



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:23 PM BST

PDB ID : 4LR8
Title : Phosphopentomutase S154A 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

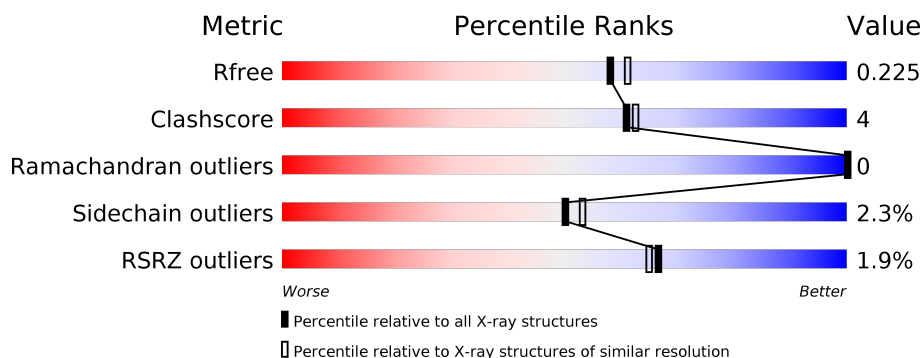
1 Overall quality at a glance

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: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 84%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 84% 10% 6% </div> </div>
1	B	416	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 84%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 84% 9% 6% </div> </div>
1	C	416	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 83%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 83% 11% 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
4	ACT	A	405	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10078 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	0	9	0
			3151	1985	525	622	1	18			
1	B	390	Total	C	N	O	P	S	4	1	0
			3067	1940	504	604	1	18			
1	C	390	Total	C	N	O	P	S	23	1	0
			3070	1941	507	604	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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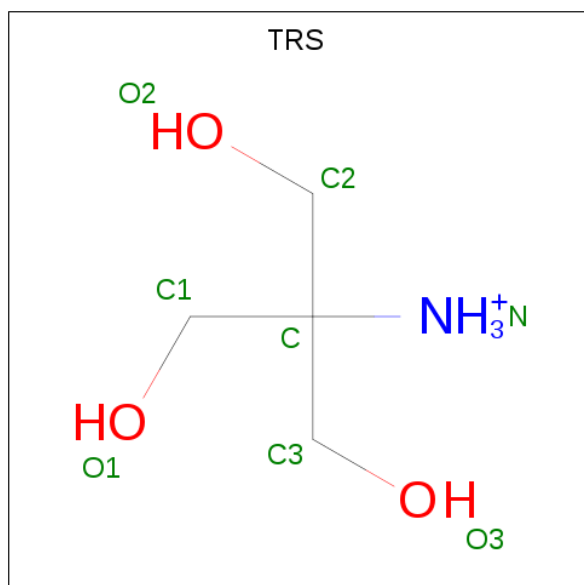
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP Q818Z9
C	-3	SER	-	expression tag	UNP Q818Z9
C	-2	HIS	-	expression tag	UNP Q818Z9
C	-1	MET	-	expression tag	UNP Q818Z9
C	0	ALA	-	expression tag	UNP Q818Z9
C	1	SER	-	expression tag	UNP Q818Z9
C	154	ALA	SER	engineered mutation	UNP Q818Z9

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

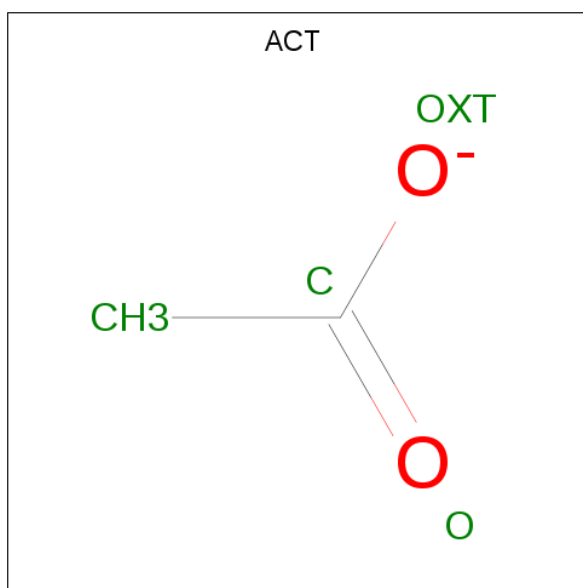
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Mn	0	0
			3	3		
2	A	3	Total	Mn	0	0
			3	3		
2	C	3	Total	Mn	0	0
			3	3		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



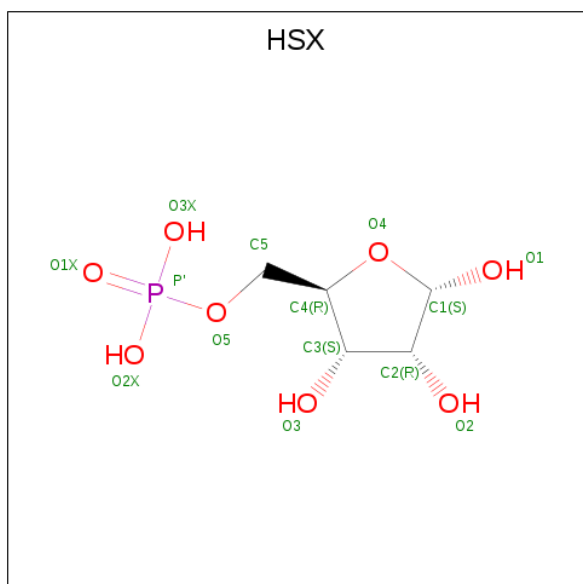
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 5-O-phosphono-alpha-D-ribofuranose (three-letter code: HSX) (formula: $\text{C}_5\text{H}_{11}\text{O}_8\text{P}$).



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

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

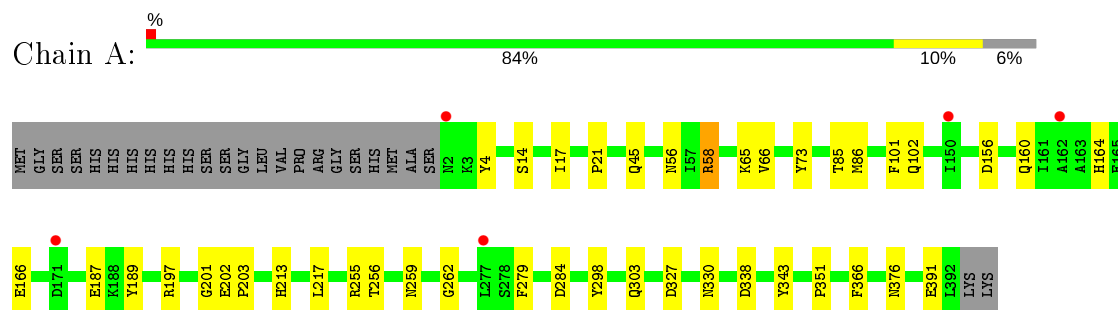
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	275	Total	O	0	0
			275	275		
6	B	320	Total	O	0	0
			320	320		
6	C	138	Total	O	0	0
			138	138		

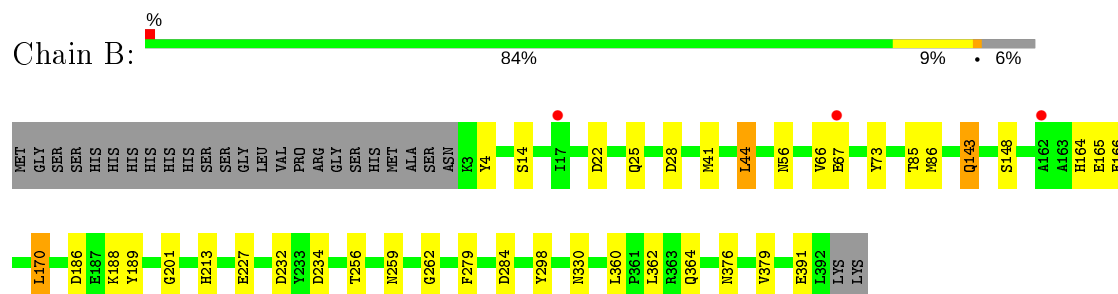
3 Residue-property plots [i](#)

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.

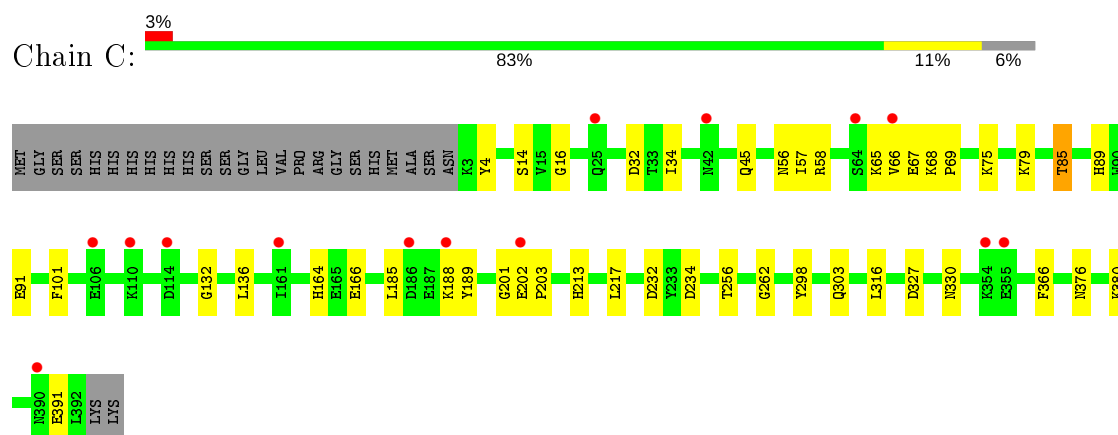
• Molecule 1: Phosphopentomutase



• 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	91.17Å 76.50Å 106.97Å 90.00° 108.89° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-2.00) 96.5 (19.96-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.164 , 0.202 0.192 , 0.225	Depositor DCC
R_{free} test set	4452 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.0	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	0.95	EDS
Total number of atoms	10078	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 4.39% 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: TPO, TRS, MN, HSX, ACT

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	0.44	0/3201	0.58	0/4319
1	B	0.46	0/3116	0.59	0/4206
1	C	0.42	0/3119	0.57	0/4210
All	All	0.44	0/9436	0.58	0/12735

There are no bond length outliers.

There are no bond angle outliers.

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	3151	0	3071	32	0
1	B	3067	0	3009	27	0
1	C	3070	0	3013	26	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
4	A	4	0	3	2	0
5	A	28	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	275	0	0	6	0
6	B	320	0	0	2	0
6	C	138	0	0	0	0
All	All	10078	0	9120	82	1

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 (82) 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:338[B]:ASP:OD2	6:A:767:HOH:O	1.73	1.06
1:C:4:TYR:H	1:C:376:ASN:HD21	1.07	0.95
1:A:4:TYR:H	1:A:376:ASN:HD21	1.17	0.92
1:A:164:HIS:HD2	1:A:166:GLU:H	1.19	0.90
1:B:4:TYR:H	1:B:376:ASN:HD21	1.19	0.87
1:A:102:GLN:HG3	6:A:707:HOH:O	1.79	0.81
1:B:56:ASN:HD21	1:B:66:VAL:H	1.26	0.79
1:C:164:HIS:HD2	1:C:166:GLU:H	1.30	0.79
1:B:227:GLU:OE1	6:B:772:HOH:O	2.01	0.77
1:B:164:HIS:HD2	1:B:166:GLU:H	1.35	0.75
1:A:56:ASN:HD21	1:A:66:VAL:H	1.33	0.73
1:B:28:ASP:OD1	6:B:690:HOH:O	2.05	0.73
1:B:227:GLU:HG3	1:B:379:VAL:HB	1.72	0.72
1:A:156[A]:ASP:CB	5:A:407[A]:HSX:O2X	2.37	0.72
1:B:143:GLN:NE2	1:B:164:HIS:H	1.91	0.69
1:A:45:GLN:H	1:A:303:GLN:HE21	1.41	0.69
1:B:164:HIS:HE1	1:B:201:GLY:O	1.76	0.69
1:A:86[B]:MET:HE3	1:A:86[B]:MET:HA	1.75	0.67
1:C:101:PHE:HE2	1:C:217:LEU:HD12	1.60	0.65
1:A:156[A]:ASP:HB3	5:A:407[A]:HSX:O2X	1.97	0.64
1:A:160:GLN:NE2	1:A:197:ARG:HE	1.98	0.61
1:C:45:GLN:H	1:C:303:GLN:HE21	1.48	0.61
1:B:56:ASN:ND2	1:B:66:VAL:H	2.00	0.59
1:C:164:HIS:HE1	1:C:201:GLY:O	1.85	0.58
1:C:14:SER:HB2	1:C:330:ASN:HB2	1.84	0.58
1:B:234:ASP:OD1	1:C:213:HIS:HD2	1.89	0.56
1:A:351:PRO:O	4:A:405:ACT:H1	2.05	0.56
1:B:213:HIS:HD2	1:C:234:ASP:OD1	1.88	0.56
1:A:101:PHE:HE2	1:A:217:LEU:HD12	1.71	0.55
1:C:4:TYR:H	1:C:376:ASN:ND2	1.91	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LEU:HD12	1:B:364:GLN:NE2	2.23	0.54
1:C:91:GLU:HG2	1:C:366:PHE:HB2	1.90	0.54
1:B:14:SER:HB2	1:B:330:ASN:HB2	1.90	0.54
1:C:256:THR:HG21	1:C:262:GLY:HA2	1.90	0.54
1:A:164:HIS:HE1	1:A:201:GLY:O	1.91	0.53
1:A:259:ASN:HD21	1:A:284:ASP:H	1.56	0.52
1:A:56:ASN:ND2	1:A:66:VAL:H	2.02	0.52
1:B:256:THR:HG21	1:B:262:GLY:HA2	1.91	0.52
1:B:232:ASP:OD1	1:C:213:HIS:HE1	1.91	0.52
4:A:405:ACT:H3	6:A:586:HOH:O	2.10	0.51
1:A:255[B]:ARG:NH2	6:A:733:HOH:O	2.42	0.49
1:B:86[B]:MET:H	1:B:86[B]:MET:HE2	1.77	0.49
1:C:56:ASN:HA	1:C:65:LYS:HG2	1.93	0.49
1:C:132:GLY:O	1:C:136:LEU:HG	2.12	0.49
1:C:56:ASN:HD21	1:C:66:VAL:H	1.61	0.48
1:A:256:THR:HG21	1:A:262:GLY:HA2	1.94	0.48
1:A:45:GLN:H	1:A:303:GLN:NE2	2.08	0.48
1:A:86[B]:MET:HG2	6:A:752:HOH:O	2.14	0.48
1:B:164:HIS:CD2	1:B:166:GLU:H	2.24	0.48
1:A:14:SER:HB2	1:A:330:ASN:HB2	1.96	0.47
1:A:164:HIS:CD2	1:A:166:GLU:H	2.12	0.47
1:A:187:GLU:O	6:A:707:HOH:O	2.21	0.47
1:B:143:GLN:HE22	1:B:164:HIS:H	1.61	0.47
1:A:160:GLN:HE22	1:A:197:ARG:HH21	1.63	0.46
1:A:56:ASN:HB3	1:A:73:TYR:CE2	2.51	0.46
1:A:160:GLN:HE21	1:A:197:ARG:HE	1.61	0.46
1:A:327:ASP:O	1:A:366:PHE:HE2	1.99	0.46
1:C:16:GLY:O	1:C:34:ILE:HG13	2.16	0.45
1:B:41:MET:HG3	1:B:44:LEU:HD13	1.98	0.45
1:B:143:GLN:HG2	1:B:148:SER:O	2.15	0.45
1:A:17:ILE:O	1:A:58:ARG:NH1	2.49	0.45
1:C:57:ILE:HG23	1:C:75:LYS:HG2	1.99	0.44
1:B:259:ASN:HD21	1:B:284:ASP:H	1.66	0.43
1:B:165:GLU:OE2	1:B:170:LEU:HG	2.18	0.43
1:A:156[A]:ASP:HB2	5:A:407[A]:HSX:O2X	2.16	0.43
1:B:186:ASP:OD1	1:B:188:LYS:HE3	2.19	0.43
1:C:14:SER:HB2	1:C:330:ASN:CB	2.48	0.43
1:A:86[B]:MET:CE	1:A:86[B]:MET:HA	2.46	0.43
1:B:22:ASP:O	1:B:25:GLN:HG2	2.19	0.43
1:B:213:HIS:HE1	1:C:232:ASP:OD1	2.02	0.42
1:C:327:ASP:O	1:C:366:PHE:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:PHE:CE2	1:A:217:LEU:HD12	2.54	0.42
1:C:101:PHE:CE2	1:C:217:LEU:HD12	2.47	0.42
1:C:32:ASP:CG	1:C:58:ARG:HH12	2.23	0.42
1:C:79:LYS:HA	1:C:79:LYS:HD2	1.84	0.41
1:A:202:GLU:HB2	1:A:203:PRO:HD2	2.02	0.41
1:B:56:ASN:HB3	1:B:73:TYR:CE2	2.56	0.41
1:C:85:TPO:O	1:C:89:HIS:HD2	2.02	0.41
1:C:67:GLU:O	1:C:69:PRO:HD3	2.21	0.40
1:A:21:PRO:HD3	1:A:343:TYR:CZ	2.56	0.40
1:B:227:GLU:CG	1:B:379:VAL:HB	2.47	0.40
1:C:202:GLU:HB2	1:C:203:PRO:HD2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:GLU:OE2	1:C:380:LYS:NZ[2_646]	2.08	0.12

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	397/416 (95%)	383 (96%)	14 (4%)	0	100	100
1	B	388/416 (93%)	376 (97%)	12 (3%)	0	100	100
1	C	388/416 (93%)	376 (97%)	12 (3%)	0	100	100
All	All	1173/1248 (94%)	1135 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	340/352 (97%)	332 (98%)	8 (2%)	49	51
1	B	331/352 (94%)	322 (97%)	9 (3%)	44	46
1	C	331/352 (94%)	324 (98%)	7 (2%)	53	57
All	All	1002/1056 (95%)	978 (98%)	24 (2%)	50	51

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	65	LYS
1	A	189	TYR
1	A	213[A]	HIS
1	A	213[B]	HIS
1	A	279	PHE
1	A	298	TYR
1	A	391	GLU
1	B	44	LEU
1	B	67	GLU
1	B	143	GLN
1	B	170	LEU
1	B	189	TYR
1	B	279	PHE
1	B	298	TYR
1	B	360	LEU
1	B	391	GLU
1	C	68	LYS
1	C	185	LEU
1	C	188	LYS
1	C	189	TYR
1	C	298	TYR
1	C	316	LEU
1	C	391	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	56	ASN
1	A	77	GLN
1	A	89	HIS
1	A	160	GLN
1	A	164	HIS
1	A	205	ASN
1	A	211	ASN
1	A	259	ASN
1	A	281	ASN
1	A	296	GLN
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	143	GLN
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	364	GLN
1	B	376	ASN
1	C	45	GLN
1	C	56	ASN
1	C	77	GLN
1	C	89	HIS
1	C	164	HIS
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	A	85	1,2	8,10,11	0.76	0	10,14,16	1.42	2 (20%)
1	TPO	C	85	1,2	8,10,11	0.85	0	10,14,16	1.13	1 (10%)
1	TPO	B	85	1,2	8,10,11	0.88	0	10,14,16	1.19	1 (10%)

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	1,2	-	2/9/11/13	-
1	TPO	C	85	1,2	-	2/9/11/13	-
1	TPO	B	85	1,2	-	2/9/11/13	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	TPO	P-OG1-CB	-2.30	116.26	123.21
1	B	85	TPO	O3P-P-O2P	2.23	116.16	107.64
1	C	85	TPO	OG1-P-O1P	-2.17	101.03	109.39
1	A	85	TPO	O-C-CA	-2.04	119.44	124.78

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	A	85	TPO	C-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
1	C	85	TPO	C-CA-CB-CG2
1	B	85	TPO	C-CA-CB-CG2
1	C	85	TPO	O-C-CA-CB
1	B	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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	TRS	A	404	-	7,7,7	0.33	0	9,9,9	0.44	0
4	ACT	A	405	-	1,3,3	1.59	0	0,3,3	0.00	-
3	TRS	B	404	-	7,7,7	0.35	0	9,9,9	0.63	0
5	HSX	A	407[A]	2	14,14,14	0.54	0	20,21,21	0.96	1 (5%)
5	HSX	A	406	-	14,14,14	0.66	0	20,21,21	1.15	2 (10%)

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	TRS	A	404	-	-	6/9/9/9	-
3	TRS	B	404	-	-	3/9/9/9	-
5	HSX	A	407[A]	2	-	4/6/22/22	0/1/1/1
5	HSX	A	406	-	-	0/6/22/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	407[A]	HSX	O4-C1-C2	2.07	107.01	104.46
5	A	406	HSX	O4-C1-C2	2.05	106.99	104.46
5	A	406	HSX	O2-C2-C1	-2.04	106.20	111.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	TRS	N-C-C1-O1
5	A	407[A]	HSX	C3-C4-C5-O5
5	A	407[A]	HSX	O4-C4-C5-O5
3	A	404	TRS	C3-C-C1-O1
3	A	404	TRS	C2-C-C3-O3
3	B	404	TRS	C3-C-C2-O2
5	A	407[A]	HSX	C4-C5-O5-P'
3	A	404	TRS	C2-C-C1-O1
3	A	404	TRS	C1-C-C3-O3
3	B	404	TRS	C1-C-C2-O2
5	A	407[A]	HSX	C5-O5-P'-O3X
3	A	404	TRS	N-C-C3-O3
3	B	404	TRS	N-C-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	ACT	2	0
5	A	407[A]	HSX	3	0

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 ⓘ

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%)	-0.15	5 (1%) 77 76	16, 24, 41, 55	1 (0%)
1	B	389/416 (93%)	-0.15	3 (0%) 86 85	13, 24, 40, 52	1 (0%)
1	C	389/416 (93%)	0.09	14 (3%) 42 42	18, 36, 64, 80	6 (1%)
All	All	1168/1248 (93%)	-0.07	22 (1%) 66 65	13, 27, 53, 80	8 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	355	GLU	3.4
1	C	188	LYS	3.0
1	C	390	ASN	2.9
1	C	186	ASP	2.8
1	C	161	ILE	2.7
1	C	25	GLN	2.7
1	A	277	LEU	2.6
1	C	106	GLU	2.5
1	C	110	LYS	2.4
1	C	42	ASN	2.4
1	B	67	GLU	2.4
1	B	162	ALA	2.3
1	C	64	SER	2.3
1	A	171[A]	ASP	2.3
1	A	150	ILE	2.2
1	A	162	ALA	2.2
1	C	66	VAL	2.2
1	A	2	ASN	2.2
1	C	354	LYS	2.2
1	B	17	ILE	2.1
1	C	114	ASP	2.1
1	C	202	GLU	2.0

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	0.93	0.14	28,29,33,33	4
1	TPO	A	85	11/12	0.94	0.14	21,24,27,29	4
1	TPO	B	85	11/12	0.94	0.16	19,22,26,26	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
4	ACT	A	405	4/4	0.66	0.26	37,37,37,38	4
3	TRS	B	404	8/8	0.75	0.25	39,41,41,42	0
5	HSX	A	406	14/14	0.86	0.14	27,28,30,30	14
3	TRS	A	404	8/8	0.87	0.20	39,40,41,41	0
5	HSX	A	407[A]	14/14	0.88	0.23	16,20,27,28	14
2	MN	B	403	1/1	0.96	0.07	36,36,36,36	1
2	MN	C	403	1/1	0.98	0.04	38,38,38,38	0
2	MN	C	401	1/1	0.99	0.07	28,28,28,28	0
2	MN	A	403	1/1	0.99	0.03	28,28,28,28	1
2	MN	B	402	1/1	0.99	0.10	18,18,18,18	0
2	MN	A	402	1/1	1.00	0.10	18,18,18,18	0
2	MN	B	401	1/1	1.00	0.10	20,20,20,20	0
2	MN	A	401	1/1	1.00	0.10	19,19,19,19	0
2	MN	C	402	1/1	1.00	0.07	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.