



# Full wwPDB X-ray Structure Validation Report

May 25, 2020 – 02:16 pm BST

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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

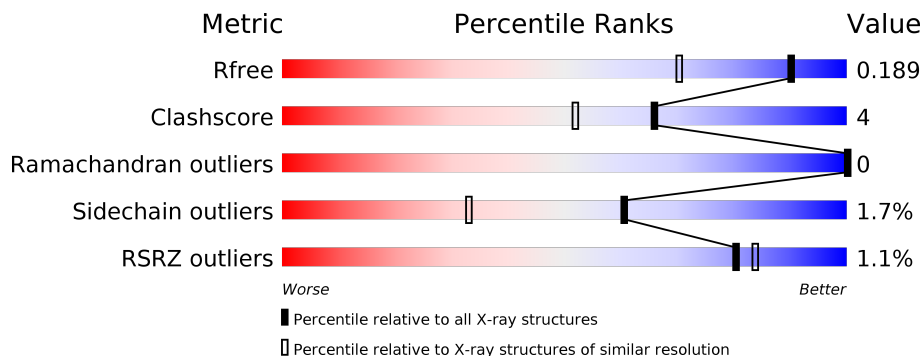
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	226	
1	B	226	
1	C	226	
1	D	226	
1	E	226	

## 2 Entry composition [i](#)

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

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

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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

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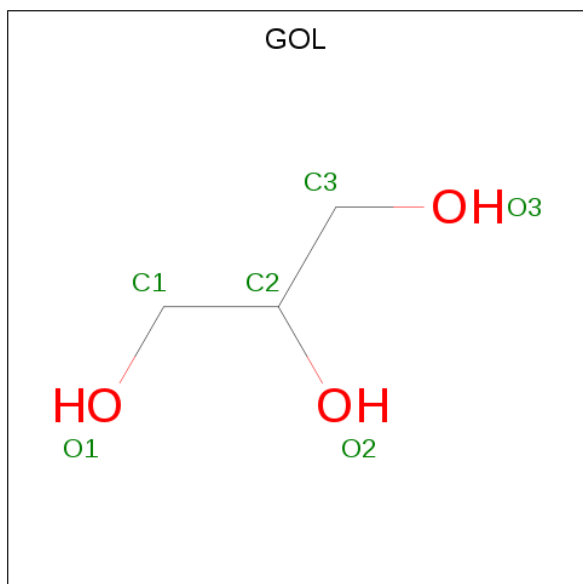
Chain	Residue	Modelled	Actual	Comment	Reference
C	137	HIS	-	expression tag	UNP A4VT01
C	138	MSE	-	expression tag	UNP A4VT01
D	118	MSE	-	expression tag	UNP A4VT01
D	119	GLY	-	expression tag	UNP A4VT01
D	120	SER	-	expression tag	UNP A4VT01
D	121	SER	-	expression tag	UNP A4VT01
D	122	HIS	-	expression tag	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

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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<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

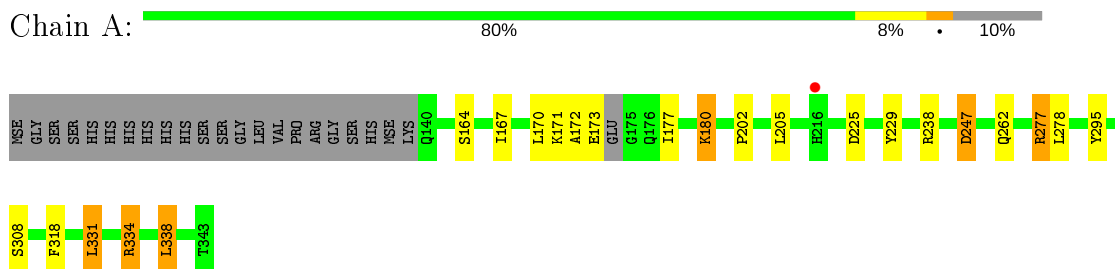
- Molecule 3 is water.

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

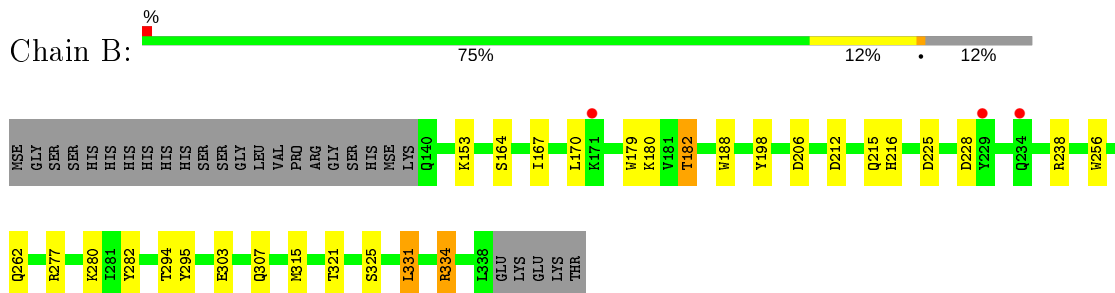
### 3 Residue-property plots [i](#)

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

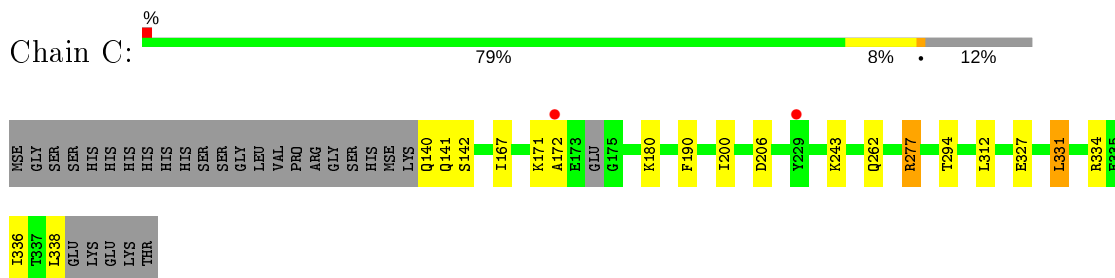
- Molecule 1: Translation initiation factor 2 (IF-2 GTPase)



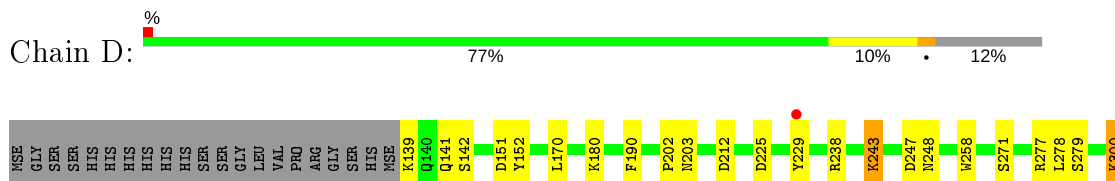
- Molecule 1: Translation initiation factor 2 (IF-2 GTPase)



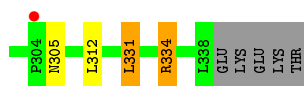
- Molecule 1: Translation initiation factor 2 (IF-2 GTPase)



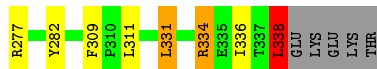
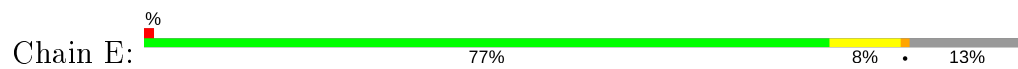
- Molecule 1: Translation initiation factor 2 (IF-2 GTPase)







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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.08 Å 77.34 Å 131.64 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 1.50 Å)	Xtrriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.161 , 0.189 0.161 , 0.189	Depositor DCC
$R_{free}$ test set	8957 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtrriage
Anisotropy	0.296	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9071	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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

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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(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 [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	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

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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

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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

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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%)	60	33
1	B	177/201 (88%)	175 (99%)	2 (1%)	73	53
1	C	178/201 (89%)	174 (98%)	4 (2%)	52	22
1	D	179/201 (89%)	176 (98%)	3 (2%)	60	33
1	E	178/201 (89%)	175 (98%)	3 (2%)	60	33
All	All	892/1005 (89%)	877 (98%)	15 (2%)	60	33

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 [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	E	403	-	5,5,5	0.47	0	5,5,5	1.58	1 (20%)
2	GOL	B	402	-	5,5,5	0.51	0	5,5,5	0.82	0
2	GOL	D	402	-	5,5,5	0.56	0	5,5,5	1.43	1 (20%)
2	GOL	B	401	-	5,5,5	0.46	0	5,5,5	1.42	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	A	401	-	5,5,5	0.79	0	5,5,5	0.53	0
2	GOL	D	401	-	5,5,5	0.55	0	5,5,5	0.69	0
2	GOL	C	401	-	5,5,5	0.40	0	5,5,5	1.41	1 (20%)
2	GOL	E	401	-	5,5,5	0.81	0	5,5,5	0.93	0
2	GOL	A	402	-	5,5,5	0.71	0	5,5,5	1.27	1 (20%)
2	GOL	E	402	-	5,5,5	0.58	0	5,5,5	1.37	1 (20%)
2	GOL	B	403	-	5,5,5	0.38	0	5,5,5	0.94	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	E	403	-	-	1/4/4/4	-
2	GOL	B	402	-	-	0/4/4/4	-
2	GOL	D	402	-	-	1/4/4/4	-
2	GOL	B	401	-	-	0/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	D	401	-	-	0/4/4/4	-
2	GOL	C	401	-	-	0/4/4/4	-
2	GOL	E	401	-	-	0/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-
2	GOL	E	402	-	-	0/4/4/4	-
2	GOL	B	403	-	-	0/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	402	GOL	O2-C2-C1	2.73	121.17	109.12
2	C	401	GOL	C3-C2-C1	-2.69	101.24	111.70
2	B	401	GOL	C3-C2-C1	-2.65	101.41	111.70
2	E	403	GOL	C3-C2-C1	-2.52	101.91	111.70
2	E	402	GOL	O3-C3-C2	-2.33	99.03	110.20
2	A	402	GOL	C3-C2-C1	-2.07	103.66	111.70

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	402	GOL	O1-C1-C2-O2
2	E	403	GOL	C1-C2-C3-O3

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	202/226 (89%)	-0.27	1 (0%) 91 93	13, 18, 32, 46	0
1	B	198/226 (87%)	-0.19	3 (1%) 73 78	13, 19, 31, 37	0
1	C	197/226 (87%)	-0.18	2 (1%) 82 85	12, 17, 30, 41	0
1	D	199/226 (88%)	-0.12	2 (1%) 82 85	11, 16, 30, 38	0
1	E	195/226 (86%)	-0.30	3 (1%) 73 78	11, 16, 27, 36	0
All	All	991/1130 (87%)	-0.21	11 (1%) 80 84	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	2.3
1	D	229	TYR	2.2
1	B	171	LYS	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	GOL	C	401	6/6	0.90	0.11	21,25,30,38	0
2	GOL	B	401	6/6	0.91	0.17	24,30,35,40	0
2	GOL	D	402	6/6	0.92	0.13	18,23,32,33	0
2	GOL	E	403	6/6	0.95	0.11	20,26,33,41	0
2	GOL	E	402	6/6	0.95	0.08	16,19,25,34	0
2	GOL	A	402	6/6	0.96	0.08	18,22,26,34	0
2	GOL	B	402	6/6	0.98	0.07	15,17,18,20	0
2	GOL	E	401	6/6	0.98	0.07	12,14,15,16	0
2	GOL	A	401	6/6	0.98	0.07	14,15,15,16	0
2	GOL	D	401	6/6	0.98	0.10	13,14,16,16	0
2	GOL	B	403	6/6	0.98	0.13	18,24,26,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.