



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2025 – 12:14 pm GMT

PDB ID : 9FHF
Title : Crystal structure of human Glucose-6-phosphate isomerase with dihydroxy-acetone phosphate ligand
Authors : Jonatansdottir, Y.Y.; Hjorleifsson, G.J.
Deposited on : 2024-05-27
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

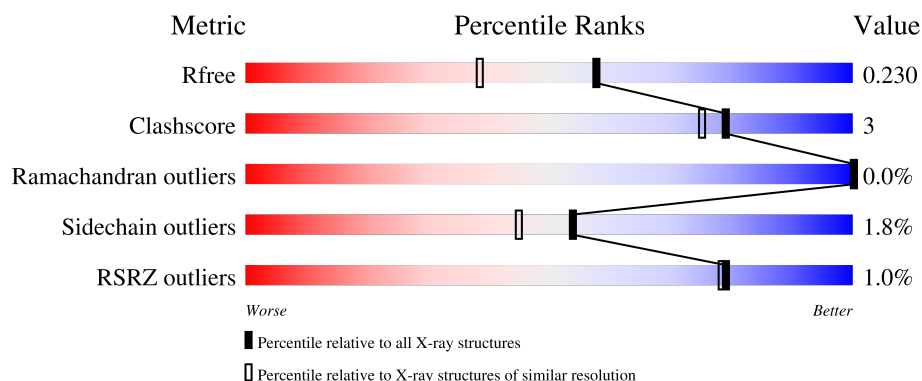
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	558	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	558	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>7%</div> <div>.</div> </div> </div>
1	C	558	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>
1	D	558	<div> <div></div> <div> <div></div> <div>90%</div> <div>9%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

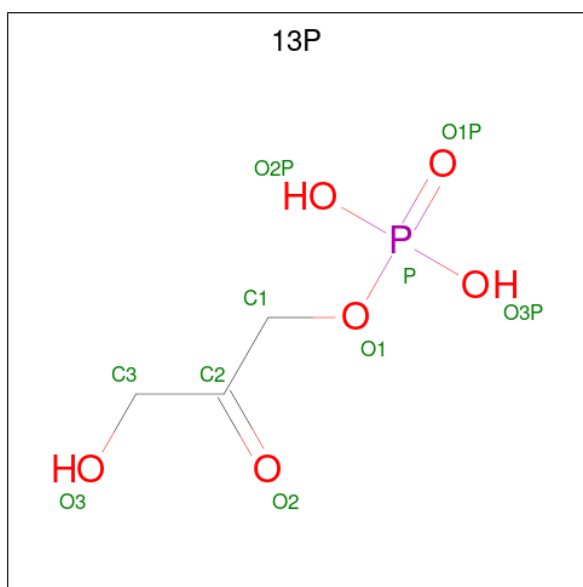
There are 4 unique types of molecules in this entry. The entry contains 36020 atoms, of which 17386 are hydrogens and 0 are deuteriums.

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 Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	552	Total	C	H	N	O	S	0	0	0
			8580	2808	4175	775	804	18			
1	A	555	Total	C	H	N	O	S	20	0	0
			8816	2822	4386	781	809	18			
1	C	555	Total	C	H	N	O	S	20	0	0
			8817	2822	4387	781	809	18			
1	B	554	Total	C	H	N	O	S	0	2	0
			8805	2820	4378	778	811	18			

- Molecule 2 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: $C_3H_7O_6P$) (labeled as "Ligand of Interest" by depositor).



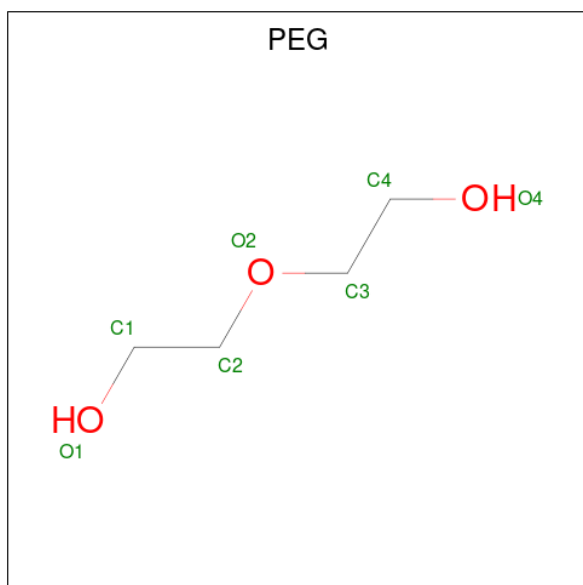
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	H	O	P	0	0
			15	3	5	6	1		
2	A	1	Total	C	H	O	P	0	0
			15	3	5	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	O	P	0	0
			15	3	5	6	1		
2	B	1	Total	C	H	O	P	0	0
			15	3	5	6	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	H	O	0	0
			17	4	10	3		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is water.

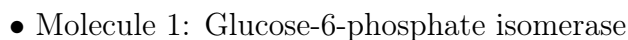
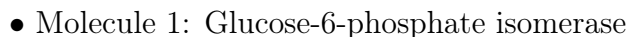
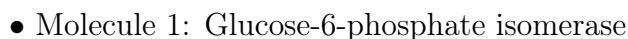
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	196	Total	O	0	0
			196	196		
4	A	228	Total	O	0	0
			228	228		
4	C	216	Total	O	0	0
			216	216		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	234	Total 234	O 234	0	0

- Molecule 1: Glucose-6-phosphate isomerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.68Å 108.31Å 271.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.05 – 1.80 45.05 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.05-1.80) 92.0 (45.05-1.80)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.79Å)	Xtriage
Refinement program	REFMAC 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.186 , 0.228 0.190 , 0.230	Depositor DCC
R_{free} test set	11099 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.849	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36020	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 34.66 % 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 6.5922e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: PEG, 13P

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	0.51	0/4538	0.69	0/6144
1	B	0.52	0/4543	0.69	1/6152 (0.0%)
1	C	0.51	0/4538	0.68	1/6144 (0.0%)
1	D	0.53	0/4513	0.69	0/6111
All	All	0.52	0/18132	0.69	2/24551 (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	B	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	ASP	CB-CG-OD1	5.77	123.49	118.30
1	C	437	MET	CG-SD-CE	-5.42	91.53	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	135	ARG	Sidechain
1	B	461	ARG	Sidechain
1	B	75	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	4430	4386	4383	31	0
1	B	4427	4378	4368	12	0
1	C	4430	4387	4383	20	0
1	D	4405	4175	4359	31	0
2	A	10	5	5	0	0
2	B	10	5	5	0	0
2	C	10	5	5	0	0
2	D	10	5	5	0	0
3	A	7	10	10	0	0
3	B	7	10	10	0	0
3	C	7	10	10	0	0
3	D	7	10	10	1	0
4	A	228	0	0	3	0
4	B	234	0	0	0	0
4	C	216	0	0	2	0
4	D	196	0	0	3	0
All	All	18634	17386	17553	92	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 3.

All (92) 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:D:120:PRO:O	4:D:701:HOH:O	2.11	0.66
1:D:62:GLU:H	1:D:62:GLU:CD	2.01	0.63
1:A:313:GLU:HG3	4:A:825:HOH:O	2.00	0.61
1:C:338:MET:HE2	4:C:821:HOH:O	2.01	0.60
1:A:259:ASP:OD2	1:A:260:PRO:HD2	2.01	0.59
1:A:27:ARG:HD2	1:A:438:ARG:NH1	2.18	0.57
1:C:526:GLU:HG2	1:B:423:LYS:HE2	1.87	0.57
1:C:353:GLN:O	1:C:357:MET:HB2	2.05	0.56
1:D:128:LYS:NZ	4:D:706:HOH:O	2.38	0.55
1:C:93:THR:CG2	1:C:513:TRP:HE1	2.20	0.55
1:C:253:VAL:HG21	1:C:263:MET:CE	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLN:HG2	1:A:19:GLU:OE2	2.09	0.53
1:D:310:THR:CG2	1:D:314:LYS:HD3	2.39	0.53
1:A:250:THR:HG22	1:A:254:LYS:HE3	1.91	0.52
1:A:370:ARG:HG2	1:A:370:ARG:HH11	1.75	0.52
1:C:408:ILE:HD13	1:C:426:LEU:HD23	1.91	0.52
1:A:259:ASP:OD2	1:A:261:GLN:HB2	2.09	0.52
1:D:401:MET:HB2	3:D:602:PEG:H31	1.93	0.51
1:A:259:ASP:OD2	1:A:261:GLN:N	2.43	0.51
1:B:261:GLN:O	1:B:261:GLN:HG3	2.11	0.51
1:D:99:LEU:HB2	1:D:269:TRP:CE3	2.46	0.51
1:A:63:ASP:O	1:A:67:MET:HG3	2.11	0.50
1:C:99:LEU:HB2	1:C:269:TRP:CE3	2.48	0.49
1:C:253:VAL:HG21	1:C:263:MET:HE2	1.94	0.49
1:A:223:GLU:OE2	4:A:701:HOH:O	2.19	0.49
1:C:219:ILE:O	1:C:223:GLU:HG3	2.12	0.49
1:D:27:ARG:NH2	1:D:444:GLU:OE2	2.43	0.48
1:A:5:THR:OG1	1:A:372:ASP:OD1	2.24	0.48
1:B:353:GLN:O	1:B:357:MET:HB2	2.13	0.48
1:A:353:GLN:O	1:A:357:MET:HB2	2.12	0.48
1:D:231:GLN:HG3	4:D:884:HOH:O	2.13	0.48
1:C:93:THR:HG21	1:C:511:ASP:OD2	2.13	0.48
1:A:260:PRO:HD2	1:A:261:GLN:H	1.78	0.48
1:A:437:MET:HE2	1:A:438:ARG:HG2	1.96	0.48
1:D:353:GLN:O	1:D:357:MET:HB2	2.13	0.47
1:D:15:GLN:OE1	1:D:18:ARG:NH2	2.42	0.47
1:D:63:ASP:OD1	1:D:66:ARG:NH1	2.47	0.47
1:D:251:THR:O	1:D:255:GLU:HG3	2.14	0.47
1:D:346:HIS:HA	1:D:383:PRO:HG3	1.97	0.47
1:B:388:GLN:HA	1:B:392:TYR:CG	2.50	0.46
1:D:531:GLY:O	1:D:550:LYS:NZ	2.44	0.46
1:D:125:VAL:O	1:D:129:MET:HG3	2.16	0.46
1:D:46:THR:O	1:D:47:ASN:HB2	2.16	0.46
1:C:249:ASN:HD22	1:C:249:ASN:C	2.18	0.46
1:D:190:THR:O	1:D:194:LYS:HG2	2.16	0.46
1:C:17:TYR:O	1:C:21:ARG:HB2	2.16	0.45
1:A:9:GLN:HG3	1:A:74:SER:HB2	1.98	0.45
1:A:27:ARG:HD2	1:A:438:ARG:CZ	2.47	0.45
1:A:408:ILE:HD13	1:A:426:LEU:HD23	1.99	0.44
1:A:145:THR:CG2	1:A:202:GLU:HG2	2.47	0.44
1:A:316:ALA:HB3	1:A:317:PRO:HD3	1.99	0.44
1:C:314:LYS:HD3	4:C:860:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:GLN:HA	1:C:392:TYR:CG	2.52	0.44
1:A:118:VAL:O	1:A:121:GLU:HG2	2.17	0.44
1:C:43:THR:C	1:C:44:LEU:HD12	2.38	0.44
1:A:388:GLN:HG2	1:A:392:TYR:CE2	2.53	0.44
1:D:394:LEU:HD13	1:A:357:MET:HG2	1.99	0.43
1:D:99:LEU:HD23	1:D:99:LEU:HA	1.85	0.43
1:D:388:GLN:HA	1:D:392:TYR:CG	2.53	0.43
1:D:248:THR:HG22	1:D:266:PHE:O	2.18	0.43
1:B:187:ILE:HB	1:B:217:GLU:CG	2.49	0.43
1:C:44:LEU:HD12	1:C:44:LEU:N	2.33	0.43
1:B:408:ILE:HD13	1:B:426:LEU:HD23	2.00	0.43
1:D:310:THR:HG23	1:D:314:LYS:HD3	2.01	0.42
1:D:144:TYR:HB3	1:D:238:ALA:HB1	2.01	0.42
1:D:284:ILE:O	1:D:288:VAL:HG22	2.19	0.42
1:A:346:HIS:HA	1:A:383:PRO:HG3	2.02	0.42
1:A:187:ILE:HB	1:A:217:GLU:CG	2.50	0.42
1:A:459:LEU:C	1:A:459:LEU:HD23	2.41	0.42
1:B:99:LEU:HB2	1:B:269:TRP:CE3	2.55	0.41
1:B:118:VAL:O	1:B:121:GLU:HG2	2.20	0.41
1:D:314:LYS:CD	1:D:314:LYS:O	2.68	0.41
1:B:233:ALA:O	1:B:235:ASP:N	2.47	0.41
1:D:406:PHE:HB3	1:D:429:PHE:CE1	2.55	0.41
1:B:449:LEU:HD13	1:B:459:LEU:HG	2.02	0.41
1:C:443:GLU:OE2	1:C:447:LYS:NZ	2.53	0.41
1:D:42:LEU:HD22	1:D:314:LYS:HG2	2.03	0.41
1:B:119:MET:N	1:B:120:PRO:CD	2.83	0.41
1:A:15:GLN:O	1:A:19:GLU:OE2	2.38	0.41
1:C:10:PHE:CE2	1:C:14:GLN:NE2	2.88	0.41
1:C:93:THR:HG21	1:C:513:TRP:HE1	1.86	0.41
1:D:219:ILE:O	1:D:223:GLU:HG3	2.20	0.41
1:A:259:ASP:OD2	1:A:260:PRO:CD	2.69	0.41
1:A:342:ASP:OD1	1:A:344:TYR:HB2	2.21	0.40
1:A:388:GLN:HA	1:A:392:TYR:CG	2.56	0.40
1:D:439:GLY:HA3	1:D:468:PHE:O	2.21	0.40
1:D:172:LYS:HD3	1:D:172:LYS:HA	1.91	0.40
1:C:26:LEU:CB	1:C:437:MET:HG2	2.52	0.40
1:A:83:ARG:HD2	4:A:865:HOH:O	2.22	0.40
1:B:246:LEU:HD13	1:B:280:ILE:HA	2.04	0.40
1:D:17:TYR:O	1:D:21:ARG:HB2	2.22	0.40
1:A:26:LEU:HD13	1:A:437:MET:HG3	2.03	0.40

There are no symmetry-related clashes.

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	553/558 (99%)	533 (96%)	20 (4%)	0	100	100
1	B	554/558 (99%)	537 (97%)	17 (3%)	0	100	100
1	C	553/558 (99%)	540 (98%)	12 (2%)	1 (0%)	44	31
1	D	550/558 (99%)	530 (96%)	20 (4%)	0	100	100
All	All	2210/2232 (99%)	2140 (97%)	69 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3	ALA

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	474/477 (99%)	465 (98%)	9 (2%)	52	43
1	B	475/477 (100%)	464 (98%)	11 (2%)	45	34
1	C	474/477 (99%)	467 (98%)	7 (2%)	60	53
1	D	472/477 (99%)	465 (98%)	7 (2%)	60	53
All	All	1895/1908 (99%)	1861 (98%)	34 (2%)	54	45

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	27	ARG
1	D	104	ARG
1	D	213	PHE
1	D	231	GLN
1	D	234	LYS
1	D	314	LYS
1	D	455	SER
1	A	19	GLU
1	A	27	ARG
1	A	35	ASP
1	A	104	ARG
1	A	116	LYS
1	A	213	PHE
1	A	231	GLN
1	A	418	LYS
1	A	466	LYS
1	C	31	ASP
1	C	104	ARG
1	C	176	SER
1	C	213	PHE
1	C	249	ASN
1	C	370	ARG
1	C	450	GLN
1	B	27	ARG
1	B	34	LYS
1	B	104	ARG
1	B	116	LYS
1	B	213	PHE
1	B	259	ASP
1	B	418	LYS
1	B	454	LYS
1	B	455	SER
1	B	466	LYS
1	B	534	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	231	GLN
1	A	9	GLN
1	C	9	GLN
1	C	11	GLN
1	C	14	GLN

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Mol	Chain	Res	Type
1	C	249	ASN
1	C	450	GLN
1	B	15	GLN
1	B	534	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	PEG	B	602	-	6,6,6	0.24	0	5,5,5	0.27	0
3	PEG	C	601	-	6,6,6	0.16	0	5,5,5	0.04	0
2	13P	A	601	-	9,9,9	1.30	1 (11%)	10,12,12	1.28	1 (10%)
3	PEG	D	602	-	6,6,6	0.38	0	5,5,5	0.29	0
3	PEG	A	602	-	6,6,6	0.26	0	5,5,5	0.29	0
2	13P	D	601	-	9,9,9	1.47	2 (22%)	10,12,12	0.69	0
2	13P	C	602	-	9,9,9	2.38	1 (11%)	10,12,12	0.97	0
2	13P	B	601	-	9,9,9	1.52	1 (11%)	10,12,12	1.19	1 (10%)

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	PEG	B	602	-	-	2/4/4/4	-
3	PEG	C	601	-	-	3/4/4/4	-
2	13P	A	601	-	-	0/7/8/8	-
3	PEG	D	602	-	-	2/4/4/4	-
3	PEG	A	602	-	-	3/4/4/4	-
2	13P	D	601	-	-	1/7/8/8	-
2	13P	C	602	-	-	5/7/8/8	-
2	13P	B	601	-	-	2/7/8/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	602	13P	O1-C1	-6.50	1.38	1.43
2	B	601	13P	O1-C1	-3.38	1.40	1.43
2	D	601	13P	O1-C1	-3.32	1.40	1.43
2	D	601	13P	O2-C2	-2.07	1.18	1.21
2	A	601	13P	O1-C1	-2.00	1.41	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	13P	O2P-P-O1	2.95	114.57	106.73
2	B	601	13P	O2-C2-C1	-2.38	116.82	120.57

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	13P	O2-C2-C3-O3
2	C	602	13P	C1-O1-P-O1P
2	C	602	13P	C1-O1-P-O2P
2	C	602	13P	C1-O1-P-O3P
2	C	602	13P	O1-C1-C2-O2
2	C	602	13P	O2-C2-C3-O3
2	B	601	13P	O2-C2-C3-O3
3	B	602	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	601	PEG	O2-C3-C4-O4
3	A	602	PEG	O2-C3-C4-O4
3	A	602	PEG	C1-C2-O2-C3
3	B	602	PEG	C1-C2-O2-C3
3	D	602	PEG	C4-C3-O2-C2
3	C	601	PEG	C1-C2-O2-C3
3	A	602	PEG	O1-C1-C2-O2
2	B	601	13P	O1-C1-C2-O2
3	C	601	PEG	O1-C1-C2-O2
3	D	602	PEG	O2-C3-C4-O4

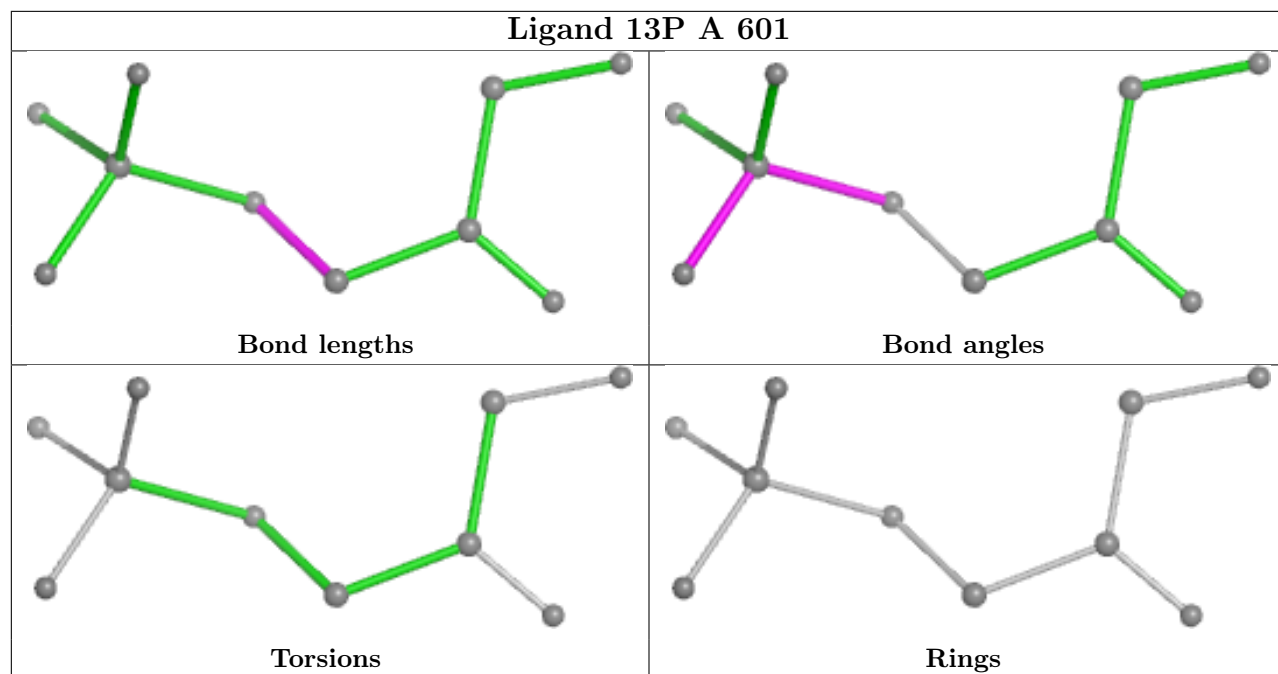
There are no ring outliers.

1 monomer is involved in 1 short contact:

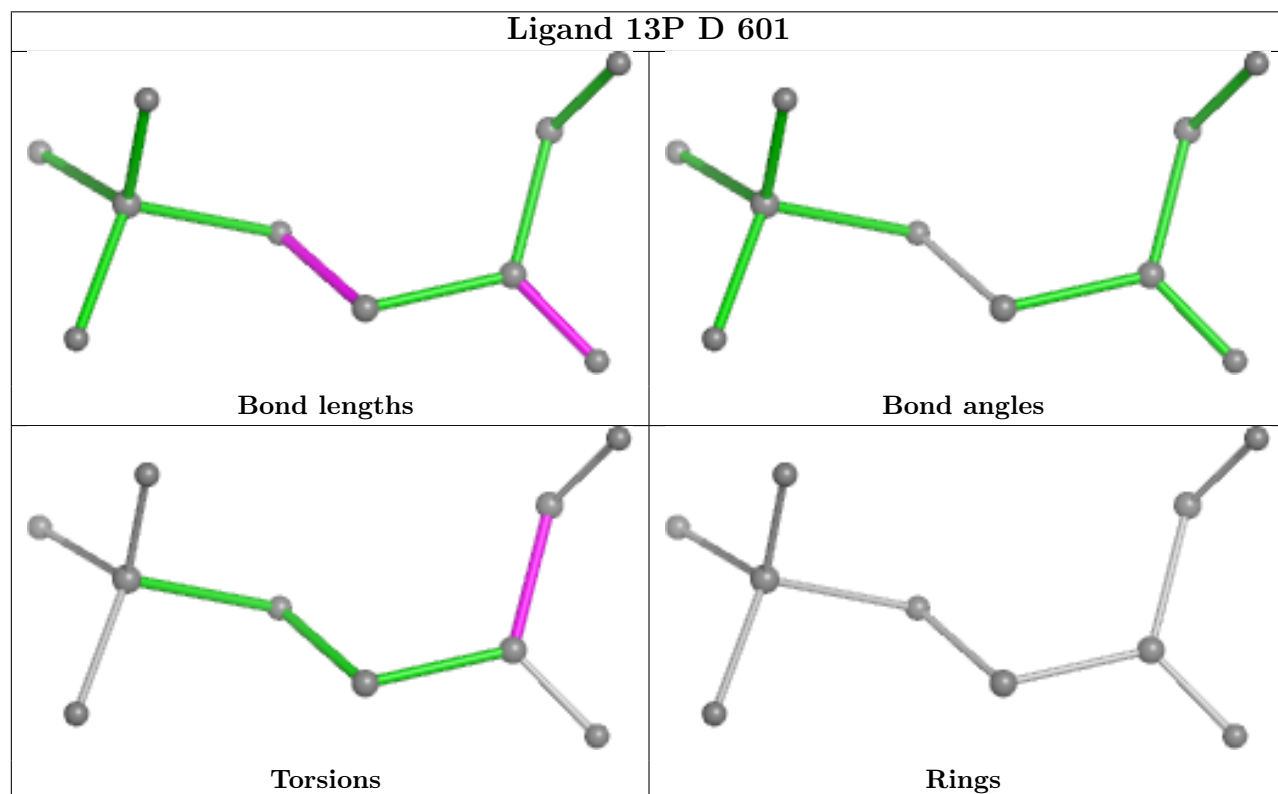
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	PEG	1	0

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.

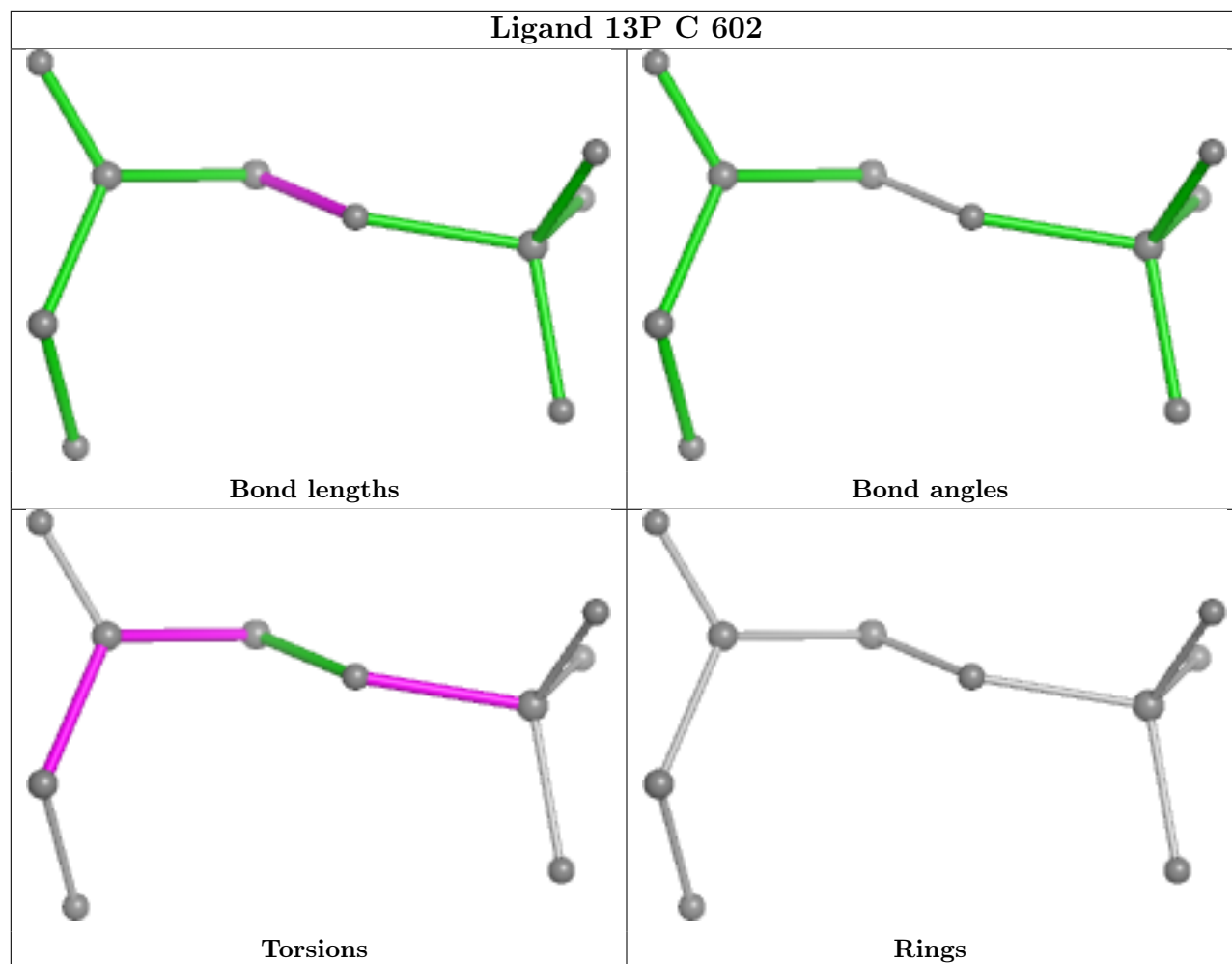
Ligand 13P A 601



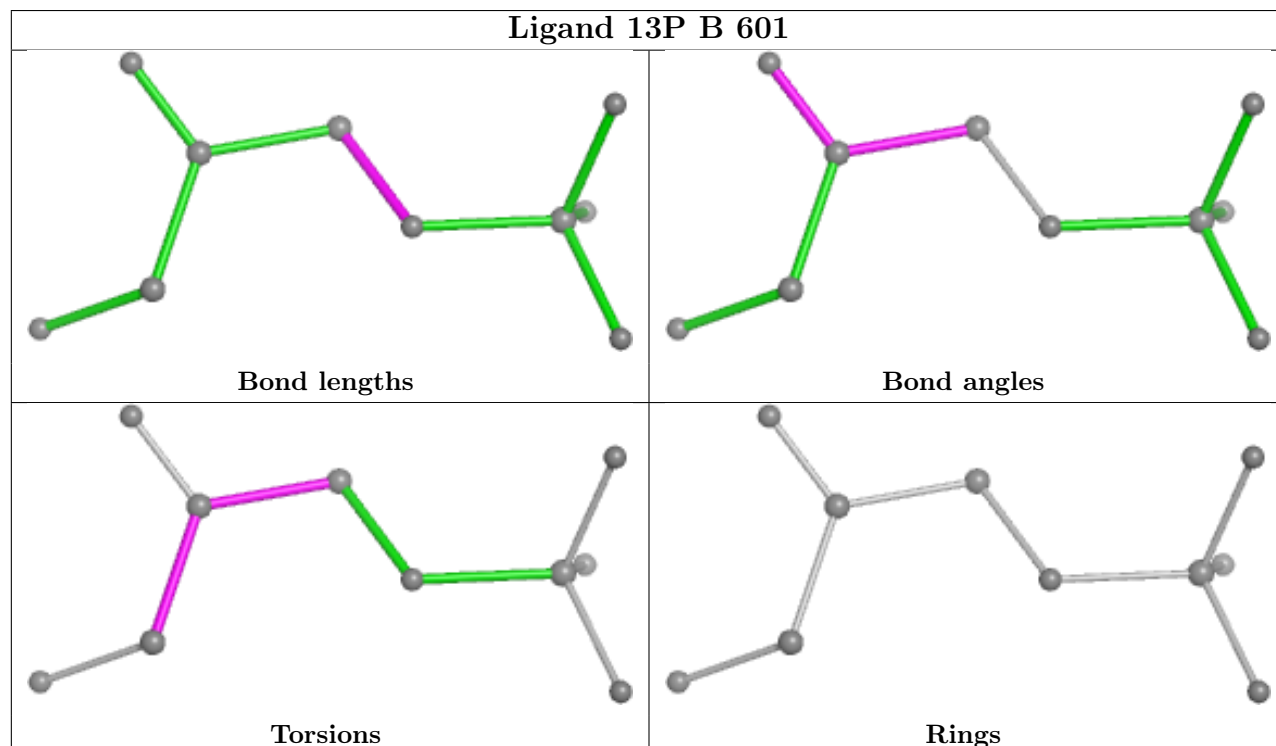
Ligand 13P D 601



Ligand 13P C 602



Ligand 13P B 601



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	555/558 (99%)	-0.08	3 (0%) 87 87	9, 29, 51, 74	1 (0%)
1	B	554/558 (99%)	-0.01	11 (1%) 64 63	16, 28, 54, 93	1 (0%)
1	C	555/558 (99%)	0.05	8 (1%) 73 72	10, 31, 53, 76	1 (0%)
1	D	552/558 (98%)	0.02	1 (0%) 92 91	18, 30, 54, 75	0
All	All	2216/2232 (99%)	-0.01	23 (1%) 79 78	9, 29, 53, 93	3 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	556	ARG	4.5
1	A	556	ARG	4.3
1	B	456	PRO	3.9
1	B	462	LEU	3.2
1	B	260	PRO	3.0
1	D	2	ALA	2.7
1	B	459	LEU	2.6
1	B	453	GLY	2.4
1	B	555	ALA	2.4
1	B	455	SER	2.4
1	B	554	GLU	2.3
1	B	452	ALA	2.3
1	C	115	GLY	2.3
1	C	554	GLU	2.3
1	C	260	PRO	2.2
1	B	454	LYS	2.2
1	C	531	GLY	2.1
1	A	115	GLY	2.1
1	A	109	THR	2.0
1	B	259	ASP	2.0
1	C	34	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	32	ALA	2.0
1	C	237	SER	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](#)

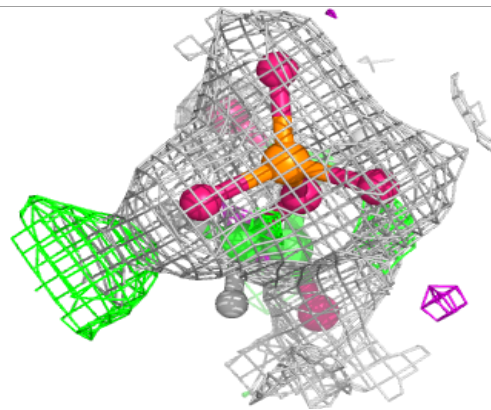
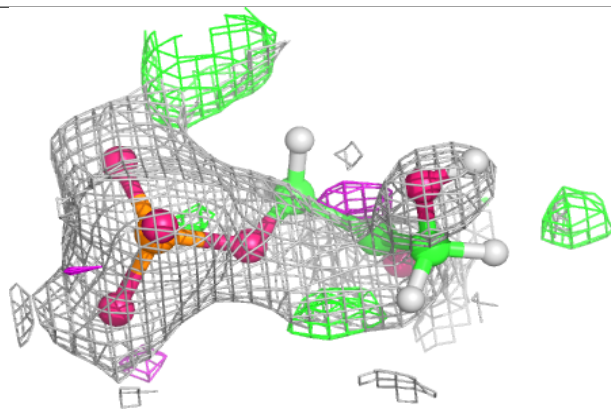
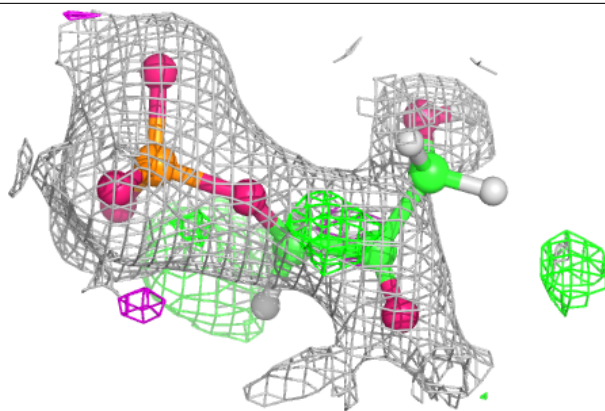
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PEG	C	601	7/7	0.86	0.10	32,44,53,54	0
3	PEG	D	602	7/7	0.87	0.11	35,43,50,50	0
3	PEG	B	602	7/7	0.87	0.13	42,51,62,65	0
3	PEG	A	602	7/7	0.89	0.12	39,47,55,60	0
2	13P	C	602	10/10	0.95	0.11	28,45,58,58	0
2	13P	D	601	10/10	0.97	0.08	24,42,53,56	0
2	13P	B	601	10/10	0.97	0.09	20,36,59,59	0
2	13P	A	601	10/10	0.98	0.07	20,34,40,43	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.

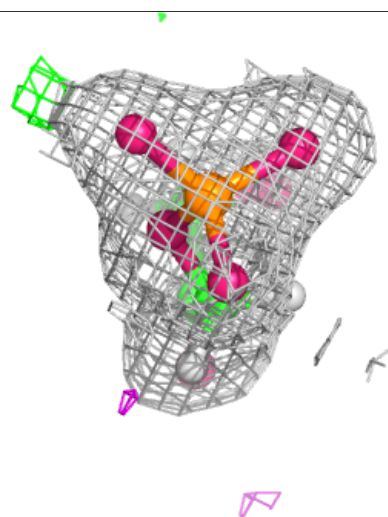
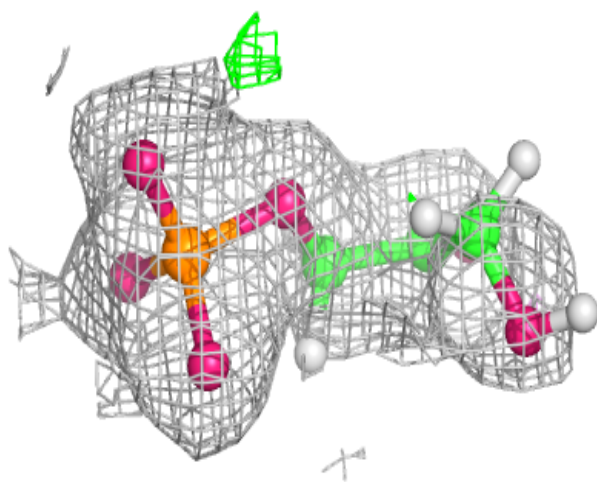
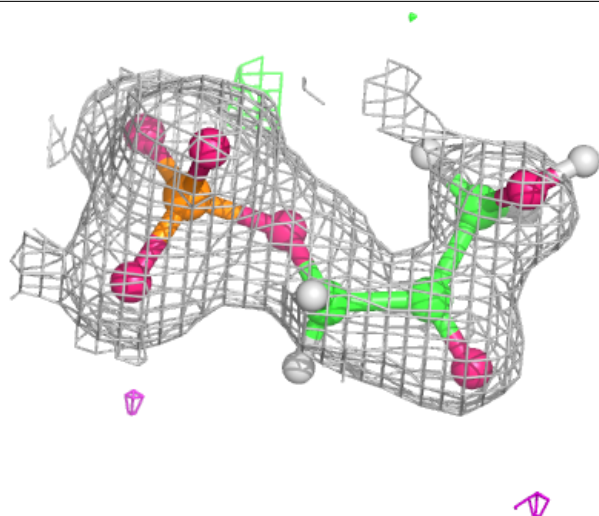
Electron density around 13P C 602:

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



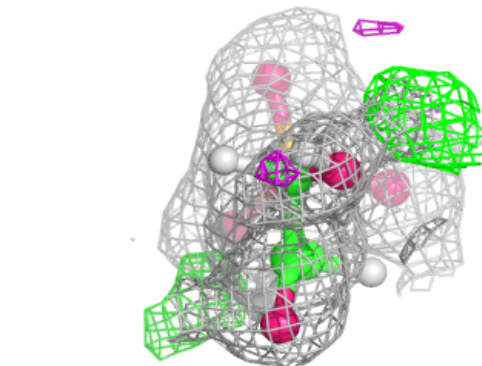
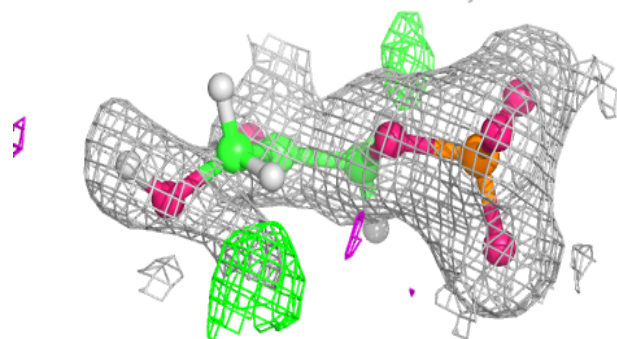
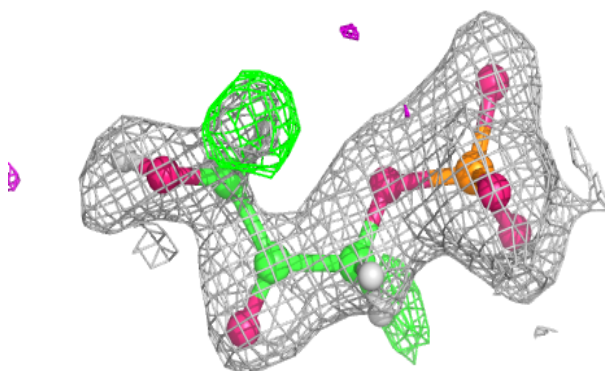
Electron density around 13P D 601:

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

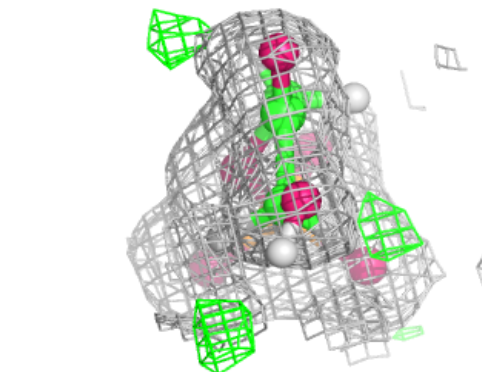
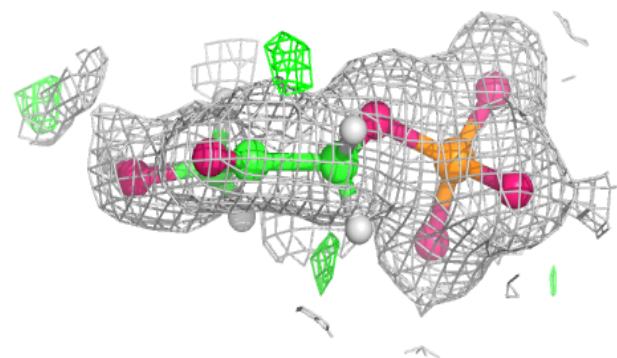
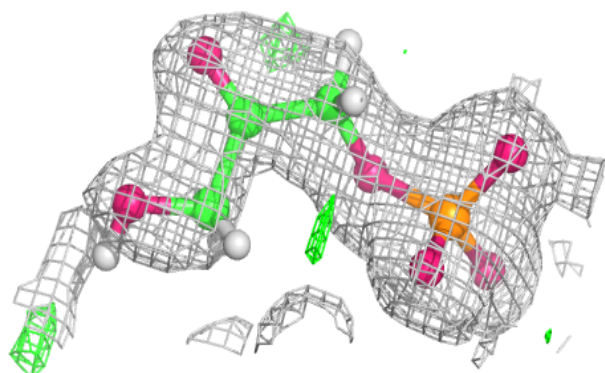


Electron density around 13P B 601:

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

**Electron density around 13P A 601:**

$2mF_o-DF_c$ (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.