



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 03:37 AM EDT

PDB ID : 4WU3 / pdb_00004wu3
Title : Structure of the PTP-like myo-inositol phosphatase from *Mitsuokella multacida* in complex with myo-inositol-(1,3,4,5)-tetrakisphosphate
Authors : Bruder, L.M.; Mosimann, S.C.
Deposited on : 2014-10-30
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

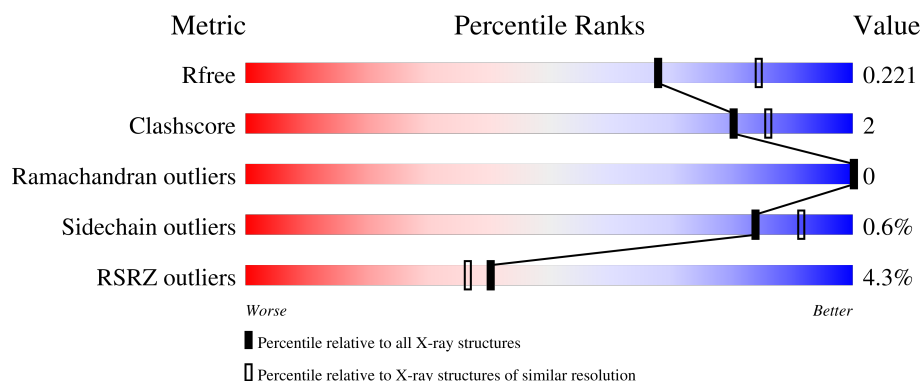
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	632	 3% 88% 5% 7%
1	B	632	 4% 87% 6% 7%
1	C	632	 3% 88% 6% 7%
1	D	632	 6% 87% 6% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21756 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 MYO-INOSITOL PHOSPHOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	1	0
			4806	3065	833	887	21			
1	B	590	Total	C	N	O	S	0	1	0
			4806	3065	833	887	21			
1	C	590	Total	C	N	O	S	0	1	0
			4806	3065	833	887	21			
1	D	590	Total	C	N	O	S	0	1	0
			4806	3065	833	887	21			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP A3QMF6
A	10	GLY	-	expression tag	UNP A3QMF6
A	11	SER	-	expression tag	UNP A3QMF6
A	12	SER	-	expression tag	UNP A3QMF6
A	13	HIS	-	expression tag	UNP A3QMF6
A	14	HIS	-	expression tag	UNP A3QMF6
A	15	HIS	-	expression tag	UNP A3QMF6
A	16	HIS	-	expression tag	UNP A3QMF6
A	17	HIS	-	expression tag	UNP A3QMF6
A	18	HIS	-	expression tag	UNP A3QMF6
A	19	SER	-	expression tag	UNP A3QMF6
A	20	SER	-	expression tag	UNP A3QMF6
A	21	GLY	-	expression tag	UNP A3QMF6
A	22	LEU	-	expression tag	UNP A3QMF6
A	23	VAL	-	expression tag	UNP A3QMF6
A	24	PRO	-	expression tag	UNP A3QMF6
A	25	ARG	-	expression tag	UNP A3QMF6
A	26	GLY	-	expression tag	UNP A3QMF6
A	27	SER	-	expression tag	UNP A3QMF6
A	28	HIS	-	expression tag	UNP A3QMF6
A	29	MET	-	expression tag	UNP A3QMF6

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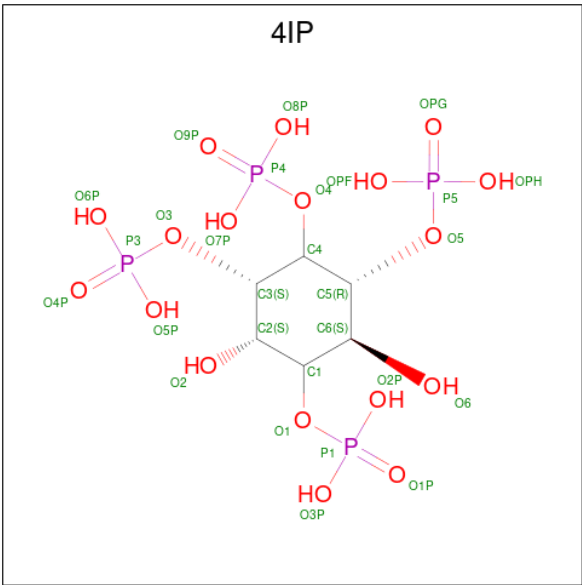
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ALA	-	expression tag	UNP A3QMF6
A	31	SER	-	expression tag	UNP A3QMF6
A	250	SER	CYS	engineered mutation	UNP A3QMF6
A	548	SER	CYS	engineered mutation	UNP A3QMF6
B	9	MET	-	initiating methionine	UNP A3QMF6
B	10	GLY	-	expression tag	UNP A3QMF6
B	11	SER	-	expression tag	UNP A3QMF6
B	12	SER	-	expression tag	UNP A3QMF6
B	13	HIS	-	expression tag	UNP A3QMF6
B	14	HIS	-	expression tag	UNP A3QMF6
B	15	HIS	-	expression tag	UNP A3QMF6
B	16	HIS	-	expression tag	UNP A3QMF6
B	17	HIS	-	expression tag	UNP A3QMF6
B	18	HIS	-	expression tag	UNP A3QMF6
B	19	SER	-	expression tag	UNP A3QMF6
B	20	SER	-	expression tag	UNP A3QMF6
B	21	GLY	-	expression tag	UNP A3QMF6
B	22	LEU	-	expression tag	UNP A3QMF6
B	23	VAL	-	expression tag	UNP A3QMF6
B	24	PRO	-	expression tag	UNP A3QMF6
B	25	ARG	-	expression tag	UNP A3QMF6
B	26	GLY	-	expression tag	UNP A3QMF6
B	27	SER	-	expression tag	UNP A3QMF6
B	28	HIS	-	expression tag	UNP A3QMF6
B	29	MET	-	expression tag	UNP A3QMF6
B	30	ALA	-	expression tag	UNP A3QMF6
B	31	SER	-	expression tag	UNP A3QMF6
B	250	SER	CYS	engineered mutation	UNP A3QMF6
B	548	SER	CYS	engineered mutation	UNP A3QMF6
C	9	MET	-	initiating methionine	UNP A3QMF6
C	10	GLY	-	expression tag	UNP A3QMF6
C	11	SER	-	expression tag	UNP A3QMF6
C	12	SER	-	expression tag	UNP A3QMF6
C	13	HIS	-	expression tag	UNP A3QMF6
C	14	HIS	-	expression tag	UNP A3QMF6
C	15	HIS	-	expression tag	UNP A3QMF6
C	16	HIS	-	expression tag	UNP A3QMF6
C	17	HIS	-	expression tag	UNP A3QMF6
C	18	HIS	-	expression tag	UNP A3QMF6
C	19	SER	-	expression tag	UNP A3QMF6
C	20	SER	-	expression tag	UNP A3QMF6
C	21	GLY	-	expression tag	UNP A3QMF6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	LEU	-	expression tag	UNP A3QMF6
C	23	VAL	-	expression tag	UNP A3QMF6
C	24	PRO	-	expression tag	UNP A3QMF6
C	25	ARG	-	expression tag	UNP A3QMF6
C	26	GLY	-	expression tag	UNP A3QMF6
C	27	SER	-	expression tag	UNP A3QMF6
C	28	HIS	-	expression tag	UNP A3QMF6
C	29	MET	-	expression tag	UNP A3QMF6
C	30	ALA	-	expression tag	UNP A3QMF6
C	31	SER	-	expression tag	UNP A3QMF6
C	250	SER	CYS	engineered mutation	UNP A3QMF6
C	548	SER	CYS	engineered mutation	UNP A3QMF6
D	9	MET	-	initiating methionine	UNP A3QMF6
D	10	GLY	-	expression tag	UNP A3QMF6
D	11	SER	-	expression tag	UNP A3QMF6
D	12	SER	-	expression tag	UNP A3QMF6
D	13	HIS	-	expression tag	UNP A3QMF6
D	14	HIS	-	expression tag	UNP A3QMF6
D	15	HIS	-	expression tag	UNP A3QMF6
D	16	HIS	-	expression tag	UNP A3QMF6
D	17	HIS	-	expression tag	UNP A3QMF6
D	18	HIS	-	expression tag	UNP A3QMF6
D	19	SER	-	expression tag	UNP A3QMF6
D	20	SER	-	expression tag	UNP A3QMF6
D	21	GLY	-	expression tag	UNP A3QMF6
D	22	LEU	-	expression tag	UNP A3QMF6
D	23	VAL	-	expression tag	UNP A3QMF6
D	24	PRO	-	expression tag	UNP A3QMF6
D	25	ARG	-	expression tag	UNP A3QMF6
D	26	GLY	-	expression tag	UNP A3QMF6
D	27	SER	-	expression tag	UNP A3QMF6
D	28	HIS	-	expression tag	UNP A3QMF6
D	29	MET	-	expression tag	UNP A3QMF6
D	30	ALA	-	expression tag	UNP A3QMF6
D	31	SER	-	expression tag	UNP A3QMF6
D	250	SER	CYS	engineered mutation	UNP A3QMF6
D	548	SER	CYS	engineered mutation	UNP A3QMF6

- Molecule 2 is INOSITOL-(1,3,4,5)-TETRAKISPHOSPHATE (CCD ID: 4IP) (formula: $C_6H_{16}O_{18}P_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			28	6	18	4		
2	A	1	Total	C	O	P	0	0
			28	6	18	4		
2	B	1	Total	C	O	P	0	0
			28	6	18	4		
2	C	1	Total	C	O	P	0	0
			28	6	18	4		
2	C	1	Total	C	O	P	0	0
			28	6	18	4		
2	D	1	Total	C	O	P	0	0
			28	6	18	4		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

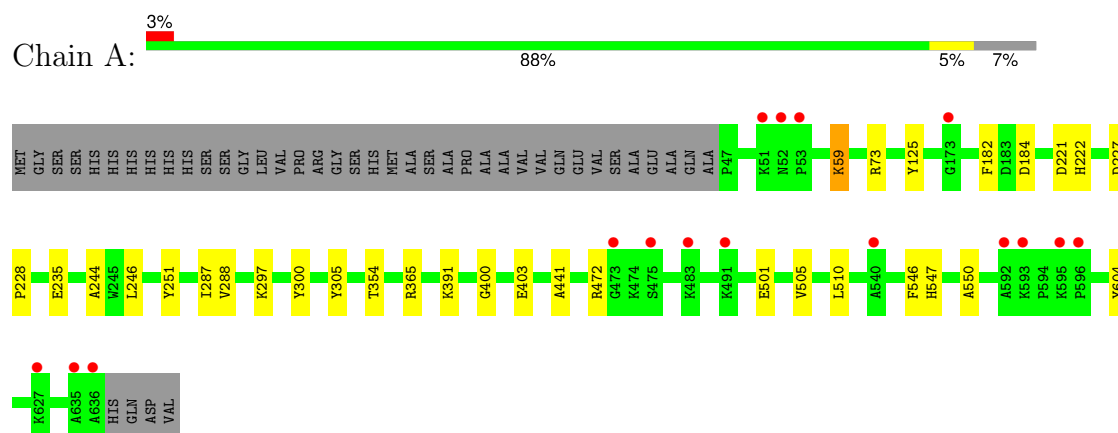
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	578	Total 578	O 578	0	0
5	B	547	Total 547	O 547	0	0
5	C	580	Total 580	O 580	0	0
5	D	557	Total 557	O 557	0	0

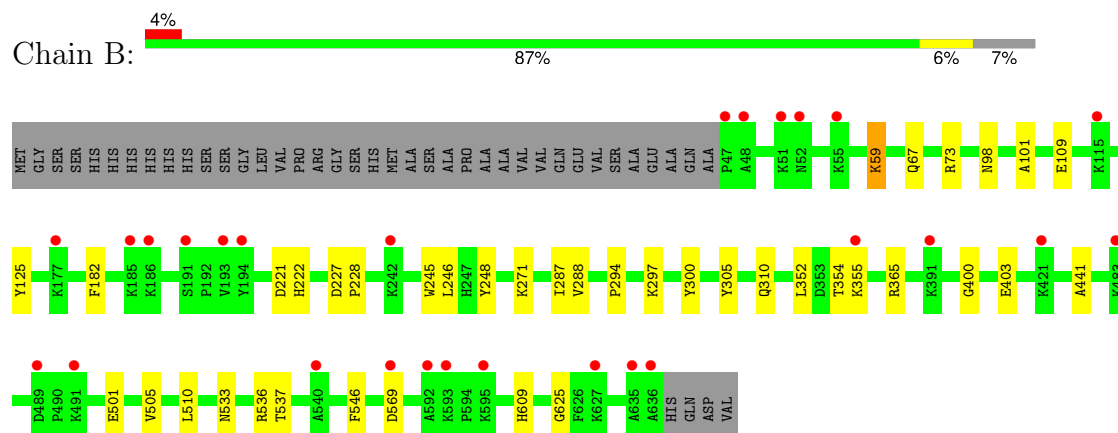
3 Residue-property plots

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

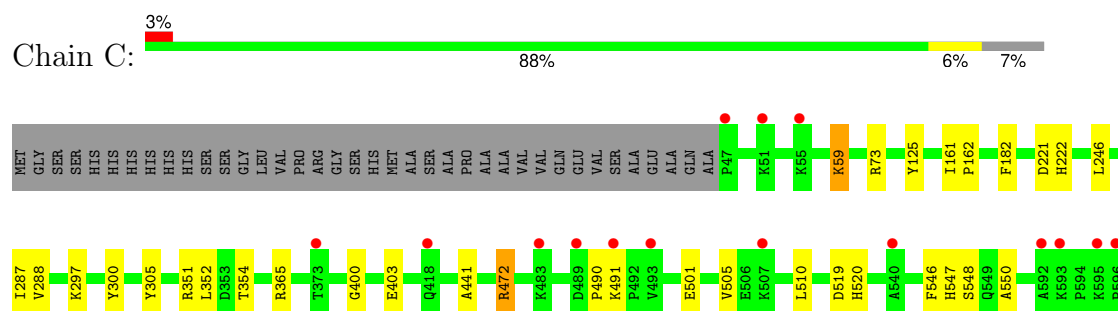
• Molecule 1: MYO-INOSITOL PHOSPHOHYDROLASE

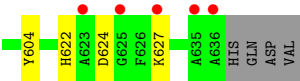


• Molecule 1: MYO-INOSITOL PHOSPHOHYDROLASE

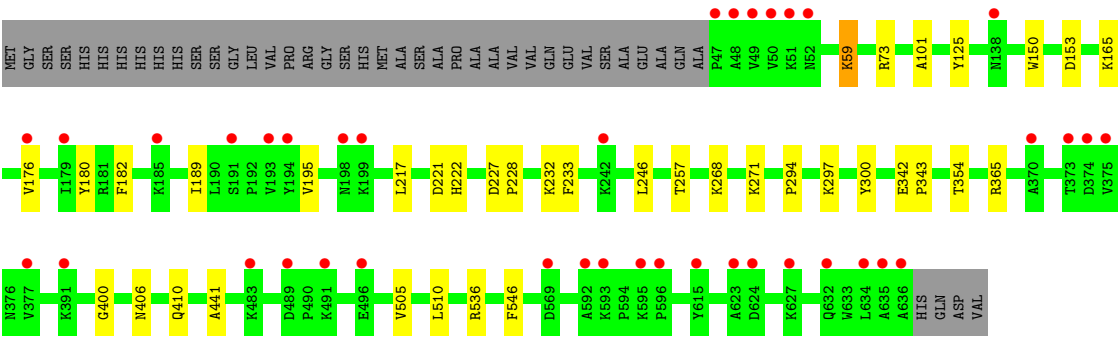
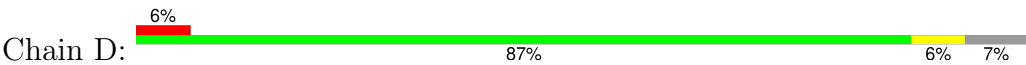


• Molecule 1: MYO-INOSITOL PHOSPHOHYDROLASE





● Molecule 1: MYO-INOSITOL PHOSPHOHYDROLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.90Å 86.68Å 124.15Å 107.27° 91.69° 90.01°	Depositor
Resolution (Å)	44.54 – 2.20 44.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (44.54-2.20) 98.1 (44.54-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.190 , 0.213 0.195 , 0.221	Depositor DCC
R_{free} test set	2118 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.836	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.087 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21756	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: PO4, GOL, 4IP

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	0.37	0/4931	0.54	0/6668
1	B	0.37	0/4931	0.54	0/6668
1	C	0.37	0/4931	0.54	1/6668 (0.0%)
1	D	0.39	0/4931	0.55	0/6668
All	All	0.38	0/19724	0.54	1/26672 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	472	ARG	NE-CZ-NH1	-5.96	117.32	120.30

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	4806	0	4723	23	0
1	B	4806	0	4723	26	0
1	C	4806	0	4723	27	0
1	D	4806	0	4723	23	0
2	A	56	0	16	4	0
2	B	28	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	56	0	16	8	0
2	D	28	0	8	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	A	18	0	24	1	0
4	B	18	0	24	0	0
4	C	18	0	24	0	0
4	D	18	0	24	2	0
5	A	578	0	0	3	0
5	B	547	0	0	3	0
5	C	580	0	0	3	0
5	D	557	0	0	3	0
All	All	21756	0	19036	96	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 2.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LYS:HE2	1:B:182:PHE:CD1	2.22	0.74
1:B:354:THR:HG22	1:B:441:ALA:HB3	1.72	0.70
1:B:352:LEU:HD21	1:B:355:LYS:HG3	1.74	0.68
1:C:550:ALA:CB	2:C:702:4IP:O2	2.43	0.67
1:D:271:LYS:HE3	5:D:1287:HOH:O	1.98	0.64
1:C:125:TYR:HB2	1:C:246:LEU:HD23	1.82	0.61
1:A:501:GLU:OE2	1:A:547:HIS:NE2	2.33	0.61
1:C:352:LEU:HD22	5:C:1215:HOH:O	2.00	0.60
1:C:550:ALA:HB2	2:C:702:4IP:O2	2.03	0.59
2:C:701:4IP:H2	2:C:701:4IP:O3P	2.03	0.58
1:D:268:LYS:NZ	4:D:705:GOL:H12	2.20	0.57
1:D:268:LYS:HZ3	4:D:705:GOL:H12	1.68	0.57
1:C:604:TYR:OH	2:C:702:4IP:OPF	2.23	0.57
1:B:271:LYS:HE3	5:B:1292:HOH:O	2.05	0.56
1:A:550:ALA:CB	2:A:702:4IP:O2	2.54	0.55
1:A:354:THR:HG22	1:A:441:ALA:HB3	1.87	0.55
1:C:490:PRO:O	1:C:491:LYS:HG2	2.07	0.54
1:C:550:ALA:HB3	2:C:702:4IP:O2	2.06	0.54
1:C:505:VAL:HG13	1:C:510:LEU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:HIS:CD2	5:B:1187:HOH:O	2.61	0.54
1:C:354:THR:HG22	1:C:441:ALA:HB3	1.89	0.54
1:D:125:TYR:HB2	1:D:246:LEU:HD23	1.91	0.53
1:B:569:ASP:OD1	1:B:569:ASP:N	2.34	0.53
1:D:232:LYS:HD2	5:D:932:HOH:O	2.07	0.53
1:A:235:GLU:HG2	5:A:827:HOH:O	2.09	0.53
1:C:59:LYS:HE2	1:C:182:PHE:CD1	2.44	0.52
1:B:294:PRO:HG2	1:B:297:LYS:HG2	1.92	0.52
1:C:300:TYR:CG	1:D:300:TYR:HB3	2.45	0.52
1:D:59:LYS:HE2	1:D:182:PHE:CD1	2.45	0.51
1:A:125:TYR:HB2	1:A:246:LEU:HD23	1.91	0.51
1:A:300:TYR:HB3	1:B:300:TYR:CG	2.46	0.50
1:A:244:ALA:HB3	4:A:705:GOL:H32	1.94	0.50
1:B:221:ASP:O	1:B:222:HIS:HB2	2.11	0.50
1:A:400:GLY:HA2	1:A:546:PHE:O	2.12	0.50
1:D:354:THR:HG22	1:D:441:ALA:HB3	1.93	0.49
1:A:550:ALA:HB2	2:A:702:4IP:O2	2.13	0.49
1:A:604:TYR:OH	2:A:702:4IP:OPG	2.31	0.49
1:A:221:ASP:O	1:A:222:HIS:HB2	2.12	0.49
1:A:297:LYS:HE2	1:A:305:TYR:CE1	2.48	0.49
1:B:59:LYS:HE2	1:B:182:PHE:CE1	2.48	0.49
1:D:536:ARG:HH11	1:D:536:ARG:HG2	1.78	0.48
1:A:505:VAL:HG13	1:A:510:LEU:HB2	1.95	0.48
1:C:297:LYS:NZ	2:C:701:4IP:O9P	2.34	0.48
1:B:403:GLU:OE1	1:B:501:GLU:OE1	2.32	0.48
1:D:342[B]:GLU:HB2	1:D:343:PRO:HD2	1.96	0.48
1:A:472:ARG:NH1	5:A:821:HOH:O	2.46	0.48
1:C:624:ASP:O	1:C:627:LYS:HG3	2.14	0.48
1:B:287:ILE:HG23	1:B:288:VAL:HG23	1.96	0.47
1:C:300:TYR:HB3	1:D:300:TYR:CG	2.48	0.47
1:B:536:ARG:NH1	1:B:625:GLY:O	2.47	0.47
1:A:287:ILE:HG23	1:A:288:VAL:HG23	1.96	0.47
1:D:180:TYR:HB3	1:D:189:ILE:HG23	1.95	0.47
1:A:550:ALA:HB3	2:A:702:4IP:O2	2.15	0.46
1:B:505:VAL:HG13	1:B:510:LEU:HB2	1.98	0.46
1:C:400:GLY:HA2	1:C:546:PHE:O	2.15	0.46
1:D:294:PRO:HG2	1:D:297:LYS:HG2	1.99	0.45
1:C:472:ARG:NH1	5:C:811:HOH:O	2.40	0.45
1:D:165:LYS:HG3	5:D:888:HOH:O	2.15	0.45
1:C:548:SER:OG	2:C:702:4IP:O2P	2.25	0.45
1:A:300:TYR:CG	1:B:300:TYR:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ARG:NH2	5:A:830:HOH:O	2.50	0.44
1:A:184:ASP:OD1	1:A:251:TYR:OH	2.33	0.44
1:B:400:GLY:HA2	1:B:546:PHE:O	2.17	0.44
1:A:391:LYS:HD3	1:A:391:LYS:C	2.37	0.44
1:B:310:GLN:OE1	5:B:801:HOH:O	2.21	0.44
1:A:403:GLU:OE2	1:A:501:GLU:OE1	2.36	0.44
1:C:351:ARG:NH2	2:C:702:4IP:O6P	2.43	0.43
1:D:400:GLY:HA2	1:D:546:PHE:O	2.18	0.43
1:C:287:ILE:HG23	1:C:288:VAL:HG23	2.00	0.43
1:C:297:LYS:HE2	1:C:305:TYR:CE1	2.53	0.43
1:C:221:ASP:O	1:C:222:HIS:HB2	2.17	0.43
1:C:501:GLU:OE2	1:C:547:HIS:NE2	2.48	0.43
1:A:59:LYS:HE2	1:A:182:PHE:CD1	2.54	0.43
1:B:98:ASN:HA	1:B:245:TRP:CZ3	2.54	0.43
1:B:67:GLN:O	1:B:109:GLU:HA	2.19	0.43
1:B:297:LYS:HE2	1:B:305:TYR:CE1	2.54	0.43
1:D:505:VAL:HG13	1:D:510:LEU:HB2	2.01	0.43
1:C:622:HIS:HE1	5:C:1194:HOH:O	2.01	0.42
1:C:403:GLU:OE1	1:C:501:GLU:OE1	2.38	0.42
1:B:227:ASP:HB2	1:B:228:PRO:HD3	2.02	0.42
1:D:176:VAL:HA	1:D:195:VAL:O	2.19	0.42
1:B:354:THR:CG2	1:B:441:ALA:HB3	2.45	0.42
1:D:101:ALA:HB1	1:D:257:THR:CG2	2.50	0.42
1:D:150:TRP:HB3	1:D:153:ASP:HB2	2.02	0.42
1:B:101:ALA:HA	1:B:248:TYR:O	2.19	0.41
1:B:533:ASN:O	1:B:537:THR:HG22	2.20	0.41
1:C:519:ASP:O	1:C:520:HIS:HB2	2.20	0.41
1:A:227:ASP:HB2	1:A:228:PRO:HD3	2.02	0.41
1:D:227:ASP:HB2	1:D:228:PRO:HD3	2.03	0.41
1:B:125:TYR:HB2	1:B:246:LEU:HD23	2.02	0.41
1:B:221:ASP:O	1:B:222:HIS:CB	2.69	0.41
1:D:221:ASP:O	1:D:222:HIS:HB2	2.21	0.41
1:C:125:TYR:HB2	1:C:246:LEU:CD2	2.48	0.40
1:D:406:ASN:O	1:D:410:GLN:HG2	2.21	0.40
1:C:161:ILE:HB	1:C:162:PRO:CD	2.51	0.40
1:D:217:LEU:HD11	1:D:233:PHE:HB2	2.02	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	589/632 (93%)	572 (97%)	17 (3%)	0	100	100
1	B	589/632 (93%)	573 (97%)	16 (3%)	0	100	100
1	C	589/632 (93%)	571 (97%)	18 (3%)	0	100	100
1	D	589/632 (93%)	572 (97%)	17 (3%)	0	100	100
All	All	2356/2528 (93%)	2288 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	516/547 (94%)	513 (99%)	3 (1%)	84	91
1	B	516/547 (94%)	513 (99%)	3 (1%)	84	91
1	C	516/547 (94%)	513 (99%)	3 (1%)	84	91
1	D	516/547 (94%)	513 (99%)	3 (1%)	84	91
All	All	2064/2188 (94%)	2052 (99%)	12 (1%)	84	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	73	ARG

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Mol	Chain	Res	Type
1	A	365	ARG
1	B	59	LYS
1	B	73	ARG
1	B	365	ARG
1	C	59	LYS
1	C	73	ARG
1	C	365	ARG
1	D	59	LYS
1	D	73	ARG
1	D	365	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	520	HIS
1	B	310	GLN
1	B	622	HIS
1	C	187	ASN
1	C	622	HIS
1	D	187	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	PO4	D	703	-	4,4,4	1.05	0	6,6,6	0.75	0
4	GOL	D	704	-	5,5,5	0.20	0	5,5,5	0.26	0
4	GOL	A	705	-	5,5,5	0.38	0	5,5,5	0.16	0
2	4IP	C	702	-	28,28,28	0.74	0	46,46,46	0.92	0
3	PO4	B	703	-	4,4,4	1.10	0	6,6,6	0.74	0
4	GOL	B	704	-	5,5,5	0.18	0	5,5,5	0.44	0
4	GOL	B	706	-	5,5,5	0.30	0	5,5,5	0.29	0
2	4IP	D	701	-	28,28,28	0.69	0	46,46,46	0.91	0
2	4IP	A	701	-	28,28,28	0.69	0	46,46,46	0.90	0
4	GOL	A	704	-	5,5,5	0.32	0	5,5,5	0.17	0
2	4IP	B	701	-	28,28,28	0.70	0	46,46,46	0.89	0
4	GOL	C	705	-	5,5,5	0.39	0	5,5,5	0.56	0
4	GOL	D	705	-	5,5,5	0.53	0	5,5,5	0.55	0
3	PO4	D	702	-	4,4,4	1.07	0	6,6,6	0.71	0
4	GOL	B	705	-	5,5,5	0.43	0	5,5,5	0.33	0
3	PO4	C	703	-	4,4,4	0.96	0	6,6,6	0.60	0
4	GOL	A	706	-	5,5,5	0.31	0	5,5,5	0.54	0
2	4IP	A	702	-	28,28,28	0.72	0	46,46,46	0.94	0
3	PO4	B	702	-	4,4,4	0.77	0	6,6,6	0.60	0
2	4IP	C	701	-	28,28,28	0.70	0	46,46,46	0.92	1 (2%)
4	GOL	C	706	-	5,5,5	0.29	0	5,5,5	0.28	0
4	GOL	C	704	-	5,5,5	0.33	0	5,5,5	0.08	0
4	GOL	D	706	-	5,5,5	0.36	0	5,5,5	0.19	0
3	PO4	A	703	-	4,4,4	0.91	0	6,6,6	0.68	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
4	GOL	B	705	-	-	4/4/4/4	-
4	GOL	D	704	-	-	0/4/4/4	-
2	4IP	C	701	-	-	3/20/44/44	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	705	-	-	4/4/4/4	-
2	4IP	B	701	-	-	4/20/44/44	0/1/1/1
4	GOL	C	705	-	-	4/4/4/4	-
4	GOL	C	706	-	-	0/4/4/4	-
2	4IP	C	702	-	-	0/20/44/44	0/1/1/1
4	GOL	C	704	-	-	2/4/4/4	-
4	GOL	B	704	-	-	2/4/4/4	-
4	GOL	D	705	-	-	1/4/4/4	-
4	GOL	A	706	-	-	4/4/4/4	-
4	GOL	D	706	-	-	1/4/4/4	-
4	GOL	B	706	-	-	3/4/4/4	-
2	4IP	D	701	-	-	4/20/44/44	0/1/1/1
2	4IP	A	702	-	-	2/20/44/44	0/1/1/1
2	4IP	A	701	-	-	4/20/44/44	0/1/1/1
4	GOL	A	704	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	4IP	O8P-P4-O7P	2.08	115.60	107.80

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	701	4IP	C2-C1-O1-P1
2	C	701	4IP	C6-C1-O1-P1
4	A	704	GOL	O1-C1-C2-O2
4	A	704	GOL	O1-C1-C2-C3
4	A	705	GOL	O1-C1-C2-C3
4	A	705	GOL	C1-C2-C3-O3
4	B	705	GOL	O1-C1-C2-C3
4	B	705	GOL	C1-C2-C3-O3
4	B	706	GOL	O1-C1-C2-C3
4	C	705	GOL	O1-C1-C2-C3
4	C	705	GOL	C1-C2-C3-O3
4	C	705	GOL	O2-C2-C3-O3

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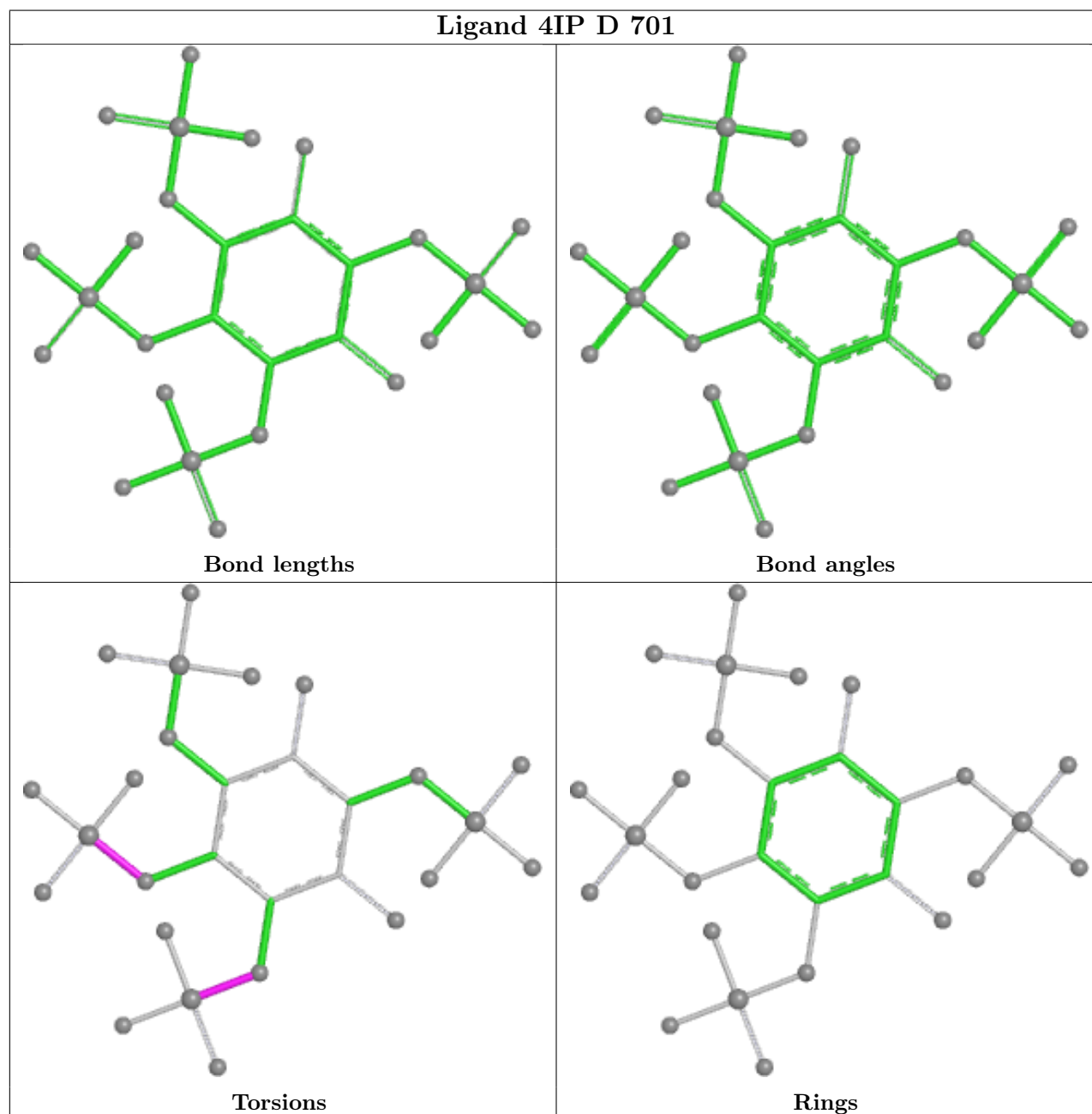
Mol	Chain	Res	Type	Atoms
4	A	705	GOL	O2-C2-C3-O3
4	A	706	GOL	C1-C2-C3-O3
4	C	704	GOL	O1-C1-C2-C3
4	A	705	GOL	O1-C1-C2-O2
4	A	706	GOL	O2-C2-C3-O3
4	B	705	GOL	O1-C1-C2-O2
4	B	706	GOL	O1-C1-C2-O2
4	C	704	GOL	O1-C1-C2-O2
4	C	705	GOL	O1-C1-C2-O2
2	A	701	4IP	C3-O3-P3-O5P
4	A	706	GOL	O1-C1-C2-O2
4	B	705	GOL	O2-C2-C3-O3
4	A	706	GOL	O1-C1-C2-C3
4	B	704	GOL	C1-C2-C3-O3
4	B	704	GOL	O2-C2-C3-O3
4	B	706	GOL	O2-C2-C3-O3
2	A	702	4IP	C3-O3-P3-O5P
2	B	701	4IP	C1-O1-P1-O3P
2	D	701	4IP	C3-O3-P3-O6P
2	D	701	4IP	C4-O4-P4-O7P
4	D	706	GOL	C1-C2-C3-O3
2	C	701	4IP	C2-C3-O3-P3
2	A	701	4IP	C3-O3-P3-O4P
2	A	702	4IP	C5-O5-P5-OPG
2	B	701	4IP	C3-O3-P3-O4P
2	D	701	4IP	C3-O3-P3-O4P
2	A	701	4IP	C3-O3-P3-O6P
2	A	701	4IP	C4-O4-P4-O7P
2	B	701	4IP	C3-O3-P3-O6P
2	D	701	4IP	C3-O3-P3-O5P
2	B	701	4IP	C4-O4-P4-O9P
4	D	705	GOL	O1-C1-C2-O2

There are no ring outliers.

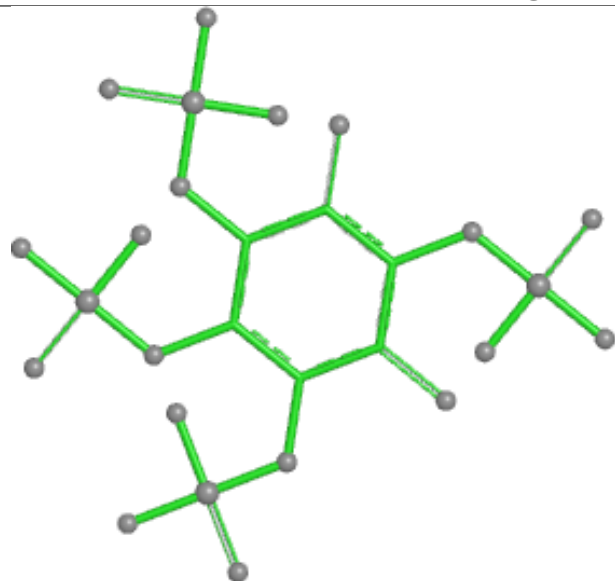
5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	GOL	1	0
2	C	702	4IP	6	0
4	D	705	GOL	2	0
2	A	702	4IP	4	0
2	C	701	4IP	2	0

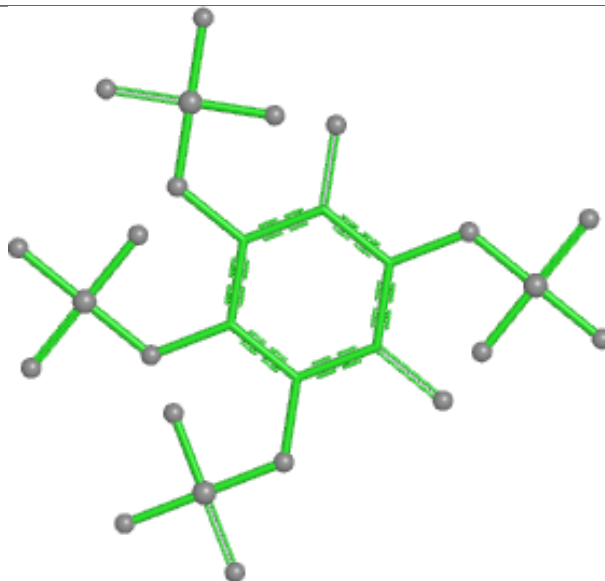
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



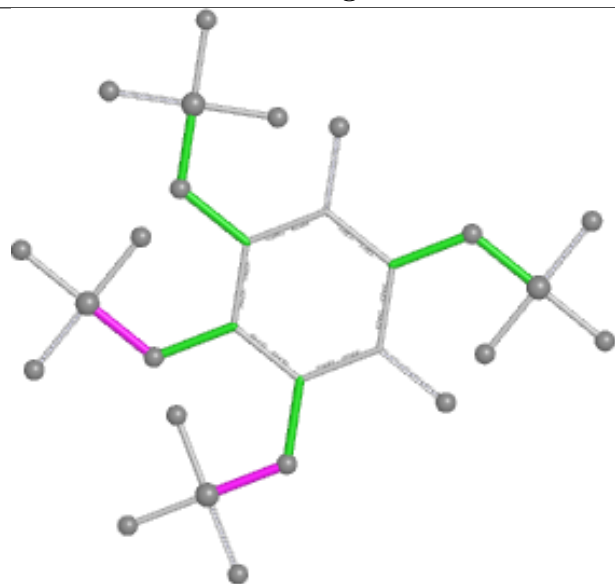
Ligand 4IP A 701



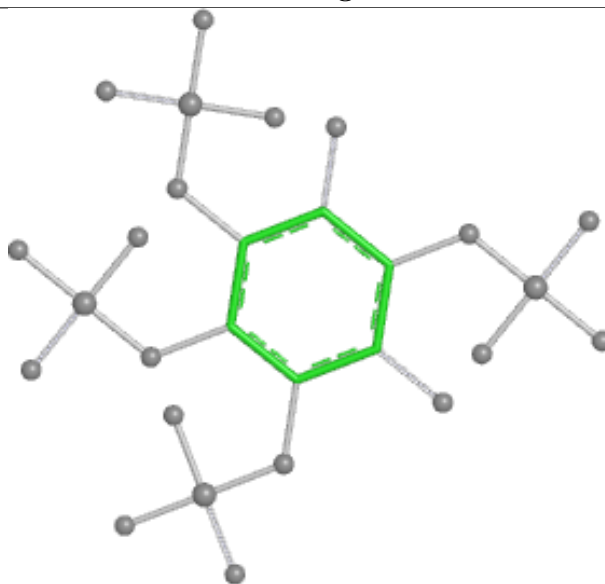
Bond lengths



Bond angles

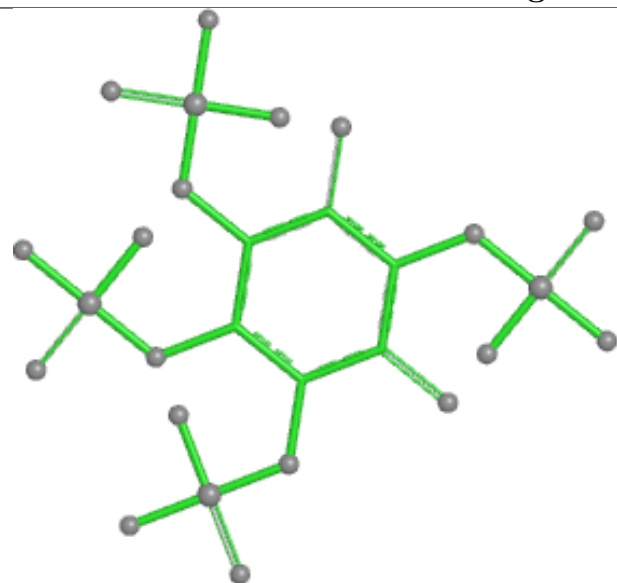


Torsions

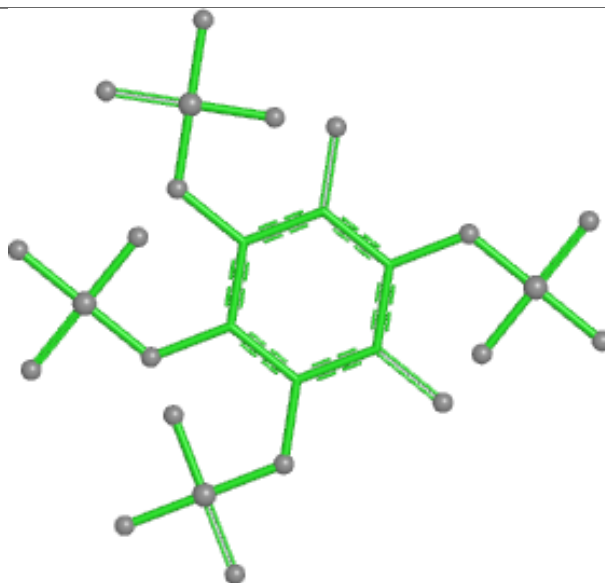


Rings

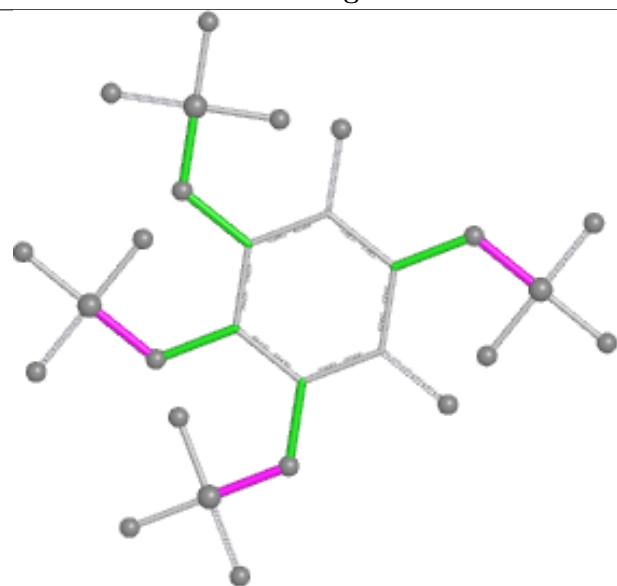
Ligand 4IP B 701



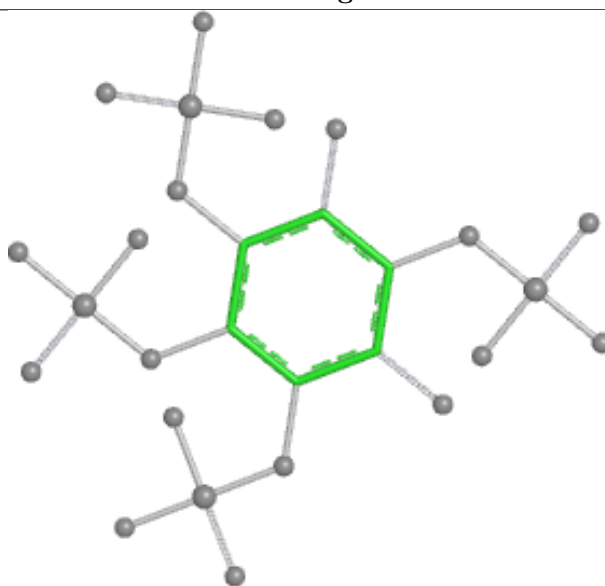
Bond lengths



Bond angles

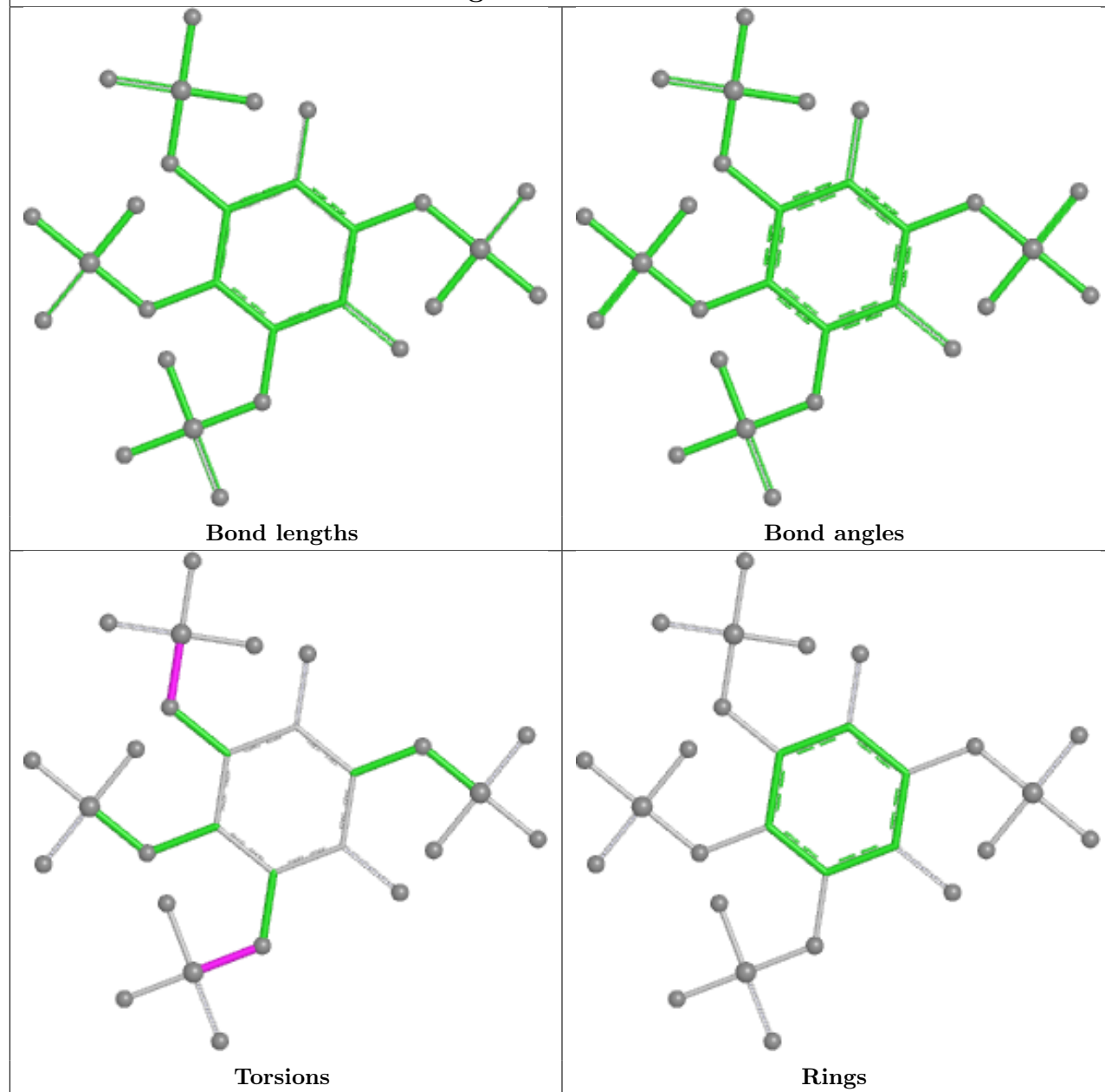


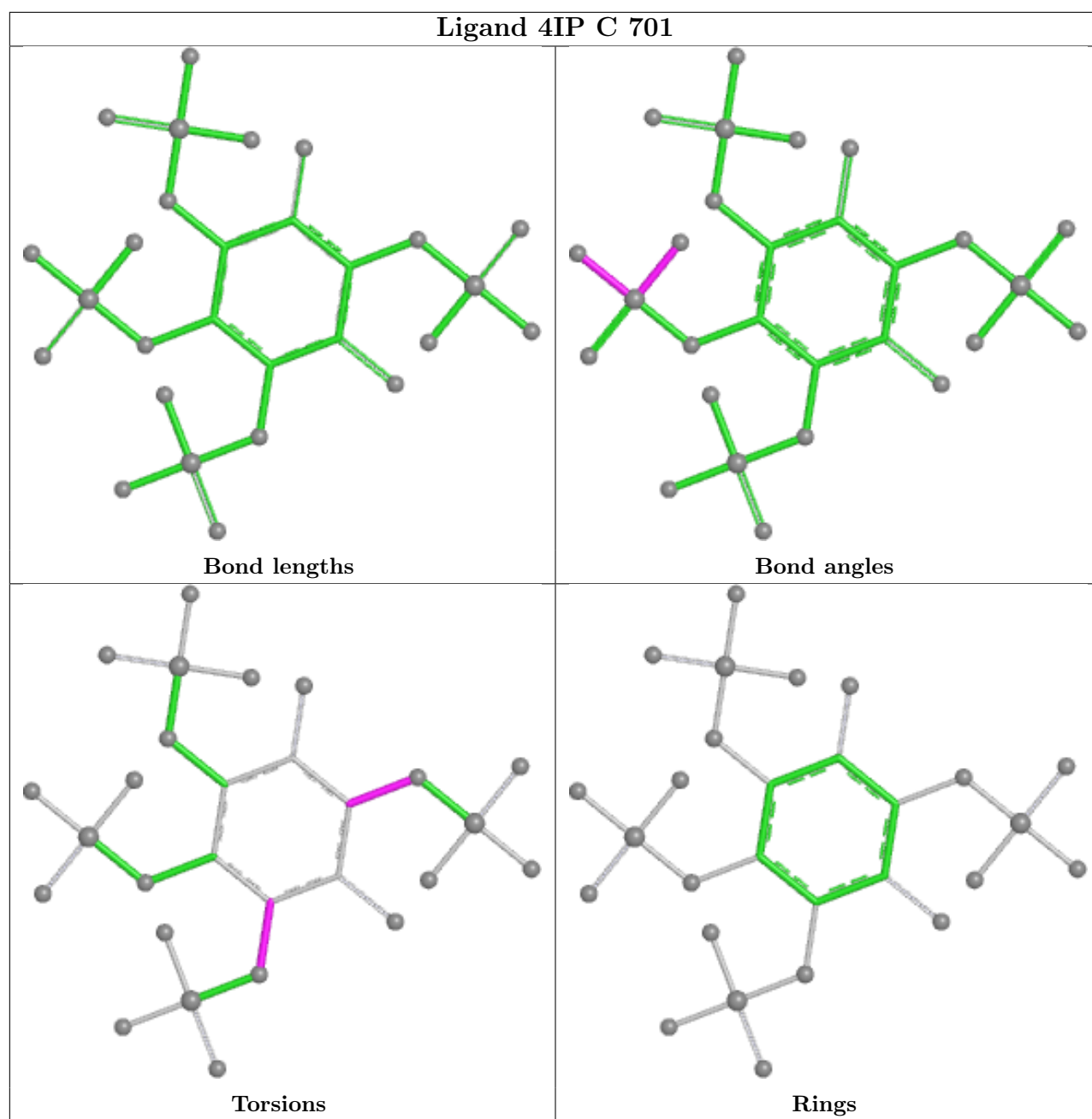
Torsions



Rings

Ligand 4IP A 702





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	590/632 (93%)	0.08	16 (2%)	56	53	5, 14, 35, 62	1 (0%)
1	B	590/632 (93%)	0.21	27 (4%)	38	35	5, 17, 39, 72	1 (0%)
1	C	590/632 (93%)	0.07	20 (3%)	48	45	6, 14, 35, 62	1 (0%)
1	D	590/632 (93%)	0.35	39 (6%)	26	23	7, 17, 41, 70	1 (0%)
All	All	2360/2528 (93%)	0.18	102 (4%)	40	36	5, 16, 38, 72	4 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	636	ALA	6.8
1	D	47	PRO	5.0
1	B	592	ALA	4.7
1	C	593	LYS	4.3
1	B	636	ALA	4.1
1	A	627	LYS	4.0
1	A	635	ALA	3.9
1	A	51	LYS	3.9
1	C	627	LYS	3.7
1	A	173	GLY	3.7
1	C	592	ALA	3.7
1	C	51	LYS	3.6
1	D	635	ALA	3.6
1	B	595	LYS	3.5
1	A	491	LYS	3.5
1	D	593	LYS	3.5
1	A	636	ALA	3.5
1	D	48	ALA	3.4
1	D	592	ALA	3.4
1	D	373	THR	3.4
1	C	55	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	595	LYS	3.3
1	D	198	ASN	3.3
1	D	632	GLN	3.2
1	D	51	LYS	3.2
1	D	242	LYS	3.2
1	D	491	LYS	3.2
1	B	194	TYR	3.2
1	B	593	LYS	3.2
1	A	596	PRO	3.2
1	C	596	PRO	3.1
1	A	593	LYS	3.0
1	B	489	ASP	3.0
1	D	569	ASP	3.0
1	C	636	ALA	3.0
1	A	483	LYS	3.0
1	D	595	LYS	3.0
1	D	489	ASP	3.0
1	C	540	ALA	2.9
1	C	595	LYS	2.8
1	D	623	ALA	2.8
1	B	47	PRO	2.8
1	D	50	VAL	2.8
1	B	115	LYS	2.7
1	B	242	LYS	2.7
1	D	52	ASN	2.7
1	D	49	VAL	2.7
1	C	623	ALA	2.7
1	B	48	ALA	2.7
1	B	52	ASN	2.6
1	B	51	LYS	2.6
1	A	473	GLY	2.6
1	B	391	LYS	2.6
1	D	375	VAL	2.6
1	A	540	ALA	2.6
1	C	635	ALA	2.6
1	C	491	LYS	2.6
1	A	592	ALA	2.6
1	B	491	LYS	2.6
1	D	176	VAL	2.5
1	D	193	VAL	2.5
1	D	496	GLU	2.5
1	B	483	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	627	LYS	2.5
1	C	483	LYS	2.4
1	B	635	ALA	2.4
1	A	52	ASN	2.4
1	B	569	ASP	2.4
1	D	483	LYS	2.4
1	C	418	GLN	2.4
1	B	540	ALA	2.3
1	B	355	LYS	2.3
1	B	177	LYS	2.3
1	D	374	ASP	2.3
1	D	624	ASP	2.3
1	D	596	PRO	2.3
1	A	475	SER	2.3
1	A	53	PRO	2.2
1	B	193	VAL	2.2
1	D	179	ILE	2.2
1	D	185	LYS	2.2
1	D	391	LYS	2.2
1	D	194	TYR	2.2
1	C	373	THR	2.2
1	C	493	VAL	2.2
1	D	377	VAL	2.2
1	D	138	ASN	2.2
1	B	55	LYS	2.2
1	D	199	LYS	2.2
1	D	627	LYS	2.2
1	B	191	SER	2.2
1	C	489	ASP	2.2
1	D	634	LEU	2.2
1	B	185	LYS	2.2
1	B	186	LYS	2.2
1	B	421	LYS	2.1
1	C	507	LYS	2.1
1	C	47	PRO	2.1
1	D	370	ALA	2.1
1	D	615	TYR	2.0
1	C	625	GLY	2.0
1	D	191	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

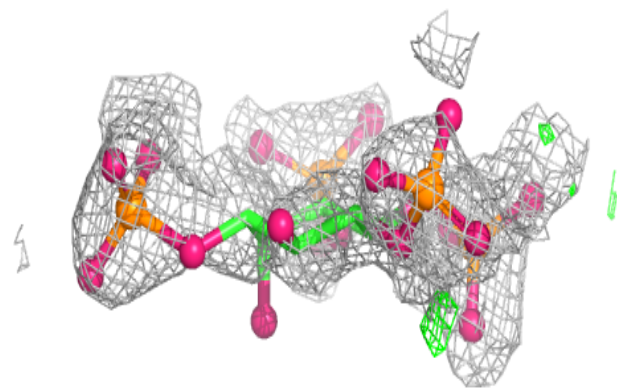
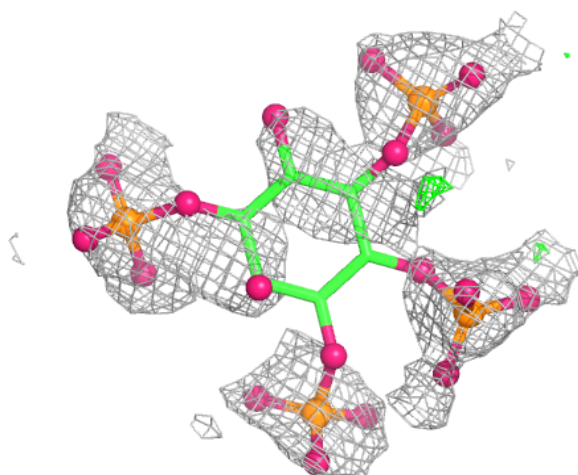
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	4IP	A	701	28/28	0.72	0.19	36,54,61,62	28
2	4IP	C	701	28/28	0.73	0.19	42,52,61,63	28
2	4IP	B	701	28/28	0.74	0.18	31,48,60,64	28
2	4IP	D	701	28/28	0.80	0.17	34,45,51,54	28
4	GOL	A	705	6/6	0.81	0.18	21,26,29,31	0
4	GOL	C	705	6/6	0.81	0.15	23,28,29,31	0
4	GOL	D	705	6/6	0.81	0.17	27,31,34,34	0
4	GOL	B	704	6/6	0.87	0.12	20,22,24,28	0
2	4IP	A	702	28/28	0.87	0.17	17,50,71,79	0
4	GOL	A	706	6/6	0.87	0.12	18,22,23,26	0
2	4IP	C	702	28/28	0.88	0.16	17,58,78,86	0
4	GOL	B	705	6/6	0.88	0.15	28,36,39,41	0
4	GOL	D	704	6/6	0.90	0.10	14,16,17,18	0
4	GOL	C	706	6/6	0.90	0.10	16,20,22,26	0
4	GOL	D	706	6/6	0.90	0.10	20,23,24,26	0
4	GOL	B	706	6/6	0.91	0.09	19,21,24,24	0
4	GOL	A	704	6/6	0.91	0.10	18,19,20,21	0
4	GOL	C	704	6/6	0.93	0.08	14,17,18,19	0
3	PO4	D	702	5/5	0.97	0.07	12,14,17,18	0
3	PO4	B	702	5/5	0.98	0.05	11,14,15,17	0
3	PO4	B	703	5/5	0.98	0.05	11,11,12,12	0
3	PO4	A	703	5/5	0.98	0.05	10,11,12,13	0
3	PO4	D	703	5/5	0.98	0.06	8,8,9,10	0
3	PO4	C	703	5/5	0.99	0.04	10,11,11,11	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.

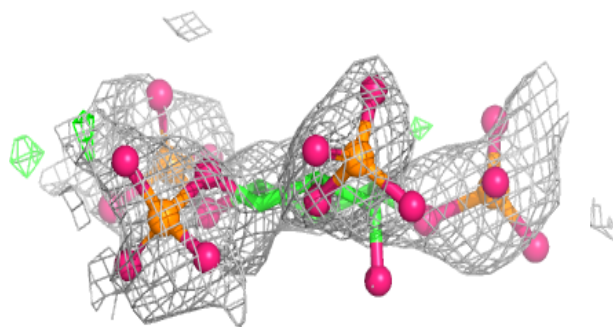
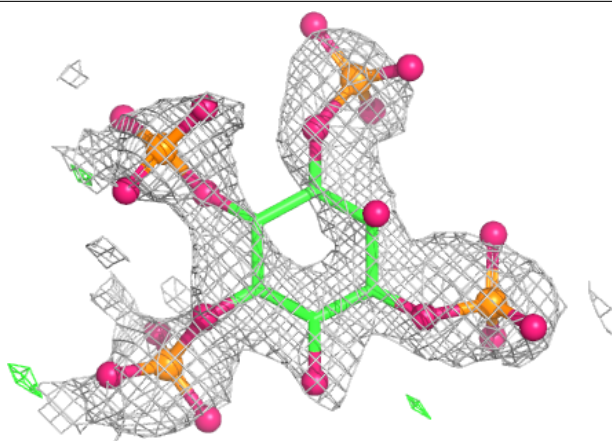
Electron density around 4IP A 701:

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



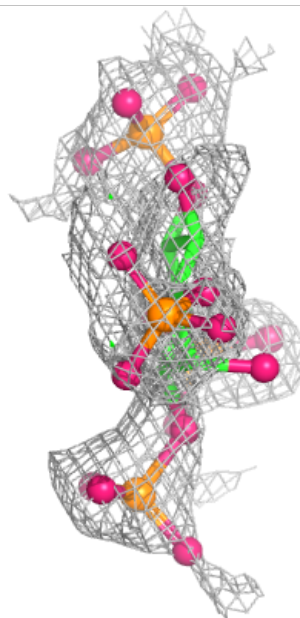
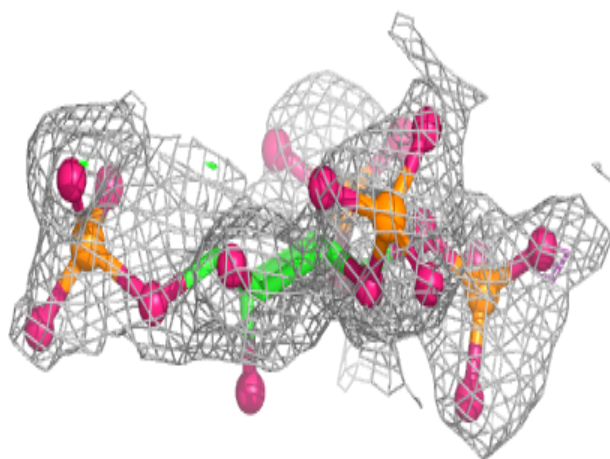
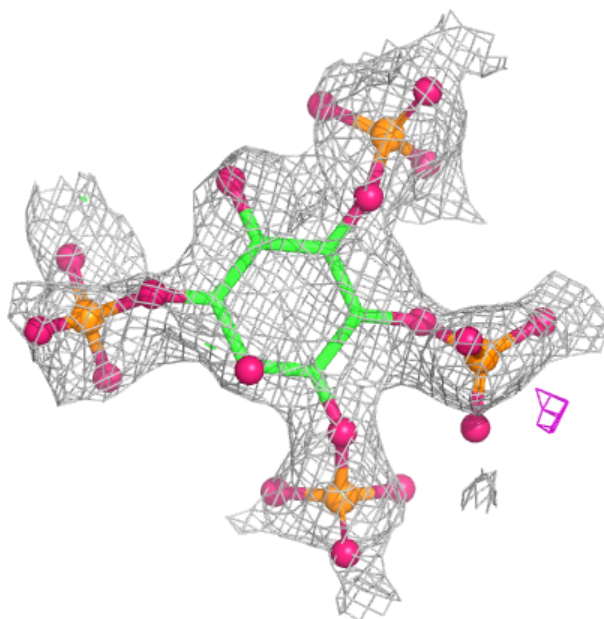
Electron density around 4IP C 701:

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



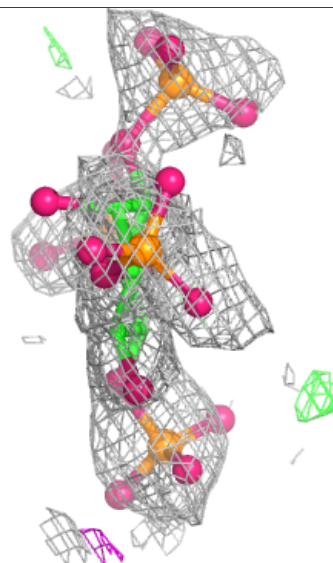
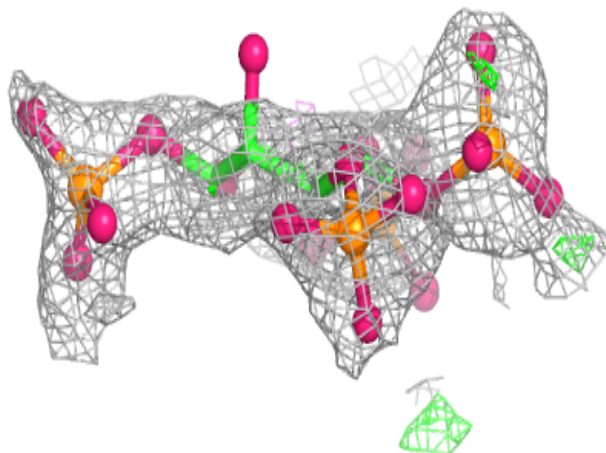
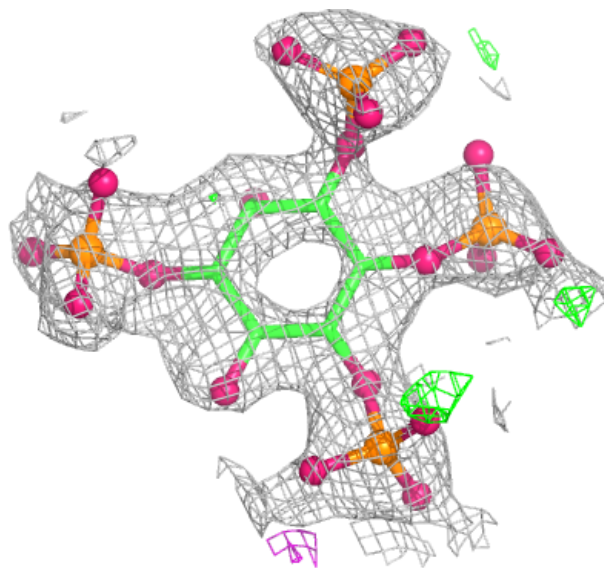
Electron density around 4IP B 701:

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



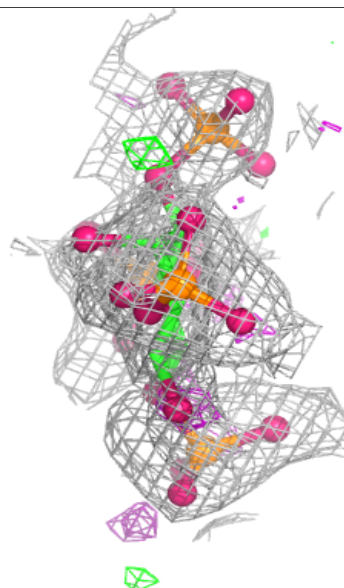
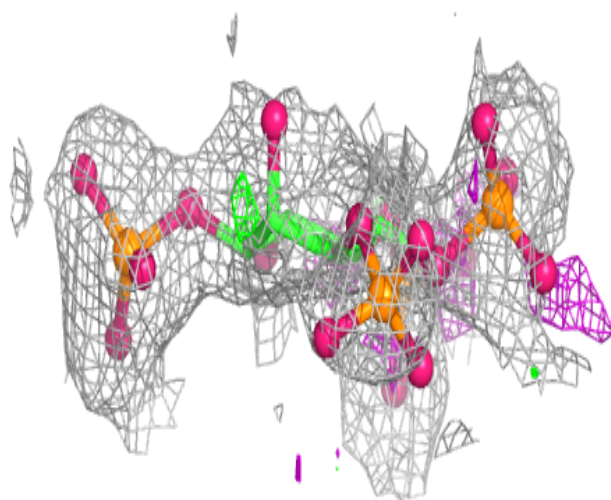
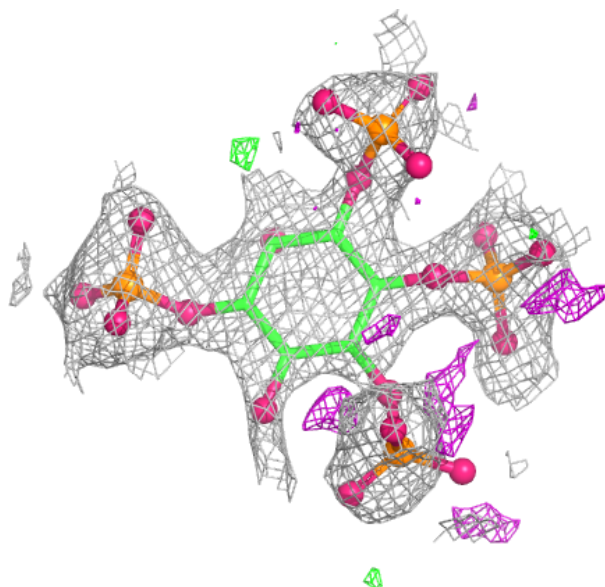
Electron density around 4IP D 701:

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



Electron density around 4IP A 702:

$2mF_o-DF_c$ (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.