



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:48 AM UTC

PDB ID : 4LR9 / pdb_00004lr9
Title : Phosphopentomutase S154A variant soaked with 2,3-dideoxyribose 5-phosphate
Authors : Birmingham, W.A.; Starbird, C.A.; Panosian, T.D.; Nannemann, D.P.; Iverson, T.M.; Bachmann, B.O.
Deposited on : 2013-07-19
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

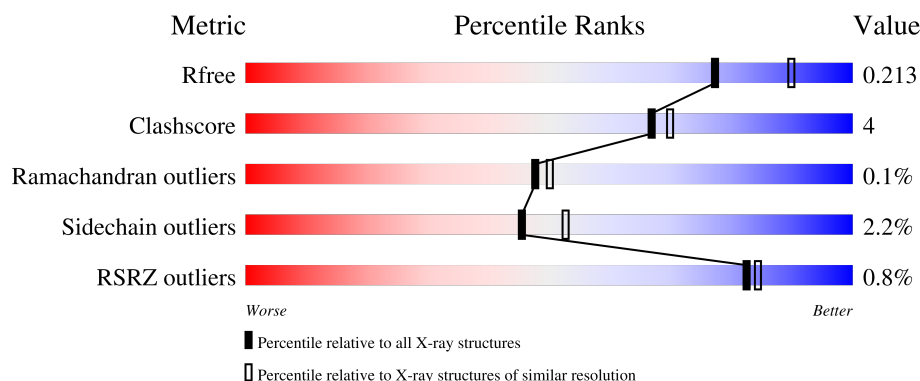
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	416	
1	B	416	
1	C	416	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9936 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 Phosphopentomutase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	P	S	11	2	0
			3085	1950	511	606	1	17			
1	B	391	Total	C	N	O	P	S	7	0	0
			3067	1939	505	605	1	17			
1	C	390	Total	C	N	O	P	S	41	0	0
			3059	1935	503	603	1	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q818Z9
A	-20	GLY	-	expression tag	UNP Q818Z9
A	-19	SER	-	expression tag	UNP Q818Z9
A	-18	SER	-	expression tag	UNP Q818Z9
A	-17	HIS	-	expression tag	UNP Q818Z9
A	-16	HIS	-	expression tag	UNP Q818Z9
A	-15	HIS	-	expression tag	UNP Q818Z9
A	-14	HIS	-	expression tag	UNP Q818Z9
A	-13	HIS	-	expression tag	UNP Q818Z9
A	-12	HIS	-	expression tag	UNP Q818Z9
A	-11	SER	-	expression tag	UNP Q818Z9
A	-10	SER	-	expression tag	UNP Q818Z9
A	-9	GLY	-	expression tag	UNP Q818Z9
A	-8	LEU	-	expression tag	UNP Q818Z9
A	-7	VAL	-	expression tag	UNP Q818Z9
A	-6	PRO	-	expression tag	UNP Q818Z9
A	-5	ARG	-	expression tag	UNP Q818Z9
A	-4	GLY	-	expression tag	UNP Q818Z9
A	-3	SER	-	expression tag	UNP Q818Z9
A	-2	HIS	-	expression tag	UNP Q818Z9
A	-1	MET	-	expression tag	UNP Q818Z9
A	0	ALA	-	expression tag	UNP Q818Z9
A	1	SER	-	expression tag	UNP Q818Z9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	154	ALA	SER	engineered mutation	UNP Q818Z9
B	-21	MET	-	expression tag	UNP Q818Z9
B	-20	GLY	-	expression tag	UNP Q818Z9
B	-19	SER	-	expression tag	UNP Q818Z9
B	-18	SER	-	expression tag	UNP Q818Z9
B	-17	HIS	-	expression tag	UNP Q818Z9
B	-16	HIS	-	expression tag	UNP Q818Z9
B	-15	HIS	-	expression tag	UNP Q818Z9
B	-14	HIS	-	expression tag	UNP Q818Z9
B	-13	HIS	-	expression tag	UNP Q818Z9
B	-12	HIS	-	expression tag	UNP Q818Z9
B	-11	SER	-	expression tag	UNP Q818Z9
B	-10	SER	-	expression tag	UNP Q818Z9
B	-9	GLY	-	expression tag	UNP Q818Z9
B	-8	LEU	-	expression tag	UNP Q818Z9
B	-7	VAL	-	expression tag	UNP Q818Z9
B	-6	PRO	-	expression tag	UNP Q818Z9
B	-5	ARG	-	expression tag	UNP Q818Z9
B	-4	GLY	-	expression tag	UNP Q818Z9
B	-3	SER	-	expression tag	UNP Q818Z9
B	-2	HIS	-	expression tag	UNP Q818Z9
B	-1	MET	-	expression tag	UNP Q818Z9
B	0	ALA	-	expression tag	UNP Q818Z9
B	1	SER	-	expression tag	UNP Q818Z9
B	154	ALA	SER	engineered mutation	UNP Q818Z9
C	-21	MET	-	expression tag	UNP Q818Z9
C	-20	GLY	-	expression tag	UNP Q818Z9
C	-19	SER	-	expression tag	UNP Q818Z9
C	-18	SER	-	expression tag	UNP Q818Z9
C	-17	HIS	-	expression tag	UNP Q818Z9
C	-16	HIS	-	expression tag	UNP Q818Z9
C	-15	HIS	-	expression tag	UNP Q818Z9
C	-14	HIS	-	expression tag	UNP Q818Z9
C	-13	HIS	-	expression tag	UNP Q818Z9
C	-12	HIS	-	expression tag	UNP Q818Z9
C	-11	SER	-	expression tag	UNP Q818Z9
C	-10	SER	-	expression tag	UNP Q818Z9
C	-9	GLY	-	expression tag	UNP Q818Z9
C	-8	LEU	-	expression tag	UNP Q818Z9
C	-7	VAL	-	expression tag	UNP Q818Z9
C	-6	PRO	-	expression tag	UNP Q818Z9
C	-5	ARG	-	expression tag	UNP Q818Z9

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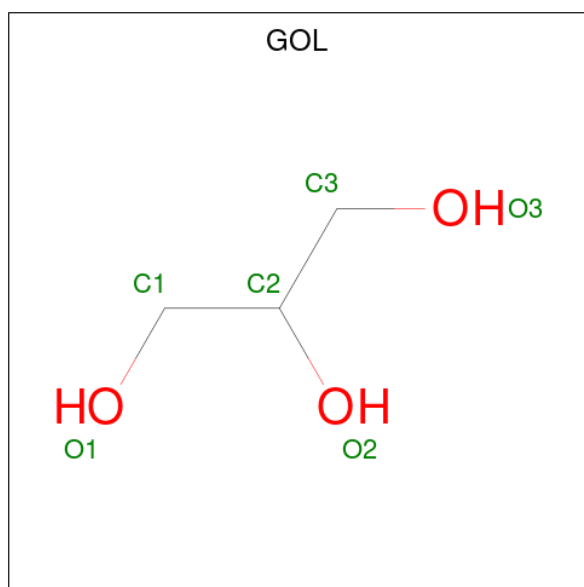
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP Q818Z9
C	-3	SER	-	expression tag	UNP Q818Z9
C	-2	HIS	-	expression tag	UNP Q818Z9
C	-1	MET	-	expression tag	UNP Q818Z9
C	0	ALA	-	expression tag	UNP Q818Z9
C	1	SER	-	expression tag	UNP Q818Z9
C	154	ALA	SER	engineered mutation	UNP Q818Z9

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

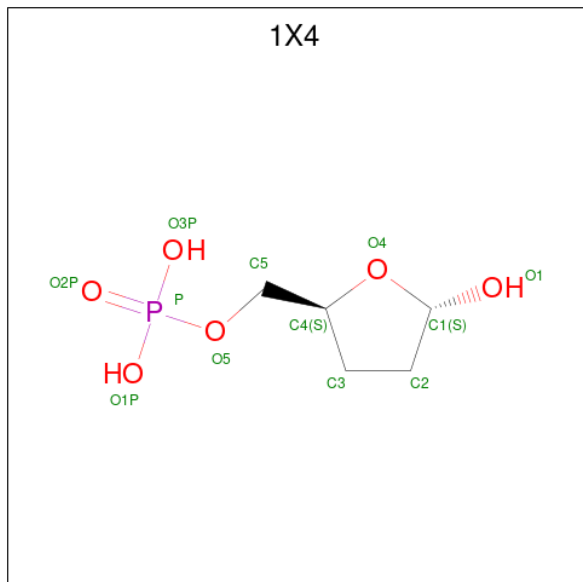
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		
2	B	4	Total	Mn	0	0
			4	4		
2	C	3	Total	Mn	0	0
			3	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is 2,3-dideoxy-5-O-phosphono-alpha-D-ribofuranose (CCD ID: 1X4) (formula: $C_5H_{11}O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			12	5	6	1		

- Molecule 5 is water.

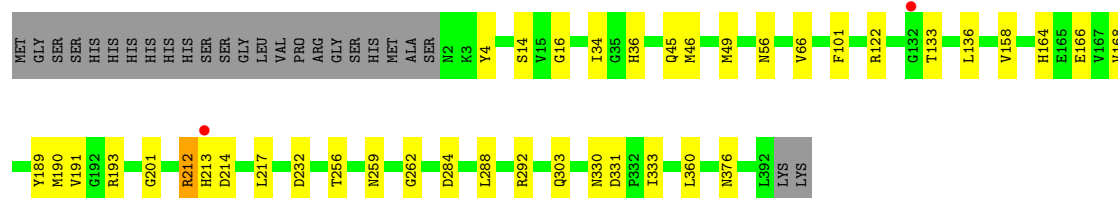
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	255	Total	O	0	0
			255	255		
5	B	272	Total	O	0	0
			272	272		
5	C	164	Total	O	0	0
			164	164		

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.

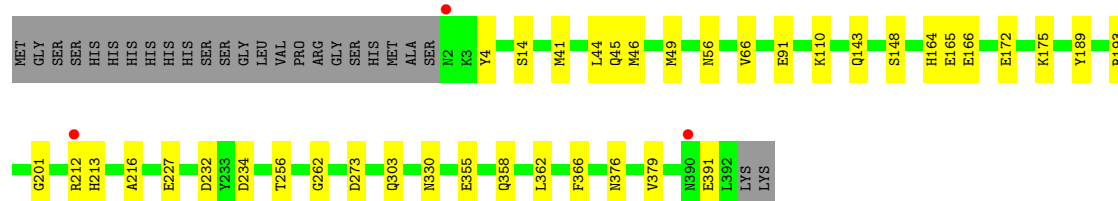
- Molecule 1: Phosphopentomutase

Chain A: 



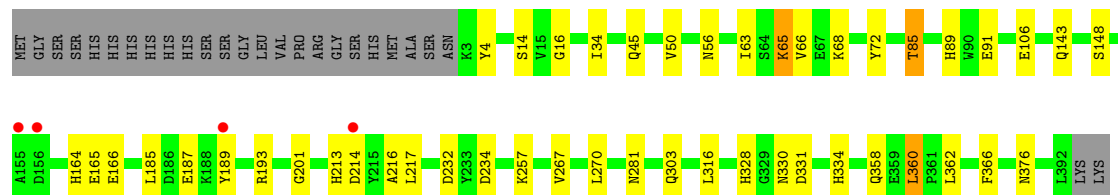
- Molecule 1: Phosphopentomutase

Chain B: 



- Molecule 1: Phosphopentomutase

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.33Å 76.61Å 107.24Å 90.00° 108.96° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.10) 98.8 (20.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.169 , 0.213 0.170 , 0.213	Depositor DCC
R_{free} test set	4084 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9936	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1X4, MN, TPO, GOL

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	0.57	0/3138	0.78	0/4236
1	B	0.57	0/3116	0.78	1/4207 (0.0%)
1	C	0.63	4/3108 (0.1%)	0.84	4/4196 (0.1%)
All	All	0.59	4/9362 (0.0%)	0.80	5/12639 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68	LYS	CB-CG	-11.63	1.17	1.52
1	C	187	GLU	CA-CB	-11.50	1.32	1.53
1	C	257	LYS	CG-CD	-7.15	1.30	1.52
1	C	65	LYS	CD-CE	-7.13	1.31	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	LYS	CA-CB-CG	12.17	138.44	114.10
1	C	106	GLU	CB-CG-CD	6.48	123.62	112.60
1	C	68	LYS	CB-CG-CD	6.38	125.98	111.30
1	C	214	ASP	N-CA-C	6.26	119.74	109.72
1	B	165	GLU	N-CA-C	5.55	118.10	111.71

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	3085	0	3026	24	0
1	B	3067	0	3007	25	0
1	C	3059	0	3001	25	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
2	C	3	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	12	0	2	0	0
5	A	255	0	0	0	0
5	B	272	0	0	0	0
5	C	164	0	0	0	0
All	All	9936	0	9052	68	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 4.

All (68) 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:4:TYR:H	1:C:376:ASN:HD21	1.15	0.91
1:B:4:TYR:H	1:B:376:ASN:HD21	1.19	0.90
1:A:164:HIS:HD2	1:A:166:GLU:H	1.23	0.86
1:A:4:TYR:H	1:A:376:ASN:HD21	1.24	0.84
1:B:164:HIS:HD2	1:B:166:GLU:H	1.27	0.81
1:C:45:GLN:H	1:C:303:GLN:HE21	1.35	0.74
1:A:56:ASN:HD21	1:A:66:VAL:H	1.35	0.74
1:A:45:GLN:H	1:A:303:GLN:HE21	1.36	0.74
1:B:56:ASN:HD21	1:B:66:VAL:H	1.33	0.73
1:C:164:HIS:HD2	1:C:166:GLU:H	1.36	0.73
1:B:45:GLN:H	1:B:303:GLN:HE21	1.37	0.69
1:C:56:ASN:HD21	1:C:66:VAL:H	1.44	0.66
1:B:213:HIS:HD2	1:C:234:ASP:OD1	1.80	0.65
1:A:36:HIS:HD2	1:A:331:ASP:OD2	1.84	0.60
1:B:234:ASP:OD1	1:C:213:HIS:HD2	1.85	0.59
1:B:227:GLU:HG3	1:B:379:VAL:HB	1.84	0.58
1:C:164:HIS:HE1	1:C:201:GLY:O	1.86	0.58
1:B:355:GLU:HA	1:B:355:GLU:OE2	2.02	0.58
1:A:212:ARG:HD3	1:A:214:ASP:OD1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ASP:OD1	1:C:213:HIS:HE1	1.88	0.57
1:B:164:HIS:CD2	1:B:166:GLU:H	2.16	0.57
1:A:164:HIS:CD2	1:A:166:GLU:H	2.14	0.56
1:B:143:GLN:HG2	1:B:148:SER:O	2.05	0.56
1:B:56:ASN:ND2	1:B:66:VAL:H	2.03	0.56
1:A:164:HIS:HE1	1:A:201:GLY:O	1.90	0.55
1:B:14:SER:HB2	1:B:330:ASN:HB2	1.89	0.54
1:A:4:TYR:N	1:A:376:ASN:HD21	2.00	0.54
1:A:14:SER:HB2	1:A:330:ASN:HB2	1.91	0.52
1:B:45:GLN:H	1:B:303:GLN:NE2	2.06	0.52
1:A:256:THR:HG21	1:A:262:GLY:HA2	1.91	0.52
1:A:36:HIS:CD2	1:A:331:ASP:OD2	2.63	0.51
1:A:45:GLN:H	1:A:303:GLN:NE2	2.06	0.51
1:A:46:MET:HE2	1:A:49:MET:HG3	1.93	0.51
1:B:164:HIS:HE1	1:B:201:GLY:O	1.93	0.51
1:C:14:SER:HB2	1:C:330:ASN:HB2	1.92	0.50
1:B:273:ASP:OD2	1:C:165:GLU:OE2	2.30	0.49
1:A:56:ASN:ND2	1:A:66:VAL:H	2.06	0.49
1:B:193:ARG:NH1	1:B:216:ALA:HB2	2.28	0.49
1:A:212:ARG:O	1:A:213[A]:HIS:HD2	1.98	0.47
1:C:91:GLU:HG2	1:C:366:PHE:HB2	1.97	0.47
1:C:72:TYR:CE1	1:C:358:GLN:HG2	2.50	0.46
1:B:213:HIS:CD2	1:C:234:ASP:OD1	2.65	0.46
1:C:85:TPO:O	1:C:89:HIS:HD2	1.99	0.46
1:B:213:HIS:HE1	1:C:232:ASP:OD1	1.99	0.46
1:C:143:GLN:HG2	1:C:148:SER:O	2.15	0.46
1:C:50:VAL:HG22	1:C:63:ILE:HG23	1.98	0.46
1:B:56:ASN:HD21	1:B:66:VAL:HG22	1.81	0.45
1:B:46:MET:HE2	1:B:49:MET:HG3	1.99	0.45
1:A:333:ILE:HG22	1:A:333:ILE:O	2.17	0.45
1:C:72:TYR:HB3	1:C:360:LEU:HD13	1.99	0.45
1:C:14:SER:HB2	1:C:330:ASN:CB	2.47	0.45
1:B:256:THR:HG21	1:B:262:GLY:HA2	1.98	0.45
1:C:45:GLN:H	1:C:303:GLN:NE2	2.11	0.45
1:C:16:GLY:O	1:C:34:ILE:HG13	2.18	0.44
1:C:267:VAL:HA	1:C:270:LEU:HD12	2.00	0.43
1:A:16:GLY:O	1:A:34:ILE:HG13	2.18	0.43
1:A:101:PHE:HE2	1:A:217:LEU:HD12	1.84	0.43
1:A:288:LEU:O	1:A:292:ARG:HD2	2.20	0.42
1:C:56:ASN:ND2	1:C:66:VAL:H	2.14	0.42
1:C:193:ARG:NH1	1:C:216:ALA:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLU:HG2	1:B:366:PHE:HB2	2.02	0.42
1:B:172:GLU:HA	1:B:175:LYS:HE2	2.01	0.41
1:B:41:MET:HG3	1:B:44:LEU:HD13	2.02	0.41
1:A:122:ARG:NH2	1:A:168:VAL:HG22	2.35	0.41
1:C:331:ASP:HB3	1:C:334:HIS:HB2	2.03	0.41
1:A:259:ASN:HD21	1:A:284:ASP:H	1.67	0.41
1:A:158:VAL:HG12	1:A:193[B]:ARG:HG2	2.03	0.40
1:A:158:VAL:HG12	1:A:193[B]:ARG:CG	2.52	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	390/416 (94%)	375 (96%)	15 (4%)	0	100	100
1	B	388/416 (93%)	375 (97%)	13 (3%)	0	100	100
1	C	387/416 (93%)	369 (95%)	17 (4%)	1 (0%)	36	36
All	All	1165/1248 (93%)	1119 (96%)	45 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	328	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	333/352 (95%)	325 (98%)	8 (2%)	43	49
1	B	331/352 (94%)	325 (98%)	6 (2%)	51	60
1	C	330/352 (94%)	322 (98%)	8 (2%)	43	49
All	All	994/1056 (94%)	972 (98%)	22 (2%)	45	53

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	THR
1	A	136	LEU
1	A	189	TYR
1	A	190	MET
1	A	191	VAL
1	A	212	ARG
1	A	232	ASP
1	A	360	LEU
1	B	110	LYS
1	B	189	TYR
1	B	212	ARG
1	B	358	GLN
1	B	362	LEU
1	B	391	GLU
1	C	65	LYS
1	C	185	LEU
1	C	189	TYR
1	C	217	LEU
1	C	281	ASN
1	C	316	LEU
1	C	360	LEU
1	C	362	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	25	GLN
1	A	36	HIS
1	A	48	ASN
1	A	56	ASN

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Mol	Chain	Res	Type
1	A	89	HIS
1	A	164	HIS
1	A	205	ASN
1	A	211	ASN
1	A	259	ASN
1	A	303	GLN
1	A	376	ASN
1	B	2	ASN
1	B	25	GLN
1	B	45	GLN
1	B	56	ASN
1	B	77	GLN
1	B	89	HIS
1	B	102	GLN
1	B	164	HIS
1	B	205	ASN
1	B	213	HIS
1	B	259	ASN
1	B	303	GLN
1	B	376	ASN
1	C	56	ASN
1	C	77	GLN
1	C	89	HIS
1	C	164	HIS
1	C	205	ASN
1	C	211	ASN
1	C	213	HIS
1	C	303	GLN
1	C	376	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	A	85	2,1	8,10,11	1.04	0	10,14,16	0.88	0
1	TPO	B	85	2,1	8,10,11	0.91	0	10,14,16	0.94	0
1	TPO	C	85	2,1	8,10,11	1.05	1 (12%)	10,14,16	1.00	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
1	TPO	A	85	2,1	-	2/9/11/13	-
1	TPO	B	85	2,1	-	3/9/11/13	-
1	TPO	C	85	2,1	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	85	TPO	P-OG1	2.03	1.63	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	85	TPO	O-C-CA-CB
1	B	85	TPO	CB-OG1-P-O1P
1	A	85	TPO	C-CA-CB-CG2
1	B	85	TPO	C-CA-CB-CG2
1	B	85	TPO	O-C-CA-CB
1	C	85	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	85	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 10 are monoatomic - leaving 3 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	$\# Z > 2$
3	GOL	B	405	-	5,5,5	0.26	0	5,5,5	0.40	0
4	1X4	A	405	-	12,12,12	1.33	1 (8%)	12,17,17	1.00	1 (8%)
3	GOL	A	404	-	5,5,5	0.28	0	5,5,5	0.32	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	GOL	B	405	-	-	0/4/4/4	-
4	1X4	A	405	-	-	3/6/15/15	0/1/1/1
3	GOL	A	404	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	1X4	P-O2P	3.64	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	1X4	O3P-P-O5	2.53	113.27	106.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	1X4	C5-O5-P-O1P
4	A	405	1X4	C5-O5-P-O2P
4	A	405	1X4	C5-O5-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	390/416 (93%)	-0.48	2 (0%) 87 88	11, 23, 38, 53	18 (4%)
1	B	390/416 (93%)	-0.41	3 (0%) 82 84	14, 24, 38, 59	12 (3%)
1	C	389/416 (93%)	-0.13	4 (1%) 79 81	18, 33, 60, 81	22 (5%)
All	All	1169/1248 (93%)	-0.34	9 (0%) 82 84	11, 26, 51, 81	52 (4%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	ARG	6.5
1	B	2	ASN	3.9
1	C	214	ASP	3.0
1	C	155	ALA	2.8
1	A	213[A]	HIS	2.5
1	C	156	ASP	2.5
1	A	132	GLY	2.4
1	C	189	TYR	2.2
1	B	390	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	C	85	11/12	0.81	0.16	25,26,26,27	4
1	TPO	B	85	11/12	0.89	0.13	21,24,26,26	4
1	TPO	A	85	11/12	0.91	0.13	20,23,26,26	4

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	405	6/6	0.82	0.22	14,14,14,15	6
3	GOL	A	404	6/6	0.85	0.27	15,16,16,17	6
2	MN	B	404	1/1	0.85	0.13	58,58,58,58	1
4	1X4	A	405	12/12	0.87	0.17	37,37,38,38	12
2	MN	A	403	1/1	0.96	0.04	44,44,44,44	1
2	MN	B	403	1/1	0.97	0.04	49,49,49,49	1
2	MN	C	401	1/1	0.99	0.03	23,23,23,23	0
2	MN	C	402	1/1	0.99	0.02	21,21,21,21	0
2	MN	C	403	1/1	0.99	0.06	45,45,45,45	0
2	MN	A	402	1/1	1.00	0.02	17,17,17,17	0
2	MN	A	401	1/1	1.00	0.02	16,16,16,16	0
2	MN	B	401	1/1	1.00	0.03	17,17,17,17	0
2	MN	B	402	1/1	1.00	0.01	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.