



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2021 – 07:12 AM BST

PDB ID : 7A3F
Title : Crystal structure of apo DPP9
Authors : Ross, B.H.; Huber, R.
Deposited on : 2020-08-18
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.20
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) : 2.20

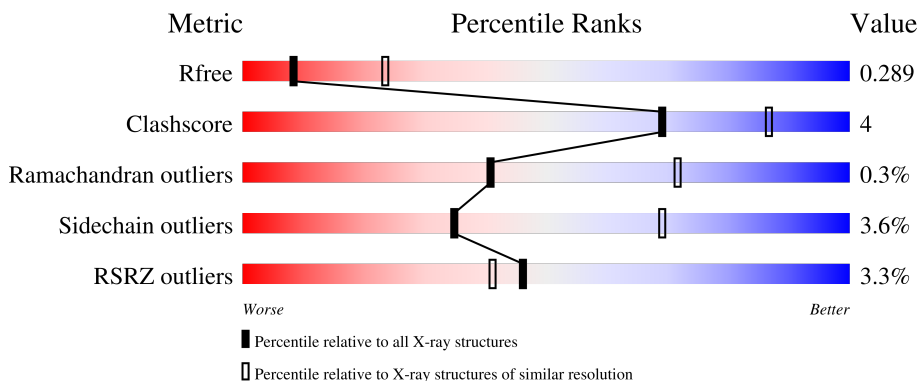
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	898	 3% 78% 10% 12%
1	B	898	 3% 75% 11% 13%
1	C	898	 3% 78% 10% 12%
1	D	898	 3% 76% 12% 12%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 25685 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 Dipeptidyl peptidase 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	782	Total 6329	C 4081	N 1070	O 1149	S 29	0	0	0
1	A	794	Total 6427	C 4136	N 1091	O 1171	S 29	0	0	0
1	C	791	Total 6389	C 4113	N 1081	O 1166	S 29	0	0	0
1	D	788	Total 6379	C 4111	N 1080	O 1159	S 29	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

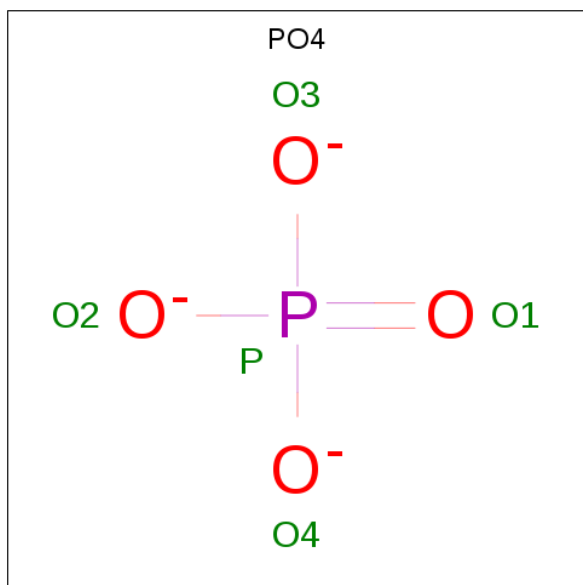
Chain	Residue	Modelled	Actual	Comment	Reference
B	864	HIS	-	expression tag	UNP Q86TI2
B	865	HIS	-	expression tag	UNP Q86TI2
B	866	HIS	-	expression tag	UNP Q86TI2
B	867	HIS	-	expression tag	UNP Q86TI2
B	868	HIS	-	expression tag	UNP Q86TI2
B	869	HIS	-	expression tag	UNP Q86TI2
A	864	HIS	-	expression tag	UNP Q86TI2
A	865	HIS	-	expression tag	UNP Q86TI2
A	866	HIS	-	expression tag	UNP Q86TI2
A	867	HIS	-	expression tag	UNP Q86TI2
A	868	HIS	-	expression tag	UNP Q86TI2
A	869	HIS	-	expression tag	UNP Q86TI2
C	864	HIS	-	expression tag	UNP Q86TI2
C	865	HIS	-	expression tag	UNP Q86TI2
C	866	HIS	-	expression tag	UNP Q86TI2
C	867	HIS	-	expression tag	UNP Q86TI2
C	868	HIS	-	expression tag	UNP Q86TI2
C	869	HIS	-	expression tag	UNP Q86TI2
D	864	HIS	-	expression tag	UNP Q86TI2
D	865	HIS	-	expression tag	UNP Q86TI2
D	866	HIS	-	expression tag	UNP Q86TI2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	867	HIS	-	expression tag	UNP Q86TI2
D	868	HIS	-	expression tag	UNP Q86TI2
D	869	HIS	-	expression tag	UNP Q86TI2

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



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

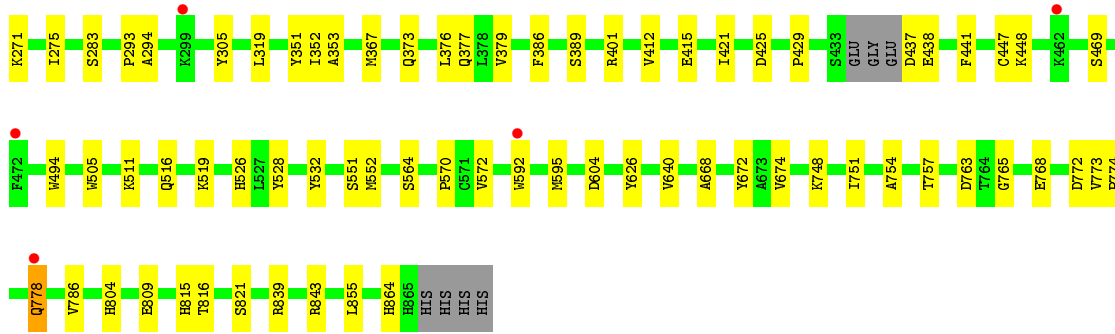
- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



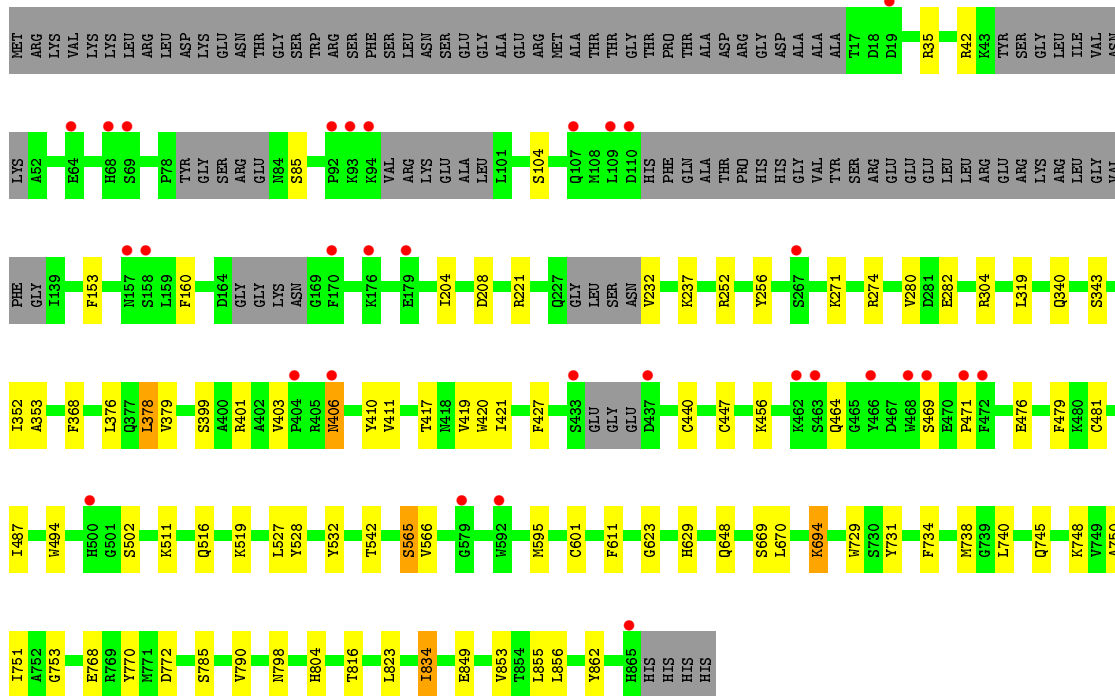
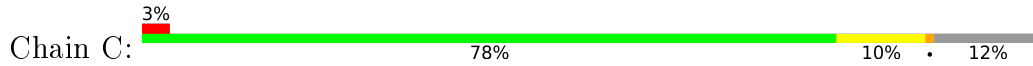
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	C O	0	0
			6	3 3		
3	A	1	Total	C O	0	0
			6	3 3		

- Molecule 4 is water.

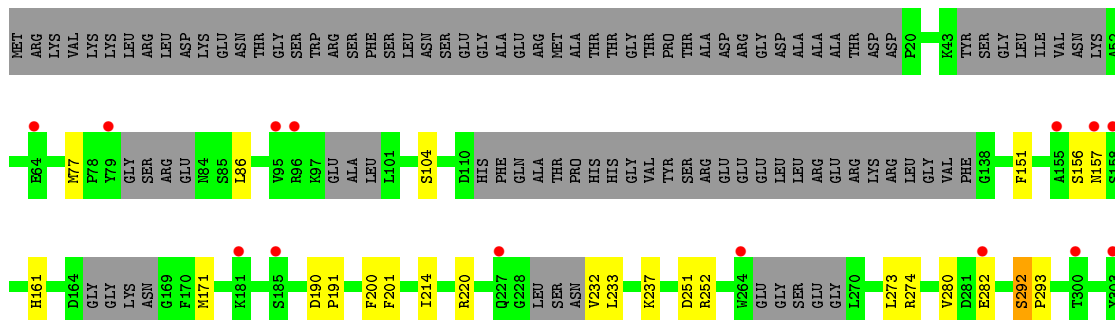
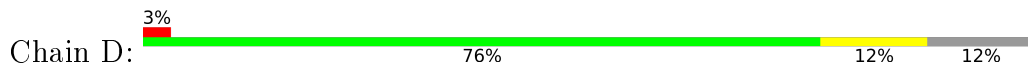
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	28	Total	O	0	0
			28	28		
4	A	36	Total	O	0	0
			36	36		
4	C	28	Total	O	0	0
			28	28		
4	D	37	Total	O	0	0
			37	37		

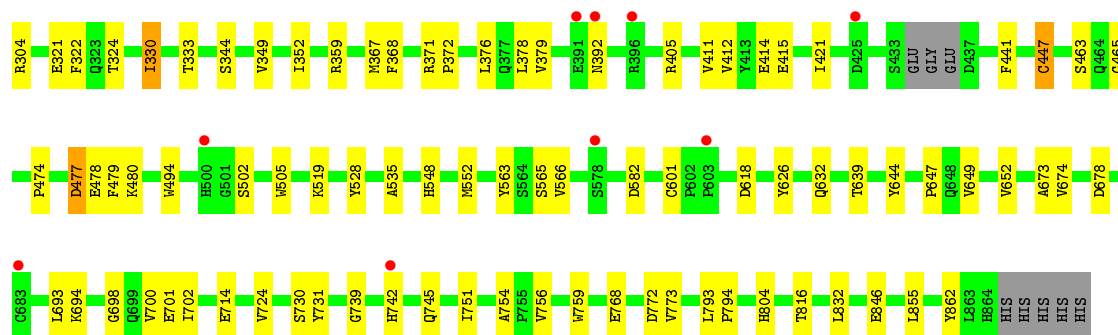


- Molecule 1: Dipeptidyl peptidase 9



- Molecule 1: Dipeptidyl peptidase 9





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.17Å 95.31Å 127.20Å 86.56° 102.54° 102.44°	Depositor
Resolution (Å)	46.89 – 2.90 46.89 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.89-2.90) 98.4 (46.89-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.223 , 0.290 0.226 , 0.289	Depositor DCC
R_{free} test set	4647 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtrriage
Anisotropy	0.219	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25685	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.00% 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: GOL, PO4

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	0.63	0/6620	0.73	0/8984
1	B	0.63	0/6518	0.74	0/8845
1	C	0.63	0/6581	0.74	0/8934
1	D	0.63	0/6570	0.73	0/8915
All	All	0.63	0/26289	0.74	0/35678

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 [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	6427	0	6219	47	0
1	B	6329	0	6128	47	0
1	C	6389	0	6162	46	0
1	D	6379	0	6176	48	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
4	A	36	0	0	3	0
4	B	28	0	0	1	0
4	C	28	0	0	2	0
4	D	37	0	0	2	0
All	All	25685	0	24701	186	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 4.

All (186) 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:C:340:GLN:HE22	1:C:471:PRO:HA	1.41	0.85
1:B:368:PHE:CE2	1:B:379:VAL:HG21	2.27	0.69
1:C:340:GLN:NE2	1:C:471:PRO:HA	2.09	0.67
1:B:415:GLU:HB3	1:B:447:CYS:SG	2.36	0.65
1:C:648:GLN:NE2	1:C:770:TYR:OH	2.30	0.64
1:B:494:TRP:CG	1:B:519:LYS:HA	2.34	0.62
1:B:602:PRO:O	1:B:604:ASP:N	2.33	0.62
1:C:252:ARG:NH1	1:C:352:ILE:O	2.34	0.61
1:C:419:VAL:O	1:C:694:LYS:HE2	1.99	0.61
1:C:494:TRP:CG	1:C:519:LYS:HA	2.36	0.60
1:A:773:VAL:HG12	1:A:774:PRO:HD2	1.83	0.60
1:D:415:GLU:HB3	1:D:447:CYS:SG	2.42	0.60
1:A:754:ALA:HA	1:A:804:HIS:CD2	2.37	0.60
1:B:768:GLU:HA	1:B:772:ASP:O	2.03	0.58
1:D:367:MET:HB3	1:D:376:LEU:HD21	1.86	0.58
1:B:716:TYR:HB3	1:B:718:PHE:CE2	2.38	0.57
1:A:305:TYR:CZ	1:A:763:ASP:HB3	2.39	0.57
1:C:785:SER:HA	4:C:1003:HOH:O	2.05	0.57
1:B:644:TYR:CE2	1:B:649:VAL:HG21	2.39	0.56
1:A:185:SER:OG	1:A:206:ASN:ND2	2.38	0.56
1:D:626:TYR:HB2	1:D:674:VAL:HB	1.89	0.55
1:A:519:LYS:HB3	1:A:528:TYR:CZ	2.42	0.55
1:A:864:HIS:HB2	4:A:1012:HOH:O	2.06	0.55
1:D:411:VAL:HG13	1:D:479:PHE:HB2	1.88	0.55
1:B:368:PHE:CZ	1:B:379:VAL:HG21	2.42	0.54
1:D:252:ARG:NH1	1:D:352:ILE:O	2.41	0.54
1:B:492:GLY:O	1:B:494:TRP:N	2.35	0.54
1:C:519:LYS:HB3	1:C:528:TYR:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:ARG:HD2	4:D:1029:HOH:O	2.06	0.54
1:D:768:GLU:HA	1:D:772:ASP:O	2.07	0.54
1:A:185:SER:HG	1:A:206:ASN:HD21	1.56	0.53
1:B:804:HIS:HD2	1:B:816:THR:OG1	1.91	0.53
1:A:252:ARG:NH1	1:A:352:ILE:O	2.42	0.53
1:D:698:GLY:N	1:D:701:GLU:OE2	2.41	0.52
1:B:804:HIS:CD2	1:B:816:THR:OG1	2.62	0.52
1:A:572:VAL:O	1:A:595:MET:HB2	2.09	0.52
1:B:71:ARG:NH1	1:B:164:ASP:OD2	2.42	0.52
1:B:153:PHE:CE1	1:B:160:PHE:HB2	2.44	0.52
1:B:378:LEU:HD21	1:B:427:PHE:CD1	2.46	0.52
1:A:66:GLY:O	1:A:93:LYS:NZ	2.36	0.51
1:A:757:THR:HA	1:A:786:VAL:HG22	1.91	0.51
1:D:151:PHE:O	1:D:161:HIS:HA	2.11	0.50
1:C:274:ARG:HB3	1:C:319:LEU:HD11	1.93	0.50
1:A:511:LYS:HA	1:A:532:TYR:CE2	2.46	0.50
1:A:778:GLN:HE21	1:A:778:GLN:HA	1.76	0.50
1:B:511:LYS:HA	1:B:532:TYR:CE2	2.47	0.50
1:C:252:ARG:HD3	1:C:353:ALA:O	2.11	0.50
1:A:367:MET:HB3	1:A:376:LEU:HD21	1.93	0.50
1:C:527:LEU:HB3	1:C:542:THR:HG23	1.94	0.50
1:A:640:VAL:O	1:A:674:VAL:HA	2.12	0.50
1:C:420:TRP:CZ3	1:C:694:LYS:HG3	2.47	0.49
1:A:401:ARG:HG3	1:A:469:SER:HB3	1.93	0.49
1:A:373:GLN:NE2	1:A:765:GLY:O	2.42	0.49
1:D:376:LEU:HB2	1:D:421:ILE:HG21	1.95	0.49
1:B:201:PHE:CD1	1:B:214:ILE:HG23	2.47	0.49
1:D:701:GLU:OE2	1:D:731:TYR:OH	2.25	0.49
1:B:60:GLN:HE21	1:B:555:ASN:ND2	2.10	0.48
1:A:151:PHE:HB2	1:A:162:CYS:SG	2.53	0.48
1:A:505:TRP:CD1	1:A:552:MET:HB2	2.48	0.48
1:C:456:LYS:HD2	1:C:487:ILE:HD12	1.95	0.48
1:C:368:PHE:CE2	1:C:379:VAL:HG21	2.49	0.48
1:A:516:GLN:HA	1:A:526:HIS:O	2.14	0.48
1:C:410:TYR:HB3	1:C:481:CYS:SG	2.54	0.48
1:C:417:THR:HB	1:C:447:CYS:SG	2.54	0.48
1:D:274:ARG:NH1	1:D:321:GLU:OE2	2.47	0.47
1:C:376:LEU:HB2	1:C:421:ILE:HG21	1.95	0.47
1:D:201:PHE:CD1	1:D:214:ILE:HG23	2.49	0.47
1:A:804:HIS:CD2	1:A:816:THR:OG1	2.68	0.47
1:C:232:VAL:O	1:C:232:VAL:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ARG:HG2	1:C:853:VAL:HG21	1.96	0.47
1:B:606:VAL:H	1:B:665:ASN:HD21	1.62	0.47
1:A:58:PHE:CE2	1:A:72:LEU:HD21	2.50	0.47
1:A:376:LEU:HB2	1:A:421:ILE:HG21	1.97	0.47
1:C:790:VAL:HG11	1:C:823:LEU:HA	1.96	0.47
1:A:415:GLU:HB3	1:A:447:CYS:SG	2.55	0.47
1:D:639:THR:O	1:D:724:VAL:HA	2.15	0.47
1:C:378:LEU:HD21	1:C:427:PHE:CZ	2.51	0.46
1:C:565:SER:OG	1:C:566:VAL:N	2.48	0.46
1:C:849:GLU:O	1:C:853:VAL:HG23	2.15	0.46
1:A:412:VAL:HG11	1:A:441:PHE:CE1	2.50	0.46
1:D:477:ASP:OD2	4:D:1001:HOH:O	2.21	0.46
1:B:201:PHE:CZ	1:B:212:ALA:HB3	2.50	0.46
1:D:200:PHE:CZ	1:D:324:THR:HG21	2.51	0.46
1:D:652:VAL:HB	1:D:678:ASP:OD2	2.16	0.46
1:D:156:SER:OG	1:D:157:ASN:N	2.49	0.46
1:D:548:HIS:CD2	1:D:563:TYR:HB3	2.51	0.46
1:A:626:TYR:HB2	1:A:674:VAL:HB	1.98	0.46
1:D:220:ARG:NH2	1:D:330:ILE:O	2.49	0.46
1:C:731:TYR:O	1:C:734:PHE:HB3	2.15	0.46
1:D:292:SER:OG	1:D:293:PRO:HD2	2.15	0.46
1:C:611:PHE:CZ	1:C:623:GLY:HA3	2.51	0.45
1:B:756:VAL:HG11	1:B:759:TRP:CZ3	2.52	0.45
1:C:411:VAL:HG23	1:C:479:PHE:HB2	1.98	0.45
1:D:273:LEU:HD12	1:D:322:PHE:CZ	2.51	0.45
1:D:644:TYR:CE2	1:D:649:VAL:HG21	2.52	0.45
1:A:95:VAL:HG22	1:A:592:TRP:CH2	2.51	0.45
1:A:376:LEU:HD13	1:A:377:GLN:N	2.31	0.45
1:B:69:SER:OG	1:B:70:HIS:N	2.50	0.45
1:B:815:HIS:HE1	4:B:1013:HOH:O	1.98	0.45
1:D:190:ASP:N	1:D:191:PRO:HD3	2.32	0.45
1:B:232:VAL:HB	1:B:233:LEU:H	1.74	0.45
1:B:542:THR:HB	1:B:548:HIS:CE1	2.51	0.45
1:C:511:LYS:HA	1:C:532:TYR:CE2	2.51	0.45
1:D:647:PRO:HD3	1:D:693:LEU:HD11	1.99	0.45
1:A:511:LYS:HA	1:A:532:TYR:CZ	2.51	0.45
1:A:429:PRO:HA	1:A:441:PHE:CB	2.46	0.45
1:C:740:LEU:HD22	1:C:750:ALA:HB3	1.97	0.45
1:C:862:TYR:HH	1:D:862:TYR:HH	1.65	0.45
1:D:349:VAL:HG22	1:D:368:PHE:HB3	1.98	0.45
1:D:804:HIS:HD2	1:D:816:THR:OG1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ARG:HB3	1:B:372:PRO:HD3	1.99	0.44
1:C:153:PHE:CE2	1:C:160:PHE:HB2	2.52	0.44
1:C:798:ASN:HB3	1:C:862:TYR:CG	2.53	0.44
1:C:804:HIS:HD2	1:C:816:THR:OG1	2.00	0.44
1:D:237:LYS:HA	1:D:280:VAL:O	2.17	0.44
1:D:751:ILE:HD13	1:D:855:LEU:CD1	2.47	0.44
1:D:494:TRP:CG	1:D:519:LYS:HA	2.52	0.44
1:B:190:ASP:N	1:B:191:PRO:CD	2.80	0.44
1:A:293:PRO:HG3	1:A:839:ARG:NH2	2.32	0.44
1:C:403:VAL:HA	4:C:1014:HOH:O	2.18	0.44
1:D:793:LEU:HB3	1:D:794:PRO:HD2	2.00	0.44
1:D:405:ARG:O	1:D:465:GLY:HA2	2.18	0.44
1:B:643:VAL:HG12	1:B:727:HIS:O	2.18	0.44
1:B:209:LEU:HD11	1:B:275:ILE:HG21	1.99	0.43
1:B:237:LYS:HA	1:B:280:VAL:O	2.17	0.43
1:D:519:LYS:HB3	1:D:528:TYR:CZ	2.53	0.43
1:B:77:MET:HB3	1:B:78:PRO:HD2	1.99	0.43
1:C:751:ILE:HD13	1:C:855:LEU:CD1	2.47	0.43
1:C:237:LYS:HA	1:C:280:VAL:O	2.19	0.43
1:C:406:ASN:OD1	1:C:406:ASN:N	2.45	0.43
1:D:322:PHE:HA	1:D:333:THR:HA	2.00	0.43
1:D:371:ARG:HB3	1:D:372:PRO:HD3	2.00	0.43
1:D:412:VAL:CG1	1:D:441:PHE:CE1	3.02	0.43
1:D:505:TRP:CG	1:D:552:MET:HB2	2.54	0.43
1:A:494:TRP:CG	1:A:519:LYS:HA	2.53	0.43
1:D:505:TRP:CD1	1:D:552:MET:HB2	2.53	0.43
1:B:274:ARG:NH1	1:B:321:GLU:OE2	2.52	0.43
1:A:252:ARG:HD3	1:A:353:ALA:O	2.19	0.43
1:A:815:HIS:HE1	4:A:1014:HOH:O	2.01	0.43
1:B:70:HIS:HB2	1:B:558:MET:HE1	2.01	0.42
1:A:668:ALA:HA	1:A:672:TYR:O	2.19	0.42
1:A:319:LEU:HD12	1:A:386:PHE:CD2	2.54	0.42
1:C:729:TRP:HA	1:C:753:GLY:O	2.19	0.42
1:B:833:GLN:HE22	1:B:850:HIS:HE1	1.67	0.42
1:A:64:GLU:HA	1:A:93:LYS:HZ1	1.84	0.42
1:D:477:ASP:HB3	1:D:480:LYS:HB2	2.02	0.42
1:B:338:LEU:HG	1:B:386:PHE:CE1	2.55	0.42
1:B:395:GLN:O	1:B:398:ALA:HB3	2.20	0.42
1:D:190:ASP:N	1:D:191:PRO:CD	2.83	0.42
1:D:474:PRO:CB	1:D:478:GLU:HG3	2.50	0.42
1:D:639:THR:HA	1:D:673:ALA:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:VAL:HG13	1:B:420:TRP:H	1.85	0.42
1:A:768:GLU:HA	1:A:772:ASP:O	2.20	0.42
1:C:401:ARG:HG2	1:C:469:SER:HB3	2.02	0.42
1:D:282:GLU:O	1:D:304:ARG:CZ	2.68	0.42
1:B:527:LEU:HB3	1:B:542:THR:HG23	2.00	0.42
1:A:188:ARG:HG2	1:A:203:PHE:CD2	2.55	0.42
1:B:380:LEU:HD11	1:B:439:LEU:CD2	2.49	0.41
1:D:756:VAL:HG11	1:D:759:TRP:CZ3	2.55	0.41
1:C:670:LEU:HD12	1:C:856:LEU:HD22	2.01	0.41
1:D:730:SER:HA	1:D:754:ALA:O	2.20	0.41
1:B:151:PHE:O	1:B:161:HIS:HA	2.20	0.41
1:B:563:TYR:CE1	1:B:571:CYS:HB2	2.55	0.41
1:B:512:LEU:HD11	1:B:584:PRO:HB2	2.02	0.41
1:A:293:PRO:HG3	1:A:839:ARG:HH22	1.86	0.41
1:B:798:ASN:HB3	1:B:862:TYR:CG	2.55	0.41
1:A:751:ILE:HD13	1:A:855:LEU:HD13	2.01	0.41
1:B:412:VAL:HG21	1:B:439:LEU:HD23	2.03	0.41
1:C:204:ILE:HD11	1:C:256:TYR:CD2	2.55	0.41
1:C:282:GLU:O	1:C:304:ARG:CZ	2.68	0.41
1:C:629:HIS:ND1	1:C:669:SER:HA	2.36	0.41
1:A:258:TRP:CH2	1:A:275:ILE:HD11	2.56	0.41
1:D:702:ILE:HD12	1:D:739:GLY:CA	2.51	0.41
1:A:225:CYS:SG	1:A:239:ALA:HB2	2.61	0.40
1:C:208:ASP:OD2	1:C:221:ARG:NH2	2.54	0.40
1:C:834:ILE:HD11	1:D:832:LEU:HD21	2.03	0.40
1:B:448:LYS:HD3	1:B:455:TYR:CE2	2.56	0.40
1:A:429:PRO:HA	1:A:441:PHE:HB3	2.03	0.40
1:A:448:LYS:HE2	4:A:1034:HOH:O	2.21	0.40
1:C:768:GLU:HA	1:C:772:ASP:O	2.21	0.40
1:B:371:ARG:N	1:B:372:PRO:CD	2.84	0.40
1:B:411:VAL:HG23	1:B:479:PHE:HB2	2.04	0.40
1:B:58:PHE:CE2	1:B:72:LEU:HD21	2.57	0.40
1:A:233:LEU:O	1:A:233:LEU:HD12	2.22	0.40
1:A:564:SER:HB3	1:A:570:PRO:HA	2.03	0.40
1:C:804:HIS:CD2	1:C:816:THR:OG1	2.75	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	780/898 (87%)	711 (91%)	68 (9%)	1 (0%)	51	82
1	B	762/898 (85%)	692 (91%)	66 (9%)	4 (0%)	29	61
1	C	775/898 (86%)	711 (92%)	63 (8%)	1 (0%)	51	82
1	D	770/898 (86%)	707 (92%)	60 (8%)	3 (0%)	34	66
All	All	3087/3592 (86%)	2821 (91%)	257 (8%)	9 (0%)	41	71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	493	GLU
1	C	476	GLU
1	B	535	ALA
1	A	294	ALA
1	D	392	ASN
1	D	535	ALA
1	B	603	PRO
1	D	330	ILE
1	B	419	VAL

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	701/785 (89%)	677 (97%)	24 (3%)	37	71
1	B	691/785 (88%)	663 (96%)	28 (4%)	30	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	696/785 (89%)	676 (97%)	20 (3%)	42	76
1	D	696/785 (89%)	667 (96%)	29 (4%)	30	63
All	All	2784/3140 (89%)	2683 (96%)	101 (4%)	35	69

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	42	ARG
1	B	147	GLU
1	B	150	LEU
1	B	164	ASP
1	B	232	VAL
1	B	233	LEU
1	B	298	ARG
1	B	343	SER
1	B	378	LEU
1	B	394	GLU
1	B	408	GLN
1	B	412	VAL
1	B	447	CYS
1	B	469	SER
1	B	477	ASP
1	B	502	SER
1	B	516	GLN
1	B	530	VAL
1	B	547	SER
1	B	557	ASP
1	B	590	ARG
1	B	595	MET
1	B	600	SER
1	B	609	GLU
1	B	669	SER
1	B	738	MET
1	B	745	GLN
1	B	795	ASN
1	A	55	ASP
1	A	95	VAL
1	A	104	SER
1	A	150	LEU
1	A	173	SER
1	A	207	SER

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Mol	Chain	Res	Type
1	A	220	ARG
1	A	232	VAL
1	A	263	SER
1	A	271	LYS
1	A	283	SER
1	A	351	TYR
1	A	379	VAL
1	A	389	SER
1	A	425	ASP
1	A	437	ASP
1	A	438	GLU
1	A	551	SER
1	A	604	ASP
1	A	748	LYS
1	A	778	GLN
1	A	809	GLU
1	A	821	SER
1	A	843	ARG
1	C	42	ARG
1	C	85	SER
1	C	104	SER
1	C	271	LYS
1	C	343	SER
1	C	378	LEU
1	C	399	SER
1	C	406	ASN
1	C	440	CYS
1	C	464	GLN
1	C	502	SER
1	C	516	GLN
1	C	565	SER
1	C	595	MET
1	C	601	CYS
1	C	694	LYS
1	C	738	MET
1	C	745	GLN
1	C	748	LYS
1	C	834	ILE
1	D	77	MET
1	D	86	LEU
1	D	104	SER
1	D	171	MET

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Mol	Chain	Res	Type
1	D	232	VAL
1	D	233	LEU
1	D	251	ASP
1	D	292	SER
1	D	344	SER
1	D	378	LEU
1	D	379	VAL
1	D	414	GLU
1	D	447	CYS
1	D	463	SER
1	D	477	ASP
1	D	502	SER
1	D	565	SER
1	D	566	VAL
1	D	582	ASP
1	D	601	CYS
1	D	618	ASP
1	D	632	GLN
1	D	694	LYS
1	D	700	VAL
1	D	714	GLU
1	D	742	HIS
1	D	745	GLN
1	D	773	VAL
1	D	846	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	60	GLN
1	B	84	ASN
1	B	206	ASN
1	B	548	HIS
1	B	555	ASN
1	B	632	GLN
1	B	665	ASN
1	B	705	GLN
1	B	804	HIS
1	B	810	ASN
1	B	815	HIS
1	B	833	GLN
1	B	860	GLN

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Mol	Chain	Res	Type
1	A	29	HIS
1	A	60	GLN
1	A	70	HIS
1	A	84	ASN
1	A	206	ASN
1	A	548	HIS
1	A	650	GLN
1	A	665	ASN
1	A	710	GLN
1	A	742	HIS
1	A	778	GLN
1	A	804	HIS
1	A	833	GLN
1	A	860	GLN
1	C	70	HIS
1	C	289	HIS
1	C	327	GLN
1	C	340	GLN
1	C	422	ASN
1	C	464	GLN
1	C	548	HIS
1	C	554	GLN
1	C	648	GLN
1	C	650	GLN
1	C	665	ASN
1	C	705	GLN
1	C	795	ASN
1	C	804	HIS
1	C	860	GLN
1	D	29	HIS
1	D	60	GLN
1	D	70	HIS
1	D	206	ASN
1	D	247	GLN
1	D	289	HIS
1	D	548	HIS
1	D	562	HIS
1	D	650	GLN
1	D	665	ASN
1	D	684	GLN
1	D	705	GLN
1	D	742	HIS

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Mol	Chain	Res	Type
1	D	804	HIS
1	D	810	ASN
1	D	831	GLN
1	D	860	GLN

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	GOL	B	902	-	5,5,5	0.11	0	5,5,5	0.32	0
2	PO4	D	901	-	4,4,4	0.75	0	6,6,6	0.42	0
2	PO4	B	901	-	4,4,4	0.76	0	6,6,6	0.36	0
2	PO4	C	901	-	4,4,4	0.76	0	6,6,6	0.43	0
2	PO4	A	901	-	4,4,4	0.66	0	6,6,6	0.48	0
3	GOL	A	902	-	5,5,5	0.11	0	5,5,5	0.36	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
3	GOL	B	902	-	-	4/4/4/4	-
3	GOL	A	902	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

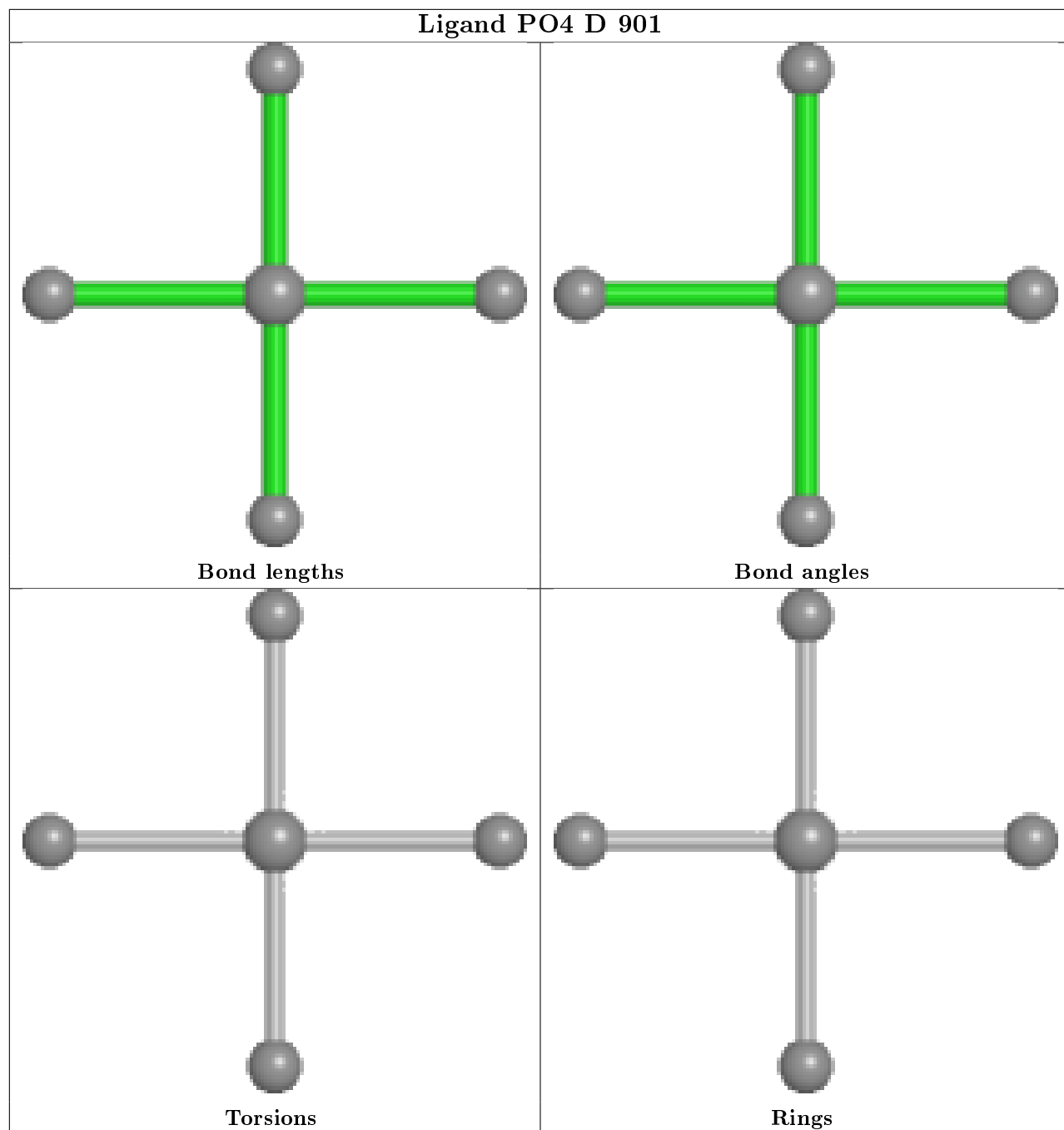
All (6) torsion outliers are listed below:

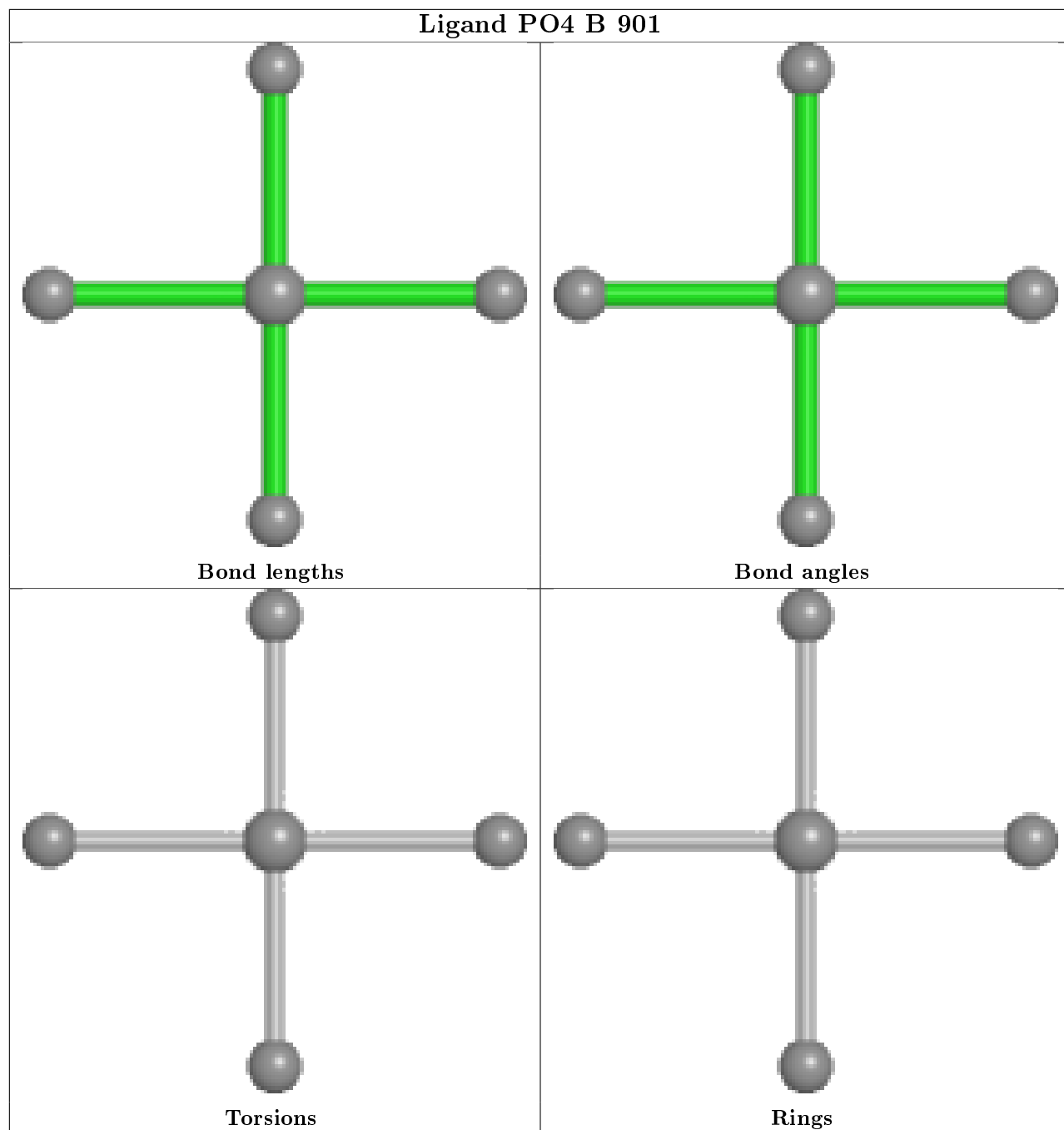
Mol	Chain	Res	Type	Atoms
3	B	902	GOL	C1-C2-C3-O3
3	A	902	GOL	O1-C1-C2-C3
3	B	902	GOL	O1-C1-C2-C3
3	B	902	GOL	O2-C2-C3-O3
3	B	902	GOL	O1-C1-C2-O2
3	A	902	GOL	O1-C1-C2-O2

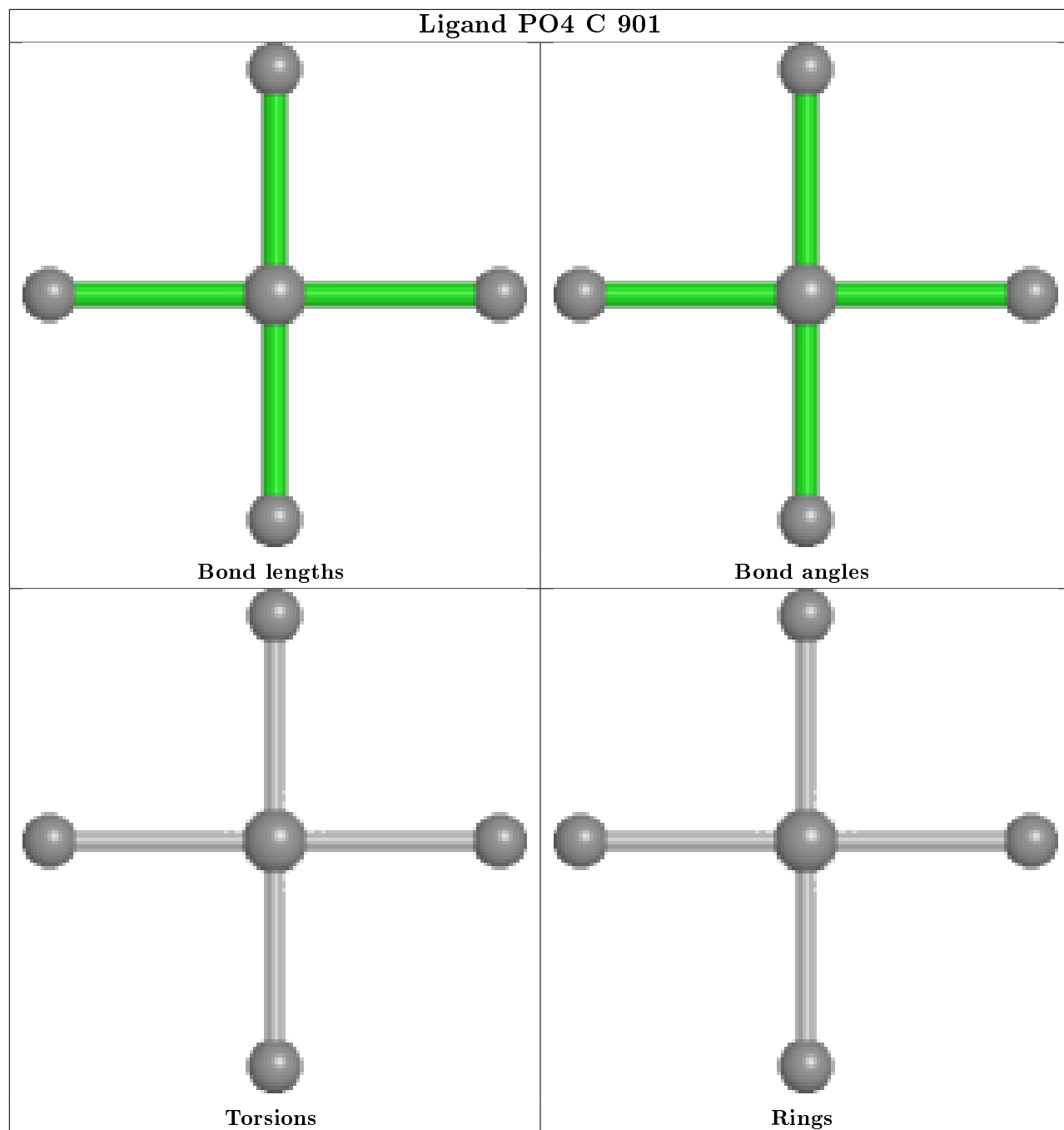
There are no ring outliers.

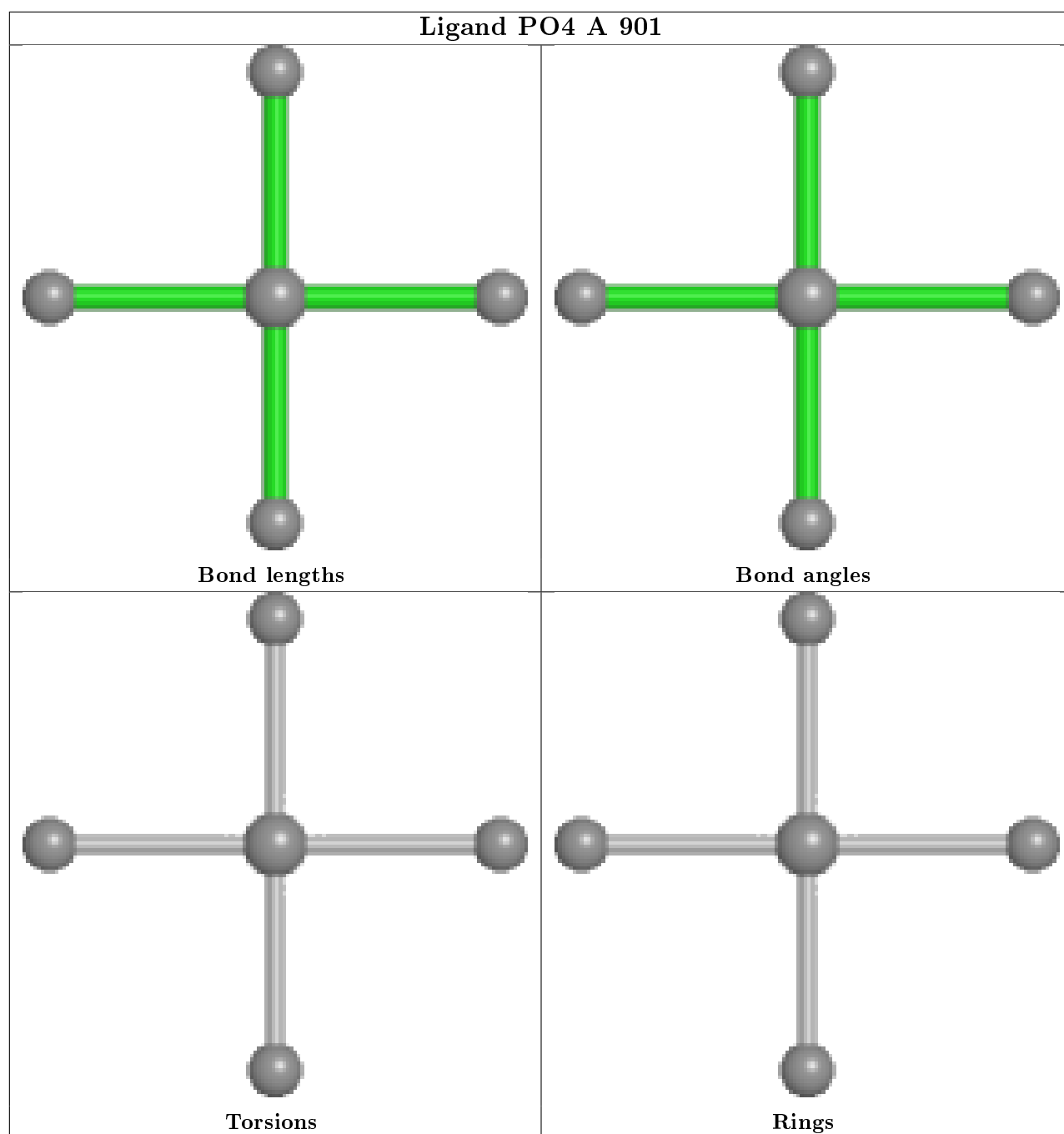
No monomer is involved in short contacts.

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	794/898 (88%)	0.20	25 (3%) 49 44	31, 62, 103, 123	0
1	B	782/898 (87%)	0.11	24 (3%) 49 44	25, 57, 96, 124	0
1	C	791/898 (88%)	0.20	31 (3%) 39 35	30, 59, 101, 134	0
1	D	788/898 (87%)	0.16	23 (2%) 51 47	38, 62, 95, 122	0
All	All	3155/3592 (87%)	0.16	103 (3%) 46 41	25, 61, 99, 134	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	185	SER	5.5
1	B	158	SER	5.1
1	B	76	GLY	4.9
1	B	110	ASP	4.5
1	C	158	SER	4.5
1	D	96	ARG	4.0
1	D	158	SER	3.9
1	A	64	GLU	3.5
1	C	157	ASN	3.5
1	A	95	VAL	3.5
1	A	98	GLU	3.5
1	A	99	ALA	3.4
1	B	599	ALA	3.4
1	B	92	PRO	3.4
1	B	183	GLN	3.3
1	A	65	SER	3.3
1	A	171	MET	3.3
1	C	437	ASP	3.3
1	D	95	VAL	3.3
1	C	68	HIS	3.3
1	A	170	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	472	PHE	3.3
1	D	227	GLN	3.3
1	D	282	GLU	3.2
1	A	96	ARG	3.2
1	C	92	PRO	3.1
1	A	181	LYS	3.1
1	C	69	SER	3.1
1	B	109	LEU	3.1
1	A	158	SER	3.1
1	A	267	SER	3.1
1	D	157	ASN	3.0
1	C	462	LYS	3.0
1	C	433	SER	3.0
1	B	433	SER	3.0
1	A	69	SER	3.0
1	C	466	TYR	2.8
1	C	170	PHE	2.8
1	D	396	ARG	2.8
1	C	19	ASP	2.8
1	A	157	ASN	2.8
1	D	155	ALA	2.8
1	A	198	PRO	2.7
1	C	468	TRP	2.7
1	C	500	HIS	2.7
1	C	463	SER	2.6
1	D	64	GLU	2.6
1	B	69	SER	2.6
1	C	109	LEU	2.6
1	D	264	TRP	2.6
1	D	181	LYS	2.6
1	B	185	SER	2.5
1	D	578	SER	2.5
1	C	579	GLY	2.5
1	B	592	TRP	2.5
1	D	79	TYR	2.5
1	B	233	LEU	2.5
1	A	778	GLN	2.4
1	A	592	TRP	2.4
1	C	110	ASP	2.4
1	D	683	CYS	2.4
1	C	469	SER	2.4
1	B	392	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	61	LYS	2.3
1	D	603	PRO	2.3
1	C	107	GLN	2.3
1	B	108	MET	2.3
1	C	592	TRP	2.3
1	A	299	LYS	2.3
1	A	97	LYS	2.3
1	A	173	SER	2.2
1	D	300	THR	2.2
1	B	93	LYS	2.2
1	C	94	LYS	2.2
1	A	185	SER	2.2
1	C	471	PRO	2.2
1	A	101	LEU	2.2
1	B	160	PHE	2.2
1	A	462	LYS	2.2
1	A	472	PHE	2.2
1	B	184	CYS	2.2
1	C	865	HIS	2.2
1	D	391	GLU	2.2
1	C	93	LYS	2.1
1	B	600	SER	2.1
1	B	62	THR	2.1
1	B	618	ASP	2.1
1	D	500	HIS	2.1
1	B	177	PRO	2.1
1	D	303	TYR	2.1
1	D	742	HIS	2.1
1	B	704	ASP	2.1
1	A	100	LEU	2.1
1	D	425	ASP	2.1
1	B	864	HIS	2.1
1	C	267	SER	2.1
1	C	179	GLU	2.1
1	A	200	PHE	2.1
1	C	64	GLU	2.0
1	C	406	ASN	2.0
1	C	176	LYS	2.0
1	D	392	ASN	2.0
1	C	404	PRO	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](#)

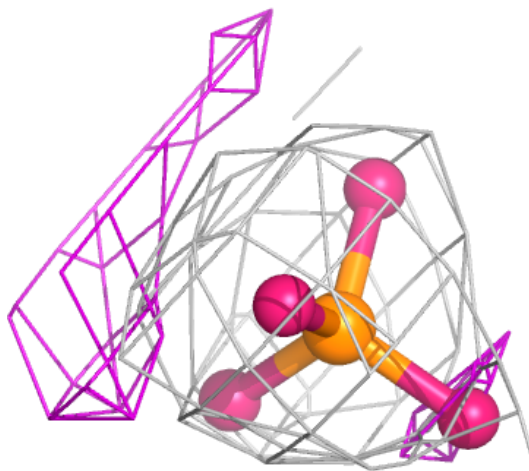
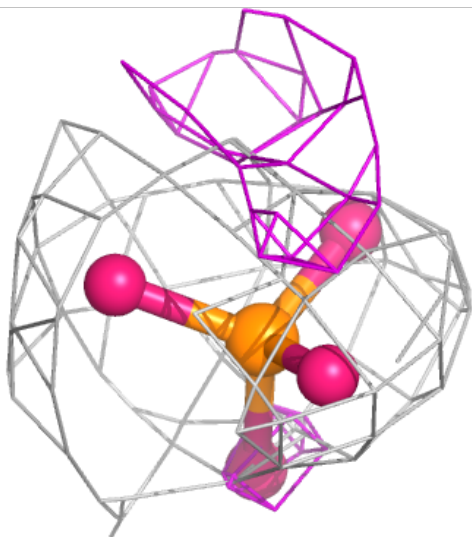
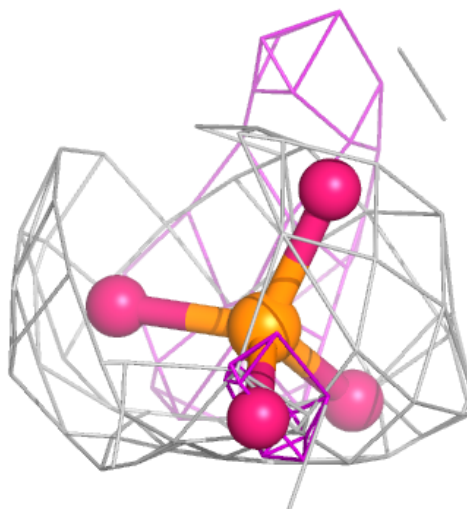
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	B	902	6/6	0.82	0.32	75,79,80,82	0
2	PO4	B	901	5/5	0.88	0.27	83,88,91,100	0
3	GOL	A	902	6/6	0.89	0.17	53,55,57,57	0
2	PO4	A	901	5/5	0.91	0.21	78,79,85,88	0
2	PO4	C	901	5/5	0.92	0.21	82,89,89,92	0
2	PO4	D	901	5/5	0.92	0.19	82,88,90,96	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.

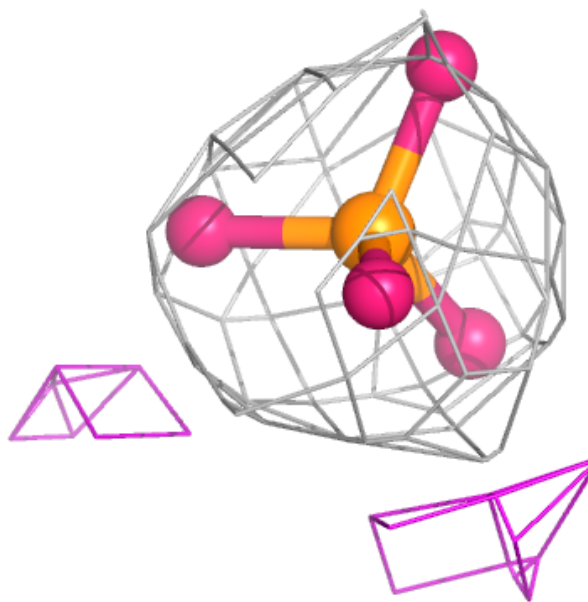
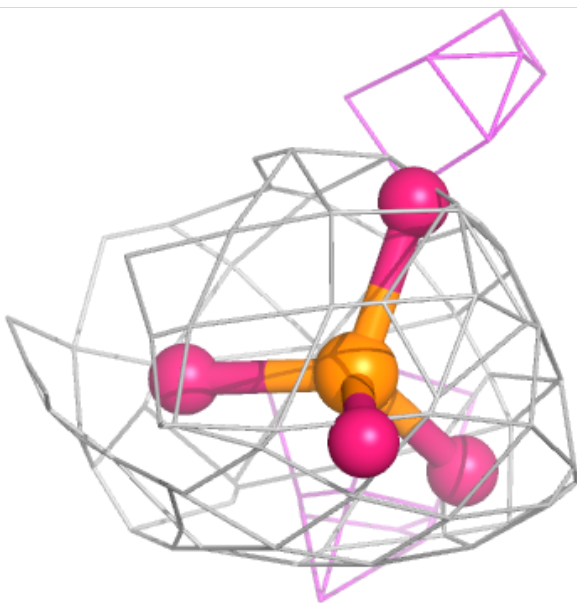
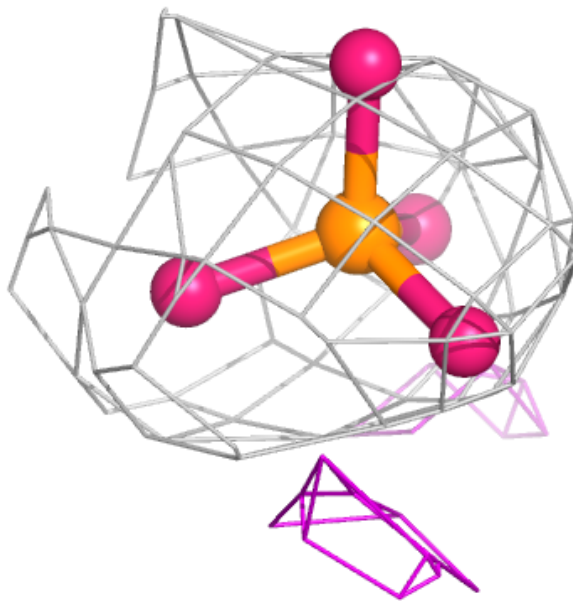
Electron density around PO4 B 901:

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



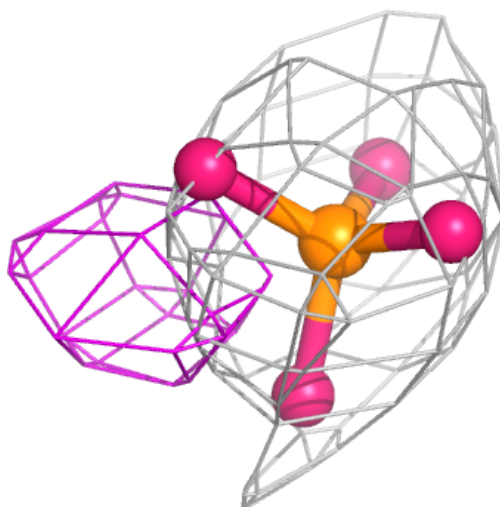
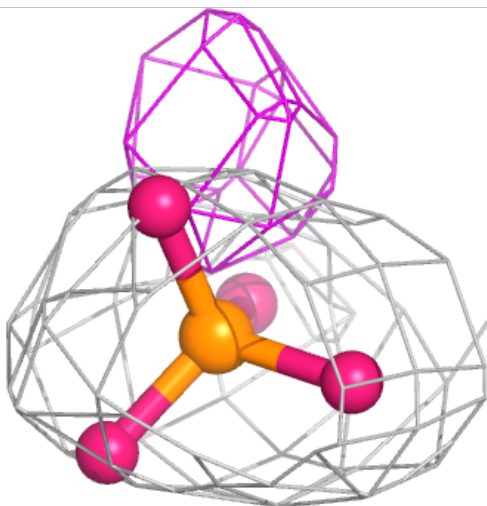
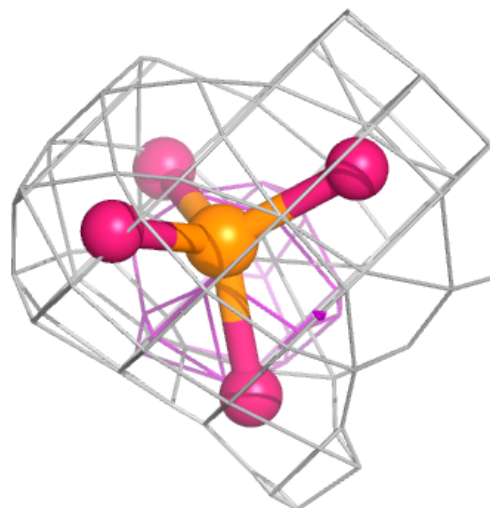
Electron density around PO4 A 901:

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



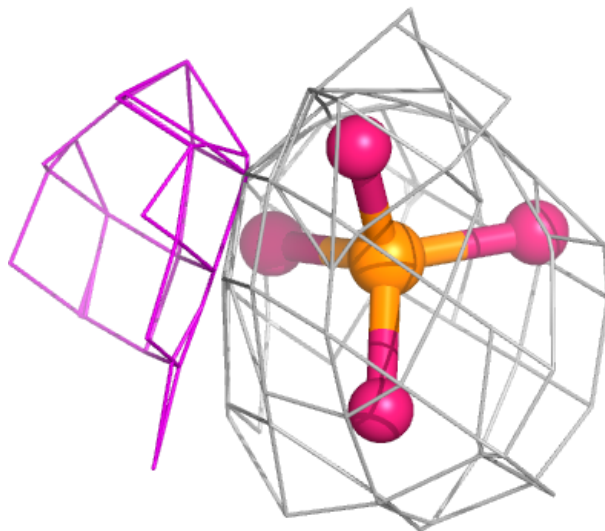
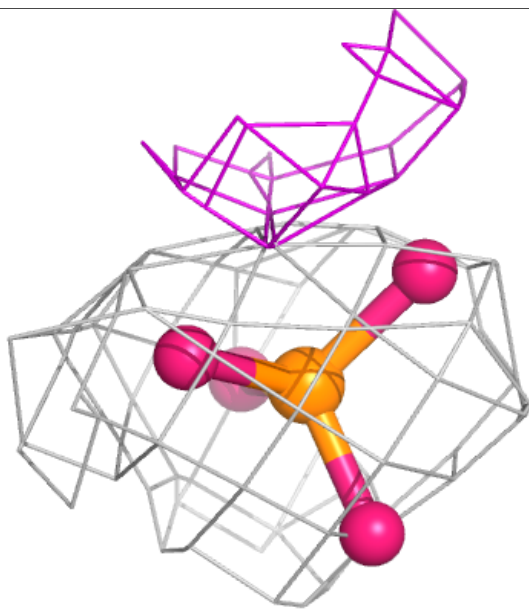
Electron density around PO4 C 901:

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



Electron density around PO4 D 901:

$2mF_o-DF_c$ (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.