Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 08:56 PM EDT

PDB ID	:	1HO4
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 (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:

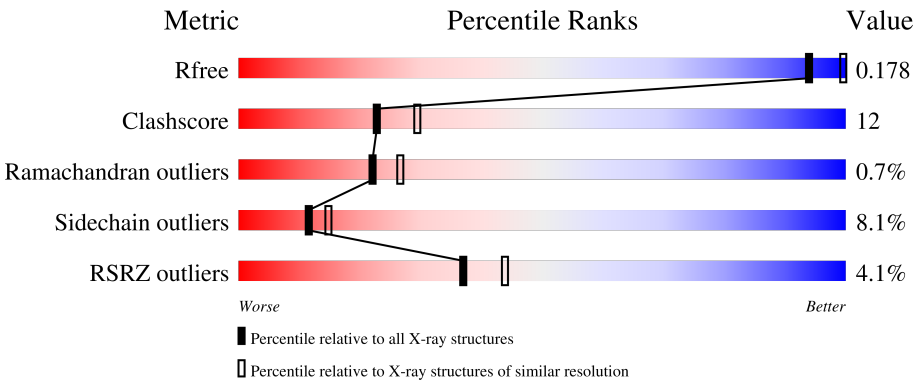
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	4% 77% 20% •
1	B	242	5% 79% 18% •
1	C	242	5% 81% 17% •
1	D	242	3% 72% 24% •

2 Entry composition (i)

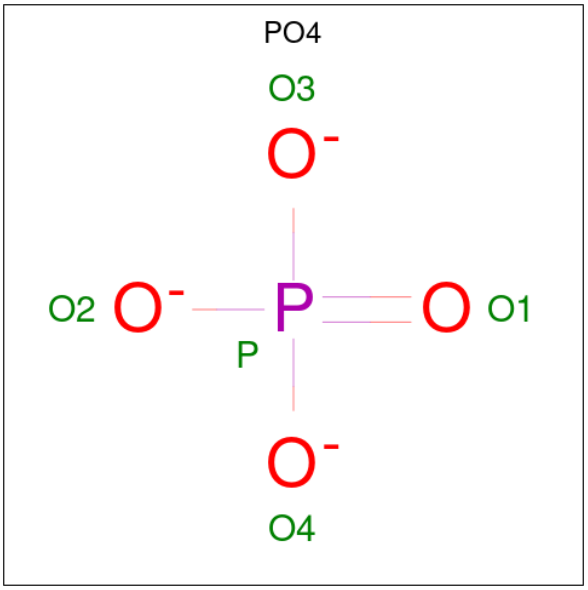
There are 4 unique types of molecules in this entry. The entry contains 8148 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	242	1833	1136	337	348	12	0	0	0
1	B	242	1837	1138	337	350	12	0	0	0
1	C	242	1837	1138	337	350	12	0	0	0
1	D	242	1827	1132	333	350	12	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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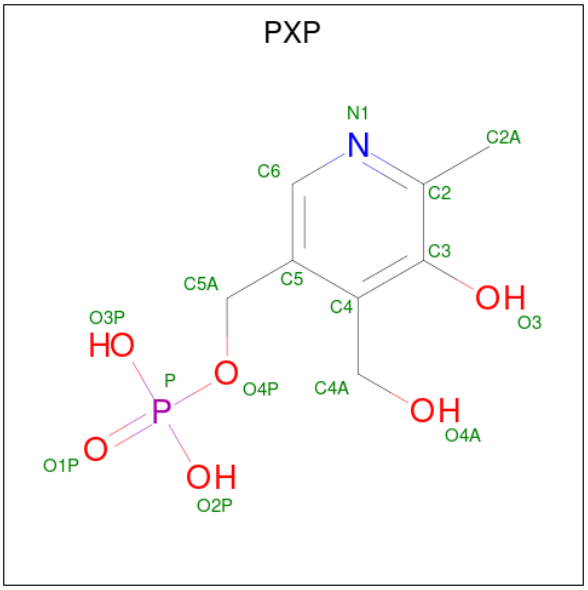
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	C	1	5	4	1	0	0

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



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

- Molecule 4 is water.

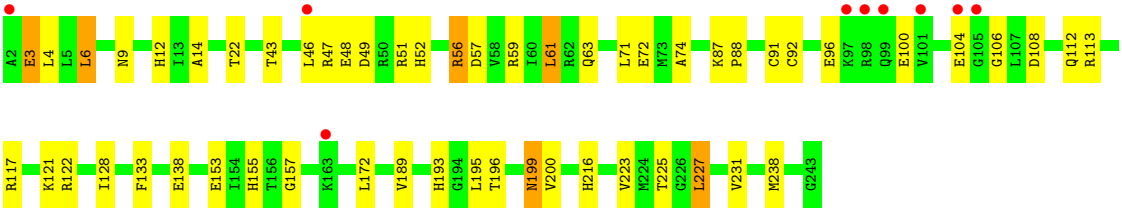
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	194	194	194	0	0
4	B	168	168	168	0	0
4	C	182	182	182	0	0
4	D	191	191	191	0	0

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.

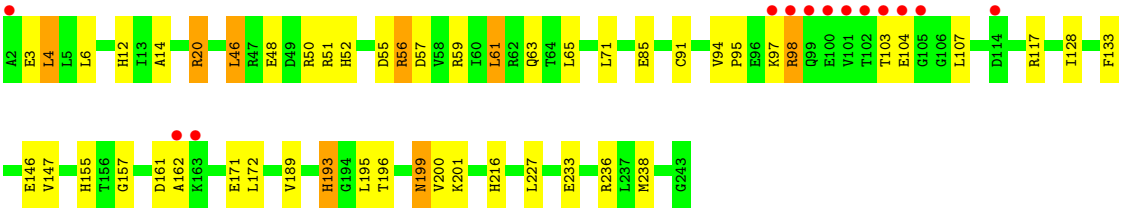
• Molecule 1: PYRIDOXINE 5'-PHOSPHATE SYNTHASE

Chain A:



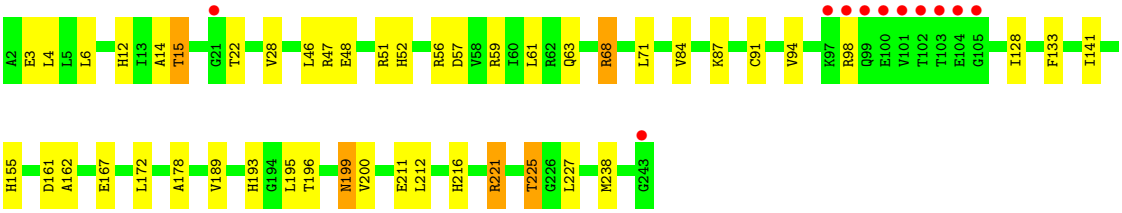
• Molecule 1: PYRIDOXINE 5'-PHOSPHATE SYNTHASE

Chain B:



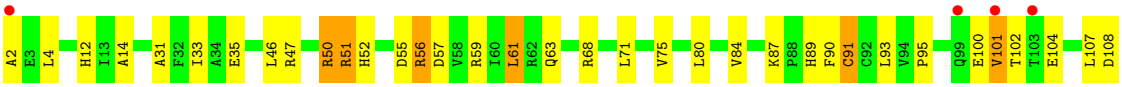
• Molecule 1: PYRIDOXINE 5'-PHOSPHATE SYNTHASE

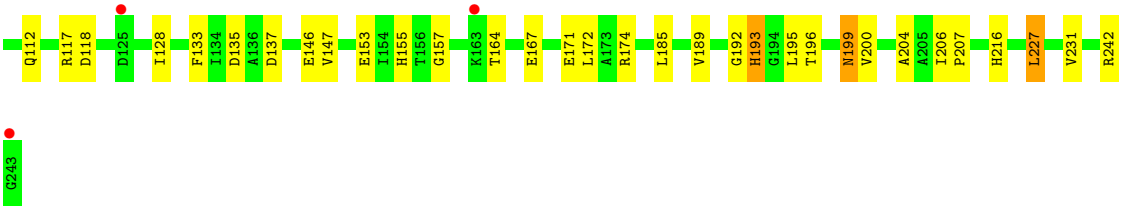
Chain C:



• Molecule 1: PYRIDOXINE 5'-PHOSPHATE SYNTHASE

Chain D:




Q112
R117
D118
D125
I128
F133
I134
D135
A136
D137
E146
V147
E153
I154
H155
T156
G157
K163
T164
E167
E171
L172
A173
R174
L185
V189
G192
H193
G194
L195
T196
N199
V200
A204
A205
I206
P207
H216
L227
V231
R242
G243

4 Data and refinement statistics (i)

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 19.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 95.9 (19.88-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [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)	0.34 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	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.*

[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: PO4, PXP

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	0.49	0/1855	0.74	0/2504
1	B	0.52	0/1859	0.72	0/2509
1	C	0.51	0/1859	0.74	0/2509
1	D	0.52	0/1849	0.75	0/2498
All	All	0.51	0/7422	0.74	0/10020

There are no bond length outliers.

There are no bond angle outliers.

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	1833	0	1850	38	0
1	B	1837	0	1854	46	0
1	C	1837	0	1854	37	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	2	0
3	B	16	0	10	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	16	0	10	2	0
3	D	16	0	10	2	0
4	A	194	0	0	6	0
4	B	168	0	0	4	0
4	C	182	0	0	3	0
4	D	191	0	0	11	0
All	All	8148	0	7430	171	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 12.

All (171) 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: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:A:199:ASN:C	1:A:199:ASN:HD22	1.79	0.85
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:221:ARG:HB2	1:C:221:ARG:HH11	1.48	0.79
1:B:199:ASN:HD22	1:B:199:ASN:C	1.86	0.78
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:C:199:ASN:C	1:C:199:ASN:HD22	1.90	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: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:D:199:ASN:C	1:D:199:ASN:HD22	1.96	0.68
1:A:14:ALA:HB3	1:A:52:HIS:HB2	1.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:PRO:HB2	1:D:101:VAL:HG22	1.76	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
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: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:B:94:VAL:HG11	3:B:804:PXP:H2A1	1.82	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:A:199:ASN:C	1:A:199:ASN:ND2	2.52	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ILE:HG21	1:D:227:LEU:HB3	1.90	0.53
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:A:133:PHE:CD2	3:A:802:PXP:H2A2	2.44	0.53
1:B:63:GLN:HE22	1:D:59:ARG:NH1	1.87	0.53
1:D:133:PHE:CD2	3:D:801:PXP:H2A2	2.43	0.53
1:C:12:HIS:HD2	1:C:216:HIS:ND1	2.06	0.53
1:C:56:ARG:HD3	1:C:56:ARG:C	2.29	0.53
1:D:56:ARG:HD3	1:D:56:ARG:C	2.28	0.53
1:B:103:THR:CB	3:B:804:PXP:H2A3	2.39	0.52
1:A:227:LEU:HD22	1:A:231:VAL:HG23	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: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:199:ASN:C	1:B:199:ASN:ND2	2.60	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:84:VAL:O	1:D:87:LYS:HD2	2.15	0.47
1:A:6:LEU:HG	1:A:238:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:199:ASN:C	1:C:199:ASN:ND2	2.63	0.46
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: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: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:4:LEU:HD13	1:B:238:MET:HE3	1.99	0.45
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:C:133:PHE:CD2	3:C:803:PXP:H2A2	2.53	0.43
1:D:171:GLU:OE2	1:D:174:ARG:NH1	2.50	0.43
1:D:199:ASN:ND2	1:D:199:ASN:C	2.66	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:C:161:ASP:O	1:C:162:ALA:C	2.55	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:B:233:GLU:CD	1:B:236:ARG:HH21	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:200:VAL:HG13	1:B:201:LYS:N	2.35	0.41
1:C:212:LEU:HD12	1:C:238:MET:HE3	2.01	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:D:50:ARG:HH12	1:D:55:ASP:CG	2.24	0.41
1:A:47:ARG:NH2	1:A:100:GLU:OE1	2.54	0.41
1:A:49:ASP:C	1:A:49:ASP:OD1	2.60	0.41
1:A:155:HIS:CE1	1:A:157:GLY:HA3	2.56	0.41
1:B:161:ASP:O	1:B:162:ALA:C	2.58	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:B:103:THR:OG1	3:B:804:PXP:H2A3	2.21	0.40
1:B:133:PHE:CZ	1:B:155:HIS:CD2	3.10	0.40
1:C:94:VAL:HG11	3:C:803:PXP:H2A1	2.04	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%)	19 23
1	B	240/242 (99%)	229 (95%)	8 (3%)	3 (1%)	12 12
1	C	240/242 (99%)	231 (96%)	8 (3%)	1 (0%)	34 42
1	D	240/242 (99%)	228 (95%)	11 (5%)	1 (0%)	34 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	960/968 (99%)	918 (96%)	35 (4%)	7 (1%)	22 26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	98	ARG
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 (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	184/185 (100%)	168 (91%)	16 (9%)	10 12
1	B	185/185 (100%)	171 (92%)	14 (8%)	13 16
1	C	185/185 (100%)	171 (92%)	14 (8%)	13 16
1	D	183/185 (99%)	167 (91%)	16 (9%)	10 12
All	All	737/740 (100%)	677 (92%)	60 (8%)	11 15

All (60) 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	56	ARG
1	A	61	LEU

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Mol	Chain	Res	Type
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
1	B	3	GLU
1	B	4	LEU
1	B	6	LEU
1	B	20	ARG
1	B	46	LEU
1	B	55	ASP
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	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	50	ARG
1	D	51	ARG
1	D	56	ARG
1	D	61	LEU

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Mol	Chain	Res	Type
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
1	D	227	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	63	GLN
1	A	89	HIS
1	A	155	HIS
1	A	199	ASN
1	A	210	HIS
1	A	216	HIS
1	B	63	GLN
1	B	89	HIS
1	B	129	GLN
1	B	155	HIS
1	B	193	HIS
1	B	199	ASN
1	B	210	HIS
1	B	216	HIS
1	C	12	HIS
1	C	63	GLN
1	C	89	HIS
1	C	155	HIS
1	C	199	ASN
1	C	210	HIS
1	D	12	HIS
1	D	63	GLN
1	D	89	HIS
1	D	155	HIS
1	D	199	ASN
1	D	210	HIS
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	A	802	-	16,16,16	1.64	4 (25%)	22,23,23	1.41	3 (13%)
3	PXP	C	803	-	16,16,16	1.79	3 (18%)	22,23,23	1.50	4 (18%)
2	PO4	C	902	-	4,4,4	0.84	0	6,6,6	0.97	0
2	PO4	B	903	-	4,4,4	0.75	0	6,6,6	0.92	0
3	PXP	D	801	-	16,16,16	1.77	5 (31%)	22,23,23	1.56	3 (13%)
3	PXP	B	804	-	16,16,16	1.82	5 (31%)	22,23,23	1.93	7 (31%)
2	PO4	A	901	-	4,4,4	0.89	0	6,6,6	0.77	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
3	PXP	D	801	-	-	0/8/8/8	0/1/1/1
3	PXP	A	802	-	-	2/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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(^{o})	Ideal(^{o})
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	PXP	2	0
3	C	803	PXP	2	0
3	D	801	PXP	2	0
3	B	804	PXP	4	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%)	-0.24	9 (3%)	41	48	21, 34, 53, 80	0
1	B	242/242 (100%)	-0.14	13 (5%)	25	32	22, 34, 58, 93	0
1	C	242/242 (100%)	-0.17	11 (4%)	33	40	20, 32, 53, 81	0
1	D	242/242 (100%)	-0.21	7 (2%)	51	58	21, 32, 50, 82	0
All	All	968/968 (100%)	-0.19	40 (4%)	37	44	20, 33, 54, 93	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	ARG	5.9
1	D	99	GLN	5.4
1	B	99	GLN	5.4
1	B	97	LYS	5.3
1	A	98	ARG	5.2
1	C	97	LYS	4.7
1	C	99	GLN	4.4
1	B	102	THR	4.3
1	C	98	ARG	4.2
1	D	103	THR	4.1
1	B	104	GLU	4.1
1	C	101	VAL	4.1
1	A	99	GLN	3.9
1	B	114	ASP	3.7
1	B	2	ALA	3.3
1	C	104	GLU	3.3
1	D	2	ALA	3.0
1	C	102	THR	3.0
1	D	101	VAL	2.9
1	A	104	GLU	2.8
1	B	163	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	105	GLY	2.7
1	D	243	GLY	2.6
1	B	103	THR	2.6
1	B	101	VAL	2.5
1	C	100	GLU	2.4
1	A	101	VAL	2.4
1	A	97	LYS	2.3
1	A	46	LEU	2.3
1	C	103	THR	2.3
1	D	163	LYS	2.3
1	C	105	GLY	2.3
1	A	163	LYS	2.3
1	D	125	ASP	2.2
1	B	162	ALA	2.2
1	A	2	ALA	2.2
1	C	21	GLY	2.1
1	C	243	GLY	2.1
1	B	100	GLU	2.1
1	A	105	GLY	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 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	PO4	B	903	5/5	0.88	0.15	67,70,72,73	0
2	PO4	C	902	5/5	0.91	0.16	60,64,67,69	0
3	PXP	B	804	16/16	0.96	0.17	30,42,47,49	0
2	PO4	A	901	5/5	0.97	0.10	51,54,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PXP	C	803	16/16	0.98	0.09	26,32,38,45	0
3	PXP	D	801	16/16	0.98	0.08	24,32,38,46	0
3	PXP	A	802	16/16	0.99	0.08	28,32,37,41	0

6.5 Other polymers (i)

There are no such residues in this entry.