Full wwPDB X-ray Structure Validation Report (i)

May 15, 2024 – 06:49 PM EDT

PDB ID	:	2X5K
Title	:	Structure of an active site mutant of the D-Erythrose-4-Phosphate Dehydrogenase from E. coli
Authors	:	Moniot, S.; Didierjean, C.; Boschi-Muller, S.; Branlant, G.; Corbier, C.
Deposited on	:	2010-02-10
Resolution	:	2.37 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:

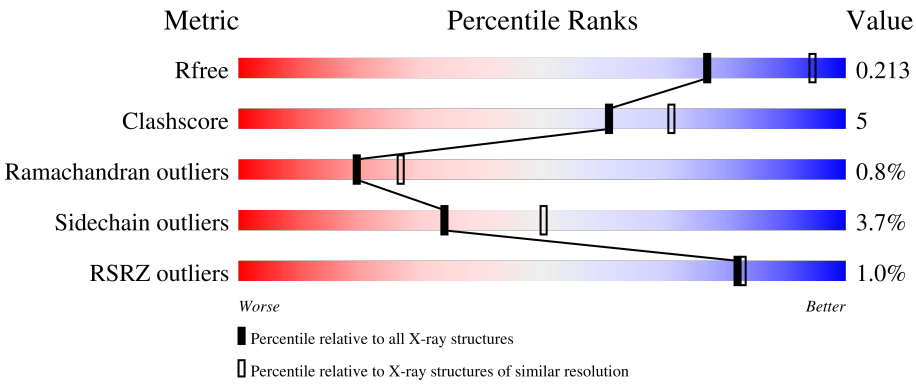
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.37 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	O	339	2% 86% 11% • •
1	P	339	% 86% 12% •
1	Q	339	% 90% 9% • •
1	R	339	% 83% 14% • •

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11575 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.

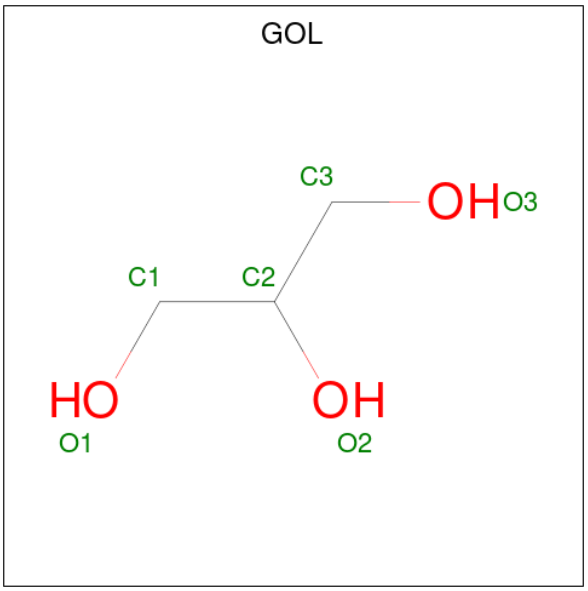
- Molecule 1 is a protein called D-ERYTHROSE-4-PHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	O	333	2641	1653	484	498	6	0	11	0
1	P	338	2636	1654	483	493	6	0	2	0
1	Q	337	2617	1641	478	492	6	0	2	0
1	R	334	2599	1635	472	486	6	0	3	0

There are 8 discrepancies between the modelled and reference sequences:

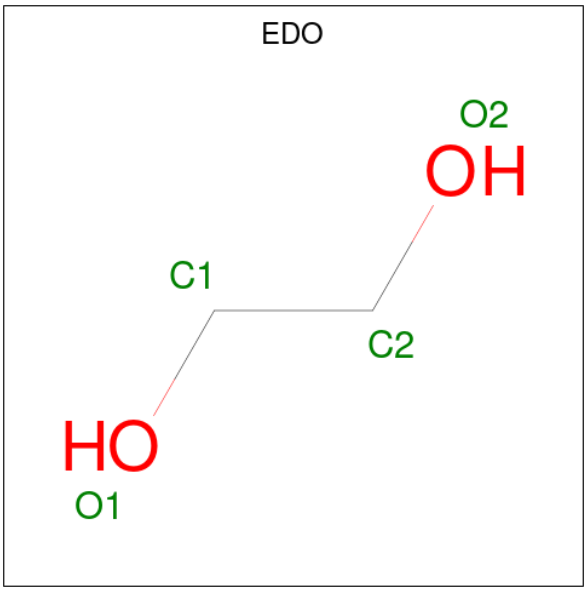
Chain	Residue	Modelled	Actual	Comment	Reference
O	149	ALA	CYS	engineered mutation	UNP P0A9B6
O	153	SER	CYS	engineered mutation	UNP P0A9B6
P	149	ALA	CYS	engineered mutation	UNP P0A9B6
P	153	SER	CYS	engineered mutation	UNP P0A9B6
Q	149	ALA	CYS	engineered mutation	UNP P0A9B6
Q	153	SER	CYS	engineered mutation	UNP P0A9B6
R	149	ALA	CYS	engineered mutation	UNP P0A9B6
R	153	SER	CYS	engineered mutation	UNP P0A9B6

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



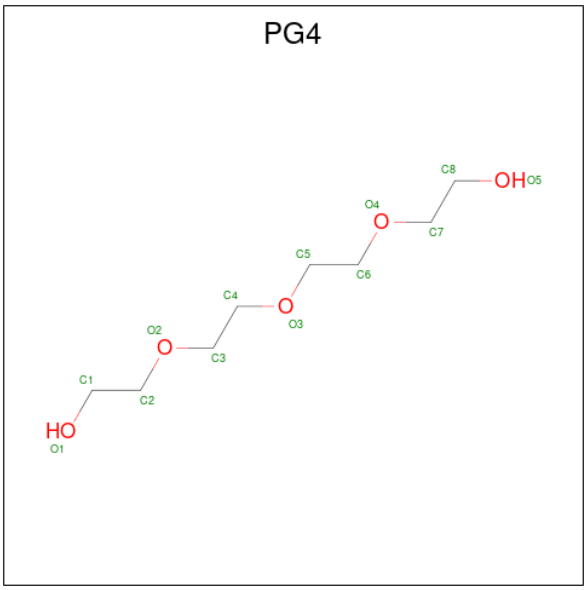
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	O	1	6	3	3	0	0
			Total	C	O		
2	O	1	6	3	3	0	0
			Total	C	O		
2	P	1	6	3	3	0	0
			Total	C	O		
2	P	1	6	3	3	0	0
			Total	C	O		
2	R	1	6	3	3	0	0
			Total	C	O		
2	R	1	6	3	3	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	O	1	4	2	2	0	0
3	P	1	4	2	2	0	0
3	Q	1	4	2	2	0	0
3	Q	1	4	2	2	0	0
3	R	1	4	2	2	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

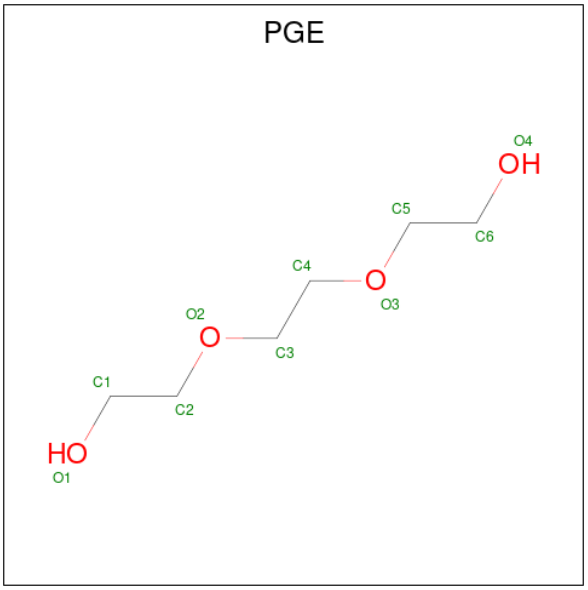


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	O	1	13	8	5	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

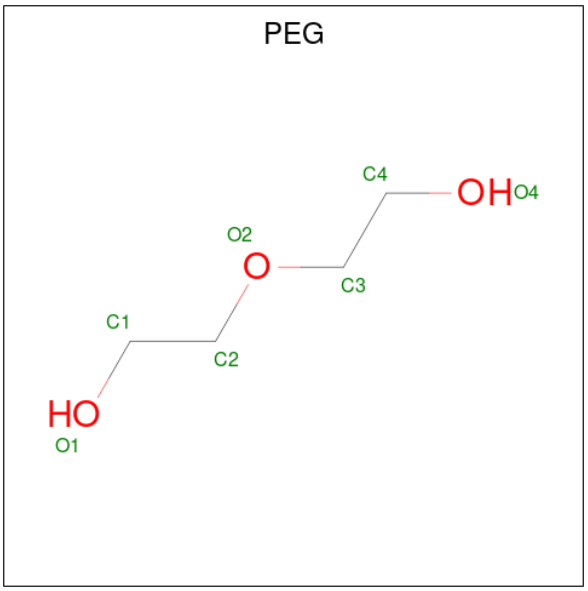
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	O	1	1	1	0	0
			Total	Cl		
5	P	1	1	1	0	0
			Total	Cl		
5	Q	1	1	1	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	O	1	10	6	4	0	0
			Total	C	O		
6	P	1	10	6	4	0	0
			Total	C	O		
6	P	1	10	6	4	0	0
			Total	C	O		
6	Q	1	10	6	4	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	P	1	7	4	3	0	0
			Total	C	O		
7	P	1	7	4	3	0	0

- Molecule 8 is water.

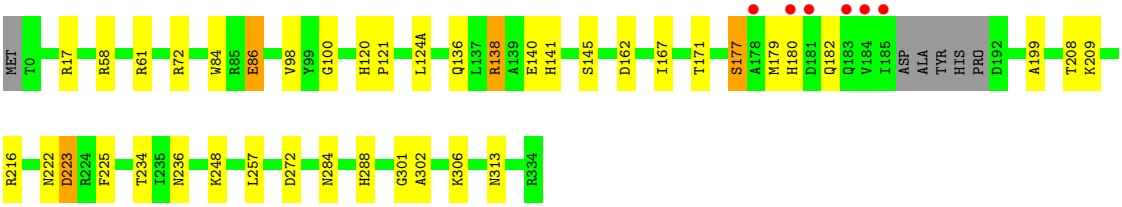
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	O	257	257	257	0	0
			Total	O		
8	P	248	248	248	0	0
			Total	O		
8	Q	248	248	248	0	0
			Total	O		
8	R	203	203	203	0	0

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.

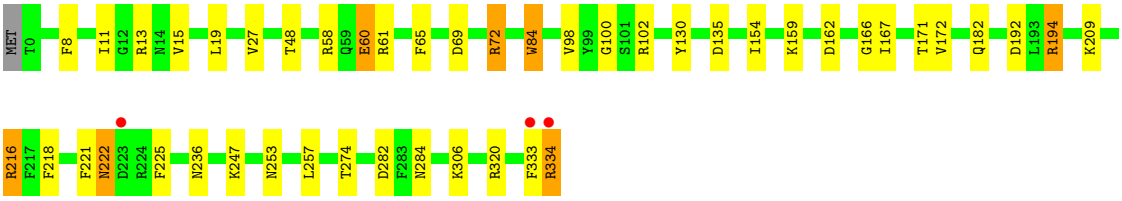
• Molecule 1: D-ERYTHROSE-4-PHOSPHATE DEHYDROGENASE

Chain O:



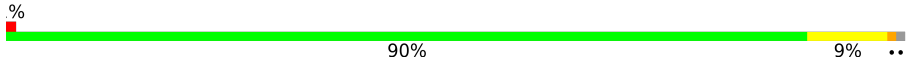
• Molecule 1: D-ERYTHROSE-4-PHOSPHATE DEHYDROGENASE

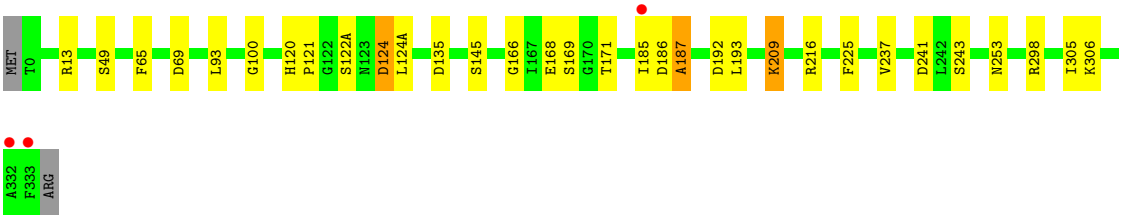
Chain P:



• Molecule 1: D-ERYTHROSE-4-PHOSPHATE DEHYDROGENASE

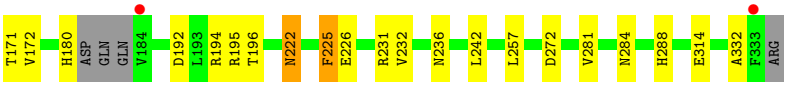
Chain Q:





• Molecule 1: D-ERYTHROSE-4-PHOSPHATE DEHYDROGENASE

Chain R:


T171
V172
H180
ASP
GLN
GLN
V184
D192
L193
R194
R195
T196
N222
F225
E226
R231
V232
N236
L242
L257
D272
V281
N284
H288
E314
A332
F333
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	134.81Å 134.81Å 246.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.97 – 2.37 55.97 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.8 (55.97-2.37) 98.8 (55.97-2.37)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.164 , 0.207 0.172 , 0.213	Depositor DCC
R_{free} test set	4571 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11575	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 2.53% 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: CL, GOL, PGE, PEG, PG4, EDO

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	O	1.13	2/2696 (0.1%)	0.98	5/3659 (0.1%)
1	P	1.07	2/2686 (0.1%)	0.96	6/3652 (0.2%)
1	Q	1.01	0/2669	0.92	4/3632 (0.1%)
1	R	1.05	3/2650 (0.1%)	0.97	8/3604 (0.2%)
All	All	1.07	7/10701 (0.1%)	0.96	23/14547 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	140	GLU	CD-OE2	5.60	1.31	1.25
1	R	231	ARG	CG-CD	5.54	1.65	1.51
1	R	232	VAL	CB-CG2	5.37	1.64	1.52
1	P	8	PHE	CB-CG	5.22	1.60	1.51
1	R	3	VAL	CB-CG2	-5.21	1.42	1.52
1	O	84	TRP	CB-CG	5.13	1.59	1.50
1	P	60	GLU	CG-CD	5.08	1.59	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	192	ASP	CB-CG-OD1	5.96	123.66	118.30
1	O	17	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	R	61	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	O	223	ASP	CB-CG-OD2	5.75	123.47	118.30
1	R	72	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	P	102	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	R	61	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	P	72	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	P	135	ASP	CB-CG-OD1	5.53	123.27	118.30
1	P	192	ASP	CB-CG-OD2	5.32	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	135[A]	ASP	CB-CG-OD2	5.28	123.06	118.30
1	Q	135[B]	ASP	CB-CG-OD2	5.28	123.06	118.30
1	R	36	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	R	28	VAL	CG1-CB-CG2	5.23	119.26	110.90
1	R	124	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	P	282	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	Q	192	ASP	CB-CG-OD1	5.17	122.95	118.30
1	R	47	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	Q	13	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	P	216	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	O	86[A]	GLU	OE1-CD-OE2	-5.02	117.27	123.30
1	O	86[B]	GLU	OE1-CD-OE2	-5.02	117.27	123.30
1	O	234	THR	CB-CA-C	-5.01	98.06	111.60

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	O	2641	0	2615	25	0
1	P	2636	0	2620	31	0
1	Q	2617	0	2601	18	0
1	R	2599	0	2587	27	0
2	O	12	0	16	1	0
2	P	12	0	16	1	0
2	R	12	0	16	0	0
3	O	4	0	6	0	0
3	P	4	0	6	0	0
3	Q	8	0	12	0	0
3	R	4	0	6	0	0
4	O	13	0	18	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
5	Q	1	0	0	0	0
6	O	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	20	0	28	1	0
6	Q	10	0	14	1	0
7	P	14	0	20	2	0
8	O	257	0	0	6	0
8	P	248	0	0	6	0
8	Q	248	0	0	2	0
8	R	203	0	0	8	0
All	All	11575	0	10595	96	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 5.

All (96) 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:P:182[B]:GLN:H	1:P:182[B]:GLN:CD	1.63	0.98
1:R:194:ARG:HD2	8:R:2135:HOH:O	1.63	0.96
1:O:138[A]:ARG:HD3	8:O:2129:HOH:O	1.69	0.92
1:R:17:ARG:NE	1:R:48:THR:HG22	1.91	0.86
1:O:177:SER:OG	1:O:180:HIS:CE1	2.30	0.85
1:Q:186:ASP:O	1:Q:187:ALA:CB	2.30	0.79
1:O:199:ALA:HB2	1:R:180:HIS:CB	2.12	0.79
1:Q:186:ASP:O	1:Q:187:ALA:HB3	1.90	0.70
1:Q:185:ILE:HD12	8:Q:2152:HOH:O	1.92	0.69
1:R:58:ARG:NH2	8:R:2036:HOH:O	2.25	0.68
1:P:58:ARG:CZ	7:P:1340:PEG:H21	2.24	0.67
1:P:182[B]:GLN:CD	1:P:182[B]:GLN:N	2.41	0.66
1:O:313[B]:ASN:H	1:O:313[B]:ASN:ND2	1.94	0.65
1:P:274:THR:HG23	8:P:2219:HOH:O	1.97	0.65
1:O:180:HIS:CE1	1:O:313[B]:ASN:OD1	2.51	0.63
1:O:177:SER:OG	1:O:180:HIS:HE1	1.79	0.63
1:P:333:PHE:C	1:P:334:ARG:HD2	2.19	0.63
1:O:208:THR:HA	8:O:2170:HOH:O	2.00	0.61
1:Q:216:ARG:NH1	8:Q:2180:HOH:O	2.34	0.60
1:R:115:LYS:HD3	8:R:2090:HOH:O	2.01	0.60
1:P:65:PHE:HA	1:P:69:ASP:O	2.02	0.60
1:P:333:PHE:O	1:P:334:ARG:OXT	2.20	0.59
1:R:115:LYS:HE3	1:R:332:ALA:HB2	1.85	0.59
1:O:301[B]:GLY:O	1:O:302[B]:ALA:HB3	2.04	0.58
1:R:17:ARG:CD	1:R:48:THR:HG22	2.33	0.58
1:P:218:PHE:HB2	1:P:221:PHE:CD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:272:ASP:HB2	1:R:288:HIS:CD2	2.40	0.57
1:O:58:ARG:NH1	8:O:2046:HOH:O	2.38	0.56
1:P:48:THR:HG23	1:R:281:VAL:HG11	1.86	0.56
2:P:1336:GOL:H31	8:P:2029:HOH:O	2.06	0.56
7:P:1341:PEG:H11	1:Q:193:LEU:CD1	2.37	0.55
1:O:177:SER:HG	1:O:180:HIS:CE1	2.24	0.55
1:P:216:ARG:HD2	8:P:2188:HOH:O	2.08	0.54
1:R:77[B]:ARG:HD2	8:R:2058:HOH:O	2.07	0.54
1:R:22(B):ARG:HD3	8:R:2011:HOH:O	2.07	0.54
1:R:19:LEU:HD22	1:R:27:VAL:HG23	1.90	0.53
1:O:162:ASP:HB2	1:O:167:ILE:HD12	1.92	0.52
1:Q:120:HIS:HB2	1:Q:121:PRO:HD2	1.92	0.52
1:Q:120:HIS:HE1	6:Q:1336:PGE:H32	1.74	0.51
1:O:171:THR:OG1	1:P:306:LYS:HE2	2.11	0.51
1:Q:93:LEU:HD12	1:Q:93:LEU:N	2.26	0.50
1:R:22(B):ARG:NH1	1:R:24:GLU:OE2	2.45	0.50
2:O:1336:GOL:H11	8:O:2147:HOH:O	2.11	0.50
1:O:236:ASN:ND2	1:O:284:ASN:OD1	2.41	0.50
1:P:334:ARG:HD2	1:P:334:ARG:N	2.27	0.50
1:R:46:TYR:CE1	1:R:52:ARG:HD3	2.47	0.49
1:Q:298:ARG:HB3	1:R:226:GLU:HG3	1.94	0.49
1:P:60:GLU:O	1:P:61:ARG:HB2	2.14	0.48
1:R:65:PHE:HA	1:R:69:ASP:O	2.14	0.47
1:P:130:TYR:HB3	1:P:320:ARG:HD3	1.97	0.47
1:O:120:HIS:HB2	1:O:121:PRO:CD	2.44	0.47
1:P:72:ARG:HD3	8:P:2063:HOH:O	2.13	0.47
1:P:221:PHE:O	1:P:222:ASN:C	2.53	0.46
1:P:194:ARG:NH1	8:P:2173:HOH:O	2.48	0.46
1:P:333:PHE:C	1:P:334:ARG:CD	2.84	0.46
1:Q:171:THR:HG22	1:Q:243:SER:HB2	1.96	0.45
1:P:236:ASN:OD1	1:P:284:ASN:ND2	2.49	0.45
1:Q:209:LYS:HD3	1:Q:209:LYS:HA	1.76	0.45
1:Q:306:LYS:HE2	1:R:171:THR:OG1	2.16	0.45
1:R:48:THR:OG1	1:R:51:GLY:O	2.23	0.45
1:R:236:ASN:HB3	1:R:284:ASN:OD1	2.17	0.45
1:P:162:ASP:HB2	1:P:167:ILE:HD12	2.00	0.44
1:P:13:ARG:NH2	8:P:2011:HOH:O	2.24	0.44
1:O:222:ASN:O	1:O:223:ASP:HB2	2.18	0.44
1:Q:243:SER:HA	1:Q:305:ILE:O	2.18	0.43
1:O:199:ALA:CB	1:R:180:HIS:CB	2.90	0.43
1:R:170:GLY:O	1:R:225:PHE:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:84:TRP:HA	1:P:84:TRP:CE3	2.54	0.43
1:P:333:PHE:O	1:P:334:ARG:HG2	2.18	0.43
1:P:11:ILE:O	1:P:15:VAL:HG23	2.19	0.42
1:R:168[B]:GLU:O	1:R:169:SER:HB3	2.18	0.42
1:P:19:LEU:HD22	1:P:27:VAL:HG23	2.01	0.42
1:R:72:ARG:HD3	8:R:2051:HOH:O	2.19	0.42
1:Q:65:PHE:HA	1:Q:69:ASP:O	2.19	0.42
1:O:138[A]:ARG:HG3	1:O:141:HIS:CE1	2.55	0.42
1:P:84:TRP:HA	1:P:84:TRP:HE3	1.83	0.41
1:P:98:VAL:HG11	6:P:1343:PGE:H2	2.01	0.41
1:P:154:ILE:HD12	1:P:154:ILE:HA	1.85	0.41
1:Q:122(A):SER:C	1:Q:124:ASP:H	2.22	0.41
1:P:209:LYS:HD3	1:P:209:LYS:HA	1.88	0.41
1:Q:241:ASP:C	1:Q:241:ASP:OD2	2.59	0.41
1:Q:186:ASP:O	1:Q:187:ALA:HB2	2.16	0.41
1:O:179:MET:HE1	1:O:236:ASN:HB2	2.01	0.41
1:O:138[A]:ARG:CD	8:O:2129:HOH:O	2.47	0.41
1:R:93:LEU:N	1:R:93:LEU:HD12	2.36	0.41
1:O:72:ARG:HH12	1:O:86[B]:GLU:CD	2.24	0.41
1:O:136:GLN:HG3	8:O:2005:HOH:O	2.21	0.41
1:R:72:ARG:CD	8:R:2051:HOH:O	2.68	0.41
1:O:236:ASN:O	1:O:236:ASN:CG	2.59	0.40
1:P:182[B]:GLN:H	1:P:182[B]:GLN:NE2	2.16	0.40
1:O:272:ASP:HB2	1:O:288:HIS:CD2	2.56	0.40
1:R:154:ILE:HD11	1:R:242:LEU:HD22	2.03	0.40
1:O:124(A):LEU:HD12	1:O:145:SER:HB2	2.04	0.40
1:Q:124(A):LEU:HD12	1:Q:145:SER:HB2	2.04	0.40
1:O:306:LYS:HE2	1:P:171:THR:OG1	2.21	0.40
1:R:222:ASN:ND2	8:R:2150:HOH:O	2.55	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	O	340/339 (100%)	320 (94%)	18 (5%)	2 (1%)	25	34
1	P	338/339 (100%)	323 (96%)	12 (4%)	3 (1%)	17	23
1	Q	337/339 (99%)	325 (96%)	8 (2%)	4 (1%)	13	17
1	R	333/339 (98%)	316 (95%)	15 (4%)	2 (1%)	25	34
All	All	1348/1356 (99%)	1284 (95%)	53 (4%)	11 (1%)	19	27

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	166	GLY
1	Q	187	ALA
1	Q	100	GLY
1	Q	237	VAL
1	R	100	GLY
1	O	100	GLY
1	P	100	GLY
1	P	222	ASN
1	O	182	GLN
1	R	166	GLY
1	P	166	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	O	279/279 (100%)	269 (96%)	10 (4%)	35	51
1	P	279/279 (100%)	270 (97%)	9 (3%)	39	56
1	Q	278/279 (100%)	271 (98%)	7 (2%)	47	65
1	R	275/279 (99%)	260 (94%)	15 (6%)	21	32
All	All	1111/1116 (100%)	1070 (96%)	41 (4%)	34	50

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	61	ARG
1	O	98	VAL
1	O	138[A]	ARG
1	O	138[B]	ARG
1	O	177	SER
1	O	209	LYS
1	O	216	ARG
1	O	225	PHE
1	O	248	LYS
1	O	257	LEU
1	P	84	TRP
1	P	159	LYS
1	P	172	VAL
1	P	194	ARG
1	P	225	PHE
1	P	247	LYS
1	P	253	ASN
1	P	257	LEU
1	P	334	ARG
1	Q	49	SER
1	Q	124	ASP
1	Q	168	GLU
1	Q	169	SER
1	Q	209	LYS
1	Q	225	PHE
1	Q	253	ASN
1	R	8	PHE
1	R	22(B)	ARG
1	R	28	VAL
1	R	72	ARG
1	R	86	GLU
1	R	98	VAL
1	R	122(A)	SER
1	R	123	ASN
1	R	172	VAL
1	R	195	ARG
1	R	196	THR
1	R	222	ASN
1	R	225	PHE
1	R	257	LEU
1	R	314	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	180	HIS
1	P	236	ASN
1	P	284	ASN
1	R	201	GLN
1	R	236	ASN

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)

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PGE	P	1343	-	9,9,9	0.64	0	8,8,8	0.62	0
7	PEG	P	1341	-	6,6,6	0.80	0	5,5,5	1.13	1 (20%)
2	GOL	O	1335	-	5,5,5	0.63	0	5,5,5	1.05	0
7	PEG	P	1340	-	6,6,6	0.78	0	5,5,5	0.78	0
2	GOL	R	1334	-	5,5,5	0.47	0	5,5,5	0.40	0
2	GOL	P	1335	-	5,5,5	0.58	0	5,5,5	0.71	0
3	EDO	O	1337	-	3,3,3	0.50	0	2,2,2	0.32	0
3	EDO	Q	1334	-	3,3,3	0.51	0	2,2,2	0.58	0
6	PGE	P	1342	-	9,9,9	0.73	0	8,8,8	0.61	0
2	GOL	O	1336	-	5,5,5	0.32	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PGE	Q	1336	-	9,9,9	0.75	0	8,8,8	0.71	0
3	EDO	P	1337	-	3,3,3	0.58	0	2,2,2	0.36	0
3	EDO	R	1336	-	3,3,3	0.46	0	2,2,2	0.30	0
6	PGE	O	1340	-	9,9,9	0.59	0	8,8,8	0.57	0
2	GOL	P	1336	-	5,5,5	0.48	0	5,5,5	0.79	0
3	EDO	Q	1335	-	3,3,3	0.50	0	2,2,2	0.64	0
4	PG4	O	1338	-	12,12,12	0.81	0	11,11,11	0.73	0
2	GOL	R	1335	-	5,5,5	0.37	0	5,5,5	1.10	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
6	PGE	P	1343	-	-	4/7/7/7	-
7	PEG	P	1341	-	-	2/4/4/4	-
2	GOL	O	1335	-	-	3/4/4/4	-
7	PEG	P	1340	-	-	1/4/4/4	-
2	GOL	R	1334	-	-	4/4/4/4	-
2	GOL	P	1335	-	-	2/4/4/4	-
3	EDO	O	1337	-	-	1/1/1/1	-
3	EDO	Q	1334	-	-	0/1/1/1	-
6	PGE	P	1342	-	-	5/7/7/7	-
2	GOL	O	1336	-	-	1/4/4/4	-
6	PGE	Q	1336	-	-	5/7/7/7	-
3	EDO	P	1337	-	-	1/1/1/1	-
3	EDO	R	1336	-	-	0/1/1/1	-
6	PGE	O	1340	-	-	2/7/7/7	-
2	GOL	P	1336	-	-	2/4/4/4	-
3	EDO	Q	1335	-	-	1/1/1/1	-
4	PG4	O	1338	-	-	3/10/10/10	-
2	GOL	R	1335	-	-	1/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	P	1341	PEG	O2-C3-C4	2.12	119.40	110.07

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	1335	GOL	O1-C1-C2-O2
2	P	1335	GOL	O1-C1-C2-C3
2	P	1336	GOL	O1-C1-C2-C3
2	R	1334	GOL	O1-C1-C2-C3
6	Q	1336	PGE	C3-C4-O3-C5
6	Q	1336	PGE	O3-C5-C6-O4
6	P	1343	PGE	O2-C3-C4-O3
6	O	1340	PGE	O2-C3-C4-O3
2	P	1336	GOL	O1-C1-C2-O2
7	P	1340	PEG	O1-C1-C2-O2
7	P	1341	PEG	O1-C1-C2-O2
6	Q	1336	PGE	O2-C3-C4-O3
4	O	1338	PG4	O4-C7-C8-O5
6	P	1342	PGE	O1-C1-C2-O2
7	P	1341	PEG	C1-C2-O2-C3
2	R	1334	GOL	O1-C1-C2-O2
3	O	1337	EDO	O1-C1-C2-O2
3	Q	1335	EDO	O1-C1-C2-O2
6	P	1342	PGE	O3-C5-C6-O4
2	O	1335	GOL	O1-C1-C2-O2
6	P	1343	PGE	O3-C5-C6-O4
3	P	1337	EDO	O1-C1-C2-O2
2	O	1335	GOL	O2-C2-C3-O3
2	R	1334	GOL	O2-C2-C3-O3
2	R	1335	GOL	O2-C2-C3-O3
6	P	1343	PGE	C4-C3-O2-C2
2	O	1335	GOL	O1-C1-C2-C3
6	P	1342	PGE	C3-C4-O3-C5
4	O	1338	PG4	C5-C6-O4-C7
6	P	1343	PGE	C6-C5-O3-C4
4	O	1338	PG4	C8-C7-O4-C6
6	Q	1336	PGE	O1-C1-C2-O2
6	O	1340	PGE	C3-C4-O3-C5
2	O	1336	GOL	O1-C1-C2-C3
2	R	1334	GOL	C1-C2-C3-O3
6	P	1342	PGE	C4-C3-O2-C2
6	P	1342	PGE	C1-C2-O2-C3
6	Q	1336	PGE	C1-C2-O2-C3

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	1343	PGE	1	0
7	P	1341	PEG	1	0
7	P	1340	PEG	1	0
2	O	1336	GOL	1	0
6	Q	1336	PGE	1	0
2	P	1336	GOL	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 (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	O	333/339 (98%)	-0.43	6 (1%)	68	70	16, 24, 49, 91	0
1	P	338/339 (99%)	-0.36	3 (0%)	84	84	15, 26, 47, 84	0
1	Q	337/339 (99%)	-0.15	3 (0%)	84	84	18, 31, 52, 77	0
1	R	334/339 (98%)	-0.09	2 (0%)	89	89	20, 33, 58, 81	0
All	All	1342/1356 (98%)	-0.26	14 (1%)	82	83	15, 28, 53, 91	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	333	PHE	6.5
1	Q	332	ALA	5.5
1	P	334	ARG	5.4
1	Q	333	PHE	4.5
1	R	333	PHE	3.8
1	R	184	VAL	3.7
1	O	184	VAL	3.4
1	O	183	GLN	3.3
1	O	178	ALA	3.0
1	Q	185	ILE	2.5
1	O	180	HIS	2.5
1	O	185	ILE	2.4
1	O	181	ASP	2.1
1	P	223	ASP	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	GOL	O	1335	6/6	0.78	0.22	53,63,64,64	0
6	PGE	O	1340	10/10	0.81	0.22	64,70,74,75	0
2	GOL	R	1334	6/6	0.82	0.18	62,67,69,69	0
2	GOL	O	1336	6/6	0.82	0.21	72,74,75,75	0
4	PG4	O	1338	13/13	0.83	0.21	63,65,68,70	0
2	GOL	P	1336	6/6	0.83	0.21	54,62,64,65	0
6	PGE	P	1342	10/10	0.84	0.22	56,72,80,81	0
3	EDO	Q	1334	4/4	0.85	0.23	67,69,69,71	0
6	PGE	P	1343	10/10	0.85	0.24	65,78,79,80	0
7	PEG	P	1340	7/7	0.85	0.28	66,67,72,72	0
2	GOL	R	1335	6/6	0.86	0.16	64,66,67,68	0
3	EDO	P	1337	4/4	0.86	0.11	56,57,60,63	0
6	PGE	Q	1336	10/10	0.87	0.18	74,75,75,77	0
3	EDO	Q	1335	4/4	0.88	0.15	50,52,52,57	0
7	PEG	P	1341	7/7	0.88	0.18	55,57,64,66	0
2	GOL	P	1335	6/6	0.89	0.13	51,57,60,60	0
3	EDO	R	1336	4/4	0.91	0.30	60,60,60,63	0
3	EDO	O	1337	4/4	0.93	0.13	52,54,55,55	0
5	CL	O	1339	1/1	0.95	0.09	47,47,47,47	0
5	CL	Q	1339	1/1	0.98	0.07	37,37,37,37	0
5	CL	P	1338	1/1	0.99	0.06	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.