



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:29 PM GMT

PDB ID : 4LR7
Title : Phosphopentomutase S154A variant
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 : 2.10 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
<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

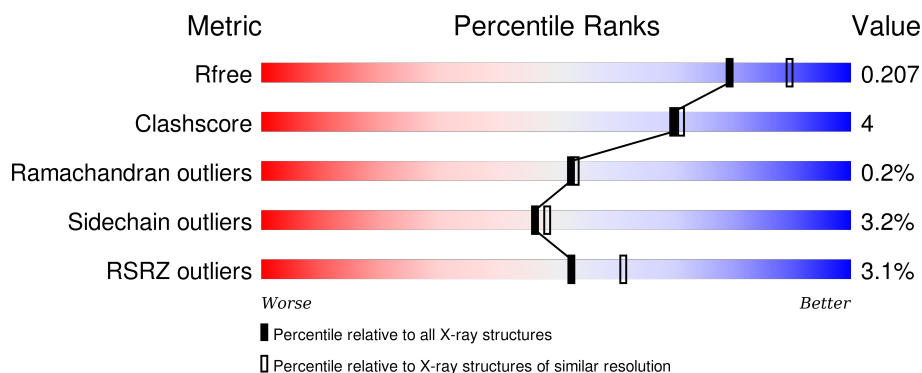
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



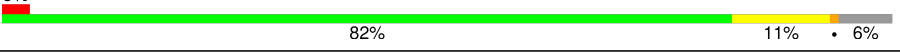
The reported resolution of this entry is 2.10 Å.

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 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	416	 4% 83% 11% • 6%
1	B	416	 2% 85% 9% 6%
1	C	416	 3% 82% 11% • 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9973 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	4	0
			3102	1958	512	613	1	18			
1	B	390	Total	C	N	O	P	S	4	4	0
			3097	1956	513	609	1	18			
1	C	390	Total	C	N	O	P	S	37	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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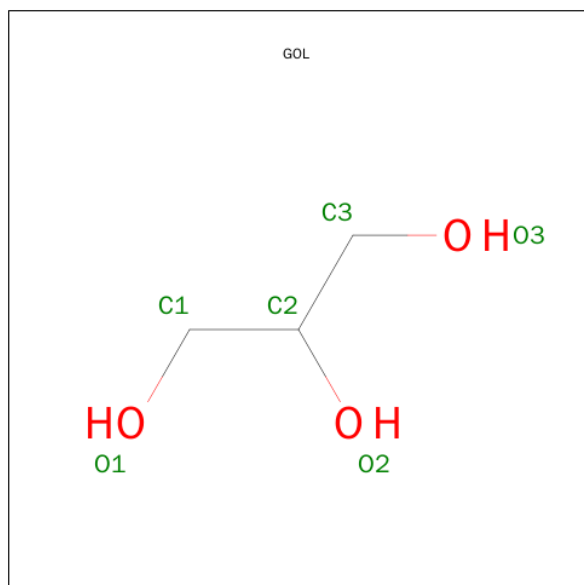
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	EXPRESSION TAG	UNP Q818Z9
C	-3	SER	-	EXPRESSION TAG	UNP Q818Z9
C	-2	HIS	-	EXPRESSION TAG	UNP Q818Z9
C	-1	MET	-	EXPRESSION TAG	UNP Q818Z9
C	0	ALA	-	EXPRESSION TAG	UNP Q818Z9
C	1	SER	-	EXPRESSION TAG	UNP Q818Z9
C	154	ALA	SER	ENGINEERED MUTATION	UNP Q818Z9

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	251	Total 251	O 251	0	0
4	B	280	Total 280	O 280	0	0
4	C	164	Total 164	O 164	0	0

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 ($\text{RSRZ} > 2$). 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.

Chain A:

Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows positions 1 to 300. A color key identifies amino acids: MET (grey), GLY (grey), SER (orange), HIS (green), LEU (yellow), VAL (yellow), PRO (grey), ARG (grey), GLY (grey), SER (orange), HIS (green), MET (grey), ALA (grey), SER (orange), P21 (yellow), H36 (yellow), Q45 (yellow), H56 (yellow), I57 (yellow), R58 (yellow), V66 (yellow), K79 (yellow), F104 (yellow), P105 (yellow), E106 (yellow), G107 (yellow), F108 (yellow), E111 (yellow), P129 (yellow), A130 (yellow), S131 (yellow), G132 (yellow), T133 (yellow), E134 (yellow), I135 (yellow), L136 (yellow), R137 (yellow), V379 (yellow), E391 (yellow), L392 (yellow), LYS (grey), LYS (grey).

Chain B:

Chain C:

82% 11% 3% 6%

• • • •

MET
GLY
SER
SER
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
LEU
VAL
PRO
ARG
ARG
GLY
SER
HIS
MET
MET
ALA
SER
ASN
K3
Y4
S14
M41
M42
G43
L44
Q45
N56
K61
K65
V66
E67
K68
Q102
P105
E111
L112
L113
D114
E115
L116
E117
I118
I124
T125
Q143
S148
H164
E165
E166
L185
D186
E187
K188
M190
V191
G192
R193
G201
G204
N205
R208
R212
H213
D214
L217
D234
T256
G262
V267
L270
F279
Y298
Q303
L316
H328
G329
N330
E355
L360
N376
K390
E391
L392
LYS
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.25Å 76.35Å 108.10Å 90.00° 108.96° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.10) 99.2 (20.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.165 , 0.206 0.166 , 0.207	Depositor DCC
R_{free} test set	4056 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 81481 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9973	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: TPO, GOL, 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	0.44	0/3151	0.59	2/4253 (0.0%)
1	B	0.42	0/3146	0.59	0/4245
1	C	0.89	5/3108 (0.2%)	0.77	7/4196 (0.2%)
All	All	0.62	5/9405 (0.1%)	0.66	9/12694 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	GLU	CG-CD	-37.11	0.96	1.51
1	C	65	LYS	CD-CE	-21.45	0.97	1.51
1	C	187	GLU	CA-CB	-8.30	1.35	1.53
1	C	67	GLU	CA-CB	-7.80	1.36	1.53
1	C	208	ARG	CB-CG	-5.71	1.37	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	GLU	CG-CD-OE1	-21.51	75.28	118.30
1	C	111	GLU	CG-CD-OE2	19.67	157.65	118.30
1	C	111	GLU	CB-CG-CD	11.72	145.85	114.20
1	C	187	GLU	N-CA-CB	8.99	126.79	110.60
1	C	67	GLU	N-CA-CB	7.97	124.94	110.60
1	C	65	LYS	CG-CD-CE	6.53	131.48	111.90
1	C	65	LYS	CD-CE-NZ	-5.59	98.84	111.70
1	A	355	GLU	CG-CD-OE1	5.35	129.00	118.30
1	A	355	GLU	CG-CD-OE2	-5.18	107.94	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3102	0	3033	32	0
1	B	3097	0	3036	27	0
1	C	3059	0	3001	27	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	4	0	0	0	0
3	A	6	0	8	0	0
4	A	251	0	0	1	0
4	B	280	0	0	3	0
4	C	164	0	0	1	0
All	All	9973	0	9078	82	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 (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:222[B]:ARG:HG2	1:A:222[B]:ARG:HH21	1.28	0.98
1:B:4:TYR:H	1:B:376:ASN:HD21	1.14	0.93
1:C:4:TYR:H	1:C:376:ASN:HD21	1.08	0.92
1:B:212[A]:ARG:O	1:B:212[A]:ARG:HG2	1.67	0.91
1:A:4:TYR:H	1:A:376:ASN:HD21	1.18	0.90
1:B:45:GLN:H	1:B:303:GLN:HE21	1.24	0.85
1:C:56:ASN:HD21	1:C:66:VAL:H	1.27	0.80
1:A:164:HIS:HD2	1:A:166:GLU:H	1.32	0.78
1:C:45:GLN:H	1:C:303:GLN:HE21	1.34	0.76
1:B:212[A]:ARG:CG	1:B:212[A]:ARG:O	2.35	0.75
1:C:164:HIS:HD2	1:C:166:GLU:H	1.33	0.74
1:A:222[B]:ARG:HG2	1:A:222[B]:ARG:NH2	2.02	0.74
1:A:56:ASN:HD21	1:A:66:VAL:H	1.36	0.73
1:B:164:HIS:HD2	1:B:166:GLU:H	1.35	0.73
1:A:36:HIS:HD2	1:A:331:ASP:OD2	1.73	0.71
1:A:104:PHE:O	1:A:153:THR:HG21	1.90	0.71
1:A:45:GLN:H	1:A:303:GLN:HE21	1.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ASN:HD21	1:B:66:VAL:H	1.42	0.67
1:A:36:HIS:CD2	1:A:331:ASP:OD2	2.52	0.61
1:C:164:HIS:HE1	1:C:201:GLY:O	1.84	0.61
1:A:222[B]:ARG:CG	1:A:222[B]:ARG:HH21	2.09	0.61
1:B:45:GLN:H	1:B:303:GLN:NE2	1.98	0.60
1:B:213:HIS:HD2	1:C:234:ASP:OD1	1.85	0.59
1:A:4:TYR:N	1:A:376:ASN:HD21	1.96	0.58
1:B:234:ASP:OD1	1:C:213:HIS:HD2	1.86	0.58
1:A:227:GLU:HG3	1:A:379:VAL:HB	1.85	0.58
1:A:212:ARG:HD3	1:A:214:ASP:OD1	2.03	0.58
1:B:164:HIS:HE1	1:B:201:GLY:O	1.86	0.57
1:C:4:TYR:N	1:C:376:ASN:HD21	1.91	0.57
1:A:164:HIS:HE1	1:A:201:GLY:O	1.88	0.57
1:A:135:ILE:HD12	1:A:136:LEU:HD13	1.87	0.57
1:C:45:GLN:H	1:C:303:GLN:NE2	2.02	0.57
1:C:56:ASN:ND2	1:C:66:VAL:H	2.01	0.56
1:C:117:GLU:HG3	1:C:124:ILE:CD1	2.36	0.55
1:C:117:GLU:CG	1:C:124:ILE:HD12	2.37	0.54
1:B:164:HIS:CD2	1:B:166:GLU:H	2.21	0.54
1:B:186:ASP:OD2	1:B:188:LYS:HE3	2.07	0.54
1:C:117:GLU:HG3	1:C:124:ILE:HD12	1.90	0.54
1:C:193:ARG:HD3	1:C:214:ASP:OD1	2.09	0.53
1:C:267:VAL:HA	1:C:270:LEU:HD12	1.91	0.53
1:A:14:SER:HB2	1:A:330:ASN:HB2	1.91	0.52
1:B:232:ASP:OD1	1:C:213:HIS:HE1	1.92	0.52
1:A:143:GLN:NE2	1:A:164:HIS:H	2.08	0.52
1:B:113:LEU:HD22	1:B:124:ILE:HG21	1.92	0.51
1:B:208:ARG:HB3	4:B:724:HOH:O	2.10	0.51
1:B:143:GLN:HG2	1:B:148:SER:O	2.10	0.50
1:A:193:ARG:HD3	1:A:214:ASP:OD2	2.11	0.50
1:A:130:ALA:CB	1:A:135:ILE:HG23	2.41	0.50
1:B:14:SER:HB2	1:B:330:ASN:HB2	1.93	0.50
1:B:256:THR:HG21	1:B:262:GLY:HA2	1.94	0.49
1:A:45:GLN:H	1:A:303:GLN:NE2	2.08	0.49
1:A:111:GLU:CD	1:A:111:GLU:H	2.16	0.49
1:A:222[B]:ARG:CG	1:A:222[B]:ARG:NH2	2.71	0.49
1:C:14:SER:HB2	1:C:330:ASN:HB2	1.95	0.48
1:B:56:ASN:ND2	1:B:66:VAL:H	2.10	0.48
1:A:56:ASN:ND2	1:A:66:VAL:H	2.07	0.48
1:A:318:GLU:HG2	4:A:563:HOH:O	2.12	0.48
1:A:132:GLY:O	1:A:136:LEU:HD22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:GLN:HE21	1:C:190:MET:H	1.61	0.47
1:A:143:GLN:HE22	1:A:164:HIS:H	1.64	0.46
1:A:256:THR:HG21	1:A:262:GLY:HA2	1.98	0.46
1:A:227:GLU:CG	1:A:379:VAL:HB	2.45	0.46
1:C:112:LEU:HD22	1:C:189:TYR:HB3	1.99	0.45
1:C:256:THR:HG21	1:C:262:GLY:HA2	1.98	0.45
1:B:133:THR:HG23	4:B:642:HOH:O	2.15	0.44
1:C:102:GLN:H	1:C:102:GLN:HG2	1.67	0.44
1:B:273:ASP:OD2	1:C:165:GLU:OE2	2.36	0.43
1:A:79:LYS:HD2	1:A:365:THR:HB	2.00	0.43
1:B:227:GLU:HG3	1:B:379:VAL:HB	1.99	0.43
1:B:227:GLU:CG	1:B:379:VAL:HB	2.48	0.43
1:B:164:HIS:HD2	1:B:166:GLU:N	2.11	0.43
1:C:102:GLN:HE21	1:C:190:MET:N	2.17	0.42
1:C:143:GLN:HG2	1:C:148:SER:O	2.19	0.42
1:B:56:ASN:HD21	1:B:66:VAL:HG22	1.84	0.41
1:C:117:GLU:HG2	1:C:124:ILE:HD12	2.02	0.41
1:B:358:GLN:NE2	4:B:726:HOH:O	2.52	0.41
1:B:41:MET:HG3	1:B:44:LEU:HD13	2.03	0.41
1:A:143:GLN:HG2	1:A:148:SER:O	2.21	0.41
1:A:108:PHE:CE1	1:A:153:THR:HB	2.57	0.40
1:C:212:ARG:HD3	4:C:512:HOH:O	2.21	0.40
1:A:21:PRO:HD3	1:A:343:TYR:CZ	2.57	0.40
1:C:41:MET:HG3	1:C:44:LEU:HD13	2.03	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	392/416 (94%)	377 (96%)	14 (4%)	1 (0%)	46 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	391/416 (94%)	380 (97%)	11 (3%)	0	100	100
1	C	387/416 (93%)	371 (96%)	15 (4%)	1 (0%)	46	45
All	All	1170/1248 (94%)	1128 (96%)	40 (3%)	2 (0%)	52	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	328	HIS
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	335/352 (95%)	323 (96%)	12 (4%)	42	43
1	B	334/352 (95%)	328 (98%)	6 (2%)	66	72
1	C	330/352 (94%)	316 (96%)	14 (4%)	36	35
All	All	999/1056 (95%)	967 (97%)	32 (3%)	46	48

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	133	THR
1	A	136	LEU
1	A	143	GLN
1	A	170	LEU
1	A	205	ASN
1	A	212	ARG
1	A	257	LYS
1	A	279	PHE
1	A	298	TYR
1	A	360	LEU
1	A	391	GLU

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Mol	Chain	Res	Type
1	B	58	ARG
1	B	67	GLU
1	B	79	LYS
1	B	189	TYR
1	B	298	TYR
1	B	362	LEU
1	C	61	LYS
1	C	65	LYS
1	C	68	LYS
1	C	102	GLN
1	C	115	GLU
1	C	185	LEU
1	C	187	GLU
1	C	188	LYS
1	C	191	VAL
1	C	217	LEU
1	C	279	PHE
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 (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	36	HIS
1	A	48	ASN
1	A	56	ASN
1	A	77	GLN
1	A	89	HIS
1	A	143	GLN
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	25	GLN
1	B	56	ASN
1	B	77	GLN

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Mol	Chain	Res	Type
1	B	89	HIS
1	B	164	HIS
1	B	211	ASN
1	B	213	HIS
1	B	259	ASN
1	B	281	ASN
1	B	303	GLN
1	B	376	ASN
1	C	56	ASN
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	0.73	0	7,14,16	1.62	2 (28%)
1	TPO	B	85	1,2	8,10,11	0.71	0	7,14,16	1.82	2 (28%)
1	TPO	C	85	1,2	8,10,11	0.78	0	7,14,16	1.25	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	1,2	-	0/8/11/13	0/0/0/0
1	TPO	B	85	1,2	-	0/8/11/13	0/0/0/0
1	TPO	C	85	1,2	-	0/8/11/13	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	TPO	OG1-P-O1P	-2.71	100.34	107.11
1	A	85	TPO	O-C-CA	-2.13	119.83	125.44
1	B	85	TPO	C-CA-N	2.39	114.82	109.83
1	A	85	TPO	C-CA-N	2.66	115.38	109.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 14 are monoatomic - leaving 1 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	A	406	-	5,5,5	0.18	0	5,5,5	0.30	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	A	406	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

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	17 (4%) 38 47	12, 22, 44, 74	15 (3%)
1	B	389/416 (93%)	-0.21	8 (2%) 67 72	12, 22, 38, 45	10 (2%)
1	C	389/416 (93%)	-0.01	11 (2%) 56 64	18, 31, 55, 72	19 (4%)
All	All	1168/1248 (93%)	-0.12	36 (3%) 52 61	12, 25, 50, 74	44 (3%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	ILE	8.6
1	A	132	GLY	7.6
1	A	133	THR	4.2
1	A	2	ASN	4.2
1	A	106	GLU	4.1
1	A	105	PRO	4.0
1	C	133	THR	3.7
1	A	131	SER	3.5
1	A	129	PRO	3.5
1	C	355	GLU	3.3
1	A	202	GLU	3.2
1	C	189	TYR	3.1
1	A	130	ALA	3.0
1	B	25	GLN	3.0
1	A	150	ILE	2.7
1	C	118	GLU	2.7
1	A	136	LEU	2.6
1	C	205	ASN	2.6
1	A	137	ASP	2.6
1	C	212	ARG	2.5
1	B	355	GLU	2.5
1	B	118	GLU	2.4
1	C	105	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	390	ASN	2.3
1	A	134	GLU	2.2
1	B	67	GLU	2.2
1	C	114	ASP	2.2
1	C	42	ASN	2.2
1	C	204	GLY	2.2
1	B	17	ILE	2.2
1	A	138	GLU	2.1
1	B	212[A]	ARG	2.1
1	C	390	ASN	2.1
1	B	133	THR	2.1
1	A	354	LYS	2.1
1	A	203	PRO	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. 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
1	TPO	B	85	11/12	0.94	0.14	-	16,19,22,22	4
1	TPO	C	85	11/12	0.96	0.12	-	21,24,26,27	4
1	TPO	A	85	11/12	0.93	0.16	-	18,21,26,27	4

6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
2	MN	A	402	1/1	1.00	0.08	-0.41	13,13,13,13	0
3	GOL	A	406	6/6	0.95	0.10	-0.42	45,49,50,52	0
2	MN	B	402	1/1	1.00	0.06	-0.84	16,16,16,16	0
2	MN	C	401	1/1	0.99	0.07	-1.25	25,25,25,25	0
2	MN	A	404	1/1	0.96	0.07	-1.60	32,32,32,32	1
2	MN	B	404	1/1	0.98	0.06	-1.66	46,46,46,46	0
2	MN	A	403	1/1	0.99	0.03	-1.77	22,22,22,22	1
2	MN	A	401	1/1	1.00	0.06	-1.80	14,14,14,14	0
2	MN	B	401	1/1	1.00	0.07	-1.87	19,19,19,19	0
2	MN	C	403	1/1	0.99	0.06	-1.93	40,40,40,40	0
2	MN	C	402	1/1	0.99	0.06	-2.02	19,19,19,19	0
2	MN	B	405	1/1	0.98	0.05	-2.23	46,46,46,46	0
2	MN	C	404	1/1	0.97	0.12	-	61,61,61,61	0
2	MN	B	403	1/1	0.96	0.06	-	37,37,37,37	1
2	MN	A	405	1/1	0.99	0.07	-	33,33,33,33	1

6.5 Other polymers [i](#)

There are no such residues in this entry.