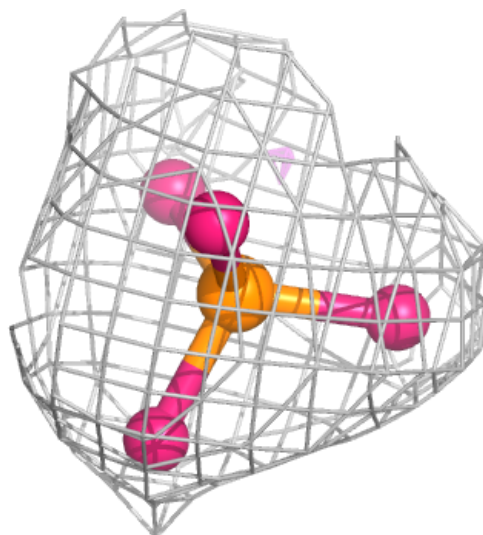
Electron density around PO4 C 501:

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



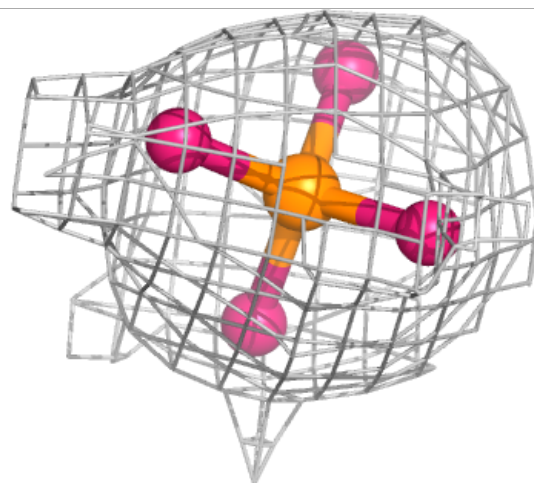
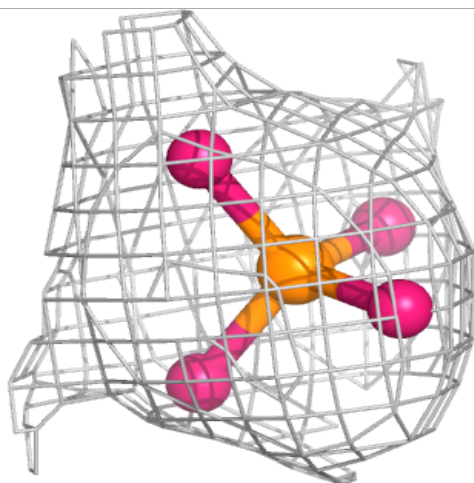
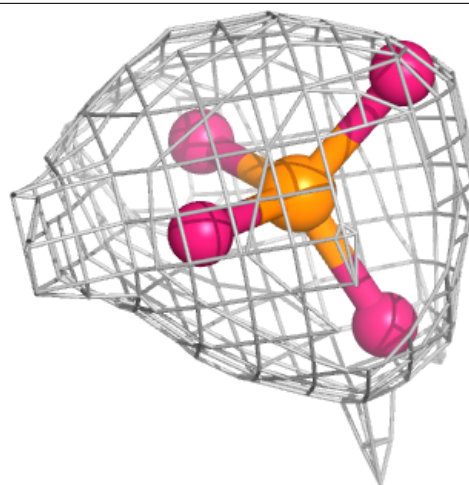
Electron density around PO4 B 501:

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



Electron density around PO4 A 503:

$2mF_o-DF_c$ (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.