Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 07:58 AM EDT

PDB ID	:	3NTL
Title	:	Crystal Structure of Glucose-1-phosphatase (AgpE) from Enterobacter cloacae
Authors	:	Grishkovskaya, I.; Hoehne, W.
Deposited on	:	2010-07-05
Resolution	:	1.88 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 (i) 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 (i)) were used in the production of this report:

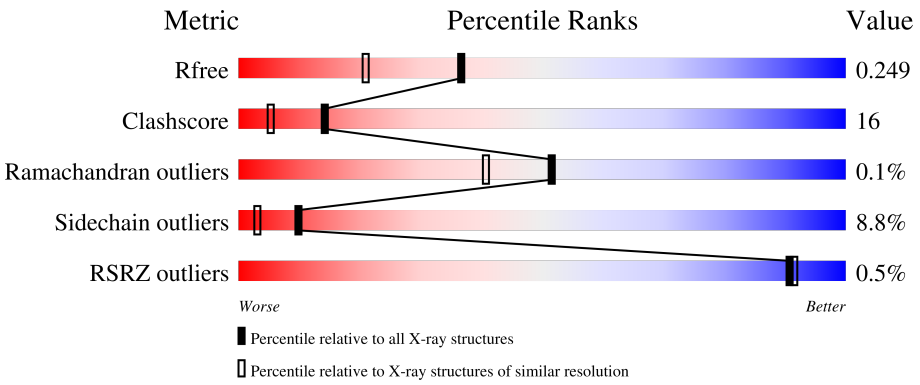
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 <=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	398	% 74% 18% 5% • •
1	B	398	74% 19% • • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IHP	A	550	-	-	X	-
2	IHP	B	551	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6947 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.

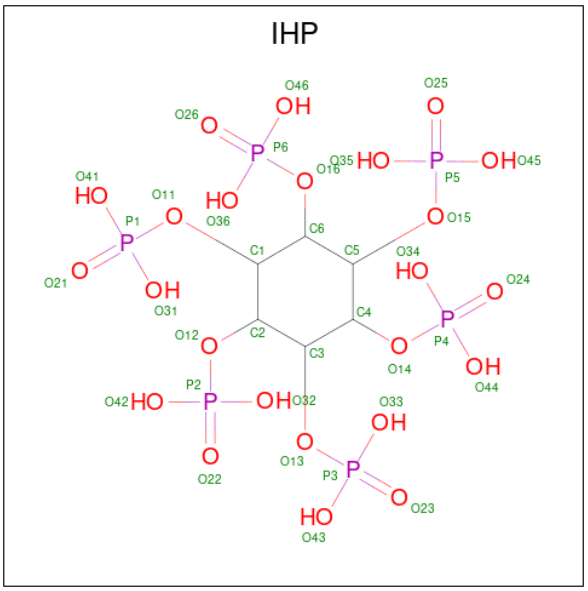
- Molecule 1 is a protein called Acid glucose-1-phosphate phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3075	1949	515	593	18	0	7	0
1	B	387	3088	1956	516	597	19	0	12	0

There are 22 discrepancies between the modelled and reference sequences:

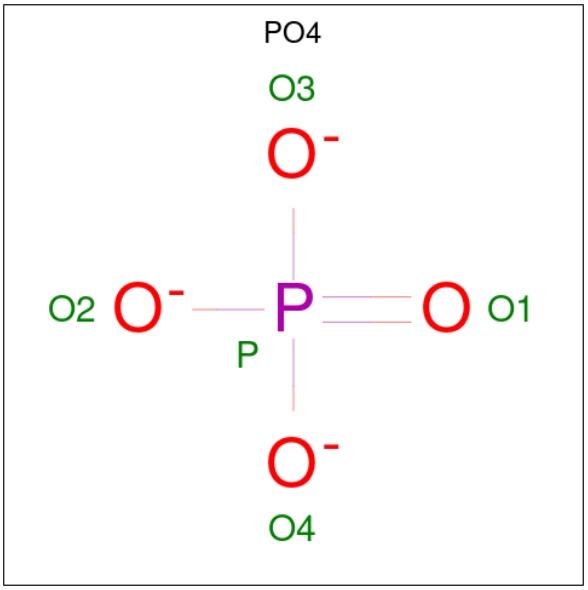
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q6EV19
A	16	ALA	HIS	engineered mutation	UNP Q6EV19
A	390	ARG	-	expression tag	UNP Q6EV19
A	391	SER	-	expression tag	UNP Q6EV19
A	392	GLY	-	expression tag	UNP Q6EV19
A	393	HIS	-	expression tag	UNP Q6EV19
A	394	HIS	-	expression tag	UNP Q6EV19
A	395	HIS	-	expression tag	UNP Q6EV19
A	396	HIS	-	expression tag	UNP Q6EV19
A	397	HIS	-	expression tag	UNP Q6EV19
A	398	HIS	-	expression tag	UNP Q6EV19
B	1	SER	-	expression tag	UNP Q6EV19
B	16	ALA	HIS	engineered mutation	UNP Q6EV19
B	390	ARG	-	expression tag	UNP Q6EV19
B	391	SER	-	expression tag	UNP Q6EV19
B	392	GLY	-	expression tag	UNP Q6EV19
B	393	HIS	-	expression tag	UNP Q6EV19
B	394	HIS	-	expression tag	UNP Q6EV19
B	395	HIS	-	expression tag	UNP Q6EV19
B	396	HIS	-	expression tag	UNP Q6EV19
B	397	HIS	-	expression tag	UNP Q6EV19
B	398	HIS	-	expression tag	UNP Q6EV19

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			36	6	24	6		
2	B	1	Total	C	O	P	0	0
			36	6	24	6		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	B	1	1	1	0	0

- Molecule 5 is water.

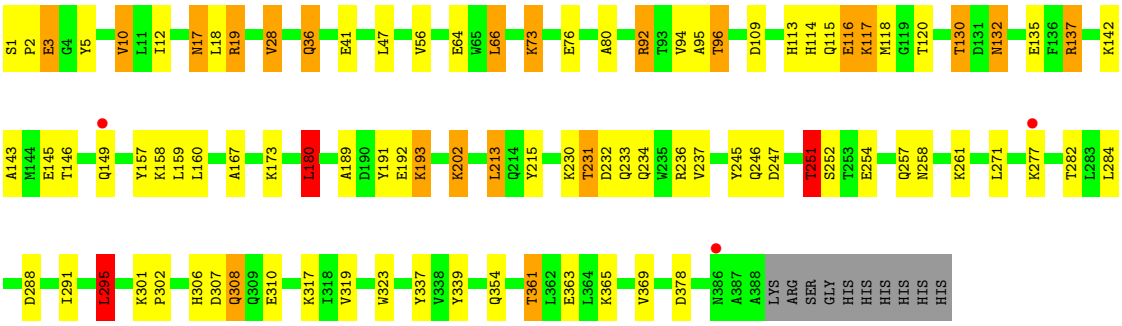
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	336	336	336	0	0
			Total	O		
5	B	370	370	370	0	0

3 Residue-property plots (i)

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.

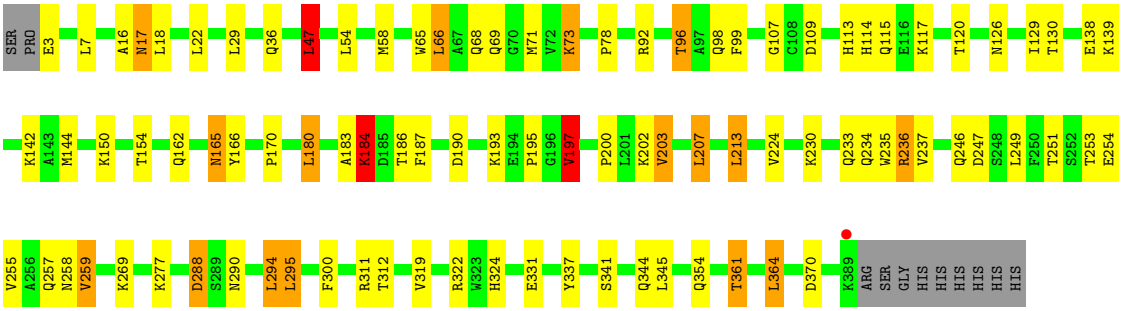
• Molecule 1: Acid glucose-1-phosphate phosphatase

Chain A:



• Molecule 1: Acid glucose-1-phosphate phosphatase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	151.08Å 151.08Å 86.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.36 – 1.88 28.36 – 1.88	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.36-1.88) 98.2 (28.36-1.88)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.74 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.181 , 0.250 0.181 , 0.249	Depositor DCC
R_{free} test set	2978 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6947	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PO4, 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	1.10	4/3163 (0.1%)	1.16	12/4290 (0.3%)
1	B	1.12	4/3190 (0.1%)	1.06	16/4326 (0.4%)
All	All	1.11	8/6353 (0.1%)	1.11	28/8616 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	LYS	CE-NZ	6.31	1.64	1.49
1	A	339	TYR	CD1-CE1	6.18	1.48	1.39
1	B	99	PHE	CD2-CE2	6.02	1.51	1.39
1	B	235	TRP	CG-CD1	5.69	1.44	1.36
1	A	56	VAL	CB-CG2	5.55	1.64	1.52
1	A	215	TYR	CD2-CE2	5.47	1.47	1.39
1	B	319	VAL	CB-CG2	5.43	1.64	1.52
1	A	251	THR	CB-CG2	-5.27	1.34	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	19	ARG	NE-CZ-NH2	-25.33	107.63	120.30
1	A	19	ARG	NE-CZ-NH1	20.39	130.50	120.30
1	B	311	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	B	197	VAL	CB-CA-C	-9.28	93.77	111.40
1	B	47	LEU	CB-CG-CD2	8.09	124.76	111.00
1	A	19	ARG	CD-NE-CZ	7.79	134.51	123.60
1	A	19	ARG	CG-CD-NE	-7.33	96.41	111.80
1	B	311	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	B	213	LEU	CB-CG-CD1	6.86	122.66	111.00
1	B	197	VAL	CG1-CB-CG2	6.73	121.66	110.90
1	A	10	VAL	CG1-CB-CG2	6.48	121.27	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	277	LYS	CD-CE-NZ	-6.39	97.01	111.70
1	A	295	LEU	CB-CG-CD1	6.30	121.72	111.00
1	B	311	ARG	CA-CB-CG	-6.30	99.53	113.40
1	A	319	VAL	CG1-CB-CG2	6.17	120.77	110.90
1	B	288	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	66	LEU	CB-CG-CD1	6.03	121.25	111.00
1	A	92	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	224	VAL	CG1-CB-CG2	5.45	119.62	110.90
1	A	180	LEU	CB-CG-CD1	5.34	120.08	111.00
1	B	203	VAL	CG1-CB-CG2	5.29	119.37	110.90
1	A	92	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	224	VAL	CA-CB-CG2	5.24	118.76	110.90
1	B	364	LEU	CB-CG-CD1	5.16	119.77	111.00
1	B	236	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	213	LEU	CA-CB-CG	5.04	126.90	115.30
1	B	224	VAL	CA-CB-CG1	5.01	118.42	110.90
1	B	322	ARG	NE-CZ-NH2	-5.00	117.80	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	3075	0	3047	103	1
1	B	3088	0	3058	87	0
2	A	36	0	6	14	0
2	B	36	0	6	2	0
3	A	5	0	0	0	0
4	B	1	0	0	0	0
5	A	336	0	0	17	0
5	B	370	0	0	23	0
All	All	6947	0	6117	193	1

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 16.

All (193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:NH2	2:A:550:IHP:H2	1.23	1.41
1:A:92:ARG:NH2	2:A:550:IHP:C2	2.20	1.03
1:B:17:ASN:HD22	1:B:18:LEU:H	1.07	1.01
1:A:94[A]:VAL:HG23	1:B:107:GLY:HA2	1.44	0.99
1:A:73:LYS:HG3	1:A:76:GLU:HG3	1.48	0.95
1:A:231:THR:HG22	1:A:234:GLN:H	1.32	0.92
1:A:92:ARG:HH22	2:A:550:IHP:H2	1.17	0.92
1:B:361:THR:HG21	5:B:532:HOH:O	1.72	0.89
1:A:64:GLU:OE1	5:A:610:HOH:O	1.93	0.86
2:A:550:IHP:O42	2:A:550:IHP:H1	1.73	0.86
1:A:17:ASN:HD22	1:A:18:LEU:H	1.21	0.85
1:A:1:SER:HB3	1:A:323:TRP:CH2	2.11	0.84
1:A:92:ARG:HH21	2:A:550:IHP:H2	1.02	0.84
1:A:117:LYS:HE3	1:A:120:THR:HG21	1.58	0.83
1:A:92:ARG:O	1:A:96:THR:HG23	1.79	0.83
1:A:73:LYS:HG3	1:A:76:GLU:CG	2.12	0.79
1:B:17:ASN:H	1:B:96:THR:HG21	1.48	0.79
1:B:257:GLN:HG3	5:B:602:HOH:O	1.81	0.79
1:B:73:LYS:HG3	5:B:765:HOH:O	1.82	0.79
1:A:130:THR:H	1:A:258:ASN:HD21	1.30	0.78
1:B:130:THR:H	1:B:258:ASN:HD21	1.30	0.78
1:A:17:ASN:H	1:A:96:THR:HG21	1.48	0.78
1:A:361:THR:HG21	5:A:539:HOH:O	1.82	0.77
1:A:92:ARG:HH21	2:A:550:IHP:C2	1.87	0.77
1:B:230:LYS:H	1:B:234:GLN:NE2	1.82	0.77
1:B:341:SER:H	1:B:344:GLN:HE21	1.32	0.77
1:B:361:THR:HG22	5:B:620:HOH:O	1.84	0.77
1:A:117:LYS:O	1:A:120:THR:OG1	2.03	0.77
1:A:137:ARG:CG	1:A:137:ARG:HH11	1.98	0.76
1:B:312:THR:HG23	1:B:312:THR:O	1.83	0.76
1:A:118[A]:MET:HE3	5:B:696:HOH:O	1.86	0.76
1:A:361:THR:HG22	5:A:552:HOH:O	1.88	0.74
1:B:183:ALA:HA	1:B:184:LYS:HE3	1.71	0.73
1:B:16:ALA:HA	1:B:96:THR:HG21	1.71	0.72
1:A:17:ASN:HD22	1:A:18:LEU:N	1.88	0.72
1:A:301:LYS:HA	1:A:301:LYS:HE2	1.72	0.71
1:B:269:LYS:HE2	5:B:641:HOH:O	1.89	0.71
1:B:66:LEU:HG	1:B:71:MET:HE3	1.72	0.71
1:B:246[A]:GLN:HE22	1:B:288:ASP:HB2	1.55	0.71
1:A:1:SER:HB3	1:A:323:TRP:CZ3	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HH22	2:A:550:IHP:C2	1.97	0.70
1:A:73:LYS:HE2	5:A:403:HOH:O	1.89	0.70
1:B:324:HIS:HD2	1:B:331:GLU:OE2	1.75	0.69
1:B:165[B]:ASN:OD1	5:B:627:HOH:O	2.11	0.69
1:B:92:ARG:O	1:B:96:THR:HG23	1.92	0.69
1:B:162:GLN:HG2	5:B:642:HOH:O	1.93	0.69
2:A:550:IHP:P2	2:A:550:IHP:H5	2.34	0.68
1:A:271:LEU:HD12	1:A:271:LEU:N	2.09	0.67
2:B:551:IHP:O42	2:B:551:IHP:H1	1.93	0.67
1:A:230:LYS:H	1:A:234:GLN:NE2	1.93	0.67
1:B:17:ASN:HD22	1:B:18:LEU:N	1.89	0.66
1:B:129:ILE:HD13	1:B:259:VAL:HG23	1.79	0.65
2:A:550:IHP:O42	2:A:550:IHP:C1	2.43	0.65
1:B:117:LYS:HD3	1:B:120:THR:HG21	1.80	0.64
1:B:190:ASP:HB2	1:B:193:LYS:HE2	1.80	0.64
1:A:301:LYS:HE3	1:A:365:LYS:HG2	1.79	0.63
1:B:246[B]:GLN:HG2	5:B:415:HOH:O	1.97	0.63
1:B:139:LYS:HE2	1:B:254:GLU:OE1	1.99	0.62
1:A:94[A]:VAL:CG2	1:B:107:GLY:HA2	2.24	0.62
1:A:137:ARG:HH11	1:A:137:ARG:HG3	1.64	0.62
1:A:137:ARG:HH21	1:A:191:TYR:N	1.97	0.61
1:A:118[A]:MET:CE	5:B:696:HOH:O	2.45	0.60
1:A:231:THR:HG22	1:A:234:GLN:N	2.10	0.60
1:B:190:ASP:CB	1:B:193:LYS:HE2	2.32	0.60
1:A:47:LEU:HD13	1:A:96:THR:HG22	1.83	0.60
1:B:142:LYS:HD2	5:B:431:HOH:O	2.02	0.59
1:A:1:SER:CB	1:A:323:TRP:CZ3	2.86	0.59
1:A:76:GLU:HB3	5:A:712:HOH:O	2.01	0.59
1:A:137:ARG:NH1	1:A:137:ARG:HG2	2.19	0.58
1:B:29[B]:LEU:HD23	1:B:207:LEU:HD13	1.84	0.58
1:B:186:THR:HG23	5:B:575:HOH:O	2.02	0.58
1:B:197:VAL:HG22	1:B:249:LEU:HD21	1.84	0.58
1:B:370:ASP:HB2	5:B:426:HOH:O	2.03	0.58
1:A:109:ASP:OD2	1:B:114:HIS:HE1	1.86	0.57
1:B:17:ASN:N	1:B:96:THR:HG21	2.17	0.56
1:A:137:ARG:CG	1:A:137:ARG:NH1	2.61	0.56
1:B:29[A]:LEU:HD13	5:B:560:HOH:O	2.06	0.56
1:A:247:ASP:O	1:A:251:THR:HB	2.06	0.56
1:A:135:GLU:HB3	5:A:543:HOH:O	2.04	0.55
1:B:247:ASP:O	1:B:251:THR:HB	2.05	0.55
1:B:16:ALA:CA	1:B:96:THR:HG21	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:550:IHP:H5	2:A:550:IHP:O32	2.06	0.55
1:A:36:GLN:HG2	5:A:516:HOH:O	2.07	0.55
1:A:17:ASN:ND2	1:A:18:LEU:H	1.99	0.55
1:A:116[A]:GLU:HG3	5:A:590:HOH:O	2.05	0.55
1:B:47:LEU:HD21	1:B:96:THR:HG22	1.89	0.55
1:B:17:ASN:ND2	1:B:18:LEU:H	1.91	0.53
1:A:2:PRO:O	1:A:5:TYR:HB2	2.08	0.53
2:A:550:IHP:O42	2:A:550:IHP:C6	2.56	0.53
1:A:17:ASN:N	1:A:96:THR:HG21	2.22	0.52
1:A:173:LYS:HE2	5:A:727:HOH:O	2.10	0.52
1:A:114:HIS:NE2	1:A:118[A]:MET:CE	2.72	0.52
1:A:306:HIS:ND1	1:A:307:ASP:OD1	2.36	0.52
1:B:312:THR:HG22	5:B:490:HOH:O	2.09	0.52
1:A:114:HIS:NE2	1:A:118[A]:MET:HE2	2.25	0.51
1:A:130:THR:N	1:A:258:ASN:HD21	2.05	0.51
1:B:78:PRO:HG2	5:B:633:HOH:O	2.10	0.51
1:A:301:LYS:HE2	1:A:302:PRO:HD2	1.92	0.51
1:A:257:GLN:HG2	5:A:477:HOH:O	2.10	0.51
1:A:117:LYS:HG2	1:A:120:THR:OG1	2.10	0.51
1:A:167:ALA:O	1:A:173:LYS:HE3	2.11	0.51
1:B:202:LYS:HD2	5:B:497:HOH:O	2.10	0.51
1:B:234:GLN:O	1:B:237[A]:VAL:HG22	2.10	0.51
1:B:113:HIS:ND1	5:B:536:HOH:O	2.34	0.51
1:B:92:ARG:O	1:B:96:THR:CG2	2.58	0.50
1:B:130:THR:N	1:B:258:ASN:HD21	2.06	0.50
1:B:295:LEU:HD12	1:B:300:PHE:CE1	2.45	0.50
1:A:301:LYS:HE3	1:A:365:LYS:CG	2.41	0.50
1:B:68:GLN:HE21	1:B:69:GLN:HE21	1.58	0.50
1:A:132:ASN:HB2	5:A:672:HOH:O	2.12	0.50
1:A:271:LEU:N	1:A:271:LEU:CD1	2.75	0.49
1:A:114:HIS:HD2	1:A:115:GLN:O	1.95	0.49
1:A:142:LYS:O	1:A:146:THR:OG1	2.19	0.49
1:A:230:LYS:H	1:A:234:GLN:HE22	1.56	0.49
1:B:230:LYS:H	1:B:234:GLN:HE22	1.55	0.49
1:A:291:ILE:HG22	1:A:295:LEU:HD22	1.95	0.49
1:A:149:GLN:HG3	5:A:604:HOH:O	2.12	0.49
1:B:3:GLU:O	1:B:3:GLU:HG2	2.12	0.49
1:A:114:HIS:HE1	1:B:109:ASP:OD2	1.96	0.49
1:A:92:ARG:HH22	2:A:550:IHP:C1	2.25	0.49
1:A:137:ARG:NH2	1:A:191:TYR:N	2.60	0.49
1:B:17:ASN:H	1:B:96:THR:CG2	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94[A]:VAL:HG23	1:A:95:ALA:N	2.28	0.48
1:B:236:ARG:HD3	5:B:585:HOH:O	2.13	0.48
1:B:129:ILE:HD13	1:B:259:VAL:CG2	2.42	0.48
1:B:312:THR:O	1:B:312:THR:CG2	2.57	0.47
2:A:550:IHP:O42	2:A:550:IHP:O16	2.32	0.47
1:B:129:ILE:HA	1:B:258:ASN:ND2	2.29	0.47
1:B:7:LEU:O	1:B:71:MET:HG3	2.14	0.47
1:A:258:ASN:HA	1:A:261:LYS:NZ	2.30	0.47
1:A:282:THR:HG22	1:A:284[A]:LEU:HD22	1.96	0.47
1:A:94[A]:VAL:HG23	1:B:107:GLY:CA	2.29	0.46
1:A:192:GLU:C	1:A:193:LYS:HE3	2.35	0.46
1:B:187:PHE:CD1	1:B:197:VAL:HG13	2.50	0.46
1:A:117:LYS:HG2	1:A:120:THR:CG2	2.46	0.46
1:A:246:GLN:HE22	1:A:288:ASP:HB2	1.80	0.46
1:B:183:ALA:HB3	1:B:200:PRO:HG3	1.98	0.45
1:A:113:HIS:CE1	5:A:500:HOH:O	2.69	0.45
1:A:113:HIS:HE1	5:A:500:HOH:O	1.99	0.45
1:B:166:TYR:CE1	1:B:180:LEU:HD13	2.52	0.45
1:B:233[B]:GLN:HG3	5:B:607:HOH:O	2.15	0.45
1:A:3:GLU:H	1:A:3:GLU:HG2	1.33	0.45
1:A:28:VAL:HG12	5:A:417:HOH:O	2.16	0.45
1:A:173:LYS:HA	1:A:173:LYS:HD3	1.58	0.44
1:A:236:ARG:NH1	5:A:464:HOH:O	2.48	0.44
1:A:73:LYS:H	1:A:73:LYS:HG2	1.37	0.44
1:B:68:GLN:HE21	1:B:69:GLN:NE2	2.14	0.44
1:B:341:SER:H	1:B:344:GLN:NE2	2.07	0.44
1:A:145:GLU:O	1:A:149:GLN:HG3	2.18	0.44
1:A:137:ARG:CZ	1:A:189:ALA:O	2.66	0.44
1:B:98:GLN:HG2	5:B:534:HOH:O	2.17	0.44
1:A:2:PRO:HD2	1:A:5:TYR:CD1	2.53	0.44
1:A:117:LYS:HG2	1:A:120:THR:HG21	2.00	0.43
1:B:36:GLN:HG3	5:B:733:HOH:O	2.18	0.43
1:B:288:ASP:HB2	1:B:312:THR:HG21	2.00	0.43
1:A:157:TYR:CD1	1:A:180:LEU:HB3	2.53	0.43
1:A:137:ARG:HH11	1:A:137:ARG:HG2	1.72	0.43
1:A:202[A]:LYS:HD2	1:A:245:TYR:CE1	2.54	0.43
1:B:16:ALA:HA	1:B:96:THR:CG2	2.46	0.43
1:A:192:GLU:O	1:A:193:LYS:HE3	2.18	0.43
1:A:363:GLU:HG3	1:A:369:VAL:HG13	2.01	0.43
1:A:12:ILE:CG2	1:A:317:LYS:HG2	2.49	0.43
1:B:195:PRO:HG3	1:B:255:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:VAL:HG23	1:B:207:LEU:HD22	2.01	0.43
1:B:114:HIS:HD2	1:B:115:GLN:O	2.02	0.42
1:B:129:ILE:HA	1:B:258:ASN:HD21	1.84	0.42
1:B:65:TRP:CE3	1:B:66:LEU:HD13	2.54	0.42
1:A:143:ALA:HB1	1:A:252:SER:HB2	2.01	0.42
1:A:282:THR:HG22	1:A:284[A]:LEU:CD2	2.50	0.42
1:A:308:GLN:HE21	1:A:310:GLU:H	1.68	0.42
1:B:58[A]:MET:CE	1:B:58[A]:MET:HA	2.49	0.42
1:A:114:HIS:CE1	1:A:118[A]:MET:HE1	2.55	0.42
1:B:66:LEU:HG	1:B:71:MET:CE	2.44	0.42
1:A:277:LYS:HA	1:A:277:LYS:HD3	1.95	0.41
1:B:18:LEU:O	1:B:47:LEU:HD22	2.19	0.41
1:A:246:GLN:NE2	1:A:288:ASP:HB2	2.36	0.41
2:A:550:IHP:O25	2:A:550:IHP:O14	2.38	0.41
1:A:202[A]:LYS:HD2	1:A:245:TYR:OH	2.19	0.41
1:B:144:MET:CE	1:B:249:LEU:HD23	2.50	0.41
1:B:65:TRP:O	1:B:69:GLN:HG2	2.20	0.41
1:B:54:LEU:HD13	1:B:345:LEU:HD22	2.02	0.41
1:B:295:LEU:HD12	1:B:300:PHE:CD1	2.55	0.41
1:B:109:ASP:HB3	5:B:736:HOH:O	2.20	0.41
1:B:290:ASN:O	1:B:294:LEU:HB2	2.20	0.41
1:A:192:GLU:HB3	5:A:625:HOH:O	2.20	0.41
1:B:144:MET:HE3	1:B:249:LEU:CD2	2.51	0.40
2:B:551:IHP:O42	2:B:551:IHP:O31	2.38	0.40
1:A:94[A]:VAL:CG2	1:B:107:GLY:CA	2.96	0.40
1:B:47:LEU:CD2	1:B:96:THR:HG22	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ALA:O	1:A:116[B]:GLU:OE2[2_555]	1.89	0.31

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	393/398 (99%)	383 (98%)	9 (2%)	1 (0%)	41	30
1	B	397/398 (100%)	389 (98%)	8 (2%)	0	100	100
All	All	790/796 (99%)	772 (98%)	17 (2%)	1 (0%)	51	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	LYS

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	339/341 (99%)	304 (90%)	35 (10%)	7	2
1	B	342/341 (100%)	316 (92%)	26 (8%)	13	4
All	All	681/682 (100%)	620 (91%)	61 (9%)	10	3

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	10	VAL
1	A	17	ASN
1	A	19	ARG
1	A	28	VAL
1	A	36	GLN
1	A	41	GLU
1	A	66	LEU
1	A	73	LYS
1	A	96	THR
1	A	116[A]	GLU
1	A	116[B]	GLU

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Mol	Chain	Res	Type
1	A	130	THR
1	A	132	ASN
1	A	137	ARG
1	A	158	LYS
1	A	159	LEU
1	A	160	LEU
1	A	180	LEU
1	A	193	LYS
1	A	202[A]	LYS
1	A	202[B]	LYS
1	A	213	LEU
1	A	231	THR
1	A	232	ASP
1	A	233	GLN
1	A	237	VAL
1	A	251	THR
1	A	254	GLU
1	A	295	LEU
1	A	308	GLN
1	A	337	TYR
1	A	354	GLN
1	A	361	THR
1	A	378	ASP
1	B	17	ASN
1	B	22	LEU
1	B	47	LEU
1	B	66	LEU
1	B	73	LYS
1	B	96	THR
1	B	126	ASN
1	B	138	GLU
1	B	150	LYS
1	B	154	THR
1	B	165[A]	ASN
1	B	165[B]	ASN
1	B	170	PRO
1	B	180	LEU
1	B	184	LYS
1	B	197	VAL
1	B	207	LEU
1	B	213	LEU
1	B	253	THR

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Mol	Chain	Res	Type
1	B	259	VAL
1	B	294	LEU
1	B	295	LEU
1	B	337	TYR
1	B	354	GLN
1	B	361	THR
1	B	364	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	113	HIS
1	A	114	HIS
1	A	126	ASN
1	A	165	ASN
1	A	234	GLN
1	A	246	GLN
1	A	258	ASN
1	A	275	GLN
1	A	308	GLN
1	A	324	HIS
1	A	347	ASN
1	A	372	ASN
1	B	17	ASN
1	B	68	GLN
1	B	114	HIS
1	B	126	ASN
1	B	234	GLN
1	B	258	ASN
1	B	324	HIS
1	B	344	GLN
1	B	347	ASN
1	B	386	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	A	550	-	36,36,36	1.79	11 (30%)	54,60,60	1.78	13 (24%)
2	IHP	B	551	-	36,36,36	1.30	6 (16%)	54,60,60	1.66	12 (22%)
3	PO4	A	399	-	4,4,4	1.21	0	6,6,6	1.21	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
2	IHP	A	550	-	-	11/30/54/54	0/1/1/1
2	IHP	B	551	-	-	9/30/54/54	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	550	IHP	P6-O16	4.53	1.67	1.59
2	A	550	IHP	P3-O13	3.87	1.66	1.59
2	A	550	IHP	C5-C4	3.48	1.59	1.52
2	A	550	IHP	P5-O15	3.27	1.65	1.59
2	A	550	IHP	C3-C2	2.94	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	550	IHP	C2-C1	2.84	1.58	1.52
2	B	551	IHP	P4-O14	2.64	1.64	1.59
2	A	550	IHP	P1-O11	2.63	1.64	1.59
2	B	551	IHP	P5-O15	2.45	1.63	1.59
2	A	550	IHP	O13-C3	2.35	1.52	1.44
2	B	551	IHP	P3-O13	2.30	1.63	1.59
2	A	550	IHP	C6-C1	2.29	1.57	1.52
2	B	551	IHP	C5-C4	2.27	1.56	1.52
2	B	551	IHP	P3-O33	-2.18	1.46	1.54
2	B	551	IHP	P2-O12	2.17	1.63	1.59
2	A	550	IHP	C6-C5	2.12	1.56	1.52
2	A	550	IHP	C4-C3	2.07	1.56	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	550	IHP	C3-C2-C1	5.13	121.64	110.41
2	A	550	IHP	C6-C5-C4	4.71	120.72	110.41
2	B	551	IHP	O13-P3-O23	-4.50	92.03	109.39
2	A	550	IHP	O11-C1-C6	4.18	118.54	108.69
2	B	551	IHP	C6-C5-C4	4.12	119.43	110.41
2	B	551	IHP	C5-C6-C1	3.80	118.72	110.41
2	A	550	IHP	O13-C3-C2	3.76	117.55	108.69
2	A	550	IHP	O15-C5-C4	3.07	115.92	108.69
2	B	551	IHP	O42-P2-O32	3.05	119.31	107.64
2	A	550	IHP	C5-C4-C3	2.86	116.67	110.41
2	B	551	IHP	O43-P3-O13	-2.69	93.95	105.99
2	A	550	IHP	O45-P5-O35	2.63	117.68	107.64
2	B	551	IHP	O14-C4-C5	2.53	114.64	108.69
2	B	551	IHP	O33-P3-O23	2.39	120.05	110.68
2	A	550	IHP	O46-P6-O36	2.38	116.72	107.64
2	A	550	IHP	O11-P1-O21	-2.36	100.28	109.39
2	A	550	IHP	O42-P2-O32	2.35	116.60	107.64
2	B	551	IHP	O15-P5-O25	-2.32	100.43	109.39
2	B	551	IHP	O43-P3-O23	2.31	119.74	110.68
2	A	550	IHP	C6-C1-C2	2.26	115.35	110.41
2	A	550	IHP	O13-C3-C4	2.23	113.94	108.69
2	B	551	IHP	C6-C1-C2	2.21	115.25	110.41
2	A	550	IHP	O12-C2-C3	2.20	113.86	108.69
2	B	551	IHP	O11-C1-C2	2.02	113.45	108.69
2	B	551	IHP	O45-P5-O35	2.01	115.33	107.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	550	IHP	C1-C2-O12-P2
2	A	550	IHP	C4-C5-O15-P5
2	A	550	IHP	C2-O12-P2-O22
2	A	550	IHP	C6-O16-P6-O26
2	B	551	IHP	C1-C2-O12-P2
2	B	551	IHP	C3-C4-O14-P4
2	B	551	IHP	C5-C4-O14-P4
2	B	551	IHP	C6-C5-O15-P5
2	B	551	IHP	C2-O12-P2-O22
2	B	551	IHP	C4-O14-P4-O24
2	B	551	IHP	C5-O15-P5-O25
2	B	551	IHP	C1-C6-O16-P6
2	A	550	IHP	C3-O13-P3-O33
2	B	551	IHP	C5-O15-P5-O45
2	A	550	IHP	C6-C1-O11-P1
2	A	550	IHP	C3-C4-O14-P4
2	A	550	IHP	C1-O11-P1-O21
2	A	550	IHP	C1-O11-P1-O31
2	A	550	IHP	C1-O11-P1-O41
2	A	550	IHP	C6-O16-P6-O36

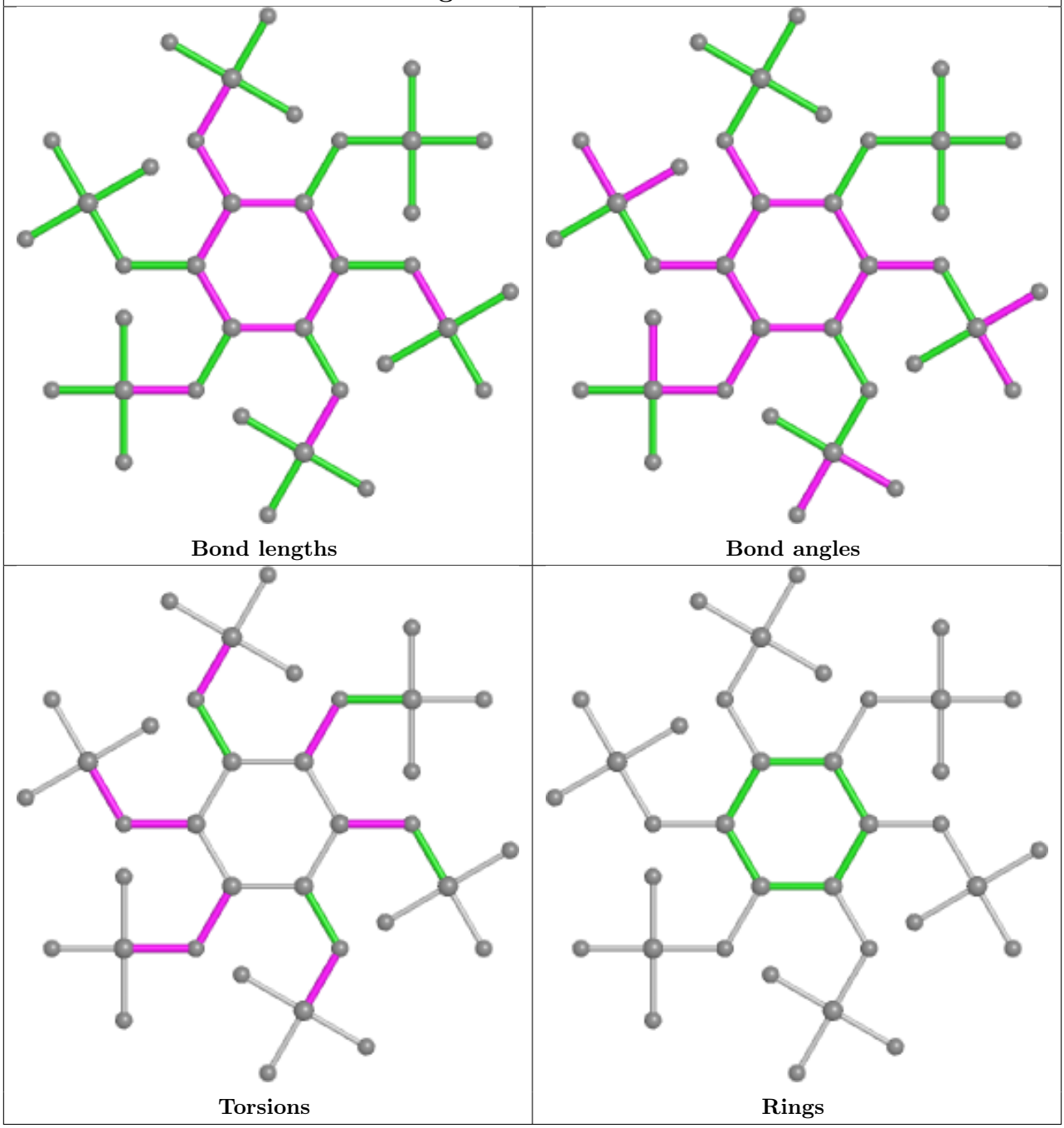
There are no ring outliers.

2 monomers are involved in 16 short contacts:

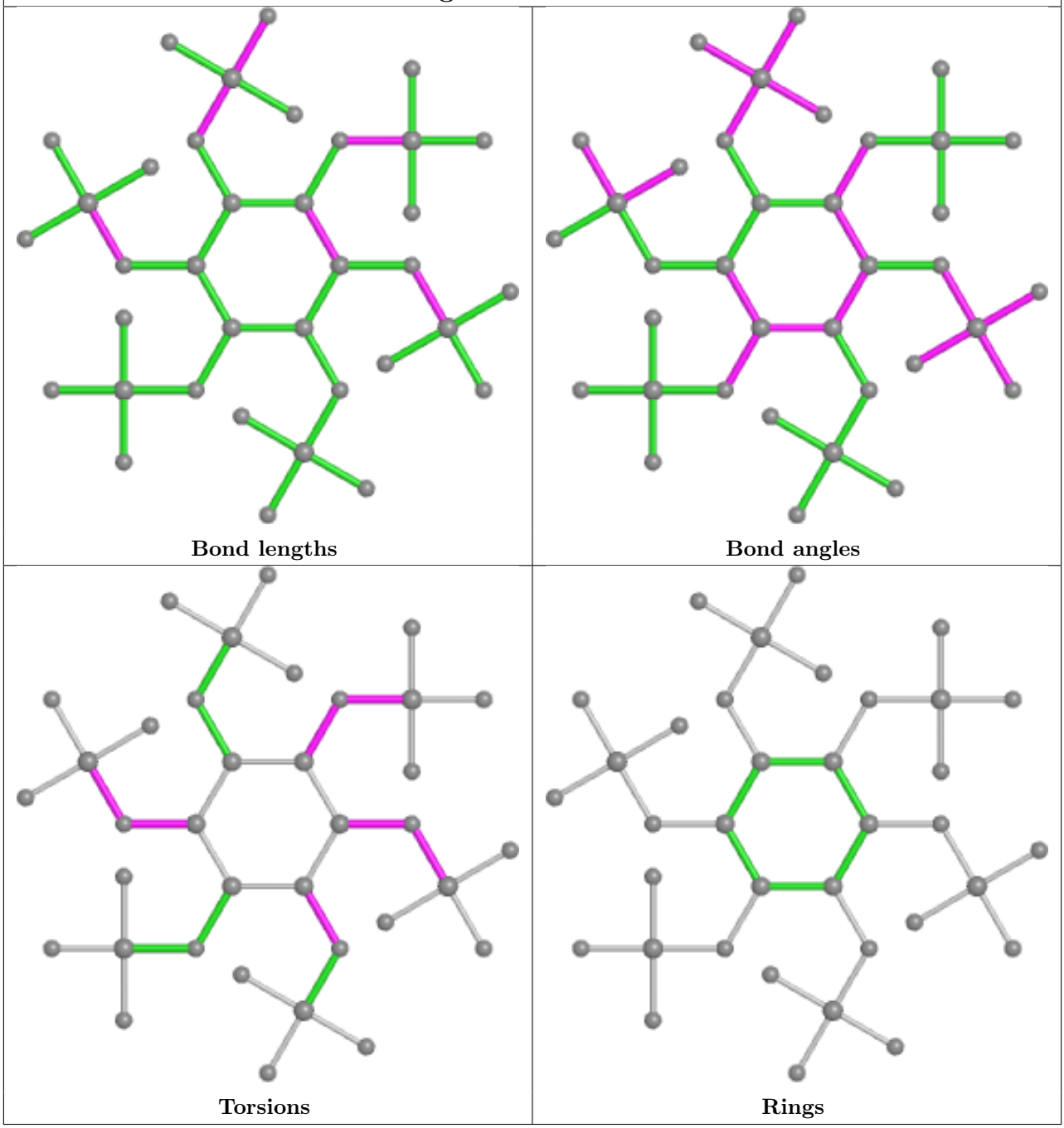
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	550	IHP	14	0
2	B	551	IHP	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand IHP A 550



Ligand IHP B 551



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	388/398 (97%)	-0.14	3 (0%)	86	87	12, 23, 42, 54	0
1	B	387/398 (97%)	-0.32	1 (0%)	94	94	12, 22, 34, 47	0
All	All	775/796 (97%)	-0.23	4 (0%)	91	91	12, 22, 40, 54	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	LYS	2.5
1	A	149	GLN	2.3
1	A	386	ASN	2.3
1	B	389	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IHP	B	551	36/36	0.78	0.41	36,79,88,89	30

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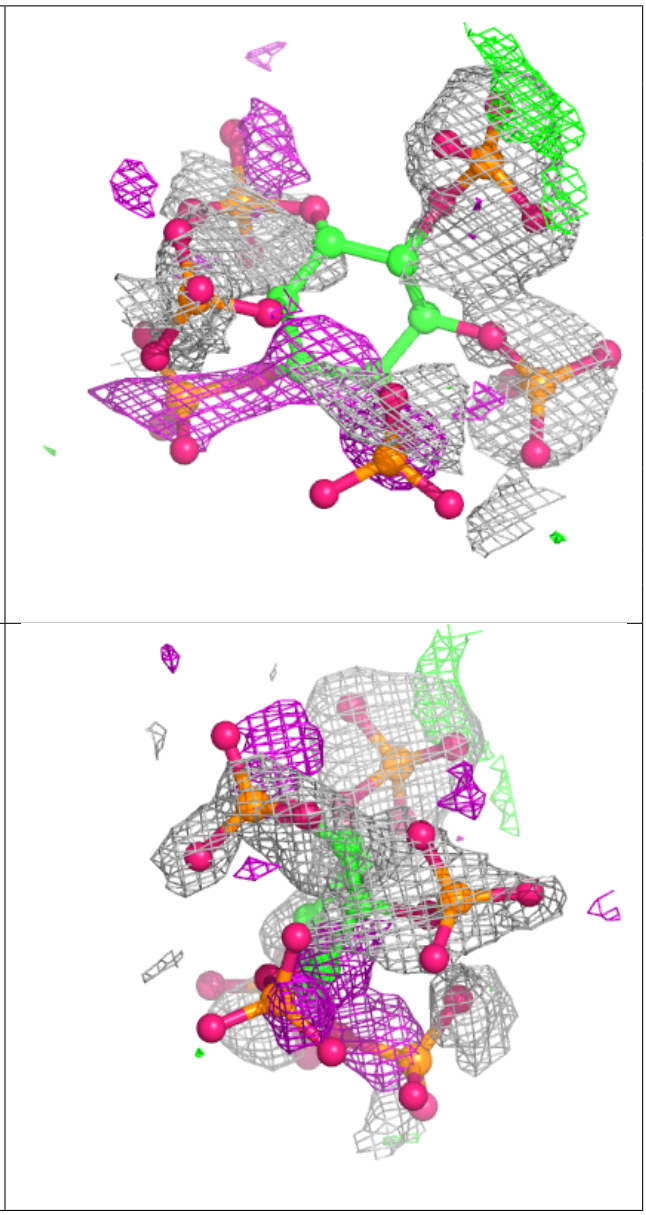
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IHP	A	550	36/36	0.82	0.27	25,56,64,64	30
4	CA	B	399	1/1	0.94	0.07	42,42,42,42	0
3	PO4	A	399	5/5	0.96	0.16	28,35,39,46	0

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.

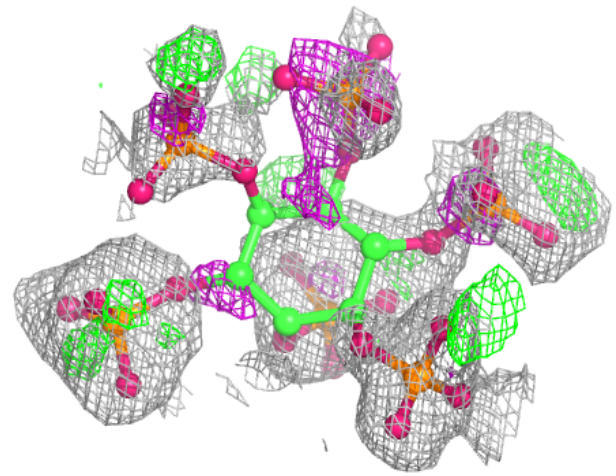
Electron density around IHP B 551:

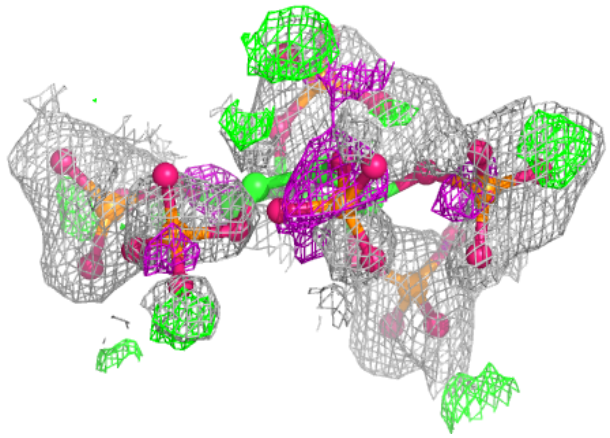
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

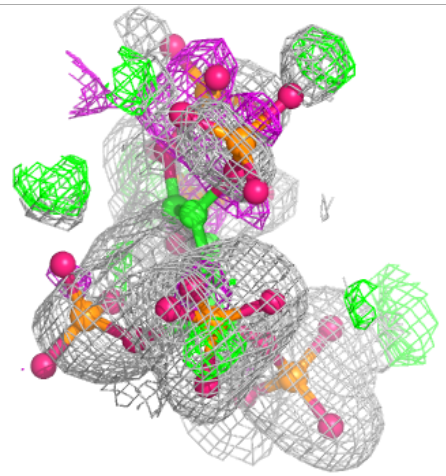


Electron density around IHP A 550:

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.