



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:15 am BST

PDB ID : 3UNY
Title : Bacillus cereus phosphopentomutase T85E variant soaked with glucose 1,6-bisphosphate
Authors : Iverson, T.M.; Birmingham, W.R.; Panosian, T.D.; Nannemann, D.P.; Bachmann, B.O.
Deposited on : 2011-11-16
Resolution : 1.95 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	:	2.11
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)	:	2.11

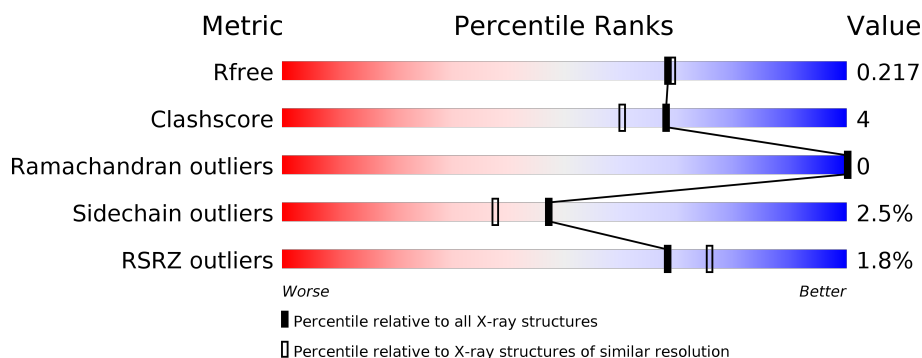
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	399	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>
1	B	399	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>•</div> </div> </div>
1	C	399	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>••</div> </div> </div>
1	D	399	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>•</div> </div> </div>
1	E	399	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>•</div> </div> </div>
1	F	399	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>•</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 20272 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	S	8	1	0
			3077	1946	509	605	17			
1	B	390	Total	C	N	O	S	4	0	0
			3058	1936	503	602	17			
1	C	390	Total	C	N	O	S	8	0	0
			3058	1936	503	602	17			
1	D	390	Total	C	N	O	S	8	1	0
			3066	1941	504	603	18			
1	E	391	Total	C	N	O	S	8	1	0
			3074	1945	506	605	18			
1	F	391	Total	C	N	O	S	8	0	0
			3066	1940	505	604	17			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	85	GLU	THR	ENGINEERED MUTATION	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	85	GLU	THR	ENGINEERED MUTATION	UNP Q818Z9
C	-4	GLY	-	EXPRESSION TAG	UNP Q818Z9
C	-3	SER	-	EXPRESSION TAG	UNP Q818Z9
C	-2	HIS	-	EXPRESSION TAG	UNP Q818Z9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	EXPRESSION TAG	UNP Q818Z9
C	0	ALA	-	EXPRESSION TAG	UNP Q818Z9
C	1	SER	-	EXPRESSION TAG	UNP Q818Z9
C	85	GLU	THR	ENGINEERED MUTATION	UNP Q818Z9
D	-4	GLY	-	EXPRESSION TAG	UNP Q818Z9
D	-3	SER	-	EXPRESSION TAG	UNP Q818Z9
D	-2	HIS	-	EXPRESSION TAG	UNP Q818Z9
D	-1	MET	-	EXPRESSION TAG	UNP Q818Z9
D	0	ALA	-	EXPRESSION TAG	UNP Q818Z9
D	1	SER	-	EXPRESSION TAG	UNP Q818Z9
D	85	GLU	THR	ENGINEERED MUTATION	UNP Q818Z9
E	-4	GLY	-	EXPRESSION TAG	UNP Q818Z9
E	-3	SER	-	EXPRESSION TAG	UNP Q818Z9
E	-2	HIS	-	EXPRESSION TAG	UNP Q818Z9
E	-1	MET	-	EXPRESSION TAG	UNP Q818Z9
E	0	ALA	-	EXPRESSION TAG	UNP Q818Z9
E	1	SER	-	EXPRESSION TAG	UNP Q818Z9
E	85	GLU	THR	ENGINEERED MUTATION	UNP Q818Z9
F	-4	GLY	-	EXPRESSION TAG	UNP Q818Z9
F	-3	SER	-	EXPRESSION TAG	UNP Q818Z9
F	-2	HIS	-	EXPRESSION TAG	UNP Q818Z9
F	-1	MET	-	EXPRESSION TAG	UNP Q818Z9
F	0	ALA	-	EXPRESSION TAG	UNP Q818Z9
F	1	SER	-	EXPRESSION TAG	UNP Q818Z9
F	85	GLU	THR	ENGINEERED MUTATION	UNP Q818Z9

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

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

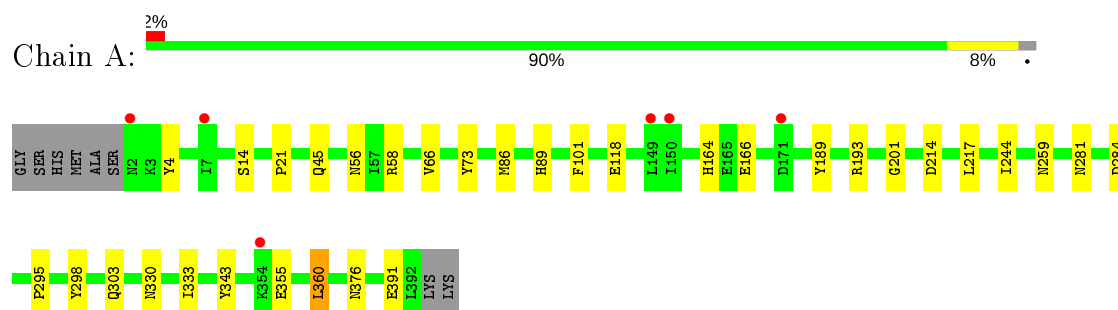
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	327	Total	O	0	0
			327	327		
4	B	271	Total	O	0	0
			271	271		
4	C	333	Total	O	0	0
			333	333		
4	D	371	Total	O	0	0
			371	371		
4	E	247	Total	O	0	0
			247	247		
4	F	290	Total	O	0	0
			290	290		

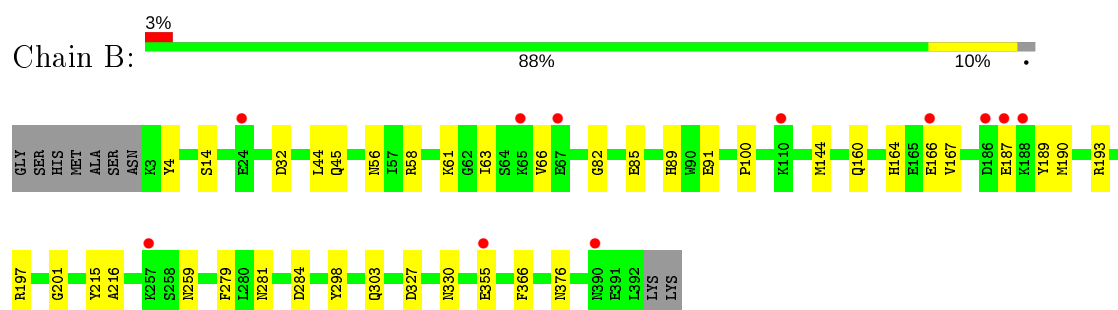
3 Residue-property plots [i](#)

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

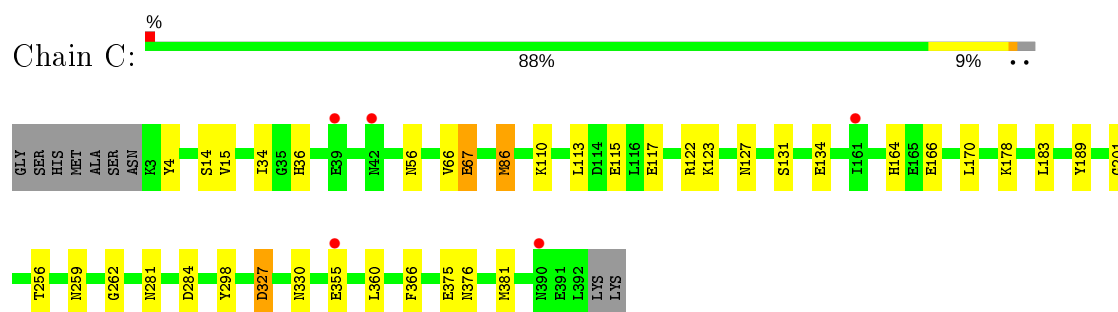
• Molecule 1: Phosphopentomutase



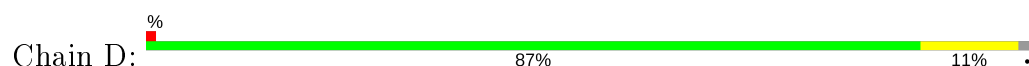
• Molecule 1: Phosphopentomutase

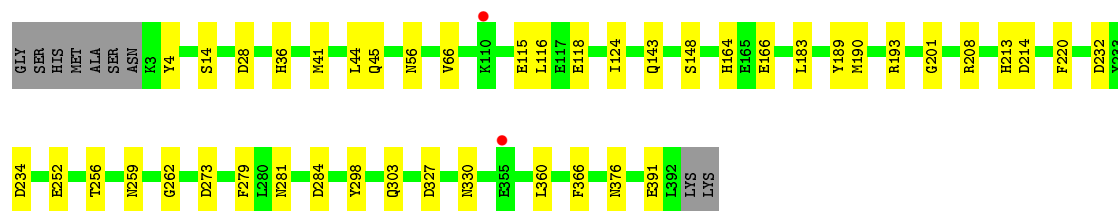


• Molecule 1: Phosphopentomutase

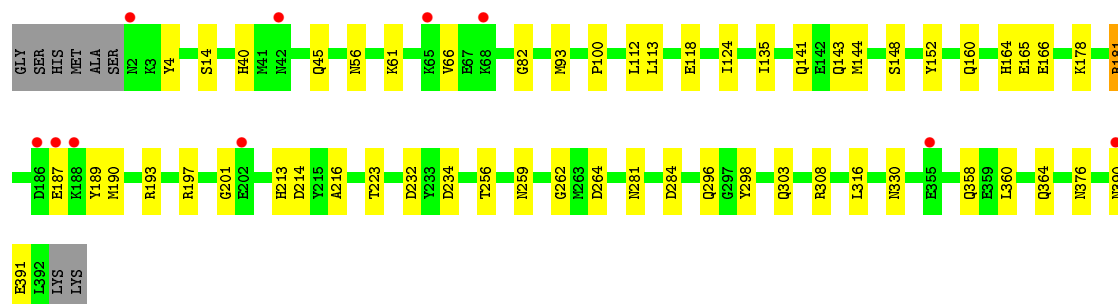
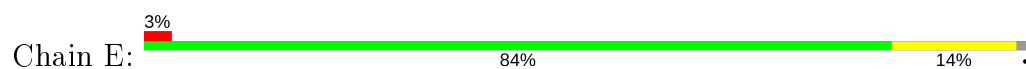


• Molecule 1: Phosphopentomutase

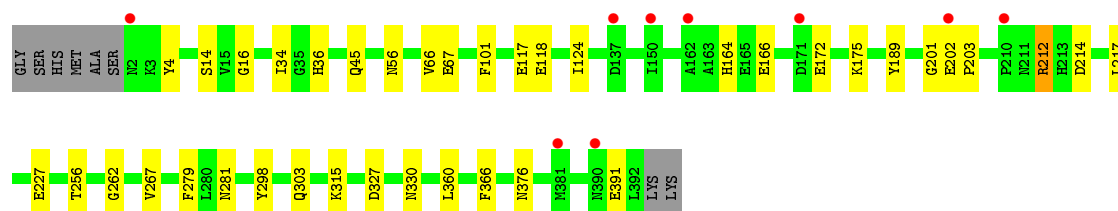
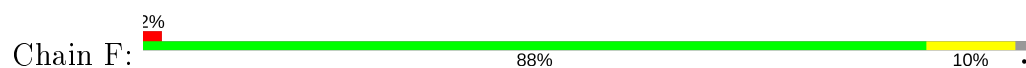




• Molecule 1: Phosphopentomutase



• 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	106.58 Å 76.79 Å 182.29 Å 90.00° 106.07° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 19.96 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-1.95) 99.3 (19.96-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.94 Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.167 , 0.199 0.190 , 0.217	Depositor DCC
R_{free} test set	10161 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20272	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0713e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 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	0.50	1/3138 (0.0%)	0.57	1/4237 (0.0%)
1	B	0.42	0/3119	0.55	0/4212
1	C	0.46	1/3119 (0.0%)	0.59	1/4212 (0.0%)
1	D	0.47	1/3127 (0.0%)	0.57	0/4222
1	E	0.48	1/3135 (0.0%)	0.57	0/4233
1	F	0.48	2/3127 (0.1%)	0.58	0/4223
All	All	0.47	6/18765 (0.0%)	0.57	2/25339 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	118	GLU	CB-CG	-13.37	1.26	1.52
1	A	118	GLU	CB-CG	-11.14	1.30	1.52
1	F	67	GLU	CB-CG	-8.64	1.35	1.52
1	C	67	GLU	CB-CG	-7.62	1.37	1.52
1	D	118	GLU	CB-CG	-6.30	1.40	1.52
1	F	118	GLU	CB-CG	-5.92	1.41	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	327	ASP	CB-CA-C	5.38	121.17	110.40
1	A	360	LEU	CA-CB-CG	5.06	126.94	115.30

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	3077	0	3019	19	0
1	B	3058	0	3001	21	0
1	C	3058	0	3001	19	0
1	D	3066	0	3009	29	0
1	E	3074	0	3015	36	0
1	F	3066	0	3007	21	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	F	6	0	8	0	0
4	A	327	0	0	1	0
4	B	271	0	0	0	1
4	C	333	0	0	1	1
4	D	371	0	0	5	0
4	E	247	0	0	0	0
4	F	290	0	0	2	0
All	All	20272	0	18076	140	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 (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:GLN:HE21	1:B:197:ARG:HE	1.09	0.96
1:A:4:TYR:H	1:A:376:ASN:HD21	1.13	0.96
1:E:160:GLN:HE21	1:E:197:ARG:HE	1.03	0.95
1:E:4:TYR:H	1:E:376:ASN:HD21	1.17	0.92
1:F:4:TYR:H	1:F:376:ASN:HD21	1.14	0.91
1:B:4:TYR:H	1:B:376:ASN:HD21	1.16	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:TYR:H	1:C:376:ASN:HD21	1.16	0.90
1:A:56:ASN:HD21	1:A:66:VAL:H	1.20	0.89
1:A:295:PRO:HG3	1:A:333:ILE:HD11	1.55	0.88
1:D:4:TYR:H	1:D:376:ASN:HD21	1.19	0.87
1:E:164:HIS:HD2	1:E:166:GLU:H	1.23	0.85
1:B:160:GLN:NE2	1:B:197:ARG:HE	1.82	0.77
1:E:160:GLN:NE2	1:E:197:ARG:HE	1.80	0.77
1:C:164:HIS:HD2	1:C:166:GLU:H	1.34	0.75
1:C:375:GLU:HA	1:C:381:MET:HE1	1.67	0.74
1:F:212:ARG:HD3	1:F:214:ASP:OD1	1.88	0.74
1:A:164:HIS:HD2	1:A:166:GLU:H	1.36	0.74
1:D:166:GLU:HG2	4:D:1644:HOH:O	1.87	0.74
1:E:45:GLN:H	1:E:303:GLN:HE21	1.36	0.73
1:A:45:GLN:H	1:A:303:GLN:HE21	1.35	0.72
1:F:164:HIS:HD2	1:F:166:GLU:H	1.38	0.72
1:B:56:ASN:HD21	1:B:66:VAL:H	1.37	0.71
1:E:181:ARG:O	1:E:181:ARG:HD3	1.90	0.71
1:B:164:HIS:HD2	1:B:166:GLU:H	1.40	0.70
1:F:56:ASN:HD21	1:F:66:VAL:H	1.39	0.68
1:F:45:GLN:H	1:F:303:GLN:HE21	1.41	0.68
1:E:56:ASN:HD21	1:E:66:VAL:H	1.38	0.68
1:D:252:GLU:HG3	4:D:1820:HOH:O	1.94	0.68
1:D:45:GLN:H	1:D:303:GLN:HE21	1.42	0.67
1:D:164:HIS:HE1	1:D:201:GLY:O	1.78	0.66
1:F:164:HIS:HE1	1:F:201:GLY:O	1.79	0.66
1:E:143:GLN:NE2	1:E:164:HIS:H	1.94	0.65
1:D:213:HIS:HD2	1:E:234:ASP:OD1	1.81	0.64
1:D:234:ASP:OD1	1:E:213:HIS:HD2	1.83	0.61
1:A:56:ASN:ND2	1:A:66:VAL:H	1.96	0.61
1:C:327:ASP:O	1:C:366:PHE:HE2	1.85	0.60
1:D:164:HIS:HD2	1:D:166:GLU:H	1.50	0.60
1:E:164:HIS:HE1	1:E:201:GLY:O	1.85	0.59
1:C:56:ASN:HD21	1:C:66:VAL:H	1.48	0.59
1:A:45:GLN:H	1:A:303:GLN:NE2	1.99	0.58
1:C:164:HIS:HE1	1:C:201:GLY:O	1.85	0.58
1:A:86:MET:SD	4:A:961:HOH:O	2.57	0.58
1:C:115:GLU:HG2	1:C:183:LEU:HD22	1.85	0.58
1:D:190:MET:CE	1:D:220:PHE:HZ	2.17	0.57
1:A:164:HIS:CD2	1:A:166:GLU:H	2.21	0.57
1:D:36:HIS:NE2	4:D:409:HOH:O	2.32	0.57
1:C:36:HIS:NE2	4:C:1378:HOH:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:PRO:HG3	1:A:333:ILE:CD1	2.34	0.56
1:F:16:GLY:O	1:F:34:ILE:HG13	2.06	0.56
1:E:40:HIS:HE1	1:E:296:GLN:HE21	1.52	0.55
1:E:4:TYR:N	1:E:376:ASN:HD21	1.97	0.55
1:D:56:ASN:HD21	1:D:66:VAL:H	1.54	0.55
1:E:181:ARG:C	1:E:181:ARG:HD3	2.25	0.55
1:E:82:GLY:HA3	1:E:100:PRO:HB3	1.88	0.55
1:B:45:GLN:NE2	1:B:303:GLN:HE22	2.05	0.55
1:F:117:GLU:HG3	1:F:124:ILE:HD12	1.88	0.55
1:E:143:GLN:HG2	1:E:148:SER:O	2.06	0.54
1:E:160:GLN:HE21	1:E:197:ARG:NE	1.88	0.54
1:E:193:ARG:NH1	1:E:216:ALA:HB2	2.23	0.54
1:D:115:GLU:HG2	1:D:183:LEU:HD22	1.90	0.54
1:F:172:GLU:HA	1:F:175:LYS:HE3	1.89	0.53
1:D:14:SER:HB2	1:D:330:ASN:HB2	1.90	0.53
1:A:295:PRO:CG	1:A:333:ILE:HD11	2.35	0.53
1:E:143:GLN:HE22	1:E:164:HIS:H	1.57	0.53
1:B:14:SER:HB2	1:B:330:ASN:HB2	1.90	0.53
1:B:164:HIS:HE1	1:B:201:GLY:O	1.92	0.52
1:A:193:ARG:HD3	1:A:214:ASP:OD2	2.10	0.52
1:F:36:HIS:NE2	4:F:405:HOH:O	2.34	0.52
1:C:113:LEU:HD11	1:C:127:ASN:ND2	2.25	0.51
1:E:264:ASP:OD2	1:E:308:ARG:NH1	2.35	0.50
1:F:101:PHE:HE2	1:F:217:LEU:HD12	1.76	0.50
1:B:56:ASN:ND2	1:B:66:VAL:H	2.08	0.50
1:D:143:GLN:HG2	1:D:148:SER:O	2.11	0.50
1:A:14:SER:HB2	1:A:330:ASN:HB2	1.94	0.49
1:C:164:HIS:CD2	1:C:166:GLU:H	2.22	0.49
1:F:227:GLU:HG3	4:F:841:HOH:O	2.12	0.49
1:F:391:GLU:N	1:F:391:GLU:OE1	2.45	0.49
1:D:45:GLN:H	1:D:303:GLN:NE2	2.08	0.49
1:C:14:SER:HB2	1:C:330:ASN:HB2	1.93	0.48
1:C:131:SER:OG	1:C:134:GLU:HB2	2.13	0.48
1:B:187:GLU:HA	1:B:190:MET:HE2	1.95	0.48
1:F:14:SER:HB2	1:F:330:ASN:HB2	1.96	0.48
1:D:213:HIS:HE1	1:E:232:ASP:OD2	1.97	0.48
1:E:164:HIS:CD2	1:E:166:GLU:H	2.14	0.47
1:E:14:SER:HB2	1:E:330:ASN:HB2	1.95	0.47
1:D:190:MET:HE2	1:D:220:PHE:HZ	1.79	0.47
1:E:45:GLN:H	1:E:303:GLN:NE2	2.08	0.47
1:D:327:ASP:O	1:D:366:PHE:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:HIS:CD2	1:F:166:GLU:H	2.25	0.46
1:D:190:MET:HE1	1:D:220:PHE:HZ	1.80	0.46
1:D:256:THR:HG21	1:D:262:GLY:HA2	1.97	0.46
1:B:91:GLU:HG2	1:B:366:PHE:HB2	1.97	0.46
1:F:256:THR:HG21	1:F:262:GLY:HA2	1.98	0.46
1:E:256:THR:HG21	1:E:262:GLY:HA2	1.98	0.46
1:A:164:HIS:HE1	1:A:201:GLY:O	1.99	0.46
1:D:208:ARG:HB3	4:D:770:HOH:O	2.15	0.45
1:D:28:ASP:OD1	4:D:1514:HOH:O	2.20	0.45
1:B:193:ARG:NH1	1:B:216:ALA:HB2	2.32	0.45
1:D:273:ASP:OD2	1:E:165:GLU:OE2	2.34	0.45
1:C:256:THR:HG21	1:C:262:GLY:HA2	1.98	0.45
1:B:45:GLN:NE2	1:B:303:GLN:NE2	2.64	0.45
1:C:375:GLU:CA	1:C:381:MET:HE1	2.44	0.45
1:D:232:ASP:OD1	1:E:213:HIS:HE1	2.00	0.45
1:E:56:ASN:ND2	1:E:66:VAL:H	2.09	0.44
1:B:327:ASP:O	1:B:366:PHE:HE2	2.01	0.44
1:B:32:ASP:OD1	1:B:58:ARG:NH2	2.48	0.44
1:C:117:GLU:HG2	1:C:122:ARG:O	2.18	0.44
1:B:144:MET:O	1:B:167:VAL:HG21	2.18	0.43
1:E:93:MET:HB3	1:E:223:THR:HB	2.01	0.43
1:A:56:ASN:HB3	1:A:73:TYR:CE2	2.53	0.43
1:A:21:PRO:HD3	1:A:343:TYR:CZ	2.54	0.43
1:F:56:ASN:ND2	1:F:66:VAL:H	2.13	0.43
1:C:86:MET:HE2	1:C:86:MET:H	1.85	0.42
1:B:44:LEU:HD23	1:B:63:ILE:HD11	2.01	0.42
1:E:164:HIS:CD2	1:E:166:GLU:HB2	2.55	0.42
1:E:187:GLU:HA	1:E:190:MET:HE2	2.02	0.42
1:E:259:ASN:HD21	1:E:284:ASP:H	1.66	0.42
1:A:259:ASN:HD21	1:A:284:ASP:H	1.67	0.42
1:D:259:ASN:HD21	1:D:284:ASP:H	1.68	0.42
1:D:41:MET:HG3	1:D:44:LEU:HD13	2.02	0.42
1:C:259:ASN:HD21	1:C:284:ASP:H	1.68	0.41
1:A:101:PHE:HE2	1:A:217:LEU:HD12	1.84	0.41
1:B:215:TYR:CD2	1:B:215:TYR:N	2.88	0.41
1:D:193:ARG:HD3	1:D:214:ASP:OD2	2.20	0.41
1:F:101:PHE:CE2	1:F:217:LEU:HD12	2.55	0.41
1:F:327:ASP:O	1:F:366:PHE:HE2	2.03	0.41
1:B:259:ASN:HD21	1:B:284:ASP:H	1.68	0.41
1:E:135:ILE:HD13	1:E:152:TYR:HB3	2.01	0.41
1:E:113:LEU:HD22	1:E:124:ILE:HG21	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:GLU:HB2	1:F:203:PRO:HD2	2.01	0.41
1:C:15:VAL:HG12	1:C:34:ILE:HD11	2.01	0.41
1:D:56:ASN:ND2	1:D:66:VAL:H	2.18	0.41
1:D:116:LEU:HB3	1:D:124:ILE:HD11	2.02	0.41
1:A:89:HIS:CG	1:A:244:ILE:HG21	2.56	0.41
1:B:85:GLU:O	1:B:89:HIS:HD2	2.03	0.41
1:E:141:GLN:HA	1:E:144:MET:HE2	2.03	0.41
1:C:327:ASP:O	1:C:366:PHE:CE2	2.70	0.40
1:B:82:GLY:HA3	1:B:100:PRO:HB3	2.02	0.40
1:E:193:ARG:HD3	1:E:214:ASP:OD2	2.20	0.40
1:F:267:VAL:HG13	1:F:315:LYS:HE2	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)
4:B:1597:HOH:O	4:C:406:HOH:O[2_555]	2.12	0.08

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	390/399 (98%)	374 (96%)	16 (4%)	0	100	100
1	B	388/399 (97%)	374 (96%)	14 (4%)	0	100	100
1	C	388/399 (97%)	376 (97%)	12 (3%)	0	100	100
1	D	389/399 (98%)	376 (97%)	13 (3%)	0	100	100
1	E	390/399 (98%)	376 (96%)	14 (4%)	0	100	100
1	F	389/399 (98%)	376 (97%)	13 (3%)	0	100	100
All	All	2334/2394 (98%)	2252 (96%)	82 (4%)	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	334/339 (98%)	327 (98%)	7 (2%)	53	46
1	B	332/339 (98%)	326 (98%)	6 (2%)	59	53
1	C	332/339 (98%)	321 (97%)	11 (3%)	38	26
1	D	333/339 (98%)	327 (98%)	6 (2%)	59	53
1	E	334/339 (98%)	321 (96%)	13 (4%)	32	19
1	F	333/339 (98%)	327 (98%)	6 (2%)	59	53
All	All	1998/2034 (98%)	1949 (98%)	49 (2%)	47	38

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	189	TYR
1	A	281	ASN
1	A	298	TYR
1	A	355	GLU
1	A	360	LEU
1	A	391	GLU
1	B	61	LYS
1	B	189	TYR
1	B	279	PHE
1	B	281	ASN
1	B	298	TYR
1	B	355	GLU
1	C	67	GLU
1	C	86	MET
1	C	110	LYS
1	C	123	LYS
1	C	170	LEU
1	C	178	LYS

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Mol	Chain	Res	Type
1	C	189	TYR
1	C	281	ASN
1	C	298	TYR
1	C	355	GLU
1	C	360	LEU
1	D	189	TYR
1	D	279	PHE
1	D	281	ASN
1	D	298	TYR
1	D	360	LEU
1	D	391	GLU
1	E	61	LYS
1	E	112	LEU
1	E	178	LYS
1	E	181	ARG
1	E	189	TYR
1	E	281	ASN
1	E	298	TYR
1	E	316	LEU
1	E	358	GLN
1	E	360	LEU
1	E	364	GLN
1	E	390	ASN
1	E	391	GLU
1	F	189	TYR
1	F	212	ARG
1	F	279	PHE
1	F	281	ASN
1	F	298	TYR
1	F	360	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) 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	164	HIS
1	A	211	ASN
1	A	259	ASN
1	A	281	ASN

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Mol	Chain	Res	Type
1	A	303	GLN
1	A	376	ASN
1	A	390	ASN
1	B	45	GLN
1	B	56	ASN
1	B	77	GLN
1	B	89	HIS
1	B	160	GLN
1	B	164	HIS
1	B	205	ASN
1	B	211	ASN
1	B	259	ASN
1	B	281	ASN
1	B	303	GLN
1	B	376	ASN
1	C	48	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	259	ASN
1	C	281	ASN
1	C	358	GLN
1	C	376	ASN
1	D	48	ASN
1	D	56	ASN
1	D	77	GLN
1	D	89	HIS
1	D	102	GLN
1	D	164	HIS
1	D	205	ASN
1	D	213	HIS
1	D	259	ASN
1	D	281	ASN
1	D	303	GLN
1	D	376	ASN
1	E	40	HIS
1	E	56	ASN
1	E	89	HIS

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Mol	Chain	Res	Type
1	E	102	GLN
1	E	143	GLN
1	E	160	GLN
1	E	164	HIS
1	E	213	HIS
1	E	259	ASN
1	E	281	ASN
1	E	296	GLN
1	E	303	GLN
1	E	376	ASN
1	F	56	ASN
1	F	89	HIS
1	F	164	HIS
1	F	211	ASN
1	F	259	ASN
1	F	281	ASN
1	F	303	GLN
1	F	376	ASN
1	F	390	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 16 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	F	398	-	5,5,5	0.38	0	5,5,5	0.38	0
3	GOL	C	397	-	5,5,5	0.41	0	5,5,5	0.30	0
3	GOL	D	397	-	5,5,5	0.43	0	5,5,5	0.40	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	F	398	-	-	0/4/4/4	-
3	GOL	C	397	-	-	0/4/4/4	-
3	GOL	D	397	-	-	0/4/4/4	-

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 [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	391/399 (97%)	-0.04	6 (1%) 73 81	10, 19, 33, 49	2 (0%)
1	B	390/399 (97%)	0.13	11 (2%) 53 62	13, 25, 44, 60	1 (0%)
1	C	390/399 (97%)	0.03	5 (1%) 77 83	10, 20, 38, 46	2 (0%)
1	D	390/399 (97%)	-0.01	2 (0%) 91 94	10, 18, 32, 40	2 (0%)
1	E	391/399 (97%)	0.13	10 (2%) 56 65	13, 25, 45, 60	2 (0%)
1	F	391/399 (97%)	0.03	9 (2%) 60 69	11, 20, 39, 66	2 (0%)
All	All	2343/2394 (97%)	0.05	43 (1%) 68 76	10, 21, 40, 66	11 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	ASN	3.9
1	A	2	ASN	3.9
1	B	186	ASP	3.7
1	B	355	GLU	3.7
1	E	187	GLU	3.4
1	F	2	ASN	3.3
1	F	171	ASP	3.2
1	B	187	GLU	3.1
1	E	65	LYS	2.9
1	E	68	LYS	2.9
1	E	355	GLU	2.8
1	B	110	LYS	2.8
1	D	110	LYS	2.7
1	F	202	GLU	2.7
1	D	355	GLU	2.6
1	E	42	ASN	2.6
1	B	65	LYS	2.5
1	C	355	GLU	2.5
1	F	150	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	162	ALA	2.3
1	C	42	ASN	2.3
1	C	161	ILE	2.3
1	B	166	GLU	2.3
1	E	186	ASP	2.3
1	A	354	LYS	2.3
1	E	188	LYS	2.3
1	E	202	GLU	2.3
1	C	39	GLU	2.2
1	B	24	GLU	2.2
1	A	150	ILE	2.2
1	B	257	LYS	2.2
1	B	67	GLU	2.2
1	A	171	ASP	2.2
1	F	137	ASP	2.2
1	F	390	ASN	2.1
1	B	188	LYS	2.1
1	F	381	MET	2.1
1	C	390	ASN	2.0
1	A	7	ILE	2.0
1	A	149	LEU	2.0
1	B	390	ASN	2.0
1	F	210	PRO	2.0
1	E	390	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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. 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(\AA^2)	Q<0.9
3	GOL	F	398	6/6	0.85	0.27	23,24,24,25	6
3	GOL	D	397	6/6	0.90	0.24	15,17,18,20	6
3	GOL	C	397	6/6	0.92	0.21	15,18,18,20	6
2	MN	F	397	1/1	0.95	0.14	39,39,39,39	0
2	MN	A	397	1/1	0.99	0.06	29,29,29,29	0
2	MN	E	395	1/1	0.99	0.07	17,17,17,17	0
2	MN	E	397	1/1	0.99	0.03	26,26,26,26	0
2	MN	B	397	1/1	0.99	0.06	32,32,32,32	0
2	MN	E	396	1/1	1.00	0.10	15,15,15,15	0
2	MN	A	395	1/1	1.00	0.10	13,13,13,13	0
2	MN	D	395	1/1	1.00	0.08	14,14,14,14	0
2	MN	B	395	1/1	1.00	0.08	16,16,16,16	0
2	MN	C	396	1/1	1.00	0.09	13,13,13,13	0
2	MN	B	396	1/1	1.00	0.10	15,15,15,15	0
2	MN	D	396	1/1	1.00	0.09	11,11,11,11	0
2	MN	F	396	1/1	1.00	0.10	11,11,11,11	0
2	MN	A	396	1/1	1.00	0.10	10,10,10,10	0
2	MN	C	395	1/1	1.00	0.10	16,16,16,16	0
2	MN	F	395	1/1	1.00	0.08	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.