



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:31 AM UTC

PDB ID : 9VA7 / pdb_00009va7
Title : Crystal structure of legionella effector Lem17 in complex with IP6
Authors : Chen, T.T.; Zheng, S.R.; Ouyang, S.Y.
Deposited on : 2025-06-02
Resolution : 2.23 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

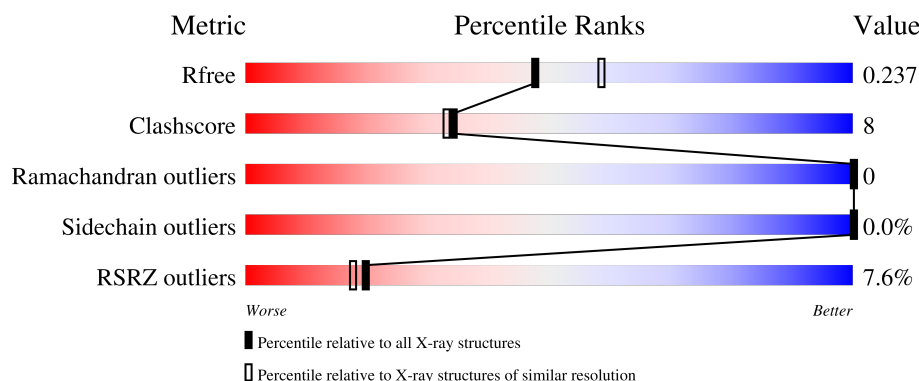
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	451	6% 74% 16% 10%
1	B	451	3% 83% 9% 8%
1	C	451	7% 75% 17% 8%
1	D	451	8% 77% 14% 8%
1	E	451	7% 77% 15% 8%

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Mol	Chain	Length	Quality of chain
1	F	451	
1	G	451	
1	H	451	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27706 atoms, of which 48 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 Dot/Icm T4SS effector Lem17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3316	2092	586	627	11			
1	B	415	Total	C	N	O	S	0	0	0
			3397	2146	599	641	11			
1	C	417	Total	C	N	O	S	0	0	0
			3414	2156	602	645	11			
1	D	413	Total	C	N	O	S	0	0	0
			3375	2129	594	641	11			
1	E	414	Total	C	N	O	S	0	0	0
			3379	2135	595	638	11			
1	F	410	Total	C	N	O	S	0	0	0
			3352	2115	592	634	11			
1	G	414	Total	C	N	O	S	0	0	0
			3386	2137	597	641	11			
1	H	407	Total	C	N	O	S	0	0	0
			3330	2101	588	630	11			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP A0AAN5PJ36
A	-3	GLY	-	expression tag	UNP A0AAN5PJ36
A	-2	SER	-	expression tag	UNP A0AAN5PJ36
A	-1	SER	-	expression tag	UNP A0AAN5PJ36
A	0	HIS	-	expression tag	UNP A0AAN5PJ36
A	1	HIS	-	expression tag	UNP A0AAN5PJ36
A	2	HIS	-	expression tag	UNP A0AAN5PJ36
A	3	HIS	-	expression tag	UNP A0AAN5PJ36
A	4	HIS	-	expression tag	UNP A0AAN5PJ36
A	5	HIS	-	expression tag	UNP A0AAN5PJ36
A	6	SER	-	expression tag	UNP A0AAN5PJ36
A	7	SER	-	expression tag	UNP A0AAN5PJ36
A	8	GLY	-	expression tag	UNP A0AAN5PJ36

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Chain	Residue	Modelled	Actual	Comment	Reference
A	9	LEU	-	expression tag	UNP A0AAN5PJ36
A	10	VAL	-	expression tag	UNP A0AAN5PJ36
A	11	PRO	-	expression tag	UNP A0AAN5PJ36
A	12	ARG	-	expression tag	UNP A0AAN5PJ36
A	13	GLY	-	expression tag	UNP A0AAN5PJ36
A	14	SER	-	expression tag	UNP A0AAN5PJ36
B	-4	MET	-	initiating methionine	UNP A0AAN5PJ36
B	-3	GLY	-	expression tag	UNP A0AAN5PJ36
B	-2	SER	-	expression tag	UNP A0AAN5PJ36
B	-1	SER	-	expression tag	UNP A0AAN5PJ36
B	0	HIS	-	expression tag	UNP A0AAN5PJ36
B	1	HIS	-	expression tag	UNP A0AAN5PJ36
B	2	HIS	-	expression tag	UNP A0AAN5PJ36
B	3	HIS	-	expression tag	UNP A0AAN5PJ36
B	4	HIS	-	expression tag	UNP A0AAN5PJ36
B	5	HIS	-	expression tag	UNP A0AAN5PJ36
B	6	SER	-	expression tag	UNP A0AAN5PJ36
B	7	SER	-	expression tag	UNP A0AAN5PJ36
B	8	GLY	-	expression tag	UNP A0AAN5PJ36
B	9	LEU	-	expression tag	UNP A0AAN5PJ36
B	10	VAL	-	expression tag	UNP A0AAN5PJ36
B	11	PRO	-	expression tag	UNP A0AAN5PJ36
B	12	ARG	-	expression tag	UNP A0AAN5PJ36
B	13	GLY	-	expression tag	UNP A0AAN5PJ36
B	14	SER	-	expression tag	UNP A0AAN5PJ36
C	-4	MET	-	initiating methionine	UNP A0AAN5PJ36
C	-3	GLY	-	expression tag	UNP A0AAN5PJ36
C	-2	SER	-	expression tag	UNP A0AAN5PJ36
C	-1	SER	-	expression tag	UNP A0AAN5PJ36
C	0	HIS	-	expression tag	UNP A0AAN5PJ36
C	1	HIS	-	expression tag	UNP A0AAN5PJ36
C	2	HIS	-	expression tag	UNP A0AAN5PJ36
C	3	HIS	-	expression tag	UNP A0AAN5PJ36
C	4	HIS	-	expression tag	UNP A0AAN5PJ36
C	5	HIS	-	expression tag	UNP A0AAN5PJ36
C	6	SER	-	expression tag	UNP A0AAN5PJ36
C	7	SER	-	expression tag	UNP A0AAN5PJ36
C	8	GLY	-	expression tag	UNP A0AAN5PJ36
C	9	LEU	-	expression tag	UNP A0AAN5PJ36
C	10	VAL	-	expression tag	UNP A0AAN5PJ36
C	11	PRO	-	expression tag	UNP A0AAN5PJ36
C	12	ARG	-	expression tag	UNP A0AAN5PJ36

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Chain	Residue	Modelled	Actual	Comment	Reference
C	13	GLY	-	expression tag	UNP A0AAN5PJ36
C	14	SER	-	expression tag	UNP A0AAN5PJ36
D	-4	MET	-	initiating methionine	UNP A0AAN5PJ36
D	-3	GLY	-	expression tag	UNP A0AAN5PJ36
D	-2	SER	-	expression tag	UNP A0AAN5PJ36
D	-1	SER	-	expression tag	UNP A0AAN5PJ36
D	0	HIS	-	expression tag	UNP A0AAN5PJ36
D	1	HIS	-	expression tag	UNP A0AAN5PJ36
D	2	HIS	-	expression tag	UNP A0AAN5PJ36
D	3	HIS	-	expression tag	UNP A0AAN5PJ36
D	4	HIS	-	expression tag	UNP A0AAN5PJ36
D	5	HIS	-	expression tag	UNP A0AAN5PJ36
D	6	SER	-	expression tag	UNP A0AAN5PJ36
D	7	SER	-	expression tag	UNP A0AAN5PJ36
D	8	GLY	-	expression tag	UNP A0AAN5PJ36
D	9	LEU	-	expression tag	UNP A0AAN5PJ36
D	10	VAL	-	expression tag	UNP A0AAN5PJ36
D	11	PRO	-	expression tag	UNP A0AAN5PJ36
D	12	ARG	-	expression tag	UNP A0AAN5PJ36
D	13	GLY	-	expression tag	UNP A0AAN5PJ36
D	14	SER	-	expression tag	UNP A0AAN5PJ36
E	-4	MET	-	initiating methionine	UNP A0AAN5PJ36
E	-3	GLY	-	expression tag	UNP A0AAN5PJ36
E	-2	SER	-	expression tag	UNP A0AAN5PJ36
E	-1	SER	-	expression tag	UNP A0AAN5PJ36
E	0	HIS	-	expression tag	UNP A0AAN5PJ36
E	1	HIS	-	expression tag	UNP A0AAN5PJ36
E	2	HIS	-	expression tag	UNP A0AAN5PJ36
E	3	HIS	-	expression tag	UNP A0AAN5PJ36
E	4	HIS	-	expression tag	UNP A0AAN5PJ36
E	5	HIS	-	expression tag	UNP A0AAN5PJ36
E	6	SER	-	expression tag	UNP A0AAN5PJ36
E	7	SER	-	expression tag	UNP A0AAN5PJ36
E	8	GLY	-	expression tag	UNP A0AAN5PJ36
E	9	LEU	-	expression tag	UNP A0AAN5PJ36
E	10	VAL	-	expression tag	UNP A0AAN5PJ36
E	11	PRO	-	expression tag	UNP A0AAN5PJ36
E	12	ARG	-	expression tag	UNP A0AAN5PJ36
E	13	GLY	-	expression tag	UNP A0AAN5PJ36
E	14	SER	-	expression tag	UNP A0AAN5PJ36
F	-4	MET	-	initiating methionine	UNP A0AAN5PJ36
F	-3	GLY	-	expression tag	UNP A0AAN5PJ36

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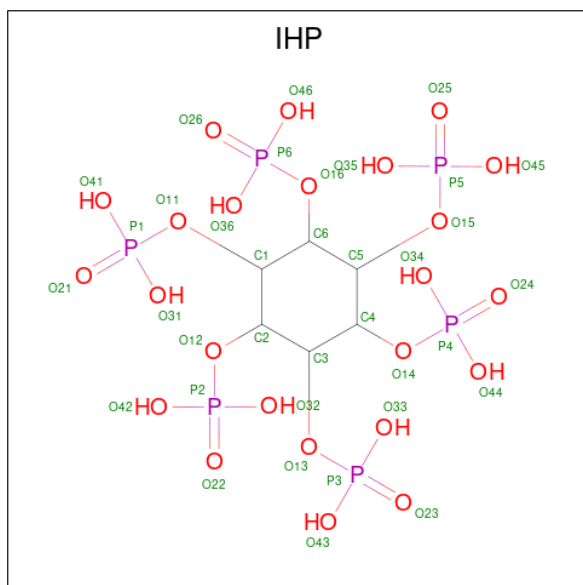
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F	-1	SER	-	expression tag	UNP A0AAN5PJ36
F	0	HIS	-	expression tag	UNP A0AAN5PJ36
F	1	HIS	-	expression tag	UNP A0AAN5PJ36
F	2	HIS	-	expression tag	UNP A0AAN5PJ36
F	3	HIS	-	expression tag	UNP A0AAN5PJ36
F	4	HIS	-	expression tag	UNP A0AAN5PJ36
F	5	HIS	-	expression tag	UNP A0AAN5PJ36
F	6	SER	-	expression tag	UNP A0AAN5PJ36
F	7	SER	-	expression tag	UNP A0AAN5PJ36
F	8	GLY	-	expression tag	UNP A0AAN5PJ36
F	9	LEU	-	expression tag	UNP A0AAN5PJ36
F	10	VAL	-	expression tag	UNP A0AAN5PJ36
F	11	PRO	-	expression tag	UNP A0AAN5PJ36
F	12	ARG	-	expression tag	UNP A0AAN5PJ36
F	13	GLY	-	expression tag	UNP A0AAN5PJ36
F	14	SER	-	expression tag	UNP A0AAN5PJ36
G	-4	MET	-	initiating methionine	UNP A0AAN5PJ36
G	-3	GLY	-	expression tag	UNP A0AAN5PJ36
G	-2	SER	-	expression tag	UNP A0AAN5PJ36
G	-1	SER	-	expression tag	UNP A0AAN5PJ36
G	0	HIS	-	expression tag	UNP A0AAN5PJ36
G	1	HIS	-	expression tag	UNP A0AAN5PJ36
G	2	HIS	-	expression tag	UNP A0AAN5PJ36
G	3	HIS	-	expression tag	UNP A0AAN5PJ36
G	4	HIS	-	expression tag	UNP A0AAN5PJ36
G	5	HIS	-	expression tag	UNP A0AAN5PJ36
G	6	SER	-	expression tag	UNP A0AAN5PJ36
G	7	SER	-	expression tag	UNP A0AAN5PJ36
G	8	GLY	-	expression tag	UNP A0AAN5PJ36
G	9	LEU	-	expression tag	UNP A0AAN5PJ36
G	10	VAL	-	expression tag	UNP A0AAN5PJ36
G	11	PRO	-	expression tag	UNP A0AAN5PJ36
G	12	ARG	-	expression tag	UNP A0AAN5PJ36
G	13	GLY	-	expression tag	UNP A0AAN5PJ36
G	14	SER	-	expression tag	UNP A0AAN5PJ36
H	-4	MET	-	initiating methionine	UNP A0AAN5PJ36
H	-3	GLY	-	expression tag	UNP A0AAN5PJ36
H	-2	SER	-	expression tag	UNP A0AAN5PJ36
H	-1	SER	-	expression tag	UNP A0AAN5PJ36
H	0	HIS	-	expression tag	UNP A0AAN5PJ36
H	1	HIS	-	expression tag	UNP A0AAN5PJ36

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Chain	Residue	Modelled	Actual	Comment	Reference
H	2	HIS	-	expression tag	UNP A0AAN5PJ36
H	3	HIS	-	expression tag	UNP A0AAN5PJ36
H	4	HIS	-	expression tag	UNP A0AAN5PJ36
H	5	HIS	-	expression tag	UNP A0AAN5PJ36
H	6	SER	-	expression tag	UNP A0AAN5PJ36
H	7	SER	-	expression tag	UNP A0AAN5PJ36
H	8	GLY	-	expression tag	UNP A0AAN5PJ36
H	9	LEU	-	expression tag	UNP A0AAN5PJ36
H	10	VAL	-	expression tag	UNP A0AAN5PJ36
H	11	PRO	-	expression tag	UNP A0AAN5PJ36
H	12	ARG	-	expression tag	UNP A0AAN5PJ36
H	13	GLY	-	expression tag	UNP A0AAN5PJ36
H	14	SER	-	expression tag	UNP A0AAN5PJ36

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			42	6	6	24	6		
2	B	1	Total	C	H	O	P	0	0
			42	6	6	24	6		
2	C	1	Total	C	H	O	P	0	0
			42	6	6	24	6		
2	D	1	Total	C	H	O	P	0	0
			42	6	6	24	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	H	O	P	0	0
			42	6	6	24	6		
2	F	1	Total	C	H	O	P	0	0
			42	6	6	24	6		
2	G	1	Total	C	H	O	P	0	0
			42	6	6	24	6		
2	H	1	Total	C	H	O	P	0	0
			42	6	6	24	6		

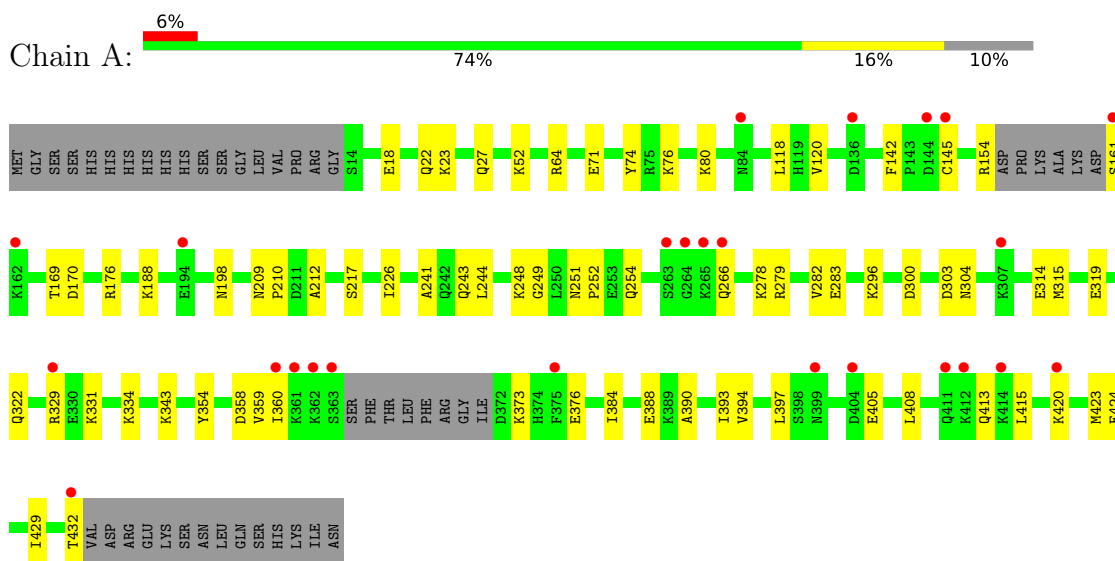
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	64	Total	O	0	0
			64	64		
3	B	95	Total	O	0	0
			95	95		
3	C	36	Total	O	0	0
			36	36		
3	D	81	Total	O	0	0
			81	81		
3	E	57	Total	O	0	0
			57	57		
3	F	52	Total	O	0	0
			52	52		
3	G	30	Total	O	0	0
			30	30		
3	H	6	Total	O	0	0
			6	6		

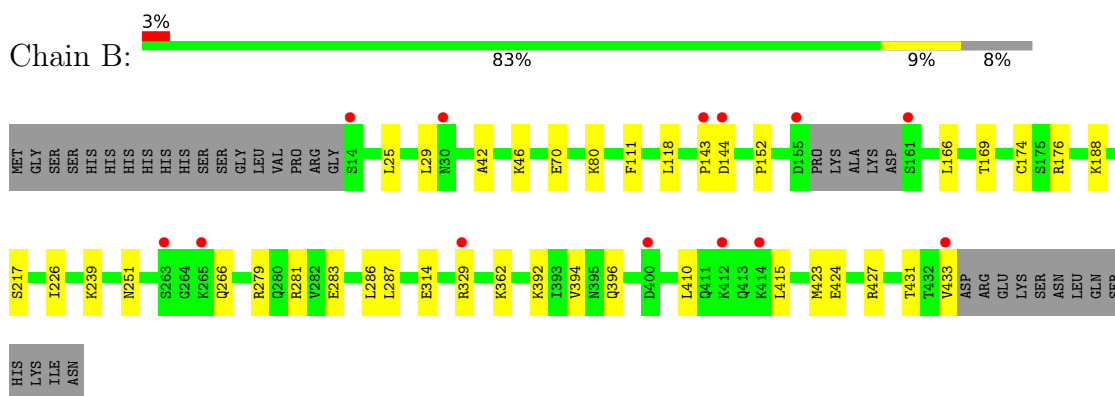
3 Residue-property plots

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.

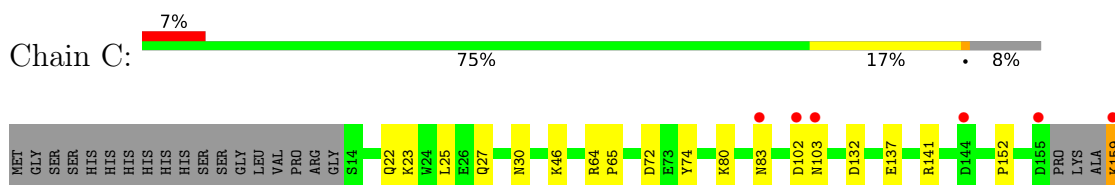
- Molecule 1: Dot/Icm T4SS effector Lem17

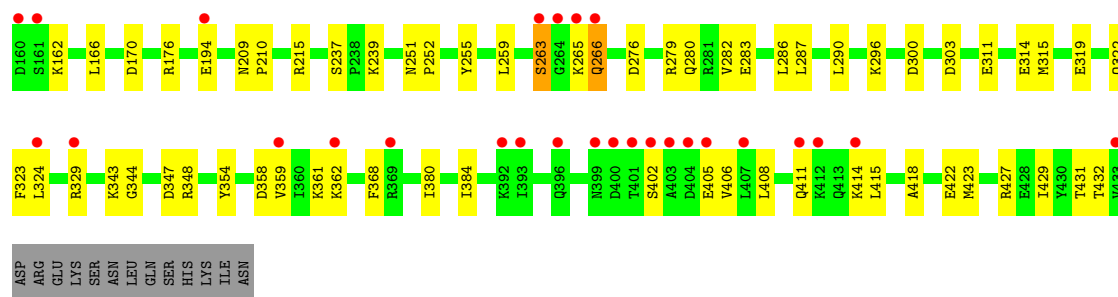


- Molecule 1: Dot/Icm T4SS effector Lem17

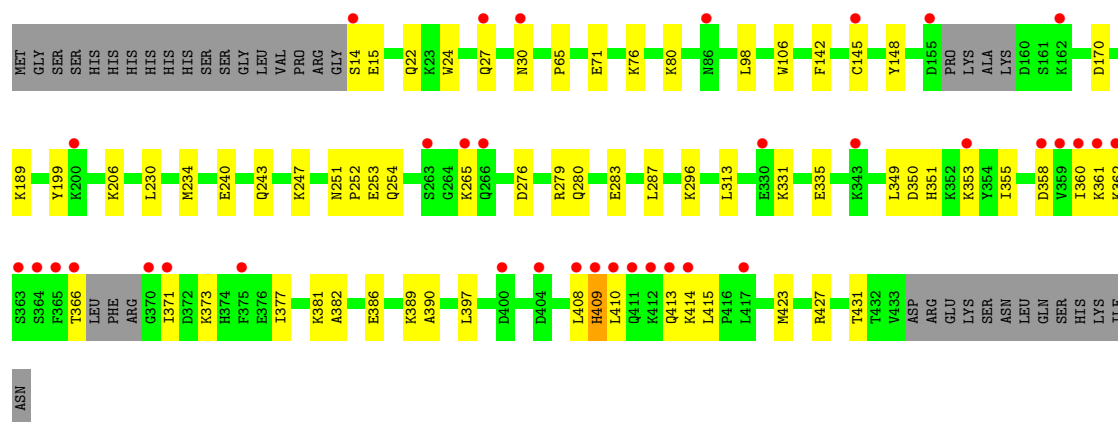
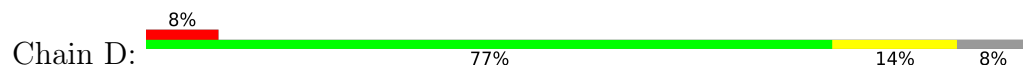


- Molecule 1: Dot/Icm T4SS effector Lem17

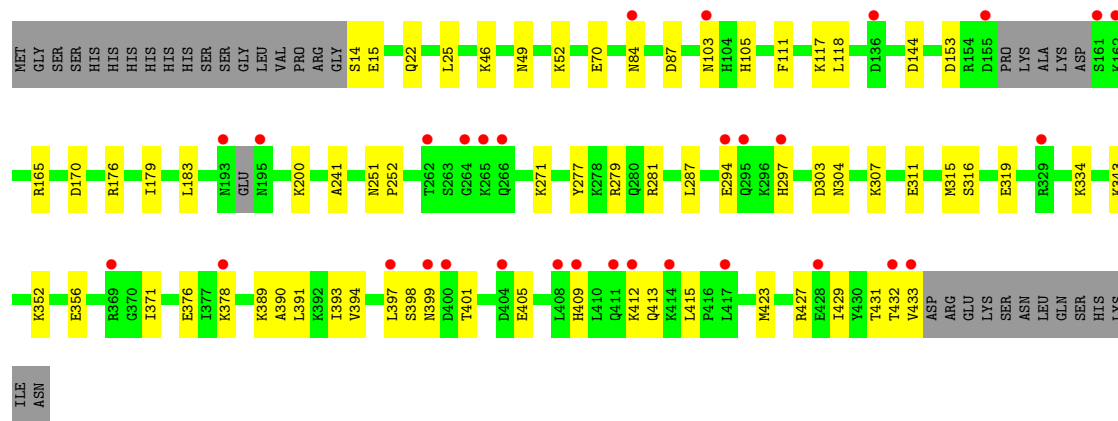
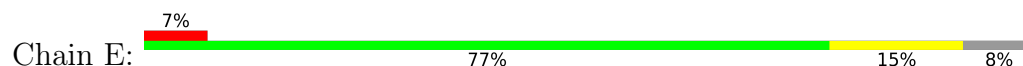




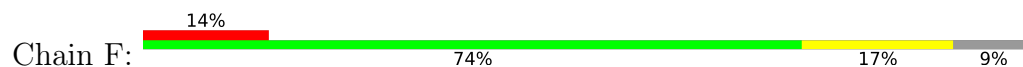
• Molecule 1: Dot/Icm T4SS effector Lem17



• Molecule 1: Dot/Icm T4SS effector Lem17

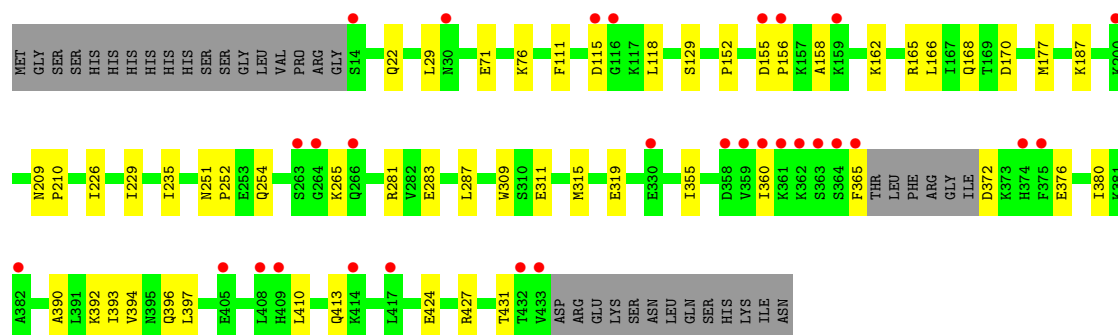
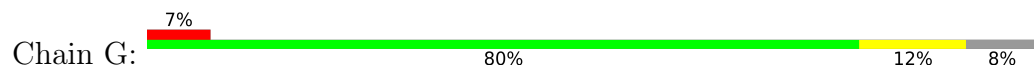


• Molecule 1: Dot/Icm T4SS effector Lem17

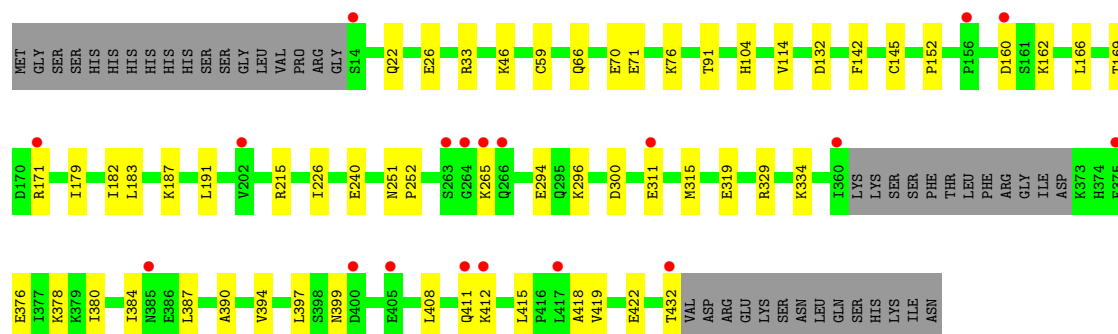
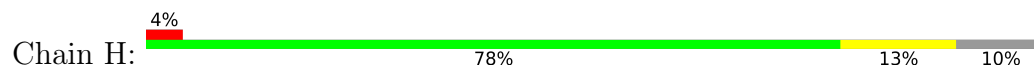




• Molecule 1: Dot/Icm T4SS effector Lem17



• Molecule 1: Dot/Icm T4SS effector Lem17



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	150.44Å 107.04Å 171.61Å 90.00° 110.11° 90.00°	Depositor
Resolution (Å)	50.07 – 2.23 50.07 – 2.23	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.07-2.23) 97.5 (50.07-2.23)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.22Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.201 , 0.237 0.202 , 0.237	Depositor DCC
R_{free} test set	1999 reflections (0.81%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27706	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.34 % 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 3.9112e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: IHP

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	0.40	0/3372	0.52	0/4522
1	B	0.48	0/3456	0.62	0/4637
1	C	0.45	0/3473	0.64	6/4659 (0.1%)
1	D	0.46	0/3432	0.62	2/4604 (0.0%)
1	E	0.41	0/3437	0.55	0/4611
1	F	0.43	1/3410 (0.0%)	0.55	0/4575
1	G	0.44	1/3445 (0.0%)	0.56	0/4622
1	H	0.40	0/3388	0.59	0/4547
All	All	0.43	2/27413 (0.0%)	0.58	8/36777 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	314	GLU	CG-CD	-6.12	1.36	1.52
1	G	115	ASP	C-N	5.09	1.40	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	263	SER	N-CA-C	13.17	129.61	108.41
1	C	263	SER	CB-CA-C	-12.06	90.92	110.81
1	D	414	LYS	CD-CE-NZ	-8.42	84.97	111.90
1	D	409	HIS	CB-CA-C	8.24	126.81	110.42
1	C	414	LYS	CG-CD-CE	-7.42	94.23	111.30
1	C	159	LYS	CD-CE-NZ	5.73	130.24	111.90
1	C	414	LYS	CD-CE-NZ	-5.58	94.06	111.90
1	C	266	GLN	CB-CG-CD	-5.31	103.58	112.60

There are no chirality outliers.

There are no planarity outliers.

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	3316	0	3326	59	0
1	B	3397	0	3408	34	0
1	C	3414	0	3425	59	0
1	D	3375	0	3378	52	0
1	E	3379	0	3381	59	0
1	F	3352	0	3362	85	0
1	G	3386	0	3396	36	0
1	H	3330	0	3338	40	0
2	A	36	6	4	3	0
2	B	36	6	3	1	0
2	C	36	6	4	1	0
2	D	36	6	4	1	0
2	E	36	6	3	1	0
2	F	36	6	3	2	0
2	G	36	6	4	2	0
2	H	36	6	4	1	0
3	A	64	0	0	2	0
3	B	95	0	0	1	0
3	C	36	0	0	0	0
3	D	81	0	0	2	0
3	E	57	0	0	0	0
3	F	52	0	0	6	0
3	G	30	0	0	1	0
3	H	6	0	0	0	0
All	All	27658	48	27043	414	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 8.

All (414) 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:E:294:GLU:OE1	1:E:297:HIS:HB2	1.62	1.00
1:A:296:LYS:H	1:A:296:LYS:HE2	1.29	0.95
1:F:413:GLN:HB3	3:F:601:HOH:O	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:410:LEU:HA	1:F:413:GLN:HG2	1.59	0.84
1:E:294:GLU:OE1	1:E:297:HIS:CB	2.25	0.84
1:A:354:TYR:HB3	1:A:359:VAL:CG2	2.07	0.84
1:F:394:VAL:HA	1:F:397:LEU:HD12	1.58	0.82
1:F:378:LYS:HA	1:F:381:LYS:HB2	1.60	0.82
1:C:354:TYR:HB3	1:C:359:VAL:HG21	1.60	0.82
1:F:402:SER:O	1:F:406:VAL:HG23	1.80	0.81
1:A:354:TYR:HB3	1:A:359:VAL:HG21	1.61	0.81
1:F:410:LEU:HA	1:F:413:GLN:CG	2.11	0.80
1:E:303:ASP:OD2	1:F:70:GLU:HG2	1.82	0.80
1:F:331:LYS:HD3	1:F:335:GLU:OE1	1.82	0.79
1:A:405:GLU:OE1	1:A:408:LEU:HD12	1.81	0.79
1:F:373:LYS:O	1:F:377:ILE:HG13	1.83	0.79
1:B:427:ARG:O	1:B:431:THR:HG23	1.83	0.78
1:F:394:VAL:HA	1:F:397:LEU:CD1	2.14	0.78
1:H:160:ASP:HB3	1:H:162:LYS:H	1.50	0.77
1:D:349:LEU:HB3	1:D:353:LYS:HE2	1.68	0.75
1:F:419:VAL:HG12	1:F:423:MET:HE2	1.69	0.75
1:A:296:LYS:H	1:A:296:LYS:CE	1.99	0.74
1:G:155:ASP:HB3	1:G:158:ALA:HB2	1.70	0.74
1:D:251:ASN:HB2	1:D:252:PRO:HD2	1.68	0.74
1:C:354:TYR:HB3	1:C:359:VAL:CG2	2.18	0.73
1:F:316:SER:OG	1:F:319:GLU:HG3	1.88	0.73
1:B:174:CYS:SG	3:B:691:HOH:O	2.46	0.73
1:F:415:LEU:HD13	1:F:423:MET:HE1	1.71	0.72
1:G:251:ASN:HB2	1:G:252:PRO:HD2	1.71	0.72
1:G:22:GLN:HG3	1:G:287:LEU:HD22	1.70	0.72
1:F:29:LEU:HD13	1:F:283:GLU:HG2	1.73	0.71
1:C:152:PRO:HG3	1:C:166:LEU:HD23	1.73	0.70
1:E:427:ARG:O	1:E:431:THR:HG23	1.91	0.70
1:A:393:ILE:HD12	1:A:413:GLN:HE21	1.57	0.70
1:H:296:LYS:HE3	1:H:300:ASP:OD1	1.90	0.70
1:F:378:LYS:HE3	1:F:382:ALA:HB2	1.74	0.69
1:A:322:GLN:HG3	1:A:329:ARG:HH12	1.57	0.69
1:A:343:LYS:NZ	2:A:501:IHP:O44	2.25	0.68
1:A:393:ILE:CD1	1:A:413:GLN:HE21	2.05	0.68
1:H:387:LEU:HD21	1:H:419:VAL:HG21	1.74	0.68
1:A:52:LYS:HA	1:A:331:LYS:HE3	1.75	0.68
1:B:281:ARG:HD3	2:B:501:IHP:O42	1.93	0.68
1:B:392:LYS:NZ	1:B:396:GLN:OE1	2.26	0.68
1:G:265:LYS:HZ2	1:G:265:LYS:HB2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:389:LYS:NZ	1:F:413:GLN:HB3	2.08	0.67
1:D:358:ASP:O	1:D:361:LYS:HE2	1.92	0.67
1:E:390:ALA:O	1:E:394:VAL:HG12	1.95	0.67
1:H:294:GLU:OE1	1:H:294:GLU:HA	1.93	0.67
1:C:362:LYS:HD2	1:C:368:PHE:O	1.95	0.67
1:B:329:ARG:HB3	1:B:433:VAL:HG22	1.76	0.66
1:H:394:VAL:HA	1:H:397:LEU:HD12	1.75	0.66
1:H:251:ASN:HB2	1:H:252:PRO:HD2	1.77	0.66
1:B:283:GLU:O	1:B:287:LEU:CD2	2.44	0.66
1:E:46:LYS:HG2	1:E:183:LEU:HD22	1.76	0.66
1:F:251:ASN:HB2	1:F:252:PRO:HD2	1.78	0.66
1:A:429:ILE:O	1:A:432:THR:HG23	1.96	0.66
1:B:424:GLU:OE2	1:B:427:ARG:NH1	2.27	0.66
1:A:296:LYS:HE2	1:A:296:LYS:N	2.09	0.65
1:F:390:ALA:CB	1:F:415:LEU:HD21	2.25	0.65
1:E:315:MET:HB3	1:E:319:GLU:HB2	1.78	0.65
1:E:49:ASN:HA	1:E:52:LYS:HE3	1.77	0.64
1:F:389:LYS:NZ	3:F:601:HOH:O	2.30	0.64
1:F:333:PHE:CD1	1:F:337:VAL:HG23	2.32	0.64
1:A:254:GLN:HE22	1:A:360:ILE:HG23	1.62	0.64
1:C:102:ASP:O	1:C:103:ASN:OD1	2.15	0.64
1:F:345:ILE:HG22	1:F:349:LEU:CD1	2.27	0.64
1:E:415:LEU:HD12	1:E:423:MET:HE1	1.80	0.64
1:D:371:ILE:HD12	1:D:371:ILE:O	1.98	0.64
1:D:373:LYS:O	1:D:377:ILE:HD12	1.98	0.64
1:D:349:LEU:O	1:D:353:LYS:HD2	1.97	0.63
1:B:283:GLU:O	1:B:287:LEU:HD23	1.99	0.63
1:F:389:LYS:O	1:F:393:ILE:HG12	1.99	0.63
1:A:384:ILE:O	1:A:388:GLU:HG3	1.99	0.63
1:D:189:LYS:HB2	1:D:189:LYS:NZ	2.12	0.63
1:A:118:LEU:HG	1:A:120:VAL:HG23	1.80	0.63
1:E:401:THR:CG2	1:E:405:GLU:HG2	2.29	0.62
1:F:46:LYS:NZ	2:F:501:IHP:O31	2.32	0.62
1:E:371:ILE:HD12	1:E:376:GLU:HG3	1.79	0.62
1:H:46:LYS:HG2	1:H:183:LEU:HD22	1.80	0.62
1:A:154:ARG:NH1	1:A:161:SER:O	2.32	0.62
1:A:188:LYS:NZ	1:A:217:SER:OG	2.33	0.62
1:D:389:LYS:NZ	1:D:413:GLN:HE22	1.98	0.62
1:B:329:ARG:HB3	1:B:433:VAL:CG2	2.30	0.62
1:C:25:LEU:HD23	1:C:287:LEU:HD23	1.82	0.61
1:F:410:LEU:CA	1:F:413:GLN:HG2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:HD13	1:A:249:GLY:HA2	1.81	0.61
1:F:249:GLY:O	1:F:360:ILE:HD13	2.01	0.61
1:D:389:LYS:HE3	1:D:413:GLN:HE22	1.65	0.60
1:F:334:LYS:HE3	1:F:394:VAL:O	2.00	0.60
1:F:345:ILE:HG22	1:F:349:LEU:HD12	1.82	0.60
1:C:315:MET:HB3	1:C:319:GLU:HB2	1.84	0.60
1:F:53:ARG:NH2	2:F:501:IHP:O45	2.34	0.60
1:A:80:LYS:HE2	1:A:314:GLU:HG3	1.83	0.60
1:C:137:GLU:HG3	1:C:141:ARG:NH1	2.17	0.60
1:E:412:LYS:HD2	1:E:412:LYS:C	2.26	0.60
1:F:390:ALA:HB2	1:F:415:LEU:HD21	1.83	0.59
1:A:393:ILE:O	1:A:397:LEU:HD13	2.03	0.59
1:C:176:ARG:HD3	1:C:176:ARG:N	2.18	0.59
1:A:413:GLN:HA	1:A:413:GLN:OE1	2.01	0.59
1:D:389:LYS:CE	1:D:413:GLN:HE22	2.15	0.59
1:D:390:ALA:HB1	1:D:410:LEU:HD22	1.85	0.59
1:H:412:LYS:HE2	1:H:412:LYS:HA	1.85	0.59
1:C:194:GLU:CD	1:C:194:GLU:H	2.11	0.59
1:F:389:LYS:HZ2	1:F:413:GLN:HB3	1.68	0.59
1:C:344:GLY:O	1:C:348:ARG:HD2	2.03	0.58
1:B:415:LEU:CD1	1:B:423:MET:HE1	2.32	0.58
1:C:402:SER:O	1:C:406:VAL:HG23	2.03	0.58
1:D:331:LYS:HD2	1:D:335:GLU:OE2	2.03	0.58
1:E:46:LYS:HE3	1:E:183:LEU:HD13	1.84	0.58
1:E:394:VAL:HA	1:E:397:LEU:HD13	1.83	0.58
1:E:200:LYS:HE3	1:G:156:PRO:O	2.03	0.58
1:F:408:LEU:HD13	1:F:411:GLN:OE1	2.04	0.57
1:D:382:ALA:O	1:D:386:GLU:HG2	2.05	0.57
1:E:111:PHE:CD2	1:E:118:LEU:HD11	2.39	0.57
1:A:354:TYR:HB3	1:A:359:VAL:HG22	1.83	0.57
1:E:70:GLU:HG2	1:F:303:ASP:OD2	2.05	0.57
1:F:345:ILE:HG23	1:F:384:ILE:HG23	1.86	0.57
1:C:296:LYS:O	1:C:296:LYS:HD3	2.05	0.57
1:G:29:LEU:HD13	1:G:283:GLU:HG2	1.87	0.56
1:D:265:LYS:O	1:D:265:LYS:HG2	2.05	0.56
1:B:266:GLN:HG3	1:E:15:GLU:HB2	1.86	0.56
1:B:188:LYS:NZ	1:B:217:SER:OG	2.39	0.56
1:D:22:GLN:HG3	1:D:287:LEU:CD2	2.35	0.56
1:G:22:GLN:HG3	1:G:287:LEU:CD2	2.35	0.56
1:F:378:LYS:O	1:F:382:ALA:N	2.29	0.55
1:H:376:GLU:OE1	1:H:376:GLU:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:22:GLN:O	1:H:26:GLU:HG3	2.07	0.55
1:C:64:ARG:HD2	1:C:72:ASP:OD2	2.07	0.55
1:C:408:LEU:HD12	1:C:411:GLN:NE2	2.21	0.55
1:A:198:ASN:ND2	1:A:212:ALA:HB2	2.21	0.55
1:A:209:ASN:HB2	1:A:210:PRO:HD2	1.89	0.55
1:A:251:ASN:HB2	1:A:252:PRO:CD	2.37	0.55
1:B:424:GLU:HA	1:B:424:GLU:OE1	2.05	0.55
1:C:323:PHE:HD2	1:C:324:LEU:HD23	1.72	0.55
1:G:251:ASN:OD1	1:G:254:GLN:HG3	2.07	0.55
1:A:420:LYS:O	1:A:424:GLU:HG2	2.06	0.54
1:F:336:ILE:O	1:F:340:ILE:HG13	2.06	0.54
1:A:243:GLN:NE2	3:A:602:HOH:O	2.40	0.54
1:B:80:LYS:NZ	1:B:314:GLU:OE2	2.40	0.54
1:C:263:SER:O	1:C:263:SER:OG	2.08	0.54
1:D:349:LEU:HB3	1:D:353:LYS:CE	2.37	0.54
1:F:386:GLU:O	1:F:389:LYS:HG3	2.07	0.54
1:C:380:ILE:O	1:C:384:ILE:HG13	2.08	0.54
1:D:14:SER:O	1:D:15:GLU:C	2.51	0.54
1:E:401:THR:HG23	1:E:405:GLU:HG2	1.90	0.54
1:F:389:LYS:HE3	3:F:601:HOH:O	2.09	0.53
1:F:404:ASP:O	1:F:408:LEU:HD23	2.07	0.53
1:E:433:VAL:HG23	1:E:433:VAL:O	2.07	0.53
1:H:311:GLU:O	1:H:315:MET:HG3	2.08	0.53
1:E:22:GLN:OE1	1:E:287:LEU:HD23	2.08	0.53
1:F:333:PHE:HD1	1:F:337:VAL:HG23	1.73	0.53
1:F:381:LYS:HE3	1:F:381:LYS:CA	2.38	0.53
1:C:343:LYS:NZ	1:C:347:ASP:OD2	2.42	0.53
1:D:148:TYR:CE2	1:D:206:LYS:HD2	2.44	0.53
1:E:241:ALA:O	1:E:252:PRO:HD2	2.09	0.53
1:B:29:LEU:HD13	1:B:283:GLU:HG2	1.91	0.52
1:D:427:ARG:O	1:D:431:THR:HG23	2.09	0.52
1:C:22:GLN:OE1	1:C:287:LEU:HD22	2.10	0.52
1:F:410:LEU:HA	1:F:413:GLN:HG3	1.88	0.52
1:A:279:ARG:O	1:A:283:GLU:HG3	2.10	0.52
1:F:80:LYS:HE2	1:F:314:GLU:OE2	2.09	0.52
1:F:288:ALA:O	1:F:292:GLU:HG3	2.08	0.52
1:B:283:GLU:O	1:B:287:LEU:HD22	2.09	0.52
1:F:381:LYS:HE3	1:F:381:LYS:HA	1.92	0.52
1:A:118:LEU:HG	1:A:120:VAL:CG2	2.39	0.51
1:C:322:GLN:HG3	1:C:329:ARG:HD3	1.91	0.51
1:F:174:CYS:SG	3:F:650:HOH:O	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:378:LYS:CE	1:F:382:ALA:HB2	2.39	0.51
1:E:22:GLN:OE1	1:E:287:LEU:CD2	2.58	0.51
1:H:334:LYS:HD3	1:H:399:ASN:HA	1.91	0.51
1:C:209:ASN:HB2	1:C:210:PRO:HD2	1.92	0.51
1:D:240:GLU:HA	1:D:243:GLN:OE1	2.11	0.51
1:F:80:LYS:CE	1:F:314:GLU:OE2	2.58	0.51
1:C:427:ARG:O	1:C:431:THR:HG23	2.11	0.51
1:F:306:GLU:HA	1:F:309:TRP:CD1	2.46	0.51
1:F:389:LYS:CE	3:F:601:HOH:O	2.59	0.51
1:F:354:TYR:HB3	1:F:359:VAL:HB	1.91	0.51
1:C:311:GLU:O	1:C:315:MET:HG3	2.11	0.51
1:D:189:LYS:HB2	1:D:189:LYS:HZ3	1.76	0.50
1:F:386:GLU:OE1	1:F:389:LYS:HE2	2.11	0.50
1:D:296:LYS:NZ	3:D:604:HOH:O	2.44	0.50
1:E:343:LYS:NZ	2:E:501:IHP:O44	2.42	0.50
1:F:387:LEU:HD21	1:F:419:VAL:HG11	1.93	0.50
1:A:266:GLN:OE1	1:F:14:SER:N	2.45	0.50
1:H:408:LEU:HA	1:H:411:GLN:HG2	1.94	0.50
1:H:296:LYS:HE3	1:H:300:ASP:CG	2.37	0.50
1:E:294:GLU:OE1	1:E:297:HIS:N	2.43	0.50
1:H:33:ARG:NH2	1:H:104:HIS:HB2	2.27	0.50
1:F:322:GLN:OE1	1:F:329:ARG:NH1	2.45	0.49
1:A:251:ASN:HB2	1:A:252:PRO:HD2	1.93	0.49
1:A:432:THR:C	3:A:631:HOH:O	2.55	0.49
1:F:318:SER:O	1:F:322:GLN:HG2	2.12	0.49
1:B:25:LEU:HD23	1:B:287:LEU:HD13	1.94	0.49
1:E:401:THR:HG22	1:E:405:GLU:HB3	1.94	0.49
1:D:24:TRP:O	1:D:27:GLN:HG3	2.13	0.49
1:H:152:PRO:HG3	1:H:166:LEU:HD23	1.95	0.49
1:H:71:GLU:OE1	1:H:76:LYS:HD2	2.12	0.49
1:C:65:PRO:HD3	1:C:72:ASP:HA	1.94	0.49
1:E:304:ASN:HA	1:E:307:LYS:HE2	1.95	0.49
1:E:389:LYS:O	1:E:393:ILE:HG13	2.12	0.49
1:F:389:LYS:HZ1	1:F:413:GLN:HB3	1.78	0.49
1:G:315:MET:HB3	1:G:319:GLU:HB2	1.95	0.49
1:H:408:LEU:HA	1:H:411:GLN:CG	2.43	0.49
1:H:169:THR:HG21	1:H:226:ILE:HD12	1.95	0.49
1:A:80:LYS:CE	1:A:314:GLU:HG3	2.42	0.48
1:C:25:LEU:HD22	1:C:290:LEU:HD22	1.95	0.48
1:E:277:TYR:CZ	1:E:281:ARG:HG3	2.48	0.48
1:E:390:ALA:HB2	1:E:415:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:GLU:O	1:F:389:LYS:HE3	2.13	0.48
1:D:80:LYS:HD3	1:D:313:LEU:HB2	1.96	0.48
1:H:179:ILE:O	1:H:183:LEU:HG	2.14	0.48
1:C:80:LYS:HE2	1:C:314:GLU:HG3	1.95	0.48
1:C:137:GLU:HG3	1:C:141:ARG:HH12	1.78	0.48
1:F:392:LYS:HE3	1:F:392:LYS:CA	2.42	0.48
1:H:329:ARG:HH22	1:H:432:THR:C	2.22	0.48
1:C:22:GLN:OE1	1:C:287:LEU:CD2	2.62	0.48
1:C:209:ASN:HB2	1:C:210:PRO:CD	2.43	0.48
1:D:279:ARG:O	1:D:283:GLU:HG3	2.13	0.48
1:D:397:LEU:HD21	1:D:409:HIS:CD2	2.49	0.48
1:F:380:ILE:O	1:F:384:ILE:HG13	2.13	0.48
1:F:415:LEU:HG	3:F:601:HOH:O	2.13	0.48
1:G:111:PHE:CD2	1:G:118:LEU:HD11	2.49	0.48
1:F:345:ILE:HG23	1:F:384:ILE:CG2	2.44	0.48
1:A:315:MET:HB3	1:A:319:GLU:HB2	1.95	0.47
1:E:412:LYS:HE3	1:E:413:GLN:OE1	2.14	0.47
1:C:83:ASN:N	1:C:83:ASN:HD22	2.12	0.47
1:E:398:SER:O	1:E:401:THR:OG1	2.27	0.47
1:H:171:ARG:HA	1:H:171:ARG:HD3	1.68	0.47
1:A:248:LYS:NZ	2:A:501:IHP:O13	2.48	0.47
1:C:279:ARG:O	1:C:283:GLU:HG3	2.14	0.47
1:D:65:PRO:HD2	3:D:640:HOH:O	2.15	0.47
1:E:378:LYS:HA	1:E:378:LYS:HD3	1.66	0.47
1:G:235:ILE:HD11	1:G:365:PHE:HD1	1.80	0.47
1:A:142:PHE:O	1:A:145:CYS:HB3	2.15	0.47
1:F:392:LYS:HE3	1:F:392:LYS:O	2.15	0.47
1:A:176:ARG:NE	1:A:279:ARG:HG3	2.30	0.47
1:A:334:LYS:HE3	1:A:394:VAL:O	2.14	0.47
1:D:170:ASP:OD1	1:D:170:ASP:C	2.57	0.47
1:F:410:LEU:C	1:F:413:GLN:HG2	2.40	0.47
1:G:424:GLU:OE2	1:G:427:ARG:NH2	2.48	0.47
1:E:84:ASN:ND2	1:E:87:ASP:HB3	2.30	0.47
1:H:380:ILE:O	1:H:384:ILE:HG13	2.14	0.47
1:D:71:GLU:CD	1:D:76:LYS:HD3	2.40	0.47
1:A:390:ALA:HB2	1:A:415:LEU:HD21	1.97	0.47
1:F:334:LYS:HD3	1:F:334:LYS:O	2.15	0.47
1:D:199:TYR:CE2	1:D:206:LYS:HD3	2.50	0.46
1:A:71:GLU:CD	1:A:76:LYS:HE3	2.40	0.46
1:C:358:ASP:O	1:C:361:LYS:HD3	2.16	0.46
1:C:415:LEU:HD12	1:C:423:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:GLU:OE1	1:D:366:THR:HG23	2.14	0.46
1:G:311:GLU:O	1:G:315:MET:HG3	2.15	0.46
1:C:266:GLN:HE21	1:C:266:GLN:HB2	1.29	0.46
1:C:276:ASP:O	1:C:280:GLN:HG3	2.15	0.46
1:F:379:LYS:HD3	1:F:383:GLU:OE2	2.15	0.46
1:G:281:ARG:HD3	2:G:501:IHP:O42	2.15	0.46
1:H:315:MET:HB3	1:H:319:GLU:HB2	1.97	0.46
1:D:371:ILE:HD12	1:D:371:ILE:C	2.41	0.46
1:F:419:VAL:HG12	1:F:423:MET:CE	2.44	0.46
1:E:176:ARG:HD3	1:E:176:ARG:N	2.30	0.46
1:G:427:ARG:O	1:G:431:THR:HG23	2.16	0.46
1:H:142:PHE:O	1:H:145:CYS:HB3	2.15	0.46
1:H:296:LYS:HD2	1:H:296:LYS:O	2.16	0.46
1:A:18:GLU:O	1:A:22:GLN:HG2	2.16	0.46
1:B:111:PHE:CD2	1:B:118:LEU:HD11	2.51	0.46
1:B:176:ARG:HD3	1:B:279:ARG:HG3	1.98	0.46
1:A:420:LYS:HD3	1:A:423:MET:HE3	1.98	0.45
1:B:424:GLU:OE1	1:B:427:ARG:NH2	2.49	0.45
1:D:389:LYS:HE3	1:D:413:GLN:NE2	2.31	0.45
1:F:350:ASP:HA	1:F:353:LYS:HE3	1.98	0.45
1:G:390:ALA:HB1	1:G:410:LEU:HD22	1.98	0.45
1:G:392:LYS:O	1:G:396:GLN:HG3	2.17	0.45
1:A:413:GLN:OE1	1:A:413:GLN:CA	2.63	0.45
1:F:170:ASP:OD1	1:F:170:ASP:C	2.59	0.45
1:F:393:ILE:O	1:F:397:LEU:HG	2.16	0.45
1:C:282:VAL:O	1:C:286:LEU:HG	2.16	0.45
1:G:372:ASP:N	3:G:602:HOH:O	2.50	0.45
1:E:179:ILE:O	1:E:183:LEU:HG	2.16	0.45
1:G:152:PRO:HG3	1:G:166:LEU:HD23	1.98	0.45
1:C:418:ALA:O	1:C:422:GLU:HG3	2.16	0.45
1:E:307:LYS:HD3	1:E:307:LYS:N	2.31	0.45
1:E:316:SER:OG	1:E:319:GLU:HG3	2.16	0.45
1:A:322:GLN:CG	1:A:329:ARG:HH22	2.29	0.45
1:C:132:ASP:OD2	1:G:162:LYS:NZ	2.39	0.45
1:C:170:ASP:OD1	1:C:170:ASP:C	2.60	0.45
1:D:408:LEU:O	1:D:409:HIS:C	2.59	0.45
1:E:46:LYS:HE3	1:E:183:LEU:CD1	2.46	0.45
1:H:418:ALA:O	1:H:422:GLU:HG3	2.17	0.45
1:B:143:PRO:O	1:B:144:ASP:HB2	2.17	0.45
1:E:429:ILE:O	1:E:432:THR:OG1	2.35	0.45
1:F:412:LYS:HD3	1:F:412:LYS:HA	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:ILE:HD11	1:G:365:PHE:CD1	2.52	0.45
1:A:358:ASP:OD1	1:A:373:LYS:HD2	2.17	0.44
1:C:23:LYS:HE2	1:H:66:GLN:OE1	2.16	0.44
1:C:239:LYS:HA	1:C:239:LYS:HD3	1.65	0.44
1:G:254:GLN:HE22	1:G:360:ILE:HG23	1.82	0.44
1:A:170:ASP:OD1	1:A:170:ASP:C	2.60	0.44
1:A:254:GLN:NE2	1:A:360:ILE:HG23	2.31	0.44
1:H:59:CYS:SG	1:H:182:ILE:HD13	2.57	0.44
1:F:391:LEU:O	1:F:394:VAL:HG22	2.17	0.44
1:G:76:LYS:HG2	1:G:309:TRP:HH2	1.82	0.44
1:A:393:ILE:CD1	1:A:413:GLN:NE2	2.77	0.44
1:F:345:ILE:HG22	1:F:349:LEU:HD11	1.99	0.44
1:F:59:CYS:SG	1:F:182:ILE:HD13	2.58	0.44
1:F:420:LYS:HA	1:F:423:MET:HE3	1.98	0.44
1:G:170:ASP:C	1:G:170:ASP:OD1	2.61	0.44
1:H:334:LYS:HD3	1:H:399:ASN:OD1	2.18	0.44
1:A:303:ASP:OD2	1:B:70:GLU:HG2	2.18	0.44
1:D:22:GLN:HG3	1:D:287:LEU:HD22	2.00	0.44
1:D:276:ASP:O	1:D:280:GLN:HG3	2.18	0.44
1:F:333:PHE:CD2	1:F:403:ALA:CB	3.01	0.44
1:B:152:PRO:HG3	1:B:166:LEU:HD23	2.00	0.44
1:D:350:ASP:HA	1:D:353:LYS:HD2	2.00	0.44
1:G:187:LYS:HE2	2:G:501:IHP:O25	2.17	0.44
1:A:23:LYS:HE3	1:A:27:GLN:NE2	2.33	0.43
1:A:300:ASP:OD1	1:A:304:ASN:ND2	2.50	0.43
1:B:176:ARG:CD	1:B:279:ARG:HG3	2.48	0.43
1:E:103:ASN:HB3	1:E:105:HIS:CB	2.48	0.43
1:E:117:LYS:NZ	1:E:144:ASP:O	2.51	0.43
1:H:132:ASP:OD1	1:H:132:ASP:N	2.50	0.43
1:G:390:ALA:HA	1:G:393:ILE:HD12	2.01	0.43
1:A:241:ALA:O	1:A:252:PRO:HD2	2.18	0.43
1:D:415:LEU:HD12	1:D:423:MET:HE1	1.99	0.43
1:G:209:ASN:HB2	1:G:210:PRO:CD	2.48	0.43
1:B:169:THR:HG21	1:B:226:ILE:HD12	2.00	0.43
1:D:390:ALA:HB2	1:D:415:LEU:HD21	2.00	0.43
1:G:168:GLN:HB2	1:G:177:MET:HE3	2.00	0.43
1:C:265:LYS:O	1:C:266:GLN:C	2.62	0.43
1:E:103:ASN:HB3	1:E:105:HIS:HB2	2.01	0.43
1:A:393:ILE:HD11	1:A:413:GLN:NE2	2.34	0.43
1:B:46:LYS:HD2	1:B:46:LYS:HA	1.80	0.43
1:F:376:GLU:O	1:F:380:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LYS:NZ	2:C:501:IHP:O31	2.50	0.43
1:G:413:GLN:HA	1:G:413:GLN:NE2	2.34	0.43
1:G:394:VAL:HA	1:G:397:LEU:HD12	2.01	0.42
1:D:351:HIS:O	1:D:355:ILE:HG13	2.19	0.42
1:E:271:LYS:HE3	1:E:271:LYS:HB3	1.80	0.42
1:F:46:LYS:HA	1:F:46:LYS:HD2	1.71	0.42
1:H:251:ASN:HB2	1:H:252:PRO:CD	2.49	0.42
1:H:390:ALA:HB2	1:H:415:LEU:HD21	2.01	0.42
1:A:64:ARG:HD3	1:A:74:TYR:HB3	2.01	0.42
1:E:397:LEU:N	1:E:397:LEU:HD12	2.35	0.42
1:C:162:LYS:HD3	1:G:129:SER:HB3	2.01	0.42
1:E:170:ASP:C	1:E:170:ASP:OD1	2.62	0.42
1:E:251:ASN:HB2	1:E:252:PRO:CD	2.49	0.42
1:A:420:LYS:HA	1:A:423:MET:HE3	2.00	0.42
1:D:98:LEU:O	1:D:106:TRP:HA	2.19	0.42
1:D:362:LYS:HB2	1:D:362:LYS:HE2	1.97	0.42
1:E:311:GLU:O	1:E:315:MET:HG3	2.19	0.42
1:F:416:PRO:HG2	1:F:419:VAL:CG2	2.49	0.42
1:E:352:LYS:HE2	1:E:356:GLU:OE2	2.19	0.42
1:D:27:GLN:O	1:D:30:ASN:HB2	2.20	0.42
1:D:254:GLN:HE22	1:D:360:ILE:HG23	1.84	0.42
1:F:333:PHE:CD2	1:F:403:ALA:HB2	2.54	0.42
1:A:278:LYS:O	1:A:282:VAL:HG23	2.20	0.42
1:A:420:LYS:HD3	1:A:420:LYS:HA	1.92	0.42
1:B:266:GLN:HB2	1:E:14:SER:OG	2.20	0.42
1:C:251:ASN:HB2	1:C:252:PRO:CD	2.49	0.42
1:C:405:GLU:OE1	1:C:408:LEU:HD22	2.20	0.42
1:E:153:ASP:OD1	1:E:165:ARG:HD3	2.19	0.42
1:H:265:LYS:HD2	1:H:265:LYS:HA	1.77	0.42
1:D:377:ILE:O	1:D:381:LYS:HG3	2.20	0.42
1:G:226:ILE:HB	1:G:229:ILE:HD12	2.01	0.42
1:G:355:ILE:CD1	1:G:380:ILE:HD12	2.50	0.42
1:B:152:PRO:HG3	1:B:166:LEU:CD2	2.50	0.41
1:C:303:ASP:OD2	1:H:70:GLU:HG2	2.20	0.41
1:H:215:ARG:HA	1:H:240:GLU:HG2	2.02	0.41
1:E:25:LEU:HD23	1:E:287:LEU:HD23	2.02	0.41
1:E:397:LEU:HD23	1:E:401:THR:HG21	2.03	0.41
1:F:410:LEU:HD23	1:F:413:GLN:HG3	2.02	0.41
1:H:91:THR:HG22	1:H:114:VAL:HG22	2.00	0.41
1:C:152:PRO:HG3	1:C:166:LEU:CD2	2.45	0.41
1:D:230:LEU:HG	1:D:234:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:HG21	1:A:226:ILE:HD12	2.03	0.41
1:C:27:GLN:O	1:C:30:ASN:HB2	2.20	0.41
1:C:159:LYS:HA	1:C:159:LYS:HD3	1.71	0.41
1:D:386:GLU:OE1	1:D:386:GLU:HA	2.21	0.41
1:D:251:ASN:HB2	1:D:252:PRO:CD	2.46	0.41
1:A:376:GLU:HA	1:A:376:GLU:OE1	2.20	0.41
1:C:429:ILE:O	1:C:432:THR:OG1	2.37	0.41
1:D:142:PHE:O	1:D:145:CYS:HB3	2.19	0.41
1:G:71:GLU:OE1	1:G:76:LYS:HD2	2.21	0.41
1:H:187:LYS:HE2	2:H:501:IHP:O35	2.20	0.41
1:C:251:ASN:OD1	1:C:251:ASN:C	2.63	0.41
1:C:296:LYS:HE3	1:C:300:ASP:OD1	2.21	0.41
1:E:294:GLU:H	1:E:294:GLU:CD	2.28	0.41
1:B:42:ALA:HA	1:B:286:LEU:HD21	2.03	0.41
1:B:176:ARG:HD2	1:B:279:ARG:HB2	2.03	0.41
1:B:251:ASN:OD1	1:B:251:ASN:C	2.64	0.41
1:C:255:TYR:CZ	1:C:259:LEU:HD12	2.55	0.41
1:D:247:LYS:HG3	2:D:501:IHP:P4	2.61	0.41
1:D:349:LEU:O	1:D:353:LYS:CD	2.68	0.41
1:F:346:LYS:NZ	1:F:347:ASP:OD1	2.51	0.41
1:G:376:GLU:O	1:G:380:ILE:HG13	2.21	0.41
1:C:64:ARG:HD3	1:C:74:TYR:HB3	2.03	0.41
1:C:83:ASN:N	1:C:83:ASN:ND2	2.68	0.41
1:E:334:LYS:HD3	1:E:399:ASN:HA	2.03	0.41
1:F:331:LYS:HE3	1:F:331:LYS:HB2	1.83	0.41
1:D:390:ALA:CB	1:D:415:LEU:HD21	2.51	0.40
1:E:391:LEU:HA	1:E:394:VAL:CG1	2.51	0.40
1:F:261:HIS:CD2	1:F:268:LYS:HE2	2.56	0.40
1:H:152:PRO:HG3	1:H:166:LEU:CD2	2.51	0.40
1:E:405:GLU:HG3	1:E:409:HIS:HE1	1.86	0.40
1:F:410:LEU:CA	1:F:413:GLN:CG	2.93	0.40
1:H:191:LEU:HD23	1:H:191:LEU:HA	1.92	0.40
1:E:176:ARG:HG2	1:E:279:ARG:HB2	2.03	0.40
1:F:265:LYS:NZ	1:F:265:LYS:HB3	2.35	0.40
1:B:239:LYS:HD3	1:B:239:LYS:C	2.47	0.40
1:B:362:LYS:HE3	1:B:362:LYS:HB2	1.82	0.40
1:C:215:ARG:NH1	1:C:237:SER:OG	2.54	0.40
1:C:296:LYS:HD3	1:C:296:LYS:C	2.46	0.40
1:E:415:LEU:CD1	1:E:423:MET:HE1	2.49	0.40
2:A:501:IHP:O43	2:A:501:IHP:O24	2.40	0.40
1:B:394:VAL:HG23	1:B:410:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:ARG:HB3	1:G:229:ILE:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/451 (88%)	394 (99%)	5 (1%)	0	100	100
1	B	411/451 (91%)	408 (99%)	3 (1%)	0	100	100
1	C	413/451 (92%)	410 (99%)	3 (1%)	0	100	100
1	D	407/451 (90%)	398 (98%)	9 (2%)	0	100	100
1	E	408/451 (90%)	405 (99%)	3 (1%)	0	100	100
1	F	406/451 (90%)	403 (99%)	3 (1%)	0	100	100
1	G	410/451 (91%)	406 (99%)	4 (1%)	0	100	100
1	H	403/451 (89%)	399 (99%)	4 (1%)	0	100	100
All	All	3257/3608 (90%)	3223 (99%)	34 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/408 (90%)	367 (100%)	0	100	100
1	B	376/408 (92%)	376 (100%)	0	100	100
1	C	378/408 (93%)	378 (100%)	0	100	100
1	D	374/408 (92%)	374 (100%)	0	100	100
1	E	373/408 (91%)	373 (100%)	0	100	100
1	F	370/408 (91%)	370 (100%)	0	100	100
1	G	375/408 (92%)	375 (100%)	0	100	100
1	H	368/408 (90%)	367 (100%)	1 (0%)	86	90
All	All	2981/3264 (91%)	2980 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	378	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	203	ASN
1	A	243	GLN
1	A	266	GLN
1	B	51	ASN
1	B	95	GLN
1	B	351	HIS
1	B	385	ASN
1	C	83	ASN
1	C	203	ASN
1	C	266	GLN
1	C	304	ASN
1	C	409	HIS
1	D	203	ASN
1	D	322	GLN
1	D	351	HIS
1	D	409	HIS
1	D	413	GLN
1	E	84	ASN
1	E	203	ASN
1	E	209	ASN

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Mol	Chain	Res	Type
1	E	242	GLN
1	E	385	ASN
1	F	22	GLN
1	F	83	ASN
1	F	84	ASN
1	F	195	ASN
1	G	58	ASN
1	G	66	GLN
1	G	104	HIS
1	G	243	GLN
1	G	266	GLN
1	G	351	HIS
1	G	399	ASN
1	G	409	HIS
1	H	84	ASN
1	H	195	ASN
1	H	385	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](#)

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
2	IHP	C	501	-	36,36,36	2.00	10 (27%)	60,60,60	3.13	13 (21%)
2	IHP	E	501	-	36,36,36	1.53	7 (19%)	60,60,60	3.34	18 (30%)
2	IHP	A	501	-	36,36,36	1.75	9 (25%)	60,60,60	3.84	21 (35%)
2	IHP	D	501	-	36,36,36	1.89	9 (25%)	60,60,60	3.31	18 (30%)
2	IHP	G	501	-	36,36,36	1.76	8 (22%)	60,60,60	4.29	14 (23%)
2	IHP	H	501	-	36,36,36	1.96	10 (27%)	60,60,60	2.59	20 (33%)
2	IHP	F	501	-	36,36,36	1.64	7 (19%)	60,60,60	4.53	17 (28%)
2	IHP	B	501	-	36,36,36	2.03	7 (19%)	60,60,60	3.52	15 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IHP	C	501	-	-	6/30/54/54	0/1/1/1
2	IHP	E	501	-	-	7/30/54/54	0/1/1/1
2	IHP	A	501	-	-	5/30/54/54	0/1/1/1
2	IHP	D	501	-	-	7/30/54/54	0/1/1/1
2	IHP	G	501	-	-	9/30/54/54	0/1/1/1
2	IHP	H	501	-	-	4/30/54/54	0/1/1/1
2	IHP	F	501	-	-	4/30/54/54	0/1/1/1
2	IHP	B	501	-	-	7/30/54/54	0/1/1/1

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	IHP	C6-C5	5.96	1.64	1.52
2	B	501	IHP	P2-O12	5.86	1.69	1.59
2	H	501	IHP	C6-C5	5.30	1.63	1.52
2	D	501	IHP	C6-C5	5.25	1.63	1.52
2	B	501	IHP	P3-O13	5.16	1.68	1.59
2	B	501	IHP	P5-O15	4.70	1.67	1.59
2	D	501	IHP	P5-O15	4.60	1.67	1.59
2	C	501	IHP	P3-O13	4.56	1.67	1.59
2	H	501	IHP	P2-O12	4.56	1.67	1.59
2	F	501	IHP	P1-O11	4.35	1.67	1.59
2	B	501	IHP	C3-C2	4.34	1.61	1.52
2	H	501	IHP	P1-O11	4.16	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	IHP	P5-O15	4.16	1.66	1.59
2	C	501	IHP	C4-C3	4.10	1.60	1.52
2	C	501	IHP	P1-O11	4.03	1.66	1.59
2	C	501	IHP	P2-O12	4.00	1.66	1.59
2	C	501	IHP	C5-C4	3.90	1.60	1.52
2	A	501	IHP	P1-O11	3.82	1.66	1.59
2	E	501	IHP	P2-O12	3.81	1.66	1.59
2	D	501	IHP	P1-O11	3.78	1.66	1.59
2	A	501	IHP	C3-C2	3.71	1.59	1.52
2	A	501	IHP	P3-O13	3.64	1.65	1.59
2	H	501	IHP	O14-C4	-3.62	1.31	1.44
2	E	501	IHP	P3-O13	3.61	1.65	1.59
2	G	501	IHP	P6-O16	3.60	1.65	1.59
2	D	501	IHP	P2-O12	3.58	1.65	1.59
2	B	501	IHP	P1-O11	3.38	1.65	1.59
2	A	501	IHP	P5-O15	3.37	1.65	1.59
2	F	501	IHP	O15-C5	-3.35	1.32	1.44
2	A	501	IHP	P2-O12	3.31	1.65	1.59
2	E	501	IHP	C6-C5	3.30	1.59	1.52
2	H	501	IHP	P3-O13	3.29	1.65	1.59
2	F	501	IHP	P6-O16	3.27	1.65	1.59
2	A	501	IHP	P6-O16	3.14	1.65	1.59
2	G	501	IHP	P1-O11	3.14	1.65	1.59
2	E	501	IHP	P1-O11	3.06	1.64	1.59
2	H	501	IHP	C3-C2	3.02	1.58	1.52
2	G	501	IHP	P5-O15	3.02	1.64	1.59
2	F	501	IHP	C5-C4	-3.02	1.46	1.52
2	D	501	IHP	P3-O13	3.01	1.64	1.59
2	F	501	IHP	C3-C2	-2.92	1.46	1.52
2	D	501	IHP	C4-C3	2.88	1.58	1.52
2	G	501	IHP	P3-O13	2.82	1.64	1.59
2	C	501	IHP	P6-O16	2.70	1.64	1.59
2	C	501	IHP	C6-C1	-2.66	1.46	1.52
2	H	501	IHP	P5-O15	2.61	1.64	1.59
2	G	501	IHP	P4-O14	2.49	1.63	1.59
2	D	501	IHP	O14-C4	-2.49	1.35	1.44
2	G	501	IHP	P2-O12	2.48	1.63	1.59
2	G	501	IHP	O13-C3	-2.39	1.35	1.44
2	E	501	IHP	O14-C4	-2.36	1.36	1.44
2	A	501	IHP	C6-C1	2.35	1.57	1.52
2	H	501	IHP	P4-O14	2.34	1.63	1.59
2	D	501	IHP	C5-C4	2.33	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	IHP	P6-O16	2.30	1.63	1.59
2	H	501	IHP	P6-O16	2.27	1.63	1.59
2	C	501	IHP	C3-C2	2.26	1.56	1.52
2	A	501	IHP	P4-O14	2.24	1.63	1.59
2	E	501	IHP	O13-C3	-2.20	1.36	1.44
2	F	501	IHP	P2-O12	2.19	1.63	1.59
2	C	501	IHP	O16-C6	-2.17	1.36	1.44
2	H	501	IHP	C5-C4	-2.17	1.47	1.52
2	B	501	IHP	C4-C3	2.15	1.56	1.52
2	B	501	IHP	P6-O16	2.10	1.63	1.59
2	A	501	IHP	C5-C4	-2.07	1.48	1.52
2	F	501	IHP	O13-C3	-2.05	1.37	1.44
2	E	501	IHP	P5-O15	2.02	1.63	1.59

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	IHP	O14-C4-C3	23.29	158.31	108.76
2	B	501	IHP	O14-C4-C5	19.84	150.97	108.76
2	A	501	IHP	O15-C5-C4	18.44	147.98	108.76
2	C	501	IHP	O14-C4-C5	18.05	147.16	108.76
2	F	501	IHP	O14-C4-C3	17.72	146.46	108.76
2	E	501	IHP	O14-C4-C5	17.71	146.43	108.76
2	D	501	IHP	O14-C4-C5	17.39	145.75	108.76
2	F	501	IHP	O13-C3-C2	13.92	138.38	108.76
2	A	501	IHP	C5-C4-C3	13.41	139.85	110.43
2	F	501	IHP	P3-O13-C3	12.98	158.11	123.43
2	F	501	IHP	O15-C5-C4	11.71	133.68	108.76
2	G	501	IHP	O15-C5-C4	11.62	133.48	108.76
2	H	501	IHP	O14-C4-C5	10.69	131.50	108.76
2	G	501	IHP	O15-C5-C6	-10.33	86.79	108.76
2	B	501	IHP	O13-C3-C4	8.94	127.77	108.76
2	F	501	IHP	O13-C3-C4	-8.79	90.05	108.76
2	F	501	IHP	C4-C3-C2	8.76	129.65	110.43
2	A	501	IHP	O13-C3-C4	8.66	127.17	108.76
2	F	501	IHP	P5-O15-C5	8.55	146.27	123.43
2	G	501	IHP	P5-O15-C5	8.49	146.11	123.43
2	E	501	IHP	O15-C5-C4	7.98	125.74	108.76
2	C	501	IHP	O16-C6-C5	-7.77	92.24	108.76
2	D	501	IHP	O16-C6-C5	-7.54	92.71	108.76
2	G	501	IHP	O12-C2-C3	-7.00	93.86	108.76
2	D	501	IHP	C4-C3-C2	6.94	125.66	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	IHP	P5-O15-C5	-6.85	105.15	123.43
2	A	501	IHP	P4-O14-C4	6.73	141.41	123.43
2	E	501	IHP	O13-C3-C4	6.72	123.05	108.76
2	A	501	IHP	P3-O13-C3	-6.71	105.51	123.43
2	H	501	IHP	O13-C3-C4	6.68	122.97	108.76
2	B	501	IHP	O16-C6-C5	-6.59	94.75	108.76
2	E	501	IHP	C6-C5-C4	6.48	124.64	110.43
2	C	501	IHP	O13-C3-C4	6.26	122.08	108.76
2	D	501	IHP	O15-C5-C4	5.96	121.44	108.76
2	C	501	IHP	C4-C3-C2	5.93	123.43	110.43
2	A	501	IHP	C4-C3-C2	-5.92	97.45	110.43
2	G	501	IHP	C6-C5-C4	5.89	123.35	110.43
2	B	501	IHP	C6-C5-C4	5.79	123.14	110.43
2	E	501	IHP	O16-C6-C5	-5.78	96.46	108.76
2	E	501	IHP	C4-C3-C2	5.58	122.67	110.43
2	F	501	IHP	C6-C5-C4	5.49	122.47	110.43
2	F	501	IHP	O12-C2-C3	-5.48	97.11	108.76
2	F	501	IHP	O12-C2-C1	5.42	120.29	108.76
2	G	501	IHP	O14-C4-C5	-5.38	97.31	108.76
2	H	501	IHP	C3-C2-C1	5.24	121.93	110.43
2	B	501	IHP	P4-O14-C4	5.17	137.25	123.43
2	D	501	IHP	O14-P4-O24	-5.11	91.11	109.33
2	B	501	IHP	O14-C4-C3	-5.04	98.05	108.76
2	B	501	IHP	O13-C3-C2	-5.01	98.10	108.76
2	B	501	IHP	C4-C3-C2	4.87	121.11	110.43
2	G	501	IHP	C3-C2-C1	4.74	120.83	110.43
2	H	501	IHP	O14-C4-C3	-4.64	98.88	108.76
2	G	501	IHP	O13-C3-C2	4.49	118.30	108.76
2	H	501	IHP	O15-C5-C6	-4.46	99.27	108.76
2	H	501	IHP	C6-C5-C4	4.37	120.00	110.43
2	D	501	IHP	C6-C1-C2	-4.34	100.91	110.43
2	F	501	IHP	O16-C6-C1	-4.24	99.74	108.76
2	H	501	IHP	O16-C6-C5	-4.24	99.75	108.76
2	H	501	IHP	O15-C5-C4	4.20	117.70	108.76
2	C	501	IHP	P5-O15-C5	-4.16	112.32	123.43
2	F	501	IHP	O15-C5-C6	-4.04	100.17	108.76
2	E	501	IHP	O15-C5-C6	-4.03	100.20	108.76
2	E	501	IHP	O14-P4-O24	-3.91	95.41	109.33
2	A	501	IHP	O35-P5-O15	3.89	121.02	105.85
2	B	501	IHP	O15-C5-C6	3.86	116.96	108.76
2	D	501	IHP	O11-C1-C2	3.77	116.78	108.76
2	G	501	IHP	C5-C6-C1	-3.73	102.25	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	IHP	O12-C2-C3	-3.73	100.84	108.76
2	D	501	IHP	O13-C3-C4	3.64	116.49	108.76
2	A	501	IHP	C3-C2-C1	3.62	118.38	110.43
2	A	501	IHP	O33-P3-O13	3.54	119.66	105.85
2	C	501	IHP	P4-O14-C4	3.41	132.53	123.43
2	H	501	IHP	O12-C2-C1	-3.40	101.53	108.76
2	H	501	IHP	O11-C1-C2	3.38	115.95	108.76
2	A	501	IHP	O13-P3-O23	-3.38	97.29	109.33
2	E	501	IHP	C3-C2-C1	3.36	117.79	110.43
2	D	501	IHP	O35-P5-O15	3.36	118.93	105.85
2	G	501	IHP	C4-C3-C2	3.34	117.76	110.43
2	C	501	IHP	O13-C3-C2	-3.29	101.75	108.76
2	A	501	IHP	O13-C3-C2	-3.21	101.93	108.76
2	E	501	IHP	C6-C1-C2	-3.20	103.40	110.43
2	A	501	IHP	O11-C1-C2	3.19	115.54	108.76
2	E	501	IHP	O33-P3-O13	3.15	118.12	105.85
2	F	501	IHP	P2-O12-C2	-3.00	115.41	123.43
2	C	501	IHP	O14-C4-C3	-2.98	102.41	108.76
2	H	501	IHP	O33-P3-O13	2.96	117.37	105.85
2	H	501	IHP	C6-C1-C2	-2.93	104.00	110.43
2	G	501	IHP	C5-C4-C3	-2.92	104.02	110.43
2	E	501	IHP	P4-O14-C4	2.91	131.21	123.43
2	C	501	IHP	C5-C6-C1	2.86	116.70	110.43
2	A	501	IHP	P5-O15-C5	-2.83	115.88	123.43
2	B	501	IHP	O14-P4-O24	-2.80	99.34	109.33
2	A	501	IHP	P1-O11-C1	-2.77	116.04	123.43
2	A	501	IHP	O41-P1-O11	2.75	116.58	105.85
2	E	501	IHP	O12-C2-C1	-2.73	102.95	108.76
2	H	501	IHP	O11-C1-C6	-2.71	102.99	108.76
2	C	501	IHP	O14-P4-O24	-2.68	99.77	109.33
2	F	501	IHP	O13-P3-O23	2.67	118.86	109.33
2	A	501	IHP	O15-C5-C6	-2.64	103.14	108.76
2	F	501	IHP	O45-P5-O15	2.64	116.14	105.85
2	D	501	IHP	P1-O11-C1	-2.63	116.41	123.43
2	B	501	IHP	O15-C5-C4	-2.61	103.21	108.76
2	D	501	IHP	O11-P1-O21	-2.61	100.04	109.33
2	H	501	IHP	P3-O13-C3	-2.60	116.49	123.43
2	D	501	IHP	O41-P1-O11	2.59	115.95	105.85
2	F	501	IHP	O44-P4-O14	2.57	115.88	105.85
2	A	501	IHP	O11-P1-O21	-2.55	100.24	109.33
2	H	501	IHP	C5-C6-C1	-2.55	104.84	110.43
2	D	501	IHP	P4-O14-C4	2.54	130.21	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	IHP	O12-C2-C1	-2.47	103.51	108.76
2	E	501	IHP	O11-C1-C6	-2.46	103.53	108.76
2	E	501	IHP	P1-O11-C1	-2.45	116.88	123.43
2	A	501	IHP	C5-C6-C1	2.45	115.80	110.43
2	D	501	IHP	O33-P3-O13	2.45	115.38	105.85
2	H	501	IHP	O13-C3-C2	-2.42	103.61	108.76
2	A	501	IHP	P6-O16-C6	-2.41	117.00	123.43
2	B	501	IHP	O11-C1-C2	2.39	113.85	108.76
2	C	501	IHP	O35-P5-O15	2.39	115.16	105.85
2	D	501	IHP	O13-C3-C2	-2.37	103.72	108.76
2	E	501	IHP	O13-C3-C2	-2.35	103.76	108.76
2	F	501	IHP	O14-C4-C5	-2.32	103.82	108.76
2	D	501	IHP	O44-P4-O14	2.30	114.82	105.85
2	H	501	IHP	O12-C2-C3	2.29	113.64	108.76
2	G	501	IHP	O33-P3-O13	2.28	114.73	105.85
2	G	501	IHP	C6-C1-C2	-2.22	105.56	110.43
2	B	501	IHP	O33-P3-O13	2.22	114.48	105.85
2	H	501	IHP	O16-C6-C1	2.16	113.36	108.76
2	H	501	IHP	O35-P5-O15	2.14	114.17	105.85
2	C	501	IHP	C6-C1-C2	-2.12	105.77	110.43
2	E	501	IHP	O11-C1-C2	2.12	113.27	108.76
2	H	501	IHP	P1-O11-C1	-2.09	117.86	123.43
2	B	501	IHP	P3-O13-C3	-2.05	117.97	123.43
2	E	501	IHP	O44-P4-O34	2.02	115.37	107.80
2	C	501	IHP	O42-P2-O32	2.02	115.37	107.80
2	B	501	IHP	O16-C6-C1	2.02	113.05	108.76
2	A	501	IHP	O43-P3-O13	2.01	113.67	105.85

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	IHP	C4-C5-O15-P5
2	B	501	IHP	C5-C4-O14-P4
2	C	501	IHP	C5-C4-O14-P4
2	D	501	IHP	C5-C4-O14-P4
2	E	501	IHP	C5-C4-O14-P4
2	E	501	IHP	C4-C5-O15-P5
2	F	501	IHP	C2-C3-O13-P3
2	F	501	IHP	C4-C5-O15-P5
2	G	501	IHP	C3-C4-O14-P4
2	G	501	IHP	C4-C5-O15-P5

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Mol	Chain	Res	Type	Atoms
2	G	501	IHP	C6-C5-O15-P5
2	G	501	IHP	C5-C6-O16-P6
2	H	501	IHP	C4-C5-O15-P5
2	E	501	IHP	C6-C5-O15-P5
2	G	501	IHP	C3-O13-P3-O43
2	B	501	IHP	C4-O14-P4-O24
2	C	501	IHP	C4-O14-P4-O24
2	C	501	IHP	C5-O15-P5-O25
2	E	501	IHP	C4-O14-P4-O24
2	F	501	IHP	C3-C4-O14-P4
2	A	501	IHP	C2-O12-P2-O42
2	B	501	IHP	C2-O12-P2-O42
2	C	501	IHP	C2-O12-P2-O42
2	D	501	IHP	C2-O12-P2-O42
2	D	501	IHP	C3-O13-P3-O43
2	E	501	IHP	C3-O13-P3-O43
2	G	501	IHP	C1-C6-O16-P6
2	A	501	IHP	C2-O12-P2-O22
2	A	501	IHP	C5-O15-P5-O25
2	B	501	IHP	C5-O15-P5-O25
2	D	501	IHP	C4-O14-P4-O24
2	D	501	IHP	C5-O15-P5-O25
2	G	501	IHP	C2-O12-P2-O22
2	H	501	IHP	C5-O15-P5-O25
2	A	501	IHP	C2-O12-P2-O32
2	B	501	IHP	C3-O13-P3-O43
2	B	501	IHP	C5-O15-P5-O45
2	C	501	IHP	C3-O13-P3-O43
2	C	501	IHP	C4-O14-P4-O44
2	D	501	IHP	C2-O12-P2-O32
2	E	501	IHP	C4-O14-P4-O44
2	F	501	IHP	C3-O13-P3-O43
2	G	501	IHP	C3-O13-P3-O33
2	H	501	IHP	C6-O16-P6-O46
2	B	501	IHP	C2-O12-P2-O22
2	D	501	IHP	C2-O12-P2-O22
2	E	501	IHP	C2-O12-P2-O22
2	G	501	IHP	C3-O13-P3-O23
2	H	501	IHP	C2-O12-P2-O22

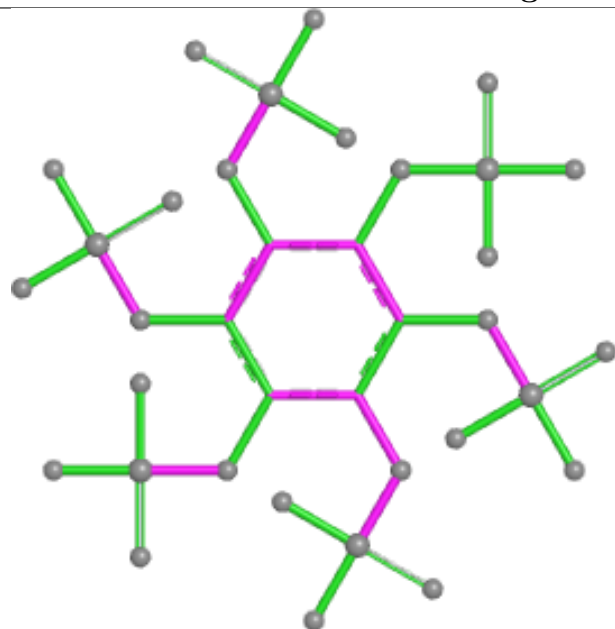
There are no ring outliers.

8 monomers are involved in 12 short contacts:

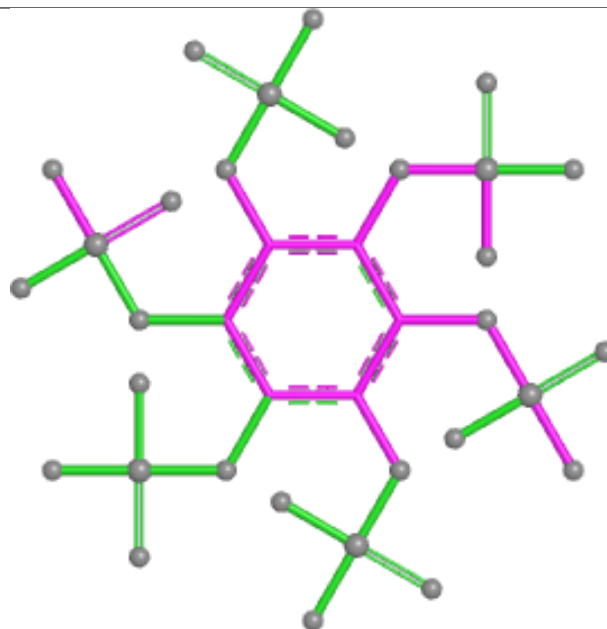
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	IHP	1	0
2	E	501	IHP	1	0
2	A	501	IHP	3	0
2	D	501	IHP	1	0
2	G	501	IHP	2	0
2	H	501	IHP	1	0
2	F	501	IHP	2	0
2	B	501	IHP	1	0

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.

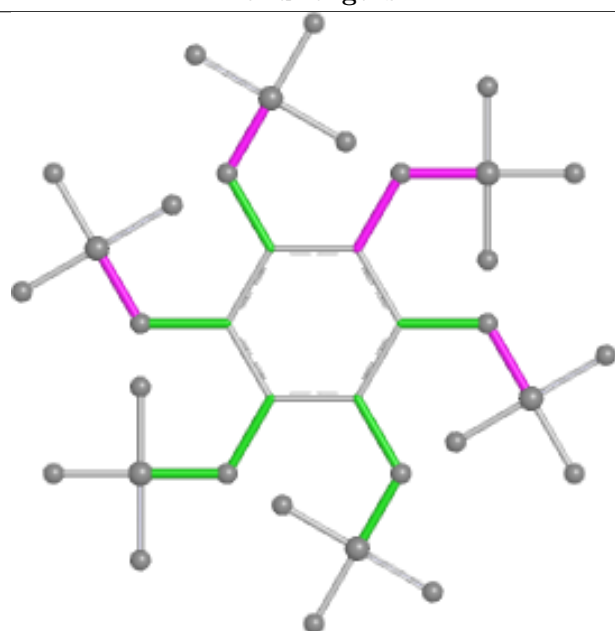
Ligand IHP C 501



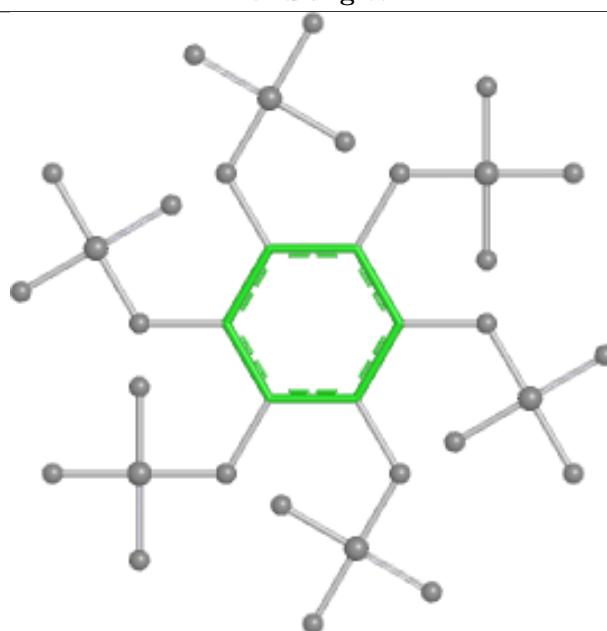
Bond lengths



Bond angles

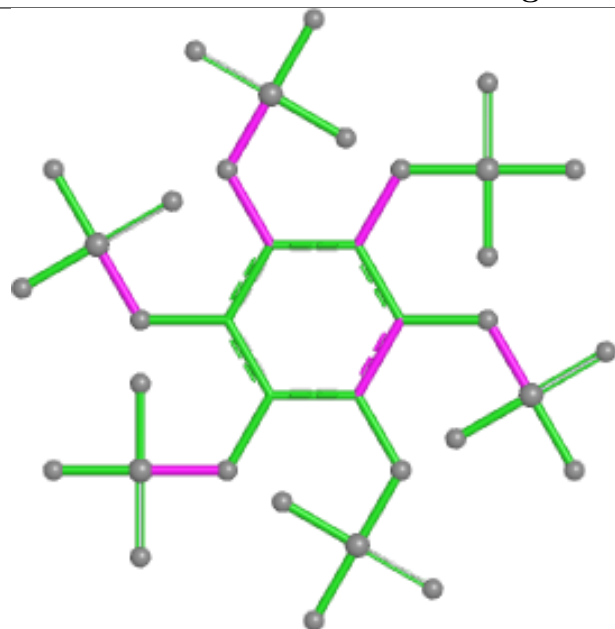


Torsions

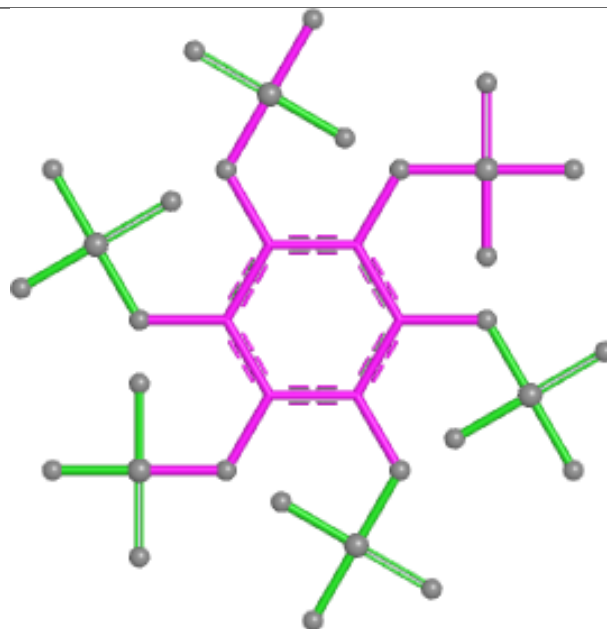


Rings

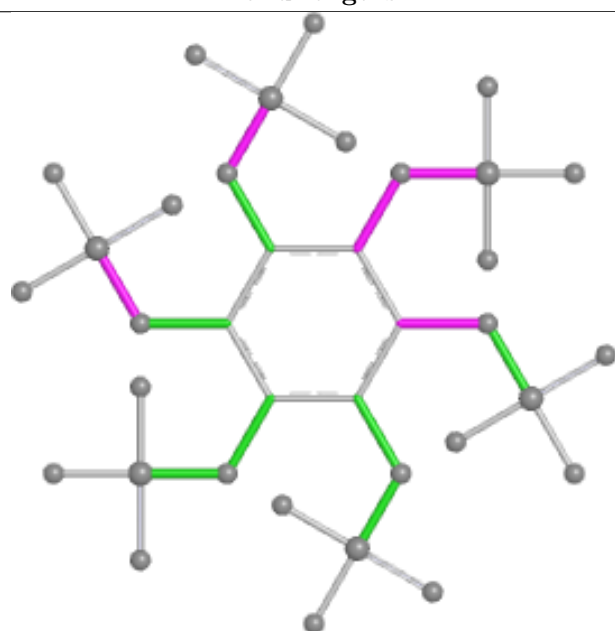
Ligand IHP E 501



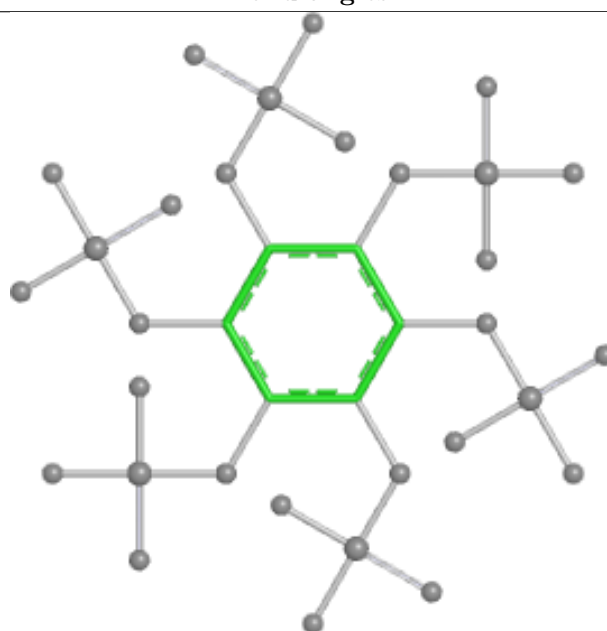
Bond lengths



Bond angles

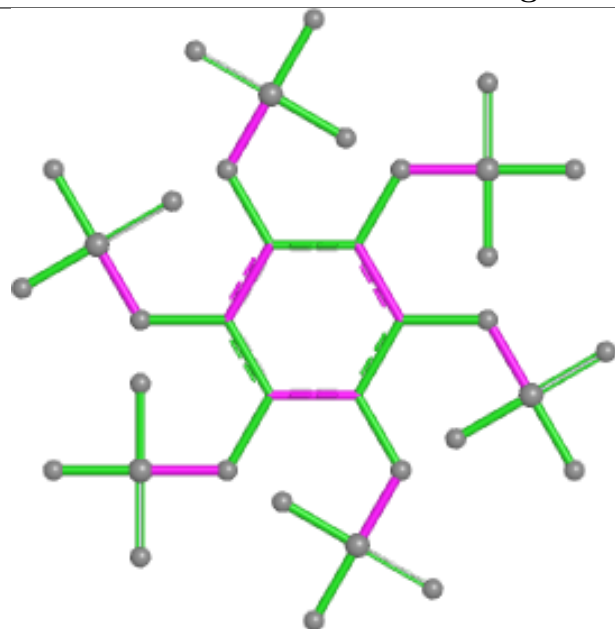


Torsions

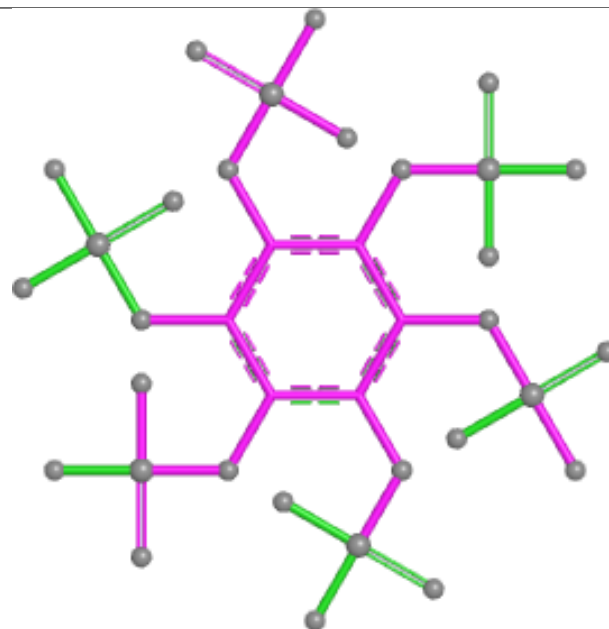


Rings

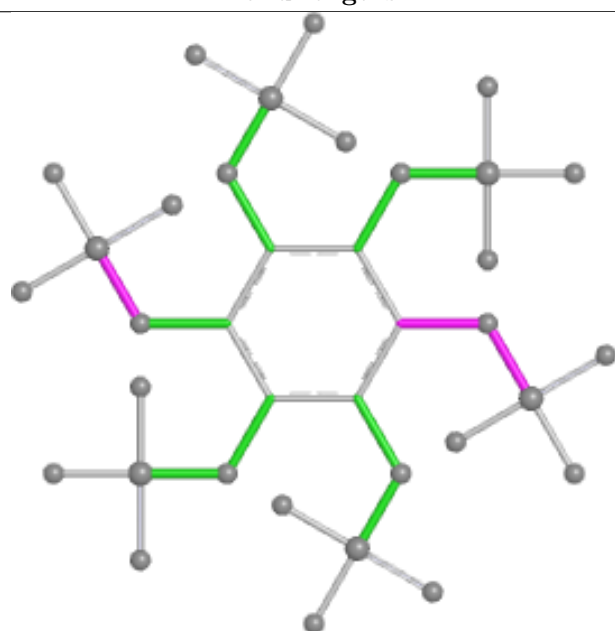
Ligand IHP A 501



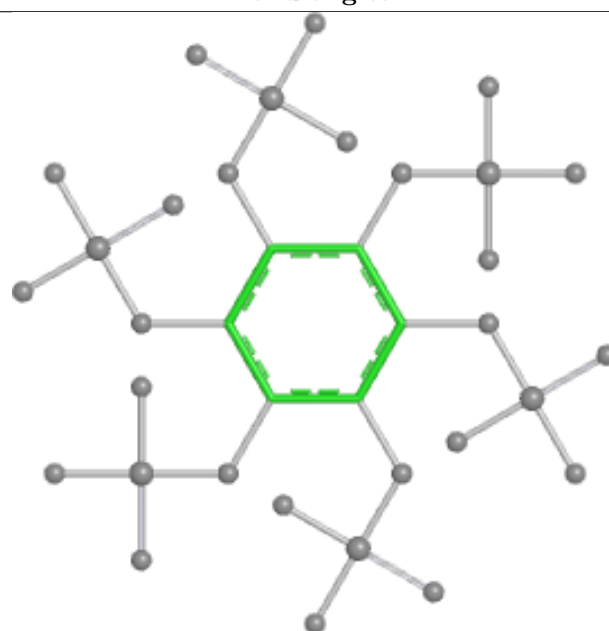
Bond lengths



Bond angles

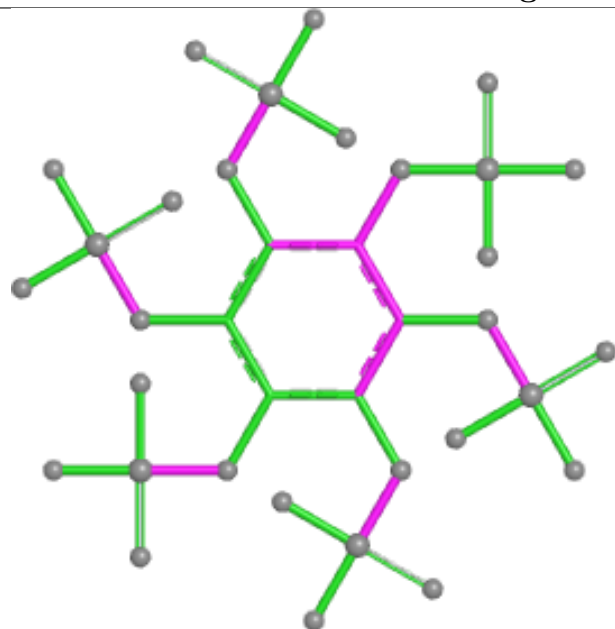


Torsions

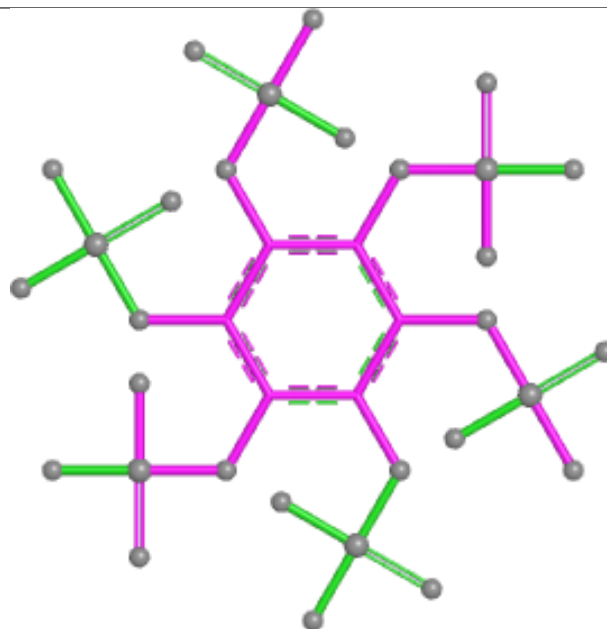


Rings

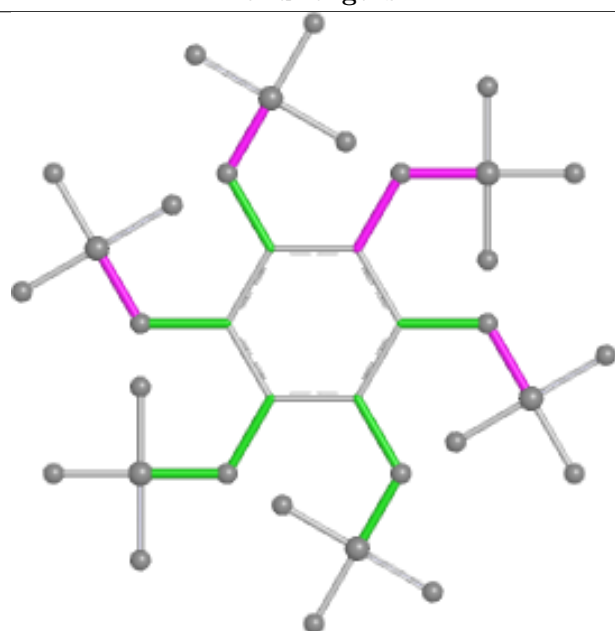
Ligand IHP D 501



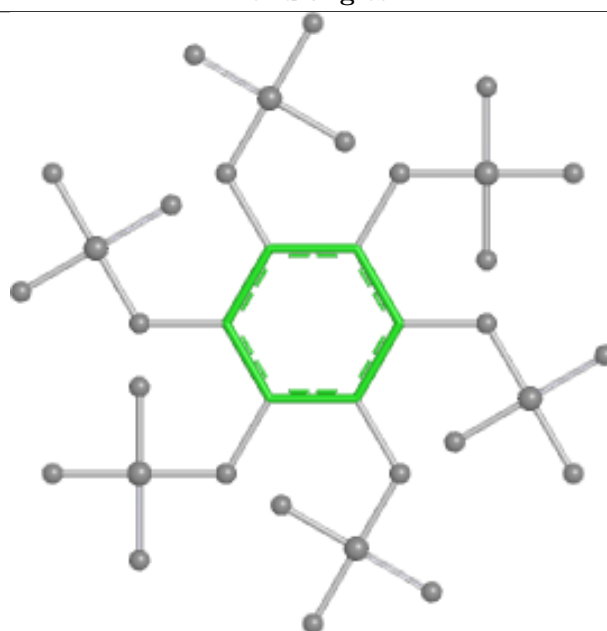
Bond lengths



Bond angles

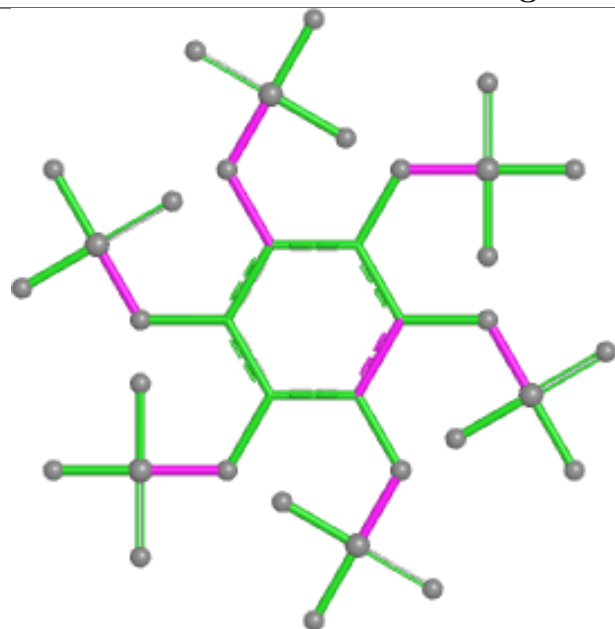


Torsions

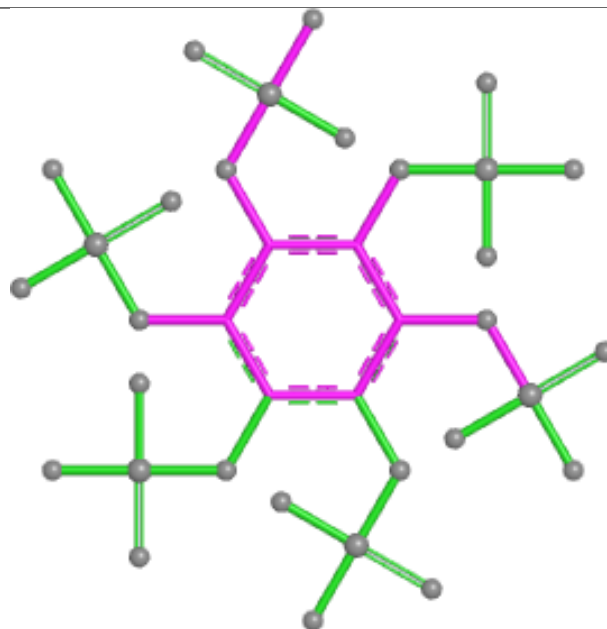


Rings

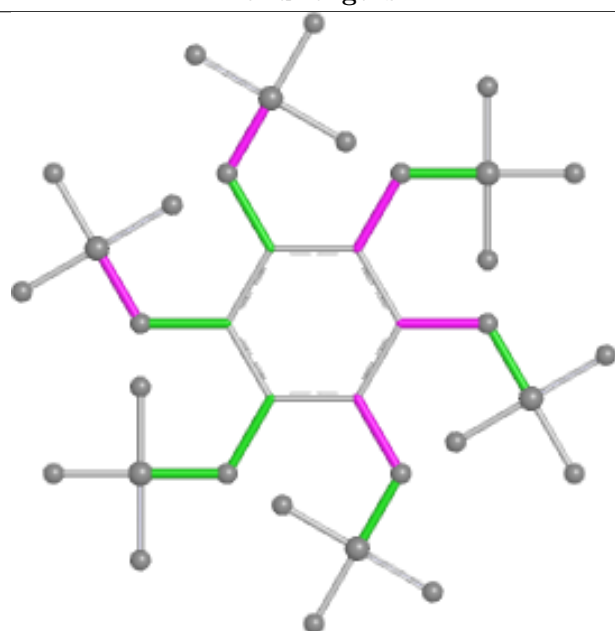
Ligand IHP G 501



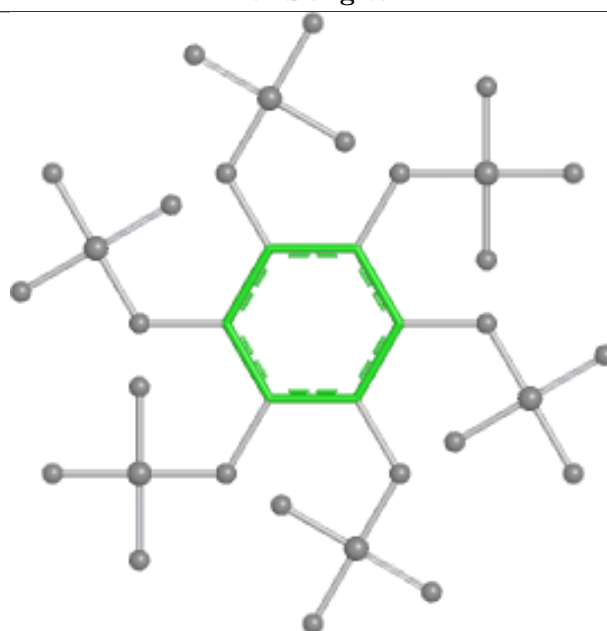
Bond lengths



Bond angles

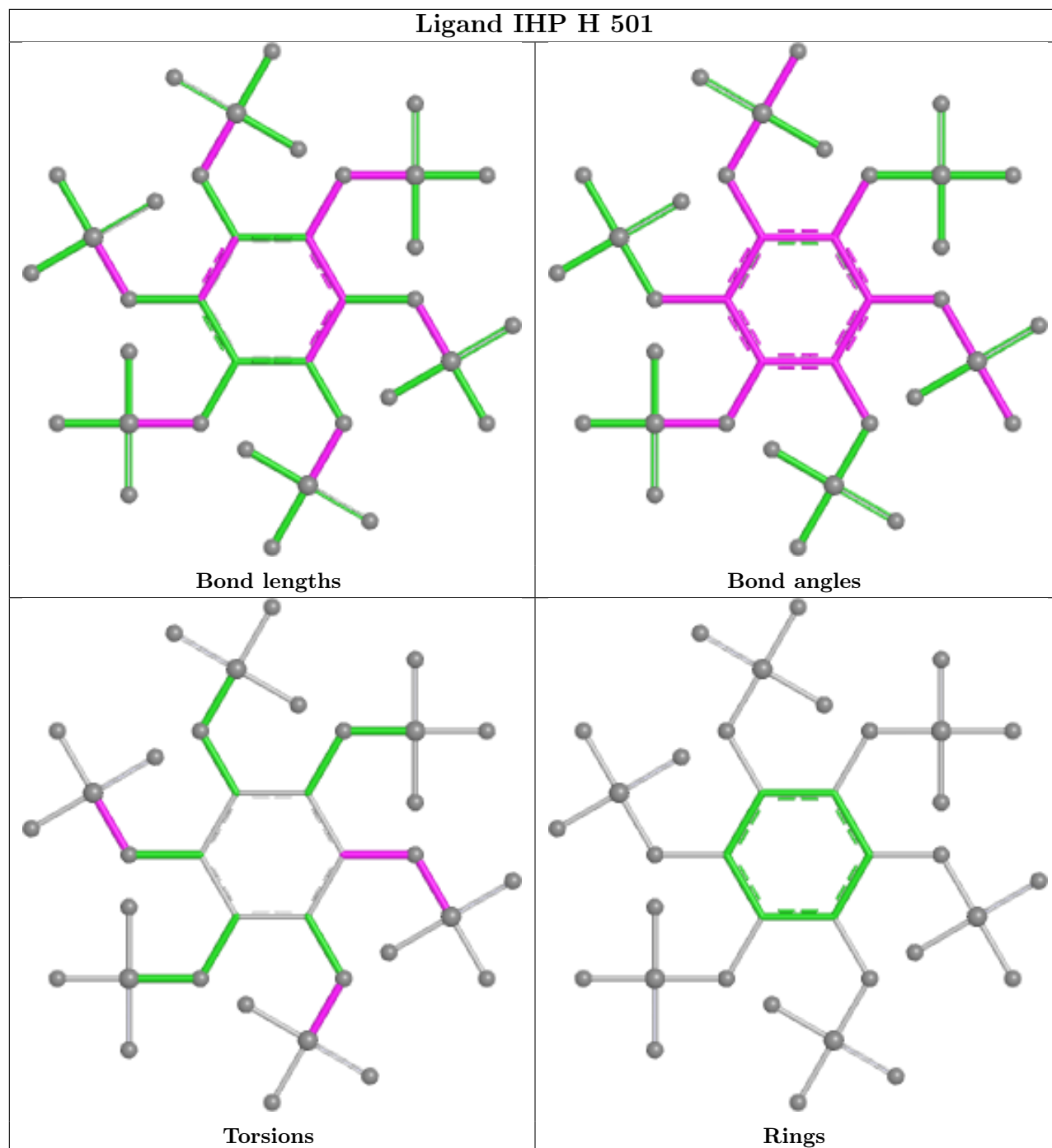


Torsions

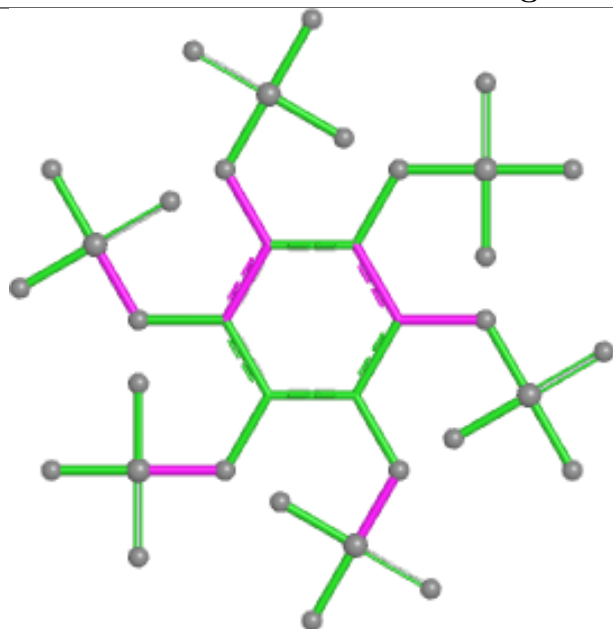


Rings

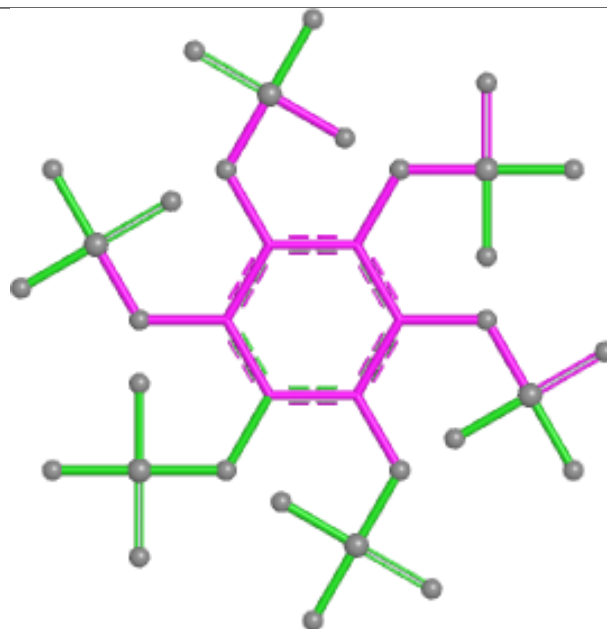
Ligand IHP H 501



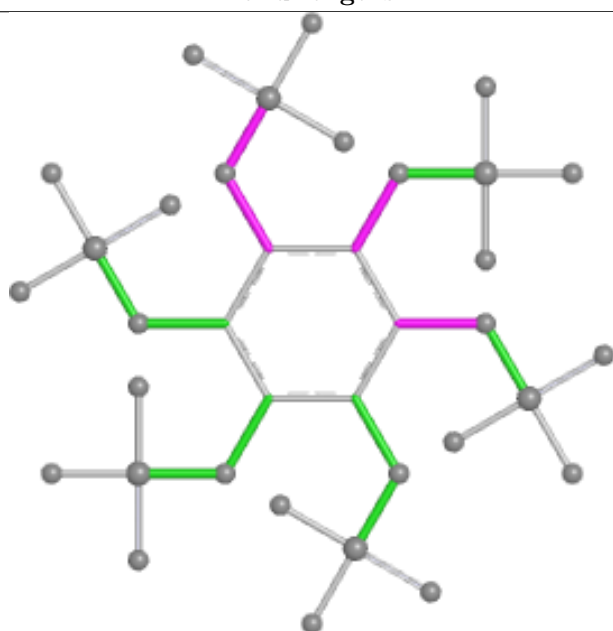
Ligand IHP F 501



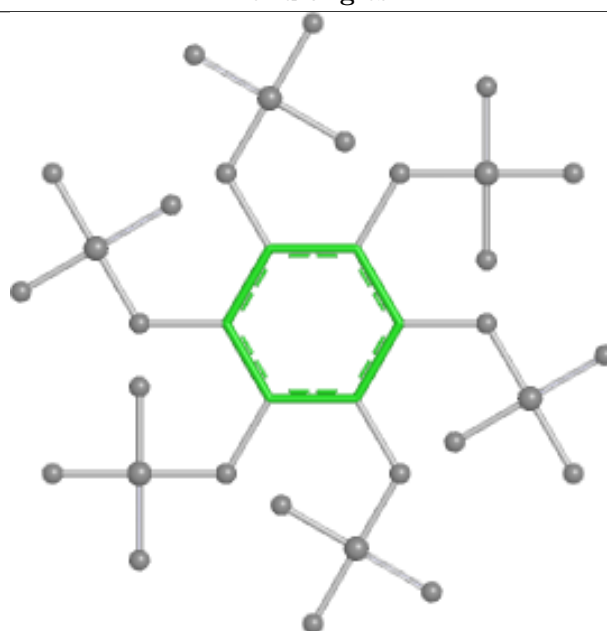
Bond lengths



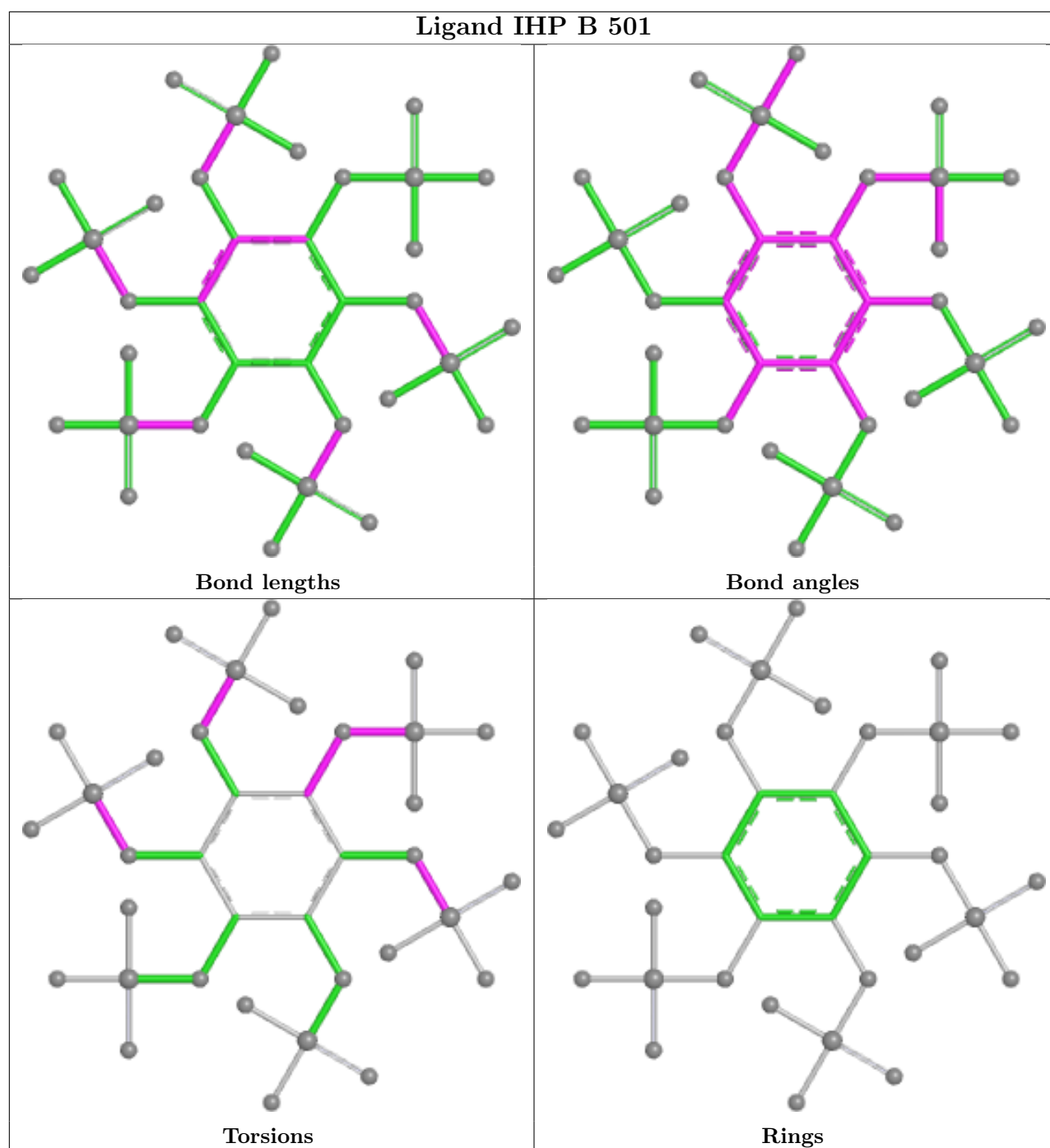
Bond angles



Torsions



Rings



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	405/451 (89%)	0.32	25 (6%)	26	24	27, 41, 66, 84	0
1	B	415/451 (92%)	-0.02	13 (3%)	51	51	23, 34, 52, 75	0
1	C	417/451 (92%)	0.38	33 (7%)	18	16	25, 41, 70, 82	0
1	D	413/451 (91%)	0.27	36 (8%)	16	14	25, 37, 65, 88	0
1	E	414/451 (91%)	0.40	31 (7%)	20	18	26, 41, 68, 82	0
1	F	410/451 (90%)	0.72	64 (15%)	5	4	26, 43, 83, 102	0
1	G	414/451 (91%)	0.39	30 (7%)	21	20	26, 41, 70, 86	0
1	H	407/451 (90%)	0.35	19 (4%)	36	35	27, 42, 66, 81	0
All	All	3295/3608 (91%)	0.35	251 (7%)	20	18	23, 40, 70, 102	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	430	TYR	6.2
1	F	332	PRO	5.4
1	F	406	VAL	5.0
1	G	115	ASP	4.9
1	F	375	PHE	4.9
1	F	392	LYS	4.8
1	E	411	GLN	4.7
1	F	401	THR	4.7
1	E	193	ASN	4.6
1	G	408	LEU	4.6
1	D	365	PHE	4.6
1	A	161	SER	4.6
1	D	364	SER	4.5
1	F	402	SER	4.5
1	D	265	LYS	4.5
1	D	359	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	400	ASP	4.4
1	B	265	LYS	4.4
1	E	195	ASN	4.4
1	A	362	LYS	4.3
1	G	363	SER	4.3
1	E	433	VAL	4.2
1	B	155	ASP	4.2
1	E	265	LYS	4.2
1	C	159	LYS	4.1
1	F	410	LEU	4.0
1	F	400	ASP	4.0
1	F	371	ILE	4.0
1	F	431	THR	3.9
1	G	365	PHE	3.9
1	H	432	THR	3.9
1	F	328	ILE	3.8
1	A	361	LYS	3.8
1	F	370	GLY	3.8
1	F	393	ILE	3.8
1	C	155	ASP	3.7
1	F	333	PHE	3.7
1	F	407	LEU	3.7
1	C	266	GLN	3.7
1	H	360	ILE	3.7
1	F	409	HIS	3.7
1	F	378	LYS	3.7
1	D	366	THR	3.6
1	F	403	ALA	3.6
1	F	412	LYS	3.6
1	D	263	SER	3.6
1	D	155	ASP	3.6
1	C	433	VAL	3.6
1	F	359	VAL	3.5
1	G	264	GLY	3.5
1	G	433	VAL	3.5
1	E	161	SER	3.5
1	G	360	ILE	3.5
1	D	14	SER	3.4
1	D	360	ILE	3.4
1	G	417	LEU	3.4
1	D	370	GLY	3.4
1	F	346	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	144	ASP	3.4
1	D	412	LYS	3.4
1	F	399	ASN	3.3
1	G	155	ASP	3.3
1	C	402	SER	3.3
1	E	103	ASN	3.3
1	F	374	HIS	3.3
1	G	266	GLN	3.3
1	C	264	GLY	3.3
1	D	363	SER	3.3
1	F	382	ALA	3.2
1	H	266	GLN	3.2
1	A	414	LYS	3.2
1	A	266	GLN	3.2
1	E	266	GLN	3.2
1	G	362	LYS	3.1
1	C	263	SER	3.1
1	C	412	LYS	3.1
1	H	156	PRO	3.1
1	E	155	ASP	3.1
1	F	266	GLN	3.0
1	C	83	ASN	3.0
1	H	264	GLY	3.0
1	D	417	LEU	3.0
1	D	353	LYS	3.0
1	A	375	PHE	3.0
1	E	84	ASN	3.0
1	C	403	ALA	2.9
1	G	364	SER	2.9
1	F	335	GLU	2.9
1	F	405	GLU	2.9
1	F	355	ILE	2.9
1	C	362	LYS	2.9
1	C	411	GLN	2.9
1	D	358	ASP	2.9
1	D	400	ASP	2.9
1	E	404	ASP	2.9
1	E	412	LYS	2.8
1	G	14	SER	2.8
1	E	294	GLU	2.8
1	A	412	LYS	2.8
1	D	361	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	361	LYS	2.8
1	B	329	ARG	2.8
1	C	161	SER	2.8
1	C	329	ARG	2.8
1	F	66	GLN	2.8
1	F	330	GLU	2.8
1	B	414	LYS	2.8
1	D	362	LYS	2.8
1	F	157	LYS	2.8
1	F	361	LYS	2.8
1	F	360	ILE	2.8
1	F	372	ASP	2.8
1	F	334	LYS	2.8
1	F	389	LYS	2.8
1	G	414	LYS	2.8
1	B	161	SER	2.8
1	F	353	LYS	2.8
1	B	14	SER	2.7
1	G	116	GLY	2.7
1	G	405	GLU	2.7
1	A	411	GLN	2.7
1	H	411	GLN	2.7
1	A	265	LYS	2.7
1	C	160	ASP	2.7
1	G	359	VAL	2.7
1	E	262	THR	2.7
1	D	27	GLN	2.6
1	B	30	ASN	2.6
1	C	401	THR	2.6
1	E	432	THR	2.6
1	F	89	SER	2.6
1	C	102	ASP	2.6
1	F	395	ASN	2.6
1	D	413	GLN	2.6
1	E	162	LYS	2.6
1	A	194	GLU	2.6
1	G	30	ASN	2.6
1	F	394	VAL	2.6
1	G	432	THR	2.6
1	D	371	ILE	2.6
1	F	384	ILE	2.6
1	G	409	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	391	LEU	2.5
1	F	408	LEU	2.5
1	F	390	ALA	2.5
1	C	404	ASP	2.5
1	H	400	ASP	2.5
1	B	412	LYS	2.5
1	B	433	VAL	2.5
1	D	266	GLN	2.5
1	C	369	ARG	2.5
1	F	358	ASP	2.5
1	A	263	SER	2.5
1	C	144	ASP	2.5
1	C	414	LYS	2.5
1	D	30	ASN	2.5
1	D	414	LYS	2.5
1	A	432	THR	2.5
1	A	360	ILE	2.5
1	F	417	LEU	2.5
1	F	352	LYS	2.5
1	G	156	PRO	2.5
1	A	363	SER	2.4
1	B	263	SER	2.4
1	F	429	ILE	2.4
1	F	354	TYR	2.4
1	F	404	ASP	2.4
1	H	375	PHE	2.4
1	C	265	LYS	2.4
1	D	162	LYS	2.4
1	E	409	HIS	2.4
1	E	295	GLN	2.4
1	C	393	ILE	2.4
1	F	331	LYS	2.4
1	B	143	PRO	2.4
1	C	407	LEU	2.4
1	H	171	ARG	2.4
1	C	399	ASN	2.3
1	G	200	LYS	2.3
1	F	337	VAL	2.3
1	A	136	ASP	2.3
1	F	379	LYS	2.3
1	E	264	GLY	2.3
1	H	263	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	330	GLU	2.3
1	E	397	LEU	2.3
1	E	417	LEU	2.3
1	G	358	ASP	2.3
1	G	374	HIS	2.3
1	A	162	LYS	2.3
1	E	408	LEU	2.3
1	F	414	LYS	2.3
1	D	145	CYS	2.3
1	H	160	ASP	2.3
1	F	338	GLY	2.3
1	D	404	ASP	2.2
1	E	400	ASP	2.2
1	D	409	HIS	2.2
1	C	396	GLN	2.2
1	C	392	LYS	2.2
1	E	378	LYS	2.2
1	H	412	LYS	2.2
1	F	336	ILE	2.2
1	D	408	LEU	2.2
1	F	83	ASN	2.2
1	E	297	HIS	2.2
1	A	420	LYS	2.2
1	G	159	LYS	2.2
1	H	14	SER	2.2
1	F	349	LEU	2.2
1	E	136	ASP	2.2
1	A	404	ASP	2.2
1	C	400	ASP	2.2
1	E	399	ASN	2.2
1	G	375	PHE	2.2
1	H	385	ASN	2.2
1	A	264	GLY	2.2
1	D	411	GLN	2.2
1	A	145	CYS	2.2
1	F	377	ILE	2.1
1	C	103	ASN	2.1
1	C	359	VAL	2.1
1	D	86	ASN	2.1
1	F	347	ASP	2.1
1	D	200	LYS	2.1
1	H	417	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	84	ASN	2.1
1	D	330	GLU	2.1
1	C	324	LEU	2.1
1	E	329	ARG	2.1
1	G	263	SER	2.1
1	D	343	LYS	2.1
1	E	414	LYS	2.1
1	F	426	ALA	2.1
1	E	428	GLU	2.1
1	H	202	VAL	2.1
1	D	375	PHE	2.1
1	A	329	ARG	2.1
1	F	318	SER	2.0
1	C	405	GLU	2.0
1	G	382	ALA	2.0
1	H	311	GLU	2.0
1	H	405	GLU	2.0
1	F	396	GLN	2.0
1	A	399	ASN	2.0
1	C	194	GLU	2.0
1	A	144	ASP	2.0
1	D	410	LEU	2.0
1	E	369	ARG	2.0
1	A	307	LYS	2.0
1	H	265	LYS	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

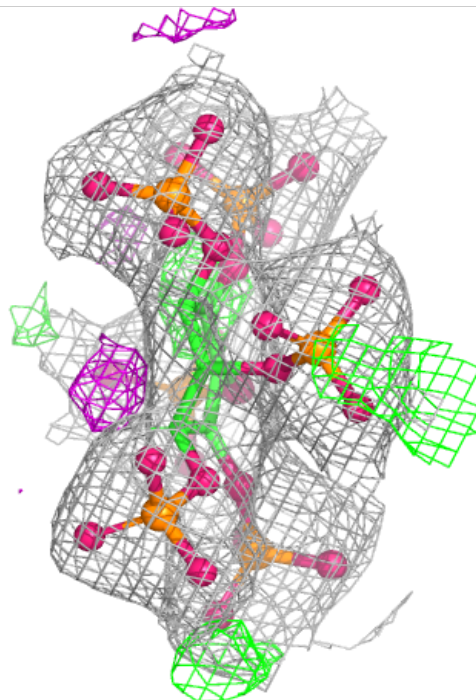
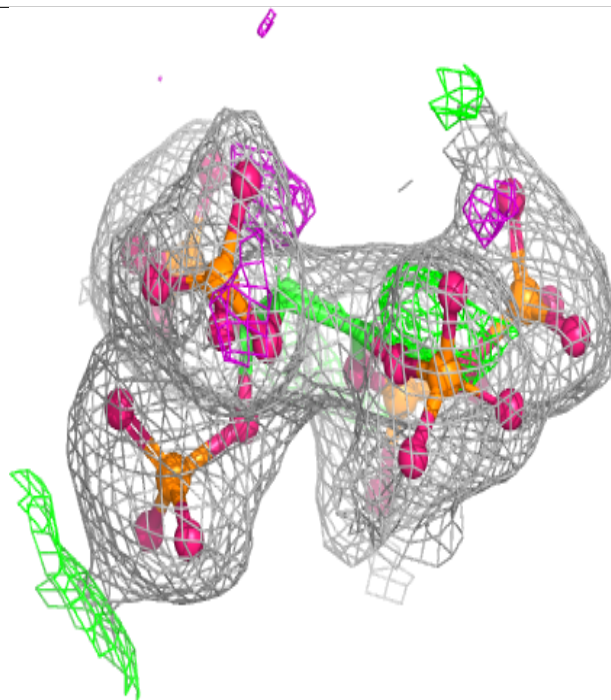
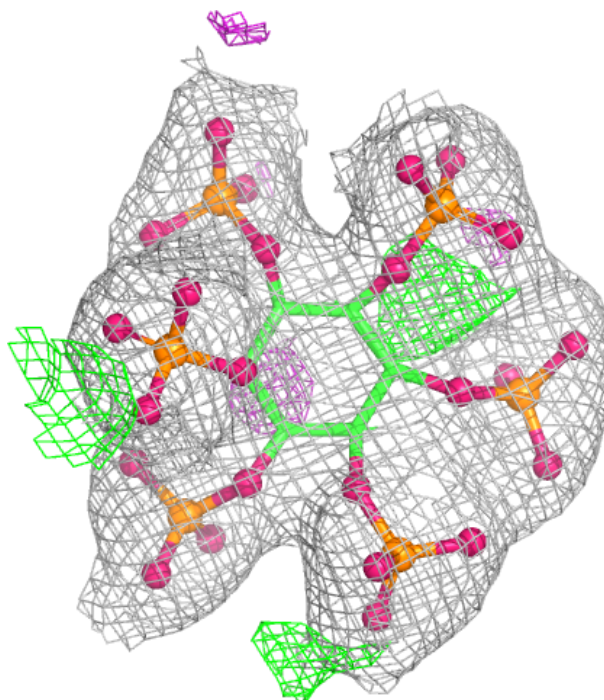
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IHP	F	501	36/36	0.95	0.09	38,46,55,57	0
2	IHP	C	501	36/36	0.97	0.06	26,35,44,47	0
2	IHP	A	501	36/36	0.97	0.06	30,37,44,52	0
2	IHP	G	501	36/36	0.97	0.06	32,38,46,50	0
2	IHP	H	501	36/36	0.97	0.07	31,36,45,46	0
2	IHP	B	501	36/36	0.98	0.05	25,31,37,41	0
2	IHP	D	501	36/36	0.98	0.06	25,33,41,44	0
2	IHP	E	501	36/36	0.98	0.06	25,33,43,48	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.

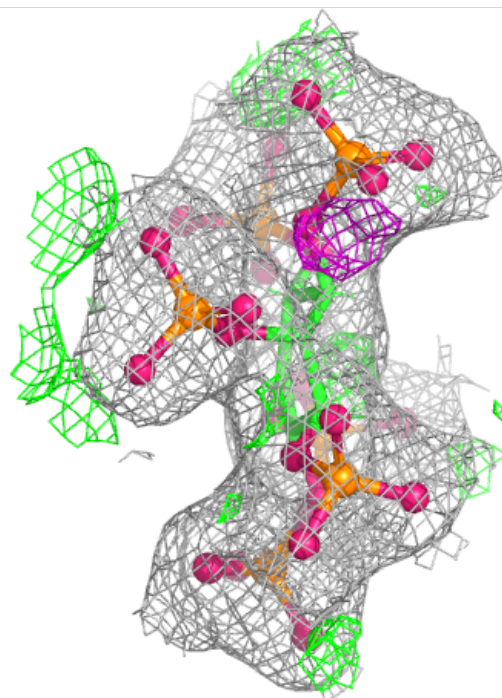
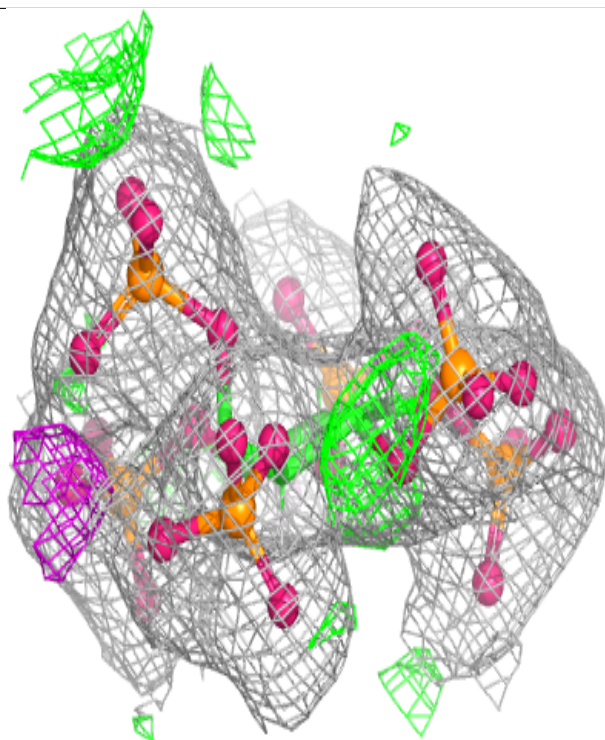
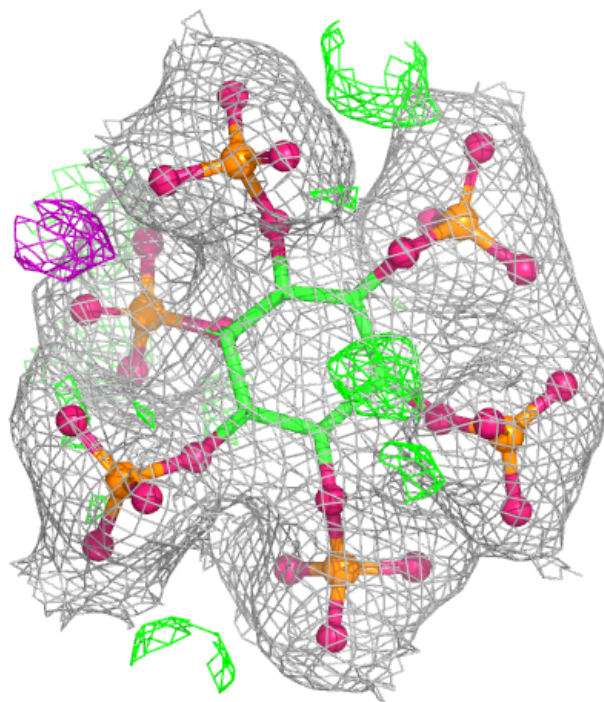
Electron density around IHP F 501:

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



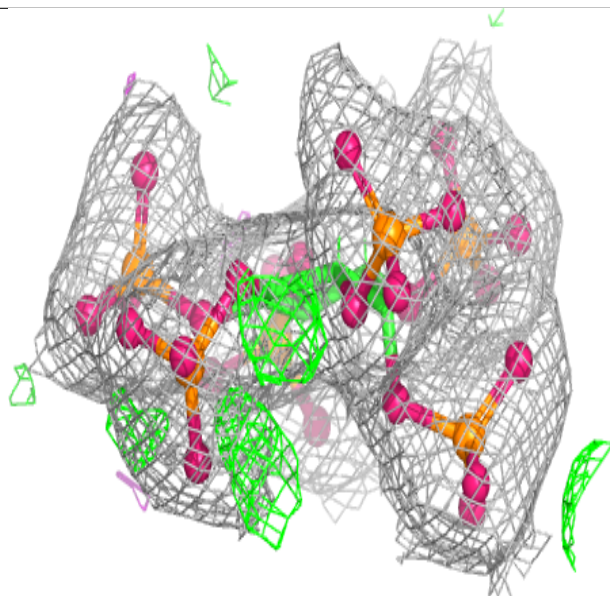
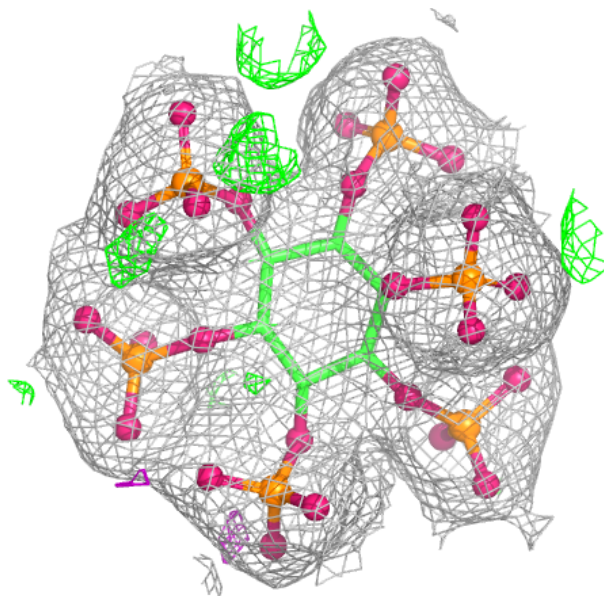
Electron density around IHP C 501:

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



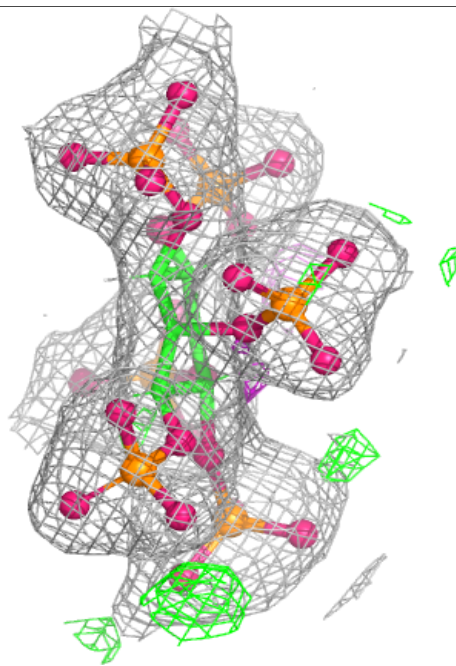
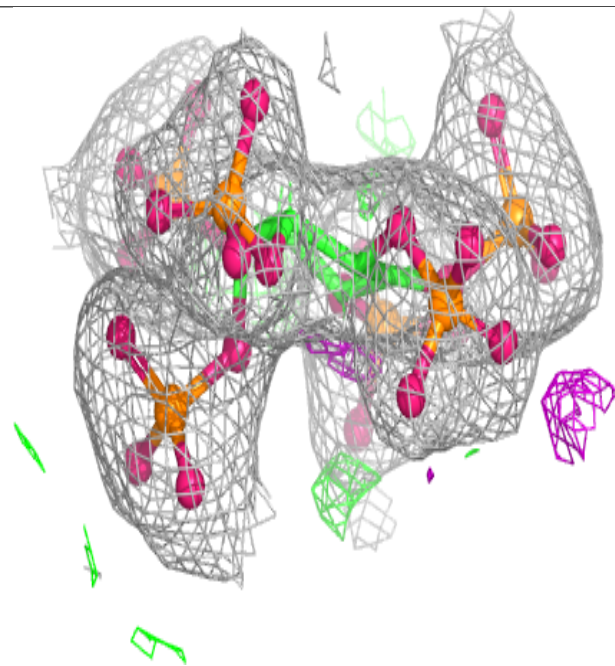
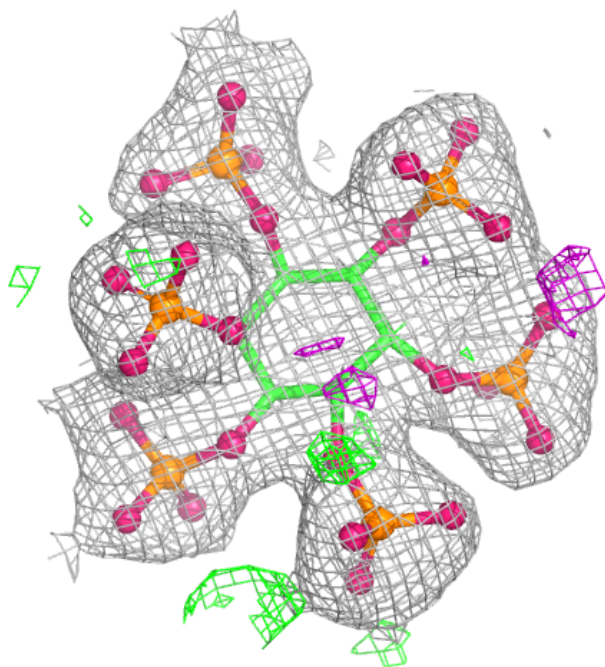
Electron density around IHP A 501:

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



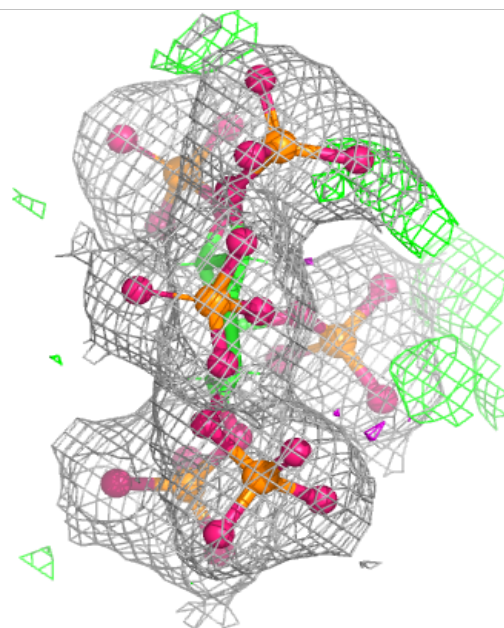
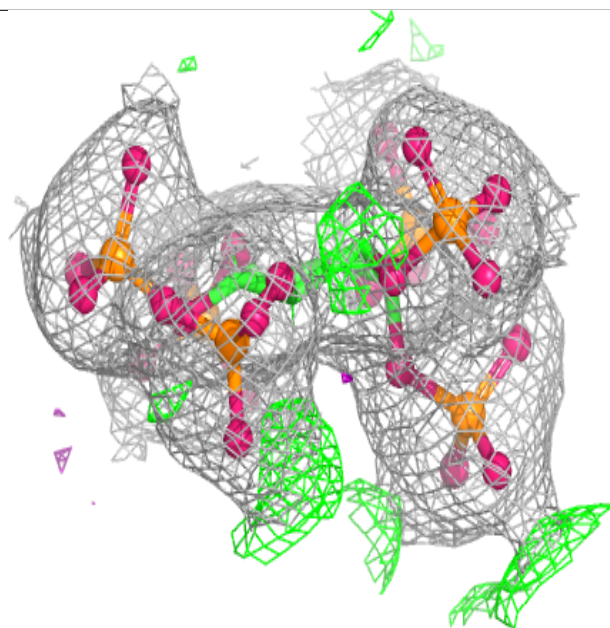
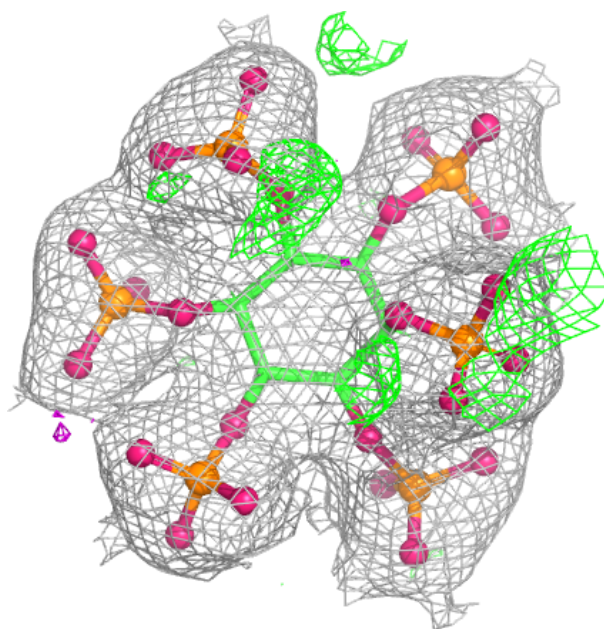
Electron density around IHP G 501:

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



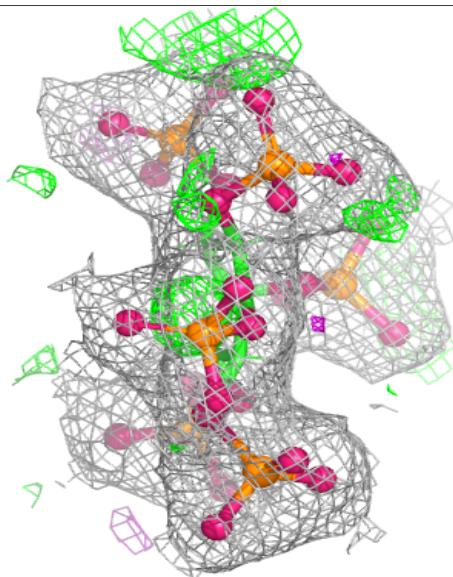
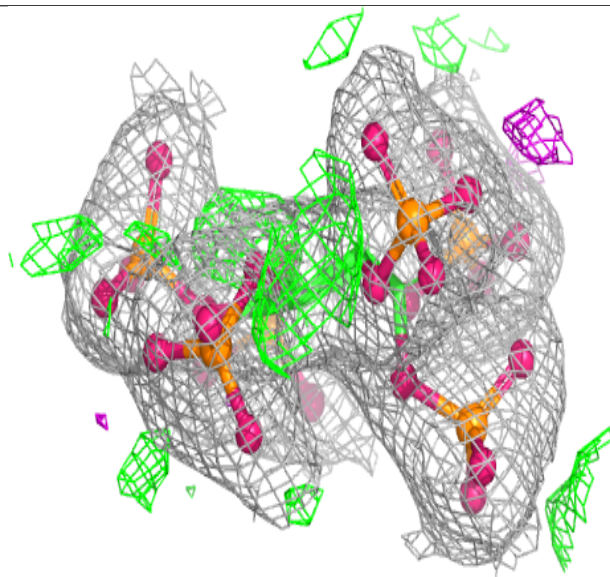
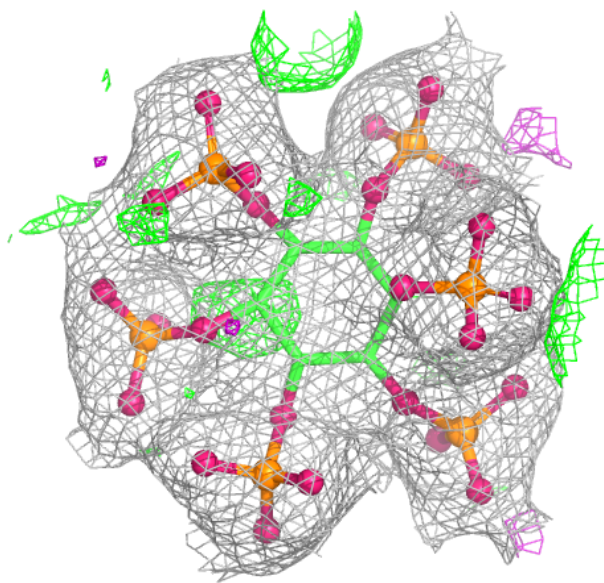
Electron density around IHP H 501:

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



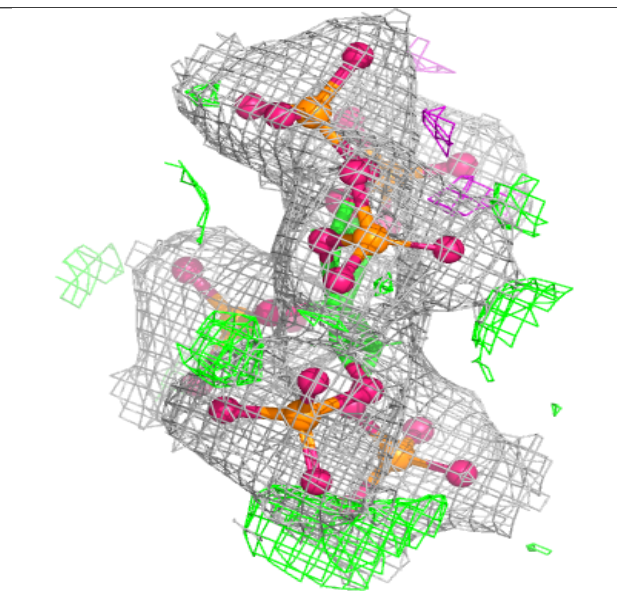
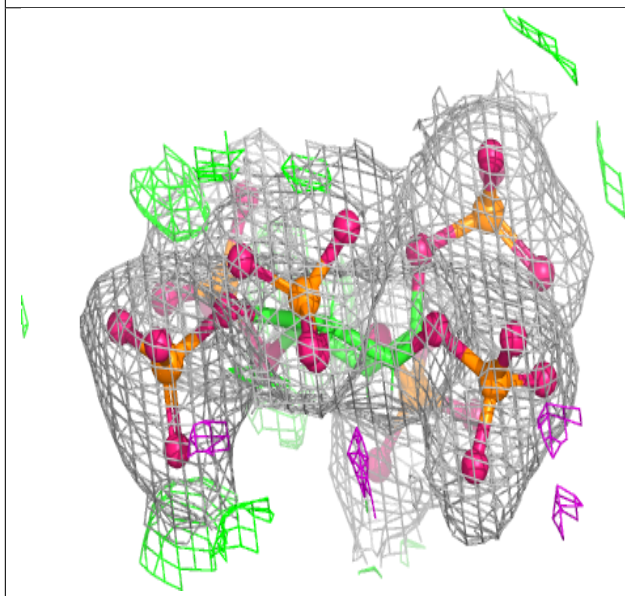
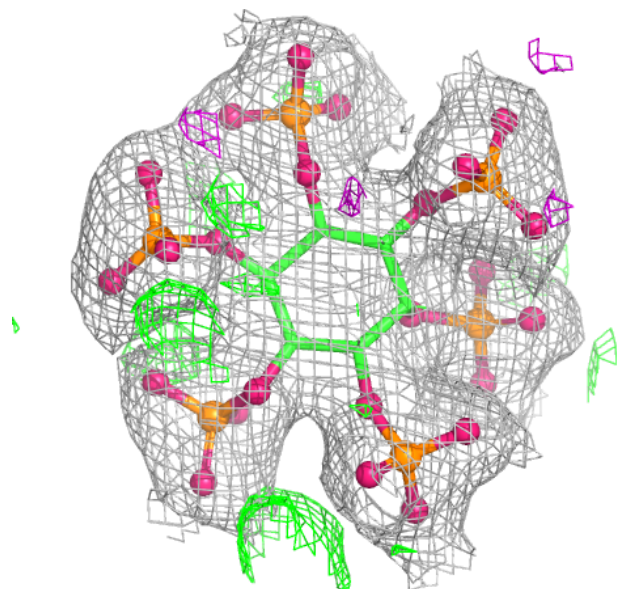
Electron density around IHP B 501:

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



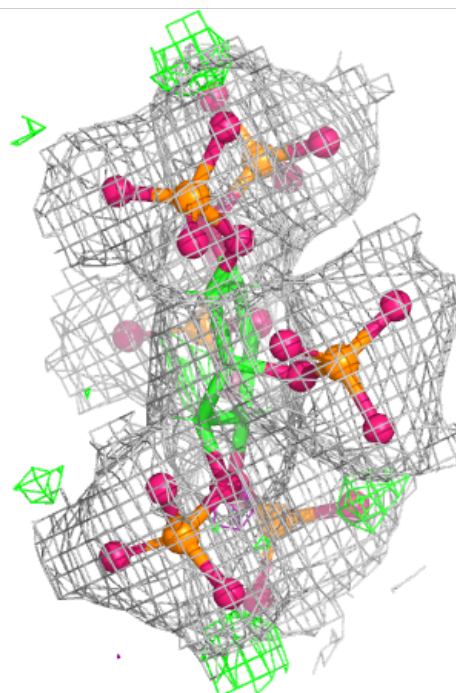
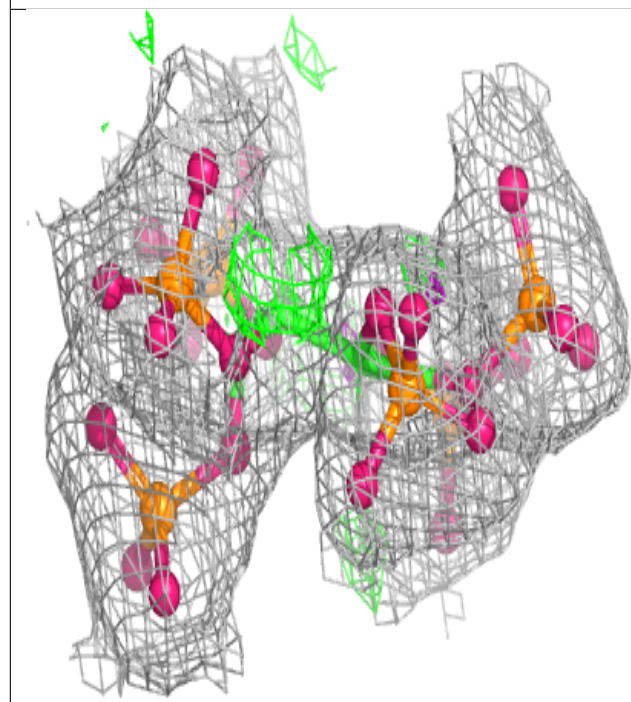
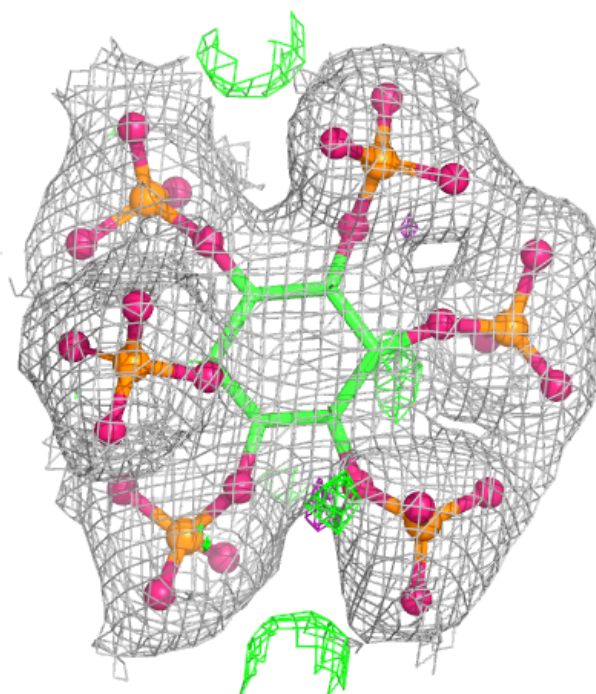
Electron density around IHP D 501:

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



Electron density around IHP E 501:

$2mF_o-DF_c$ (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.