



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:15 AM BST

PDB ID : 4LRF
Title : Phosphopentomutase S154G variant soaked with ribose 5-phosphate
Authors : Birmingham, W.A.; Starbird, C.A.; Panosian, T.D.; Nannemann, D.P.; Iversen, T.M.; Bachmann, B.O.
Deposited on : 2013-07-19
Resolution : 2.00 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 : 2.13.1
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) : 2.13.1

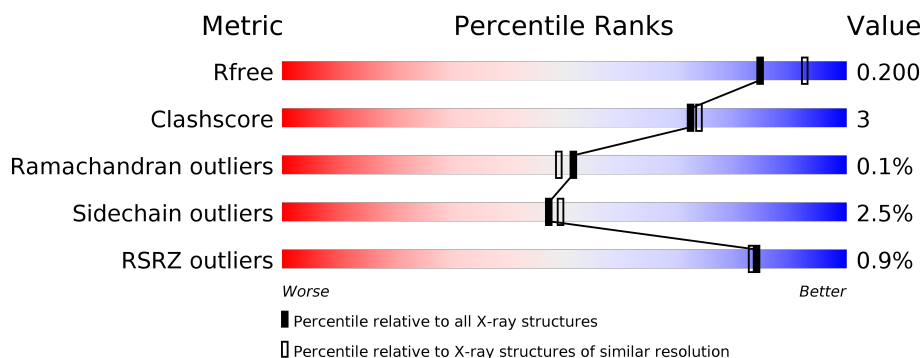
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. 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	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 86%; height: 10px; background-color: green;"></div> <div style="width: 7%; height: 10px; background-color: yellow;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 86% 7% 6% </div> </div>
1	B	416	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 86%; height: 10px; background-color: green;"></div> <div style="width: 7%; height: 10px; background-color: yellow;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 86% 7% 6% </div> </div>
1	C	416	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 9%; height: 10px; background-color: yellow;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 84% 9% 6% </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10203 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	3	6	0
			3122	1968	519	617	1	17			
1	B	390	Total	C	N	O	P	S	7	2	0
			3077	1945	508	605	1	18			
1	C	390	Total	C	N	O	P	S	47	0	0
			3058	1934	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	GLY	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	GLY	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

Continued on next page...

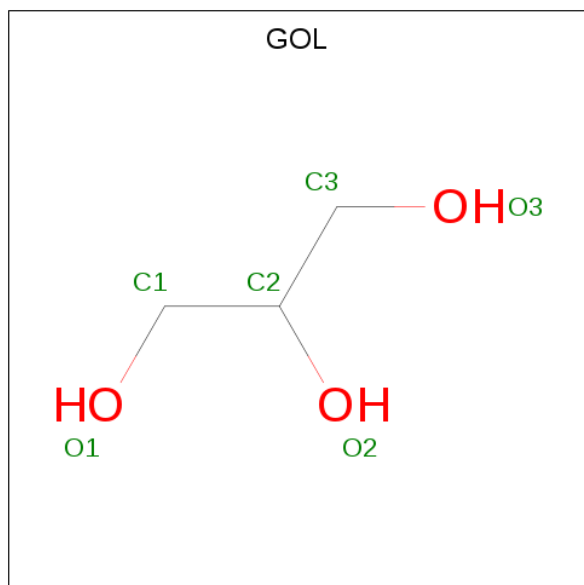
Continued from previous page...

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	GLY	SER	engineered mutation	UNP Q818Z9

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

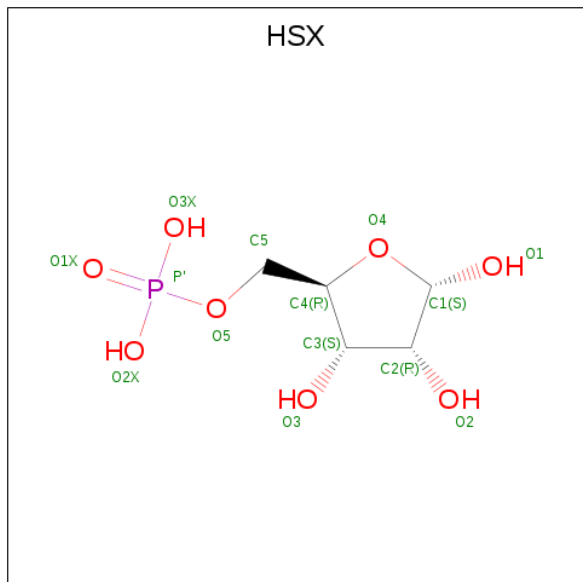
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	5	Total Mn 5 5	0	0
2	A	4	Total Mn 4 4	0	0
2	C	3	Total Mn 3 3	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is 5-O-phosphono-alpha-D-ribofuranose (three-letter code: HSX) (formula: $C_5H_{11}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			14	5	8	1		
4	A	1	Total	C	O	P	0	1
			14	5	8	1		

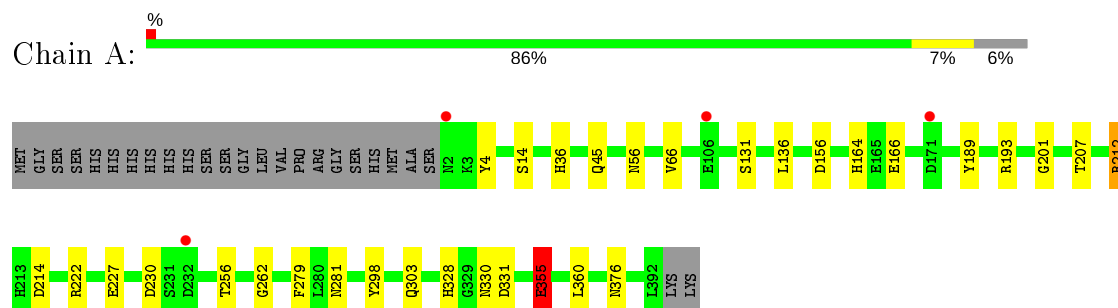
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	318	Total	O	0	0
			318	318		
5	B	354	Total	O	0	0
			354	354		
5	C	222	Total	O	0	0
			222	222		

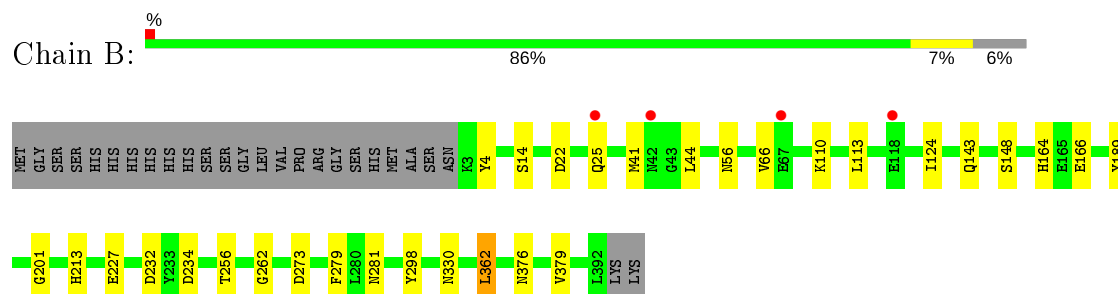
3 Residue-property plots [i](#)

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.

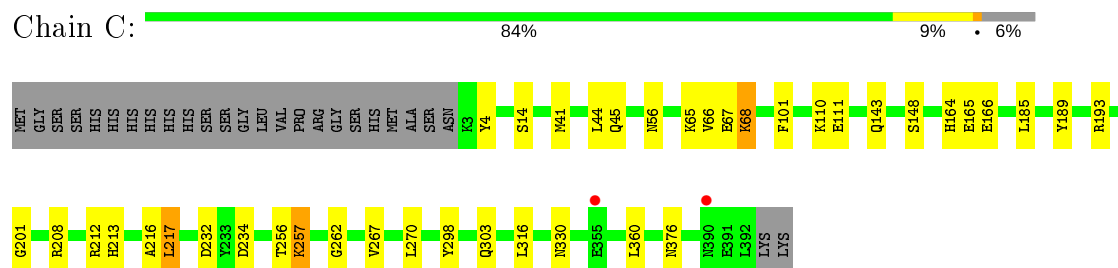
• Molecule 1: Phosphopentomutase



• Molecule 1: Phosphopentomutase



• Molecule 1: Phosphopentomutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.92Å 76.77Å 107.53Å 90.00° 108.72° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.00) 99.9 (19.90-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117, CNS	Depositor
R, R_{free}	0.163 , 0.200 0.164 , 0.200	Depositor DCC
R_{free} test set	4633 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 54.2	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	10203	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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

5.1 Standard geometry

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

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	0.54	1/3172 (0.0%)	0.62	2/4281 (0.0%)
1	B	0.41	0/3126	0.57	1/4218 (0.0%)
1	C	0.50	2/3107 (0.1%)	0.59	5/4194 (0.1%)
All	All	0.48	3/9405 (0.0%)	0.60	8/12693 (0.1%)

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	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	GLU	CG-CD	-20.69	1.21	1.51
1	C	65	LYS	CD-CE	-14.97	1.13	1.51
1	C	67	GLU	CA-CB	-8.54	1.35	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	GLU	CG-CD-OE2	-12.76	92.78	118.30
1	A	355	GLU	CG-CD-OE1	9.44	137.18	118.30
1	C	67	GLU	N-CA-CB	6.34	122.02	110.60
1	C	111	GLU	CG-CD-OE1	-5.86	106.58	118.30
1	C	111	GLU	CG-CD-OE2	5.76	129.82	118.30
1	C	257	LYS	CG-CD-CE	5.51	128.43	111.90
1	C	68	LYS	CA-CB-CG	5.48	125.45	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	362	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	GLU	Sidechain

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	3122	0	3044	22	0
1	B	3077	0	3019	20	0
1	C	3058	0	2999	23	0
2	A	4	0	0	0	0
2	B	5	0	0	1	0
2	C	3	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	28	0	0	1	0
5	A	318	0	0	3	0
5	B	354	0	0	1	0
5	C	222	0	0	0	0
All	All	10203	0	9078	62	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 3.

All (62) 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:A:222[B]:ARG:NH2	1:A:227:GLU:OE2	1.76	1.16
1:A:4:TYR:H	1:A:376:ASN:HD21	1.14	0.93
1:C:4:TYR:H	1:C:376:ASN:HD21	1.13	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:TYR:H	1:B:376:ASN:HD21	1.16	0.89
1:A:222[B]:ARG:NH1	1:A:230:ASP:OD2	2.08	0.87
1:B:164:HIS:HD2	1:B:166:GLU:H	1.24	0.86
1:A:164:HIS:HD2	1:A:166:GLU:H	1.26	0.82
1:C:164:HIS:HD2	1:C:166:GLU:H	1.26	0.81
1:A:56:ASN:HD21	1:A:66:VAL:H	1.32	0.78
1:C:45:GLN:H	1:C:303:GLN:HE21	1.34	0.76
1:A:45:GLN:H	1:A:303:GLN:HE21	1.35	0.75
4:A:407[A]:HSX:O3X	5:A:575:HOH:O	2.07	0.73
1:B:56:ASN:HD21	1:B:66:VAL:H	1.36	0.72
1:C:56:ASN:HD21	1:C:66:VAL:H	1.38	0.71
1:A:212:ARG:HD3	1:A:214:ASP:OD1	1.91	0.70
1:B:227:GLU:HG3	1:B:379:VAL:HB	1.75	0.69
1:C:212:ARG:HG3	1:C:212:ARG:HH21	1.63	0.64
1:A:222[B]:ARG:HH22	1:A:227:GLU:CD	2.02	0.62
2:B:404:MN:MN	5:B:844:HOH:O	1.60	0.60
1:A:36:HIS:HD2	1:A:331:ASP:OD2	1.85	0.60
1:B:164:HIS:CD2	1:B:166:GLU:H	2.13	0.59
1:B:213:HIS:HD2	1:C:234:ASP:OD1	1.87	0.57
1:B:164:HIS:HE1	1:B:201:GLY:O	1.88	0.56
1:C:164:HIS:CD2	1:C:166:GLU:H	2.17	0.56
1:B:234:ASP:OD1	1:C:213:HIS:HD2	1.89	0.55
1:A:164:HIS:HE1	1:A:201:GLY:O	1.91	0.54
1:A:156[B]:ASP:OD2	1:A:193[B]:ARG:NH2	2.41	0.54
1:A:56:ASN:ND2	1:A:66:VAL:H	2.02	0.54
1:C:164:HIS:HE1	1:C:201:GLY:O	1.91	0.54
1:B:56:ASN:ND2	1:B:66:VAL:H	2.06	0.54
1:B:227:GLU:CG	1:B:379:VAL:HB	2.37	0.54
1:B:113:LEU:HD22	1:B:124:ILE:HG21	1.90	0.53
1:A:45:GLN:H	1:A:303:GLN:NE2	2.03	0.53
1:A:207:THR:HG22	5:A:627:HOH:O	2.10	0.51
1:C:4:TYR:N	1:C:376:ASN:HD21	1.96	0.51
1:C:212:ARG:NH2	1:C:212:ARG:HG3	2.24	0.51
1:C:14:SER:HB2	1:C:330:ASN:HB2	1.93	0.50
1:B:22:ASP:O	1:B:25:GLN:HG2	2.14	0.48
1:A:164:HIS:CD2	1:A:166:GLU:H	2.18	0.47
1:C:56:ASN:ND2	1:C:66:VAL:H	2.07	0.47
1:A:256:THR:HG21	1:A:262:GLY:HA2	1.95	0.47
1:C:256:THR:HG21	1:C:262:GLY:HA2	1.97	0.47
1:A:14:SER:HB2	1:A:330:ASN:HB2	1.97	0.47
1:B:256:THR:HG21	1:B:262:GLY:HA2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:HIS:HE1	1:C:232:ASP:OD1	1.99	0.46
1:B:14:SER:HB2	1:B:330:ASN:HB2	1.96	0.46
1:B:273:ASP:OD2	1:C:165:GLU:OE2	2.34	0.46
1:C:267:VAL:HA	1:C:270:LEU:HD12	1.99	0.45
1:C:41:MET:HG3	1:C:44:LEU:HD13	1.98	0.45
1:B:164:HIS:HD2	1:B:166:GLU:N	2.04	0.45
1:C:45:GLN:H	1:C:303:GLN:NE2	2.10	0.44
1:B:232:ASP:OD1	1:C:213:HIS:HE1	2.00	0.44
1:A:36:HIS:CD2	1:A:331:ASP:OD2	2.69	0.44
1:A:193[A]:ARG:HD3	1:A:214:ASP:HB3	2.00	0.43
1:C:193:ARG:NH1	1:C:216:ALA:HB2	2.34	0.42
1:A:4:TYR:N	1:A:376:ASN:HD21	1.97	0.42
1:A:222[B]:ARG:NH2	5:A:814:HOH:O	2.54	0.41
1:B:41:MET:HG3	1:B:44:LEU:HD13	2.03	0.41
1:B:143:GLN:HG2	1:B:148:SER:O	2.19	0.41
1:A:193[A]:ARG:HH11	1:A:214:ASP:HB3	1.86	0.41
1:C:101:PHE:HE2	1:C:217:LEU:HD23	1.84	0.41
1:C:143:GLN:HG2	1:C:148:SER:O	2.22	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	394/416 (95%)	377 (96%)	16 (4%)	1 (0%)	41	37
1	B	389/416 (94%)	377 (97%)	12 (3%)	0	100	100
1	C	387/416 (93%)	374 (97%)	13 (3%)	0	100	100
All	All	1170/1248 (94%)	1128 (96%)	41 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	HIS

5.3.2 Protein sidechains ⓘ

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	337/352 (96%)	328 (97%)	9 (3%)	44	46
1	B	332/352 (94%)	326 (98%)	6 (2%)	59	63
1	C	330/352 (94%)	320 (97%)	10 (3%)	41	41
All	All	999/1056 (95%)	974 (98%)	25 (2%)	47	49

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	SER
1	A	136	LEU
1	A	189	TYR
1	A	212	ARG
1	A	279	PHE
1	A	281	ASN
1	A	298	TYR
1	A	355	GLU
1	A	360	LEU
1	B	110	LYS
1	B	189	TYR
1	B	279	PHE
1	B	281	ASN
1	B	298	TYR
1	B	362	LEU
1	C	68	LYS
1	C	110	LYS
1	C	185	LEU
1	C	189	TYR
1	C	208	ARG
1	C	217	LEU
1	C	257	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	298	TYR
1	C	316	LEU
1	C	360	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	48	ASN
1	A	56	ASN
1	A	77	GLN
1	A	89	HIS
1	A	164	HIS
1	A	205	ASN
1	A	211	ASN
1	A	259	ASN
1	A	281	ASN
1	A	303	GLN
1	A	376	ASN
1	A	390	ASN
1	B	45	GLN
1	B	48	ASN
1	B	56	ASN
1	B	77	GLN
1	B	89	HIS
1	B	164	HIS
1	B	205	ASN
1	B	211	ASN
1	B	213	HIS
1	B	259	ASN
1	B	281	ASN
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	213	HIS
1	C	259	ASN
1	C	281	ASN
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	B	85	1,2	8,10,11	0.95	0	10,14,16	0.95	0
1	TPO	A	85	1,2	8,10,11	0.76	0	10,14,16	1.11	0
1	TPO	C	85	1,2	8,10,11	0.95	0	10,14,16	0.97	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	B	85	1,2	-	1/9/11/13	-
1	TPO	A	85	1,2	-	2/9/11/13	-
1	TPO	C	85	1,2	-	1/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	$\# Z > 2$
4	HSX	A	407[A]	2	14,14,14	0.61	0	20,21,21	0.92	1 (5%)
3	GOL	B	406	-	5,5,5	0.23	0	5,5,5	0.37	0
4	HSX	A	406	-	14,14,14	0.61	0	20,21,21	1.06	1 (5%)
3	GOL	A	405	-	5,5,5	0.34	0	5,5,5	0.37	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
4	HSX	A	407[A]	2	-	6/6/22/22	0/1/1/1
3	GOL	B	406	-	-	0/4/4/4	-
4	HSX	A	406	-	-	0/6/22/22	0/1/1/1
3	GOL	A	405	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	406	HSX	C1-C2-C3	2.41	105.32	102.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	407[A]	HSX	O4-C1-C2	2.02	106.95	104.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	407[A]	HSX	C3-C4-C5-O5
4	A	407[A]	HSX	C5-O5-P'-O3X
3	A	405	GOL	O1-C1-C2-C3
3	A	405	GOL	O1-C1-C2-O2
4	A	407[A]	HSX	O4-C4-C5-O5
4	A	407[A]	HSX	C5-O5-P'-O1X
4	A	407[A]	HSX	C5-O5-P'-O2X
4	A	407[A]	HSX	C4-C5-O5-P'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	407[A]	HSX	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	390/416 (93%)	-0.49	4 (1%) 82 81	9, 17, 30, 42	12 (3%)
1	B	389/416 (93%)	-0.49	4 (1%) 82 81	9, 17, 30, 39	11 (2%)
1	C	389/416 (93%)	-0.28	2 (0%) 91 90	13, 26, 48, 64	23 (5%)
All	All	1168/1248 (93%)	-0.42	10 (0%) 84 83	9, 20, 39, 64	46 (3%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	390	ASN	3.0
1	B	67	GLU	2.7
1	C	355	GLU	2.5
1	A	2	ASN	2.2
1	A	106	GLU	2.2
1	B	118	GLU	2.1
1	B	42	ASN	2.1
1	A	232[A]	ASP	2.1
1	A	171	ASP	2.0
1	B	25	GLN	2.0

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

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	B	85	11/12	0.93	0.13	13,15,19,19	4
1	TPO	C	85	11/12	0.94	0.11	18,20,23,23	4
1	TPO	A	85	11/12	0.98	0.10	16,17,20,21	4

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
3	GOL	A	405	6/6	0.84	0.16	35,38,40,40	0
4	HSX	A	407[A]	14/14	0.90	0.20	18,19,21,22	14
2	MN	B	404	1/1	0.95	0.10	33,33,33,33	1
4	HSX	A	406	14/14	0.96	0.10	18,20,21,22	14
3	GOL	B	406	6/6	0.97	0.14	25,26,26,27	0
2	MN	A	404	1/1	0.98	0.07	48,48,48,48	0
2	MN	B	403	1/1	0.98	0.05	36,36,36,36	1
2	MN	B	405	1/1	0.99	0.07	28,28,28,28	1
2	MN	A	403	1/1	0.99	0.04	16,16,16,16	1
2	MN	C	402	1/1	0.99	0.05	15,15,15,15	0
2	MN	A	402	1/1	1.00	0.06	11,11,11,11	0
2	MN	C	403	1/1	1.00	0.04	30,30,30,30	0
2	MN	B	401	1/1	1.00	0.05	14,14,14,14	0
2	MN	C	401	1/1	1.00	0.04	18,18,18,18	0
2	MN	A	401	1/1	1.00	0.04	13,13,13,13	0
2	MN	B	402	1/1	1.00	0.04	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.