



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:04 PM UTC

PDB ID : 1IXP / pdb_00001ixp
Title : Enzyme-phosphate Complex of Pyridoxine 5'-Phosphate synthase
Authors : Garrido-Franco, M.; Laber, B.; Huber, R.; Clausen, T.
Deposited on : 2002-06-28
Resolution : 2.30 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
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

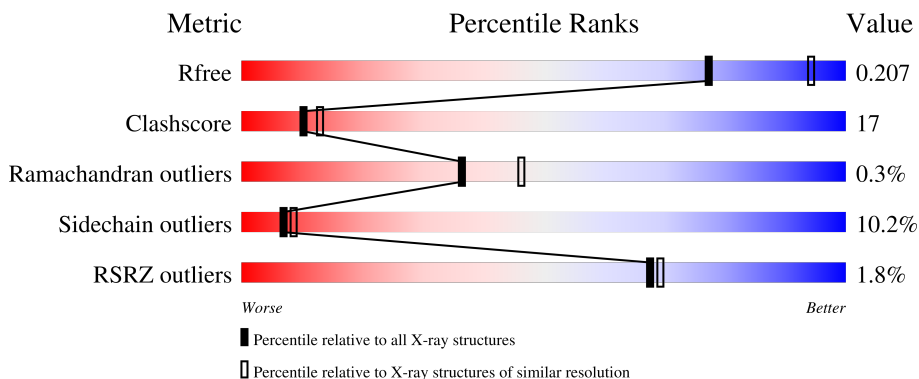
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	242	
1	B	242	
1	C	242	
1	D	242	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7882 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 Pyridoxine 5'-Phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1825	1131	333	349	12			
1	B	242	Total	C	N	O	S	0	0	0
			1821	1129	332	348	12			
1	C	242	Total	C	N	O	S	0	0	0
			1825	1131	333	349	12			
1	D	242	Total	C	N	O	S	0	0	0
			1827	1132	333	350	12			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

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

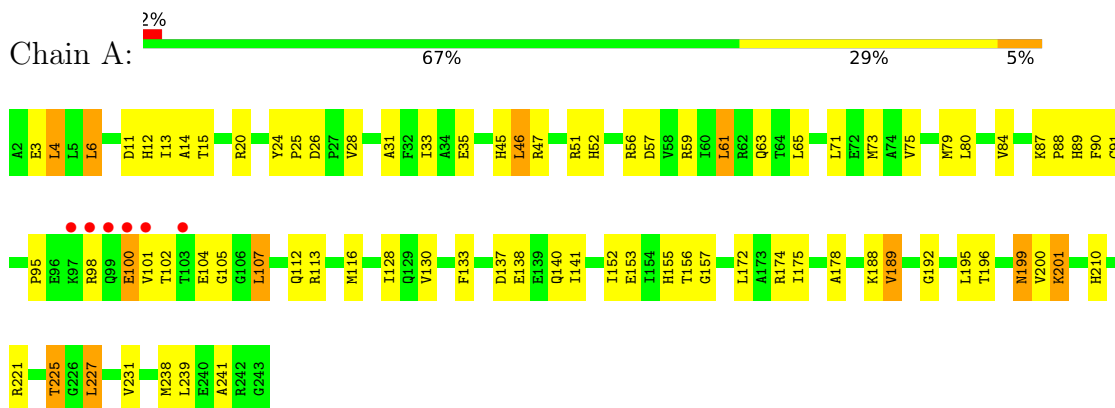
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	125	Total	O	0	0
			125	125		
3	B	128	Total	O	0	0
			128	128		
3	C	139	Total	O	0	0
			139	139		
3	D	152	Total	O	0	0
			152	152		

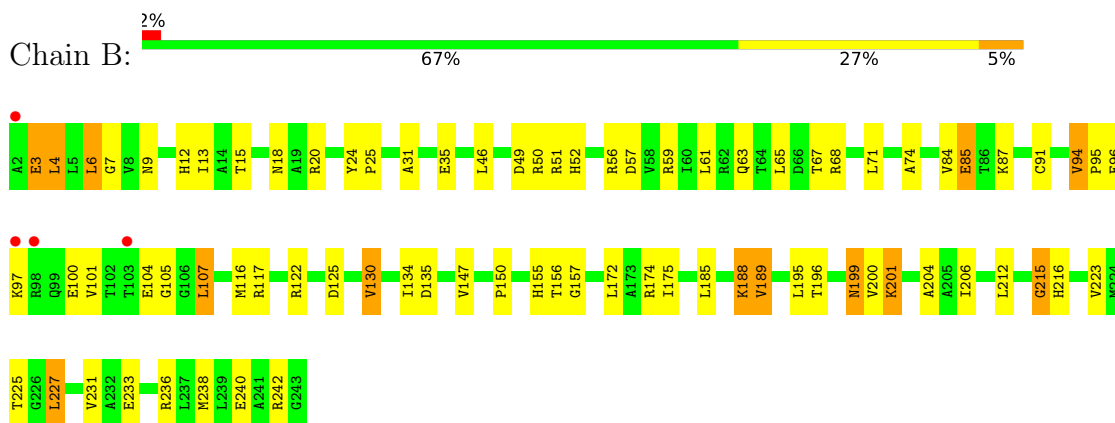
3 Residue-property plots [i](#)

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.

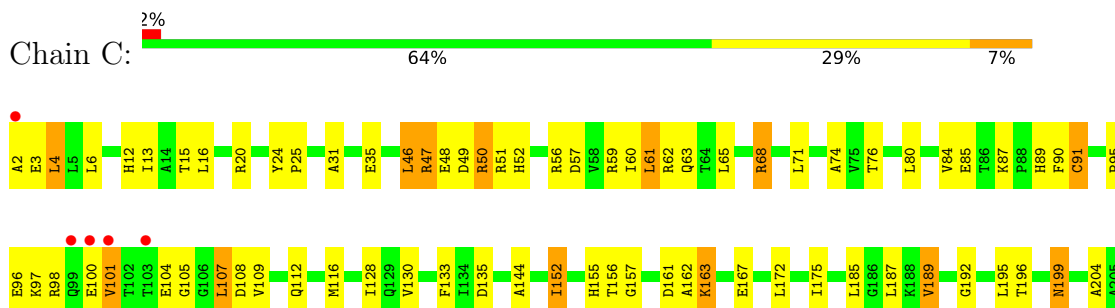
• Molecule 1: Pyridoxine 5'-Phosphate synthase

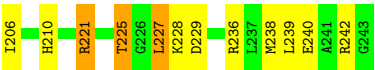


• Molecule 1: Pyridoxine 5'-Phosphate synthase

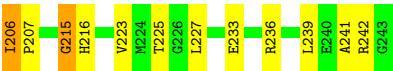
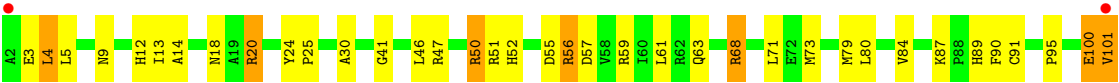


• Molecule 1: Pyridoxine 5'-Phosphate synthase





● Molecule 1: Pyridoxine 5'-Phosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.00Å 154.80Å 130.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 94.0 (20.00-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.30Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.266 0.214 , 0.207	Depositor DCC
R_{free} test set	2818 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7882	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.55	0/1847	1.03	9/2495 (0.4%)
1	B	0.54	0/1843	1.03	9/2490 (0.4%)
1	C	0.55	0/1847	1.02	8/2495 (0.3%)
1	D	0.55	0/1849	1.06	8/2498 (0.3%)
All	All	0.55	0/7386	1.03	34/9978 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	13	ILE	N-CA-C	-10.19	100.93	110.82
1	B	13	ILE	N-CA-C	-9.84	100.78	110.72
1	A	13	ILE	N-CA-C	-9.03	101.60	110.72
1	A	189	VAL	N-CA-C	8.19	119.92	108.12
1	C	189	VAL	N-CA-C	7.86	119.12	108.11
1	C	225	THR	N-CA-C	7.33	122.51	112.90
1	C	13	ILE	N-CA-C	-7.20	103.51	110.42
1	A	188	LYS	N-CA-C	-7.14	98.05	109.76
1	D	206	ILE	CA-C-N	6.53	126.76	119.32
1	D	206	ILE	C-N-CA	6.53	126.76	119.32
1	D	189	VAL	N-CA-C	6.45	117.77	108.48
1	C	206	ILE	CA-C-N	6.37	126.12	119.05
1	C	206	ILE	C-N-CA	6.37	126.12	119.05
1	B	206	ILE	CA-C-N	6.25	127.66	119.84
1	B	206	ILE	C-N-CA	6.25	127.66	119.84
1	B	189	VAL	N-CA-C	6.22	117.44	108.48
1	C	130	VAL	N-CA-C	6.12	118.17	108.87
1	B	188	LYS	N-CA-C	-5.82	100.21	109.76
1	A	225	THR	N-CA-C	5.81	120.37	113.28
1	B	96	GLU	N-CA-C	-5.80	106.83	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	ILE	N-CA-C	-5.79	99.43	108.81
1	A	130	VAL	N-CA-C	5.62	117.41	108.87
1	B	130	VAL	N-CA-C	5.54	117.29	108.87
1	B	201	LYS	N-CA-C	5.54	117.75	111.11
1	D	134	ILE	N-CA-C	5.53	116.82	108.96
1	D	201	LYS	N-CA-C	5.45	117.22	111.28
1	B	134	ILE	N-CA-C	5.39	116.61	108.96
1	A	152	ILE	N-CA-C	-5.38	101.24	108.35
1	C	144	ALA	N-CA-C	-5.38	105.31	111.07
1	A	221	ARG	N-CA-C	-5.32	105.14	111.69
1	A	113	ARG	N-CA-C	5.22	117.65	111.33
1	D	101	VAL	N-CA-C	5.18	117.15	109.17
1	D	130	VAL	N-CA-C	5.11	116.33	108.71
1	A	201	LYS	N-CA-C	5.11	117.24	111.11

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	1825	0	1827	67	0
1	B	1821	0	1821	54	0
1	C	1825	0	1827	58	0
1	D	1827	0	1832	76	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
3	A	125	0	0	10	0
3	B	128	0	0	4	0
3	C	139	0	0	3	0
3	D	152	0	0	12	0
All	All	7882	0	7307	251	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 17.

All (251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:THR:HG22	1:D:104:GLU:H	1.20	1.04
1:B:12:HIS:HA	1:B:15:THR:HG23	1.42	0.99
1:D:79:MET:HA	1:D:79:MET:HE3	1.45	0.98
1:D:117:ARG:HA	1:D:147:VAL:HG13	1.51	0.92
1:D:47:ARG:HH12	1:D:51:ARG:NH1	1.68	0.92
1:D:50:ARG:HG3	1:D:50:ARG:HH11	1.38	0.88
1:B:117:ARG:HA	1:B:147:VAL:HG13	1.53	0.88
1:B:85:GLU:HG2	3:B:1040:HOH:O	1.73	0.88
1:A:59:ARG:HH12	1:C:63:GLN:HE22	1.20	0.86
1:D:199:ASN:C	1:D:199:ASN:HD22	1.85	0.85
1:A:196:THR:H	1:A:199:ASN:HD21	1.20	0.84
1:A:63:GLN:HE22	1:C:59:ARG:HH12	1.22	0.84
1:D:95:PRO:HB2	1:D:101:VAL:HG22	1.59	0.83
1:D:118:ASP:HB3	3:D:1045:HOH:O	1.79	0.83
1:B:225:THR:HG22	3:B:1010:HOH:O	1.79	0.81
1:A:196:THR:H	1:A:199:ASN:ND2	1.78	0.79
1:A:56:ARG:HD2	3:A:1029:HOH:O	1.82	0.78
1:A:199:ASN:C	1:A:199:ASN:HD22	1.90	0.78
1:D:50:ARG:HH11	1:D:50:ARG:CG	1.96	0.78
1:C:199:ASN:C	1:C:199:ASN:HD22	1.92	0.77
1:C:80:LEU:O	1:C:84:VAL:HG23	1.86	0.75
1:A:95:PRO:HG3	1:A:107:LEU:HA	1.68	0.75
1:D:233:GLU:CD	1:D:236:ARG:HH21	1.96	0.74
1:B:196:THR:H	1:B:199:ASN:ND2	1.86	0.73
1:D:56:ARG:HD3	1:D:56:ARG:C	2.13	0.73
1:A:14:ALA:HB3	1:A:52:HIS:HB2	1.70	0.73
1:C:15:THR:HG22	1:C:52:HIS:HB3	1.72	0.72
1:C:95:PRO:HG3	1:C:107:LEU:HA	1.71	0.72
1:B:155:HIS:CD2	1:B:157:GLY:H	2.08	0.72
1:B:84:VAL:O	1:B:87:LYS:HD2	1.91	0.71
1:D:47:ARG:O	1:D:50:ARG:HD2	1.90	0.71
1:B:199:ASN:C	1:B:199:ASN:HD22	1.98	0.70
1:B:130:VAL:O	1:B:150:PRO:HD2	1.91	0.70
1:D:12:HIS:CD2	1:D:216:HIS:HD2	2.09	0.69
1:A:3:GLU:HB3	3:A:1075:HOH:O	1.93	0.69
1:C:196:THR:H	1:C:199:ASN:ND2	1.91	0.69
1:C:155:HIS:CD2	1:C:157:GLY:H	2.12	0.68
1:D:95:PRO:HB2	1:D:101:VAL:CG2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:VAL:HG12	1:D:102:THR:O	1.93	0.68
1:B:196:THR:H	1:B:199:ASN:HD21	1.41	0.68
1:D:225:THR:HG22	3:D:1021:HOH:O	1.93	0.67
1:C:163:LYS:HD2	1:C:167:GLU:OE1	1.94	0.67
1:D:139:GLU:HG3	3:D:1124:HOH:O	1.94	0.67
1:B:31:ALA:O	1:B:35:GLU:HG3	1.95	0.67
1:A:98:ARG:HA	1:A:101:VAL:HG12	1.76	0.67
1:B:95:PRO:HG3	1:B:107:LEU:HA	1.76	0.66
1:B:59:ARG:HH12	1:D:63:GLN:HE22	1.44	0.66
1:D:233:GLU:HG2	3:D:1042:HOH:O	1.95	0.66
1:D:47:ARG:HH12	1:D:51:ARG:HH11	1.42	0.66
1:D:199:ASN:HD22	1:D:200:VAL:N	1.93	0.66
1:B:61:LEU:O	1:B:65:LEU:HG	1.95	0.65
1:A:192:GLY:HA2	1:A:195:LEU:HD12	1.77	0.65
1:C:84:VAL:O	1:C:87:LYS:HD2	1.97	0.65
1:D:47:ARG:NH1	1:D:51:ARG:NH1	2.44	0.64
1:C:161:ASP:O	1:C:163:LYS:HE2	1.98	0.64
1:B:212:LEU:HD12	1:B:238:MET:HE3	1.80	0.63
1:C:89:HIS:HD2	1:C:90:PHE:CE1	2.17	0.63
1:D:196:THR:H	1:D:199:ASN:ND2	1.96	0.63
1:D:84:VAL:O	1:D:87:LYS:HD2	1.99	0.63
1:D:204:ALA:O	1:D:242:ARG:HD3	1.98	0.63
1:A:46:LEU:HB3	1:A:79:MET:HE1	1.79	0.63
1:A:98:ARG:HA	1:A:101:VAL:CG1	2.29	0.63
1:D:196:THR:H	1:D:199:ASN:HD21	1.45	0.62
1:C:196:THR:H	1:C:199:ASN:HD21	1.46	0.62
1:C:98:ARG:HA	1:C:101:VAL:HG23	1.82	0.62
1:D:117:ARG:CA	1:D:147:VAL:HG13	2.24	0.62
1:A:101:VAL:CG2	1:A:105:GLY:HA2	2.29	0.62
1:B:199:ASN:HD22	1:B:200:VAL:N	1.97	0.62
1:C:236:ARG:O	1:C:240:GLU:HG3	2.01	0.61
1:A:101:VAL:HG23	1:A:105:GLY:HA2	1.81	0.61
1:D:155:HIS:CD2	1:D:157:GLY:H	2.19	0.61
1:B:156:THR:HG22	1:B:175:ILE:HD13	1.82	0.61
1:D:137:ASP:O	1:D:141:ILE:HG13	2.01	0.60
1:A:91:CYS:HB2	1:A:128:ILE:HG21	1.82	0.60
1:D:56:ARG:HD3	1:D:57:ASP:N	2.17	0.60
1:B:3:GLU:H	1:B:3:GLU:CD	2.08	0.60
1:C:4:LEU:HD13	1:C:238:MET:HE3	1.84	0.59
1:B:227:LEU:HD22	1:B:231:VAL:HG23	1.85	0.59
1:B:63:GLN:HE22	1:D:59:ARG:HH12	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:HD11	1:A:178:ALA:HB1	1.83	0.59
1:B:15:THR:HG22	1:B:52:HIS:HB3	1.84	0.59
1:A:196:THR:N	1:A:199:ASN:HD21	1.96	0.59
1:A:107:LEU:HB2	1:A:133:PHE:O	2.03	0.59
1:D:79:MET:HE3	1:D:79:MET:CA	2.26	0.58
1:B:57:ASP:O	1:B:61:LEU:HD23	2.03	0.58
1:C:56:ARG:HD3	1:C:56:ARG:C	2.29	0.58
1:D:50:ARG:CG	1:D:50:ARG:NH1	2.63	0.58
1:A:155:HIS:CD2	1:A:157:GLY:H	2.21	0.58
1:C:210:HIS:HE1	3:C:1083:HOH:O	1.87	0.57
1:D:104:GLU:HG3	3:D:1153:HOH:O	2.04	0.57
1:C:74:ALA:HB2	1:C:96:GLU:HG3	1.86	0.57
1:C:101:VAL:HG12	1:C:105:GLY:HA2	1.86	0.57
1:A:100:GLU:OE2	1:A:116:MET:HE1	2.05	0.56
1:A:192:GLY:HA2	1:A:195:LEU:CD1	2.35	0.56
1:D:47:ARG:CZ	3:D:1056:HOH:O	2.53	0.56
1:D:50:ARG:HH12	1:D:55:ASP:CG	2.14	0.56
1:A:199:ASN:ND2	1:A:199:ASN:C	2.61	0.56
1:C:57:ASP:O	1:C:61:LEU:HB2	2.06	0.56
1:B:117:ARG:HA	1:B:147:VAL:CG1	2.31	0.55
1:A:210:HIS:HD2	3:A:1027:HOH:O	1.89	0.55
1:C:107:LEU:HD22	1:C:116:MET:HE3	1.89	0.55
1:D:101:VAL:HG12	1:D:102:THR:N	2.22	0.55
1:D:9:ASN:HB3	1:D:215:GLY:HA3	1.87	0.55
1:A:91:CYS:HB2	1:A:128:ILE:CG2	2.37	0.55
1:B:188:LYS:HA	3:B:1072:HOH:O	2.07	0.55
1:B:236:ARG:NH1	1:B:240:GLU:OE2	2.37	0.55
1:A:57:ASP:O	1:A:61:LEU:HB2	2.07	0.54
1:D:156:THR:HG22	1:D:175:ILE:HD13	1.89	0.54
1:B:56:ARG:HD2	3:D:1014:HOH:O	2.07	0.54
1:D:101:VAL:CG1	1:D:102:THR:N	2.70	0.54
1:B:101:VAL:HG23	1:B:105:GLY:O	2.08	0.54
1:C:104:GLU:HB3	1:C:135:ASP:OD1	2.08	0.54
1:C:95:PRO:HB3	1:C:100:GLU:HB3	1.89	0.53
1:A:225:THR:HG22	3:A:1042:HOH:O	2.07	0.53
1:C:91:CYS:HB2	1:C:128:ILE:HG21	1.91	0.53
1:D:50:ARG:N	1:D:50:ARG:CD	2.71	0.53
1:A:47:ARG:NH1	1:A:51:ARG:HB2	2.24	0.53
1:A:51:ARG:HD2	1:A:51:ARG:O	2.09	0.53
1:A:80:LEU:O	1:A:84:VAL:HG23	2.09	0.53
1:A:101:VAL:HG22	1:A:102:THR:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:HIS:CD2	1:B:216:HIS:HD2	2.27	0.52
1:B:12:HIS:HA	1:B:15:THR:CG2	2.26	0.52
1:C:97:LYS:O	1:C:100:GLU:HB2	2.08	0.52
1:C:204:ALA:O	1:C:242:ARG:HD3	2.10	0.52
1:C:192:GLY:HA2	1:C:195:LEU:HD12	1.90	0.52
1:A:26:ASP:OD1	1:A:28:VAL:HG23	2.10	0.52
1:C:56:ARG:NE	1:C:60:ILE:HD12	2.25	0.52
1:A:201:LYS:HG2	1:A:241:ALA:HB2	1.92	0.51
1:C:12:HIS:HA	1:C:15:THR:HG23	1.93	0.51
1:B:18:ASN:C	1:B:20:ARG:H	2.19	0.51
1:D:199:ASN:C	1:D:199:ASN:ND2	2.58	0.50
1:A:225:THR:CG2	3:A:1042:HOH:O	2.60	0.50
1:B:12:HIS:ND1	1:B:15:THR:HG21	2.26	0.50
1:B:49:ASP:O	1:B:50:ARG:C	2.54	0.50
1:B:117:ARG:CA	1:B:147:VAL:HG13	2.34	0.50
1:D:41:GLY:HA3	1:D:68:ARG:HH11	1.76	0.50
1:D:73:MET:HE1	1:D:80:LEU:HD23	1.93	0.50
1:D:102:THR:HG21	1:D:135:ASP:OD2	2.12	0.50
1:B:204:ALA:O	1:B:242:ARG:NE	2.45	0.50
1:C:68:ARG:HD3	1:C:68:ARG:N	2.26	0.50
1:C:221:ARG:HD3	3:C:1103:HOH:O	2.10	0.50
1:D:104:GLU:OE2	1:D:174:ARG:NH2	2.40	0.50
1:B:199:ASN:ND2	1:B:199:ASN:C	2.69	0.49
1:C:3:GLU:CG	1:C:239:LEU:HD22	2.43	0.49
1:A:227:LEU:HD22	1:A:231:VAL:HG23	1.94	0.49
1:B:104:GLU:OE1	1:B:135:ASP:HB3	2.11	0.49
1:B:6:LEU:HD22	1:B:7:GLY:N	2.27	0.49
1:B:195:LEU:HA	1:B:199:ASN:HD21	1.78	0.49
1:C:101:VAL:CG1	1:C:105:GLY:HA2	2.42	0.49
1:D:24:TYR:HA	1:D:25:PRO:C	2.37	0.49
1:B:122:ARG:HG3	3:B:1056:HOH:O	2.13	0.48
1:B:200:VAL:HG13	1:B:201:LYS:N	2.28	0.48
1:A:46:LEU:HD12	1:A:79:MET:HE1	1.96	0.48
1:A:101:VAL:HG22	1:A:102:THR:N	2.28	0.48
1:D:215:GLY:H	2:D:1008:PO4:P	2.35	0.48
1:A:137:ASP:O	1:A:141:ILE:HG13	2.13	0.48
1:D:30:ALA:HB1	1:D:227:LEU:HD11	1.96	0.48
1:A:95:PRO:HG3	1:A:107:LEU:CA	2.41	0.48
1:D:14:ALA:HB3	1:D:52:HIS:HB2	1.96	0.48
1:A:87:LYS:N	1:A:88:PRO:HD3	2.29	0.47
1:B:74:ALA:HA	1:B:94:VAL:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:O	1:A:65:LEU:HG	2.15	0.47
1:C:91:CYS:HB2	1:C:128:ILE:CG2	2.44	0.47
1:D:89:HIS:HD2	1:D:90:PHE:CE1	2.32	0.47
1:A:47:ARG:HH11	1:A:51:ARG:CB	2.28	0.47
1:A:89:HIS:HD2	1:A:90:PHE:CE1	2.32	0.47
1:A:47:ARG:HH11	1:A:51:ARG:HB2	1.79	0.47
1:A:98:ARG:CA	1:A:101:VAL:HG12	2.43	0.47
1:C:109:VAL:HG13	1:C:116:MET:HG3	1.97	0.47
1:C:195:LEU:HA	1:C:199:ASN:HD21	1.80	0.47
1:D:47:ARG:NH1	1:D:51:ARG:HD2	2.29	0.47
1:A:225:THR:HG22	3:A:1022:HOH:O	2.15	0.46
1:A:156:THR:HG22	1:A:175:ILE:HD13	1.97	0.46
1:D:195:LEU:HD21	1:D:203:ILE:HG13	1.96	0.46
1:B:50:ARG:HH11	1:B:50:ARG:HG2	1.80	0.46
1:D:151:PHE:CE1	1:D:188:LYS:HD2	2.50	0.46
1:D:155:HIS:HD2	1:D:157:GLY:H	1.61	0.46
1:C:47:ARG:NH1	1:C:49:ASP:OD1	2.49	0.46
1:D:146:GLU:HG2	1:D:147:VAL:N	2.27	0.46
1:A:26:ASP:CG	1:A:56:ARG:HH22	2.22	0.46
1:A:153:GLU:HB2	3:A:1036:HOH:O	2.16	0.46
1:A:210:HIS:HE1	3:A:1067:HOH:O	1.98	0.46
1:A:199:ASN:HD22	1:A:200:VAL:N	2.13	0.45
1:C:61:LEU:O	1:C:65:LEU:HG	2.15	0.45
1:D:206:ILE:HA	1:D:207:PRO:HD3	1.82	0.45
1:A:137:ASP:OD2	1:A:140:GLN:HG2	2.17	0.45
1:D:100:GLU:HB3	3:D:1065:HOH:O	2.17	0.45
1:D:110:ALA:O	1:D:113:ARG:NH1	2.49	0.45
1:B:24:TYR:HA	1:B:25:PRO:C	2.41	0.45
1:D:79:MET:HA	1:D:79:MET:CE	2.29	0.45
1:D:18:ASN:C	1:D:20:ARG:H	2.24	0.45
1:A:6:LEU:HG	1:A:238:MET:SD	2.57	0.45
1:D:122:ARG:NH2	3:D:1072:HOH:O	2.50	0.45
1:A:12:HIS:HA	1:A:15:THR:OG1	2.17	0.45
1:A:51:ARG:HD2	1:A:51:ARG:C	2.42	0.45
1:D:102:THR:HG22	1:D:103:THR:N	2.32	0.45
1:D:47:ARG:NE	3:D:1056:HOH:O	2.49	0.45
1:A:98:ARG:C	1:A:101:VAL:HG12	2.42	0.44
1:A:100:GLU:OE1	1:A:107:LEU:HD21	2.18	0.44
1:B:18:ASN:C	1:B:20:ARG:N	2.75	0.44
1:B:4:LEU:HD12	1:B:204:ALA:HB1	2.00	0.44
1:C:46:LEU:CD2	1:C:50:ARG:HD3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:THR:CG2	1:D:103:THR:N	2.81	0.44
1:D:192:GLY:HA2	1:D:195:LEU:HD12	2.00	0.44
1:B:51:ARG:HG3	1:B:52:HIS:N	2.33	0.44
1:C:152:ILE:HG21	1:C:187:LEU:HD13	1.99	0.44
1:B:67:THR:OG1	1:B:68:ARG:N	2.51	0.44
1:D:201:LYS:HG2	1:D:241:ALA:HB2	2.00	0.44
1:D:47:ARG:HD2	3:D:1123:HOH:O	2.18	0.43
1:C:104:GLU:HB3	1:C:135:ASP:CG	2.43	0.43
1:D:12:HIS:HD2	1:D:216:HIS:HD2	1.64	0.43
1:B:97:LYS:O	1:B:100:GLU:HG3	2.19	0.43
1:C:95:PRO:HG3	1:C:107:LEU:CA	2.43	0.43
1:A:4:LEU:HD13	1:A:238:MET:HE3	2.00	0.43
1:A:24:TYR:HA	1:A:25:PRO:C	2.43	0.43
1:A:31:ALA:O	1:A:35:GLU:HG3	2.18	0.43
1:C:161:ASP:O	1:C:162:ALA:C	2.61	0.43
1:C:15:THR:CG2	1:C:52:HIS:HB3	2.46	0.43
1:D:4:LEU:HD22	1:D:5:LEU:N	2.34	0.43
1:C:49:ASP:O	1:C:50:ARG:C	2.61	0.43
1:D:41:GLY:HA3	1:D:68:ARG:NH1	2.34	0.42
1:C:24:TYR:HA	1:C:25:PRO:C	2.44	0.42
1:C:76:THR:O	1:C:80:LEU:HG	2.19	0.42
1:C:227:LEU:O	1:C:228:LYS:C	2.62	0.42
1:C:108:ASP:HB3	1:C:112:GLN:HE21	1.83	0.42
1:D:50:ARG:N	1:D:50:ARG:HD3	2.35	0.42
1:C:107:LEU:HB2	1:C:133:PHE:O	2.20	0.42
1:B:4:LEU:HD13	1:B:238:MET:HE2	2.01	0.42
1:A:100:GLU:OE1	3:A:1055:HOH:O	2.22	0.42
1:A:100:GLU:HG2	1:A:112:GLN:HE22	1.85	0.42
1:A:33:ILE:HG21	1:A:227:LEU:HB3	2.03	0.41
1:C:47:ARG:NH2	1:C:51:ARG:CZ	2.83	0.41
1:A:104:GLU:CD	1:A:174:ARG:HH22	2.28	0.41
1:B:233:GLU:CD	1:B:236:ARG:HH21	2.29	0.41
1:C:62:ARG:HG3	1:C:62:ARG:HH11	1.85	0.41
1:A:11:ASP:OD2	1:A:45:HIS:HB3	2.21	0.41
1:A:239:LEU:HD22	3:A:1061:HOH:O	2.21	0.41
1:B:3:GLU:CD	1:B:3:GLU:N	2.76	0.41
1:C:2:ALA:HB3	3:C:1139:HOH:O	2.20	0.41
1:C:31:ALA:O	1:C:35:GLU:HG3	2.21	0.41
1:B:9:ASN:HB3	1:B:215:GLY:HA3	2.02	0.41
1:B:104:GLU:CD	1:B:174:ARG:HH22	2.28	0.40
1:C:156:THR:HG22	1:C:175:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:PHE:CD2	1:D:129:GLN:HB2	2.56	0.40
1:D:102:THR:HG22	1:D:104:GLU:N	2.05	0.40
1:B:107:LEU:HD11	1:B:116:MET:HE3	2.03	0.40
1:C:225:THR:CG2	1:C:229:ASP:HB2	2.51	0.40
1:D:225:THR:HG22	3:D:1019:HOH:O	2.22	0.40
1:A:195:LEU:HA	1:A:199:ASN:HD21	1.86	0.40
1:C:4:LEU:HD23	1:C:4:LEU:HA	1.90	0.40
1:D:117:ARG:HA	1:D:147:VAL:CG1	2.37	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	240/242 (99%)	232 (97%)	8 (3%)	0	100	100
1	B	240/242 (99%)	228 (95%)	11 (5%)	1 (0%)	30	38
1	C	240/242 (99%)	228 (95%)	11 (5%)	1 (0%)	30	38
1	D	240/242 (99%)	229 (95%)	10 (4%)	1 (0%)	30	38
All	All	960/968 (99%)	917 (96%)	40 (4%)	3 (0%)	36	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	215	GLY
1	C	50	ARG
1	B	215	GLY

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	182/185 (98%)	167 (92%)	15 (8%)	10	14
1	B	181/185 (98%)	165 (91%)	16 (9%)	9	12
1	C	182/185 (98%)	161 (88%)	21 (12%)	5	6
1	D	183/185 (99%)	161 (88%)	22 (12%)	5	5
All	All	728/740 (98%)	654 (90%)	74 (10%)	7	8

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	6	LEU
1	A	20	ARG
1	A	46	LEU
1	A	61	LEU
1	A	71	LEU
1	A	73	MET
1	A	75	VAL
1	A	100	GLU
1	A	107	LEU
1	A	138	GLU
1	A	172	LEU
1	A	189	VAL
1	A	199	ASN
1	A	227	LEU
1	B	3	GLU
1	B	4	LEU
1	B	6	LEU
1	B	46	LEU
1	B	71	LEU
1	B	85	GLU
1	B	91	CYS
1	B	94	VAL
1	B	107	LEU

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Mol	Chain	Res	Type
1	B	125	ASP
1	B	172	LEU
1	B	185	LEU
1	B	189	VAL
1	B	199	ASN
1	B	223	VAL
1	B	227	LEU
1	C	4	LEU
1	C	6	LEU
1	C	16	LEU
1	C	20	ARG
1	C	46	LEU
1	C	47	ARG
1	C	48	GLU
1	C	61	LEU
1	C	68	ARG
1	C	71	LEU
1	C	85	GLU
1	C	91	CYS
1	C	101	VAL
1	C	107	LEU
1	C	163	LYS
1	C	172	LEU
1	C	185	LEU
1	C	189	VAL
1	C	199	ASN
1	C	221	ARG
1	C	227	LEU
1	D	3	GLU
1	D	4	LEU
1	D	20	ARG
1	D	46	LEU
1	D	50	ARG
1	D	56	ARG
1	D	61	LEU
1	D	68	ARG
1	D	71	LEU
1	D	91	CYS
1	D	100	GLU
1	D	114	ASP
1	D	122	ARG
1	D	146	GLU

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Mol	Chain	Res	Type
1	D	158	CYS
1	D	170	GLN
1	D	172	LEU
1	D	185	LEU
1	D	189	VAL
1	D	199	ASN
1	D	223	VAL
1	D	239	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	36	GLN
1	A	63	GLN
1	A	89	HIS
1	A	112	GLN
1	A	155	HIS
1	A	198	HIS
1	A	199	ASN
1	A	210	HIS
1	A	213	ASN
1	B	36	GLN
1	B	63	GLN
1	B	70	ASN
1	B	89	HIS
1	B	129	GLN
1	B	155	HIS
1	B	199	ASN
1	B	213	ASN
1	B	216	HIS
1	C	36	GLN
1	C	63	GLN
1	C	70	ASN
1	C	89	HIS
1	C	112	GLN
1	C	155	HIS
1	C	198	HIS
1	C	199	ASN
1	C	210	HIS
1	D	12	HIS
1	D	29	GLN

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Mol	Chain	Res	Type
1	D	63	GLN
1	D	89	HIS
1	D	129	GLN
1	D	155	HIS
1	D	170	GLN
1	D	199	ASN
1	D	210	HIS
1	D	213	ASN
1	D	216	HIS

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	PO4	B	1006	-	4,4,4	1.14	0	6,6,6	0.70	0
2	PO4	C	1003	-	4,4,4	0.88	0	6,6,6	0.90	0
2	PO4	A	1002	-	4,4,4	0.95	0	6,6,6	0.85	0
2	PO4	A	1001	-	4,4,4	0.99	0	6,6,6	0.79	0
2	PO4	C	1004	-	4,4,4	0.94	0	6,6,6	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	D	1007	-	4,4,4	0.91	0	6,6,6	0.90	0
2	PO4	D	1008	-	4,4,4	1.08	0	6,6,6	0.84	0
2	PO4	B	1005	-	4,4,4	0.99	0	6,6,6	0.86	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1008	PO4	1	0

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	242/242 (100%)	-0.43	6 (2%) 58 60	13, 25, 48, 70	0
1	B	242/242 (100%)	-0.39	4 (1%) 69 70	14, 27, 49, 71	0
1	C	242/242 (100%)	-0.44	5 (2%) 63 65	14, 25, 48, 66	0
1	D	242/242 (100%)	-0.46	2 (0%) 82 83	15, 26, 45, 57	0
All	All	968/968 (100%)	-0.43	17 (1%) 67 69	13, 26, 47, 71	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	THR	4.1
1	B	103	THR	4.0
1	A	98	ARG	3.9
1	A	97	LYS	3.8
1	B	2	ALA	3.5
1	A	100	GLU	3.4
1	A	101	VAL	3.1
1	B	97	LYS	3.0
1	C	2	ALA	2.9
1	C	103	THR	2.8
1	C	100	GLU	2.4
1	A	99	GLN	2.2
1	C	101	VAL	2.2
1	B	98	ARG	2.2
1	D	2	ALA	2.0
1	C	99	GLN	2.0
1	D	101	VAL	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 [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PO4	B	1006	5/5	0.86	0.15	76,77,79,81	0
2	PO4	C	1004	5/5	0.86	0.15	79,81,82,83	0
2	PO4	C	1003	5/5	0.87	0.24	74,76,79,79	0
2	PO4	D	1008	5/5	0.87	0.28	83,84,85,86	0
2	PO4	D	1007	5/5	0.88	0.14	76,78,80,82	0
2	PO4	A	1001	5/5	0.89	0.11	69,69,73,73	0
2	PO4	B	1005	5/5	0.90	0.31	89,90,94,94	0
2	PO4	A	1002	5/5	0.91	0.24	77,80,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.