



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 01:53 AM GMT

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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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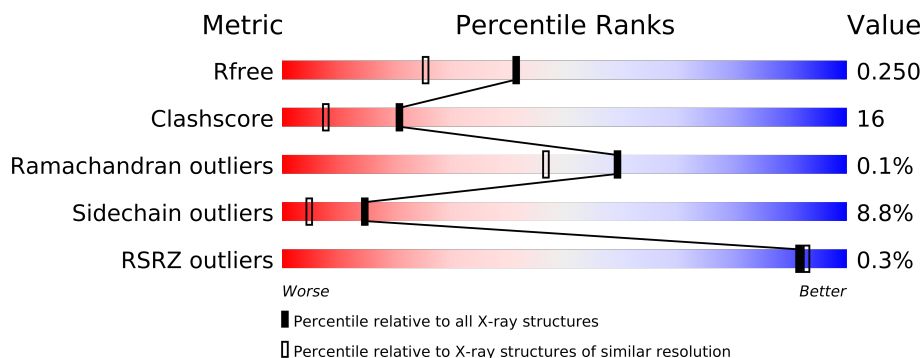
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	5260 (1.90-1.86)
Clashscore	79885	6268 (1.90-1.86)
Ramachandran outliers	78287	6195 (1.90-1.86)
Sidechain outliers	78261	6196 (1.90-1.86)
RSRZ outliers	66119	5262 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	398	
1	B	398	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	IHP	A	550	-	X
2	IHP	B	551	-	X
3	PO4	A	399	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6947 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

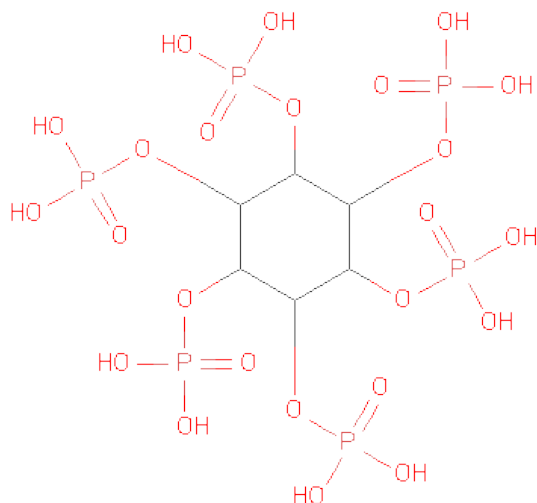
- Molecule 1 is a protein called Acid glucose-1-phosphate phosphatase.

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

There are 22 discrepancies between the modelled and reference sequences:

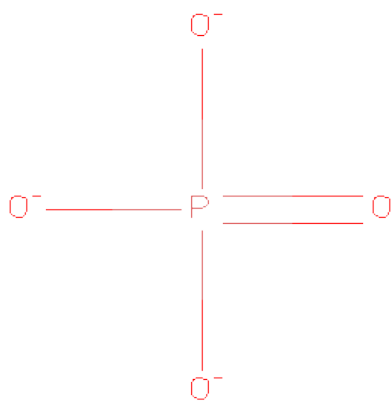
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q6EV19
A	16	ALA	HIS	ENGINEERED MUTATION	UNP Q6EV19
A	390	ARG	-	EXPRESSION TAG	UNP Q6EV19
A	391	SER	-	EXPRESSION TAG	UNP Q6EV19
A	392	GLY	-	EXPRESSION TAG	UNP Q6EV19
A	393	HIS	-	EXPRESSION TAG	UNP Q6EV19
A	394	HIS	-	EXPRESSION 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:  $\text{O}_4\text{P}$ ).



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
4	B	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

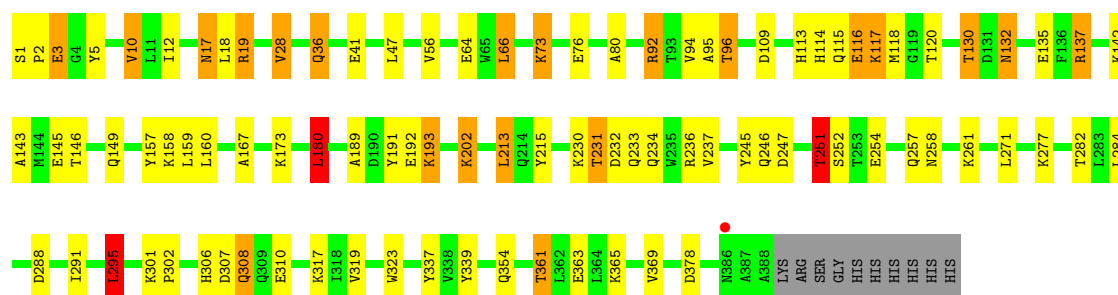
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	336	Total 336	O 336	0	0
5	B	370	Total 370	O 370	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

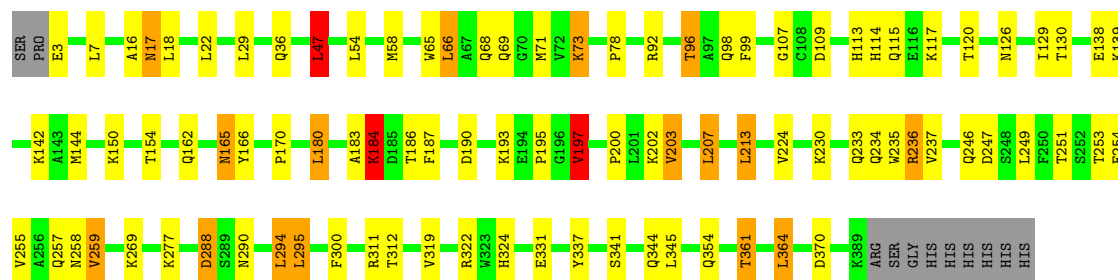
- Molecule 1: Acid glucose-1-phosphate phosphatase

Chain A: 



- Molecule 1: Acid glucose-1-phosphate phosphatase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.74 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.181 , 0.250 0.181 , 0.250	Depositor DCC
$R_{free}$ test set	2978 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 31.9	EDS
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 58835 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6947	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, IHP, CA

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(°)	Ideal(°)
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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	1
5	B	370	0	0	23	1
All	All	6947	0	6117	193	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (193) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:H1	2:A:550:IHP:O42	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:B:17:ASN:H	1:B:96:THR:HG21	1.48	0.79
1:A:73:LYS:HG3	1:A:76:GLU:CG	2.12	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:HH11	1:A:137:ARG:CG	1.98	0.76
1:B:312:THR:O	1:B:312:THR:HG23	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:246[A]:GLN:HE22	1:B:288:ASP:HB2	1.55	0.71
1:B:66:LEU:HG	1:B:71:MET:HE3	1.72	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1:SER:HB3	1:A:323:TRP:CZ3	2.26	0.70
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:H5	2:A:550:IHP:P2	2.34	0.68
1:A:271:LEU:HD12	1:A:271:LEU:N	2.09	0.67
2:B:551:IHP:H1	2:B:551:IHP:O42	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:C1	2:A:550:IHP:O42	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:B:246[B]:GLN:HG2	5:B:415:HOH:O	1.97	0.63
1:A:301:LYS:HE3	1:A:365:LYS:HG2	1.79	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:231:THR:HG22	1:A:234:GLN:N	2.10	0.60
1:A:118[A]:MET:CE	5:B:696:HOH:O	2.45	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:186:THR:HG23	5:B:575:HOH:O	2.02	0.58
1:B:29[B]:LEU:HD23	1:B:207:LEU:HD13	1.84	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:NH1	1:A:137:ARG:CG	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	Distance(Å)	Clash(Å)
2:A:550:IHP:O32	2:A:550:IHP:H5	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:B:47:LEU:HD21	1:B:96:THR:HG22	1.89	0.55
1:A:116[A]:GLU:HG3	5:A:590:HOH:O	2.05	0.55
1:B:17:ASN:ND2	1:B:18:LEU:H	1.91	0.53
2:A:550:IHP:C6	2:A:550:IHP:O42	2.56	0.53
1:A:2:PRO:O	1:A:5:TYR:HB2	2.08	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:130:THR:N	1:A:258:ASN:HD21	2.05	0.51
1:A:114:HIS:NE2	1:A:118[A]:MET:HE2	2.25	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:CD1	1:A:271:LEU:N	2.75	0.49
1:A:230:LYS:H	1:A:234:GLN:HE22	1.56	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: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:B:17:ASN:H	1:B:96:THR:CG2	2.24	0.49
1:A:137:ARG:NH2	1:A:191:TYR:N	2.60	0.49
1:A:94[A]:VAL:HG23	1:A:95:ALA:N	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:O16	2:A:550:IHP:O42	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:B:187:PHE:CD1	1:B:197:VAL:HG13	2.50	0.46
1:A:192:GLU:C	1:A:193:LYS:HE3	2.35	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:HD3	1:A:173:LYS:HA	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:341:SER:H	1:B:344:GLN:NE2	2.07	0.44
1:B:68:GLN:HE21	1:B:69:GLN:NE2	2.14	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:B:203:VAL:HG23	1:B:207:LEU:HD22	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
1:B:114:HIS:HD2	1:B:115:GLN:O	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:A:550:IHP:O14	2:A:550:IHP:O25	2.38	0.41
1:A:246:GLN:NE2	1:A:288:ASP:HB2	2.36	0.41
1:B:144:MET:CE	1:B:249:LEU:HD23	2.50	0.41
1:A:202[A]:LYS:HD2	1:A:245:TYR:OH	2.19	0.41
1:B:65:TRP:O	1:B:69:GLN:HG2	2.20	0.41
1:B:295:LEU:HD12	1:B:300:PHE:CD1	2.55	0.41
1:B:54:LEU:HD13	1:B:345:LEU:HD22	2.02	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:O31	2:B:551:IHP:O42	2.38	0.40
1:B:47:LEU:CD2	1:B:96:THR:HG22	2.51	0.40
1:A:94[A]:VAL:CG2	1:B:107:GLY:CA	2.96	0.40

All (2) 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	Distance(Å)	Clash(Å)
5:A:698:HOH:O	5:B:719:HOH:O[6_454]	1.54	0.66
1:A:80:ALA:O	1:A:116[B]:GLU:OE2[2_555]	1.89	0.31

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	393/398 (99%)	383 (98%)	9 (2%)	1 (0%)	50	36
1	B	397/398 (100%)	389 (98%)	8 (2%)	0	100	100
All	All	790/796 (99%)	772 (98%)	17 (2%)	1 (0%)	59	47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/341 (99%)	304 (90%)	35 (10%)	10	3
1	B	342/341 (100%)	316 (92%)	26 (8%)	19	7
All	All	681/682 (100%)	620 (91%)	61 (9%)	14	4

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
1	A	130	THR
1	A	132	ASN
1	A	137	ARG
1	A	158	LYS

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Mol	Chain	Res	Type
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
1	B	259	VAL
1	B	294	LEU
1	B	295	LEU
1	B	337	TYR

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Mol	Chain	Res	Type
1	B	354	GLN
1	B	361	THR
1	B	364	LEU

Some 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 ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
3	PO4	A	399	-	4,4,4	0.41	0	6,6,6	0.33	0
2	IHP	A	550	-	36,36,36	1.50	9 (25%)	60,60,60	2.52	18 (30%)
2	IHP	B	551	-	36,36,36	1.05	2 (5%)	60,60,60	1.97	17 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	399	-	-	0/0/0/0	0/0/0/0
2	IHP	A	550	-	-	0/30/54/54	1/1/1/1
2	IHP	B	551	-	-	0/30/54/54	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	550	IHP	C5-C4	3.61	1.59	1.52
2	A	550	IHP	C3-C2	3.05	1.58	1.52
2	A	550	IHP	C2-C1	2.95	1.58	1.52
2	A	550	IHP	O13-C3	2.71	1.52	1.44
2	A	550	IHP	P6-O16	2.59	1.67	1.59
2	A	550	IHP	C6-C1	2.38	1.57	1.52
2	B	551	IHP	C5-C4	2.36	1.56	1.52
2	B	551	IHP	P3-O33	-2.26	1.46	1.54
2	A	550	IHP	C6-C5	2.20	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	550	IHP	P3-O13	2.19	1.66	1.59
2	A	550	IHP	C4-C3	2.15	1.56	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	550	IHP	P3-O13-C3	9.76	142.50	121.96
2	A	550	IHP	P1-O11-C1	5.60	133.75	121.96
2	A	550	IHP	C3-C2-C1	5.46	121.64	110.44
2	B	551	IHP	O13-P3-O23	-5.28	92.03	106.79
2	A	550	IHP	C6-C5-C4	5.01	120.72	110.44
2	A	550	IHP	O11-C1-C6	4.89	118.54	108.45
2	B	551	IHP	O43-P3-O13	-4.56	93.95	107.09
2	A	550	IHP	O13-C3-C2	4.41	117.55	108.45
2	B	551	IHP	C6-C5-C4	4.38	119.43	110.44
2	B	551	IHP	C5-C6-C1	4.04	118.72	110.44
2	A	550	IHP	P6-O16-C6	4.02	130.43	121.96
2	A	550	IHP	P5-O15-C5	3.98	130.33	121.96
2	A	550	IHP	O15-C5-C4	3.62	115.92	108.45
2	B	551	IHP	P5-O15-C5	3.33	128.97	121.96
2	A	550	IHP	C5-C4-C3	3.04	116.67	110.44
2	B	551	IHP	O42-P2-O32	3.00	119.31	107.61
2	B	551	IHP	O14-C4-C5	3.00	114.64	108.45
2	B	551	IHP	O33-P3-O23	2.94	120.05	110.44
2	B	551	IHP	P3-O13-C3	2.85	127.96	121.96
2	B	551	IHP	O43-P3-O23	2.84	119.74	110.44
2	B	551	IHP	O32-P2-O12	-2.70	99.31	107.09
2	A	550	IHP	O13-C3-C4	2.66	113.94	108.45
2	A	550	IHP	O12-C2-C3	2.62	113.86	108.45
2	A	550	IHP	O45-P5-O35	2.59	117.68	107.61
2	A	550	IHP	O32-P2-O12	-2.53	99.80	107.09
2	B	551	IHP	O11-C1-C2	2.43	113.45	108.45
2	A	550	IHP	C6-C1-C2	2.39	115.35	110.44
2	B	551	IHP	C6-C1-C2	2.34	115.25	110.44
2	A	550	IHP	O46-P6-O36	2.34	116.72	107.61
2	A	550	IHP	O11-P1-O21	-2.33	100.28	106.79
2	A	550	IHP	O42-P2-O32	2.31	116.60	107.61
2	B	551	IHP	P4-O14-C4	2.28	126.76	121.96
2	B	551	IHP	O15-P5-O25	-2.28	100.43	106.79
2	B	551	IHP	O12-C2-C3	2.18	112.95	108.45
2	B	551	IHP	C5-C4-C3	2.01	114.56	110.44

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	550	IHP	C1-C2-C3-C4-C5-C6

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	388/398 (97%)	-0.12	1 (0%) 91 93	12, 23, 42, 54	0
1	B	387/398 (97%)	-0.27	0 100 100	12, 22, 34, 47	0
All	All	775/796 (97%)	-0.19	1 (0%) 91 94	12, 22, 40, 54	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	386	ASN	2.2

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	IHP	B	551	36/36	0.35	9.26	36,79,88,89	30
2	IHP	A	550	36/36	0.25	6.21	25,56,64,64	30

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	A	399	5/5	0.15	4.47	28,35,39,46	0
4	CA	B	399	1/1	0.07	-0.39	42,42,42,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.