Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 12:03 AM EST

PDB ID	:	3UN5
Title	:	Bacillus cereus phosphopentomutase T85E variant
Authors	:	Iverson, T.M.; Birmingham, W.R.; Panosian, T.D.; Nannemann, D.P.; Bachmann, B.O.
Deposited on	:	2011-11-15
Resolution	:	1.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

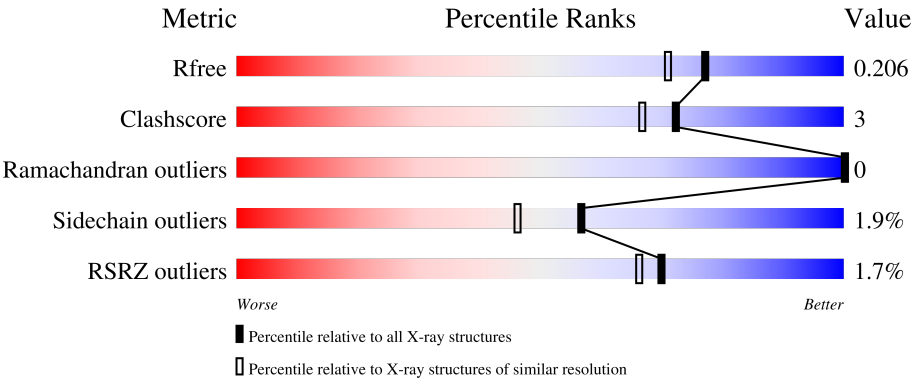
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	91% 7%
1	B	399	4% 87% 11%
1	C	399	90% 7%
1	D	399	88% 9%
1	E	399	3% 85% 12%

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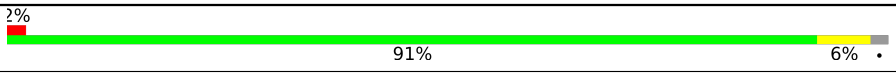
Mol	Chain	Length	Quality of chain
1	F	399	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20431 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	0	2	0
			3082	1949	507	608	18			
1	B	390	Total	C	N	O	S	4	2	0
			3077	1947	508	604	18			
1	C	390	Total	C	N	O	S	6	6	0
			3117	1969	518	612	18			
1	D	390	Total	C	N	O	S	8	4	0
			3097	1958	513	608	18			
1	E	390	Total	C	N	O	S	4	2	0
			3075	1946	505	606	18			
1	F	390	Total	C	N	O	S	3	2	0
			3077	1947	508	604	18			

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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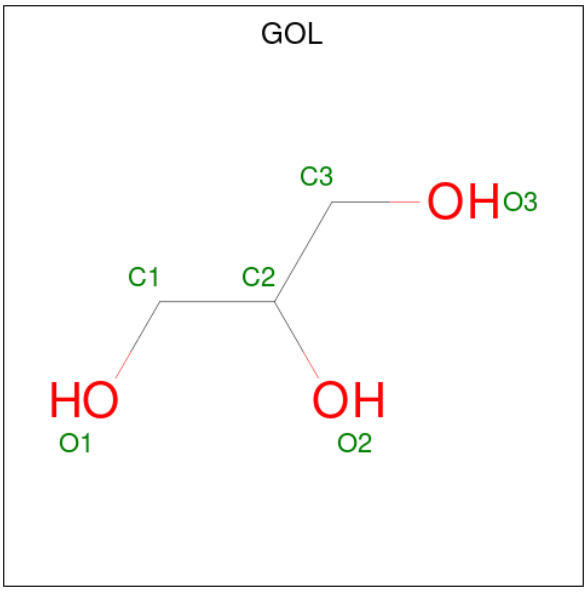
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	expression tag	UNP Q818Z9
C	0	ALA	-	expression tag	UNP Q818Z9
C	1	SER	-	expression tag	UNP Q818Z9
C	85	GLU	THR	engineered mutation	UNP Q818Z9
D	-4	GLY	-	expression tag	UNP Q818Z9
D	-3	SER	-	expression tag	UNP Q818Z9
D	-2	HIS	-	expression tag	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	A	5	Total Mn 5 5	0	0
2	B	3	Total Mn 3 3	0	0
2	C	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	E	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: $C_3H_8O_3$).



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

- Molecule 4 is water.

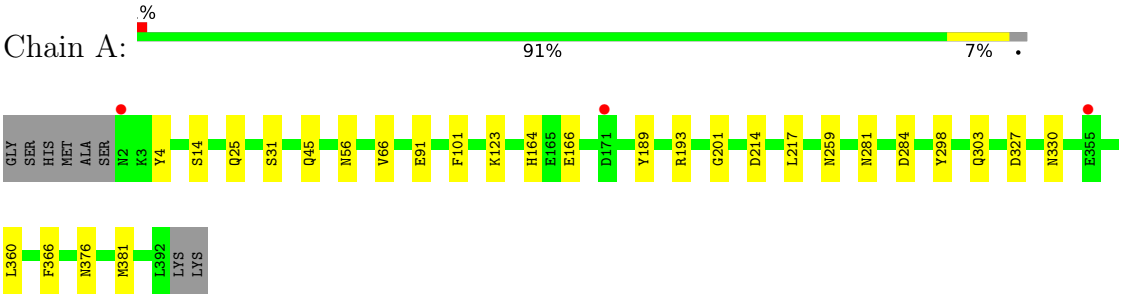
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	348	Total O 348 348	0	0
4	B	239	Total O 239 239	0	0
4	C	336	Total O 336 336	0	0
4	D	356	Total O 356 356	0	0
4	E	273	Total O 273 273	0	0
4	F	312	Total O 312 312	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

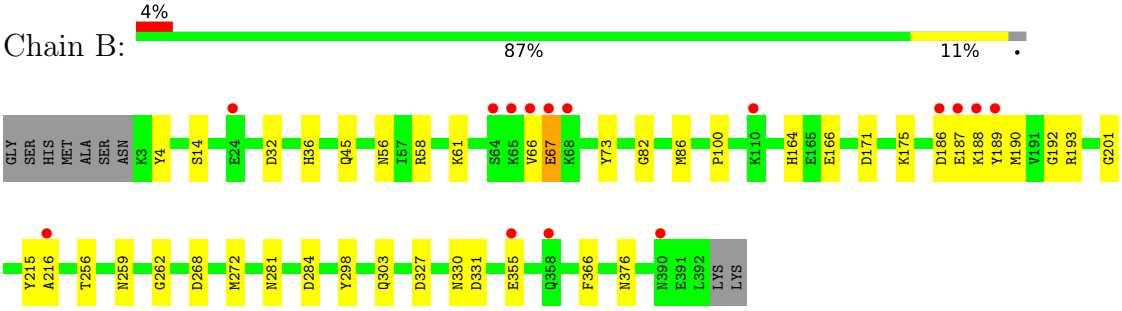
• Molecule 1: Phosphopentomutase

Chain A:



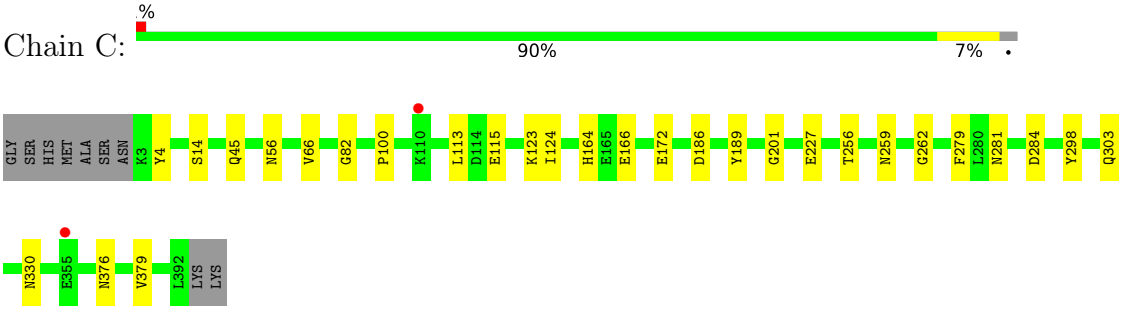
• Molecule 1: Phosphopentomutase

Chain B:



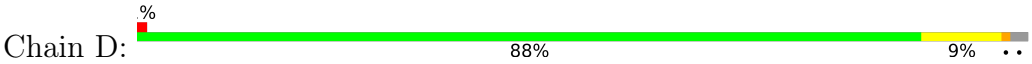
• Molecule 1: Phosphopentomutase

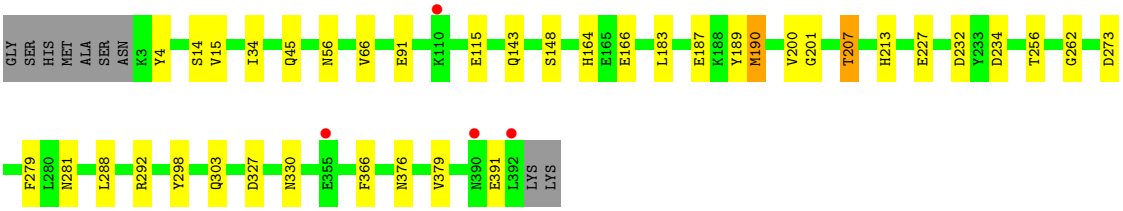
Chain C:



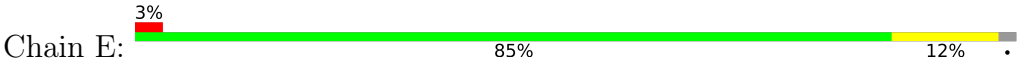
• Molecule 1: Phosphopentomutase

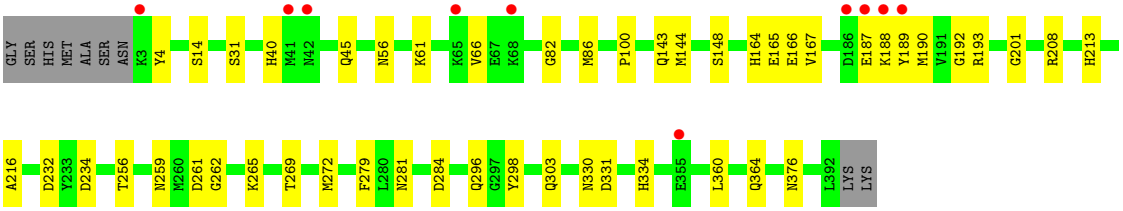
Chain D:



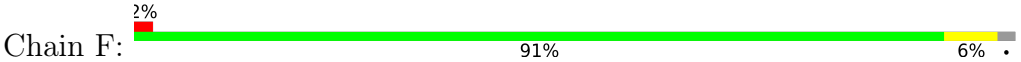


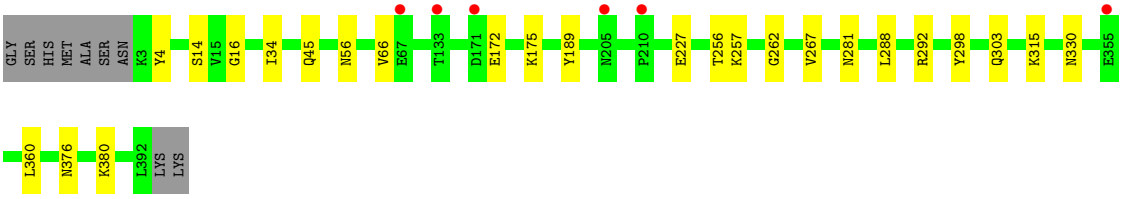
• Molecule 1: Phosphopentomutase





• Molecule 1: Phosphopentomutase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.45Å 76.83Å 182.84Å 90.00° 105.99° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 19.86 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.80) 97.2 (19.86-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.167 , 0.193 0.179 , 0.206	Depositor DCC
R_{free} test set	12792 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20431	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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 35.87 % 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 5.4567e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MN, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.40	0/3143	0.57	1/4245 (0.0%)
1	B	0.39	1/3138 (0.0%)	0.54	1/4236 (0.0%)
1	C	0.40	0/3178	0.54	1/4288 (0.0%)
1	D	0.42	0/3158	0.55	0/4262
1	E	0.39	0/3136	0.56	1/4234 (0.0%)
1	F	0.41	0/3138	0.56	0/4237
All	All	0.40	1/18891 (0.0%)	0.55	4/25502 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	GLU	CB-CG	-6.04	1.40	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	67	GLU	CA-CB-CG	9.50	134.29	113.40
1	E	31	SER	CB-CA-C	-6.18	98.36	110.10
1	A	31	SER	CB-CA-C	-5.66	99.35	110.10
1	C	186	ASP	N-CA-C	-5.08	97.28	111.00

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	3082	0	3019	19	0
1	B	3077	0	3021	26	0
1	C	3117	0	3055	15	0
1	D	3097	0	3038	28	0
1	E	3075	0	3014	30	0
1	F	3077	0	3022	12	0
2	A	5	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	A	6	0	8	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	348	0	0	3	0
4	B	239	0	0	2	0
4	C	336	0	0	1	0
4	D	356	0	0	0	0
4	E	273	0	0	2	0
4	F	312	0	0	0	0
All	All	20431	0	18201	124	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 (124) 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:186:ASP:OD1	1:B:188:LYS:HB2	1.50	1.10
1:A:4:TYR:H	1:A:376:ASN:HD21	1.15	0.95
1:F:4:TYR:H	1:F:376:ASN:HD21	1.16	0.94
1:B:4:TYR:H	1:B:376:ASN:HD21	1.13	0.89
1:D:4:TYR:H	1:D:376:ASN:HD21	1.21	0.88
1:B:86:MET:HE2	4:B:1325:HOH:O	1.74	0.87
1:E:4:TYR:H	1:E:376:ASN:HD21	1.17	0.87
1:A:56:ASN:HD21	1:A:66:VAL:H	1.22	0.86
1:C:4:TYR:H	1:C:376:ASN:HD21	1.19	0.84
1:B:86:MET:HE1	1:B:192:GLY:HA3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:MET:HE1	1:E:192:GLY:HA3	1.64	0.80
1:E:164:HIS:HD2	1:E:166:GLU:H	1.29	0.79
1:C:164:HIS:HD2	1:C:166:GLU:H	1.32	0.77
1:F:45:GLN:H	1:F:303:GLN:HE21	1.33	0.75
1:A:164:HIS:HD2	1:A:166:GLU:H	1.35	0.74
1:F:227:GLU:OE2	1:F:380:LYS:O	2.05	0.74
1:F:56:ASN:HD21	1:F:66:VAL:H	1.33	0.73
1:B:187:GLU:HA	1:B:190:MET:HE2	1.71	0.72
1:D:45:GLN:H	1:D:303:GLN:HE21	1.35	0.71
1:E:45:GLN:H	1:E:303:GLN:HE21	1.39	0.70
1:B:164:HIS:HD2	1:B:166:GLU:H	1.40	0.70
1:D:56:ASN:HD21	1:D:66:VAL:H	1.40	0.69
1:C:56:ASN:HD21	1:C:66:VAL:H	1.39	0.69
1:B:56:ASN:HD21	1:B:66:VAL:H	1.40	0.69
1:C:227[B]:GLU:HG3	1:C:379:VAL:HB	1.74	0.68
1:B:36:HIS:HD2	1:B:331:ASP:OD2	1.76	0.68
1:D:213:HIS:HD2	1:E:234:ASP:OD1	1.77	0.68
1:A:45:GLN:H	1:A:303:GLN:HE21	1.38	0.68
1:D:227[B]:GLU:HG3	1:D:379:VAL:HB	1.76	0.66
1:D:164:HIS:HD2	1:D:166:GLU:H	1.43	0.66
1:E:86:MET:HE2	4:E:898:HOH:O	1.96	0.66
1:E:86:MET:CE	4:E:898:HOH:O	2.47	0.63
1:D:234:ASP:OD1	1:E:213:HIS:HD2	1.82	0.63
1:D:164:HIS:HE1	1:D:201:GLY:O	1.83	0.61
1:F:172:GLU:HA	1:F:175:LYS:HE3	1.82	0.61
1:E:143:GLN:NE2	1:E:164:HIS:H	1.98	0.60
1:D:115:GLU:HG2	1:D:183:LEU:HD22	1.84	0.60
1:A:56:ASN:ND2	1:A:66:VAL:H	1.98	0.59
1:E:56:ASN:HD21	1:E:66:VAL:H	1.50	0.58
1:B:171:ASP:O	1:B:175:LYS:HG2	2.02	0.58
1:A:164:HIS:CD2	1:A:166:GLU:H	2.20	0.57
1:D:14:SER:HB2	1:D:330:ASN:HB2	1.85	0.57
1:D:288:LEU:O	1:D:292[A]:ARG:HD2	2.05	0.56
1:E:40:HIS:HE1	1:E:296:GLN:HE21	1.53	0.56
1:E:164:HIS:HE1	1:E:201:GLY:O	1.89	0.56
1:C:164:HIS:HE1	1:C:201:GLY:O	1.91	0.54
1:B:14:SER:HB2	1:B:330:ASN:HB2	1.89	0.53
1:B:164:HIS:HE1	1:B:201:GLY:O	1.91	0.53
1:E:164:HIS:CD2	1:E:166:GLU:H	2.18	0.53
1:D:187:GLU:HA	1:D:190:MET:HG3	1.91	0.52
1:D:273:ASP:OD2	1:E:165:GLU:OE2	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227[B]:GLU:CG	1:C:379:VAL:HB	2.39	0.51
1:D:200:VAL:HG23	1:D:207:THR:HG23	1.92	0.51
1:D:213:HIS:HE1	1:E:232:ASP:OD2	1.93	0.51
1:A:14:SER:HB2	1:A:330:ASN:HB2	1.92	0.51
1:C:164:HIS:CD2	1:C:166:GLU:H	2.20	0.51
1:B:193:ARG:NH1	1:B:216:ALA:HB2	2.26	0.50
1:D:227[B]:GLU:CG	1:D:379:VAL:HB	2.41	0.50
1:D:232:ASP:OD1	1:E:213:HIS:HE1	1.95	0.50
1:F:14:SER:HB2	1:F:330:ASN:HB2	1.94	0.49
1:A:193:ARG:HD3	1:A:214:ASP:OD2	2.13	0.49
1:B:256:THR:HG21	1:B:262:GLY:HA2	1.94	0.49
1:F:56:ASN:ND2	1:F:66:VAL:H	2.06	0.49
1:C:14:SER:HB2	1:C:330:ASN:HB2	1.94	0.48
1:A:327:ASP:O	1:A:366:PHE:HE2	1.96	0.48
1:E:14:SER:HB2	1:E:330:ASN:HB2	1.94	0.48
1:B:45:GLN:H	1:B:303:GLN:HE21	1.59	0.48
1:E:269:THR:HA	1:E:272[A]:MET:HE2	1.94	0.48
1:A:164:HIS:HE1	1:A:201:GLY:O	1.96	0.48
1:D:56:ASN:ND2	1:D:66:VAL:H	2.08	0.47
1:E:82:GLY:HA3	1:E:100:PRO:HB3	1.97	0.47
1:A:25:GLN:HG3	4:A:1004:HOH:O	2.14	0.47
1:C:56:ASN:ND2	1:C:66:VAL:H	2.08	0.46
1:C:172[B]:GLU:HG3	4:C:1955:HOH:O	2.15	0.46
1:B:56:ASN:ND2	1:B:66:VAL:H	2.11	0.46
1:C:256:THR:HG21	1:C:262:GLY:HA2	1.97	0.46
1:E:187:GLU:HA	1:E:190:MET:HE2	1.98	0.46
1:A:123:LYS:HE2	4:A:1531:HOH:O	2.15	0.46
1:A:45:GLN:H	1:A:303:GLN:NE2	2.11	0.45
1:B:86:MET:CE	4:B:1325:HOH:O	2.45	0.45
1:B:186:ASP:OD1	1:B:188:LYS:CB	2.42	0.45
1:F:288:LEU:O	1:F:292:ARG:HB2	2.17	0.45
1:A:259:ASN:HD21	1:A:284:ASP:H	1.65	0.45
1:D:15:VAL:HG12	1:D:34:ILE:HD11	1.98	0.44
1:E:193:ARG:NH1	1:E:216:ALA:HB2	2.33	0.44
1:D:143:GLN:HG2	1:D:148:SER:O	2.17	0.44
1:D:45:GLN:H	1:D:303:GLN:NE2	2.08	0.44
1:D:327:ASP:O	1:D:366:PHE:HE2	2.01	0.44
1:F:16:GLY:O	1:F:34:ILE:HG13	2.18	0.44
1:D:91:GLU:HG2	1:D:366:PHE:HB2	2.00	0.44
1:C:259:ASN:HD21	1:C:284:ASP:H	1.66	0.43
1:B:187:GLU:HA	1:B:190:MET:CE	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:LEU:HD22	1:C:124:ILE:HG21	2.00	0.43
1:E:14:SER:HB2	1:E:330:ASN:CB	2.49	0.43
1:E:331:ASP:HB3	1:E:334:HIS:HB2	1.99	0.43
1:F:267:VAL:HG13	1:F:315:LYS:HE2	1.99	0.43
1:D:256:THR:HG21	1:D:262:GLY:HA2	2.00	0.43
1:F:256:THR:HG21	1:F:262:GLY:HA2	2.02	0.42
1:E:256:THR:HG21	1:E:262:GLY:HA2	2.02	0.42
1:D:164:HIS:CD2	1:D:166:GLU:H	2.30	0.42
1:A:381[A]:MET:HE2	4:A:1913:HOH:O	2.19	0.42
1:E:143:GLN:HE22	1:E:164:HIS:H	1.63	0.42
1:E:143:GLN:HG2	1:E:148:SER:O	2.20	0.42
1:C:45:GLN:O	1:C:303:GLN:HG2	2.19	0.42
1:A:91:GLU:HG2	1:A:366:PHE:HB2	2.02	0.41
1:B:164:HIS:CD2	1:B:166:GLU:H	2.28	0.41
1:B:259:ASN:HD21	1:B:284:ASP:H	1.68	0.41
1:A:4:TYR:N	1:A:376:ASN:HD21	1.98	0.41
1:B:215:TYR:CD2	1:B:215:TYR:N	2.88	0.41
1:E:261:ASP:O	1:E:265:LYS:HG2	2.20	0.41
1:B:268:ASP:O	1:B:272[B]:MET:HG3	2.21	0.41
1:B:327:ASP:O	1:B:366:PHE:HE2	2.03	0.41
1:C:82:GLY:HA3	1:C:100:PRO:HB3	2.03	0.41
1:D:45:GLN:O	1:D:303:GLN:HG2	2.20	0.41
1:D:213:HIS:CD2	1:E:234:ASP:OD1	2.65	0.41
1:E:259:ASN:HD21	1:E:284:ASP:H	1.68	0.40
1:A:101:PHE:HE2	1:A:217:LEU:HD12	1.85	0.40
1:E:144:MET:HB2	1:E:167:VAL:HG21	2.03	0.40
1:B:32:ASP:OD1	1:B:58:ARG:NH2	2.53	0.40
1:B:82:GLY:HA3	1:B:100:PRO:HB3	2.02	0.40
1:B:56:ASN:HB3	1:B:73:TYR:CE2	2.57	0.40
1:D:14:SER:HB2	1:D:330:ASN:CB	2.51	0.40
1:F:4:TYR:N	1:F:376:ASN:HD21	1.99	0.40
1:A:14:SER:HB2	1:A:330:ASN:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/399 (98%)	378 (97%)	13 (3%)	0	100	100
1	B	390/399 (98%)	377 (97%)	13 (3%)	0	100	100
1	C	394/399 (99%)	383 (97%)	11 (3%)	0	100	100
1	D	392/399 (98%)	380 (97%)	12 (3%)	0	100	100
1	E	390/399 (98%)	380 (97%)	10 (3%)	0	100	100
1	F	390/399 (98%)	378 (97%)	12 (3%)	0	100	100
All	All	2347/2394 (98%)	2276 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/339 (99%)	331 (99%)	4 (1%)	71	65
1	B	334/339 (98%)	328 (98%)	6 (2%)	59	48
1	C	338/339 (100%)	332 (98%)	6 (2%)	59	48
1	D	336/339 (99%)	329 (98%)	7 (2%)	53	42
1	E	334/339 (98%)	325 (97%)	9 (3%)	44	31
1	F	334/339 (98%)	329 (98%)	5 (2%)	65	56
All	All	2011/2034 (99%)	1974 (98%)	37 (2%)	57	48

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	TYR
1	A	281	ASN
1	A	298	TYR

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Mol	Chain	Res	Type
1	A	360	LEU
1	B	61	LYS
1	B	67	GLU
1	B	189	TYR
1	B	281	ASN
1	B	298	TYR
1	B	355	GLU
1	C	115	GLU
1	C	123	LYS
1	C	189	TYR
1	C	279	PHE
1	C	281	ASN
1	C	298	TYR
1	D	189	TYR
1	D	190	MET
1	D	207	THR
1	D	279	PHE
1	D	281	ASN
1	D	298	TYR
1	D	391	GLU
1	E	61	LYS
1	E	188	LYS
1	E	189	TYR
1	E	208	ARG
1	E	279	PHE
1	E	281	ASN
1	E	298	TYR
1	E	360	LEU
1	E	364	GLN
1	F	189	TYR
1	F	257	LYS
1	F	281	ASN
1	F	298	TYR
1	F	360	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) 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

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Mol	Chain	Res	Type
1	A	164	HIS
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	36	HIS
1	B	56	ASN
1	B	77	GLN
1	B	89	HIS
1	B	164	HIS
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	102	GLN
1	C	164	HIS
1	C	205	ASN
1	C	211	ASN
1	C	259	ASN
1	C	281	ASN
1	C	376	ASN
1	D	48	ASN
1	D	56	ASN
1	D	77	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	102	GLN

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Mol	Chain	Res	Type
1	E	143	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	364	GLN
1	E	376	ASN
1	F	48	ASN
1	F	56	ASN
1	F	77	GLN
1	F	89	HIS
1	F	102	GLN
1	F	259	ASN
1	F	281	ASN
1	F	303	GLN
1	F	376	ASN
1	F	390	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 18 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	$\#\|Z\| > 2$
3	GOL	C	397	-	5,5,5	0.38	0	5,5,5	0.33	0
3	GOL	F	398	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	A	400	-	5,5,5	0.40	0	5,5,5	0.28	0
3	GOL	D	397	-	5,5,5	0.35	0	5,5,5	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	397	-	-	0/4/4/4	-
3	GOL	F	398	-	-	0/4/4/4	-
3	GOL	A	400	-	-	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, 95^{th} 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%)	-0.36	3 (0%) 86 84	9, 17, 29, 40	0
1	B	390/399 (97%)	-0.10	15 (3%) 40 35	14, 24, 40, 52	1 (0%)
1	C	390/399 (97%)	-0.29	2 (0%) 91 89	11, 19, 33, 39	2 (0%)
1	D	390/399 (97%)	-0.33	4 (1%) 82 80	10, 16, 28, 33	2 (0%)
1	E	390/399 (97%)	-0.13	10 (2%) 56 51	12, 23, 39, 48	2 (0%)
1	F	390/399 (97%)	-0.26	6 (1%) 73 70	11, 18, 35, 52	1 (0%)
All	All	2341/2394 (97%)	-0.24	40 (1%) 70 66	9, 20, 36, 52	8 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	ASP	4.6
1	B	355	GLU	4.5
1	F	210	PRO	3.7
1	E	355	GLU	3.4
1	E	68	LYS	3.3
1	E	188	LYS	2.9
1	A	355	GLU	2.8
1	E	186	ASP	2.8
1	F	171	ASP	2.8
1	B	66	VAL	2.8
1	A	2	ASN	2.7
1	B	187	GLU	2.7
1	B	24	GLU	2.7
1	D	355	GLU	2.6
1	B	358	GLN	2.6
1	F	355	GLU	2.6
1	B	110	LYS	2.5
1	B	65	LYS	2.5
1	C	355	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	42	ASN	2.5
1	B	68	LYS	2.4
1	A	171	ASP	2.4
1	E	187	GLU	2.4
1	F	205	ASN	2.4
1	B	64	SER	2.3
1	D	110	LYS	2.3
1	E	65	LYS	2.3
1	B	216	ALA	2.3
1	E	3	LYS	2.2
1	B	390	ASN	2.2
1	B	188	LYS	2.2
1	F	133	THR	2.2
1	B	189	TYR	2.2
1	B	67	GLU	2.1
1	E	41	MET	2.1
1	E	189	TYR	2.1
1	C	110	LYS	2.0
1	D	392	LEU	2.0
1	F	67	GLU	2.0
1	D	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 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, 95^{th} 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
2	MN	A	399	1/1	0.90	0.15	48,48,48,48	0
2	MN	A	398	1/1	0.93	0.07	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	400	6/6	0.94	0.07	33,34,35,35	0
3	GOL	F	398	6/6	0.94	0.15	37,37,37,37	0
3	GOL	D	397	6/6	0.95	0.09	28,28,29,29	0
2	MN	F	397	1/1	0.96	0.10	36,36,36,36	0
3	GOL	C	397	6/6	0.97	0.10	28,29,30,30	0
2	MN	B	397	1/1	0.98	0.04	34,34,34,34	0
2	MN	E	397	1/1	0.99	0.03	27,27,27,27	0
2	MN	E	395	1/1	0.99	0.07	17,17,17,17	0
2	MN	D	395	1/1	1.00	0.06	13,13,13,13	0
2	MN	D	396	1/1	1.00	0.07	11,11,11,11	0
2	MN	A	395	1/1	1.00	0.08	12,12,12,12	0
2	MN	E	396	1/1	1.00	0.09	15,15,15,15	0
2	MN	A	396	1/1	1.00	0.10	10,10,10,10	0
2	MN	F	395	1/1	1.00	0.06	13,13,13,13	0
2	MN	F	396	1/1	1.00	0.10	11,11,11,11	0
2	MN	B	395	1/1	1.00	0.06	16,16,16,16	0
2	MN	B	396	1/1	1.00	0.08	16,16,16,16	0
2	MN	A	397	1/1	1.00	0.07	14,14,14,14	1
2	MN	C	395	1/1	1.00	0.07	15,15,15,15	0
2	MN	C	396	1/1	1.00	0.09	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.