Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:53 PM GMT

PDB ID	:	5BOB
Title	:	Crystal Structure of the Meningitis Pathogen Streptococcus suis adhesion Fhb
Authors	:	Jiang, Y.; Zhang, C.; Yu, Y.
Deposited on	:	2015-05-27
Resolution	:	1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

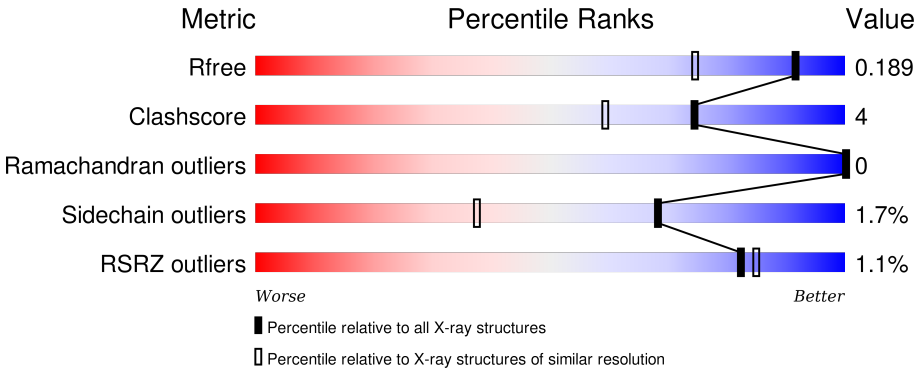
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	226	80% 8% • 10%
1	B	226	% 75% 12% • 12%
1	C	226	% 79% 8% • 12%
1	D	226	% 77% 10% • 12%
1	E	226	% 77% 8% • 13%

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	A	402	-	-	-	X
2	GOL	B	401	-	-	-	X
2	GOL	C	401	-	-	-	X
2	GOL	D	401	-	-	-	X
2	GOL	D	402	-	-	-	X
2	GOL	E	402	-	-	-	X
2	GOL	E	403	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9071 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 Translation initiation factor 2 (IF-2 GTPase).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	Se	0	1	0
			1606	1008	272	325	1			
1	B	199	Total	C	N	O	Se	0	0	0
			1579	993	268	317	1			
1	C	198	Total	C	N	O	Se	0	1	0
			1579	995	267	316	1			
1	D	200	Total	C	N	O	Se	0	1	0
			1590	999	270	320	1			
1	E	196	Total	C	N	O	Se	0	1	0
			1573	989	267	316	1			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	MSE	-	expression tag	UNP A4VT01
A	119	GLY	-	expression tag	UNP A4VT01
A	120	SER	-	expression tag	UNP A4VT01
A	121	SER	-	expression tag	UNP A4VT01
A	122	HIS	-	expression tag	UNP A4VT01
A	123	HIS	-	expression tag	UNP A4VT01
A	124	HIS	-	expression tag	UNP A4VT01
A	125	HIS	-	expression tag	UNP A4VT01
A	126	HIS	-	expression tag	UNP A4VT01
A	127	HIS	-	expression tag	UNP A4VT01
A	128	SER	-	expression tag	UNP A4VT01
A	129	SER	-	expression tag	UNP A4VT01
A	130	GLY	-	expression tag	UNP A4VT01
A	131	LEU	-	expression tag	UNP A4VT01
A	132	VAL	-	expression tag	UNP A4VT01
A	133	PRO	-	expression tag	UNP A4VT01
A	134	ARG	-	expression tag	UNP A4VT01
A	135	GLY	-	expression tag	UNP A4VT01
A	136	SER	-	expression tag	UNP A4VT01

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	HIS	-	expression tag	UNP A4VT01
A	138	MSE	-	expression tag	UNP A4VT01
B	118	MSE	-	expression tag	UNP A4VT01
B	119	GLY	-	expression tag	UNP A4VT01
B	120	SER	-	expression tag	UNP A4VT01
B	121	SER	-	expression tag	UNP A4VT01
B	122	HIS	-	expression tag	UNP A4VT01
B	123	HIS	-	expression tag	UNP A4VT01
B	124	HIS	-	expression tag	UNP A4VT01
B	125	HIS	-	expression tag	UNP A4VT01
B	126	HIS	-	expression tag	UNP A4VT01
B	127	HIS	-	expression tag	UNP A4VT01
B	128	SER	-	expression tag	UNP A4VT01
B	129	SER	-	expression tag	UNP A4VT01
B	130	GLY	-	expression tag	UNP A4VT01
B	131	LEU	-	expression tag	UNP A4VT01
B	132	VAL	-	expression tag	UNP A4VT01
B	133	PRO	-	expression tag	UNP A4VT01
B	134	ARG	-	expression tag	UNP A4VT01
B	135	GLY	-	expression tag	UNP A4VT01
B	136	SER	-	expression tag	UNP A4VT01
B	137	HIS	-	expression tag	UNP A4VT01
B	138	MSE	-	expression tag	UNP A4VT01
C	118	MSE	-	expression tag	UNP A4VT01
C	119	GLY	-	expression tag	UNP A4VT01
C	120	SER	-	expression tag	UNP A4VT01
C	121	SER	-	expression tag	UNP A4VT01
C	122	HIS	-	expression tag	UNP A4VT01
C	123	HIS	-	expression tag	UNP A4VT01
C	124	HIS	-	expression tag	UNP A4VT01
C	125	HIS	-	expression tag	UNP A4VT01
C	126	HIS	-	expression tag	UNP A4VT01
C	127	HIS	-	expression tag	UNP A4VT01
C	128	SER	-	expression tag	UNP A4VT01
C	129	SER	-	expression tag	UNP A4VT01
C	130	GLY	-	expression tag	UNP A4VT01
C	131	LEU	-	expression tag	UNP A4VT01
C	132	VAL	-	expression tag	UNP A4VT01
C	133	PRO	-	expression tag	UNP A4VT01
C	134	ARG	-	expression tag	UNP A4VT01
C	135	GLY	-	expression tag	UNP A4VT01
C	136	SER	-	expression tag	UNP A4VT01

Continued on next page...

Continued from previous page...

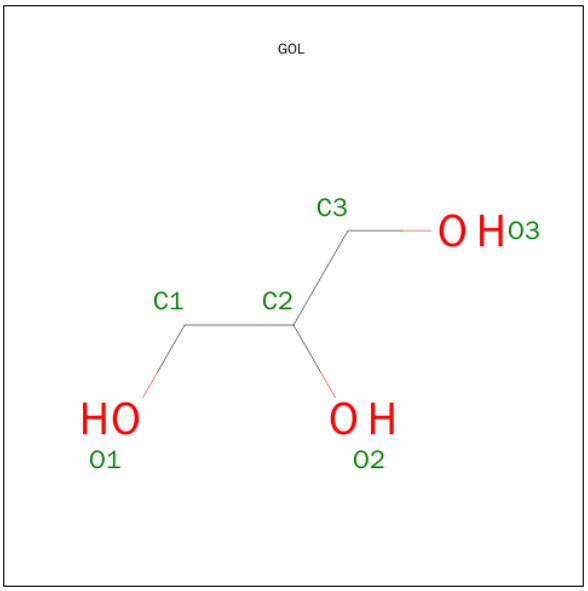
Chain	Residue	Modelled	Actual	Comment	Reference
C	137	HIS	-	expression tag	UNP A4VT01
C	138	MSE	-	expression tag	UNP A4VT01
D	118	MSE	-	expression tag	UNP A4VT01
D	119	GLY	-	expression tag	UNP A4VT01
D	120	SER	-	expression tag	UNP A4VT01
D	121	SER	-	expression tag	UNP A4VT01
D	122	HIS	-	expression tag	UNP A4VT01
D	123	HIS	-	expression tag	UNP A4VT01
D	124	HIS	-	expression tag	UNP A4VT01
D	125	HIS	-	expression tag	UNP A4VT01
D	126	HIS	-	expression tag	UNP A4VT01
D	127	HIS	-	expression tag	UNP A4VT01
D	128	SER	-	expression tag	UNP A4VT01
D	129	SER	-	expression tag	UNP A4VT01
D	130	GLY	-	expression tag	UNP A4VT01
D	131	LEU	-	expression tag	UNP A4VT01
D	132	VAL	-	expression tag	UNP A4VT01
D	133	PRO	-	expression tag	UNP A4VT01
D	134	ARG	-	expression tag	UNP A4VT01
D	135	GLY	-	expression tag	UNP A4VT01
D	136	SER	-	expression tag	UNP A4VT01
D	137	HIS	-	expression tag	UNP A4VT01
D	138	MSE	-	expression tag	UNP A4VT01
E	118	MSE	-	expression tag	UNP A4VT01
E	119	GLY	-	expression tag	UNP A4VT01
E	120	SER	-	expression tag	UNP A4VT01
E	121	SER	-	expression tag	UNP A4VT01
E	122	HIS	-	expression tag	UNP A4VT01
E	123	HIS	-	expression tag	UNP A4VT01
E	124	HIS	-	expression tag	UNP A4VT01
E	125	HIS	-	expression tag	UNP A4VT01
E	126	HIS	-	expression tag	UNP A4VT01
E	127	HIS	-	expression tag	UNP A4VT01
E	128	SER	-	expression tag	UNP A4VT01
E	129	SER	-	expression tag	UNP A4VT01
E	130	GLY	-	expression tag	UNP A4VT01
E	131	LEU	-	expression tag	UNP A4VT01
E	132	VAL	-	expression tag	UNP A4VT01
E	133	PRO	-	expression tag	UNP A4VT01
E	134	ARG	-	expression tag	UNP A4VT01
E	135	GLY	-	expression tag	UNP A4VT01
E	136	SER	-	expression tag	UNP A4VT01

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	137	HIS	-	expression tag	UNP A4VT01
E	138	MSE	-	expression tag	UNP A4VT01

- 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	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is water.

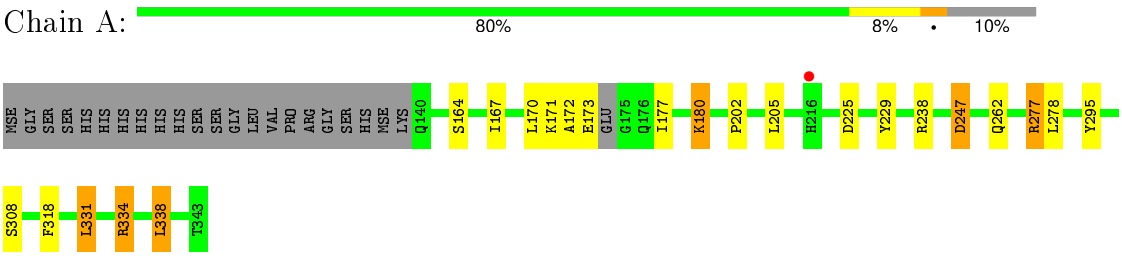
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	209	Total	O	0	0
			209	209		
3	B	183	Total	O	0	0
			183	183		
3	C	219	Total	O	0	0
			219	219		
3	D	227	Total	O	0	0
			227	227		
3	E	240	Total	O	0	0
			240	240		

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

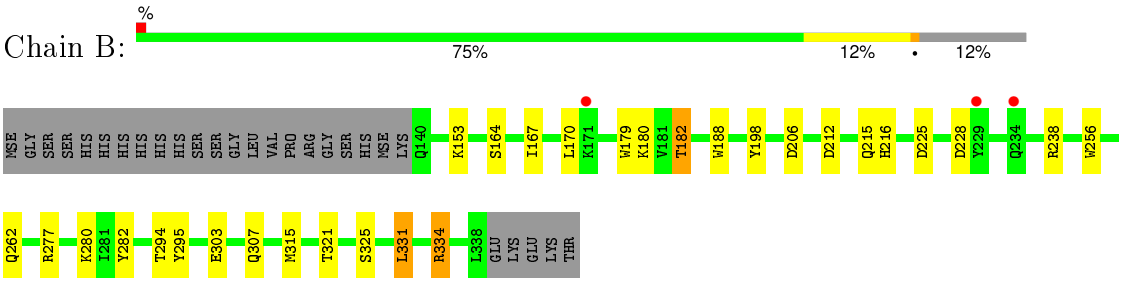
- Molecule 1: Translation initiation factor 2 (IF-2 GTPase)

Chain A:



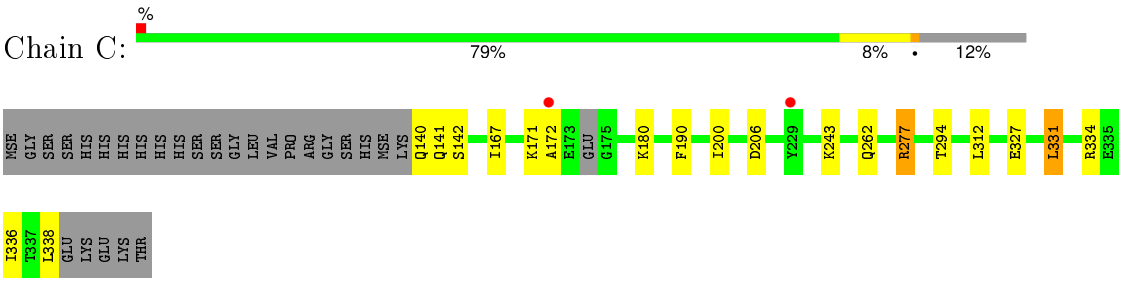
- Molecule 1: Translation initiation factor 2 (IF-2 GTPase)

Chain B:



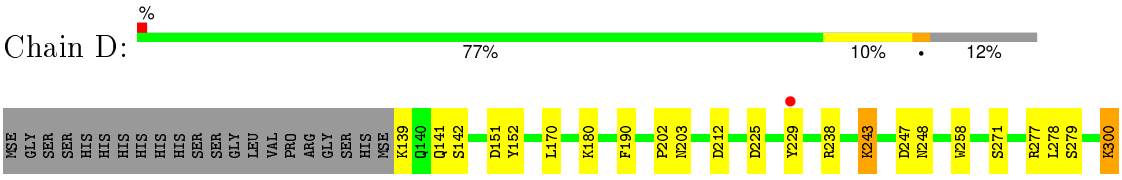
- Molecule 1: Translation initiation factor 2 (IF-2 GTPase)

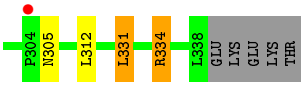
Chain C:



- Molecule 1: Translation initiation factor 2 (IF-2 GTPase)

Chain D:





• Molecule 1: Translation initiation factor 2 (IF-2 GTPase)

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.08Å 77.34Å 131.64Å 90.00° 115.93° 90.00°	Depositor
Resolution (Å)	39.46 – 1.50 39.46 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (39.46-1.50) 97.0 (39.46-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.161 , 0.189 0.161 , 0.189	Depositor DCC
R_{free} test set	8926 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.6	EDS
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 178754 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9071	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.42	6/1645 (0.4%)	1.45	19/2231 (0.9%)
1	B	1.40	7/1612 (0.4%)	1.27	12/2187 (0.5%)
1	C	1.38	5/1614 (0.3%)	1.34	10/2188 (0.5%)
1	D	1.51	10/1629 (0.6%)	1.47	20/2210 (0.9%)
1	E	1.39	3/1605 (0.2%)	1.26	12/2176 (0.6%)
All	All	1.42	31/8105 (0.4%)	1.36	73/10992 (0.7%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	262	GLN	CB-CG	-11.85	1.20	1.52
1	A	262	GLN	CB-CG	-10.45	1.24	1.52
1	D	334	ARG	CB-CG	-8.99	1.28	1.52
1	C	262	GLN	CB-CG	-7.87	1.31	1.52
1	D	334	ARG	CD-NE	-7.66	1.33	1.46
1	C	334	ARG	CB-CG	-7.01	1.33	1.52
1	A	308	SER	CB-OG	-6.96	1.33	1.42
1	E	232	SER	CB-OG	6.84	1.51	1.42
1	A	180	LYS	CB-CG	-6.74	1.34	1.52
1	D	258	TRP	CE3-CZ3	6.67	1.49	1.38
1	C	142	SER	CB-OG	6.39	1.50	1.42
1	C	334	ARG	CD-NE	-6.34	1.35	1.46
1	D	305	ASN	C-O	6.29	1.35	1.23
1	D	229	TYR	CG-CD1	6.19	1.47	1.39
1	D	229	TYR	CE2-CZ	6.19	1.46	1.38
1	D	271	SER	CB-OG	6.16	1.50	1.42
1	D	229	TYR	CA-CB	6.15	1.67	1.53
1	B	303	GLU	CB-CG	-6.14	1.40	1.52
1	A	247	ASP	CA-C	6.08	1.68	1.52
1	B	295	TYR	CE2-CZ	5.78	1.46	1.38
1	B	256	TRP	CZ3-CH2	5.50	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	TYR	CG-CD2	5.48	1.46	1.39
1	D	300	LYS	CD-CE	5.48	1.65	1.51
1	E	186	SER	CB-OG	-5.36	1.35	1.42
1	C	327	GLU	CD-OE2	5.29	1.31	1.25
1	B	262	GLN	CB-CG	-5.28	1.38	1.52
1	A	334	ARG	CG-CD	-5.26	1.38	1.51
1	B	164	SER	CB-OG	5.20	1.49	1.42
1	D	152	TYR	CE1-CZ	-5.16	1.31	1.38
1	B	334	ARG	CB-CG	-5.00	1.39	1.52
1	A	164	SER	CB-OG	5.00	1.48	1.42

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277	ARG	NE-CZ-NH2	-27.96	106.32	120.30
1	D	334	ARG	NE-CZ-NH2	-18.30	111.15	120.30
1	C	277	ARG	NE-CZ-NH2	-17.26	111.67	120.30
1	A	277	ARG	NE-CZ-NH1	16.40	128.50	120.30
1	C	334	ARG	NE-CZ-NH2	-15.74	112.43	120.30
1	D	334	ARG	CG-CD-NE	-15.33	79.60	111.80
1	C	277	ARG	NE-CZ-NH1	13.28	126.94	120.30
1	A	277	ARG	CD-NE-CZ	10.91	138.88	123.60
1	E	225	ASP	CB-CG-OD1	10.47	127.72	118.30
1	A	225	ASP	CB-CG-OD1	9.81	127.13	118.30
1	D	334	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	C	334	ARG	NE-CZ-NH1	9.43	125.01	120.30
1	E	277	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	D	277	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	D	312[A]	LEU	CA-CB-CG	8.86	135.67	115.30
1	D	312[B]	LEU	CA-CB-CG	8.86	135.67	115.30
1	E	338	LEU	CB-CG-CD1	8.70	125.79	111.00
1	D	225	ASP	CB-CG-OD1	8.56	126.00	118.30
1	D	238	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	C	277	ARG	CD-NE-CZ	8.32	135.25	123.60
1	B	277	ARG	NE-CZ-NH2	8.03	124.31	120.30
1	A	247	ASP	CB-CA-C	7.86	126.12	110.40
1	A	238	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	B	225	ASP	CB-CG-OD1	7.39	124.95	118.30
1	C	334	ARG	CG-CD-NE	-7.26	96.55	111.80
1	D	190	PHE	CB-CG-CD2	-7.22	115.75	120.80
1	B	212	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	D	331	LEU	CB-CG-CD1	7.19	123.23	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	206	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	D	151	ASP	CB-CG-OD2	-7.01	112.00	118.30
1	B	334	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	D	312[A]	LEU	CB-CG-CD1	-6.84	99.37	111.00
1	D	312[B]	LEU	CB-CG-CD1	-6.84	99.37	111.00
1	D	334	ARG	CD-NE-CZ	6.66	132.92	123.60
1	A	225	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	B	331	LEU	CA-CB-CG	6.49	130.23	115.30
1	E	331	LEU	CB-CG-CD1	6.39	121.87	111.00
1	E	157	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	E	162	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	D	247	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	334	ARG	CG-CD-NE	-6.24	98.69	111.80
1	A	331	LEU	CA-CB-CG	6.21	129.58	115.30
1	A	318	PHE	CB-CG-CD1	-6.19	116.47	120.80
1	C	190	PHE	CB-CG-CD2	-6.17	116.48	120.80
1	D	151	ASP	CB-CG-OD1	6.16	123.84	118.30
1	E	282	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	B	282	TYR	CB-CG-CD1	-5.99	117.41	121.00
1	D	212	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	229	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	B	238	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	295	TYR	CD1-CE1-CZ	-5.87	114.51	119.80
1	A	295	TYR	CB-CG-CD2	-5.79	117.52	121.00
1	E	238	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	277	ARG	CG-CD-NE	5.58	123.52	111.80
1	A	247	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	334	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	229	TYR	CA-CB-CG	5.51	123.88	113.40
1	D	334	ARG	CB-CA-C	-5.50	99.40	110.40
1	C	206	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	331	LEU	CA-CB-CG	5.37	127.65	115.30
1	D	334	ARG	CA-CB-CG	5.36	125.19	113.40
1	B	282	TYR	CG-CD1-CE1	-5.30	117.06	121.30
1	E	247	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	262	GLN	CB-CA-C	-5.24	99.92	110.40
1	C	262	GLN	CB-CA-C	-5.21	99.97	110.40
1	E	334	ARG	CG-CD-NE	-5.20	100.88	111.80
1	E	277	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	229	TYR	CG-CD2-CE2	-5.17	117.17	121.30
1	A	247	ASP	N-CA-C	-5.13	97.16	111.00
1	E	190	PHE	CB-CG-CD2	-5.09	117.24	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	331	LEU	CB-CG-CD2	5.06	119.60	111.00
1	A	277	ARG	NH1-CZ-NH2	5.04	124.95	119.40
1	B	225	ASP	CB-CG-OD2	-5.04	113.76	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1606	0	1521	10	0
1	B	1579	0	1516	18	0
1	C	1579	0	1524	8	0
1	D	1590	0	1514	10	0
1	E	1573	0	1513	15	0
2	A	12	0	16	0	0
2	B	18	0	24	0	0
2	C	6	0	8	0	0
2	D	12	0	16	0	0
2	E	18	0	24	3	0
3	A	209	0	0	3	0
3	B	183	0	0	5	0
3	C	219	0	0	2	0
3	D	227	0	0	3	0
3	E	240	0	0	5	0
All	All	9071	0	7676	62	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 (62) 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:C:243:LYS:HG2	3:C:513:HOH:O	1.57	1.05
1:D:142:SER:O	1:D:334:ARG:HD3	1.57	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:LEU:HD13	1:B:179:TRP:HA	1.57	0.84
1:D:142:SER:O	1:D:334:ARG:CD	2.27	0.82
1:A:247:ASP:O	3:A:502:HOH:O	1.96	0.81
1:E:311:LEU:HD11	1:E:336:ILE:CD1	2.20	0.72
1:D:139:LYS:N	3:D:501:HOH:O	2.21	0.72
1:E:311:LEU:CD1	1:E:336:ILE:HD11	2.21	0.71
1:B:307:GLN:H	1:E:276[B]:ASN:HD21	1.39	0.68
1:E:156:LYS:NZ	3:E:503:HOH:O	2.28	0.67
1:B:170:LEU:HD13	1:B:179:TRP:CA	2.26	0.66
1:E:169:LEU:HD13	1:E:336:ILE:HD13	1.79	0.64
1:A:170:LEU:HD21	1:A:180:LYS:HE2	1.80	0.64
2:E:403:GOL:C3	3:E:501:HOH:O	2.42	0.63
1:B:215:GLN:NE2	3:B:501:HOH:O	2.32	0.63
1:E:311:LEU:HD11	1:E:336:ILE:HD12	1.81	0.61
1:B:182:THR:HG23	3:B:557:HOH:O	1.99	0.61
1:E:160:LYS:NZ	3:E:505:HOH:O	2.33	0.61
2:E:403:GOL:H31	3:E:501:HOH:O	1.99	0.60
1:B:170:LEU:N	1:B:170:LEU:HD12	2.17	0.60
1:E:311:LEU:HD12	1:E:336:ILE:HD11	1.84	0.59
1:B:216:HIS:HB3	3:B:660:HOH:O	2.03	0.59
1:C:140:GLN:CB	3:C:703:HOH:O	2.50	0.59
1:E:311:LEU:CD1	1:E:336:ILE:CD1	2.81	0.58
1:D:170:LEU:HD11	1:D:180:LYS:HG3	1.85	0.58
3:D:680:HOH:O	1:E:156:LYS:HE2	2.04	0.57
1:B:228:ASP:CG	3:B:502:HOH:O	2.44	0.56
1:B:307:GLN:H	1:E:276[B]:ASN:ND2	2.03	0.55
1:E:167:ILE:O	1:E:334:ARG:HD2	2.06	0.55
1:D:203:ASN:ND2	1:D:243:LYS:NZ	2.54	0.55
1:B:167:ILE:O	1:B:334:ARG:HD2	2.06	0.55
1:C:172:ALA:HB1	1:C:338:LEU:CD2	2.38	0.53
1:C:141:GLN:HG2	1:C:336:ILE:HD12	1.91	0.53
1:B:180:LYS:HG3	1:B:294:THR:HG23	1.91	0.52
1:B:170:LEU:CD1	1:B:179:TRP:HA	2.33	0.52
1:E:311:LEU:HD11	1:E:336:ILE:HD11	1.83	0.52
1:D:141:GLN:HB2	1:D:334:ARG:HD2	1.92	0.52
1:B:321:THR:OG1	1:B:325:SER:C	2.48	0.52
1:A:247:ASP:CB	3:A:501:HOH:O	2.57	0.49
1:A:171:LYS:NZ	1:A:173:GLU:OE2	2.38	0.48
1:A:172:ALA:HB1	1:A:338:LEU:CD2	2.43	0.48
1:A:167:ILE:O	1:A:334:ARG:HD2	2.14	0.48
1:A:247:ASP:HB3	3:A:501:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:403:GOL:H32	3:E:521:HOH:O	2.13	0.47
1:B:188:TRP:CE2	1:B:315:MSE:HE2	2.49	0.46
1:A:172:ALA:HB1	1:A:338:LEU:HD21	1.97	0.46
1:A:177:ILE:HD12	1:A:205:LEU:HD21	1.96	0.46
1:B:280:LYS:NZ	3:B:505:HOH:O	2.48	0.46
1:A:202:PRO:HA	1:A:278:LEU:HA	1.99	0.45
1:D:203:ASN:ND2	1:D:279:SER:HB3	2.31	0.45
1:C:172:ALA:HB1	1:C:338:LEU:HD21	1.99	0.44
1:E:309:PHE:HE2	1:E:338:LEU:HD22	1.83	0.44
1:C:200:ILE:HB	1:C:312[B]:LEU:HB3	2.00	0.44
1:B:180:LYS:HG3	1:B:294:THR:CG2	2.48	0.44
1:B:170:LEU:N	1:B:170:LEU:CD1	2.79	0.43
1:C:141:GLN:HG2	1:C:336:ILE:CD1	2.48	0.43
1:E:171:LYS:HE3	1:E:171:LYS:HB2	1.83	0.43
1:C:180:LYS:HG3	1:C:294:THR:HG23	2.01	0.43
1:D:203:ASN:ND2	1:D:243:LYS:HZ1	2.16	0.43
1:B:153:LYS:NZ	1:B:321:THR:HG23	2.34	0.42
1:D:202:PRO:HA	1:D:278:LEU:HA	2.02	0.41
1:D:248:ASN:HB3	3:D:642:HOH:O	2.22	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	200/226 (88%)	194 (97%)	6 (3%)	0	100	100
1	B	197/226 (87%)	191 (97%)	6 (3%)	0	100	100
1	C	195/226 (86%)	187 (96%)	8 (4%)	0	100	100
1	D	199/226 (88%)	193 (97%)	6 (3%)	0	100	100
1	E	193/226 (85%)	187 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	984/1130 (87%)	952 (97%)	32 (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	180/201 (90%)	177 (98%)	3 (2%)	68 37
1	B	177/201 (88%)	175 (99%)	2 (1%)	80 58
1	C	178/201 (89%)	174 (98%)	4 (2%)	60 25
1	D	179/201 (89%)	176 (98%)	3 (2%)	68 37
1	E	178/201 (89%)	175 (98%)	3 (2%)	68 37
All	All	892/1005 (89%)	877 (98%)	15 (2%)	68 37

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	ARG
1	A	331	LEU
1	A	338	LEU
1	B	182	THR
1	B	331	LEU
1	C	167	ILE
1	C	171	LYS
1	C	277	ARG
1	C	331	LEU
1	D	243	LYS
1	D	300	LYS
1	D	331	LEU
1	E	171	LYS
1	E	331	LEU
1	E	338	LEU

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

Mol	Chain	Res	Type
1	A	178	GLN
1	A	262	GLN
1	B	255	GLN
1	C	262	GLN
1	D	203	ASN
1	E	234	GLN
1	E	262	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

11 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	401	-	5,5,5	0.75	0	5,5,5	0.45	0
2	GOL	A	402	-	5,5,5	0.67	0	5,5,5	1.13	0
2	GOL	B	401	-	5,5,5	0.41	0	5,5,5	1.29	1 (20%)
2	GOL	B	402	-	5,5,5	0.52	0	5,5,5	0.73	0
2	GOL	B	403	-	5,5,5	0.33	0	5,5,5	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	C	401	-	5,5,5	0.41	0	5,5,5	1.27	1 (20%)
2	GOL	D	401	-	5,5,5	0.51	0	5,5,5	0.59	0
2	GOL	D	402	-	5,5,5	0.63	0	5,5,5	1.41	1 (20%)
2	GOL	E	401	-	5,5,5	0.78	0	5,5,5	0.84	0
2	GOL	E	402	-	5,5,5	0.54	0	5,5,5	1.23	1 (20%)
2	GOL	E	403	-	5,5,5	0.53	0	5,5,5	1.42	1 (20%)

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	401	-	-	0/4/4/4	0/0/0/0
2	GOL	A	402	-	-	0/4/4/4	0/0/0/0
2	GOL	B	401	-	-	0/4/4/4	0/0/0/0
2	GOL	B	402	-	-	0/4/4/4	0/0/0/0
2	GOL	B	403	-	-	0/4/4/4	0/0/0/0
2	GOL	C	401	-	-	0/4/4/4	0/0/0/0
2	GOL	D	401	-	-	0/4/4/4	0/0/0/0
2	GOL	D	402	-	-	0/4/4/4	0/0/0/0
2	GOL	E	401	-	-	0/4/4/4	0/0/0/0
2	GOL	E	402	-	-	0/4/4/4	0/0/0/0
2	GOL	E	403	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	GOL	C3-C2-C1	-2.33	101.24	111.06
2	B	401	GOL	C3-C2-C1	-2.29	101.41	111.06
2	E	403	GOL	C3-C2-C1	-2.17	101.91	111.06
2	E	402	GOL	O3-C3-C2	-2.16	99.03	109.97
2	D	402	GOL	O2-C2-C1	2.64	121.17	108.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	403	GOL	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	202/226 (89%)	-0.28	1 (0%)	91	93	13, 18, 32, 46	0
1	B	198/226 (87%)	-0.20	3 (1%)	76	79	13, 19, 31, 37	0
1	C	197/226 (87%)	-0.18	2 (1%)	84	86	12, 17, 30, 41	0
1	D	199/226 (88%)	-0.12	2 (1%)	84	86	11, 16, 30, 38	0
1	E	195/226 (86%)	-0.31	3 (1%)	76	79	11, 16, 27, 36	0
All	All	991/1130 (87%)	-0.22	11 (1%)	82	85	11, 17, 30, 46	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	TYR	3.6
1	C	172	ALA	3.4
1	D	304	PRO	3.4
1	C	229	TYR	3.3
1	B	234	GLN	2.7
1	A	216	HIS	2.6
1	E	215	GLN	2.5
1	E	214	ASN	2.5
1	E	171	LYS	2.2
1	D	229	TYR	2.2
1	B	171	LYS	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	B	401	6/6	0.91	0.17	7.19	24,30,35,40	0
2	GOL	E	403	6/6	0.95	0.11	4.96	20,26,33,41	0
2	GOL	D	402	6/6	0.92	0.13	3.08	18,23,32,33	0
2	GOL	D	401	6/6	0.98	0.10	2.94	13,14,16,16	0
2	GOL	A	402	6/6	0.96	0.08	2.84	18,22,26,34	0
2	GOL	C	401	6/6	0.90	0.11	2.77	21,25,30,38	0
2	GOL	E	402	6/6	0.95	0.08	2.27	16,19,25,34	0
2	GOL	B	403	6/6	0.98	0.13	1.99	18,24,26,33	0
2	GOL	E	401	6/6	0.98	0.07	1.15	12,14,15,16	0
2	GOL	A	401	6/6	0.98	0.07	0.46	14,15,15,16	0
2	GOL	B	402	6/6	0.98	0.07	-0.56	15,17,18,20	0

6.5 Other polymers

There are no such residues in this entry.