



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:57 PM GMT

PDB ID : 3S9Y
Title : Crystal Structure of *P. falciparum* orotidine 5'-monophosphate decarboxylase complexed with 5-fluoro-6-amino-UMP in space group P21, produced from 5-fluoro-6-azido-UMP
Authors : Liu, Y.; Kotra, L.P.; Pai, E.F.
Deposited on : 2011-06-02
Resolution : 1.70 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

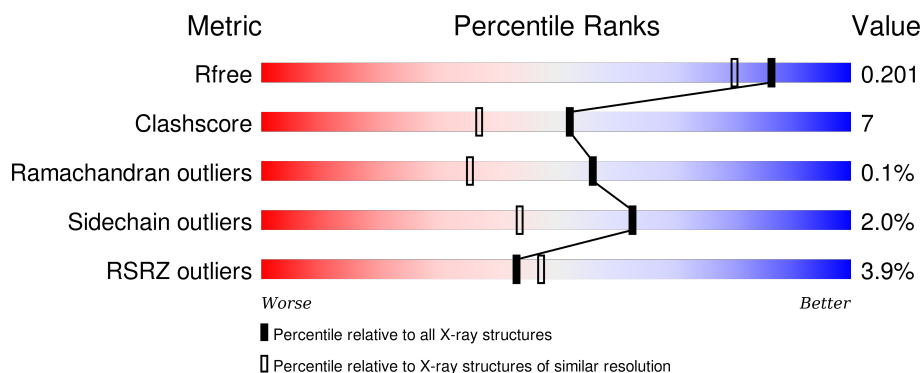
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	342	<div> <div>4%</div> <div>81% 14% • •</div> </div>
1	B	342	<div> <div>2%</div> <div>85% 8% • 6%</div> </div>
1	C	342	<div> <div>3%</div> <div>82% 12% • 6%</div> </div>
1	D	342	<div> <div>5%</div> <div>80% 14% 6%</div> </div>

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	B	3001	-	-	X	X
6	P6G	B	3003	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12383 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 Orotidine 5'-phosphate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	23	0
			2902	1862	470	552	18			
1	B	323	Total	C	N	O	S	0	12	0
			2758	1774	446	519	19			
1	C	321	Total	C	N	O	S	0	9	0
			2719	1752	440	510	17			
1	D	320	Total	C	N	O	S	0	10	0
			2721	1755	440	510	16			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP Q8IJH3
A	-17	GLY	-	EXPRESSION TAG	UNP Q8IJH3
A	-16	SER	-	EXPRESSION TAG	UNP Q8IJH3
A	-15	SER	-	EXPRESSION TAG	UNP Q8IJH3
A	-14	HIS	-	EXPRESSION TAG	UNP Q8IJH3
A	-13	HIS	-	EXPRESSION TAG	UNP Q8IJH3
A	-12	HIS	-	EXPRESSION TAG	UNP Q8IJH3
A	-11	HIS	-	EXPRESSION TAG	UNP Q8IJH3
A	-10	HIS	-	EXPRESSION TAG	UNP Q8IJH3
A	-9	HIS	-	EXPRESSION TAG	UNP Q8IJH3
A	-8	SER	-	EXPRESSION TAG	UNP Q8IJH3
A	-7	SER	-	EXPRESSION TAG	UNP Q8IJH3
A	-6	GLY	-	EXPRESSION TAG	UNP Q8IJH3
A	-5	LEU	-	EXPRESSION TAG	UNP Q8IJH3
A	-4	VAL	-	EXPRESSION TAG	UNP Q8IJH3
A	-3	PRO	-	EXPRESSION TAG	UNP Q8IJH3
A	-2	ARG	-	EXPRESSION TAG	UNP Q8IJH3
A	-1	GLY	-	EXPRESSION TAG	UNP Q8IJH3
A	0	SER	-	EXPRESSION TAG	UNP Q8IJH3
B	-18	MET	-	EXPRESSION TAG	UNP Q8IJH3
B	-17	GLY	-	EXPRESSION TAG	UNP Q8IJH3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP Q8IJH3
B	-15	SER	-	EXPRESSION TAG	UNP Q8IJH3
B	-14	HIS	-	EXPRESSION TAG	UNP Q8IJH3
B	-13	HIS	-	EXPRESSION TAG	UNP Q8IJH3
B	-12	HIS	-	EXPRESSION TAG	UNP Q8IJH3
B	-11	HIS	-	EXPRESSION TAG	UNP Q8IJH3
B	-10	HIS	-	EXPRESSION TAG	UNP Q8IJH3
B	-9	HIS	-	EXPRESSION TAG	UNP Q8IJH3
B	-8	SER	-	EXPRESSION TAG	UNP Q8IJH3
B	-7	SER	-	EXPRESSION TAG	UNP Q8IJH3
B	-6	GLY	-	EXPRESSION TAG	UNP Q8IJH3
B	-5	LEU	-	EXPRESSION TAG	UNP Q8IJH3
B	-4	VAL	-	EXPRESSION TAG	UNP Q8IJH3
B	-3	PRO	-	EXPRESSION TAG	UNP Q8IJH3
B	-2	ARG	-	EXPRESSION TAG	UNP Q8IJH3
B	-1	GLY	-	EXPRESSION TAG	UNP Q8IJH3
B	0	SER	-	EXPRESSION TAG	UNP Q8IJH3
C	-18	MET	-	EXPRESSION TAG	UNP Q8IJH3
C	-17	GLY	-	EXPRESSION TAG	UNP Q8IJH3
C	-16	SER	-	EXPRESSION TAG	UNP Q8IJH3
C	-15	SER	-	EXPRESSION TAG	UNP Q8IJH3
C	-14	HIS	-	EXPRESSION TAG	UNP Q8IJH3
C	-13	HIS	-	EXPRESSION TAG	UNP Q8IJH3
C	-12	HIS	-	EXPRESSION TAG	UNP Q8IJH3
C	-11	HIS	-	EXPRESSION TAG	UNP Q8IJH3
C	-10	HIS	-	EXPRESSION TAG	UNP Q8IJH3
C	-9	HIS	-	EXPRESSION TAG	UNP Q8IJH3
C	-8	SER	-	EXPRESSION TAG	UNP Q8IJH3
C	-7	SER	-	EXPRESSION TAG	UNP Q8IJH3
C	-6	GLY	-	EXPRESSION TAG	UNP Q8IJH3
C	-5	LEU	-	EXPRESSION TAG	UNP Q8IJH3
C	-4	VAL	-	EXPRESSION TAG	UNP Q8IJH3
C	-3	PRO	-	EXPRESSION TAG	UNP Q8IJH3
C	-2	ARG	-	EXPRESSION TAG	UNP Q8IJH3
C	-1	GLY	-	EXPRESSION TAG	UNP Q8IJH3
C	0	SER	-	EXPRESSION TAG	UNP Q8IJH3
D	-18	MET	-	EXPRESSION TAG	UNP Q8IJH3
D	-17	GLY	-	EXPRESSION TAG	UNP Q8IJH3
D	-16	SER	-	EXPRESSION TAG	UNP Q8IJH3
D	-15	SER	-	EXPRESSION TAG	UNP Q8IJH3
D	-14	HIS	-	EXPRESSION TAG	UNP Q8IJH3
D	-13	HIS	-	EXPRESSION TAG	UNP Q8IJH3

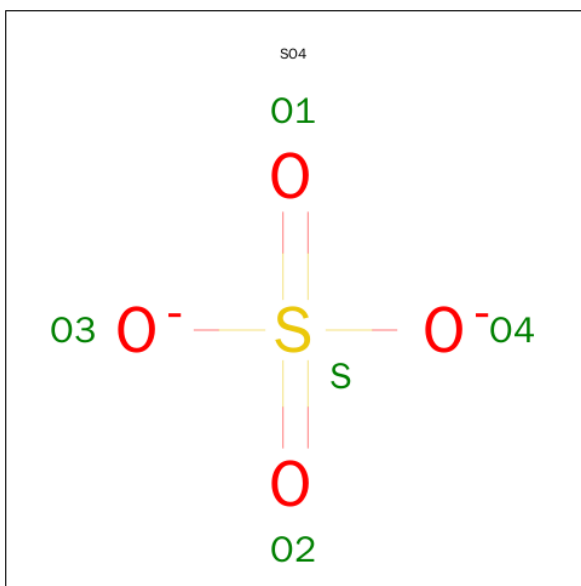
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	EXPRESSION TAG	UNP Q8IJH3
D	-11	HIS	-	EXPRESSION TAG	UNP Q8IJH3
D	-10	HIS	-	EXPRESSION TAG	UNP Q8IJH3
D	-9	HIS	-	EXPRESSION TAG	UNP Q8IJH3
D	-8	SER	-	EXPRESSION TAG	UNP Q8IJH3
D	-7	SER	-	EXPRESSION TAG	UNP Q8IJH3
D	-6	GLY	-	EXPRESSION TAG	UNP Q8IJH3
D	-5	LEU	-	EXPRESSION TAG	UNP Q8IJH3
D	-4	VAL	-	EXPRESSION TAG	UNP Q8IJH3
D	-3	PRO	-	EXPRESSION TAG	UNP Q8IJH3
D	-2	ARG	-	EXPRESSION TAG	UNP Q8IJH3
D	-1	GLY	-	EXPRESSION TAG	UNP Q8IJH3
D	0	SER	-	EXPRESSION TAG	UNP Q8IJH3

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- The chemical structure of FNU is shown. It consists of a pyrimidine ring (uracil) substituted with a fluorine atom at the 5-position (C5) and a methyl group at the 2-position (C2). The base is attached to a deoxyribose sugar at the C1' position. The sugar has a phosphate group at the 5' position (C5') and a hydroxyl group at the 3' position (C3'). The structure is labeled with atom names: N1, N2, N3, C2, C4, C5, C6 for the base; C1', C2', C3', C4', C5' for the sugar; and O1P, O2P, O3P, O4, O5 for the phosphate and carbonyl groups. The fluorine atom is labeled F24.

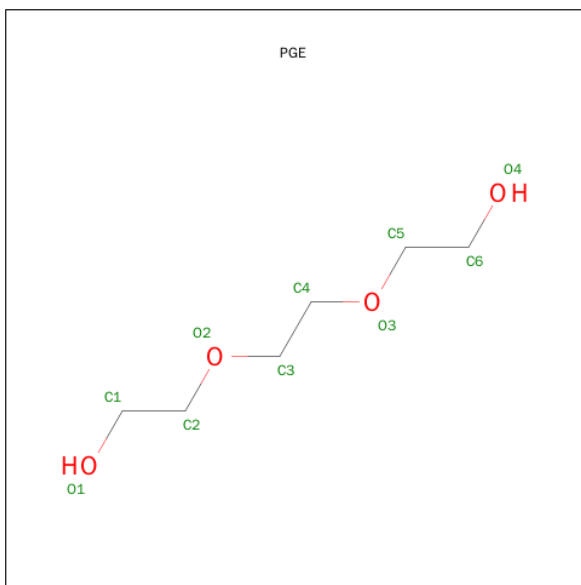
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 23	C 9	F 1	N 3	O 9	P 1	0	0
2	B	1	Total 23	C 9	F 1	N 3	O 9	P 1	0	0
2	C	1	Total 23	C 9	F 1	N 3	O 9	P 1	0	0
2	D	1	Total 23	C 9	F 1	N 3	O 9	P 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



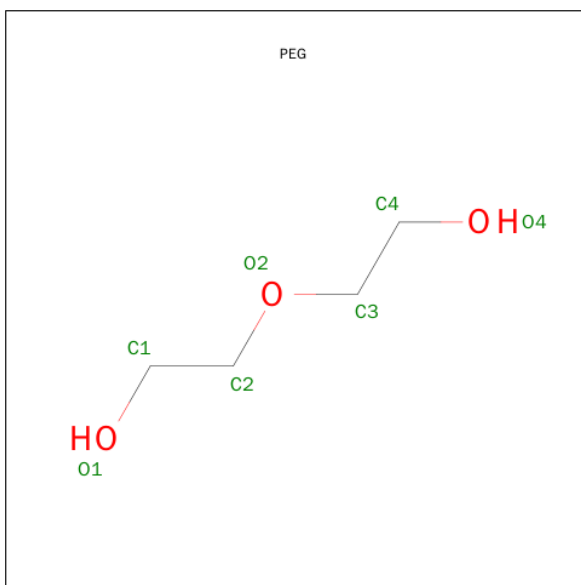
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



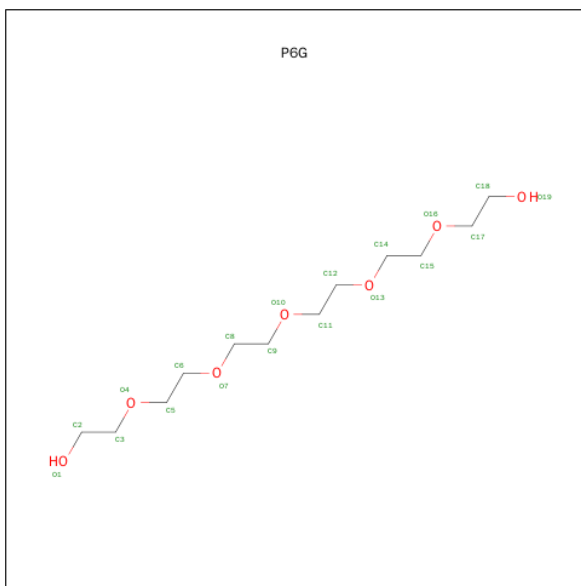
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 6 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			19	12	7		
6	C	1	Total	C	O	0	0
			19	12	7		

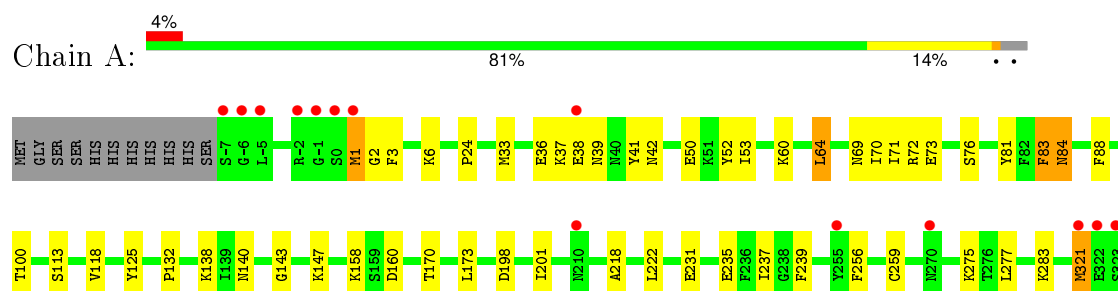
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	289	Total 289	O 289	0	0
7	B	331	Total 331	O 331	0	0
7	C	279	Total 279	O 279	0	0
7	D	232	Total 232	O 232	0	0

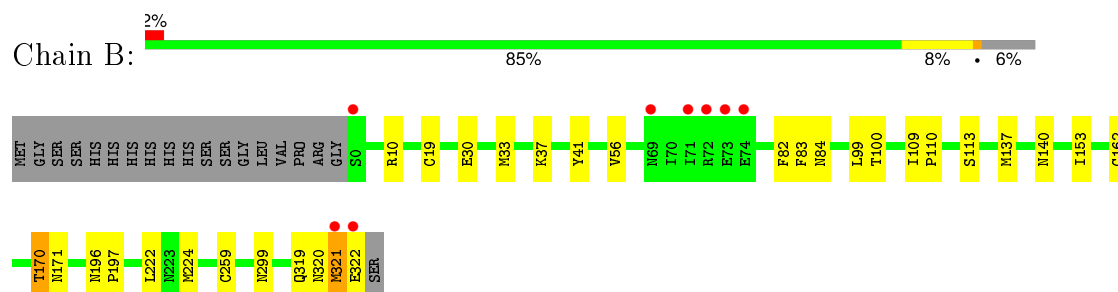
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

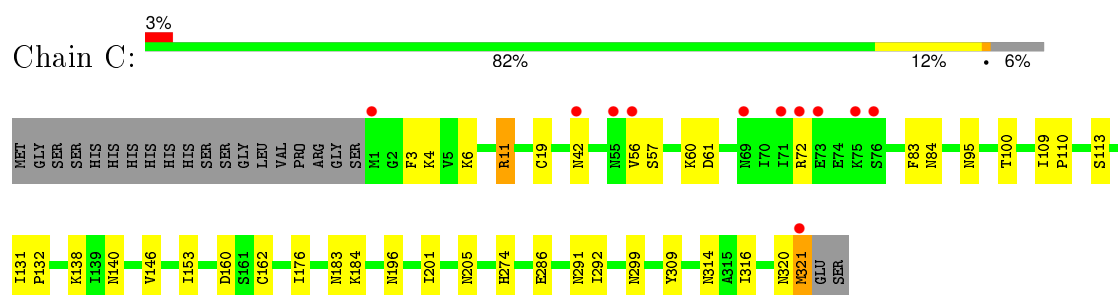
- Molecule 1: Orotidine 5'-phosphate decarboxylase



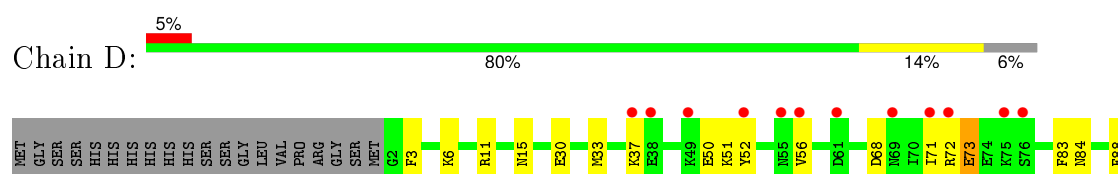
- Molecule 1: Orotidine 5'-phosphate decarboxylase

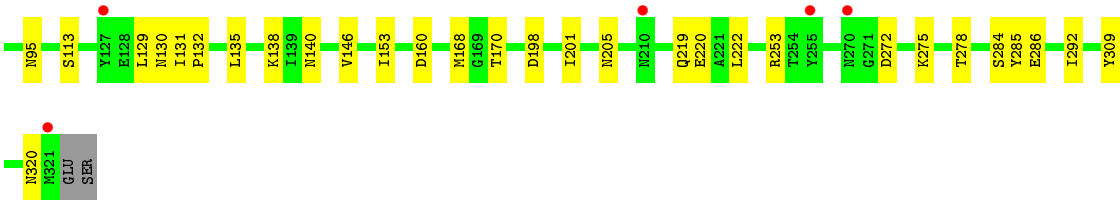


- Molecule 1: Orotidine 5'-phosphate decarboxylase



- Molecule 1: Orotidine 5'-phosphate decarboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.59Å 82.91Å 91.73Å 90.00° 90.93° 90.00°	Depositor
Resolution (Å)	25.99 – 1.70 25.99 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.99-1.70) 99.4 (25.99-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.163 , 0.201 0.163 , 0.201	Depositor DCC
R_{free} test set	7010 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.4	EDS
Estimated twinning fraction	0.008 for k,h,-l 0.011 for -k,-h,-l 0.066 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 139703 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12383	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PEG, FNU, PGE, SO4, P6G

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	0.59	0/2961	0.75	0/3992
1	B	0.60	0/2814	0.75	0/3792
1	C	0.56	0/2775	0.72	1/3741 (0.0%)
1	D	0.52	0/2778	0.69	1/3745 (0.0%)
All	All	0.57	0/11328	0.73	2/15270 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	253	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	C	11	ARG	NE-CZ-NH1	5.46	123.03	120.30

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	2902	0	2851	54	0
1	B	2758	0	2726	32	0
1	C	2719	0	2691	30	0
1	D	2721	0	2691	32	0
2	A	23	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	23	0	11	0	0
2	C	23	0	11	2	0
2	D	23	0	11	1	0
3	B	5	0	0	0	0
4	B	10	0	14	3	0
5	B	7	0	10	10	0
6	B	19	0	26	0	0
6	C	19	0	26	2	0
7	A	289	0	0	16	0
7	B	331	0	0	15	0
7	C	279	0	0	11	0
7	D	232	0	0	5	0
All	All	12383	0	11079	150	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 7.

All (150) 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:299:ASN:HD21	4:B:3000:PGE:H22	1.32	0.93
1:A:222[B]:LEU:HD11	1:A:239:PHE:HZ	1.34	0.93
1:A:1:MET:HG2	7:A:1042:HOH:O	1.66	0.93
1:B:170[A]:THR:HG21	7:B:456:HOH:O	1.70	0.90
1:D:37:LYS:HE2	1:D:71:ILE:HD12	1.52	0.90
1:B:259:CYS:HB3	7:B:444:HOH:O	1.72	0.87
1:B:33[B]:MET:SD	7:B:795:HOH:O	2.31	0.87
1:A:218:ALA:O	1:A:222[B]:LEU:HD12	1.77	0.84
1:D:72:ARG:HG2	1:D:72:ARG:O	1.79	0.82
1:A:113:SER:HB2	1:B:113:SER:HB2	1.62	0.81
1:A:222[B]:LEU:CD1	1:A:239:PHE:HZ	1.95	0.80
1:B:170[A]:THR:HG23	1:B:224:MET:HE3	1.66	0.78
1:D:6[A]:LYS:HE3	7:D:837:HOH:O	1.84	0.78
1:A:222[B]:LEU:HD21	7:A:350:HOH:O	1.84	0.76
1:A:53[B]:ILE:HD13	1:A:53[B]:ILE:O	1.88	0.74
1:A:222[B]:LEU:HD11	1:A:239:PHE:CZ	2.21	0.74
1:C:113:SER:HB2	1:D:113:SER:HB2	1.70	0.72
1:A:259:CYS:HB3	7:A:350:HOH:O	1.88	0.71
1:B:33[A]:MET:O	1:B:37[A]:LYS:HG3	1.91	0.70
1:B:197:PRO:HD3	5:B:3001:PEG:H31	1.75	0.68
1:A:283:LYS:NZ	7:A:903:HOH:O	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:O	1:A:201[B]:ILE:HG13	1.95	0.66
4:B:3000:PGE:H52	1:C:299:ASN:HD21	1.59	0.66
1:B:170[A]:THR:HG23	1:B:224:MET:CE	2.25	0.66
1:C:320:ASN:O	1:C:321:MET:HB2	1.96	0.65
1:A:33:MET:O	1:A:37:LYS:HD3	1.96	0.65
1:A:6[A]:LYS:HE3	7:A:480:HOH:O	1.97	0.64
1:D:11:ARG:HD3	1:D:286:GLU:OE2	1.97	0.63
1:A:143:GLY:H	5:B:3001:PEG:H11	1.63	0.63
1:C:19:CYS:SG	1:C:100:THR:HG23	2.38	0.63
1:D:278:THR:HG23	1:D:320:ASN:HD21	1.64	0.62
1:B:10:ARG:HG2	1:B:99:LEU:HD12	1.83	0.61
1:A:158:LYS:NZ	7:A:516:HOH:O	2.33	0.61
1:A:6[A]:LYS:HE2	1:A:132:PRO:HA	1.82	0.61
1:B:56:VAL:HG13	7:B:402:HOH:O	2.00	0.60
1:B:259:CYS:CB	7:B:444:HOH:O	2.36	0.60
1:A:6[B]:LYS:HD3	7:A:932:HOH:O	2.02	0.60
1:A:143:GLY:N	5:B:3001:PEG:H11	2.17	0.59
1:C:11:ARG:HD3	1:C:286:GLU:OE2	2.03	0.58
5:B:3001:PEG:H32	7:B:605:HOH:O	2.04	0.58
1:B:321:MET:HE1	7:B:1054:HOH:O	2.03	0.58
1:B:196:ASN:HB3	5:B:3001:PEG:H21	1.87	0.56
1:D:6[A]:LYS:HE2	1:D:132:PRO:HA	1.88	0.56
1:D:201[B]:ILE:HD11	7:D:870:HOH:O	2.06	0.56
1:A:53[B]:ILE:HD12	1:A:64:LEU:HD13	1.88	0.55
1:C:146[B]:VAL:HG21	1:C:176:ILE:HD11	1.89	0.55
1:C:61:ASP:HB2	7:C:618:HOH:O	2.07	0.55
1:B:299:ASN:ND2	4:B:3000:PGE:H22	2.13	0.55
1:B:196:ASN:HB3	5:B:3001:PEG:C2	2.38	0.54
1:A:72:ARG:HG3	1:A:73:GLU:HG3	1.89	0.54
1:C:138:LYS:NZ	2:C:324:FNU:N3	2.56	0.54
1:B:19:CYS:SG	1:B:100[B]:THR:HG23	2.48	0.54
6:C:3002:P6G:H152	7:C:416:HOH:O	2.09	0.53
6:C:3002:P6G:H21	7:C:386:HOH:O	2.07	0.53
1:A:259:CYS:CB	7:A:350:HOH:O	2.54	0.52
1:A:100[B]:THR:HG22	1:A:132:PRO:HB2	1.92	0.52
1:D:138:LYS:NZ	2:D:324:FNU:N3	2.58	0.52
1:A:198:ASP:HB2	1:A:201[B]:ILE:HD11	1.91	0.52
1:B:320:ASN:ND2	7:B:850:HOH:O	2.42	0.52
1:A:38:GLU:HG3	7:A:800:HOH:O	2.09	0.52
1:B:222:LEU:HD11	7:B:444:HOH:O	2.10	0.52
1:A:222[B]:LEU:HG	7:A:693:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:THR:HG21	1:D:220:GLU:HB3	1.91	0.51
1:D:15[B]:ASN:OD1	1:D:285:TYR:OH	2.27	0.51
1:A:60:LYS:HG2	1:A:64:LEU:HD22	1.93	0.51
1:C:196:ASN:ND2	1:D:168:MET:O	2.34	0.50
1:B:33[B]:MET:HG2	1:B:82:PHE:CG	2.46	0.50
1:C:320:ASN:ND2	7:C:948:HOH:O	2.34	0.50
1:B:197:PRO:HD2	7:B:468:HOH:O	2.13	0.49
1:C:201[A]:ILE:O	1:C:205:ASN:HB2	2.12	0.49
1:A:52[B]:TYR:HB2	1:A:125:TYR:CE1	2.48	0.49
1:A:138:LYS:NZ	2:A:324:FNU:N3	2.61	0.49
1:D:3:PHE:CD1	1:D:160:ASP:HB3	2.49	0.48
1:B:196:ASN:CB	5:B:3001:PEG:H22	2.43	0.48
1:A:37:LYS:HE2	1:A:71:ILE:HD11	1.95	0.48
1:A:173:LEU:HD13	1:A:237:ILE:HD13	1.96	0.48
1:D:198:ASP:O	1:D:201[B]:ILE:HG13	2.13	0.48
1:D:219:GLN:OE1	1:D:222[B]:LEU:HD23	2.13	0.48
1:A:76[A]:SER:HB2	7:A:446:HOH:O	2.14	0.48
1:D:56:VAL:HG11	1:D:88:PHE:HZ	1.79	0.47
1:C:3:PHE:HE1	1:C:132:PRO:HB3	1.79	0.47
1:C:314:ASN:ND2	7:C:336:HOH:O	2.47	0.47
1:A:170[A]:THR:CG2	7:B:410:HOH:O	2.63	0.47
1:A:170[A]:THR:HG21	7:A:688:HOH:O	2.14	0.47
1:A:69:ASN:HD21	1:A:72:ARG:HH21	1.62	0.47
1:A:275:LYS:HE2	7:A:744:HOH:O	2.15	0.46
1:A:3:PHE:HE1	1:A:132:PRO:HB3	1.79	0.46
1:D:11:ARG:NH1	1:D:284:SER:HA	2.31	0.46
5:B:3001:PEG:C3	7:B:605:HOH:O	2.63	0.46
1:D:170:THR:HG21	1:D:220:GLU:OE2	2.16	0.46
1:A:84[A]:ASN:ND2	1:A:88:PHE:CZ	2.84	0.46
1:C:72:ARG:NH1	7:C:964:HOH:O	2.48	0.46
1:B:30:GLU:HG2	7:B:1159:HOH:O	2.15	0.46
1:A:24:PRO:HG2	1:A:83:PHE:HE2	1.81	0.45
1:B:137[A]:MET:HB3	7:B:403:HOH:O	2.16	0.45
1:C:183:ASN:ND2	7:C:897:HOH:O	2.49	0.45
1:D:135:LEU:CD2	1:D:153:ILE:HG12	2.47	0.45
1:A:84[B]:ASN:ND2	1:A:118:VAL:HG22	2.32	0.45
1:A:222[B]:LEU:HD13	1:A:256:PHE:CE1	2.52	0.45
1:D:3:PHE:HE1	1:D:132:PRO:HB3	1.82	0.44
1:D:68:ASP:OD2	1:D:72:ARG:NH2	2.50	0.44
1:C:4:LYS:HE2	7:C:1102:HOH:O	2.17	0.44
1:C:6[A]:LYS:HG2	1:C:132:PRO:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201[B]:ILE:O	1:D:205:ASN:HB2	2.18	0.43
1:A:70:ILE:HG13	1:A:81:TYR:CE1	2.52	0.43
1:A:143:GLY:H	5:B:3001:PEG:C1	2.29	0.43
1:C:132:PRO:HA	1:C:160:ASP:OD2	2.18	0.43
1:B:196:ASN:CB	5:B:3001:PEG:C2	2.96	0.43
1:C:274:HIS:HA	1:C:316:ILE:HD13	1.99	0.43
2:C:324:FNU:HN3	2:C:324:FNU:H1'	1.59	0.43
1:B:19:CYS:SG	1:B:100[B]:THR:CG2	3.07	0.43
1:D:292[A]:ILE:HD13	1:D:309:TYR:CD1	2.54	0.43
1:B:37[A]:LYS:HG2	1:B:41:TYR:OH	2.19	0.43
1:B:109:ILE:N	1:B:110:PRO:CD	2.82	0.43
1:A:53[B]:ILE:HD12	1:A:64:LEU:CD1	2.49	0.42
1:C:3:PHE:CD1	1:C:160:ASP:HB3	2.54	0.42
1:A:36:GLU:HB3	1:A:41:TYR:CD2	2.53	0.42
1:D:95:ASN:HB2	1:D:131:ILE:CD1	2.49	0.42
1:B:30:GLU:HG3	7:B:451:HOH:O	2.19	0.42
1:D:33:MET:HG2	1:D:37:LYS:HE3	2.01	0.42
1:D:15[A]:ASN:ND2	7:D:448:HOH:O	2.22	0.42
1:C:60:LYS:HG3	7:C:1029:HOH:O	2.19	0.42
1:A:2:GLY:HA2	1:A:235:GLU:OE2	2.19	0.42
1:B:153:ILE:HG21	1:B:162:CYS:HB3	2.02	0.42
1:B:319[A]:GLN:O	1:B:322:GLU:HG3	2.18	0.42
1:A:3:PHE:CD1	1:A:160:ASP:HB3	2.53	0.42
1:C:153:ILE:HG21	1:C:162:CYS:HB3	2.02	0.42
1:C:95:ASN:HB2	1:C:131:ILE:CD1	2.50	0.41
1:D:272:ASP:OD2	1:D:275:LYS:HG3	2.20	0.41
1:D:37:LYS:HE2	1:D:71:ILE:CD1	2.36	0.41
1:C:57:SER:HB3	7:C:503:HOH:O	2.20	0.41
1:A:70:ILE:HG13	1:A:81:TYR:CD1	2.56	0.41
1:C:56:VAL:O	1:C:60:LYS:HE3	2.21	0.41
1:A:39:ASN:CG	1:A:42[B]:ASN:HD22	2.23	0.41
1:C:292[B]:ILE:HD13	1:C:309:TYR:CD1	2.56	0.41
1:C:184:LYS:HA	1:C:184:LYS:HD2	1.91	0.41
1:D:6[A]:LYS:HG3	7:D:837:HOH:O	2.19	0.41
1:A:198:ASP:HB2	1:A:201[B]:ILE:CD1	2.51	0.41
1:C:19:CYS:O	1:C:291:ASN:HA	2.21	0.41
1:A:231:GLU:HG2	1:A:235:GLU:O	2.21	0.41
1:C:109:ILE:N	1:C:110:PRO:CD	2.84	0.41
1:D:50:GLU:HB3	1:D:52[B]:TYR:CE1	2.55	0.41
1:A:147:LYS:HE2	7:A:479:HOH:O	2.20	0.41
1:C:314:ASN:OD1	7:C:1181:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:MET:HB2	7:A:500:HOH:O	2.21	0.40
7:A:360:HOH:O	1:B:170[A]:THR:HG22	2.21	0.40
1:A:50:GLU:O	1:A:53[A]:ILE:HG22	2.22	0.40
1:D:129:LEU:O	1:D:130:ASN:HB2	2.21	0.40
1:A:6[A]:LYS:HE2	1:A:132:PRO:CA	2.50	0.40
1:D:30:GLU:HG3	7:D:447:HOH:O	2.20	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	352/342 (103%)	343 (97%)	9 (3%)	0	100	100
1	B	333/342 (97%)	327 (98%)	6 (2%)	0	100	100
1	C	328/342 (96%)	321 (98%)	7 (2%)	0	100	100
1	D	328/342 (96%)	317 (97%)	10 (3%)	1 (0%)	46	26
All	All	1341/1368 (98%)	1308 (98%)	32 (2%)	1 (0%)	56	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	73	GLU

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	324/311 (104%)	316 (98%)	8 (2%)	55	34
1	B	307/311 (99%)	300 (98%)	7 (2%)	58	37
1	C	302/311 (97%)	297 (98%)	5 (2%)	68	51
1	D	302/311 (97%)	296 (98%)	6 (2%)	63	44
All	All	1235/1244 (99%)	1209 (98%)	26 (2%)	63	42

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	64	LEU
1	A	83	PHE
1	A	84[A]	ASN
1	A	84[B]	ASN
1	A	140	ASN
1	A	277	LEU
1	A	321	MET
1	B	83	PHE
1	B	84	ASN
1	B	140	ASN
1	B	170[A]	THR
1	B	170[B]	THR
1	B	171	ASN
1	B	321	MET
1	C	42	ASN
1	C	83	PHE
1	C	84	ASN
1	C	140	ASN
1	C	321	MET
1	D	51	LYS
1	D	73	GLU
1	D	83	PHE
1	D	84	ASN
1	D	140	ASN
1	D	146	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	183	ASN
1	A	274	HIS
1	A	303	GLN
1	B	223	ASN
1	B	312	GLN
1	B	320	ASN
1	C	42	ASN
1	C	55	ASN
1	C	130	ASN
1	C	183	ASN
1	C	223	ASN
1	C	269	GLN
1	C	303	GLN
1	C	314	ASN
1	D	223	ASN
1	D	291	ASN
1	D	320	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

9 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	FNU	A	324	-	19,24,24	1.18	1 (5%)	21,37,37	1.83	4 (19%)
3	SO4	B	2000	-	4,4,4	0.31	0	6,6,6	0.33	0
4	PGE	B	3000	-	9,9,9	0.47	0	8,8,8	0.43	0
5	PEG	B	3001	-	6,6,6	0.75	0	5,5,5	1.85	2 (40%)
6	P6G	B	3003	-	18,18,18	0.53	0	17,17,17	0.54	0
2	FNU	B	324	-	19,24,24	1.09	1 (5%)	21,37,37	1.57	3 (14%)
6	P6G	C	3002	-	18,18,18	0.58	0	17,17,17	0.68	1 (5%)
2	FNU	C	324	-	19,24,24	1.13	1 (5%)	21,37,37	1.55	4 (19%)
2	FNU	D	324	-	19,24,24	1.14	1 (5%)	21,37,37	1.27	2 (9%)

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	FNU	A	324	-	-	0/6/26/26	0/2/2/2
3	SO4	B	2000	-	-	0/0/0/0	0/0/0/0
4	PGE	B	3000	-	-	0/7/7/7	0/0/0/0
5	PEG	B	3001	-	-	0/4/4/4	0/0/0/0
6	P6G	B	3003	-	-	0/16/16/16	0/0/0/0
2	FNU	B	324	-	-	0/6/26/26	0/2/2/2
6	P6G	C	3002	-	-	0/16/16/16	0/0/0/0
2	FNU	C	324	-	-	0/6/26/26	0/2/2/2
2	FNU	D	324	-	-	0/6/26/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	324	FNU	O4-C4	3.67	1.33	1.24
2	C	324	FNU	O4-C4	3.70	1.33	1.24
2	B	324	FNU	O4-C4	3.94	1.34	1.24
2	A	324	FNU	O4-C4	3.95	1.34	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	324	FNU	N3-C6-N1	-4.83	117.50	120.71
2	B	324	FNU	N3-C6-N1	-3.92	118.10	120.71
2	C	324	FNU	N3-C6-N1	-3.03	118.69	120.71
2	A	324	FNU	O3P-P-O5'	-2.28	99.99	106.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	324	FNU	F24-C5-C6	2.07	121.52	119.11
6	C	3002	P6G	O16-C15-C14	2.18	120.06	110.36
2	C	324	FNU	O3P-P-O2P	2.18	115.69	107.38
5	B	3001	PEG	O2-C2-C1	2.56	122.22	110.43
2	B	324	FNU	F24-C5-C6	2.68	122.23	119.11
5	B	3001	PEG	C3-O2-C2	2.86	125.59	113.31
2	A	324	FNU	F24-C5-C6	2.91	122.50	119.11
2	D	324	FNU	C4-N2-C2	3.30	118.10	115.25
2	D	324	FNU	F24-C5-C6	3.34	123.00	119.11
2	B	324	FNU	C4-N2-C2	3.37	118.16	115.25
2	A	324	FNU	C4-N2-C2	4.24	118.91	115.25
2	C	324	FNU	C4-N2-C2	4.35	119.01	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	324	FNU	1	0
4	B	3000	PGE	3	0
5	B	3001	PEG	10	0
6	C	3002	P6G	2	0
2	C	324	FNU	2	0
2	D	324	FNU	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	331/342 (96%)	0.04	14 (4%) 40 44	7, 13, 29, 54	0
1	B	323/342 (94%)	-0.10	8 (2%) 61 65	6, 13, 29, 49	0
1	C	321/342 (93%)	0.06	11 (3%) 49 53	8, 15, 34, 50	0
1	D	320/342 (93%)	0.20	17 (5%) 30 32	9, 18, 37, 49	0
All	All	1295/1368 (94%)	0.05	50 (3%) 43 47	6, 15, 34, 54	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	SER	6.8
1	D	270	ASN	6.2
1	B	72	ARG	5.3
1	D	71	ILE	5.3
1	A	-7	SER	5.3
1	A	322	GLU	5.2
1	D	72	ARG	4.9
1	C	72	ARG	4.6
1	C	73	GLU	4.6
1	D	56	VAL	4.1
1	B	73	GLU	4.0
1	B	321	MET	3.9
1	A	-6	GLY	3.7
1	C	71	ILE	3.6
1	A	210	ASN	3.5
1	C	1	MET	3.5
1	A	1	MET	3.5
1	D	321	MET	3.4
1	D	69	ASN	3.3
1	C	75	LYS	3.2
1	D	55	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	-2	ARG	3.2
1	A	-5	LEU	3.2
1	B	322	GLU	3.2
1	C	69	ASN	3.1
1	D	75	LYS	3.1
1	B	71	ILE	2.9
1	A	-1	GLY	2.8
1	D	255	TYR	2.8
1	D	210	ASN	2.7
1	B	0	SER	2.7
1	D	52[A]	TYR	2.7
1	A	38	GLU	2.6
1	C	321	MET	2.5
1	D	38	GLU	2.5
1	A	270	ASN	2.5
1	A	321	MET	2.5
1	C	76	SER	2.5
1	B	69[A]	ASN	2.4
1	D	127	TYR	2.4
1	B	74	GLU	2.3
1	A	0	SER	2.3
1	C	56	VAL	2.3
1	A	255	TYR	2.3
1	D	49	LYS	2.2
1	D	61	ASP	2.2
1	D	37	LYS	2.2
1	C	42	ASN	2.1
1	C	55	ASN	2.0
1	D	76	SER	2.0

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

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

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	PEG	B	3001	7/7	0.87	0.20	5.88	13,17,22,25	0
6	P6G	B	3003	19/19	0.90	0.16	2.61	22,25,32,34	0
4	PGE	B	3000	10/10	0.82	0.12	1.62	35,37,39,39	0
3	SO4	B	2000	5/5	0.94	0.16	1.42	25,27,29,30	0
6	P6G	C	3002	19/19	0.84	0.15	1.32	26,31,40,41	0
2	FNU	B	324	23/23	0.99	0.07	-0.68	5,7,8,10	0
2	FNU	C	324	23/23	0.98	0.06	-0.85	8,10,11,12	0
2	FNU	A	324	23/23	0.98	0.06	-0.95	6,8,9,10	0
2	FNU	D	324	23/23	0.98	0.06	-1.06	8,10,11,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.