Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2016 – 04:30 AM EDT

PDB ID	:	5BOA
Title	:	Crystal Structure of the Meningitis Pathogen Streptococcus suis adhesion Fhb bound to the disaccharide receptor Gb2
Authors	:	Zhang, C.; Yu, Y.; Yang, M.; Jiang, Y.
Deposited on	:	2015-05-27
Resolution	:	2.71 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:

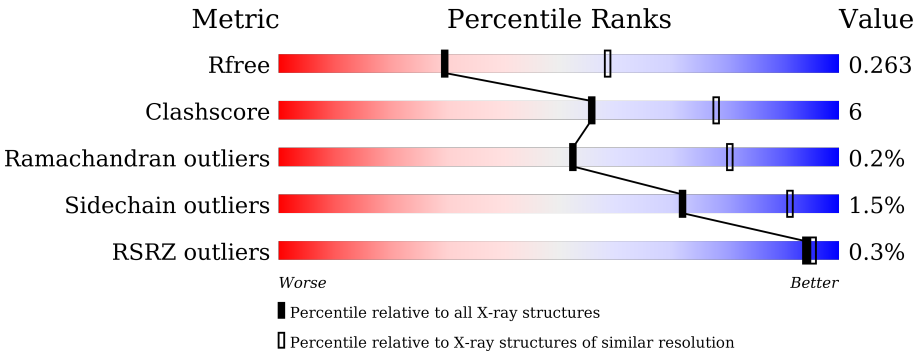
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027257
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027257

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 2.71 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	68% 18% 14%
1	B	226	77% 11% 12%
1	C	226	74% 12% • 12%
1	D	226	75% 12% 13%
1	E	226	75% 10% 15%
1	F	226	65% 19% • 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9415 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	194	Total	C	N	O	S	0	0	0
			1549	975	261	312	1			
1	B	198	Total	C	N	O	S	0	0	0
			1570	987	265	317	1			
1	C	198	Total	C	N	O	S	0	0	0
			1565	982	265	317	1			
1	D	196	Total	C	N	O	S	0	0	0
			1561	983	264	313	1			
1	E	191	Total	C	N	O	S	0	0	0
			1515	954	256	304	1			
1	F	192	Total	C	N	O	S	0	0	0
			1517	953	258	305	1			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	MET	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	135	GLY	-	expression tag	UNP A4VT01
A	136	SER	-	expression tag	UNP A4VT01
A	137	HIS	-	expression tag	UNP A4VT01
A	138	MET	-	expression tag	UNP A4VT01
B	118	MET	-	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	MET	-	expression tag	UNP A4VT01
C	118	MET	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	135	GLY	-	expression tag	UNP A4VT01
C	136	SER	-	expression tag	UNP A4VT01
C	137	HIS	-	expression tag	UNP A4VT01
C	138	MET	-	expression tag	UNP A4VT01
D	118	MET	-	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	MET	-	expression tag	UNP A4VT01
E	118	MET	-	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

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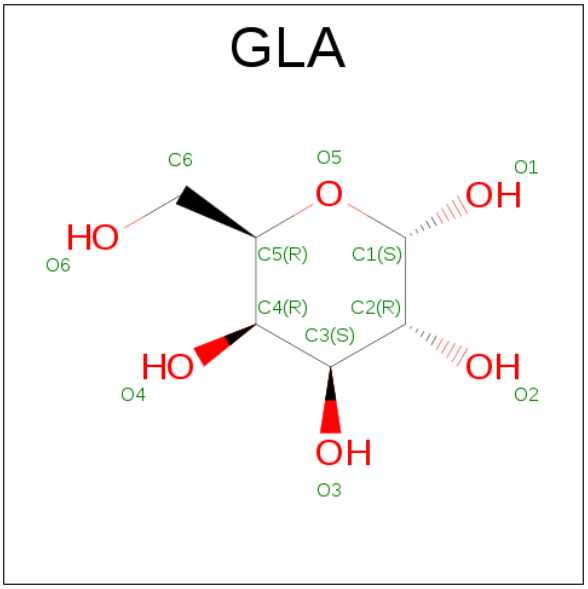
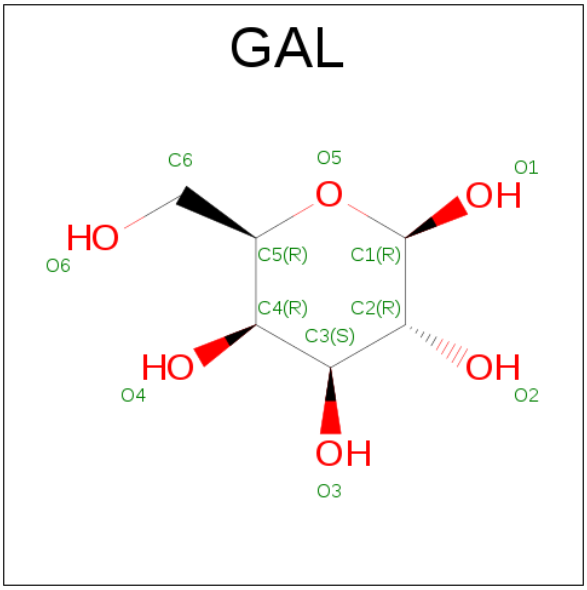
Chain	Residue	Modelled	Actual	Comment	Reference
E	135	GLY	-	expression tag	UNP A4VT01
E	136	SER	-	expression tag	UNP A4VT01
E	137	HIS	-	expression tag	UNP A4VT01
E	138	MET	-	expression tag	UNP A4VT01
F	118	MET	-	expression tag	UNP A4VT01
F	119	GLY	-	expression tag	UNP A4VT01
F	120	SER	-	expression tag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

- Molecule 2 is ALPHA D-GALACTOSE (three-letter code: GLA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 11 6 5	0	0
2	B	1	Total C O 11 6 5	0	0
2	C	1	Total C O 11 6 5	0	0
2	D	1	Total C O 11 6 5	0	0
2	E	1	Total C O 11 6 5	0	0
2	F	1	Total C O 11 6 5	0	0

- Molecule 3 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



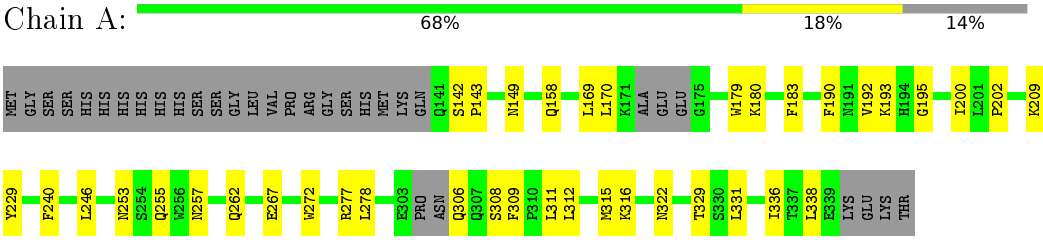
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0
3	B	1	Total C O 12 6 6	0	0
3	C	1	Total C O 12 6 6	0	0
3	D	1	Total C O 12 6 6	0	0
3	E	1	Total C O 12 6 6	0	0
3	F	1	Total C O 12 6 6	0	0

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 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.

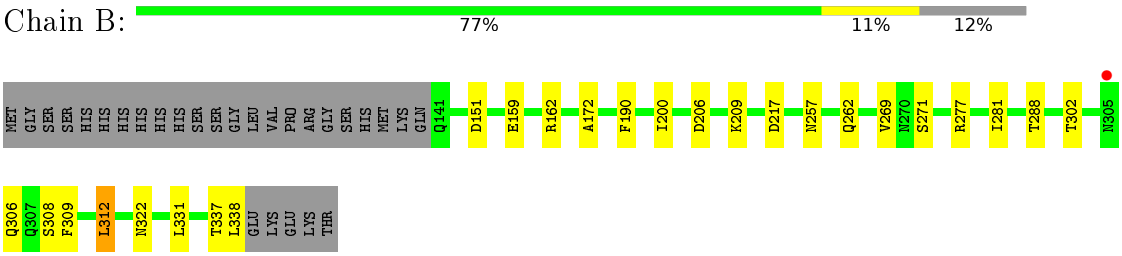
- Molecule 1: Translation initiation factor 2 (IF-2 GTPase)

Chain A:



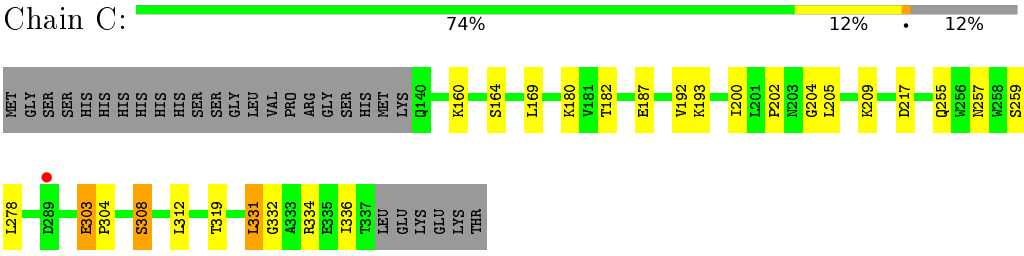
- Molecule 1: Translation initiation factor 2 (IF-2 GTPase)

Chain B:



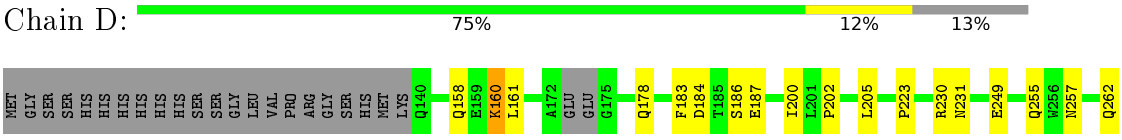
- Molecule 1: Translation initiation factor 2 (IF-2 GTPase)

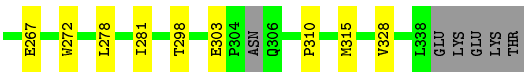
Chain C:



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

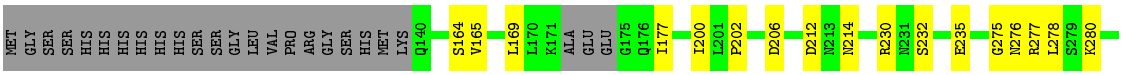
Chain D:

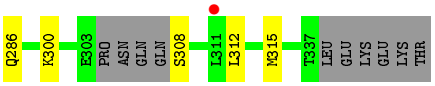




• Molecule 1: Translation initiation factor 2 (IF-2 GTPase)

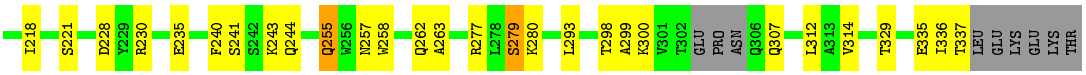
Chain E:





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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	126.49Å 136.57Å 75.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.49 – 2.71 48.50 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.49-2.71) 99.5 (48.50-2.71)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.20 (at 2.73Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.264 0.185 , 0.263	Depositor DCC
R_{free} test set	1805 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.856	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9415	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: GLA, GAL

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	0.48	0/1580	0.61	0/2140
1	B	0.42	0/1604	0.59	0/2179
1	C	0.43	0/1598	0.62	1/2169 (0.0%)
1	D	0.41	0/1593	0.57	0/2159
1	E	0.44	0/1546	0.61	0/2096
1	F	0.43	0/1547	0.62	0/2097
All	All	0.43	0/9468	0.60	1/12840 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	331	LEU	CA-CB-CG	6.20	129.56	115.30

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	1549	0	1490	25	0
1	B	1570	0	1501	12	0
1	C	1565	0	1496	17	0
1	D	1561	0	1504	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1515	0	1450	15	0
1	F	1517	0	1451	33	0
2	A	11	0	10	0	0
2	B	11	0	10	0	0
2	C	11	0	10	0	0
2	D	11	0	10	1	0
2	E	11	0	10	0	0
2	F	11	0	10	0	0
3	A	12	0	11	0	0
3	B	12	0	10	0	0
3	C	12	0	10	0	0
3	D	12	0	10	0	0
3	E	12	0	10	0	0
3	F	12	0	10	1	0
All	All	9415	0	9013	114	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 6.

All (114) 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:A:183:PHE:HD1	1:A:315:MET:HE2	1.36	0.89
1:D:160:LYS:HE3	1:D:187:GLU:HG3	1.68	0.75
1:A:277:ARG:NH2	1:A:308:SER:OG	2.24	0.70
1:B:277:ARG:NH2	1:B:308:SER:OG	2.24	0.70
1:F:184:ASP:OD1	1:F:186:SER:OG	2.09	0.68
1:C:169:LEU:HD22	1:C:336:ILE:HD12	1.76	0.68
1:A:316:LYS:HB3	1:A:329:THR:HG23	1.77	0.67
1:D:184:ASP:OD1	1:D:186:SER:OG	2.11	0.67
1:E:206:ASP:OD1	1:E:280:LYS:NZ	2.26	0.67
1:F:263:ALA:HB2	1:F:329:THR:HG22	1.77	0.65
1:E:164:SER:HB2	1:E:315:MET:HE1	1.78	0.64
1:F:178:GLN:OE1	1:F:298:THR:OG1	2.16	0.64
1:E:165:VAL:HG23	1:E:315:MET:HE2	1.78	0.64
1:F:240:PHE:CD2	1:F:255:GLN:HG3	2.33	0.63
1:A:183:PHE:CD1	1:A:315:MET:HE2	2.27	0.62
1:D:200:ILE:HG12	1:D:281:ILE:HG12	1.83	0.60
1:F:177:ILE:HD12	1:F:205:LEU:HD21	1.84	0.59
1:F:277:ARG:HH11	1:F:277:ARG:HG2	1.68	0.58
1:B:269:VAL:HG13	1:B:312:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:VAL:CG2	1:E:315:MET:HE2	2.34	0.56
1:F:228:ASP:OD1	1:F:230:ARG:NH2	2.37	0.56
1:F:243:LYS:NZ	1:F:244:GLN:HE21	2.03	0.56
1:F:142:SER:HB3	1:F:335:GLU:HB3	1.88	0.55
1:B:151:ASP:OD2	1:B:322:ASN:HB2	2.07	0.55
1:F:170:LEU:HB2	1:F:178:GLN:HG2	1.89	0.54
1:C:259:SER:OG	1:C:260:ALA:N	2.40	0.54
1:E:202:PRO:HA	1:E:278:LEU:HA	1.90	0.53
1:F:279:SER:HB2	1:F:280:LYS:HD2	1.90	0.53
1:E:200:ILE:HB	1:E:312:LEU:HB2	1.91	0.53
1:F:240:PHE:CE2	1:F:255:GLN:HG3	2.44	0.53
1:B:190:PHE:HB3	1:B:288:THR:HA	1.90	0.53
1:D:178:GLN:HG3	1:D:298:THR:OG1	2.09	0.52
1:F:255:GLN:OE1	1:F:258:TRP:HE3	1.93	0.52
1:C:160:LYS:HE3	1:C:187:GLU:HG3	1.91	0.51
1:B:306:GLN:HB3	1:B:309:PHE:CZ	2.46	0.51
1:E:277:ARG:NH2	1:E:308:SER:OG	2.38	0.50
1:F:210:ILE:HG23	1:F:218:ILE:HG13	1.93	0.50
1:B:200:ILE:HG12	1:B:281:ILE:HG12	1.93	0.50
1:F:241:SER:OG	1:F:243:LYS:HE3	2.10	0.49
1:F:157:ASP:O	1:F:161:LEU:HG	2.12	0.49
1:F:241:SER:OG	1:F:243:LYS:HG2	2.12	0.49
1:A:202:PRO:HA	1:A:278:LEU:HA	1.94	0.49
1:A:246:LEU:HB3	1:A:253:ASN:ND2	2.28	0.49
1:C:277:ARG:NH2	1:C:308:SER:OG	2.39	0.49
1:D:183:PHE:CD1	1:D:315:MET:HB3	2.48	0.49
1:D:249:GLU:HB2	1:E:232:SER:HB3	1.95	0.48
1:C:255:GLN:O	1:C:259:SER:HB3	2.13	0.48
1:A:142:SER:HB2	1:A:143:PRO:HD2	1.96	0.48
1:A:170:LEU:HD11	1:A:180:LYS:HB3	1.95	0.48
1:A:190:PHE:CE1	1:A:195:GLY:HA3	2.49	0.48
1:C:202:PRO:HA	1:C:278:LEU:HA	1.95	0.48
1:F:169:LEU:HD22	1:F:336:ILE:HD12	1.96	0.48
1:C:303:GLU:HA	1:C:304:PRO:HD3	1.74	0.47
1:F:168:ASN:HB2	1:F:180:LYS:HE3	1.95	0.47
1:C:209:LYS:HE2	1:C:217:ASP:OD2	2.14	0.47
1:D:255:GLN:NE2	2:D:401:GLA:O6	2.26	0.47
1:C:180:LYS:HE2	1:C:182:THR:OG1	2.14	0.47
1:B:172:ALA:HB1	1:B:338:LEU:HD21	1.97	0.47
1:F:307:GLN:O	1:F:337:THR:HA	2.14	0.47
1:C:193:LYS:HG3	1:C:319:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ASN:O	1:D:262:GLN:HG3	2.15	0.46
1:F:300:LYS:HB3	1:F:300:LYS:HE2	1.59	0.46
1:D:202:PRO:HA	1:D:278:LEU:HA	1.97	0.46
1:A:257:ASN:O	1:A:262:GLN:HG3	2.16	0.46
1:A:192:VAL:O	1:A:193:LYS:HG2	2.16	0.46
1:A:240:PHE:CG	1:A:255:GLN:HG3	2.51	0.45
1:E:315:MET:HB3	1:E:315:MET:HE3	1.70	0.45
1:C:160:LYS:O	1:C:164:SER:OG	2.31	0.45
1:A:240:PHE:CD2	1:A:255:GLN:HG3	2.52	0.45
1:F:198:TYR:HB2	1:F:314:VAL:HB	2.00	0.44
1:A:200:ILE:HB	1:A:312:LEU:HB2	2.00	0.44
1:D:272:TRP:CE3	1:D:310:PRO:HB3	2.53	0.44
1:F:205:LEU:HA	1:F:205:LEU:HD23	1.79	0.44
1:F:230:ARG:C	1:F:235:GLU:HG3	2.38	0.44
1:A:272:TRP:CE3	1:A:312:LEU:HD11	2.52	0.44
1:E:230:ARG:C	1:E:235:GLU:HG3	2.38	0.44
1:F:200:ILE:HB	1:F:312:LEU:HB2	1.98	0.44
1:C:204:GLY:O	1:C:205:LEU:HD23	2.16	0.44
1:A:267:GLU:HB2	1:D:158:GLN:HB3	2.00	0.44
1:A:149:ASN:O	1:A:322:ASN:ND2	2.44	0.43
1:B:206:ASP:OD2	1:B:302:THR:HG21	2.18	0.43
1:B:257:ASN:O	1:B:262:GLN:HG3	2.17	0.43
1:F:243:LYS:HZ1	1:F:244:GLN:HE21	1.66	0.43
1:F:258:TRP:CG	3:F:402:GAL:H3	2.54	0.43
1:A:169:LEU:HD13	1:A:336:ILE:HD12	2.00	0.43
1:C:200:ILE:HB	1:C:312:LEU:HB2	2.01	0.43
1:E:275:GLY:O	1:E:277:ARG:HB2	2.19	0.43
1:F:277:ARG:HH11	1:F:277:ARG:CG	2.32	0.43
1:A:158:GLN:HB3	1:D:267:GLU:HB2	2.01	0.42
1:D:161:LEU:HD13	1:D:328:VAL:HG11	2.01	0.42
1:F:257:ASN:O	1:F:262:GLN:HG3	2.19	0.42
1:A:209:LYS:HE3	1:A:217:ASP:OD2	2.18	0.42
1:A:309:PHE:HE2	1:A:338:LEU:HD12	1.85	0.42
1:E:164:SER:CB	1:E:315:MET:HE1	2.47	0.42
1:C:192:VAL:HG12	1:C:193:LYS:HG2	2.02	0.42
1:E:230:ARG:O	1:E:235:GLU:HG3	2.20	0.42
1:B:209:LYS:HE3	1:B:217:ASP:OD2	2.20	0.42
1:A:179:TRP:CG	1:A:311:LEU:HD13	2.55	0.41
1:B:269:VAL:HG11	1:B:331:LEU:HD11	2.01	0.41
1:A:338:LEU:HA	1:A:338:LEU:HD23	1.71	0.41
1:B:159:GLU:OE2	1:B:162:ARG:NH2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:LEU:HD23	1:C:332:GLY:N	2.35	0.41
1:F:183:PHE:HB2	1:F:293:LEU:HB2	2.03	0.41
1:F:240:PHE:CG	1:F:255:GLN:HG3	2.56	0.41
1:F:190:PHE:HA	1:F:193:LYS:O	2.21	0.41
1:D:205:LEU:HD23	1:D:205:LEU:HA	1.85	0.41
1:E:169:LEU:HD11	1:E:177:ILE:HD11	2.03	0.41
1:E:212:ASP:OD1	1:E:214:ASN:N	2.54	0.40
1:F:205:LEU:HD22	1:F:299:ALA:HB1	2.02	0.40
1:A:228:ASP:OD2	1:A:229:TYR:N	2.55	0.40
1:D:223:PRO:HG2	1:D:231:ASN:OD1	2.22	0.40
1:A:272:TRP:HE3	1:A:312:LEU:HD11	1.87	0.40
1:C:160:LYS:HE2	1:C:160:LYS:HB2	1.82	0.40
1:C:257:ASN:O	1:C:262:GLN:HG3	2.21	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	188/226 (83%)	177 (94%)	11 (6%)	0	100	100
1	B	196/226 (87%)	182 (93%)	14 (7%)	0	100	100
1	C	196/226 (87%)	178 (91%)	18 (9%)	0	100	100
1	D	190/226 (84%)	179 (94%)	10 (5%)	1 (0%)	34	63
1	E	185/226 (82%)	173 (94%)	11 (6%)	1 (0%)	34	63
1	F	186/226 (82%)	172 (92%)	14 (8%)	0	100	100
All	All	1141/1356 (84%)	1061 (93%)	78 (7%)	2 (0%)	52	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	276	ASN
1	D	303	GLU

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	175/204 (86%)	173 (99%)	2 (1%)	80	94
1	B	176/204 (86%)	173 (98%)	3 (2%)	68	90
1	C	175/204 (86%)	172 (98%)	3 (2%)	68	90
1	D	176/204 (86%)	174 (99%)	2 (1%)	80	94
1	E	170/204 (83%)	168 (99%)	2 (1%)	78	93
1	F	170/204 (83%)	166 (98%)	4 (2%)	57	85
All	All	1042/1224 (85%)	1026 (98%)	16 (2%)	72	91

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	GLN
1	A	331	LEU
1	B	271	SER
1	B	312	LEU
1	B	337	THR
1	C	303	GLU
1	C	308	SER
1	C	334	ARG
1	D	160	LYS
1	D	230	ARG
1	E	286	GLN
1	E	300	LYS
1	F	186	SER
1	F	221	SER
1	F	255	GLN
1	F	279	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	HIS
1	A	306	GLN
1	D	255	GLN
1	E	255	GLN
1	F	214	ASN
1	F	244	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)

12 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	GLA	A	401	3	11,11,12	1.96	2 (18%)	15,15,17	1.41	4 (26%)
3	GAL	A	402	2	12,12,12	1.21	2 (16%)	17,17,17	1.07	1 (5%)
2	GLA	B	401	3	11,11,12	1.52	2 (18%)	15,15,17	1.45	3 (20%)
3	GAL	B	402	2	12,12,12	1.42	2 (16%)	17,17,17	0.92	0
2	GLA	C	401	3	11,11,12	1.83	3 (27%)	15,15,17	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GAL	C	402	2	12,12,12	1.36	2 (16%)	17,17,17	1.06	0
2	GLA	D	401	3	11,11,12	1.75	2 (18%)	15,15,17	1.31	1 (6%)
3	GAL	D	402	2	12,12,12	1.37	2 (16%)	17,17,17	1.42	3 (17%)
2	GLA	E	401	3	11,11,12	1.55	1 (9%)	15,15,17	1.10	1 (6%)
3	GAL	E	402	2	12,12,12	1.37	2 (16%)	17,17,17	1.03	0
2	GLA	F	401	3	11,11,12	1.68	2 (18%)	15,15,17	1.03	0
3	GAL	F	402	2	12,12,12	1.31	1 (8%)	17,17,17	0.86	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	GLA	A	401	3	-	0/2/19/22	0/1/1/1
3	GAL	A	402	2	-	0/2/22/22	0/1/1/1
2	GLA	B	401	3	-	0/2/19/22	0/1/1/1
3	GAL	B	402	2	-	0/2/22/22	0/1/1/1
2	GLA	C	401	3	-	0/2/19/22	0/1/1/1
3	GAL	C	402	2	-	0/2/22/22	0/1/1/1
2	GLA	D	401	3	-	0/2/19/22	0/1/1/1
3	GAL	D	402	2	-	0/2/22/22	0/1/1/1
2	GLA	E	401	3	-	0/2/19/22	0/1/1/1
3	GAL	E	402	2	-	0/2/22/22	0/1/1/1
2	GLA	F	401	3	-	0/2/19/22	0/1/1/1
3	GAL	F	402	2	-	0/2/22/22	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GLA	C2-C3	-5.05	1.45	1.52
2	C	401	GLA	C2-C3	-4.82	1.46	1.52
2	D	401	GLA	C2-C3	-4.51	1.46	1.52
2	F	401	GLA	C2-C3	-4.44	1.46	1.52
2	E	401	GLA	C2-C3	-3.98	1.47	1.52
2	B	401	GLA	C2-C3	-3.56	1.47	1.52
3	E	402	GAL	C4-C3	-2.57	1.45	1.52
2	D	401	GLA	C4-C3	-2.51	1.45	1.52
3	F	402	GAL	C4-C3	-2.45	1.45	1.52
2	A	401	GLA	C4-C3	-2.41	1.46	1.52
3	C	402	GAL	C4-C3	-2.38	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	GAL	C4-C3	-2.34	1.46	1.52
3	B	402	GAL	C3-C2	-2.34	1.46	1.52
3	C	402	GAL	C3-C2	-2.33	1.46	1.52
3	B	402	GAL	C4-C3	-2.27	1.46	1.52
3	E	402	GAL	C3-C2	-2.23	1.46	1.52
2	F	401	GLA	C4-C3	-2.21	1.46	1.52
3	D	402	GAL	C1-C2	-2.18	1.48	1.52
3	A	402	GAL	C3-C2	-2.18	1.46	1.52
2	C	401	GLA	C4-C3	-2.12	1.46	1.52
2	B	401	GLA	C4-C5	-2.11	1.48	1.53
3	A	402	GAL	C4-C3	-2.04	1.47	1.52
2	C	401	GLA	C4-C5	-2.01	1.48	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	GLA	C3-C4-C5	-3.07	104.76	110.23
2	B	401	GLA	O2-C2-C1	-3.06	103.11	109.23
3	D	402	GAL	O2-C2-C1	-2.69	103.85	109.74
2	A	401	GLA	O2-C2-C3	-2.07	106.01	110.19
2	A	401	GLA	C1-C2-C3	2.07	112.06	109.55
2	B	401	GLA	C2-C3-C4	2.23	114.94	111.05
3	D	402	GAL	O5-C1-C2	2.29	114.00	110.00
2	C	401	GLA	O5-C5-C4	2.47	114.22	110.13
2	A	401	GLA	O5-C5-C4	2.48	114.24	110.13
3	A	402	GAL	O6-C6-C5	2.58	119.93	111.30
3	D	402	GAL	C4-C3-C2	2.94	116.20	110.79
2	E	401	GLA	C1-C2-C3	2.96	113.14	109.55
2	B	401	GLA	C1-C2-C3	3.37	113.64	109.55
2	D	401	GLA	C1-C2-C3	3.54	113.84	109.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	GLA	1	0
3	F	402	GAL	1	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	194/226 (85%)	-0.22	0 100 100	24, 33, 48, 74	0
1	B	198/226 (87%)	-0.17	1 (0%) 91 93	26, 36, 59, 70	0
1	C	198/226 (87%)	-0.12	1 (0%) 91 93	30, 40, 54, 68	0
1	D	196/226 (86%)	-0.19	0 100 100	29, 40, 59, 72	0
1	E	191/226 (84%)	0.08	1 (0%) 91 93	28, 41, 56, 63	0
1	F	192/226 (84%)	-0.13	0 100 100	29, 40, 59, 67	0
All	All	1169/1356 (86%)	-0.13	3 (0%) 94 95	24, 38, 57, 74	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	305	ASN	2.7
1	C	289	ASP	2.3
1	E	311	LEU	2.3

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
3	GAL	B	402	12/12	0.97	0.15	-0.22	30,33,35,36	0
2	GLA	A	401	11/12	0.97	0.14	-0.51	27,29,33,37	0
2	GLA	D	401	11/12	0.95	0.16	-0.65	36,39,45,46	0
3	GAL	A	402	12/12	0.97	0.14	-0.72	20,29,31,35	0
2	GLA	C	401	11/12	0.95	0.14	-0.93	36,38,43,44	0
3	GAL	C	402	12/12	0.96	0.12	-1.27	37,42,47,47	0
3	GAL	E	402	12/12	0.96	0.15	-1.32	34,36,41,43	0
2	GLA	B	401	11/12	0.95	0.14	-1.53	28,35,39,41	0
3	GAL	D	402	12/12	0.97	0.14	-1.67	33,35,38,39	0
2	GLA	E	401	11/12	0.93	0.12	-1.84	35,38,41,42	0
3	GAL	F	402	12/12	0.97	0.12	-2.01	30,36,40,41	0
2	GLA	F	401	11/12	0.97	0.13	-2.11	31,35,39,45	0

6.5 Other polymers (i)

There are no such residues in this entry.