Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:22 am BST

PDB ID	:	1IXN
Title	:	Enzyme-Substrate 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 following versions of software and data (see references ⓘ) were used in the production of this report:

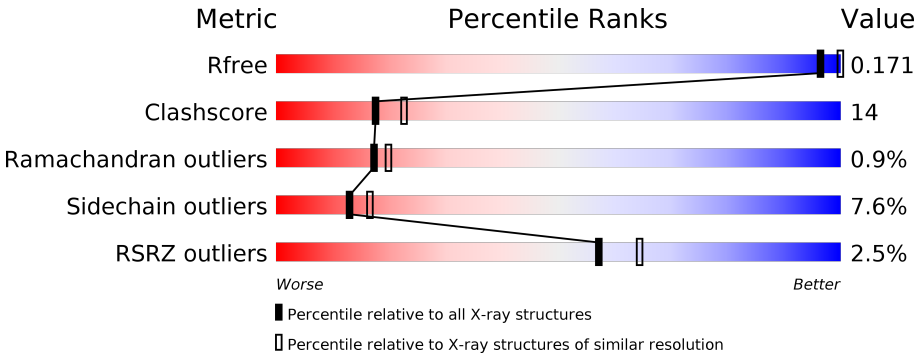
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 on 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	% 78% 18% ·
1	B	242	3% 77% 19% ·
1	C	242	% 75% 23% ·
1	D	242	5% 74% 21% 5%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DXP	A	2001	-	-	X	-
2	DXP	B	2002	-	-	X	-
2	DXP	C	2003	-	-	X	-
3	G3P	A	1001	-	-	X	-
3	G3P	B	1002	-	X	X	-
3	G3P	C	1003	-	X	X	-
3	G3P	D	1004	-	X	-	-

2 Entry composition

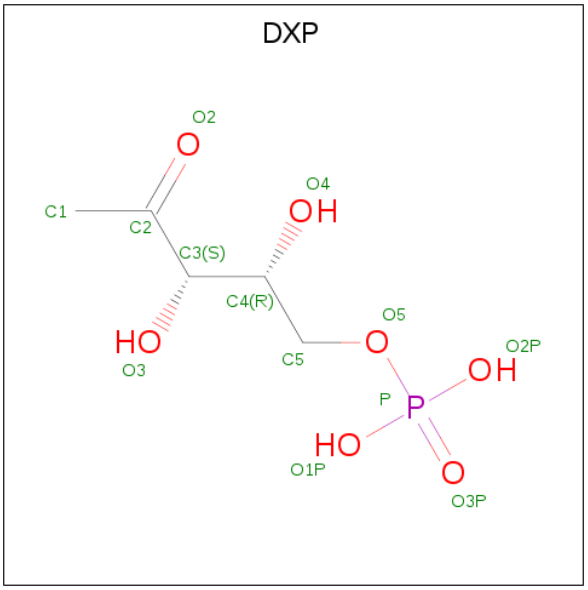
There are 4 unique types of molecules in this entry. The entry contains 8149 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			1833	1135	336	350	12			

- Molecule 2 is 1-DEOXY-D-XYLULOSE-5-PHOSPHATE (three-letter code: DXP) (formula: $C_5H_{11}O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			13	5	7	1		
2	B	1	Total	C	O	P	0	0
			13	5	7	1		

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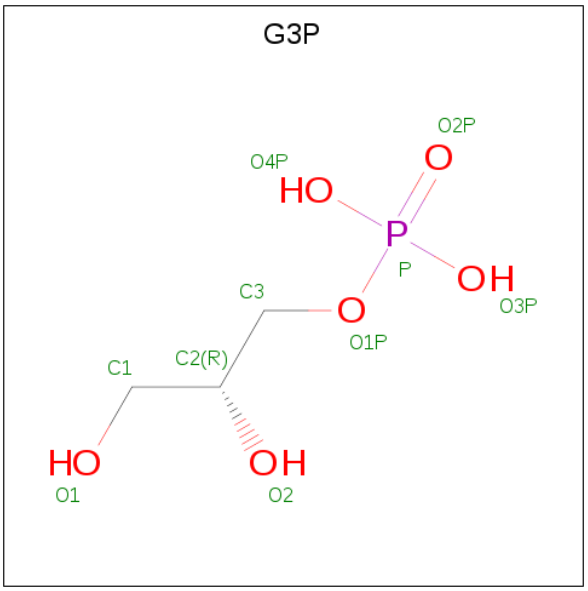
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O P 13 5 7 1	0	0
2	D	1	Total C O P 13 5 7 1	0	0

- Molecule 3 is SN-GLYCEROL-3-PHOSPHATE (three-letter code: G3P) (formula: $C_3H_9O_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 10 3 6 1	0	0
3	B	1	Total C O P 10 3 6 1	0	0
3	C	1	Total C O P 10 3 6 1	0	0
3	D	1	Total C O P 10 3 6 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	177	Total O 177 177	0	0
4	B	181	Total O 181 181	0	0
4	C	188	Total O 188 188	0	0

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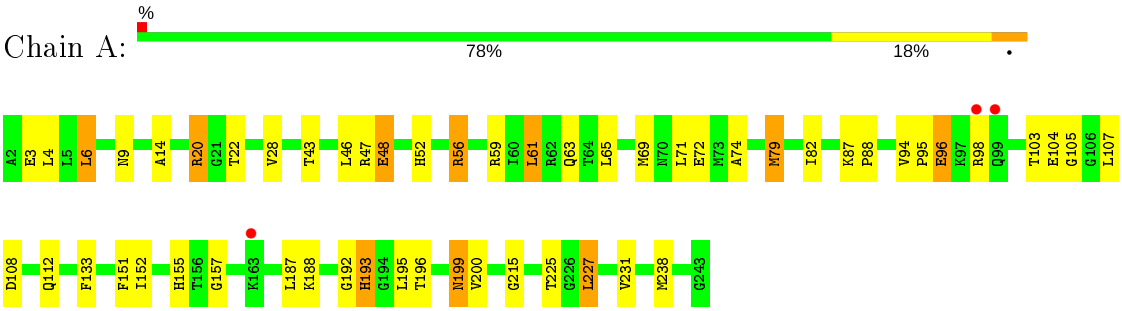
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	171	Total	O	0	0
			171	171		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

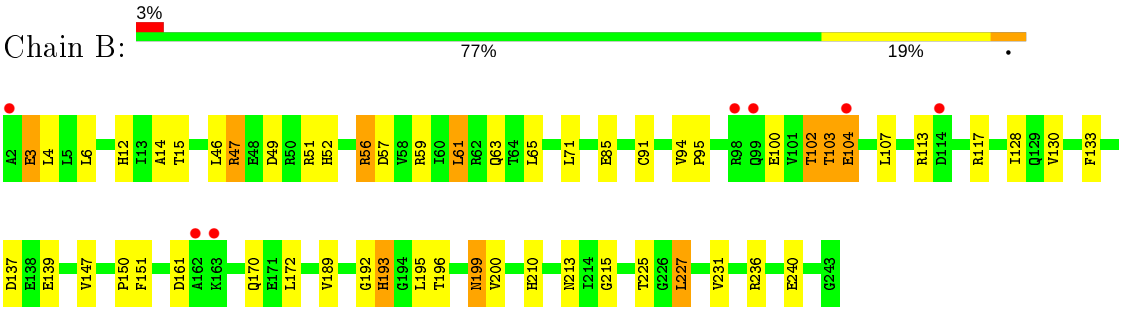
- Molecule 1: Pyridoxine 5'-Phosphate Synthase

Chain A:



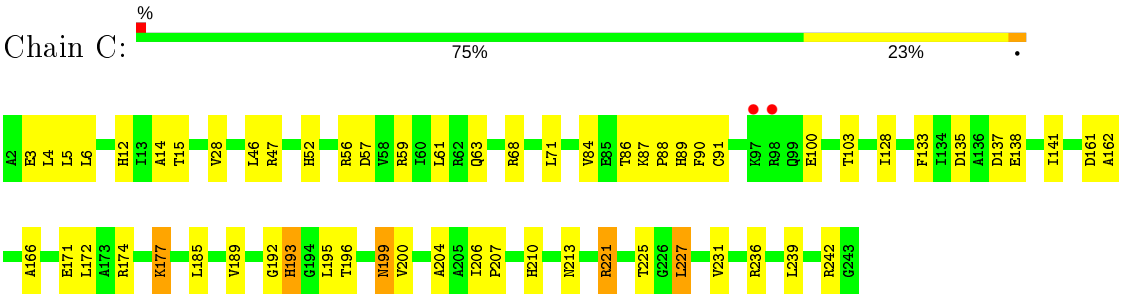
- Molecule 1: Pyridoxine 5'-Phosphate Synthase

Chain B:



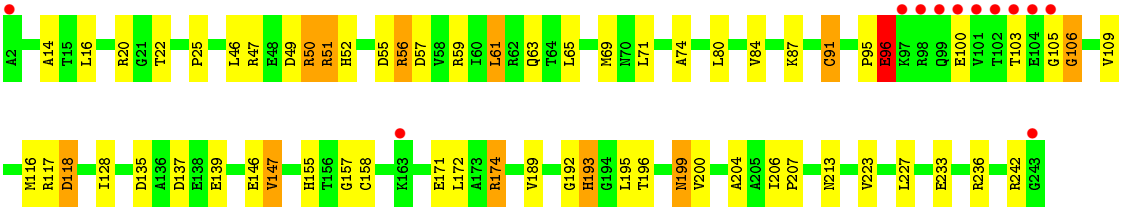
- Molecule 1: Pyridoxine 5'-Phosphate Synthase

Chain C:



- Molecule 1: Pyridoxine 5'-Phosphate Synthase

Chain D:


A2
A14
T15
L16
R20
G21
T22
P25
L46
R47
E48
D49
R50
R51
H52
D55
R56
D57
V58
R59
I60
L61
R62
Q63
T64
L65
M69
N70
L71
A74
L80
V84
K87
C91
P95
E96
K97
R98
Q99
E100
V101
T102
T103
E104
G105
G106
V109
M116
R117
D118
I128
D135
A136
D137
E138
E139
E146
V147
H155
T156
G157
C158
K163
E171
L172
A173
R174
V189
G192
H193
G194
L195
T196
N199
V200
A204
A205
I206
P207
M213
V223
L227
E233
R236
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	128.90Å 156.30Å 127.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 87.6 (19.89-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.30Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.180 , 0.224 0.179 , 0.171	Depositor DCC
R_{free} test set	2563 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.688	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.9	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	8149	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.39% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G3P, DXP

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	0.38	0/1855	0.67	0/2504
1	B	0.40	0/1859	0.68	0/2509
1	C	0.39	0/1859	0.69	0/2509
1	D	0.46	1/1855 (0.1%)	1.45	1/2505 (0.0%)
All	All	0.41	1/7428 (0.0%)	0.93	1/10027 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	96	GLU	C-N	8.45	1.53	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	96	GLU	O-C-N	-63.54	21.04	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	96	GLU	Mainchain

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	50	0
1	B	1837	0	1854	45	0
1	C	1837	0	1854	53	0
1	D	1833	0	1843	58	0
2	A	13	0	9	7	0
2	B	13	0	9	6	0
2	C	13	0	9	6	0
2	D	13	0	9	2	0
3	A	10	0	6	4	0
3	B	10	0	6	4	0
3	C	10	0	6	7	0
3	D	10	0	6	3	0
4	A	177	0	0	3	0
4	B	181	0	0	8	0
4	C	188	0	0	7	0
4	D	171	0	0	2	0
All	All	8149	0	7461	204	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 14.

All (204) 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:B:12:HIS:HA	1:B:15:THR:HG23	1.38	1.05
1:A:79:MET:HA	1:A:79:MET:HE3	1.42	1.02
1:B:59:ARG:HH12	1:D:63:GLN:HE22	1.18	0.90
1:D:103:THR:O	1:D:193:HIS:HE1	1.55	0.89
1:A:63:GLN:HE22	1:C:59:ARG:HH12	1.22	0.88
1:A:48:GLU:CD	1:A:48:GLU:H	1.76	0.87
1:A:103:THR:HB	2:A:2001:DXP:HC12	1.56	0.86
1:B:3:GLU:HB2	4:B:2011:HOH:O	1.75	0.85
1:C:103:THR:HB	2:C:2003:DXP:HC12	1.57	0.85
1:C:199:ASN:C	1:C:199:ASN:HD22	1.82	0.83
1:A:59:ARG:HH12	1:C:63:GLN:HE22	1.24	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLN:HE22	1:D:59:ARG:HH12	1.26	0.80
1:A:199:ASN:C	1:A:199:ASN:HD22	1.87	0.79
1:D:199:ASN:HD22	1:D:199:ASN:C	1.87	0.78
1:B:199:ASN:HD22	1:B:199:ASN:C	1.85	0.78
1:C:174:ARG:O	1:C:177:LYS:HD3	1.84	0.78
1:D:95:PRO:HG3	1:D:105:GLY:O	1.84	0.78
1:C:12:HIS:HA	1:C:15:THR:HG23	1.64	0.76
1:D:103:THR:O	1:D:193:HIS:CE1	2.38	0.76
1:A:79:MET:CE	1:A:79:MET:HA	2.16	0.76
1:D:50:ARG:HG2	1:D:50:ARG:HH11	1.51	0.75
1:B:57:ASP:O	1:B:61:LEU:HB2	1.86	0.75
1:D:233:GLU:CD	1:D:236:ARG:HH21	1.91	0.73
1:D:51:ARG:HB2	1:D:51:ARG:HH11	1.54	0.72
1:B:95:PRO:HG3	1:B:107:LEU:HA	1.72	0.72
1:D:51:ARG:NH2	1:D:100:GLU:O	2.23	0.71
1:B:12:HIS:ND1	1:B:15:THR:HG21	2.05	0.71
1:A:79:MET:CA	1:A:79:MET:HE3	2.19	0.70
1:B:213:ASN:HB3	3:B:1002:G3P:H11	1.74	0.69
1:A:196:THR:H	1:A:199:ASN:ND2	1.90	0.69
1:D:50:ARG:N	1:D:50:ARG:HD2	2.07	0.69
1:C:193:HIS:CG	2:C:2003:DXP:HC13	2.29	0.67
1:D:158:CYS:HB3	1:D:171:GLU:OE1	1.94	0.66
1:A:193:HIS:CG	2:A:2001:DXP:HC13	2.30	0.66
1:D:105:GLY:O	1:D:106:GLY:O	2.13	0.66
1:C:174:ARG:HD2	4:C:2173:HOH:O	1.93	0.66
1:D:105:GLY:O	1:D:106:GLY:C	2.33	0.64
1:D:118:ASP:HB3	4:D:2044:HOH:O	1.96	0.64
1:D:20:ARG:HG3	1:D:22:THR:HG23	1.79	0.63
1:D:50:ARG:H	1:D:50:ARG:HD2	1.62	0.63
1:B:56:ARG:HD2	4:B:2032:HOH:O	1.97	0.63
1:C:5:LEU:HD13	1:C:68:ARG:HH22	1.63	0.63
1:B:117:ARG:HA	1:B:147:VAL:HG13	1.80	0.63
1:B:195:LEU:HA	1:B:199:ASN:HD21	1.62	0.63
1:A:103:THR:CB	2:A:2001:DXP:HC12	2.28	0.62
1:B:14:ALA:HB3	1:B:52:HIS:HB2	1.80	0.62
1:D:84:VAL:O	1:D:87:LYS:HD2	1.99	0.62
1:A:56:ARG:HD2	4:C:2025:HOH:O	1.99	0.62
1:C:91:CYS:HB2	1:C:128:ILE:HG21	1.82	0.62
1:B:91:CYS:HB2	1:B:128:ILE:HG21	1.83	0.61
1:C:204:ALA:O	1:C:242:ARG:HD3	2.01	0.61
1:C:86:THR:HG22	1:C:88:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ARG:HH11	1:B:47:ARG:HG3	1.65	0.61
1:D:117:ARG:NH1	1:D:146:GLU:OE2	2.31	0.60
1:D:105:GLY:C	1:D:106:GLY:O	2.36	0.60
1:C:14:ALA:HB3	1:C:52:HIS:HB2	1.84	0.60
1:C:12:HIS:ND1	1:C:15:THR:HG21	2.17	0.59
1:C:138:GLU:OE1	1:C:177:LYS:HE3	2.02	0.59
1:B:213:ASN:HB3	3:B:1002:G3P:C1	2.32	0.59
1:C:103:THR:CB	2:C:2003:DXP:HC12	2.33	0.58
1:B:103:THR:HG21	2:B:2002:DXP:HC12	1.84	0.58
1:A:95:PRO:HG3	1:A:107:LEU:HA	1.86	0.58
1:D:56:ARG:C	1:D:56:ARG:HD3	2.25	0.58
1:C:193:HIS:HD2	3:C:1003:G3P:O2P	1.86	0.57
1:B:196:THR:H	1:B:199:ASN:ND2	2.02	0.57
1:A:199:ASN:C	1:A:199:ASN:ND2	2.57	0.56
1:A:195:LEU:HA	1:A:199:ASN:HD21	1.70	0.56
1:A:196:THR:H	1:A:199:ASN:HD21	1.53	0.56
1:B:210:HIS:HD2	4:B:2089:HOH:O	1.88	0.56
1:C:166:ALA:HA	4:C:2102:HOH:O	2.06	0.55
1:A:6:LEU:HG	1:A:238:MET:SD	2.47	0.55
1:D:91:CYS:HB2	1:D:128:ILE:CG2	2.37	0.55
1:A:14:ALA:HB3	1:A:52:HIS:HB2	1.89	0.55
1:D:91:CYS:HB2	1:D:128:ILE:HG21	1.89	0.55
1:A:225:THR:HG22	4:A:2176:HOH:O	2.07	0.54
1:B:102:THR:O	1:B:103:THR:O	2.26	0.54
1:C:199:ASN:HD22	1:C:200:VAL:N	2.04	0.54
1:D:50:ARG:HH12	1:D:55:ASP:CG	2.10	0.54
1:B:130:VAL:O	1:B:150:PRO:HD2	2.08	0.53
1:D:80:LEU:O	1:D:84:VAL:HG23	2.08	0.53
1:C:199:ASN:C	1:C:199:ASN:ND2	2.55	0.53
1:D:196:THR:H	1:D:199:ASN:ND2	2.07	0.53
1:C:195:LEU:HA	1:C:199:ASN:HD21	1.74	0.53
1:B:227:LEU:HD22	1:B:231:VAL:HG23	1.90	0.52
1:D:14:ALA:HB3	1:D:52:HIS:HB2	1.91	0.52
1:A:9:ASN:HA	1:A:43:THR:O	2.10	0.52
1:D:137:ASP:OD2	1:D:139:GLU:HB3	2.09	0.52
1:D:20:ARG:CG	1:D:22:THR:HG23	2.39	0.52
1:D:51:ARG:CB	1:D:51:ARG:HH11	2.23	0.52
1:C:103:THR:O	1:C:193:HIS:HE1	1.93	0.51
1:D:155:HIS:CD2	1:D:157:GLY:H	2.28	0.51
1:D:199:ASN:ND2	1:D:199:ASN:C	2.57	0.51
1:B:133:PHE:CZ	2:B:2002:DXP:HC11	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ARG:HG3	4:C:2041:HOH:O	2.10	0.51
1:D:57:ASP:O	1:D:61:LEU:HB2	2.10	0.51
1:B:104:GLU:HG2	4:B:2157:HOH:O	2.09	0.51
1:A:98:ARG:HD3	4:A:2174:HOH:O	2.11	0.50
1:D:199:ASN:HD22	1:D:200:VAL:N	2.09	0.50
1:C:137:ASP:O	1:C:141:ILE:HG13	2.11	0.50
1:C:196:THR:H	1:C:199:ASN:ND2	2.09	0.50
1:B:113:ARG:NH2	4:B:2117:HOH:O	2.40	0.50
1:A:48:GLU:OE2	1:A:96:GLU:OE1	2.29	0.49
1:C:56:ARG:HD3	1:C:56:ARG:C	2.32	0.49
1:C:84:VAL:O	1:C:87:LYS:HD2	2.12	0.49
1:D:135:ASP:O	1:D:137:ASP:N	2.41	0.49
1:B:193:HIS:CG	2:B:2002:DXP:HC13	2.47	0.49
1:D:171:GLU:OE2	1:D:174:ARG:NH1	2.45	0.49
1:B:61:LEU:O	1:B:65:LEU:HG	2.11	0.49
1:D:193:HIS:HD2	3:D:1004:G3P:O3P	1.95	0.49
1:A:20:ARG:HG3	1:A:22:THR:HG23	1.94	0.49
1:D:103:THR:HB	2:D:2004:DXP:HC13	1.95	0.49
1:D:56:ARG:HD3	1:D:57:ASP:N	2.28	0.49
1:B:236:ARG:O	1:B:240:GLU:HG3	2.12	0.49
1:B:102:THR:HG23	1:B:102:THR:O	2.13	0.48
1:B:199:ASN:C	1:B:199:ASN:ND2	2.57	0.48
1:A:47:ARG:NH1	2:A:2001:DXP:O1P	2.45	0.48
1:D:74:ALA:HB2	1:D:96:GLU:HB2	1.94	0.48
1:D:213:ASN:CB	3:D:1004:G3P:H11	2.43	0.48
1:A:199:ASN:HD22	1:A:200:VAL:N	2.11	0.48
1:C:213:ASN:CB	3:C:1003:G3P:H11	2.43	0.48
1:D:16:LEU:HD23	1:D:25:PRO:HG3	1.94	0.48
1:B:192:GLY:O	1:B:193:HIS:CB	2.62	0.48
1:D:47:ARG:O	1:D:50:ARG:HD2	2.14	0.48
2:A:2001:DXP:O3	3:A:1001:G3P:H32	2.13	0.48
1:B:100:GLU:HB2	1:B:104:GLU:OE2	2.14	0.48
1:B:199:ASN:HD22	1:B:200:VAL:N	2.12	0.48
1:C:68:ARG:NH1	1:C:90:PHE:HE1	2.12	0.48
1:C:227:LEU:HD22	1:C:231:VAL:HG23	1.96	0.47
1:D:103:THR:CB	2:D:2004:DXP:HC13	2.44	0.47
1:A:193:HIS:HA	3:A:1001:G3P:H31	1.95	0.47
1:B:103:THR:OG1	2:B:2002:DXP:HC4	2.15	0.47
1:A:20:ARG:NH1	4:A:2105:HOH:O	2.47	0.47
1:A:61:LEU:O	1:A:65:LEU:HG	2.15	0.47
1:B:94:VAL:HG12	1:B:95:PRO:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:HIS:HA	3:C:1003:G3P:O2P	2.15	0.46
1:D:213:ASN:HB3	3:D:1004:G3P:H11	1.96	0.46
1:A:193:HIS:HA	3:A:1001:G3P:O2P	2.14	0.46
1:A:87:LYS:N	1:A:88:PRO:HD3	2.30	0.46
1:D:49:ASP:OD2	1:D:51:ARG:HB2	2.15	0.46
1:C:3:GLU:CD	1:C:239:LEU:HD22	2.36	0.46
1:B:225:THR:HG22	4:B:2068:HOH:O	2.14	0.46
1:C:135:ASP:O	1:C:137:ASP:N	2.48	0.46
1:C:89:HIS:HD2	1:C:90:PHE:CE1	2.32	0.46
1:A:155:HIS:CE1	1:A:157:GLY:HA3	2.50	0.46
1:A:63:GLN:HE22	1:C:59:ARG:NH1	2.03	0.46
1:C:213:ASN:HB3	3:C:1003:G3P:H11	1.98	0.46
1:C:193:HIS:HA	3:C:1003:G3P:H31	1.97	0.45
1:C:221:ARG:NH1	4:C:2024:HOH:O	2.36	0.45
1:C:28:VAL:HG22	1:C:61:LEU:HD12	1.98	0.45
1:C:196:THR:O	1:C:200:VAL:HB	2.16	0.45
1:D:233:GLU:HG2	4:D:2123:HOH:O	2.16	0.45
1:A:48:GLU:OE2	1:A:96:GLU:OE2	2.35	0.45
1:A:192:GLY:O	1:A:193:HIS:CB	2.65	0.45
1:B:150:PRO:HB2	1:B:151:PHE:HD1	1.82	0.45
1:A:103:THR:OG1	2:A:2001:DXP:HC4	2.17	0.44
1:A:79:MET:CE	1:A:82:ILE:HD12	2.47	0.44
1:A:74:ALA:HB2	1:A:96:GLU:HB2	1.99	0.44
1:C:210:HIS:HE1	4:C:2101:HOH:O	2.01	0.44
1:B:225:THR:CG2	4:B:2010:HOH:O	2.64	0.44
1:A:28:VAL:HG22	1:A:61:LEU:HD13	1.99	0.44
1:C:133:PHE:CZ	2:C:2003:DXP:HC11	2.52	0.44
1:A:105:GLY:HA2	1:A:133:PHE:HE1	1.83	0.44
1:D:195:LEU:HA	1:D:199:ASN:HD21	1.83	0.44
2:B:2002:DXP:O3	3:B:1002:G3P:O2	2.28	0.43
1:D:204:ALA:O	1:D:242:ARG:HD3	2.18	0.43
1:D:196:THR:H	1:D:199:ASN:HD21	1.66	0.43
1:A:65:LEU:HD12	1:A:69:MET:HB2	2.01	0.43
1:B:103:THR:CG2	2:B:2002:DXP:HC12	2.48	0.43
1:D:117:ARG:NH2	1:D:146:GLU:OE2	2.52	0.43
1:C:57:ASP:O	1:C:61:LEU:HD13	2.19	0.43
2:C:2003:DXP:O3	3:C:1003:G3P:H32	2.19	0.42
1:D:117:ARG:CA	1:D:147:VAL:HG22	2.49	0.42
1:A:227:LEU:HD22	1:A:231:VAL:HG23	2.00	0.42
1:C:47:ARG:NH2	1:C:100:GLU:OE1	2.53	0.42
1:A:133:PHE:CZ	2:A:2001:DXP:HC11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:GLU:CG	1:C:239:LEU:HD22	2.49	0.42
1:D:109:VAL:HG13	1:D:116:MET:HG3	2.02	0.42
1:C:161:ASP:O	1:C:162:ALA:C	2.57	0.42
1:C:210:HIS:HD2	4:C:2055:HOH:O	2.02	0.42
1:B:3:GLU:HG3	1:B:3:GLU:H	1.58	0.42
1:D:65:LEU:HD12	1:D:69:MET:HB2	2.01	0.42
1:B:193:HIS:HA	3:B:1002:G3P:O3P	2.19	0.41
1:A:72:GLU:OE2	3:A:1001:G3P:O1	2.38	0.41
1:D:20:ARG:HG3	1:D:20:ARG:O	2.20	0.41
1:A:94:VAL:HG12	1:A:133:PHE:CB	2.50	0.41
1:C:171:GLU:OE2	1:C:171:GLU:HA	2.20	0.41
1:A:108:ASP:O	1:A:112:GLN:HG3	2.21	0.41
1:A:48:GLU:OE2	1:A:96:GLU:CD	2.58	0.41
1:C:192:GLY:O	1:C:193:HIS:CB	2.68	0.41
1:A:152:ILE:CG2	1:A:187:LEU:HD13	2.51	0.41
1:B:47:ARG:HB3	1:B:49:ASP:OD1	2.20	0.41
1:C:206:ILE:HA	1:C:207:PRO:HD3	1.82	0.41
1:A:151:PHE:CZ	1:A:188:LYS:HD2	2.55	0.41
1:D:206:ILE:HA	1:D:207:PRO:HD3	1.80	0.41
1:B:137:ASP:OD2	1:B:139:GLU:HB3	2.20	0.41
1:B:47:ARG:NH1	4:B:2084:HOH:O	2.54	0.41
1:D:50:ARG:HG2	1:D:50:ARG:NH1	2.27	0.41
1:B:49:ASP:OD1	1:B:51:ARG:HB2	2.21	0.41
1:D:192:GLY:O	1:D:193:HIS:CB	2.69	0.41
1:A:104:GLU:HA	1:A:104:GLU:OE2	2.21	0.40
1:A:152:ILE:HG21	1:A:187:LEU:HD13	2.03	0.40
1:C:236:ARG:HH11	1:C:236:ARG:HG2	1.85	0.40
1:C:213:ASN:HB2	3:C:1003:G3P:H11	2.04	0.40
1:C:103:THR:OG1	2:C:2003:DXP:HC4	2.21	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%)	228 (95%)	10 (4%)	2 (1%)	19 23
1	B	240/242 (99%)	229 (95%)	7 (3%)	4 (2%)	9 8
1	C	240/242 (99%)	228 (95%)	11 (5%)	1 (0%)	34 42
1	D	240/242 (99%)	231 (96%)	7 (3%)	2 (1%)	19 23
All	All	960/968 (99%)	916 (95%)	35 (4%)	9 (1%)	17 20

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	103	THR
1	D	193	HIS
1	B	102	THR
1	C	193	HIS
1	D	106	GLY
1	A	193	HIS
1	B	193	HIS
1	B	215	GLY
1	A	215	GLY

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%)	171 (93%)	13 (7%)	14 19
1	B	185/185 (100%)	169 (91%)	16 (9%)	10 12
1	C	185/185 (100%)	173 (94%)	12 (6%)	17 23
1	D	184/185 (100%)	169 (92%)	15 (8%)	11 14
All	All	738/740 (100%)	682 (92%)	56 (8%)	13 16

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	LEU

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Mol	Chain	Res	Type
1	A	6	LEU
1	A	20	ARG
1	A	46	LEU
1	A	48	GLU
1	A	56	ARG
1	A	61	LEU
1	A	71	LEU
1	A	79	MET
1	A	96	GLU
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	47	ARG
1	B	56	ARG
1	B	61	LEU
1	B	71	LEU
1	B	85	GLU
1	B	104	GLU
1	B	161	ASP
1	B	170	GLN
1	B	172	LEU
1	B	189	VAL
1	B	199	ASN
1	B	227	LEU
1	C	4	LEU
1	C	6	LEU
1	C	46	LEU
1	C	71	LEU
1	C	172	LEU
1	C	177	LYS
1	C	185	LEU
1	C	189	VAL
1	C	199	ASN
1	C	221	ARG
1	C	225	THR
1	C	227	LEU
1	D	46	LEU
1	D	50	ARG
1	D	51	ARG

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Mol	Chain	Res	Type
1	D	56	ARG
1	D	61	LEU
1	D	71	LEU
1	D	91	CYS
1	D	118	ASP
1	D	147	VAL
1	D	172	LEU
1	D	174	ARG
1	D	189	VAL
1	D	199	ASN
1	D	223	VAL
1	D	227	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	89	HIS
1	A	198	HIS
1	A	199	ASN
1	A	210	HIS
1	B	63	GLN
1	B	89	HIS
1	B	193	HIS
1	B	199	ASN
1	B	210	HIS
1	C	63	GLN
1	C	89	HIS
1	C	193	HIS
1	C	199	ASN
1	C	210	HIS
1	D	63	GLN
1	D	89	HIS
1	D	193	HIS
1	D	199	ASN
1	D	210	HIS

5.3.3 RNA

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 carbohydrates 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	DXP	D	2004	-	11,12,12	1.98	3 (27%)	13,17,17	2.43	5 (38%)
3	G3P	A	1001	-	9,9,9	2.17	3 (33%)	11,12,12	2.16	3 (27%)
2	DXP	A	2001	-	11,12,12	1.97	3 (27%)	13,17,17	1.64	5 (38%)
3	G3P	B	1002	-	9,9,9	2.44	3 (33%)	11,12,12	2.15	6 (54%)
2	DXP	B	2002	-	11,12,12	2.31	3 (27%)	13,17,17	2.16	5 (38%)
3	G3P	C	1003	-	9,9,9	2.25	3 (33%)	11,12,12	2.91	6 (54%)
2	DXP	C	2003	-	11,12,12	1.83	3 (27%)	13,17,17	1.34	2 (15%)
3	G3P	D	1004	-	9,9,9	1.94	2 (22%)	11,12,12	2.95	7 (63%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DXP	D	2004	-	-	8/14/14/14	-
3	G3P	A	1001	-	-	5/8/8/8	-
2	DXP	A	2001	-	-	2/14/14/14	-
3	G3P	B	1002	-	-	6/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DXP	B	2002	-	-	2/14/14/14	-
3	G3P	C	1003	-	-	4/8/8/8	-
2	DXP	C	2003	-	-	7/14/14/14	-
3	G3P	D	1004	-	-	6/8/8/8	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	G3P	P-O4P	-5.28	1.34	1.54
2	B	2002	DXP	C3-C2	-5.07	1.48	1.52
2	A	2001	DXP	P-O3P	-4.70	1.35	1.50
2	D	2004	DXP	P-O3P	-4.53	1.35	1.50
2	C	2003	DXP	P-O3P	-4.41	1.36	1.50
3	C	1003	G3P	P-O4P	-4.39	1.37	1.54
2	B	2002	DXP	P-O3P	-4.29	1.36	1.50
3	A	1001	G3P	P-O4P	-4.18	1.38	1.54
3	C	1003	G3P	O1-C1	-4.15	1.24	1.42
3	D	1004	G3P	P-O4P	-4.15	1.38	1.54
3	A	1001	G3P	O1-C1	-4.05	1.25	1.42
3	B	1002	G3P	O1-C1	-3.81	1.26	1.42
3	D	1004	G3P	O1-C1	-3.40	1.28	1.42
2	D	2004	DXP	C3-C2	-3.20	1.50	1.52
2	D	2004	DXP	P-O5	-3.13	1.50	1.60
2	C	2003	DXP	P-O5	-3.09	1.50	1.60
2	B	2002	DXP	P-O5	-3.09	1.50	1.60
2	A	2001	DXP	P-O5	-3.03	1.50	1.60
2	A	2001	DXP	C3-C2	-2.68	1.50	1.52
2	C	2003	DXP	C3-C2	-2.38	1.50	1.52
3	B	1002	G3P	P-O1P	-2.35	1.52	1.60
3	C	1003	G3P	P-O1P	-2.25	1.53	1.60
3	A	1001	G3P	P-O1P	-2.21	1.53	1.60

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1003	G3P	O1P-P-O2P	7.32	127.02	106.47
2	D	2004	DXP	C1-C2-C3	6.60	122.91	118.39
3	D	1004	G3P	O2-C2-C3	5.49	128.81	109.56
3	A	1001	G3P	O1P-P-O2P	5.25	121.20	106.47
2	B	2002	DXP	O3-C3-C2	-4.72	103.46	111.04
3	D	1004	G3P	O3P-P-O1P	4.12	117.71	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1004	G3P	O1P-P-O2P	3.95	117.57	106.47
2	B	2002	DXP	O2P-P-O5	3.53	116.13	106.73
3	B	1002	G3P	O3P-P-O1P	3.51	116.08	106.73
2	D	2004	DXP	O3-C3-C2	-3.34	105.67	111.04
3	D	1004	G3P	C3-C2-C1	-3.24	100.13	111.67
3	C	1003	G3P	O2-C2-C3	3.18	120.72	109.56
3	B	1002	G3P	O2-C2-C3	3.12	120.50	109.56
3	D	1004	G3P	O3P-P-O2P	-3.07	98.65	110.68
3	C	1003	G3P	C3-C2-C1	-2.87	101.45	111.67
3	B	1002	G3P	C3-C2-C1	-2.83	101.61	111.67
3	C	1003	G3P	O4P-P-O1P	-2.83	99.21	106.73
3	B	1002	G3P	O3P-P-O2P	-2.68	100.20	110.68
3	A	1001	G3P	O4P-P-O1P	-2.58	99.86	106.73
2	B	2002	DXP	O2-C2-C3	2.57	121.94	118.98
3	A	1001	G3P	C3-C2-C1	-2.56	102.57	111.67
2	C	2003	DXP	C1-C2-C3	2.52	120.12	118.39
3	D	1004	G3P	O4P-P-O1P	-2.52	100.03	106.73
3	B	1002	G3P	O4P-P-O2P	2.46	120.31	110.68
2	B	2002	DXP	P-O5-C5	-2.46	111.53	118.30
2	C	2003	DXP	O2-C2-C3	2.33	121.67	118.98
2	D	2004	DXP	P-O5-C5	-2.33	111.89	118.30
2	A	2001	DXP	P-O5-C5	-2.29	111.98	118.30
2	A	2001	DXP	C1-C2-C3	2.26	119.94	118.39
3	C	1003	G3P	O1-C1-C2	2.24	120.92	110.20
2	A	2001	DXP	O2P-P-O5	2.23	112.67	106.73
2	A	2001	DXP	O2-C2-C3	2.22	121.54	118.98
2	D	2004	DXP	O2P-P-O5	2.17	112.51	106.73
2	B	2002	DXP	O2P-P-O3P	-2.15	102.27	110.68
2	A	2001	DXP	O3-C3-C2	-2.10	107.67	111.04
3	B	1002	G3P	O1P-P-O2P	2.09	112.33	106.47
2	D	2004	DXP	O2P-P-O3P	-2.04	102.70	110.68
3	C	1003	G3P	O3P-P-O1P	-2.04	101.31	106.73
3	D	1004	G3P	O4P-P-O2P	2.00	118.52	110.68

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2004	DXP	C1-C2-C3-O3
2	D	2004	DXP	O2-C2-C3-C4
2	D	2004	DXP	O2-C2-C3-O3
2	D	2004	DXP	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	D	2004	DXP	C2-C3-C4-O4
2	D	2004	DXP	O3-C3-C4-C5
2	D	2004	DXP	O3-C3-C4-O4
3	A	1001	G3P	O1-C1-C2-C3
3	A	1001	G3P	C3-O1P-P-O4P
3	A	1001	G3P	C3-O1P-P-O2P
3	A	1001	G3P	C3-O1P-P-O3P
3	B	1002	G3P	C3-O1P-P-O4P
3	B	1002	G3P	C3-O1P-P-O3P
2	B	2002	DXP	O2-C2-C3-O3
3	C	1003	G3P	C3-O1P-P-O4P
3	C	1003	G3P	C3-O1P-P-O2P
3	C	1003	G3P	C3-O1P-P-O3P
2	C	2003	DXP	C2-C3-C4-O4
2	C	2003	DXP	O3-C3-C4-O4
3	D	1004	G3P	O2-C2-C3-O1P
3	D	1004	G3P	C3-O1P-P-O3P
3	B	1002	G3P	O2-C2-C3-O1P
3	B	1002	G3P	C1-C2-C3-O1P
3	B	1002	G3P	O1-C1-C2-C3
3	C	1003	G3P	O1-C1-C2-C3
3	D	1004	G3P	O1-C1-C2-C3
3	A	1001	G3P	O1-C1-C2-O2
3	D	1004	G3P	C1-C2-C3-O1P
3	B	1002	G3P	C3-O1P-P-O2P
2	D	2004	DXP	C1-C2-C3-C4
2	C	2003	DXP	O2-C2-C3-O3
2	C	2003	DXP	O3-C3-C4-C5
2	A	2001	DXP	C1-C2-C3-O3
2	C	2003	DXP	C1-C2-C3-O3
3	D	1004	G3P	C3-O1P-P-O4P
2	B	2002	DXP	C1-C2-C3-O3
3	D	1004	G3P	O1-C1-C2-O2
2	A	2001	DXP	O2-C2-C3-C4
2	C	2003	DXP	O2-C2-C3-C4
2	C	2003	DXP	C2-C3-C4-C5

There are no ring outliers.

8 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2004	DXP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	G3P	4	0
2	A	2001	DXP	7	0
3	B	1002	G3P	4	0
2	B	2002	DXP	6	0
3	C	1003	G3P	7	0
2	C	2003	DXP	6	0
3	D	1004	G3P	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

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^{th} 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%)	-0.46	3 (1%)	79	83	19, 31, 47, 67	0
1	B	242/242 (100%)	-0.38	7 (2%)	51	58	17, 30, 49, 74	0
1	C	242/242 (100%)	-0.42	2 (0%)	86	89	18, 28, 44, 61	0
1	D	242/242 (100%)	-0.25	12 (4%)	28	35	19, 29, 48, 100	0
All	All	968/968 (100%)	-0.37	24 (2%)	57	64	17, 29, 48, 100	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	8.2
1	D	104	GLU	6.7
1	D	99	GLN	5.5
1	D	103	THR	5.4
1	D	98	ARG	5.4
1	D	105	GLY	5.3
1	D	97	LYS	4.7
1	B	99	GLN	4.0
1	D	100	GLU	3.9
1	D	102	THR	3.7
1	D	2	ALA	3.6
1	B	104	GLU	3.5
1	D	101	VAL	3.4
1	C	97	LYS	3.1
1	A	98	ARG	2.9
1	A	99	GLN	2.8
1	B	98	ARG	2.5
1	D	163	LYS	2.4
1	D	243	GLY	2.2
1	B	163	LYS	2.1
1	B	162	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	163	LYS	2.1
1	B	114	ASP	2.0
1	C	98	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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, 95^{th} 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	DXP	D	2004	13/13	0.88	0.20	77,79,80,81	0
2	DXP	A	2001	13/13	0.97	0.12	34,41,51,51	0
2	DXP	B	2002	13/13	0.97	0.12	40,49,54,56	0
3	G3P	C	1003	10/10	0.97	0.11	25,31,38,42	0
2	DXP	C	2003	13/13	0.97	0.10	29,41,44,45	0
3	G3P	D	1004	10/10	0.97	0.12	30,38,44,45	0
3	G3P	A	1001	10/10	0.98	0.09	29,34,43,44	0
3	G3P	B	1002	10/10	0.99	0.08	25,32,41,44	0

6.5 Other polymers (i)

There are no such residues in this entry.