Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 03:28 AM EDT

PDB ID	:	2QYH
Title	:	Crystal structure of the hypothetical protein (gk1056) from geobacillus kaustophilus HTA426
Authors	:	Jeyakanthan, J.; Kanaujia, S.P.; Sekar, K.; Ebihara, A.; Shinkai, A.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-08-15
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

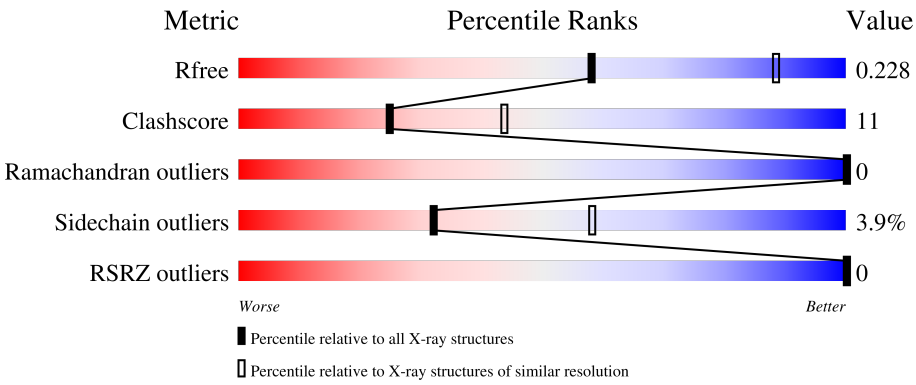
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	258	73% 24% • •
1	B	258	79% 19% •
1	C	258	78% 20% • •
1	D	258	77% 21% •

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
2	GOL	B	259	-	-	X	-
2	GOL	D	259	-	-	X	-

2 Entry composition (i)

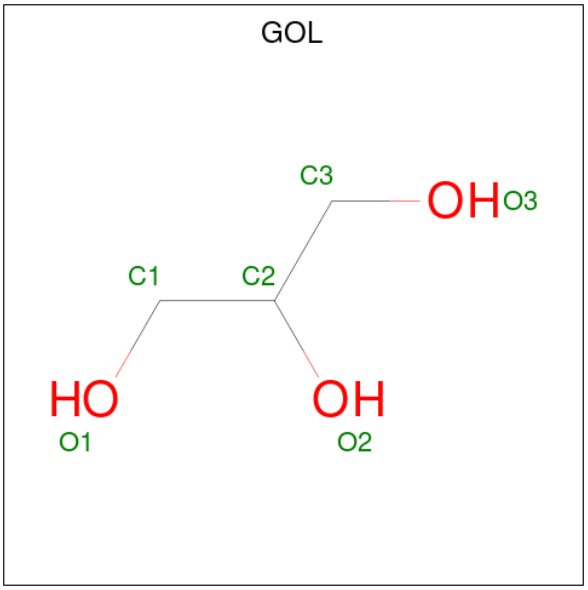
There are 3 unique types of molecules in this entry. The entry contains 8855 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hypothetical conserved protein, GK1056.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	256	2056	1321	355	371	1	8	0	0	0
1	B	258	2075	1332	360	373	1	9	0	0	0
1	C	256	2056	1321	355	371	1	8	0	0	0
1	D	257	2064	1326	356	372	1	9	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 3 is water.

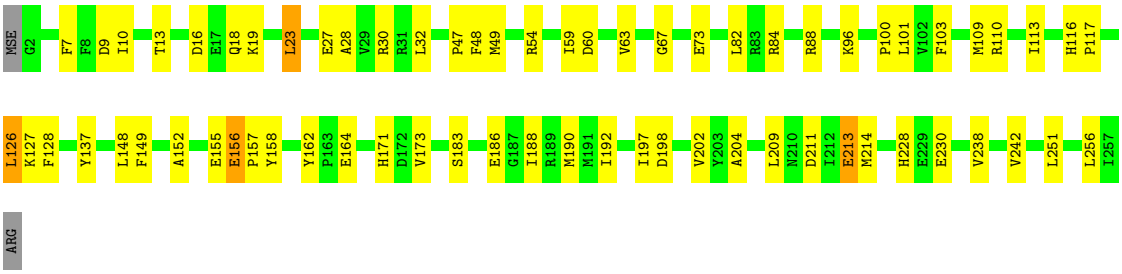
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	115	115	115	0	0
3	B	140	140	140	0	0
3	C	113	113	113	0	0
3	D	140	140	140	0	0

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.

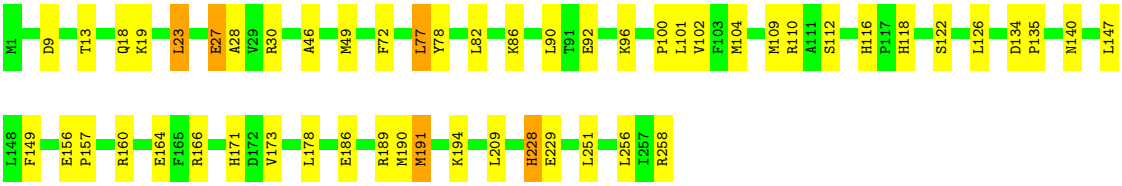
• Molecule 1: Hypothetical conserved protein, GK1056

Chain A:



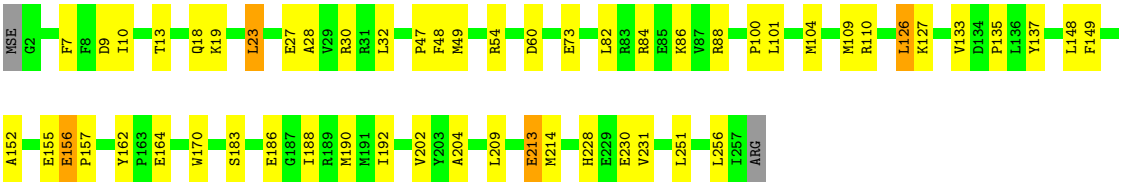
• Molecule 1: Hypothetical conserved protein, GK1056

Chain B:



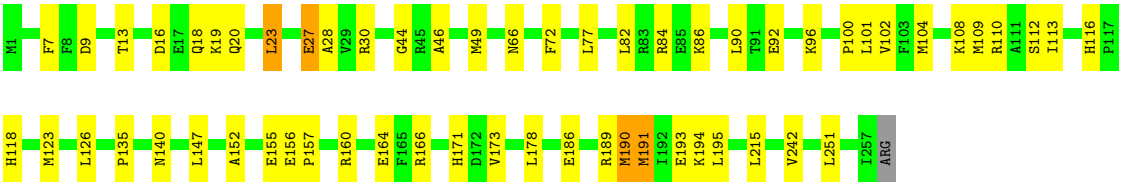
• Molecule 1: Hypothetical conserved protein, GK1056

Chain C:



• Molecule 1: Hypothetical conserved protein, GK1056

Chain D:


M1
F7
F8
D9
T13
D16
E17
Q18
K19
Q20
L23
E27
A28
V29
R30
G44
R45
A46
M49
N66
F72
L77
L82
R83
R84
E85
K86
L90
T91
E92
K96
P100
L101
V102
F103
M104
K108
M109
R110
A111
S112
I113
H116
P117
H118
M123
L126
P135
N140
L147
A152
E155
E156
P157
R160
E164
F165
R166
H171
D172
V173
L178
E186
R189
M190
M191
I192
E193
K194
L195
L215
V242
L251
I257
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.99Å 113.91Å 182.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.24 – 2.60 25.24 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (25.24-2.60) 94.9 (25.24-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 2.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.231 0.193 , 0.228	Depositor DCC
R_{free} test set	3543 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 27.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.487 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8855	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.36	0/2097	0.59	0/2816
1	B	0.37	0/2116	0.60	0/2840
1	C	0.37	0/2097	0.59	0/2816
1	D	0.37	0/2105	0.60	0/2826
All	All	0.37	0/8415	0.60	0/11298

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	2056	0	2045	47	0
1	B	2075	0	2070	40	0
1	C	2056	0	2045	42	0
1	D	2064	0	2057	51	0
2	A	18	0	24	1	0
2	B	30	0	40	6	0
2	C	18	0	24	2	0
2	D	30	0	40	9	0
3	A	115	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	140	0	0	1	0
3	C	113	0	0	0	0
3	D	140	0	0	2	0
All	All	8855	0	8345	180	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 11.

All (180) 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:D:23:LEU:H	2:D:259:GOL:H12	1.20	1.02
1:D:77:LEU:HD22	1:D:191:MSE:HE3	1.38	1.02
1:B:23:LEU:H	2:B:259:GOL:H12	1.27	0.99
1:B:72:PHE:HB2	1:B:191:MSE:HE1	1.49	0.94
1:D:72:PHE:HB2	1:D:191:MSE:HE1	1.47	0.94
1:A:49:MSE:HA	1:A:49:MSE:HE2	1.51	0.92
1:B:104:MSE:HE3	1:B:109:MSE:HE3	1.52	0.90
1:D:104:MSE:HE3	1:D:109:MSE:HE3	1.53	0.90
1:C:23:LEU:H	2:C:259:GOL:H12	1.43	0.82
1:B:209:LEU:HD21	1:B:228:HIS:CD2	2.16	0.81
1:C:48:PHE:CD2	1:C:49:MSE:HE3	2.16	0.80
1:D:23:LEU:N	2:D:259:GOL:H12	1.96	0.80
1:D:23:LEU:HB2	2:D:259:GOL:H11	1.64	0.79
1:D:189:ARG:HH11	1:D:189:ARG:HB3	1.47	0.79
1:D:100:PRO:HB3	1:D:113:ILE:HD12	1.63	0.77
1:C:49:MSE:HA	1:C:49:MSE:HE2	1.68	0.75
1:B:23:LEU:N	2:B:259:GOL:H12	2.01	0.73
1:D:23:LEU:H	2:D:259:GOL:C1	2.00	0.72
1:A:100:PRO:HG2	1:A:149:PHE:HB2	1.70	0.72
1:A:84:ARG:NE	1:A:88:ARG:HH22	1.90	0.70
1:A:152:ALA:O	1:A:155:GLU:HG2	1.91	0.69
1:C:152:ALA:O	1:C:155:GLU:HG2	1.91	0.69
1:D:156:GLU:HB3	1:D:157:PRO:HD3	1.75	0.69
1:A:213:GLU:HG3	1:A:214:MSE:N	2.07	0.68
1:C:213:GLU:HG3	1:C:214:MSE:N	2.09	0.67
1:B:189:ARG:HB3	1:B:189:ARG:HH11	1.59	0.67
1:C:48:PHE:HD2	1:C:49:MSE:HE3	1.58	0.66
1:D:104:MSE:HE3	1:D:109:MSE:CE	2.25	0.66
1:D:110:ARG:HH22	2:D:263:GOL:H32	1.62	0.65
1:A:49:MSE:HA	1:A:49:MSE:CE	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LEU:HD22	1:B:191:MSE:HE3	1.81	0.62
1:A:54:ARG:HG2	1:A:59:ILE:O	1.99	0.61
1:B:23:LEU:HB2	2:B:259:GOL:H11	1.82	0.61
1:D:86:LYS:HG3	1:D:164:GLU:HG3	1.83	0.61
1:C:213:GLU:HG3	1:C:214:MSE:H	1.64	0.61
1:B:104:MSE:HE3	1:B:109:MSE:CE	2.26	0.60
1:B:27:GLU:OE1	1:B:30:ARG:HD3	2.02	0.60
1:B:166:ARG:HH11	1:B:166:ARG:HA	1.66	0.60
1:B:186:GLU:OE2	1:B:189:ARG:NH1	2.34	0.59
1:A:47:PRO:O	1:A:54:ARG:NH2	2.35	0.59
1:D:27:GLU:OE1	1:D:30:ARG:HD3	2.02	0.59
1:B:23:LEU:H	2:B:259:GOL:C1	2.09	0.59
1:C:28:ALA:HB1	1:C:251:LEU:HD12	1.83	0.58
1:B:46:ALA:HB2	1:B:104:MSE:HE2	1.85	0.58
1:D:190:MSE:HA	1:D:193:GLU:HB2	1.86	0.58
1:A:213:GLU:HG3	1:A:214:MSE:H	1.67	0.58
1:A:48:PHE:CD2	1:A:49:MSE:HE3	2.39	0.57
1:C:104:MSE:HG2	1:C:109:MSE:HG2	1.86	0.57
1:C:100:PRO:HG2	1:C:149:PHE:HB2	1.87	0.57
1:A:28:ALA:HB1	1:A:251:LEU:HD12	1.87	0.56
1:A:18:GLN:O	1:A:19:LYS:HB2	2.05	0.56
1:B:110:ARG:HG3	1:B:134:ASP:HB3	1.87	0.56
1:D:186:GLU:OE2	1:D:189:ARG:NH1	2.39	0.56
1:C:186:GLU:O	1:C:190:MSE:HG3	2.05	0.55
1:D:101:LEU:HA	1:D:147:LEU:O	2.05	0.55
1:D:77:LEU:HD21	1:D:194:LYS:HB2	1.89	0.55
1:D:116:HIS:CE1	1:D:118:HIS:HB2	2.41	0.55
1:C:27:GLU:OE2	1:C:30:ARG:HD3	2.06	0.55
1:A:7:PHE:CE2	1:A:188:ILE:HG23	2.42	0.55
1:D:84:ARG:HD3	3:D:773:HOH:O	2.07	0.55
1:A:183:SER:HB2	1:A:213:GLU:OE1	2.08	0.54
1:D:92:GLU:O	1:D:96:LYS:HG3	2.08	0.54
1:A:23:LEU:HB2	2:A:259:GOL:H31	1.90	0.54
1:D:46:ALA:HB2	1:D:104:MSE:HE2	1.90	0.54
1:D:110:ARG:HH12	2:D:263:GOL:H12	1.72	0.53
1:A:204:ALA:HB1	1:A:214:MSE:HE3	1.90	0.53
1:C:10:ILE:HD12	1:C:10:ILE:N	2.25	0.52
1:A:156:GLU:CB	1:A:157:PRO:HD3	2.39	0.52
1:D:189:ARG:HH11	1:D:189:ARG:CB	2.18	0.52
1:D:18:GLN:O	1:D:19:LYS:HB2	2.09	0.52
1:A:27:GLU:OE2	1:A:30:ARG:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:PHE:HB2	1:D:191:MSE:CE	2.31	0.52
1:B:112:SER:O	1:B:135:PRO:HG3	2.10	0.51
1:C:7:PHE:CE2	1:C:188:ILE:HG23	2.45	0.51
1:A:186:GLU:O	1:A:190:MSE:HG3	2.10	0.51
1:B:171:HIS:CE1	1:B:173:VAL:HG22	2.45	0.51
1:C:84:ARG:HH21	1:C:88:ARG:NH2	2.08	0.51
1:C:47:PRO:O	1:C:54:ARG:NH2	2.44	0.51
1:D:104:MSE:HG2	1:D:109:MSE:HG3	1.92	0.51
1:C:204:ALA:HB1	1:C:214:MSE:HE3	1.92	0.51
1:C:183:SER:HB2	1:C:213:GLU:OE1	2.12	0.50
1:C:162:TYR:HA	1:C:164:GLU:OE2	2.12	0.50
1:D:112:SER:O	1:D:135:PRO:HG3	2.11	0.50
1:A:16:ASP:HA	1:A:242:VAL:HG11	1.94	0.50
1:A:162:TYR:HA	1:A:164:GLU:OE2	2.11	0.50
1:B:49:MSE:HE1	2:B:261:GOL:O3	2.12	0.50
1:B:228:HIS:ND1	1:B:229:GLU:N	2.61	0.49
1:B:18:GLN:O	1:B:19:LYS:HB2	2.12	0.49
1:C:101:LEU:HD23	1:C:148:LEU:HA	1.95	0.49
1:B:122:SER:OG	1:B:149:PHE:HE2	1.96	0.49
1:C:84:ARG:HH21	1:C:84:ARG:HG2	1.78	0.49
1:D:100:PRO:C	1:D:101:LEU:HD12	2.33	0.49
1:D:166:ARG:HA	1:D:166:ARG:HH11	1.78	0.48
1:A:10:ILE:HD12	1:A:10:ILE:N	2.28	0.48
1:D:49:MSE:HE1	2:D:261:GOL:O3	2.12	0.48
1:C:228:HIS:HE1	1:C:230:GLU:HG2	1.79	0.48
1:A:48:PHE:HD2	1:A:49:MSE:HE3	1.77	0.48
1:C:18:GLN:O	1:C:19:LYS:HB2	2.14	0.48
1:D:123:MSE:HE3	1:D:123:MSE:HA	1.95	0.48
1:B:77:LEU:HD21	1:B:194:LYS:HB2	1.94	0.48
1:B:101:LEU:HA	1:B:147:LEU:O	2.12	0.48
1:B:86:LYS:HG3	1:B:164:GLU:HG3	1.95	0.47
1:B:104:MSE:CE	1:B:109:MSE:HE3	2.37	0.47
1:D:108:LYS:HD3	1:D:110:ARG:NH2	2.29	0.47
1:D:190:MSE:HE2	1:D:194:LYS:NZ	2.30	0.47
1:B:166:ARG:HA	1:B:166:ARG:NH1	2.30	0.46
1:C:133:VAL:HG22	1:C:135:PRO:HD3	1.96	0.46
1:D:102:VAL:HB	1:D:147:LEU:HB2	1.97	0.46
1:A:156:GLU:CG	1:A:157:PRO:HD3	2.45	0.46
1:D:190:MSE:O	1:D:194:LYS:HG2	2.16	0.46
1:B:102:VAL:HA	1:B:110:ARG:O	2.16	0.46
1:C:126:LEU:O	1:C:127:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:O	1:A:127:LYS:HB2	2.16	0.46
1:A:238:VAL:O	1:B:160:ARG:NH2	2.47	0.46
1:C:156:GLU:CB	1:C:157:PRO:HD3	2.45	0.46
1:D:108:LYS:HD3	1:D:110:ARG:CZ	2.46	0.46
1:C:126:LEU:HD13	1:C:170:TRP:CZ3	2.51	0.45
1:A:101:LEU:HD23	1:A:148:LEU:HA	1.99	0.45
1:D:152:ALA:O	1:D:155:GLU:HG2	2.16	0.45
1:A:28:ALA:O	1:A:32:LEU:HB2	2.16	0.45
1:A:100:PRO:HB3	1:A:113:ILE:HD12	1.98	0.45
1:B:28:ALA:HB1	1:B:251:LEU:HD12	1.98	0.45
1:C:84:ARG:NH2	1:C:88:ARG:HH22	2.15	0.45
1:C:28:ALA:O	1:C:32:LEU:HB2	2.16	0.45
1:D:171:HIS:CE1	1:D:173:VAL:HG22	2.52	0.45
1:C:84:ARG:HH21	1:C:88:ARG:HH22	1.63	0.45
1:A:60:ASP:OD2	1:A:73:GLU:HA	2.17	0.45
2:B:262:GOL:H31	3:B:745:HOH:O	2.16	0.45
1:C:110:ARG:HH12	2:C:261:GOL:H11	1.82	0.45
1:D:44:GLY:HA2	1:D:66:ASN:H	1.82	0.44
1:B:156:GLU:HB3	1:B:157:PRO:HD3	1.97	0.44
1:C:228:HIS:HB3	1:C:231:VAL:HG23	2.00	0.44
1:A:103:PHE:O	1:A:109:MSE:HA	2.17	0.44
1:B:78:TYR:CZ	1:B:190:MSE:HE3	2.52	0.44
1:A:49:MSE:HE1	1:A:128:PHE:CZ	2.51	0.44
1:C:192:ILE:HG21	1:C:202:VAL:HG21	2.00	0.44
1:D:23:LEU:HB2	2:D:259:GOL:C1	2.39	0.44
1:B:72:PHE:HB2	1:B:191:MSE:CE	2.35	0.44
1:A:16:ASP:HB2	3:A:718:HOH:O	2.18	0.43
1:B:109:MSE:O	1:B:110:ARG:HD3	2.19	0.43
1:A:116:HIS:HA	1:A:117:PRO:HD3	1.89	0.43
1:A:197:ILE:HG22	1:A:198:ASP:N	2.33	0.43
1:B:100:PRO:HG2	1:B:149:PHE:HB2	2.00	0.43
1:A:228:HIS:HE1	1:A:230:GLU:HG2	1.84	0.43
1:C:110:ARG:HG3	1:C:137:TYR:CD2	2.54	0.42
1:C:156:GLU:HB2	1:C:157:PRO:HD3	2.00	0.42
1:B:110:ARG:CG	1:B:134:ASP:HB3	2.48	0.42
1:A:19:LYS:HD2	3:D:506:HOH:O	2.18	0.42
1:B:9:ASP:O	1:B:13:THR:HB	2.19	0.42
1:D:102:VAL:CG1	1:D:109:MSE:HG2	2.49	0.42
1:A:63:VAL:HG13	1:A:67:GLY:HA2	2.01	0.42
1:A:156:GLU:HB2	1:A:157:PRO:HD3	2.01	0.42
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:MSE:HE2	1:D:195:LEU:HD11	2.02	0.42
1:A:192:ILE:HG21	1:A:202:VAL:HG21	2.02	0.42
1:C:7:PHE:O	1:C:204:ALA:HA	2.20	0.42
1:C:86:LYS:HA	1:C:86:LYS:HD3	1.85	0.42
1:D:100:PRO:HB3	1:D:113:ILE:CD1	2.44	0.42
1:A:148:LEU:HD21	1:A:158:TYR:CD2	2.55	0.42
1:A:171:HIS:CE1	1:A:173:VAL:HG22	2.54	0.42
1:C:60:ASP:OD2	1:C:73:GLU:HA	2.19	0.41
1:A:110:ARG:HG3	1:A:137:TYR:CD2	2.55	0.41
1:C:9:ASP:O	1:C:13:THR:HB	2.19	0.41
1:C:48:PHE:CZ	1:C:109:MSE:HG3	2.56	0.41
1:C:48:PHE:CE2	1:C:49:MSE:HE3	2.56	0.41
1:D:16:ASP:OD2	1:D:20:GLN:HB2	2.20	0.41
1:A:96:LYS:HE3	1:A:96:LYS:HB2	1.92	0.41
1:D:9:ASP:O	1:D:13:THR:HB	2.21	0.41
1:D:28:ALA:HB1	1:D:251:LEU:HD12	2.02	0.41
1:D:16:ASP:HA	1:D:242:VAL:HG11	2.02	0.41
1:A:9:ASP:OD2	1:A:211:ASP:OD1	2.39	0.41
1:B:102:VAL:HB	1:B:147:LEU:HB2	2.03	0.40
1:D:7:PHE:HZ	1:D:191:MSE:HG2	1.85	0.40
1:D:116:HIS:CE1	1:D:118:HIS:H	2.38	0.40
1:A:9:ASP:O	1:A:13:THR:HB	2.21	0.40
1:B:256:LEU:HD23	1:B:256:LEU:HA	1.90	0.40
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.94	0.40
1:D:110:ARG:HH22	2:D:263:GOL:C3	2.33	0.40
1:B:92:GLU:O	1:B:96:LYS:HG3	2.21	0.40
1:B:116:HIS:CE1	1:B:118:HIS:HB2	2.57	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	254/258 (98%)	244 (96%)	10 (4%)	0	100	100
1	B	256/258 (99%)	245 (96%)	11 (4%)	0	100	100
1	C	254/258 (98%)	243 (96%)	11 (4%)	0	100	100
1	D	255/258 (99%)	249 (98%)	6 (2%)	0	100	100
All	All	1019/1032 (99%)	981 (96%)	38 (4%)	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	218/211 (103%)	212 (97%)	6 (3%)	43	69
1	B	220/211 (104%)	209 (95%)	11 (5%)	24	47
1	C	218/211 (103%)	212 (97%)	6 (3%)	43	69
1	D	219/211 (104%)	208 (95%)	11 (5%)	24	47
All	All	875/844 (104%)	841 (96%)	34 (4%)	32	58

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	82	LEU
1	A	126	LEU
1	A	156	GLU
1	A	209	LEU
1	A	213	GLU
1	B	23	LEU
1	B	27	GLU
1	B	77	LEU
1	B	82	LEU
1	B	90	LEU
1	B	126	LEU
1	B	140	ASN

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Mol	Chain	Res	Type
1	B	178	LEU
1	B	191	MSE
1	B	228	HIS
1	B	258	ARG
1	C	23	LEU
1	C	82	LEU
1	C	126	LEU
1	C	156	GLU
1	C	209	LEU
1	C	213	GLU
1	D	23	LEU
1	D	27	GLU
1	D	82	LEU
1	D	90	LEU
1	D	126	LEU
1	D	140	ASN
1	D	160	ARG
1	D	178	LEU
1	D	190	MSE
1	D	191	MSE
1	D	215	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	161	ASN
1	C	97	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands 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	$\#\|Z\| > 2$
2	GOL	A	261	-	5,5,5	0.29	0	5,5,5	0.22	0
2	GOL	A	259	-	5,5,5	0.33	0	5,5,5	0.23	0
2	GOL	B	262	-	5,5,5	0.33	0	5,5,5	0.26	0
2	GOL	B	260	-	5,5,5	0.35	0	5,5,5	0.25	0
2	GOL	D	259	-	5,5,5	0.31	0	5,5,5	0.28	0
2	GOL	D	263	-	5,5,5	0.28	0	5,5,5	0.27	0
2	GOL	C	261	-	5,5,5	0.28	0	5,5,5	0.21	0
2	GOL	D	261	-	5,5,5	0.28	0	5,5,5	0.27	0
2	GOL	B	259	-	5,5,5	0.30	0	5,5,5	0.31	0
2	GOL	C	260	-	5,5,5	0.32	0	5,5,5	0.31	0
2	GOL	D	262	-	5,5,5	0.29	0	5,5,5	0.16	0
2	GOL	C	259	-	5,5,5	0.32	0	5,5,5	0.18	0
2	GOL	A	260	-	5,5,5	0.33	0	5,5,5	0.21	0
2	GOL	B	261	-	5,5,5	0.28	0	5,5,5	0.28	0
2	GOL	B	263	-	5,5,5	0.30	0	5,5,5	0.35	0
2	GOL	D	260	-	5,5,5	0.33	0	5,5,5	0.21	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
2	GOL	A	261	-	-	0/4/4/4	-
2	GOL	A	259	-	-	0/4/4/4	-
2	GOL	B	262	-	-	0/4/4/4	-
2	GOL	B	260	-	-	0/4/4/4	-
2	GOL	D	259	-	-	0/4/4/4	-
2	GOL	D	263	-	-	0/4/4/4	-
2	GOL	C	261	-	-	0/4/4/4	-
2	GOL	D	261	-	-	0/4/4/4	-
2	GOL	B	259	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	260	-	-	2/4/4/4	-
2	GOL	D	262	-	-	0/4/4/4	-
2	GOL	C	259	-	-	2/4/4/4	-
2	GOL	A	260	-	-	0/4/4/4	-
2	GOL	B	261	-	-	0/4/4/4	-
2	GOL	B	263	-	-	0/4/4/4	-
2	GOL	D	260	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	259	GOL	C1-C2-C3-O3
2	C	259	GOL	O2-C2-C3-O3
2	C	260	GOL	O1-C1-C2-O2
2	C	260	GOL	O1-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	259	GOL	1	0
2	B	262	GOL	1	0
2	D	259	GOL	5	0
2	D	263	GOL	3	0
2	C	261	GOL	1	0
2	D	261	GOL	1	0
2	B	259	GOL	4	0
2	C	259	GOL	1	0
2	B	261	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	248/258 (96%)	-0.29	0	100	100	24, 40, 73, 86	0
1	B	249/258 (96%)	-0.34	0	100	100	20, 37, 66, 84	0
1	C	248/258 (96%)	-0.26	0	100	100	22, 40, 69, 90	0
1	D	248/258 (96%)	-0.35	0	100	100	21, 37, 69, 84	0
All	All	993/1032 (96%)	-0.31	0	100	100	20, 39, 71, 90	0

There are no RSRZ outliers to report.

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, 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
2	GOL	A	259	6/6	0.85	0.16	63,65,66,66	0
2	GOL	B	261	6/6	0.86	0.25	54,55,56,56	0
2	GOL	C	261	6/6	0.86	0.19	52,53,54,55	0
2	GOL	D	260	6/6	0.86	0.13	66,67,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	C	259	6/6	0.87	0.17	54,56,58,58	0
2	GOL	A	261	6/6	0.87	0.19	51,53,56,56	0
2	GOL	B	263	6/6	0.87	0.20	51,55,57,58	0
2	GOL	B	260	6/6	0.88	0.12	59,62,62,63	0
2	GOL	B	262	6/6	0.90	0.23	52,54,56,57	0
2	GOL	D	263	6/6	0.92	0.20	53,56,58,59	0
2	GOL	D	261	6/6	0.93	0.23	52,54,56,56	0
2	GOL	D	262	6/6	0.95	0.21	50,52,54,55	0
2	GOL	B	259	6/6	0.96	0.19	48,50,51,52	0
2	GOL	D	259	6/6	0.96	0.18	48,48,49,50	0
2	GOL	C	260	6/6	0.96	0.22	47,50,51,53	0
2	GOL	A	260	6/6	0.97	0.22	46,49,50,52	0

6.5 Other polymers (i)

There are no such residues in this entry.