Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:06 pm BST

PDB ID	:	6FW5
Title	:	TesA a major thioesterase from Mycobacterium tuberculosis
Authors	:	Cambillau, C.; Nguyen, V.S.; Canaan, S.
Deposited on	:	2018-03-05
Resolution	:	2.75 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:

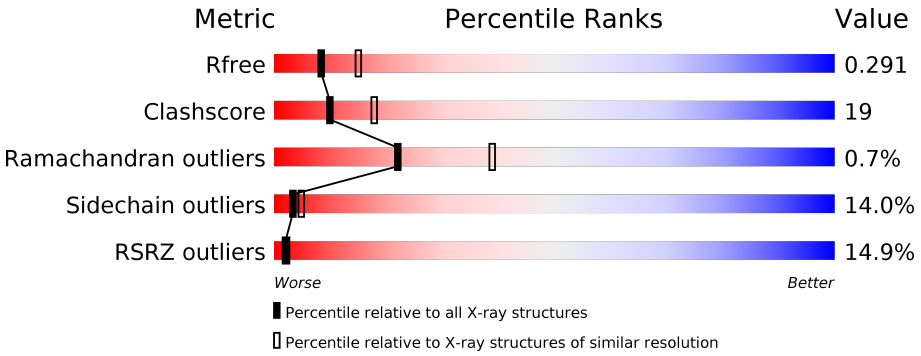
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 on 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 <=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	261	6% 67% 16% 6% 11%
1	B	261	11% 64% 18% • 15%
1	C	261	18% 46% 28% 6% 20%
1	D	261	15% 60% 21% • 14%

2 Entry composition

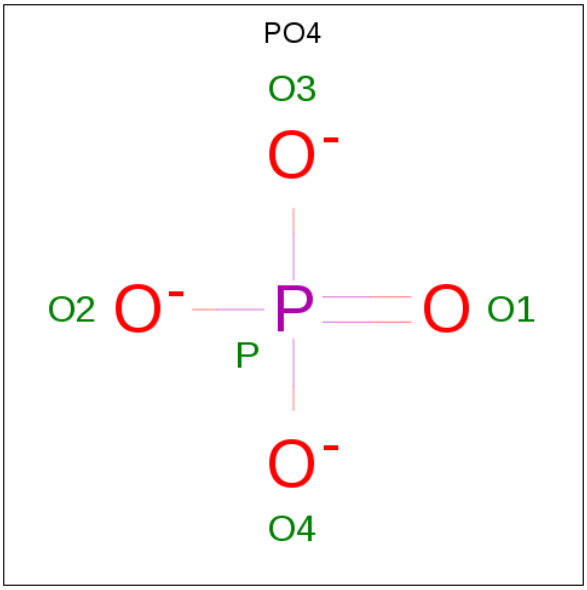
There are 3 unique types of molecules in this entry. The entry contains 6870 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Probable thioesterase TesA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	1	0
			1799	1145	305	339	10			
1	B	223	Total	C	N	O	S	0	0	0
			1704	1088	286	321	9			
1	C	208	Total	C	N	O	S	0	0	0
			1601	1032	264	295	10			
1	D	224	Total	C	N	O	S	0	0	0
			1666	1069	276	313	8			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by author).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 water.

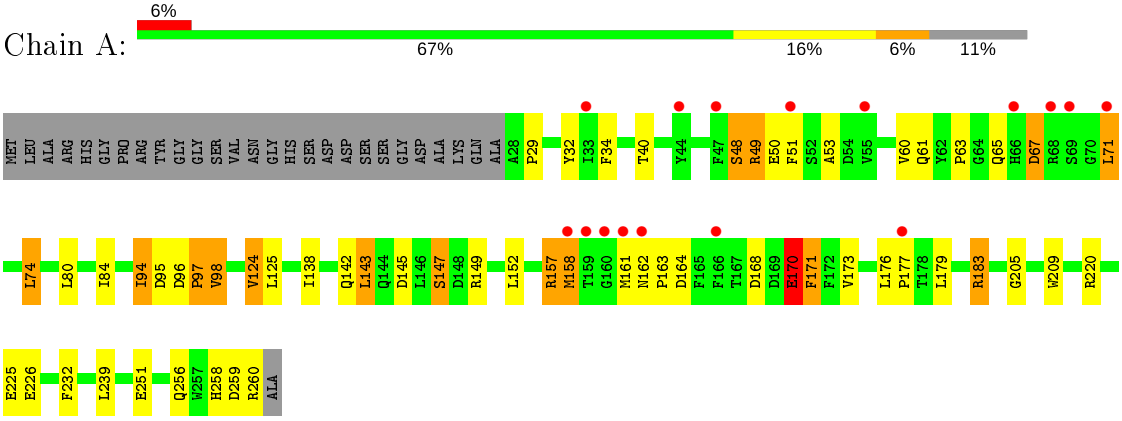
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	34	Total O 34 34	0	0
3	B	22	Total O 22 22	0	0
3	C	10	Total O 10 10	0	0
3	D	14	Total O 14 14	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

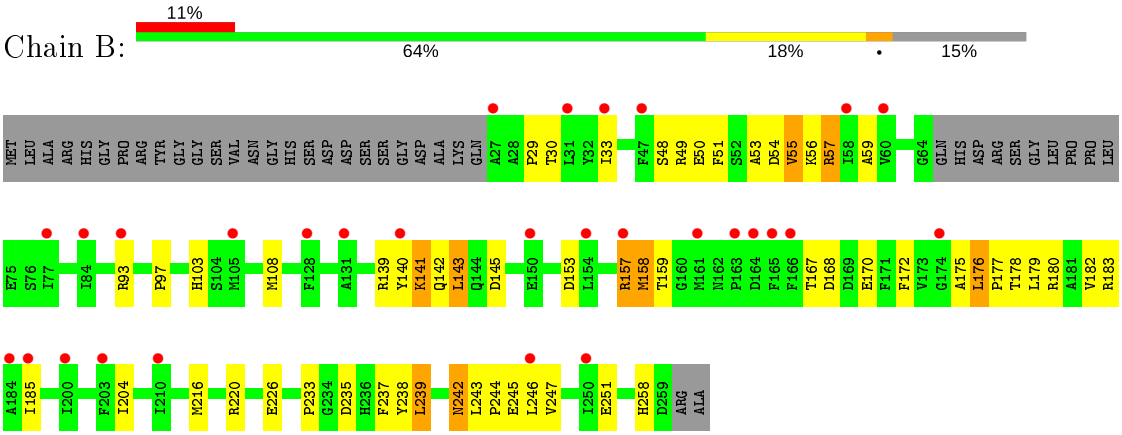
- Molecule 1: Probable thioesterase TesA

Chain A:



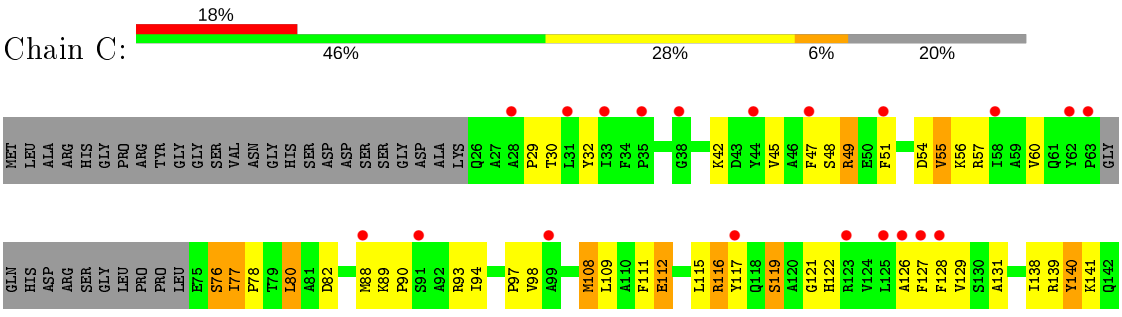
- Molecule 1: Probable thioesterase TesA

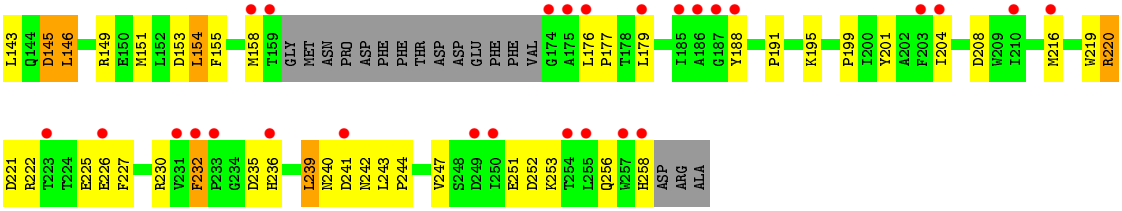
Chain B:



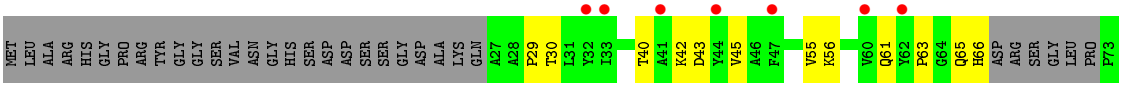
- Molecule 1: Probable thioesterase TesA

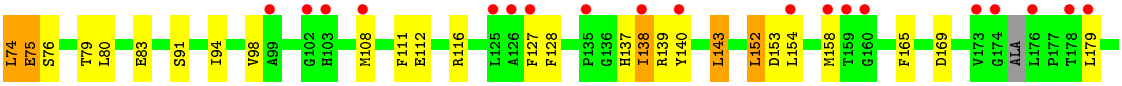
Chain C:

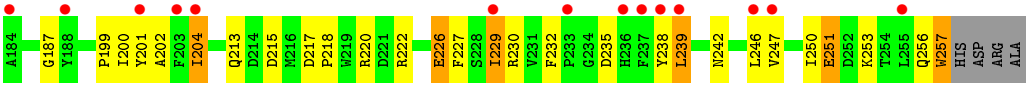




- Molecule 1: Probable thioesterase TesA







4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	77.58Å 224.65Å 226.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.89 – 2.75 39.89 – 2.75	Depositor EDS
% Data completeness (in resolution range)	93.1 (39.89-2.75) 91.0 (39.89-2.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.271 , 0.281 0.272 , 0.291	Depositor DCC
R_{free} test set	1216 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	112.3	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 123.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.055 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6870	wwPDB-VP
Average B, all atoms (Å^2)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1678e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.70	4/1854 (0.2%)	0.87	7/2528 (0.3%)
1	B	0.47	0/1751	0.71	0/2386
1	C	0.53	0/1646	0.76	0/2243
1	D	0.50	0/1712	0.75	1/2340 (0.0%)
All	All	0.56	4/6963 (0.1%)	0.78	8/9497 (0.1%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	SER	C-O	8.91	1.40	1.23
1	A	49[A]	ARG	CA-C	-8.39	1.31	1.52
1	A	49[B]	ARG	CA-C	-8.39	1.31	1.52
1	A	50	GLU	CA-CB	-5.08	1.42	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	49[A]	ARG	C-N-CA	8.17	142.13	121.70
1	A	49[B]	ARG	C-N-CA	8.17	142.13	121.70
1	A	50	GLU	N-CA-CB	-7.09	97.84	110.60
1	A	49[A]	ARG	CA-C-O	-6.26	106.96	120.10
1	A	49[B]	ARG	CA-C-O	-6.26	106.96	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	147	SER	CB-CA-C	-5.04	100.52	110.10
1	A	170	GLU	CA-C-O	-5.04	109.51	120.10
1	D	222	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	GLU	Mainchain

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	1799	0	1661	53	2
1	B	1704	0	1577	63	2
1	C	1601	0	1499	91	0
1	D	1666	0	1514	53	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	34	0	0	0	0
3	B	22	0	0	0	0
3	C	10	0	0	0	0
3	D	14	0	0	0	0
All	All	6870	0	6251	249	4

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 19.

All (249) 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:220:ARG:NH1	1:B:220:ARG:NH1	1.77	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ARG:HA	1:C:119:SER:OG	1.33	1.27
1:A:220:ARG:HH11	1:B:220:ARG:NH1	1.28	1.26
1:B:51:PHE:HB2	1:B:57:ARG:NH1	1.56	1.19
1:C:77:ILE:CD1	1:C:188:TYR:HB2	1.75	1.14
1:A:220:ARG:NH1	1:B:220:ARG:HH12	1.36	1.11
1:C:77:ILE:HD11	1:C:188:TYR:HB2	1.19	1.11
1:D:65:GLN:HB2	1:D:74:LEU:HB3	1.20	1.10
1:B:93:ARG:HH21	1:C:54:ASP:HB2	1.18	1.06
1:D:202:ALA:HB3	1:D:229:ILE:HD13	1.46	0.97
1:B:143:LEU:H	1:B:143:LEU:HD23	1.29	0.97
1:C:116:ARG:CA	1:C:119:SER:OG	2.17	0.91
1:A:170:GLU:HA	1:A:173:VAL:HG22	1.53	0.90
1:C:108:MET:HE2	1:C:188:TYR:CE2	2.07	0.89
1:D:65:GLN:CD	1:D:83:GLU:OE2	2.10	0.89
1:C:116:ARG:HA	1:C:119:SER:HG	1.35	0.87
1:C:220:ARG:N	1:C:227:PHE:HE2	1.72	0.87
1:A:220:ARG:NH1	1:B:220:ARG:HH11	1.72	0.87
1:A:125:LEU:HD11	1:A:258:HIS:HB2	1.58	0.86
1:B:93:ARG:NH2	1:C:54:ASP:HB2	1.90	0.85
1:B:51:PHE:HB2	1:B:57:ARG:HH11	1.37	0.84
1:A:29:PRO:HA	1:A:97:PRO:HB2	1.60	0.84
1:B:176:LEU:N	1:B:177:PRO:HD2	1.93	0.83
1:A:53:ALA:HB3	1:A:251:GLU:OE1	1.78	0.83
1:C:220:ARG:N	1:C:227:PHE:CE2	2.46	0.83
1:A:147:SER:CA	1:A:183:ARG:HH12	1.92	0.82
1:A:96:ASP:HB3	1:A:97:PRO:HD2	1.62	0.82
1:A:94:ILE:HD12	1:A:94:ILE:H	1.45	0.81
1:D:65:GLN:HB2	1:D:74:LEU:CB	2.08	0.81
1:D:65:GLN:H	1:D:74:LEU:HD22	1.45	0.81
1:D:230:ARG:NH1	1:D:232:PHE:CZ	2.49	0.80
1:A:147:SER:OG	1:A:183:ARG:NH2	2.13	0.80
1:A:220:ARG:HH12	1:B:220:ARG:NH1	1.79	0.80
1:A:125:LEU:CD1	1:A:258:HIS:HB2	2.11	0.79
1:B:176:LEU:HD11	1:B:180:ARG:CZ	2.14	0.77
1:C:77:ILE:CD1	1:C:188:TYR:CB	2.62	0.76
1:A:147:SER:HG	1:A:183:ARG:HH22	1.33	0.76
1:C:219:TRP:C	1:C:227:PHE:HE2	1.88	0.76
1:C:108:MET:CE	1:C:188:TYR:CE2	2.69	0.75
1:C:108:MET:CE	1:C:188:TYR:CD2	2.71	0.74
1:D:202:ALA:CB	1:D:229:ILE:HD13	2.17	0.74
1:B:153:ASP:O	1:B:157:ARG:HG2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:SER:OG	1:A:183:ARG:NH1	2.21	0.73
1:B:157:ARG:CZ	1:B:157:ARG:HA	2.20	0.72
1:D:65:GLN:CG	1:D:83:GLU:OE2	2.37	0.71
1:C:77:ILE:HD12	1:C:188:TYR:HB2	1.69	0.71
1:D:239:LEU:HD11	1:D:246:LEU:HD23	1.72	0.71
1:A:48:SER:O	1:A:51:PHE:HB2	1.90	0.70
1:C:145:ASP:HA	1:C:149:ARG:HD2	1.73	0.70
1:A:220:ARG:HH11	1:B:220:ARG:HH12	0.71	0.69
1:C:126:ALA:HB3	1:C:128:PHE:CZ	2.28	0.69
1:C:220:ARG:CA	1:C:227:PHE:CE2	2.76	0.69
1:C:252:ASP:O	1:C:256:GLN:HB2	1.91	0.69
1:D:76:SER:HB3	1:D:79:THR:HG23	1.75	0.69
1:B:176:LEU:HD21	1:B:180:ARG:NH1	2.09	0.68
1:B:29:PRO:O	1:B:55:VAL:HG23	1.94	0.68
1:A:226:GLU:HB3	1:B:226:GLU:HB3	1.76	0.67
1:B:176:LEU:N	1:B:177:PRO:CD	2.57	0.67
1:A:96:ASP:CB	1:A:97:PRO:HD2	2.25	0.66
1:A:71:LEU:HG	1:A:147:SER:HB2	1.77	0.66
1:B:243:LEU:H	1:B:243:LEU:HD23	1.59	0.66
1:B:204:ILE:HB	1:B:216:MET:CE	2.26	0.66
1:B:180:ARG:HD3	1:B:183:ARG:HH22	1.61	0.66
1:C:108:MET:HE1	1:C:188:TYR:CD2	2.31	0.65
1:C:94:ILE:O	1:C:122:HIS:HA	1.97	0.65
1:C:77:ILE:HG13	1:C:78:PRO:HD3	1.80	0.64
1:C:32:TYR:HE2	1:C:98:VAL:CG2	2.10	0.64
1:B:51:PHE:HB2	1:B:57:ARG:CZ	2.26	0.64
1:C:204:ILE:HD11	1:C:216:MET:CE	2.28	0.64
1:C:220:ARG:HA	1:C:227:PHE:CE2	2.33	0.64
1:C:77:ILE:HD11	1:C:188:TYR:CB	2.12	0.64
1:A:147:SER:CB	1:A:183:ARG:HH12	2.10	0.64
1:D:127:PHE:HD2	1:D:200:ILE:HG12	1.63	0.64
1:B:239:LEU:HD22	1:B:239:LEU:H	1.61	0.63
1:B:33:ILE:HG13	1:B:59:ALA:HA	1.80	0.63
1:B:51:PHE:CG	1:B:57:ARG:HD2	2.34	0.63
1:D:143:LEU:HB3	1:D:187:GLY:HA2	1.81	0.63
1:B:108:MET:HE1	1:B:185:ILE:HG12	1.80	0.62
1:B:48:SER:O	1:B:57:ARG:NH1	2.33	0.62
1:C:154:LEU:HD22	1:C:158:MET:HB2	1.81	0.62
1:C:204:ILE:HD11	1:C:216:MET:HE1	1.82	0.62
1:D:108:MET:CE	1:D:138:ILE:HD11	2.30	0.62
1:D:65:GLN:OE1	1:D:83:GLU:OE2	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:MET:H	1:B:158:MET:HE3	1.65	0.61
1:C:80:LEU:HD21	1:C:109:LEU:HD21	1.83	0.61
1:D:227:PHE:CZ	1:D:229:ILE:HD11	2.35	0.61
1:D:40:THR:HG22	1:D:43:ASP:OD1	1.99	0.61
1:D:227:PHE:HZ	1:D:229:ILE:HD11	1.66	0.61
1:C:177:PRO:HA	1:C:179:LEU:HD23	1.82	0.60
1:C:77:ILE:HD12	1:C:188:TYR:CB	2.30	0.60
1:A:147:SER:OG	1:A:183:ARG:CZ	2.50	0.59
1:A:96:ASP:HB3	1:A:97:PRO:CD	2.31	0.59
1:A:220:ARG:HH12	1:B:220:ARG:HH11	1.41	0.59
1:A:63:PRO:HD2	1:A:80:LEU:HD11	1.85	0.59
1:B:157:ARG:NH2	1:B:157:ARG:HA	2.18	0.58
1:A:157:ARG:NH1	1:A:157:ARG:HG3	2.17	0.58
1:B:53:ALA:HB3	1:B:251:GLU:OE1	2.02	0.58
1:C:131:ALA:HB1	1:C:236:HIS:CE1	2.38	0.58
1:C:220:ARG:HB3	1:C:227:PHE:CD2	2.38	0.58
1:C:154:LEU:HD11	1:C:158:MET:SD	2.44	0.58
1:B:172:PHE:HA	1:B:176:LEU:HB2	1.85	0.58
1:B:180:ARG:HD3	1:B:183:ARG:NH2	2.19	0.58
1:C:128:PHE:HD1	1:C:201:TYR:HB2	1.68	0.57
1:C:49:ARG:HB2	1:C:49:ARG:CZ	2.35	0.57
1:C:51:PHE:O	1:C:251:GLU:OE2	2.22	0.57
1:B:243:LEU:N	1:B:244:PRO:HD2	2.19	0.57
1:C:219:TRP:C	1:C:227:PHE:CE2	2.74	0.57
1:A:157:ARG:HH11	1:A:157:ARG:CG	2.18	0.57
1:C:199:PRO:HB3	1:C:226:GLU:OE1	2.05	0.57
1:D:217:ASP:O	1:D:220:ARG:HG3	2.04	0.57
1:D:63:PRO:HG2	1:D:83:GLU:OE1	2.05	0.57
1:B:176:LEU:HD11	1:B:180:ARG:NE	2.18	0.57
1:D:75:GLU:OE1	1:D:75:GLU:HA	2.01	0.57
1:C:220:ARG:HA	1:C:227:PHE:CD2	2.40	0.56
1:D:111:PHE:HB2	1:D:127:PHE:CZ	2.40	0.56
1:C:219:TRP:HB2	1:C:227:PHE:HZ	1.69	0.56
1:A:53:ALA:CB	1:A:251:GLU:OE1	2.50	0.56
1:C:230:ARG:O	1:C:232:PHE:CE2	2.58	0.56
1:A:147:SER:HA	1:A:183:ARG:HH12	1.67	0.56
1:C:230:ARG:O	1:C:232:PHE:HE2	1.88	0.56
1:A:170:GLU:CA	1:A:173:VAL:HG22	2.32	0.56
1:B:176:LEU:H	1:B:177:PRO:HD2	1.70	0.55
1:C:141:LYS:HB3	1:C:143:LEU:CD1	2.36	0.55
1:D:138:ILE:HG22	1:D:140:TYR:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ARG:CA	1:C:227:PHE:HE2	2.16	0.54
1:C:220:ARG:HD3	1:C:221:ASP:OD1	2.06	0.54
1:D:165:PHE:O	1:D:169:ASP:CB	2.55	0.54
1:C:146:LEU:H	1:C:149:ARG:HB3	1.72	0.54
1:C:60:VAL:HG22	1:C:88:MET:SD	2.48	0.53
1:D:152:LEU:O	1:D:152:LEU:HD12	2.09	0.53
1:C:131:ALA:HA	1:C:204:ILE:HD11	1.90	0.53
1:D:128:PHE:HD2	1:D:201:TYR:HB2	1.74	0.53
1:A:147:SER:CA	1:A:183:ARG:NH1	2.69	0.53
1:B:167:THR:HG22	1:B:170:GLU:H	1.74	0.53
1:D:108:MET:HE1	1:D:138:ILE:HD11	1.89	0.53
1:C:93:ARG:O	1:C:122:HIS:CD2	2.62	0.53
1:B:97:PRO:HG3	1:B:258:HIS:CE1	2.44	0.52
1:C:191:PRO:O	1:C:222:ARG:NH1	2.41	0.52
1:C:195:LYS:CB	1:C:222:ARG:O	2.58	0.52
1:D:204:ILE:CD1	1:D:213:GLN:HA	2.40	0.52
1:D:40:THR:HA	1:D:61:GLN:HE22	1.75	0.52
1:D:253:LYS:O	1:D:257:TRP:NE1	2.43	0.51
1:A:157:ARG:HH11	1:A:157:ARG:HG3	1.74	0.51
1:B:175:ALA:HA	1:B:177:PRO:HD2	1.93	0.51
1:C:111:PHE:HB2	1:C:127:PHE:CZ	2.45	0.51
1:B:103:HIS:CE1	1:B:239:LEU:HD11	2.45	0.51
1:B:243:LEU:HA	1:B:246:LEU:HB3	1.93	0.51
1:C:29:PRO:HB3	1:C:97:PRO:HB2	1.93	0.51
1:A:98:VAL:HG23	1:A:124:VAL:HA	1.93	0.51
1:D:199:PRO:HG3	1:D:257:TRP:CH2	2.46	0.50
1:B:176:LEU:H	1:B:177:PRO:CD	2.24	0.50
1:B:233:PRO:HG2	1:B:242:ASN:HD21	1.76	0.50
1:C:32:TYR:CE2	1:C:98:VAL:CG2	2.94	0.50
1:D:116:ARG:HG3	1:D:116:ARG:HH11	1.76	0.50
1:C:117:TYR:O	1:C:121:GLY:O	2.30	0.49
1:B:176:LEU:HD11	1:B:180:ARG:NH2	2.26	0.49
1:C:76:SER:O	1:C:80:LEU:HD22	2.11	0.49
1:A:170:GLU:O	1:A:171:PHE:C	2.50	0.49
1:D:108:MET:HE3	1:D:138:ILE:HD11	1.95	0.49
1:D:127:PHE:O	1:D:200:ILE:HA	2.12	0.49
1:A:157:ARG:NH1	1:A:157:ARG:CG	2.75	0.49
1:B:33:ILE:CG1	1:B:59:ALA:HA	2.42	0.49
1:A:40:THR:HA	1:A:61:GLN:HE22	1.77	0.49
1:C:131:ALA:HA	1:C:204:ILE:CD1	2.42	0.49
1:A:162:ASN:N	1:A:163:PRO:HD2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LYS:HB3	1:C:143:LEU:HD12	1.94	0.48
1:B:53:ALA:HB3	1:B:251:GLU:CD	2.33	0.48
1:C:140:TYR:HD1	1:C:140:TYR:O	1.96	0.48
1:C:108:MET:HE1	1:C:188:TYR:HD2	1.74	0.48
1:C:32:TYR:HE2	1:C:98:VAL:HG23	1.78	0.48
1:D:232:PHE:CD1	1:D:242:ASN:ND2	2.81	0.48
1:C:94:ILE:HA	1:C:122:HIS:CD2	2.49	0.48
1:D:76:SER:HB3	1:D:79:THR:CG2	2.43	0.48
1:B:239:LEU:O	1:B:243:LEU:HB3	2.14	0.48
1:C:151:MET:HB3	1:C:155:PHE:CZ	2.49	0.48
1:D:112:GLU:HG3	1:D:116:ARG:NH1	2.28	0.48
1:A:34:PHE:HA	1:A:60:VAL:HG22	1.96	0.47
1:C:158:MET:O	1:C:158:MET:HG2	2.14	0.47
1:D:42:LYS:HA	1:D:45:VAL:HG13	1.96	0.47
1:C:97:PRO:HG2	1:C:258:HIS:NE2	2.28	0.47
1:B:140:TYR:HB2	1:B:142:GLN:OE1	2.15	0.47
1:B:243:LEU:N	1:B:244:PRO:CD	2.78	0.47
1:B:235:ASP:O	1:B:238:TYR:HB3	2.14	0.47
1:D:232:PHE:HD1	1:D:242:ASN:ND2	2.13	0.47
1:D:30:THR:HG23	1:D:56:LYS:HE2	1.95	0.47
1:A:147:SER:N	1:A:183:ARG:NH1	2.63	0.47
1:A:32:TYR:HE2	1:A:98:VAL:HG12	1.79	0.47
1:A:97:PRO:HG3	1:A:258:HIS:CE1	2.50	0.47
1:C:108:MET:HE1	1:C:188:TYR:CE2	2.50	0.47
1:C:108:MET:HE2	1:C:108:MET:HB2	1.63	0.46
1:C:42:LYS:HA	1:C:45:VAL:HG13	1.97	0.46
1:A:125:LEU:HD13	1:A:258:HIS:HB2	1.97	0.46
1:C:127:PHE:CZ	1:C:129:VAL:CG1	2.99	0.46
1:D:247:VAL:O	1:D:251:GLU:HB2	2.16	0.46
1:B:30:THR:HG22	1:B:56:LYS:HB2	1.97	0.46
1:D:30:THR:OG1	1:D:98:VAL:HG12	2.15	0.46
1:A:170:GLU:O	1:A:173:VAL:N	2.48	0.46
1:C:30:THR:HG22	1:C:56:LYS:HE2	1.98	0.46
1:B:204:ILE:HB	1:B:216:MET:HE1	1.99	0.45
1:D:220:ARG:HG2	1:D:227:PHE:CD1	2.52	0.45
1:B:57:ARG:NH2	1:C:90:PRO:HB3	2.32	0.45
1:C:55:VAL:HB	1:C:57:ARG:HD2	1.98	0.45
1:D:235:ASP:O	1:D:238:TYR:HB3	2.16	0.45
1:B:141:LYS:HG2	1:B:143:LEU:HD21	1.97	0.45
1:C:77:ILE:HD12	1:C:188:TYR:CG	2.52	0.45
1:C:93:ARG:O	1:C:122:HIS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ILE:HA	1:C:80:LEU:CD2	2.47	0.45
1:C:30:THR:HG22	1:C:56:LYS:CE	2.47	0.44
1:B:176:LEU:HD21	1:B:180:ARG:HH12	1.83	0.44
1:C:244:PRO:HA	1:C:247:VAL:HG22	1.99	0.44
1:B:30:THR:HA	1:B:56:LYS:O	2.17	0.44
1:B:178:THR:O	1:B:182:VAL:HG23	2.18	0.43
1:C:112:GLU:C	1:C:116:ARG:HH11	2.20	0.43
1:C:235:ASP:HB2	1:C:236:HIS:H	1.67	0.43
1:C:232:PHE:N	1:C:232:PHE:CD2	2.86	0.43
1:D:152:LEU:C	1:D:152:LEU:HD12	2.39	0.43
1:C:239:LEU:O	1:C:243:LEU:HG	2.19	0.43
1:A:158:MET:HG3	1:A:158:MET:H	1.56	0.43
1:A:74:LEU:HG	1:A:74:LEU:H	1.52	0.43
1:C:219:TRP:HB2	1:C:227:PHE:CZ	2.52	0.43
1:B:50:GLU:HB3	1:B:247:VAL:HG11	2.01	0.42
1:D:128:PHE:CD2	1:D:201:TYR:HB2	2.53	0.42
1:C:177:PRO:HA	1:C:179:LEU:CD2	2.47	0.42
1:C:154:LEU:HD22	1:C:154:LEU:O	2.20	0.42
1:D:253:LYS:O	1:D:257:TRP:CD1	2.72	0.42
1:C:216:MET:HE3	1:C:216:MET:HB2	1.93	0.42
1:D:199:PRO:HB3	1:D:226:GLU:HB3	2.01	0.42
1:C:77:ILE:H	1:C:77:ILE:HG12	1.58	0.42
1:C:154:LEU:CD2	1:C:158:MET:HB2	2.49	0.42
1:D:137:HIS:CD2	1:D:218:PRO:HG2	2.55	0.42
1:A:147:SER:HA	1:A:183:ARG:NH1	2.32	0.42
1:C:47:PHE:O	1:C:51:PHE:CE2	2.73	0.42
1:A:80:LEU:O	1:A:84:ILE:HG12	2.20	0.42
1:B:176:LEU:HD22	1:B:176:LEU:O	2.20	0.41
1:C:204:ILE:HD11	1:C:216:MET:HE3	2.01	0.41
1:A:258:HIS:O	1:A:258:HIS:ND1	2.53	0.41
1:D:220:ARG:HG2	1:D:227:PHE:CE1	2.55	0.41
1:C:108:MET:HB3	1:C:108:MET:HE3	1.72	0.41
1:B:141:LYS:CG	1:B:143:LEU:HD21	2.50	0.41
1:A:176:LEU:HA	1:A:179:LEU:HB2	2.02	0.41
1:B:175:ALA:C	1:B:177:PRO:HD2	2.40	0.41
1:A:143:LEU:H	1:A:143:LEU:CD2	2.33	0.41
1:D:80:LEU:O	1:D:80:LEU:HD12	2.20	0.41
1:D:65:GLN:HG3	1:D:83:GLU:OE2	2.18	0.41
1:A:147:SER:N	1:A:183:ARG:HH12	2.19	0.41
1:A:205:GLY:HA2	1:A:232:PHE:O	2.21	0.41
1:D:200:ILE:O	1:D:227:PHE:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:PHE:CB	1:B:57:ARG:HH11	2.19	0.40
1:D:29:PRO:HG2	1:D:55:VAL:HG12	2.03	0.40

All (4) 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:B:157:ARG:NH1	1:B:237:PHE:CE2[3_455]	1.50	0.70
1:A:164:ASP:OD2	1:A:170:GLU:OE2[3_455]	1.62	0.58
1:A:157:ARG:NH2	1:A:209:TRP:CZ2[3_455]	1.87	0.33
1:B:157:ARG:NH1	1:B:237:PHE:CZ[3_455]	1.90	0.30

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	232/261 (89%)	208 (90%)	20 (9%)	4 (2%)	9 16
1	B	219/261 (84%)	201 (92%)	18 (8%)	0	100 100
1	C	202/261 (77%)	182 (90%)	20 (10%)	0	100 100
1	D	218/261 (84%)	198 (91%)	18 (8%)	2 (1%)	17 31
All	All	871/1044 (83%)	789 (91%)	76 (9%)	6 (1%)	22 39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	GLU
1	A	171	PHE
1	D	94	ILE
1	A	97	PRO
1	A	67	ASP

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Mol	Chain	Res	Type
1	D	158	MET

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	182/216 (84%)	154 (85%)	28 (15%)	2 3
1	B	170/216 (79%)	153 (90%)	17 (10%)	7 13
1	C	161/216 (74%)	131 (81%)	30 (19%)	1 2
1	D	161/216 (74%)	141 (88%)	20 (12%)	4 7
All	All	674/864 (78%)	579 (86%)	95 (14%)	3 4

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49[A]	ARG
1	A	49[B]	ARG
1	A	65	GLN
1	A	67	ASP
1	A	71	LEU
1	A	74	LEU
1	A	94	ILE
1	A	95	ASP
1	A	98	VAL
1	A	124	VAL
1	A	138	ILE
1	A	142	GLN
1	A	143	LEU
1	A	145	ASP
1	A	149	ARG
1	A	152	LEU
1	A	157	ARG
1	A	158	MET
1	A	161	MET
1	A	168	ASP

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Mol	Chain	Res	Type
1	A	170	GLU
1	A	177	PRO
1	A	183	ARG
1	A	225	GLU
1	A	239	LEU
1	A	256	GLN
1	A	259	ASP
1	A	260	ARG
1	B	49	ARG
1	B	54	ASP
1	B	55	VAL
1	B	57	ARG
1	B	139	ARG
1	B	141	LYS
1	B	143	LEU
1	B	145	ASP
1	B	157	ARG
1	B	158	MET
1	B	159	THR
1	B	168	ASP
1	B	176	LEU
1	B	179	LEU
1	B	239	LEU
1	B	242	ASN
1	B	245	GLU
1	C	48	SER
1	C	49	ARG
1	C	55	VAL
1	C	76	SER
1	C	77	ILE
1	C	80	LEU
1	C	82	ASP
1	C	89	LYS
1	C	108	MET
1	C	112	GLU
1	C	115	LEU
1	C	116	ARG
1	C	119	SER
1	C	138	ILE
1	C	139	ARG
1	C	140	TYR
1	C	145	ASP

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Mol	Chain	Res	Type
1	C	146	LEU
1	C	153	ASP
1	C	154	LEU
1	C	176	LEU
1	C	208	ASP
1	C	220	ARG
1	C	225	GLU
1	C	232	PHE
1	C	239	LEU
1	C	240	ASN
1	C	241	ASP
1	C	242	ASN
1	C	253	LYS
1	D	66	HIS
1	D	74	LEU
1	D	75	GLU
1	D	91	SER
1	D	138	ILE
1	D	139	ARG
1	D	143	LEU
1	D	152	LEU
1	D	153	ASP
1	D	154	LEU
1	D	179	LEU
1	D	204	ILE
1	D	215	ASP
1	D	226	GLU
1	D	229	ILE
1	D	239	LEU
1	D	250	ILE
1	D	251	GLU
1	D	256	GLN
1	D	257	TRP

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

Mol	Chain	Res	Type
1	A	142	GLN
1	B	242	ASN
1	C	122	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	A	301	1	4,4,4	2.46	1 (25%)	6,6,6	0.48	0
2	PO4	D	301	1	4,4,4	2.02	1 (25%)	6,6,6	0.42	0
2	PO4	B	301	1	4,4,4	1.98	3 (75%)	6,6,6	0.59	0
2	PO4	C	301	1	4,4,4	2.05	1 (25%)	6,6,6	0.38	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	PO4	P-O1	4.08	1.60	1.50
2	C	301	PO4	P-O1	2.27	1.56	1.50
2	D	301	PO4	P-O1	2.19	1.56	1.50
2	B	301	PO4	P-O4	2.09	1.60	1.54
2	B	301	PO4	P-O2	2.05	1.60	1.54
2	B	301	PO4	P-O3	2.05	1.60	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 then 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.

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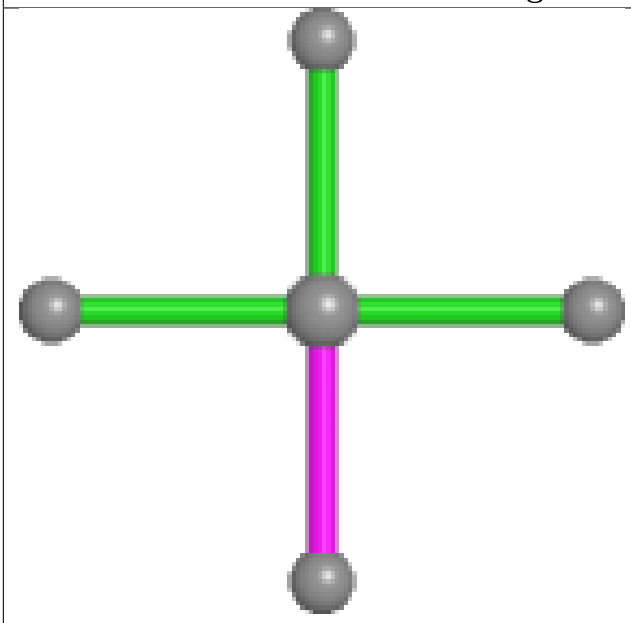
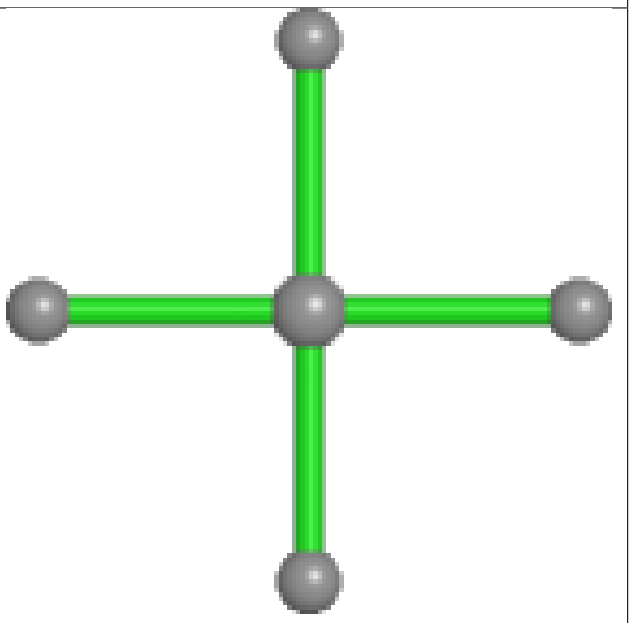
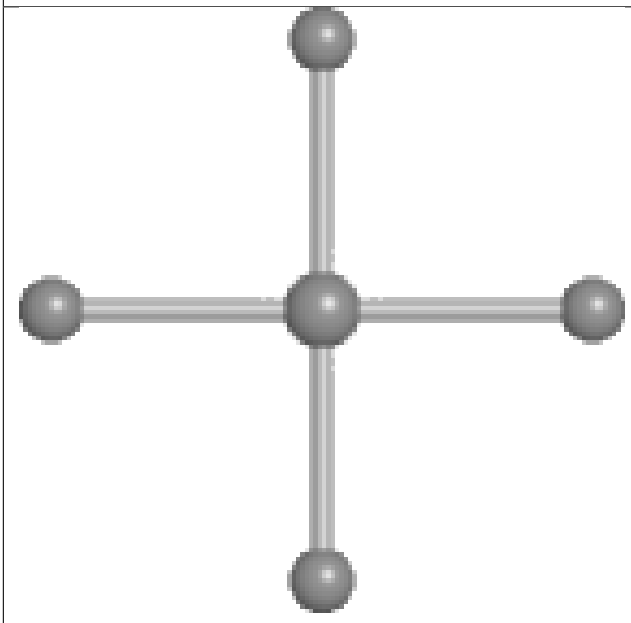


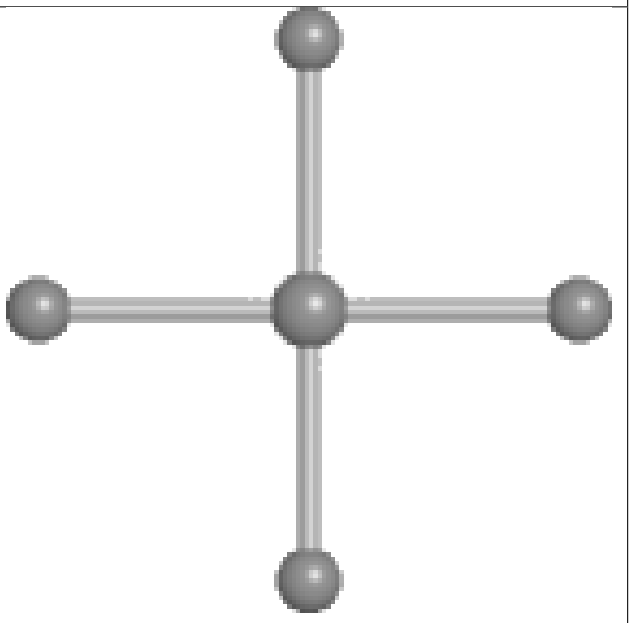
Bond lengths



Bond angles

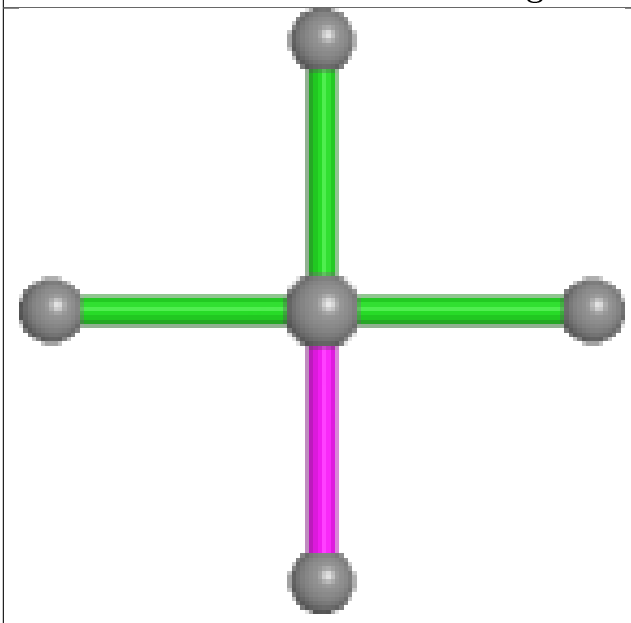


Torsions

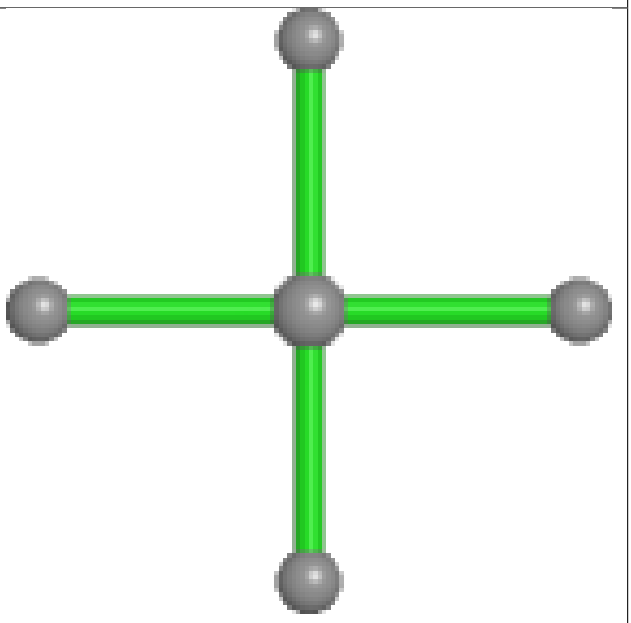


Rings

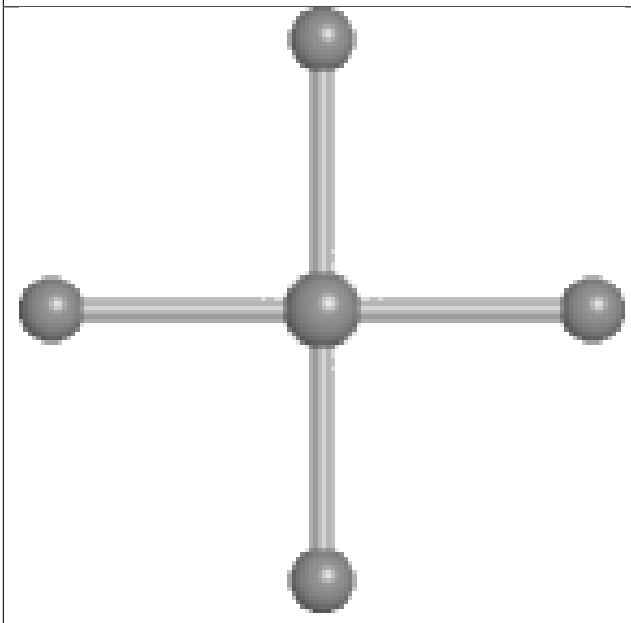
Ligand PO4 D 301



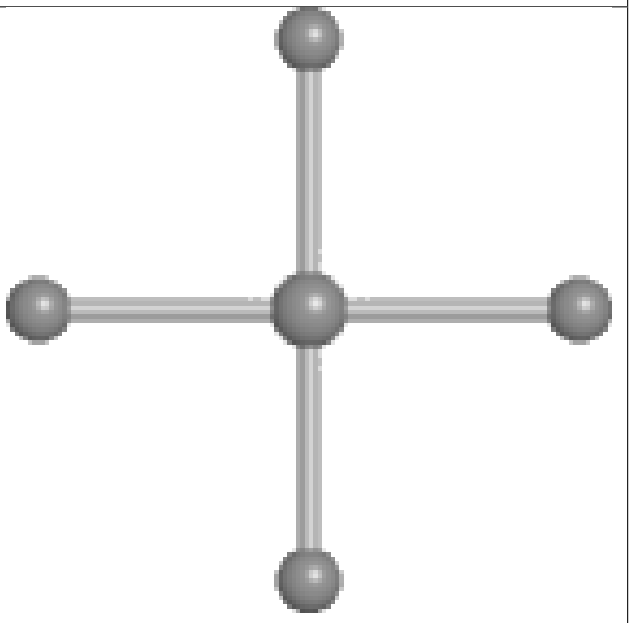
Bond lengths



Bond angles

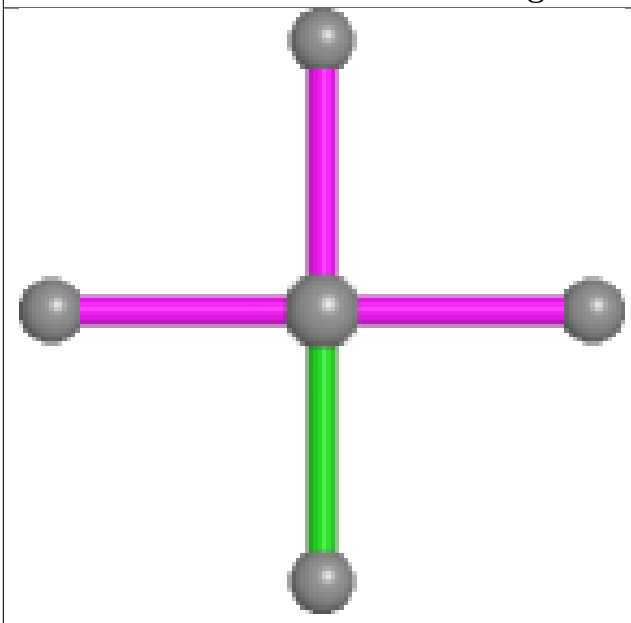


Torsions

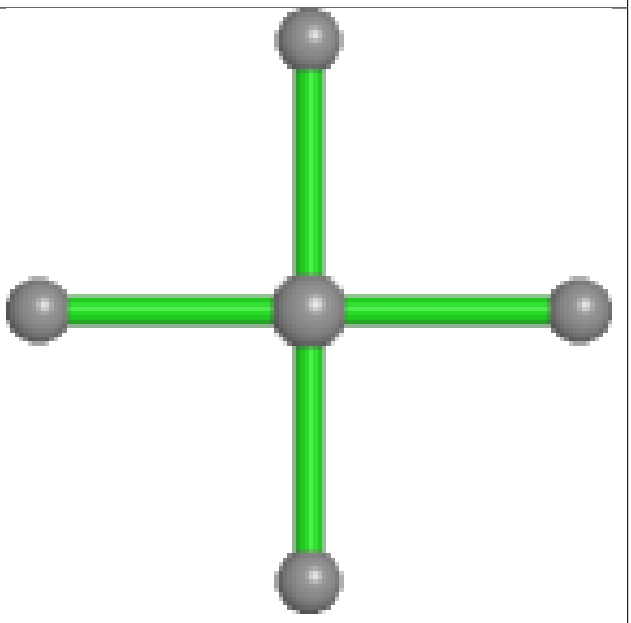


Rings

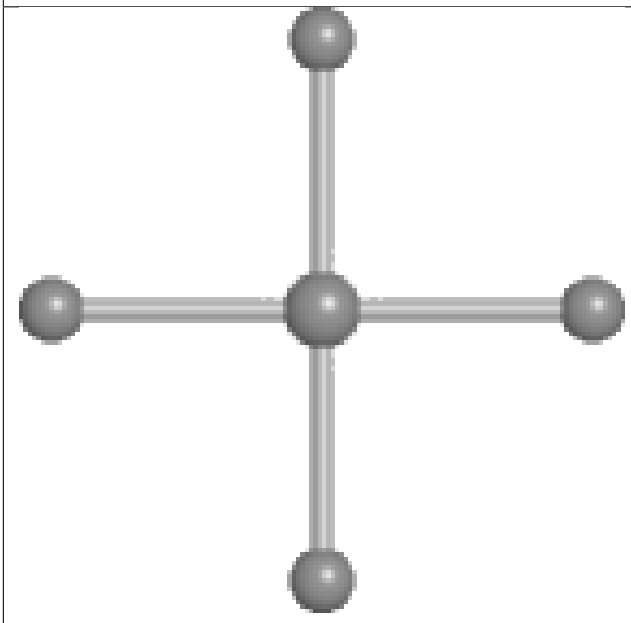
Ligand PO4 B 301



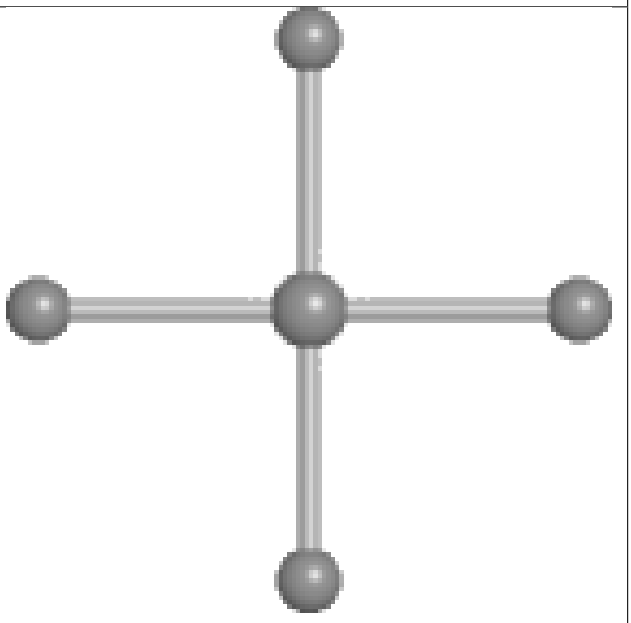
Bond lengths



Bond angles

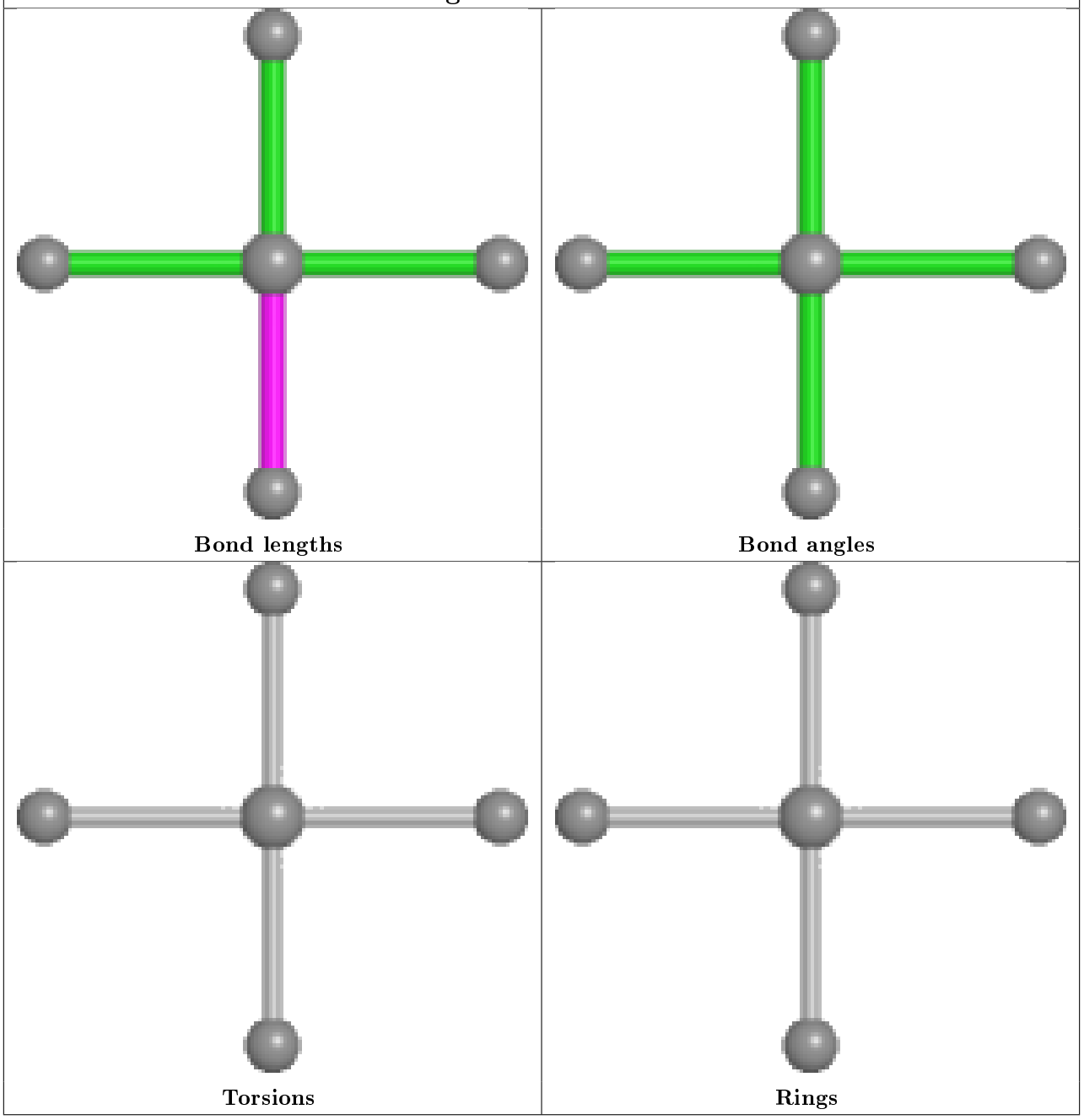


Torsions



Rings

Ligand PO4 C 301



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, 95^{th} 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	233/261 (89%)	0.54	16 (6%) 16 20	76, 103, 220, 243	0
1	B	223/261 (85%)	0.72	29 (13%) 3 4	76, 112, 249, 277	0
1	C	208/261 (79%)	1.08	47 (22%) 0 0	95, 131, 226, 275	0
1	D	224/261 (85%)	0.96	40 (17%) 1 1	99, 136, 262, 276	0
All	All	888/1044 (85%)	0.82	132 (14%) 2 2	76, 125, 238, 277	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	176	LEU	10.2
1	D	159	THR	7.0
1	C	187	GLY	6.2
1	D	178	THR	6.1
1	D	47	PHE	5.8
1	C	159	THR	5.8
1	A	159	THR	5.7
1	C	174	GLY	4.7
1	D	233	PRO	4.6
1	B	140	TYR	4.4
1	C	175	ALA	4.4
1	C	62	TYR	4.3
1	B	174	GLY	4.3
1	D	127	PHE	4.2
1	C	216	MET	4.1
1	C	158	MET	4.0
1	B	47	PHE	4.0
1	C	44	TYR	4.0
1	C	123	ARG	3.9
1	C	236	HIS	3.8
1	C	51	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	246	LEU	3.7
1	C	255	LEU	3.7
1	C	258	HIS	3.7
1	C	249	ASP	3.7
1	B	185	ILE	3.6
1	B	165	PHE	3.6
1	C	31	LEU	3.6
1	D	32	TYR	3.6
1	A	177	PRO	3.6
1	B	164	ASP	3.5
1	D	188	TYR	3.5
1	D	238	TYR	3.4
1	D	108	MET	3.4
1	D	239	LEU	3.4
1	B	250	ILE	3.3
1	C	125	LEU	3.3
1	C	188	TYR	3.3
1	B	77	ILE	3.3
1	D	201	TYR	3.3
1	A	162	ASN	3.2
1	D	236	HIS	3.2
1	B	200	ILE	3.2
1	C	186	ALA	3.2
1	C	203	PHE	3.2
1	D	158	MET	3.1
1	C	127	PHE	3.1
1	C	254	THR	3.1
1	C	250	ILE	3.0
1	C	58	ILE	3.0
1	A	66	HIS	3.0
1	C	233	PRO	2.9
1	D	138	ILE	2.9
1	A	68	ARG	2.9
1	B	31	LEU	2.9
1	D	102	GLY	2.9
1	B	33	ILE	2.9
1	D	204	ILE	2.9
1	D	44	TYR	2.8
1	A	33	ILE	2.8
1	C	126	ALA	2.7
1	D	103	HIS	2.7
1	B	154	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	161	MET	2.7
1	A	47	PHE	2.7
1	B	60	VAL	2.7
1	C	117	TYR	2.7
1	D	229	ILE	2.7
1	B	27	ALA	2.6
1	B	166	PHE	2.6
1	C	33	ILE	2.6
1	B	105	MET	2.6
1	B	246	LEU	2.6
1	D	203	PHE	2.6
1	A	161	MET	2.6
1	C	63	PRO	2.6
1	B	184	ALA	2.6
1	B	58	ILE	2.6
1	D	99	ALA	2.6
1	C	28	ALA	2.5
1	C	204	ILE	2.5
1	C	179	LEU	2.5
1	D	125	LEU	2.5
1	A	166	PHE	2.5
1	C	257	TRP	2.4
1	D	173	VAL	2.4
1	C	226	GLU	2.4
1	C	185	ILE	2.4
1	D	255	LEU	2.4
1	C	88	MET	2.4
1	D	62	TYR	2.4
1	C	47	PHE	2.4
1	D	176	LEU	2.4
1	D	33	ILE	2.4
1	A	44	TYR	2.3
1	D	41	ALA	2.3
1	D	179	LEU	2.3
1	A	51	PHE	2.3
1	C	223	THR	2.3
1	A	69	SER	2.3
1	A	71	LEU	2.3
1	C	210	ILE	2.3
1	C	91	SER	2.2
1	D	154	LEU	2.2
1	B	203	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	99	ALA	2.2
1	D	160	GLY	2.2
1	D	184	ALA	2.2
1	D	247	VAL	2.2
1	B	157	ARG	2.2
1	B	163	PRO	2.2
1	A	55	VAL	2.2
1	B	210	ILE	2.2
1	C	232	PHE	2.2
1	A	160	GLY	2.1
1	D	60	VAL	2.1
1	C	38	GLY	2.1
1	C	241	ASP	2.1
1	B	150	GLU	2.1
1	C	128	PHE	2.1
1	B	84	ILE	2.1
1	D	174	GLY	2.1
1	D	140	TYR	2.1
1	B	128	PHE	2.0
1	B	131	ALA	2.0
1	D	126	ALA	2.0
1	A	158	MET	2.0
1	D	237	PHE	2.0
1	B	93	ARG	2.0
1	C	35	PRO	2.0
1	C	231	VAL	2.0
1	D	135	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 carbohydrates 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,

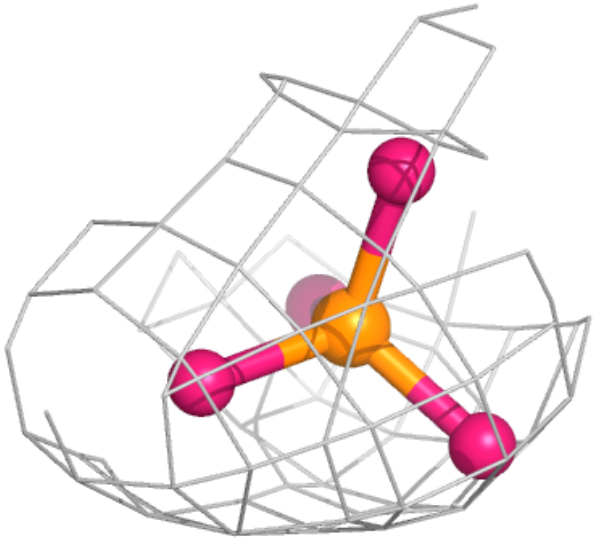
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

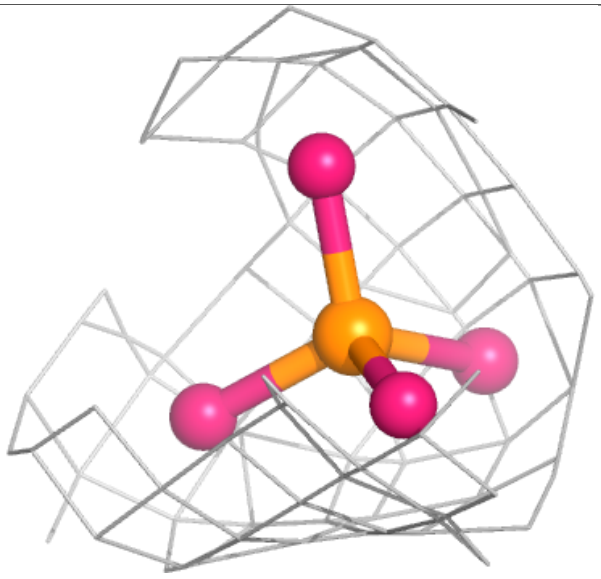
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	D	301	5/5	0.84	0.13	109,109,110,111	0
2	PO4	C	301	5/5	0.95	0.16	103,104,105,105	0
2	PO4	B	301	5/5	0.96	0.11	86,86,88,88	0
2	PO4	A	301	5/5	0.97	0.16	76,76,78,79	0

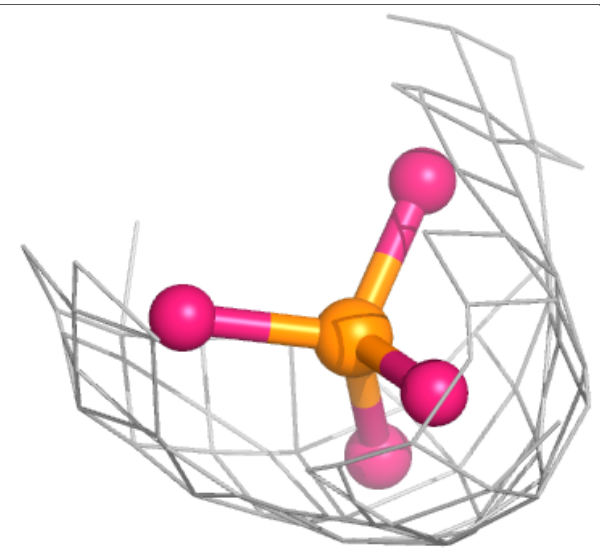
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PO4 D 301:

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

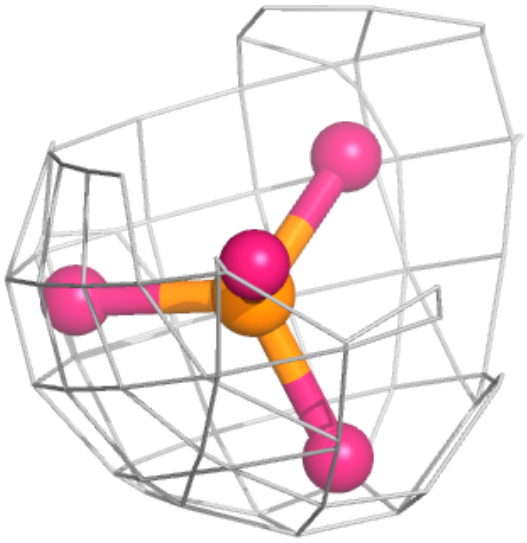


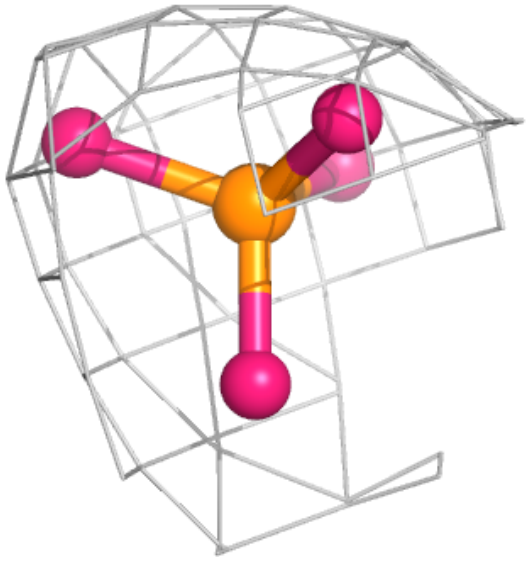


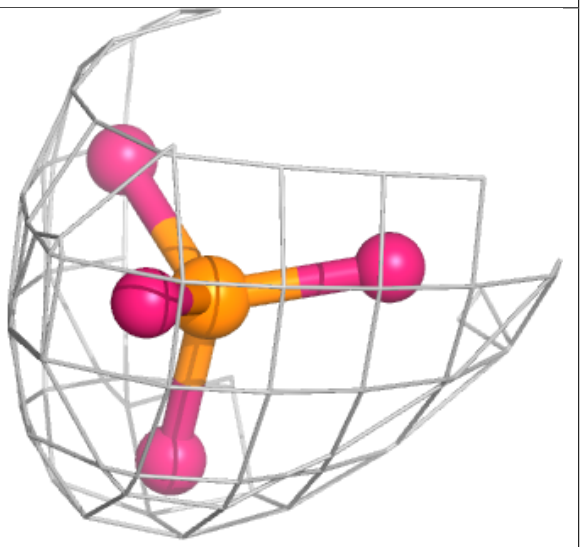


Electron density around PO4 C 301:

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

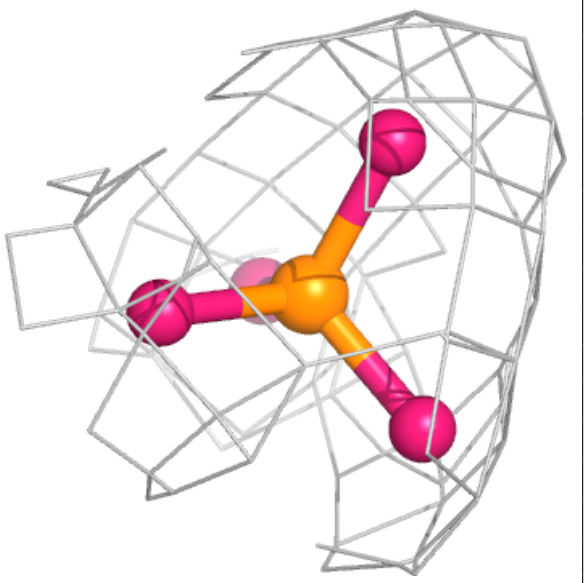


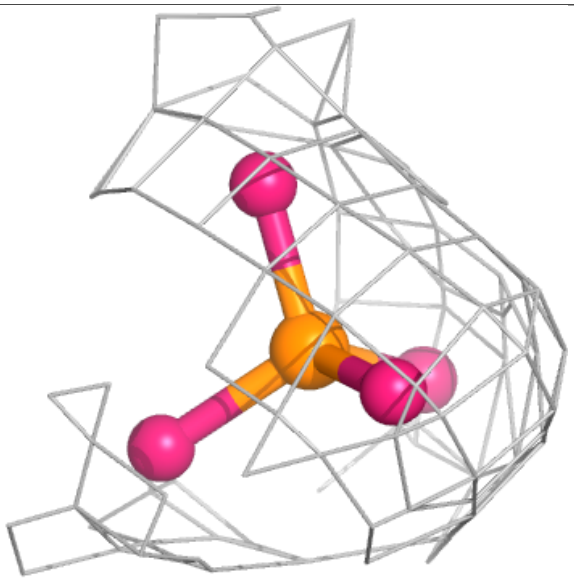


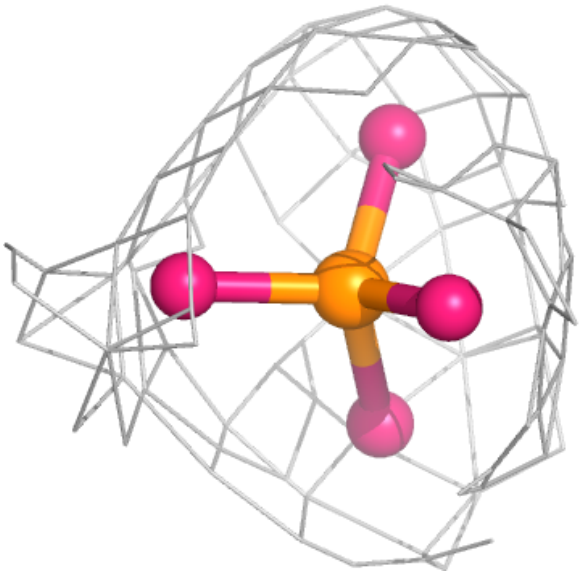


Electron density around PO4 B 301:

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

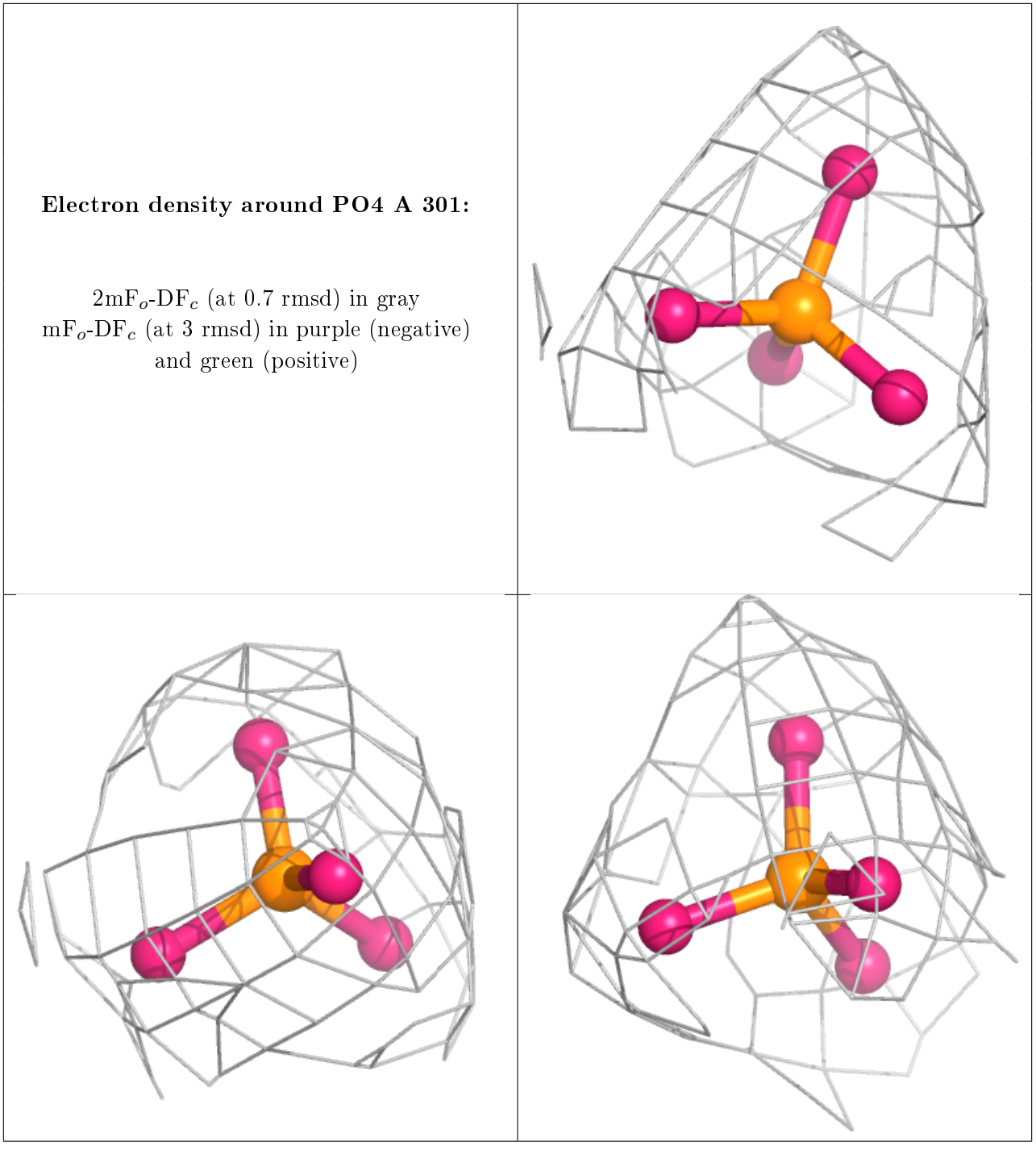






Electron density around PO4 A 301:

$2mF_o$-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

There are no such residues in this entry.