Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 02:42 AM EDT

PDB ID	:	3KJJ
Title	:	Crystal structure of NMB1025, a member of YjgF protein family, from Neisseria meningitidis (hexagonal crystal form)
Authors	:	Ren, J.; Sainsbury, S.; Owens, R.J.; Oxford Protein Production Facility (OPPF)
Deposited on	:	2009-11-03
Resolution	:	1.90 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:

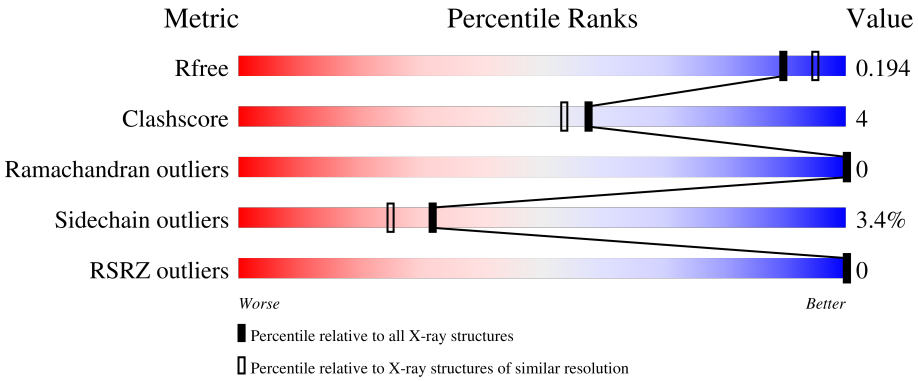
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	128	77% 13% • 9%
1	B	128	83% 10% 7%
1	C	128	79% 12% • 7%
1	D	128	73% 17% • 8%
1	E	128	82% 9% 9%

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Mol	Chain	Length	Quality of chain
1	F	128	
1	G	128	
1	H	128	
1	I	128	
1	J	128	
1	K	128	
1	L	128	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11793 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 NMB1025 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	Se	0	0	0
			905	567	161	171	2	4			
1	B	119	Total	C	N	O	S	Se	0	3	0
			940	590	171	173	2	4			
1	C	119	Total	C	N	O	S	Se	0	1	0
			926	581	166	173	2	4			
1	D	118	Total	C	N	O	S	Se	0	1	0
			919	576	164	173	2	4			
1	E	116	Total	C	N	O	S	Se	0	0	0
			897	563	160	168	2	4			
1	F	117	Total	C	N	O	S	Se	0	1	0
			909	571	161	171	2	4			
1	G	115	Total	C	N	O	S	Se	0	4	0
			916	578	163	169	2	4			
1	H	116	Total	C	N	O	S	Se	0	0	0
			902	566	162	168	2	4			
1	I	117	Total	C	N	O	S	Se	0	3	0
			924	579	164	175	2	4			
1	J	119	Total	C	N	O	S	Se	0	0	0
			925	579	167	173	2	4			
1	K	119	Total	C	N	O	S	Se	0	1	0
			921	577	163	175	2	4			
1	L	115	Total	C	N	O	S	Se	0	1	0
			896	563	159	168	2	4			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MSE	-	expression tag	UNP Q9JZJ4
A	-6	ALA	-	expression tag	UNP Q9JZJ4
A	-5	HIS	-	expression tag	UNP Q9JZJ4
A	-4	HIS	-	expression tag	UNP Q9JZJ4
A	-3	HIS	-	expression tag	UNP Q9JZJ4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	HIS	-	expression tag	UNP Q9JZJ4
A	-1	HIS	-	expression tag	UNP Q9JZJ4
A	0	HIS	-	expression tag	UNP Q9JZJ4
B	-7	MSE	-	expression tag	UNP Q9JZJ4
B	-6	ALA	-	expression tag	UNP Q9JZJ4
B	-5	HIS	-	expression tag	UNP Q9JZJ4
B	-4	HIS	-	expression tag	UNP Q9JZJ4
B	-3	HIS	-	expression tag	UNP Q9JZJ4
B	-2	HIS	-	expression tag	UNP Q9JZJ4
B	-1	HIS	-	expression tag	UNP Q9JZJ4
B	0	HIS	-	expression tag	UNP Q9JZJ4
C	-7	MSE	-	expression tag	UNP Q9JZJ4
C	-6	ALA	-	expression tag	UNP Q9JZJ4
C	-5	HIS	-	expression tag	UNP Q9JZJ4
C	-4	HIS	-	expression tag	UNP Q9JZJ4
C	-3	HIS	-	expression tag	UNP Q9JZJ4
C	-2	HIS	-	expression tag	UNP Q9JZJ4
C	-1	HIS	-	expression tag	UNP Q9JZJ4
C	0	HIS	-	expression tag	UNP Q9JZJ4
D	-7	MSE	-	expression tag	UNP Q9JZJ4
D	-6	ALA	-	expression tag	UNP Q9JZJ4
D	-5	HIS	-	expression tag	UNP Q9JZJ4
D	-4	HIS	-	expression tag	UNP Q9JZJ4
D	-3	HIS	-	expression tag	UNP Q9JZJ4
D	-2	HIS	-	expression tag	UNP Q9JZJ4
D	-1	HIS	-	expression tag	UNP Q9JZJ4
D	0	HIS	-	expression tag	UNP Q9JZJ4
E	-7	MSE	-	expression tag	UNP Q9JZJ4
E	-6	ALA	-	expression tag	UNP Q9JZJ4
E	-5	HIS	-	expression tag	UNP Q9JZJ4
E	-4	HIS	-	expression tag	UNP Q9JZJ4
E	-3	HIS	-	expression tag	UNP Q9JZJ4
E	-2	HIS	-	expression tag	UNP Q9JZJ4
E	-1	HIS	-	expression tag	UNP Q9JZJ4
E	0	HIS	-	expression tag	UNP Q9JZJ4
F	-7	MSE	-	expression tag	UNP Q9JZJ4
F	-6	ALA	-	expression tag	UNP Q9JZJ4
F	-5	HIS	-	expression tag	UNP Q9JZJ4
F	-4	HIS	-	expression tag	UNP Q9JZJ4
F	-3	HIS	-	expression tag	UNP Q9JZJ4
F	-2	HIS	-	expression tag	UNP Q9JZJ4
F	-1	HIS	-	expression tag	UNP Q9JZJ4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP Q9JZJ4
G	-7	MSE	-	expression tag	UNP Q9JZJ4
G	-6	ALA	-	expression tag	UNP Q9JZJ4
G	-5	HIS	-	expression tag	UNP Q9JZJ4
G	-4	HIS	-	expression tag	UNP Q9JZJ4
G	-3	HIS	-	expression tag	UNP Q9JZJ4
G	-2	HIS	-	expression tag	UNP Q9JZJ4
G	-1	HIS	-	expression tag	UNP Q9JZJ4
G	0	HIS	-	expression tag	UNP Q9JZJ4
H	-7	MSE	-	expression tag	UNP Q9JZJ4
H	-6	ALA	-	expression tag	UNP Q9JZJ4
H	-5	HIS	-	expression tag	UNP Q9JZJ4
H	-4	HIS	-	expression tag	UNP Q9JZJ4
H	-3	HIS	-	expression tag	UNP Q9JZJ4
H	-2	HIS	-	expression tag	UNP Q9JZJ4
H	-1	HIS	-	expression tag	UNP Q9JZJ4
H	0	HIS	-	expression tag	UNP Q9JZJ4
I	-7	MSE	-	expression tag	UNP Q9JZJ4
I	-6	ALA	-	expression tag	UNP Q9JZJ4
I	-5	HIS	-	expression tag	UNP Q9JZJ4
I	-4	HIS	-	expression tag	UNP Q9JZJ4
I	-3	HIS	-	expression tag	UNP Q9JZJ4
I	-2	HIS	-	expression tag	UNP Q9JZJ4
I	-1	HIS	-	expression tag	UNP Q9JZJ4
I	0	HIS	-	expression tag	UNP Q9JZJ4
J	-7	MSE	-	expression tag	UNP Q9JZJ4
J	-6	ALA	-	expression tag	UNP Q9JZJ4
J	-5	HIS	-	expression tag	UNP Q9JZJ4
J	-4	HIS	-	expression tag	UNP Q9JZJ4
J	-3	HIS	-	expression tag	UNP Q9JZJ4
J	-2	HIS	-	expression tag	UNP Q9JZJ4
J	-1	HIS	-	expression tag	UNP Q9JZJ4
J	0	HIS	-	expression tag	UNP Q9JZJ4
K	-7	MSE	-	expression tag	UNP Q9JZJ4
K	-6	ALA	-	expression tag	UNP Q9JZJ4
K	-5	HIS	-	expression tag	UNP Q9JZJ4
K	-4	HIS	-	expression tag	UNP Q9JZJ4
K	-3	HIS	-	expression tag	UNP Q9JZJ4
K	-2	HIS	-	expression tag	UNP Q9JZJ4
K	-1	HIS	-	expression tag	UNP Q9JZJ4
K	0	HIS	-	expression tag	UNP Q9JZJ4
L	-7	MSE	-	expression tag	UNP Q9JZJ4

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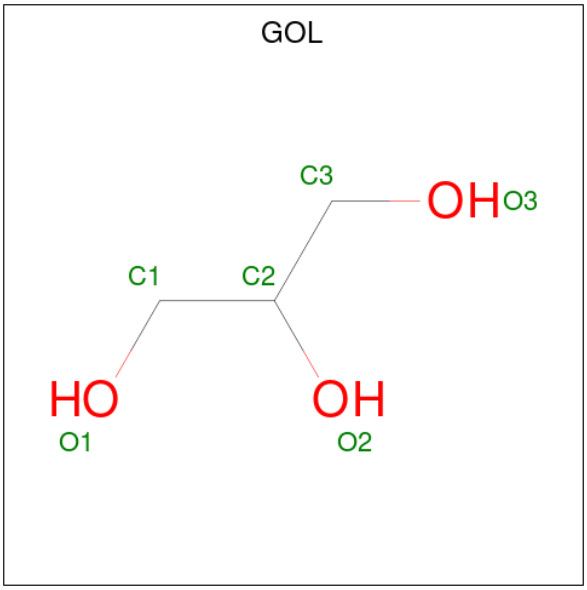
Chain	Residue	Modelled	Actual	Comment	Reference
L	-6	ALA	-	expression tag	UNP Q9JZJ4
L	-5	HIS	-	expression tag	UNP Q9JZJ4
L	-4	HIS	-	expression tag	UNP Q9JZJ4
L	-3	HIS	-	expression tag	UNP Q9JZJ4
L	-2	HIS	-	expression tag	UNP Q9JZJ4
L	-1	HIS	-	expression tag	UNP Q9JZJ4
L	0	HIS	-	expression tag	UNP Q9JZJ4

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	86	Total O 86 86	0	0
3	B	91	Total O 91 91	0	0
3	C	73	Total O 73 73	0	0
3	D	51	Total O 51 51	0	0

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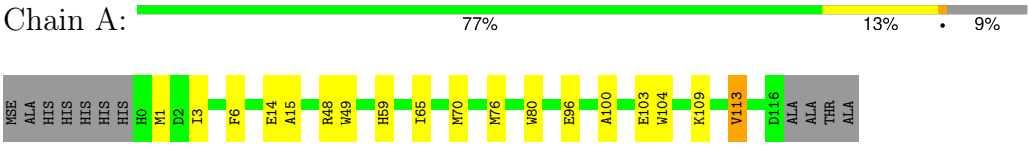
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	42	Total O 42 42	0	0
3	F	60	Total O 60 60	0	0
3	G	76	Total O 76 76	0	0
3	H	81	Total O 81 81	0	0
3	I	67	Total O 67 67	0	0
3	J	92	Total O 92 92	0	0
3	K	50	Total O 50 50	0	0
3	L	32	Total O 32 32	0	0

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.

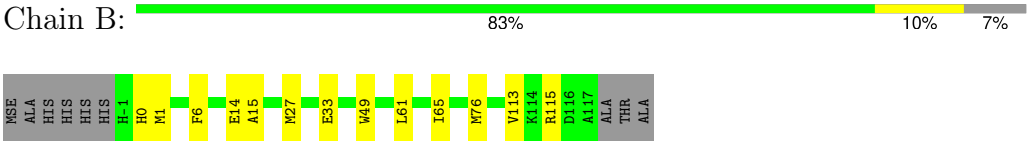
• Molecule 1: NMB1025 protein

Chain A:



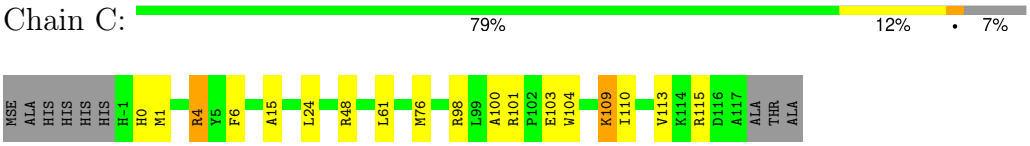
• Molecule 1: NMB1025 protein

Chain B:



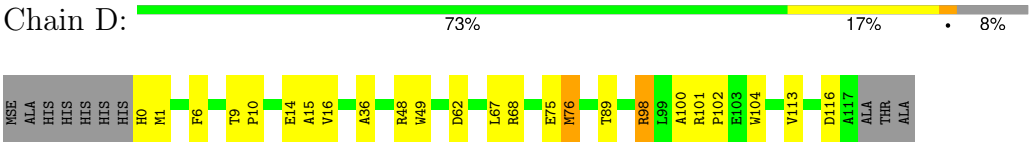
• Molecule 1: NMB1025 protein

Chain C:



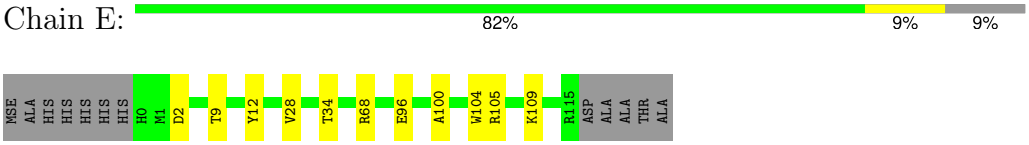
• Molecule 1: NMB1025 protein

Chain D:



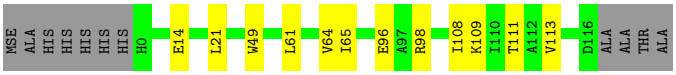
• Molecule 1: NMB1025 protein

Chain E:



• Molecule 1: NMB1025 protein

Chain F:

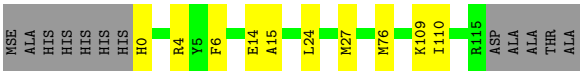


• Molecule 1: NMB1025 protein

Chain G:

• Molecule 1: NMB1025 protein

Chain H:

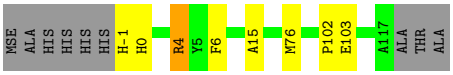


• Molecule 1: NMB1025 protein

Chain I:

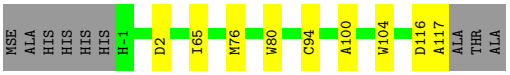
• Molecule 1: NMB1025 protein

Chain J:



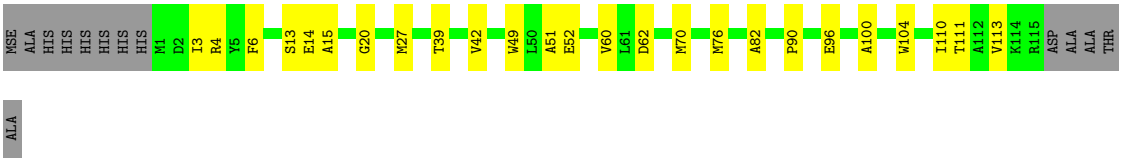
• Molecule 1: NMB1025 protein

Chain K:



• Molecule 1: NMB1025 protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	155.61Å 155.61Å 116.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.88 – 1.90 29.88 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.88-1.90) 100.0 (29.88-1.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.166 , 0.206 0.166 , 0.194	Depositor DCC
R_{free} test set	6301 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 17.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.407 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.422 for H, K, L 0.578 for h+k,-k,-l	Depositor
Outliers	2 of 126574 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11793	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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 40.62 % 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 2.6648e-04.*

[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: 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	0.43	0/919	0.58	0/1242
1	B	0.43	0/964	0.57	0/1302
1	C	0.44	0/944	0.57	0/1275
1	D	0.38	0/937	0.53	0/1268
1	E	0.38	0/911	0.55	0/1231
1	F	0.40	0/926	0.54	0/1252
1	G	0.44	0/943	0.58	0/1275
1	H	0.43	0/917	0.56	0/1239
1	I	0.40	0/948	0.58	0/1282
1	J	0.45	0/941	0.57	0/1272
1	K	0.39	0/938	0.54	0/1268
1	L	0.36	0/914	0.50	0/1237
All	All	0.41	0/11202	0.56	0/15143

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

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	905	0	879	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	940	0	926	13	0
1	C	926	0	904	14	0
1	D	919	0	896	18	0
1	E	897	0	875	10	0
1	F	909	0	888	9	0
1	G	916	0	914	5	0
1	H	902	0	880	5	0
1	I	924	0	905	4	0
1	J	925	0	896	4	0
1	K	921	0	892	5	0
1	L	896	0	880	12	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
3	A	86	0	0	1	0
3	B	91	0	0	0	0
3	C	73	0	0	2	0
3	D	51	0	0	0	0
3	E	42	0	0	1	0
3	F	60	0	0	2	0
3	G	76	0	0	0	0
3	H	81	0	0	0	0
3	I	67	0	0	0	0
3	J	92	0	0	0	0
3	K	50	0	0	0	0
3	L	32	0	0	1	0
All	All	11793	0	10751	96	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 (96) 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:115[B]:ARG:HG2	1:B:115[B]:ARG:HH11	0.88	1.05
1:B:115[B]:ARG:HG2	1:B:115[B]:ARG:NH1	1.63	0.98
1:B:115[B]:ARG:HH11	1:B:115[B]:ARG:CG	1.79	0.93
1:E:34:THR:HA	1:E:105:ARG:HH21	1.43	0.82
1:D:101:ARG:HG2	1:D:101:ARG:HH11	1.53	0.73
1:C:115:ARG:HH22	1:L:82:ALA:HB1	1.58	0.69
1:A:6:PHE:HB2	1:A:15:ALA:HB3	1.76	0.68
1:J:0:HIS:H	1:J:0:HIS:CD2	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4:ARG:HG2	1:J:6:PHE:CZ	2.32	0.65
1:B:61:LEU:HD11	1:B:113[B]:VAL:HG23	1.81	0.63
1:L:27:MSE:HB3	1:L:42:VAL:HG13	1.81	0.62
1:A:113:VAL:HG21	1:C:1:MSE:HB3	1.81	0.61
1:E:68:ARG:NH2	1:E:105:ARG:HD3	2.16	0.60
1:D:16:VAL:HG21	1:F:61:LEU:O	2.02	0.59
1:D:1:MSE:HB3	1:F:113[A]:VAL:HG21	1.84	0.59
1:B:115[B]:ARG:NH1	1:B:115[B]:ARG:CG	2.47	0.59
1:B:65:ILE:HD13	1:B:76:MSE:CE	2.35	0.57
1:B:6:PHE:HB2	1:B:15:ALA:HB3	1.85	0.57
1:C:4:ARG:HG2	1:C:6:PHE:CZ	2.40	0.57
1:A:96:GLU:OE1	1:C:98:ARG:HD2	2.05	0.56
1:I:62[A]:ASP:OD1	1:I:111:THR:HB	2.06	0.55
1:L:14:GLU:HG2	1:L:49:TRP:CE2	2.40	0.55
1:E:100:ALA:HB3	1:E:104:TRP:CZ3	2.43	0.54
1:E:2:ASP:HB3	3:E:672:HOH:O	2.08	0.54
1:E:68:ARG:HH21	1:E:105:ARG:HD3	1.73	0.52
1:D:101:ARG:HG2	1:D:101:ARG:NH1	2.21	0.52
1:L:39[B]:THR:HG21	1:L:76:MSE:HG2	1.93	0.51
1:F:21:LEU:HD22	3:F:662:HOH:O	2.10	0.51
1:F:111:THR:HG22	3:F:662:HOH:O	2.11	0.51
1:A:14:GLU:HG3	1:A:49:TRP:CZ2	2.46	0.51
1:G:1:MSE:SE	1:G:19:ASN:HB2	2.62	0.50
1:G:6:PHE:HB2	1:G:15:ALA:HB3	1.93	0.50
1:B:14:GLU:HG3	1:B:49:TRP:CZ2	2.47	0.50
1:E:100:ALA:HB3	1:E:104:TRP:HZ3	1.77	0.50
1:A:1:MSE:HB3	1:B:113[B]:VAL:CG1	2.40	0.50
1:C:0:HIS:CD2	1:C:1:MSE:HE2	2.47	0.50
1:A:65:ILE:HD13	1:A:76:MSE:CE	2.42	0.50
1:D:68:ARG:NH1	1:D:102:PRO:O	2.44	0.50
1:L:6:PHE:HB2	1:L:15:ALA:HB3	1.93	0.49
1:D:67:LEU:HD21	1:D:76:MSE:HG3	1.94	0.49
1:G:64:VAL:CG2	1:I:109:LYS:HE3	2.43	0.49
1:K:116:ASP:O	1:K:117:ALA:HB2	2.13	0.48
1:K:76:MSE:HE1	1:K:80:TRP:CE3	2.48	0.48
3:A:656:HOH:O	1:C:1:MSE:HE3	2.13	0.48
1:D:101:ARG:HD3	1:D:104:TRP:CZ2	2.47	0.48
1:J:6:PHE:HB2	1:J:15:ALA:HB3	1.95	0.48
1:A:3:ILE:HD11	1:B:113[A]:VAL:CG1	2.44	0.48
1:D:76:MSE:SE	1:D:76:MSE:C	3.02	0.48
1:D:89[B]:THR:OG1	1:E:12:TYR:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:GLU:HG3	1:F:49:TRP:CZ2	2.49	0.48
1:C:109[A]:LYS:HE3	3:C:706:HOH:O	2.14	0.47
1:F:65:ILE:HG12	1:F:108:ILE:HG12	1.97	0.47
1:L:62:ASP:OD1	1:L:111:THR:HB	2.14	0.47
1:C:6:PHE:HB2	1:C:15:ALA:HB3	1.96	0.46
1:A:59:HIS:HB3	1:A:113:VAL:HG12	1.98	0.46
1:A:1:MSE:HB3	1:B:113[B]:VAL:HG11	1.97	0.45
1:C:61:LEU:HD11	1:C:113:VAL:HG13	1.99	0.45
1:L:70:MSE:HE2	1:L:96:GLU:HB2	1.98	0.45
1:I:6:PHE:HB2	1:I:15:ALA:HB3	1.97	0.45
1:L:20:GLY:O	1:L:113:VAL:HA	2.16	0.45
1:C:24:LEU:HD12	1:C:110:ILE:HB	1.99	0.44
1:G:67:LEU:HD21	1:G:76:MSE:HG3	1.99	0.44
1:A:3:ILE:HD11	1:B:113[A]:VAL:HG12	2.00	0.44
1:L:51:ALA:HA	3:L:531:HOH:O	2.17	0.44
1:A:113:VAL:CG2	1:C:1:MSE:HB3	2.45	0.44
1:E:96:GLU:HB3	1:F:98:ARG:HB2	2.00	0.44
1:F:64:VAL:HB	1:F:109:LYS:HB3	1.99	0.44
1:D:98:ARG:HB3	1:F:96:GLU:HB3	1.99	0.44
1:D:100:ALA:HB3	1:D:104:TRP:CZ3	2.53	0.44
1:D:62:ASP:OD1	1:E:109:LYS:HE2	2.18	0.43
1:C:98:ARG:NE	3:C:417:HOH:O	2.51	0.43
1:D:100:ALA:HB3	1:D:104:TRP:HZ3	1.84	0.43
1:D:89[B]:THR:HG21	1:E:9:THR:O	2.18	0.43
1:H:24:LEU:HD12	1:H:110:ILE:HB	2.01	0.43
1:L:60:VAL:HG13	1:L:110:ILE:HG23	2.01	0.43
1:D:9:THR:HB	1:D:10:PRO:HD2	2.01	0.43
1:D:14:GLU:HG3	1:D:49:TRP:CZ2	2.55	0.42
1:H:4:ARG:HD3	1:H:6:PHE:CZ	2.54	0.42
1:J:102:PRO:HD2	1:J:103:GLU:OE2	2.19	0.42
1:C:101:ARG:HG3	1:C:104:TRP:CZ2	2.53	0.42
1:H:14:GLU:OE1	1:H:27:MSE:HE1	2.20	0.42
1:K:65:ILE:HD13	1:K:76:MSE:CE	2.49	0.42
1:H:76:MSE:SE	1:H:76:MSE:C	3.08	0.42
1:D:36:ALA:HB2	1:D:75:GLU:HG2	2.02	0.41
1:B:27:MSE:HE1	1:B:49:TRP:CD1	2.55	0.41
1:G:113[B]:VAL:HG12	1:G:114:LYS:O	2.20	0.41
1:L:60:VAL:HG12	1:L:90:PRO:HB3	2.03	0.41
1:D:6:PHE:HB2	1:D:15:ALA:HB3	2.03	0.41
1:I:67:LEU:HD21	1:I:76:MSE:HG3	2.03	0.41
1:L:100:ALA:HB3	1:L:104:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:PHE:HB2	1:H:15:ALA:HB3	2.03	0.41
1:K:65:ILE:O	1:K:94:CYS:HA	2.20	0.41
1:A:70:MSE:SE	1:C:100:ALA:HA	2.71	0.41
1:A:100:ALA:HB3	1:A:104:TRP:CZ3	2.56	0.41
1:K:100:ALA:HB3	1:K:104:TRP:CZ3	2.56	0.40
1:A:76:MSE:HE1	1:A:80:TRP:CE3	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	115/128 (90%)	115 (100%)	0	0	100	100
1	B	120/128 (94%)	119 (99%)	1 (1%)	0	100	100
1	C	118/128 (92%)	118 (100%)	0	0	100	100
1	D	117/128 (91%)	117 (100%)	0	0	100	100
1	E	114/128 (89%)	111 (97%)	3 (3%)	0	100	100
1	F	116/128 (91%)	116 (100%)	0	0	100	100
1	G	117/128 (91%)	116 (99%)	1 (1%)	0	100	100
1	H	114/128 (89%)	114 (100%)	0	0	100	100
1	I	118/128 (92%)	117 (99%)	1 (1%)	0	100	100
1	J	117/128 (91%)	117 (100%)	0	0	100	100
1	K	118/128 (92%)	118 (100%)	0	0	100	100
1	L	114/128 (89%)	111 (97%)	3 (3%)	0	100	100
All	All	1398/1536 (91%)	1389 (99%)	9 (1%)	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	89/92 (97%)	85 (96%)	4 (4%)	23 16
1	B	93/92 (101%)	90 (97%)	3 (3%)	34 27
1	C	91/92 (99%)	85 (93%)	6 (7%)	14 7
1	D	91/92 (99%)	85 (93%)	6 (7%)	14 7
1	E	88/92 (96%)	87 (99%)	1 (1%)	70 71
1	F	90/92 (98%)	90 (100%)	0	100 100
1	G	92/92 (100%)	90 (98%)	2 (2%)	47 43
1	H	89/92 (97%)	87 (98%)	2 (2%)	47 43
1	I	92/92 (100%)	86 (94%)	6 (6%)	14 7
1	J	91/92 (99%)	88 (97%)	3 (3%)	33 26
1	K	90/92 (98%)	89 (99%)	1 (1%)	70 71
1	L	89/92 (97%)	85 (96%)	4 (4%)	23 16
All	All	1085/1104 (98%)	1047 (96%)	38 (4%)	32 24

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	103	GLU
1	A	109	LYS
1	A	113	VAL
1	B	0	HIS
1	B	1	MSE
1	B	33	GLU
1	C	4	ARG
1	C	48	ARG
1	C	76	MSE
1	C	103	GLU
1	C	109[A]	LYS
1	C	109[B]	LYS
1	D	0	HIS

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Mol	Chain	Res	Type
1	D	48	ARG
1	D	76	MSE
1	D	98	ARG
1	D	113	VAL
1	D	116	ASP
1	E	28	VAL
1	G	19	ASN
1	G	52	GLU
1	H	0	HIS
1	H	109	LYS
1	I	1	MSE
1	I	2	ASP
1	I	4	ARG
1	I	48	ARG
1	I	62[A]	ASP
1	I	62[B]	ASP
1	J	-1	HIS
1	J	4	ARG
1	J	76	MSE
1	K	2	ASP
1	L	3	ILE
1	L	4	ARG
1	L	13	SER
1	L	52	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	0	HIS
1	F	31	ASN
1	G	19	ASN
1	I	19	ASN
1	J	-1	HIS
1	J	0	HIS
1	J	19	ASN

5.3.3 RNA

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	B	950	-	5,5,5	0.38	0	5,5,5	0.22	0
2	GOL	A	951	-	5,5,5	0.35	0	5,5,5	0.51	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	B	950	-	-	4/4/4/4	-
2	GOL	A	951	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	951	GOL	C1-C2-C3-O3
2	B	950	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	951	GOL	O2-C2-C3-O3
2	B	950	GOL	C1-C2-C3-O3
2	B	950	GOL	O1-C1-C2-O2
2	A	951	GOL	O1-C1-C2-O2
2	B	950	GOL	O2-C2-C3-O3

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	113/128 (88%)	-1.24	0	100	100	14, 19, 32, 40	0
1	B	115/128 (89%)	-1.24	0	100	100	12, 19, 34, 53	3 (2%)
1	C	115/128 (89%)	-1.22	0	100	100	12, 21, 34, 51	1 (0%)
1	D	114/128 (89%)	-1.07	0	100	100	15, 26, 39, 55	1 (0%)
1	E	112/128 (87%)	-1.07	0	100	100	15, 27, 40, 53	0
1	F	113/128 (88%)	-1.17	0	100	100	14, 23, 35, 47	1 (0%)
1	G	111/128 (86%)	-1.32	0	100	100	10, 18, 27, 40	4 (3%)
1	H	112/128 (87%)	-1.29	0	100	100	12, 19, 32, 54	0
1	I	113/128 (88%)	-1.24	0	100	100	12, 21, 34, 54	3 (2%)
1	J	115/128 (89%)	-1.25	0	100	100	10, 18, 35, 51	0
1	K	115/128 (89%)	-1.14	0	100	100	17, 25, 40, 60	1 (0%)
1	L	111/128 (86%)	-0.86	0	100	100	16, 33, 43, 51	1 (0%)
All	All	1359/1536 (88%)	-1.18	0	100	100	10, 22, 39, 60	15 (1%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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	GOL	B	950	6/6	0.96	0.08	52,53,57,63	0
2	GOL	A	951	6/6	0.98	0.05	35,40,41,45	0

6.5 Other polymers

There are no such residues in this entry.