



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:58 PM UTC

PDB ID : 1HO4 / pdb_00001ho4
Title : CRYSTAL STRUCTURE OF PYRIDOXINE 5'-PHOSPHATE SYNTHASE
IN COMPLEX WITH PYRIDOXINE 5'-PHOSPHATE AND INORGANIC
PHOSPHATE
Authors : Garrido-Franco, M.; Laber, B.; Huber, R.; Clausen, T.
Deposited on : 2000-12-08
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

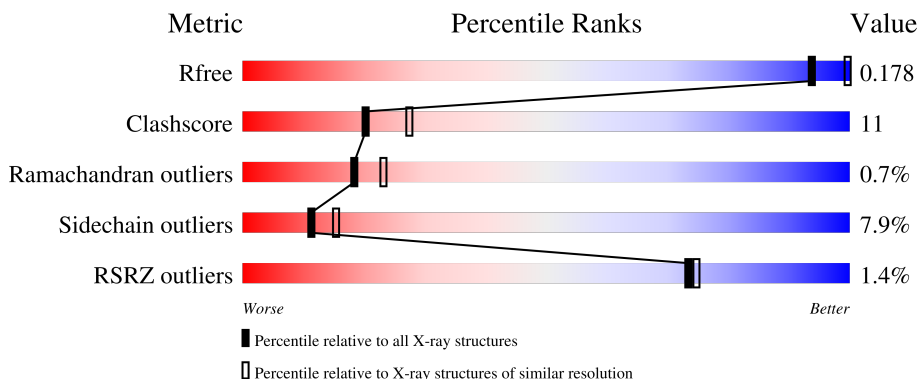
1 Overall quality at a glance

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	0% 76% 20% •
1	B	242	2% 77% 19% 5%
1	C	242	2% 79% 19% •
1	D	242	70% 24% 6%

2 Entry composition [i](#)

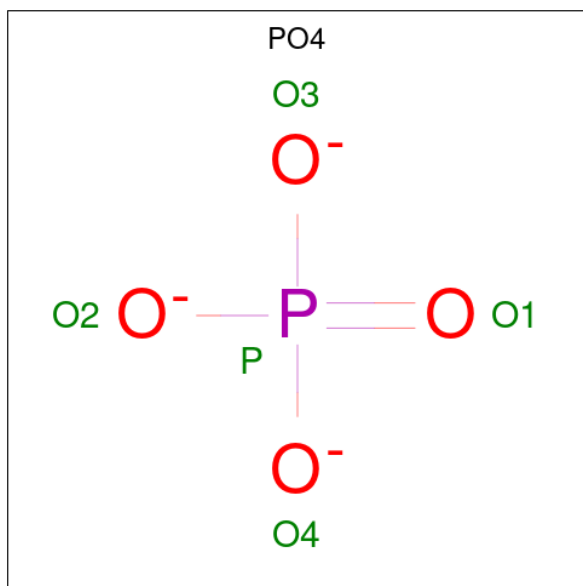
There are 4 unique types of molecules in this entry. The entry contains 8148 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			1833	1136	337	348	12			
1	B	242	Total	C	N	O	S	0	0	0
			1837	1138	337	350	12			
1	C	242	Total	C	N	O	S	0	0	0
			1837	1138	337	350	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).



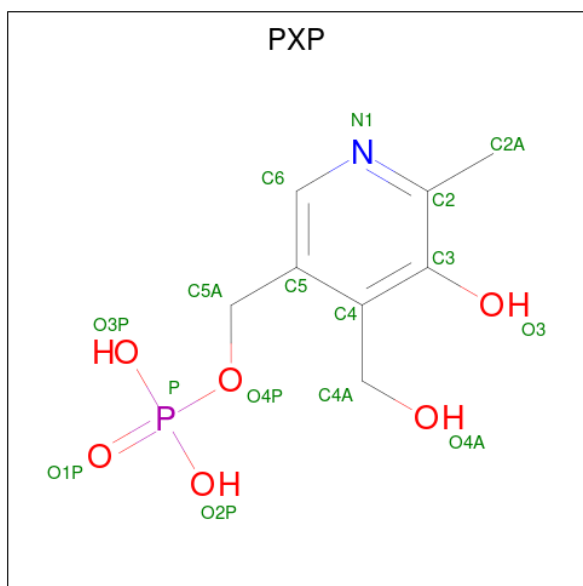
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 3 is PYRIDOXINE-5'-PHOSPHATE (CCD ID: PXP) (formula: $C_8H_{12}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

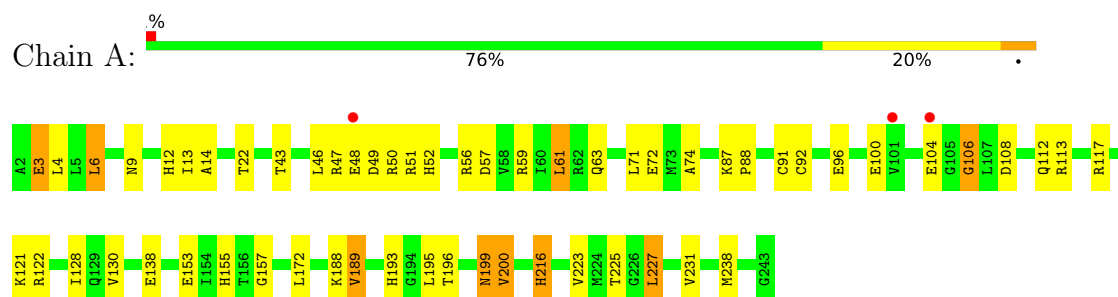
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	194	Total	O	0	0
			194	194		
4	B	168	Total	O	0	0
			168	168		
4	C	182	Total	O	0	0
			182	182		
4	D	191	Total	O	0	0
			191	191		

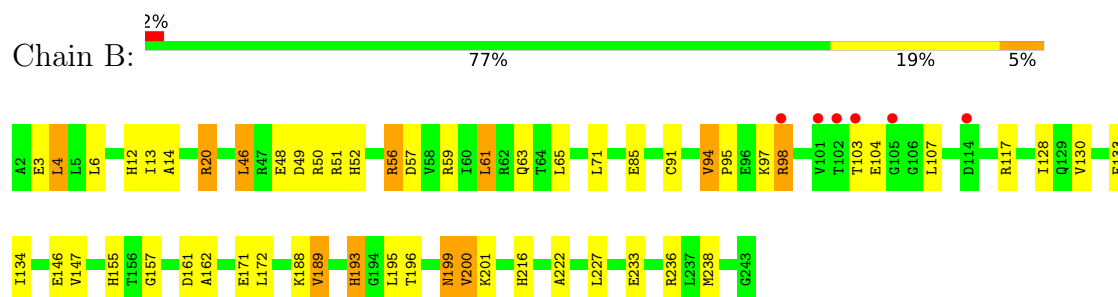
3 Residue-property plots [i](#)

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.

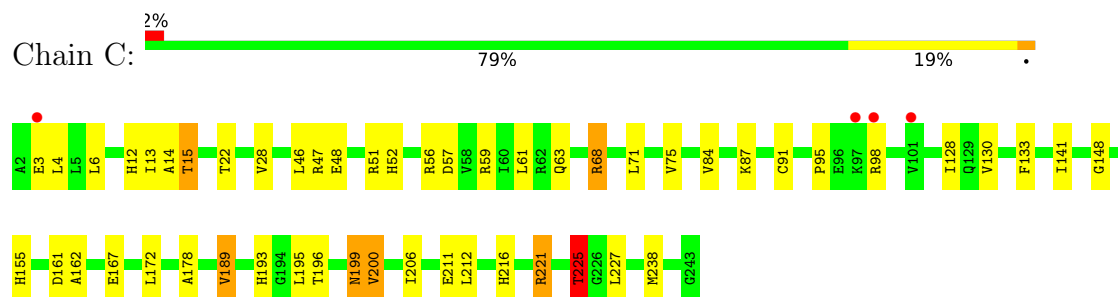
• Molecule 1: PYRIDOXINE 5'-PHOSPHATE SYNTHASE



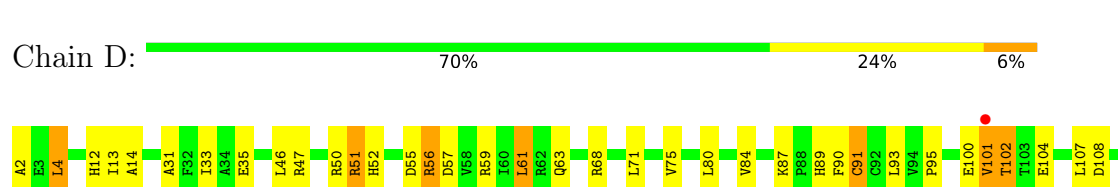
• Molecule 1: PYRIDOXINE 5'-PHOSPHATE SYNTHASE

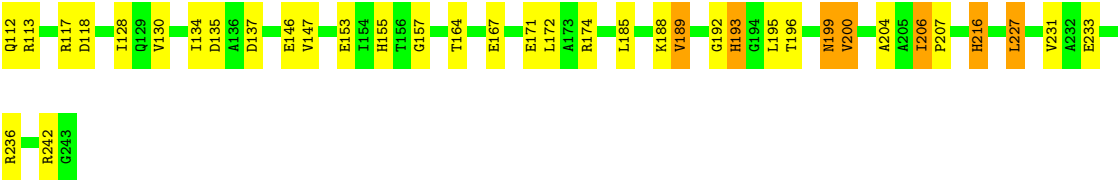


• Molecule 1: PYRIDOXINE 5'-PHOSPHATE SYNTHASE



• 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	128.80Å 156.30Å 127.50Å 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) 95.7 (20.00-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.30Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.187 , 0.245 0.180 , 0.178	Depositor DCC
R_{free} test set	2782 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.815	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8148	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.92% 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: PXP, 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	0.63	0/1855	1.03	7/2504 (0.3%)
1	B	0.63	0/1859	1.05	8/2509 (0.3%)
1	C	0.64	0/1859	1.07	9/2509 (0.4%)
1	D	0.65	0/1849	1.09	12/2498 (0.5%)
All	All	0.64	0/7422	1.06	36/10020 (0.4%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	13	ILE	N-CA-C	-12.40	98.87	110.53
1	B	13	ILE	N-CA-C	-9.89	101.23	110.53
1	C	13	ILE	N-CA-C	-9.30	101.33	110.72
1	A	13	ILE	N-CA-C	-8.84	101.79	110.72
1	C	189	VAL	N-CA-C	8.34	120.12	108.12
1	C	225	THR	N-CA-C	7.77	122.87	113.23
1	A	189	VAL	N-CA-C	7.59	118.84	107.75
1	D	189	VAL	N-CA-C	7.54	118.97	108.12
1	B	130	VAL	N-CA-C	7.48	119.06	108.36
1	B	189	VAL	N-CA-C	7.06	117.99	108.11
1	C	130	VAL	N-CA-C	6.90	119.35	108.87
1	C	200	VAL	N-CA-C	6.76	117.55	110.72
1	A	216	HIS	N-CA-C	6.74	119.20	111.11
1	D	206	ILE	CA-C-N	6.37	126.12	119.05
1	D	206	ILE	C-N-CA	6.37	126.12	119.05
1	B	200	VAL	N-CA-C	6.01	116.79	110.72
1	D	200	VAL	N-CA-C	5.92	118.49	111.09
1	D	188	LYS	N-CA-C	-5.78	101.12	110.32
1	A	200	VAL	N-CA-C	5.66	118.16	111.09
1	A	130	VAL	N-CA-C	5.62	117.41	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	LYS	N-CA-C	-5.55	100.66	109.76
1	D	102	THR	N-CA-C	-5.51	101.81	110.36
1	C	148	GLY	N-CA-C	5.47	122.03	114.92
1	C	206	ILE	CA-C-N	5.37	125.44	119.32
1	C	206	ILE	C-N-CA	5.37	125.44	119.32
1	D	130	VAL	N-CA-C	5.37	116.71	108.71
1	C	95	PRO	N-CA-C	-5.31	103.49	111.57
1	D	113	ARG	N-CA-C	5.28	118.51	111.75
1	B	222	ALA	N-CA-C	5.21	116.96	111.28
1	D	134	ILE	N-CA-C	5.20	116.19	108.65
1	A	188	LYS	N-CA-C	-5.19	101.25	109.76
1	D	4	LEU	N-CA-C	-5.17	102.73	110.23
1	B	134	ILE	N-CA-C	5.11	116.06	108.65
1	B	94	VAL	N-CA-C	5.08	114.55	108.45
1	D	216	HIS	N-CA-C	5.06	117.19	111.11
1	A	106	GLY	N-CA-C	5.04	125.13	113.18

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	1833	0	1850	38	0
1	B	1837	0	1854	46	0
1	C	1837	0	1854	34	0
1	D	1827	0	1832	56	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	16	0	10	1	0
3	B	16	0	10	3	0
3	C	16	0	10	0	0
3	D	16	0	10	1	0
4	A	194	0	0	6	0
4	B	168	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	182	0	0	3	0
4	D	191	0	0	11	0
All	All	8148	0	7430	168	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 11.

All (168) 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:C:12:HIS:HA	1:C:15:THR:HG23	1.20	1.15
1:B:63:GLN:HE22	1:D:59:ARG:HH12	1.02	0.95
1:A:199:ASN:C	1:A:199:ASN:HD22	1.79	0.90
1:D:102:THR:HG23	4:D:870:HOH:O	1.69	0.90
1:A:63:GLN:HE22	1:C:59:ARG:HH12	0.93	0.89
1:B:59:ARG:HH12	1:D:63:GLN:HE22	1.18	0.88
1:D:155:HIS:HD2	1:D:157:GLY:H	1.17	0.88
1:C:12:HIS:HA	1:C:15:THR:CG2	2.02	0.86
1:B:199:ASN:HD22	1:B:199:ASN:C	1.86	0.82
1:A:59:ARG:HH12	1:C:63:GLN:HE22	1.28	0.81
1:D:155:HIS:CD2	1:D:157:GLY:H	1.98	0.81
1:C:199:ASN:C	1:C:199:ASN:HD22	1.90	0.79
1:C:221:ARG:HB2	1:C:221:ARG:HH11	1.48	0.79
1:A:63:GLN:HE22	1:C:59:ARG:NH1	1.77	0.77
1:A:63:GLN:NE2	1:C:59:ARG:HH12	1.79	0.76
1:B:56:ARG:HD2	4:B:906:HOH:O	1.85	0.75
1:A:196:THR:H	1:A:199:ASN:ND2	1.85	0.75
1:A:12:HIS:CD2	1:A:216:HIS:HD2	2.04	0.74
1:B:97:LYS:O	1:B:98:ARG:HB2	1.87	0.74
1:D:199:ASN:C	1:D:199:ASN:HD22	1.96	0.73
1:C:162:ALA:HA	1:C:167:GLU:OE2	1.91	0.71
1:D:196:THR:H	1:D:199:ASN:ND2	1.88	0.71
1:B:57:ASP:O	1:B:61:LEU:HB2	1.91	0.70
1:B:155:HIS:CE1	1:B:157:GLY:HA3	2.26	0.69
1:A:225:THR:HG22	4:A:921:HOH:O	1.93	0.68
1:D:50:ARG:N	1:D:50:ARG:HD2	2.09	0.68
1:A:14:ALA:HB3	1:A:52:HIS:HB2	1.73	0.67
1:D:95:PRO:HB2	1:D:101:VAL:HG22	1.76	0.67
1:C:212:LEU:HD12	1:C:238:MET:HE3	1.75	0.67
1:B:117:ARG:HA	1:B:147:VAL:HG13	1.78	0.66
1:A:12:HIS:HD2	1:A:216:HIS:HD2	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:VAL:HG11	3:B:804:PXP:H2A3	1.78	0.64
1:D:100:GLU:HG2	4:D:893:HOH:O	1.97	0.63
1:C:195:LEU:HA	1:C:199:ASN:HD21	1.63	0.63
1:D:89:HIS:HD2	1:D:90:PHE:CE1	2.17	0.63
1:A:196:THR:H	1:A:199:ASN:HD21	1.45	0.62
1:A:199:ASN:C	1:A:199:ASN:ND2	2.52	0.62
1:A:12:HIS:CD2	1:A:216:HIS:CD2	2.87	0.62
1:A:74:ALA:HB2	1:A:96:GLU:HB2	1.82	0.62
1:D:107:LEU:HD12	4:D:832:HOH:O	1.98	0.61
1:A:12:HIS:HD2	1:A:216:HIS:CD2	2.19	0.61
1:B:95:PRO:HG3	1:B:107:LEU:HA	1.81	0.61
1:D:102:THR:HG23	4:D:842:HOH:O	1.99	0.61
1:C:48:GLU:OE1	1:C:98:ARG:HB2	2.00	0.61
1:A:47:ARG:HD3	1:A:51:ARG:HG2	1.84	0.60
1:C:12:HIS:CA	1:C:15:THR:HG23	2.14	0.60
1:B:14:ALA:HB3	1:B:52:HIS:HB2	1.83	0.60
1:B:51:ARG:NH2	1:B:98:ARG:O	2.35	0.59
1:C:14:ALA:HB3	1:C:52:HIS:HB2	1.85	0.59
1:B:195:LEU:HA	1:B:199:ASN:HD21	1.67	0.58
1:C:57:ASP:O	1:C:61:LEU:HD13	2.03	0.58
1:D:112:GLN:NE2	4:D:832:HOH:O	2.36	0.58
1:D:50:ARG:NH1	1:D:55:ASP:OD1	2.37	0.58
1:D:56:ARG:HD3	1:D:56:ARG:C	2.28	0.58
1:C:221:ARG:NH1	4:C:934:HOH:O	2.37	0.57
1:A:91:CYS:HB2	1:A:128:ILE:HG21	1.86	0.57
1:C:56:ARG:HD3	1:C:56:ARG:C	2.29	0.57
1:D:195:LEU:HA	1:D:199:ASN:HD21	1.70	0.57
1:B:97:LYS:O	1:B:98:ARG:CB	2.53	0.56
1:B:199:ASN:HD22	1:B:200:VAL:N	2.03	0.56
1:C:28:VAL:HG22	1:C:61:LEU:HD12	1.87	0.56
1:D:196:THR:H	1:D:199:ASN:HD21	1.50	0.56
1:C:84:VAL:O	1:C:87:LYS:HD2	2.06	0.56
1:D:12:HIS:CD2	1:D:216:HIS:HD2	2.23	0.56
1:D:102:THR:N	4:D:870:HOH:O	2.38	0.56
1:C:68:ARG:NH2	1:C:211:GLU:OE1	2.39	0.55
1:A:199:ASN:HD22	1:A:200:VAL:N	2.04	0.55
1:C:196:THR:H	1:C:199:ASN:ND2	2.05	0.55
1:A:108:ASP:O	1:A:112:GLN:HG3	2.07	0.54
1:D:199:ASN:HD22	1:D:200:VAL:N	2.04	0.54
1:C:199:ASN:HD22	1:C:200:VAL:N	2.04	0.54
1:D:33:ILE:HG21	1:D:227:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ARG:HB2	1:C:221:ARG:NH1	2.19	0.53
1:A:122:ARG:NE	4:A:984:HOH:O	2.36	0.53
1:B:63:GLN:HE22	1:D:59:ARG:NH1	1.87	0.53
1:C:12:HIS:HD2	1:C:216:HIS:ND1	2.06	0.53
1:A:227:LEU:HD22	1:A:231:VAL:HG23	1.92	0.52
1:B:4:LEU:HD13	1:B:238:MET:HE3	1.92	0.52
1:A:56:ARG:HD2	4:C:947:HOH:O	2.10	0.52
1:B:20:ARG:HG2	1:B:20:ARG:HH11	1.75	0.52
1:B:46:LEU:HD21	1:B:50:ARG:CD	2.40	0.52
1:D:108:ASP:HB2	4:D:870:HOH:O	2.10	0.52
1:A:195:LEU:HA	1:A:199:ASN:HD21	1.74	0.51
1:B:196:THR:H	1:B:199:ASN:ND2	2.07	0.51
1:C:225:THR:HG21	4:C:919:HOH:O	2.10	0.51
1:D:100:GLU:O	4:D:832:HOH:O	2.19	0.51
1:A:57:ASP:O	1:A:61:LEU:HB2	2.10	0.51
1:B:199:ASN:C	1:B:199:ASN:ND2	2.60	0.50
1:B:51:ARG:HG2	4:B:1024:HOH:O	2.12	0.50
1:D:164:THR:OG1	1:D:167:GLU:HB2	2.11	0.50
1:A:87:LYS:N	1:A:88:PRO:HD3	2.25	0.50
1:B:12:HIS:CD2	1:B:216:HIS:HD2	2.30	0.50
1:B:95:PRO:HG3	1:B:107:LEU:HD23	1.93	0.50
1:B:91:CYS:HB2	1:B:128:ILE:HG21	1.94	0.50
1:D:57:ASP:O	1:D:61:LEU:HB2	2.12	0.49
1:A:3:GLU:HB3	4:A:1032:HOH:O	2.11	0.49
1:D:75:VAL:HG22	1:D:93:LEU:HD13	1.94	0.49
1:C:12:HIS:CD2	1:C:216:HIS:ND1	2.81	0.49
1:B:133:PHE:HZ	1:B:155:HIS:HD2	1.61	0.48
1:D:50:ARG:HH11	1:D:50:ARG:HG2	1.78	0.48
1:C:91:CYS:HB2	1:C:128:ILE:HG21	1.95	0.48
1:D:47:ARG:NE	1:D:51:ARG:NH1	2.60	0.48
1:B:20:ARG:HG2	1:B:20:ARG:NH1	2.28	0.48
1:C:28:VAL:HG22	1:C:61:LEU:CD1	2.43	0.48
1:D:117:ARG:NH1	1:D:146:GLU:OE2	2.44	0.48
1:B:61:LEU:O	1:B:65:LEU:HG	2.14	0.47
1:D:199:ASN:C	1:D:199:ASN:ND2	2.66	0.47
1:D:84:VAL:O	1:D:87:LYS:HD2	2.15	0.47
1:C:161:ASP:O	1:C:162:ALA:C	2.55	0.47
1:A:6:LEU:HG	1:A:238:MET:SD	2.55	0.47
1:B:133:PHE:CZ	1:B:155:HIS:HD2	2.32	0.47
1:D:91:CYS:HB2	1:D:128:ILE:HG21	1.95	0.47
1:B:147:VAL:O	1:B:147:VAL:CG1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:HIS:CD2	1:D:216:HIS:CD2	3.03	0.46
1:D:227:LEU:HD22	1:D:231:VAL:HG23	1.96	0.46
1:D:242:ARG:NH2	4:D:913:HOH:O	2.46	0.46
1:D:14:ALA:HB3	1:D:52:HIS:HB2	1.97	0.46
1:D:50:ARG:HH12	1:D:55:ASP:CG	2.24	0.46
1:A:49:ASP:OD1	1:A:49:ASP:C	2.60	0.45
1:C:141:ILE:HD11	1:C:178:ALA:HB1	1.99	0.45
1:D:153:GLU:OE1	3:D:801:PXP:N1	2.49	0.45
1:B:48:GLU:OE1	1:B:98:ARG:HD2	2.16	0.45
1:B:161:ASP:O	1:B:162:ALA:C	2.58	0.45
1:C:133:PHE:HZ	1:C:155:HIS:HD2	1.63	0.45
1:D:117:ARG:NH2	1:D:146:GLU:OE2	2.49	0.45
1:B:233:GLU:CD	1:B:236:ARG:HH21	2.24	0.44
1:D:233:GLU:CD	1:D:236:ARG:HH21	2.26	0.44
1:B:103:THR:HG21	3:B:804:PXP:H2A2	2.00	0.44
1:D:95:PRO:HD3	1:D:107:LEU:HB2	2.00	0.44
1:D:104:GLU:OE2	1:D:174:ARG:NH2	2.41	0.44
1:D:2:ALA:HB2	4:D:901:HOH:O	2.18	0.44
1:B:193:HIS:CD2	4:B:972:HOH:O	2.70	0.44
1:A:9:ASN:HA	1:A:43:THR:O	2.18	0.43
1:A:113:ARG:HD3	4:A:992:HOH:O	2.18	0.43
1:D:171:GLU:OE2	1:D:174:ARG:NH1	2.50	0.43
1:D:80:LEU:O	1:D:84:VAL:HG23	2.18	0.43
1:A:72:GLU:HG2	1:A:92:CYS:HB3	2.00	0.43
1:B:46:LEU:CD2	1:B:50:ARG:HD3	2.49	0.43
1:B:46:LEU:HD21	1:B:50:ARG:NE	2.34	0.43
1:D:135:ASP:O	1:D:137:ASP:N	2.47	0.42
1:B:49:ASP:O	1:B:50:ARG:C	2.62	0.42
1:B:146:GLU:HG2	4:B:1044:HOH:O	2.19	0.42
1:C:221:ARG:HH11	1:C:221:ARG:CB	2.25	0.42
1:C:47:ARG:HD3	1:C:51:ARG:HB3	2.01	0.42
1:A:121:LYS:HE3	4:A:1086:HOH:O	2.19	0.42
1:B:20:ARG:HD3	1:B:20:ARG:HA	1.87	0.42
1:D:91:CYS:HB2	1:D:128:ILE:CG2	2.49	0.42
1:C:12:HIS:ND1	1:C:15:THR:HG21	2.34	0.42
1:D:155:HIS:CD2	1:D:157:GLY:N	2.79	0.42
1:D:31:ALA:O	1:D:35:GLU:HG3	2.19	0.41
1:D:204:ALA:O	1:D:242:ARG:HD3	2.19	0.41
1:A:113:ARG:O	1:A:117:ARG:HB2	2.20	0.41
1:A:153:GLU:OE1	3:A:802:PXP:N1	2.53	0.41
1:B:20:ARG:HH11	1:B:20:ARG:CG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:VAL:HG13	1:B:201:LYS:N	2.35	0.41
1:D:206:ILE:HA	1:D:207:PRO:HD3	1.75	0.41
1:B:12:HIS:CD2	1:B:216:HIS:CD2	3.08	0.41
1:B:171:GLU:OE2	1:B:171:GLU:HA	2.20	0.41
1:A:47:ARG:NH2	1:A:100:GLU:OE1	2.54	0.41
1:A:155:HIS:CE1	1:A:157:GLY:HA3	2.56	0.41
1:B:196:THR:H	1:B:199:ASN:HD21	1.69	0.41
1:D:68:ARG:HG2	4:D:963:HOH:O	2.20	0.41
1:D:192:GLY:O	1:D:193:HIS:CB	2.68	0.41
1:A:49:ASP:O	1:A:50:ARG:C	2.65	0.40
1:B:133:PHE:CZ	1:B:155:HIS:CD2	3.10	0.40
1:A:225:THR:CG2	4:A:942:HOH:O	2.70	0.40
3:B:804:PXP:H4A1	3:B:804:PXP:H5A2	1.88	0.40
1:D:89:HIS:CD2	1:D:90:PHE:CE1	3.04	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%)	230 (96%)	8 (3%)	2 (1%)	16	20
1	B	240/242 (99%)	229 (95%)	8 (3%)	3 (1%)	9	10
1	C	240/242 (99%)	231 (96%)	8 (3%)	1 (0%)	30	38
1	D	240/242 (99%)	228 (95%)	11 (5%)	1 (0%)	30	38
All	All	960/968 (99%)	918 (96%)	35 (4%)	7 (1%)	18	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	98	ARG

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Mol	Chain	Res	Type
1	A	106	GLY
1	B	104	GLU
1	C	193	HIS
1	D	193	HIS
1	B	193	HIS
1	A	193	HIS

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	184/185 (100%)	169 (92%)	15 (8%)	10	14
1	B	185/185 (100%)	172 (93%)	13 (7%)	14	19
1	C	185/185 (100%)	170 (92%)	15 (8%)	11	14
1	D	183/185 (99%)	168 (92%)	15 (8%)	10	14
All	All	737/740 (100%)	679 (92%)	58 (8%)	11	15

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	LEU
1	A	6	LEU
1	A	22	THR
1	A	46	LEU
1	A	48	GLU
1	A	61	LEU
1	A	71	LEU
1	A	104	GLU
1	A	138	GLU
1	A	172	LEU
1	A	189	VAL
1	A	199	ASN
1	A	223	VAL
1	A	227	LEU

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Mol	Chain	Res	Type
1	B	3	GLU
1	B	4	LEU
1	B	6	LEU
1	B	20	ARG
1	B	46	LEU
1	B	56	ARG
1	B	61	LEU
1	B	71	LEU
1	B	85	GLU
1	B	172	LEU
1	B	189	VAL
1	B	199	ASN
1	B	227	LEU
1	C	3	GLU
1	C	4	LEU
1	C	6	LEU
1	C	15	THR
1	C	22	THR
1	C	46	LEU
1	C	68	ARG
1	C	71	LEU
1	C	75	VAL
1	C	172	LEU
1	C	189	VAL
1	C	199	ASN
1	C	221	ARG
1	C	225	THR
1	C	227	LEU
1	D	4	LEU
1	D	46	LEU
1	D	51	ARG
1	D	56	ARG
1	D	61	LEU
1	D	71	LEU
1	D	91	CYS
1	D	101	VAL
1	D	118	ASP
1	D	147	VAL
1	D	172	LEU
1	D	185	LEU
1	D	189	VAL
1	D	199	ASN

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Mol	Chain	Res	Type
1	D	227	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	12	HIS
1	A	63	GLN
1	A	89	HIS
1	A	112	GLN
1	A	155	HIS
1	A	199	ASN
1	A	210	HIS
1	A	216	HIS
1	B	29	GLN
1	B	36	GLN
1	B	63	GLN
1	B	155	HIS
1	B	170	GLN
1	B	193	HIS
1	B	198	HIS
1	B	199	ASN
1	B	210	HIS
1	B	213	ASN
1	B	216	HIS
1	C	12	HIS
1	C	63	GLN
1	C	70	ASN
1	C	129	GLN
1	C	155	HIS
1	C	199	ASN
1	C	210	HIS
1	D	12	HIS
1	D	29	GLN
1	D	36	GLN
1	D	63	GLN
1	D	70	ASN
1	D	89	HIS
1	D	129	GLN
1	D	155	HIS
1	D	193	HIS
1	D	199	ASN
1	D	210	HIS

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Mol	Chain	Res	Type
1	D	213	ASN
1	D	216	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PXP	C	803	-	16,16,16	1.79	3 (18%)	22,23,23	1.50	4 (18%)
2	PO4	A	901	-	4,4,4	0.89	0	6,6,6	0.77	0
3	PXP	A	802	-	16,16,16	1.64	4 (25%)	22,23,23	1.41	3 (13%)
3	PXP	D	801	-	16,16,16	1.77	5 (31%)	22,23,23	1.56	3 (13%)
2	PO4	B	903	-	4,4,4	0.75	0	6,6,6	0.92	0
2	PO4	C	902	-	4,4,4	0.84	0	6,6,6	0.97	0
3	PXP	B	804	-	16,16,16	1.82	5 (31%)	22,23,23	1.93	7 (31%)

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	PXP	A	802	-	-	2/8/8/8	0/1/1/1
3	PXP	D	801	-	-	0/8/8/8	0/1/1/1
3	PXP	B	804	-	-	4/8/8/8	0/1/1/1
3	PXP	C	803	-	-	2/8/8/8	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	801	PXP	C2A-C2	3.68	1.56	1.50
3	B	804	PXP	C2-N1	3.52	1.40	1.33
3	C	803	PXP	C2-N1	3.49	1.40	1.33
3	C	803	PXP	C2A-C2	3.35	1.55	1.50
3	D	801	PXP	C2-N1	3.19	1.39	1.33
3	A	802	PXP	C2-N1	2.89	1.39	1.33
3	B	804	PXP	C4A-C4	-2.85	1.48	1.51
3	A	802	PXP	C6-N1	2.80	1.40	1.34
3	B	804	PXP	P-O3P	-2.77	1.44	1.54
3	D	801	PXP	C6-N1	2.51	1.39	1.34
3	A	802	PXP	C2A-C2	2.42	1.54	1.50
3	C	803	PXP	P-O3P	-2.27	1.46	1.54
3	B	804	PXP	C6-N1	2.24	1.39	1.34
3	B	804	PXP	P-O4P	-2.22	1.53	1.60
3	A	802	PXP	P-O3P	-2.21	1.46	1.54
3	D	801	PXP	P-O3P	-2.16	1.46	1.54
3	D	801	PXP	C5-C4	2.02	1.43	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	804	PXP	O3P-P-O4P	4.30	117.88	106.67
3	B	804	PXP	O4P-P-O1P	-3.62	96.65	106.44
3	D	801	PXP	O3P-P-O4P	3.57	115.99	106.67
3	B	804	PXP	O4P-C5A-C5	-3.41	102.96	109.36
3	A	802	PXP	O3P-P-O4P	3.33	115.36	106.67
3	C	803	PXP	O3P-P-O4P	2.99	114.47	106.67
3	B	804	PXP	O4A-C4A-C4	-2.51	105.16	111.60
3	B	804	PXP	C5-C6-N1	-2.48	119.79	123.83
3	D	801	PXP	C5-C6-N1	-2.45	119.84	123.83
3	C	803	PXP	C5-C6-N1	-2.39	119.95	123.83
3	C	803	PXP	O2P-P-O4P	-2.33	100.58	106.67
3	B	804	PXP	C3-C4-C5	2.29	120.80	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	PXP	C5-C6-N1	-2.26	120.15	123.83
3	A	802	PXP	O4P-P-O1P	-2.18	100.56	106.44
3	B	804	PXP	O2P-P-O4P	-2.17	101.02	106.67
3	D	801	PXP	O2P-P-O4P	-2.16	101.03	106.67
3	C	803	PXP	O4P-P-O1P	-2.00	101.03	106.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	804	PXP	C5A-O4P-P-O1P
3	B	804	PXP	C5A-O4P-P-O3P
3	A	802	PXP	C5-C4-C4A-O4A
3	C	803	PXP	C5-C4-C4A-O4A
3	B	804	PXP	C5A-O4P-P-O2P
3	C	803	PXP	C3-C4-C4A-O4A
3	B	804	PXP	C4-C5-C5A-O4P
3	A	802	PXP	C3-C4-C4A-O4A

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	PXP	1	0
3	D	801	PXP	1	0
3	B	804	PXP	3	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 [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	242/242 (100%)	-0.44	3 (1%) 76 77	21, 34, 53, 80	0
1	B	242/242 (100%)	-0.31	6 (2%) 58 60	22, 34, 58, 93	0
1	C	242/242 (100%)	-0.44	4 (1%) 69 70	20, 32, 53, 81	0
1	D	242/242 (100%)	-0.48	1 (0%) 88 89	21, 32, 50, 82	0
All	All	968/968 (100%)	-0.42	14 (1%) 73 75	20, 33, 54, 93	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	THR	4.5
1	B	103	THR	3.5
1	C	101	VAL	3.1
1	A	101	VAL	3.0
1	B	98	ARG	2.9
1	B	105	GLY	2.9
1	B	101	VAL	2.9
1	D	101	VAL	2.5
1	C	98	ARG	2.3
1	C	97	LYS	2.3
1	A	48	GLU	2.3
1	A	104	GLU	2.1
1	B	114	ASP	2.1
1	C	3	GLU	2.1

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 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	C	902	5/5	0.84	0.13	60,64,67,69	0
2	PO4	B	903	5/5	0.87	0.14	67,70,72,73	0
3	PXP	B	804	16/16	0.95	0.11	30,42,47,49	0
2	PO4	A	901	5/5	0.96	0.09	51,54,55,56	0
3	PXP	A	802	16/16	0.98	0.05	28,32,37,41	0
3	PXP	C	803	16/16	0.98	0.06	26,32,38,45	0
3	PXP	D	801	16/16	0.98	0.05	24,32,38,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.