



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:49 AM GMT

PDB ID : 3C6S  
Title : Crystal structure of Fab F22-4 in complex with a Shigella flexneri 2a O-Ag pentadecasaccharide  
Authors : Saul, F.A.; Vulliez-le-Normand, B.; Bentley, G.A.  
Deposited on : 2008-02-05  
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

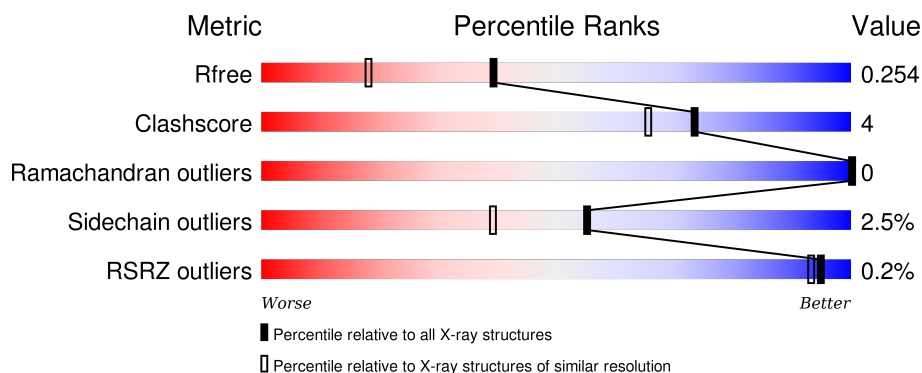
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. 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	219	<div> <div>89%</div> <div>9% ..</div> </div>
1	C	219	<div> <div>91%</div> <div>8%</div> </div>
1	E	219	<div> <div>90%</div> <div>9% .</div> </div>
1	G	219	<div> <div>89%</div> <div>8% ..</div> </div>
2	B	217	<div> <div>87%</div> <div>9% . .</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	217	 83%12% . .
2	F	217	 85%10% . .
2	H	217	 86%8% . .

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15755 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 Fab F22-4 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	1	0
			1680	1051	288	335	6			
1	C	218	Total	C	N	O	S	0	0	0
			1690	1056	288	340	6			
1	E	216	Total	C	N	O	S	0	0	0
			1673	1047	285	335	6			
1	G	216	Total	C	N	O	S	0	0	0
			1673	1047	285	335	6			

- Molecule 2 is a protein called Fab F22-4 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	209	Total	C	N	O	S	0	0	0
			1604	1021	260	314	9			
2	D	209	Total	C	N	O	S	0	2	0
			1616	1029	261	317	9			
2	F	209	Total	C	N	O	S	0	1	0
			1610	1025	260	316	9			
2	H	209	Total	C	N	O	S	0	0	0
			1604	1021	260	314	9			

- Molecule 3 is a polymer of unknown type called SUGAR (11-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	11	Total	C	N	O	0	0
			120	70	2	48		
3	D	11	Total	C	N	O	0	0
			120	70	2	48		
3	F	11	Total	C	N	O	0	0
			120	70	2	48		
3	H	11	Total	C	N	O	0	0
			120	70	2	48		

- Molecule 4 is PALLADIUM ION (three-letter code: PD) (formula: Pd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Pd	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	273	Total	O	0	0
			273	273		
5	B	211	Total	O	0	0
			211	211		
5	C	260	Total	O	0	0
			260	260		
5	D	280	Total	O	0	0
			280	280		
5	E	271	Total	O	0	0
			271	271		
5	F	312	Total	O	0	0
			312	312		
5	G	256	Total	O	0	0
			256	256		
5	H	261	Total	O	0	0
			261	261		

### 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: Fab F22-4 light chain

Chain A: 



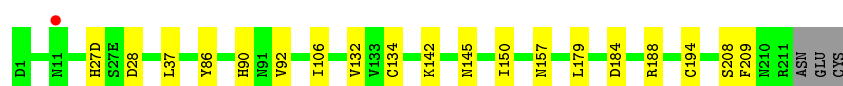
- Molecule 1: Fab F22-4 light chain

Chain C: 



- Molecule 1: Fab F22-4 light chain

Chain E: 




- Molecule 1: Fab F22-4 light chain

Chain G: 




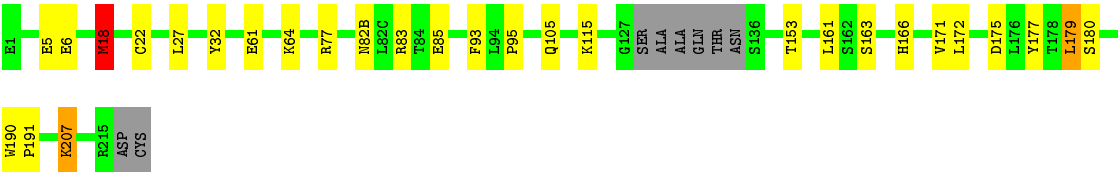
- Molecule 2: Fab F22-4 heavy chain

Chain B: 



- Molecule 2: Fab F22-4 heavy chain

Chain D: 



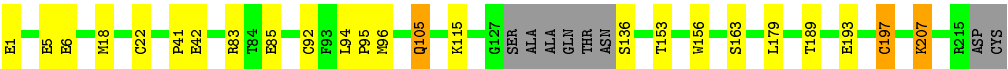
- Molecule 2: Fab F22-4 heavy chain

Chain F: 

85%

10%

• •



- Molecule 2: Fab F22-4 heavy chain

Chain H: 

86%

8%

• •



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.86Å 137.15Å 109.38Å 90.00° 94.97° 90.00°	Depositor
Resolution (Å)	44.79 – 1.80 44.79 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.79-1.80) 98.0 (44.79-1.74)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.191 , 0.251 0.199 , 0.254	Depositor DCC
$R_{free}$ test set	2670 reflections (1.51%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.5	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 195949 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15755	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GLC, RAM, NAG, PD

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	0.68	0/1723	0.79	2/2340 (0.1%)
1	C	0.66	0/1729	0.77	0/2349
1	E	0.72	2/1712 (0.1%)	0.75	0/2326
1	G	0.70	0/1712	0.74	1/2326 (0.0%)
2	B	0.68	0/1646	0.73	0/2245
2	D	0.73	0/1664	0.80	2/2269 (0.1%)
2	F	0.77	2/1655 (0.1%)	0.80	2/2257 (0.1%)
2	H	0.74	0/1646	0.78	0/2245
All	All	0.71	4/13487 (0.0%)	0.77	7/18357 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	194	CYS	CB-SG	-7.00	1.70	1.82
2	F	92	CYS	CB-SG	-5.37	1.73	1.81
2	F	197	CYS	CB-SG	-5.21	1.73	1.81
1	E	134	CYS	CB-SG	-5.08	1.73	1.81

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	ASP	CB-CG-OD1	6.89	124.51	118.30
2	F	18	MET	CG-SD-CE	-6.61	89.62	100.20
2	D	179	LEU	CA-CB-CG	6.44	130.12	115.30
2	F	179	LEU	CA-CB-CG	6.30	129.80	115.30
2	D	18	MET	CG-SD-CE	-5.92	90.73	100.20

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	1680	0	1625	13	0
1	C	1690	0	1628	12	0
1	E	1673	0	1616	11	0
1	G	1673	0	1616	13	0
2	B	1604	0	1574	10	1
2	D	1616	0	1588	20	0
2	F	1610	0	1580	11	0
2	H	1604	0	1574	17	1
3	B	120	0	106	0	0
3	D	120	0	106	2	0
3	F	120	0	106	3	0
3	H	120	0	106	1	0
4	A	1	0	0	0	0
5	A	273	0	0	6	0
5	B	211	0	0	1	1
5	C	260	0	0	2	0
5	D	280	0	0	7	2
5	E	271	0	0	3	1
5	F	312	0	0	6	1
5	G	256	0	0	2	0
5	H	261	0	0	8	1
All	All	15755	0	13225	110	4

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.

The worst 5 of 110 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)
2:H:18:MET:CG	5:H:514:HOH:O	1.76	1.28
2:D:171:VAL:HB	5:D:532:HOH:O	1.55	1.07
2:H:18:MET:HE3	5:H:514:HOH:O	1.53	1.05
2:H:18:MET:CE	5:H:514:HOH:O	2.00	1.04
1:A:134:CYS:SG	5:A:424:HOH:O	2.17	1.03

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:136:SER:N	5:E:372:HOH:O[2_545]	1.80	0.40
2:B:188:SER:N	5:D:513:HOH:O[2_645]	1.99	0.21
5:B:335:HOH:O	5:D:509:HOH:O[2_645]	2.02	0.18
5:F:420:HOH:O	5:H:354:HOH:O[2_655]	2.11	0.09

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	215/219 (98%)	209 (97%)	6 (3%)	0	100	100
1	C	216/219 (99%)	211 (98%)	5 (2%)	0	100	100
1	E	214/219 (98%)	211 (99%)	3 (1%)	0	100	100
1	G	214/219 (98%)	209 (98%)	5 (2%)	0	100	100
2	B	205/217 (94%)	203 (99%)	2 (1%)	0	100	100
2	D	207/217 (95%)	204 (99%)	3 (1%)	0	100	100
2	F	206/217 (95%)	204 (99%)	2 (1%)	0	100	100
2	H	205/217 (94%)	201 (98%)	4 (2%)	0	100	100
All	All	1682/1744 (96%)	1652 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	192/194 (99%)	189 (98%)	3 (2%)	70	59
1	C	193/194 (100%)	190 (98%)	3 (2%)	70	59
1	E	191/194 (98%)	189 (99%)	2 (1%)	82	77
1	G	191/194 (98%)	186 (97%)	5 (3%)	54	37
2	B	185/191 (97%)	179 (97%)	6 (3%)	46	29
2	D	187/191 (98%)	178 (95%)	9 (5%)	31	14
2	F	186/191 (97%)	181 (97%)	5 (3%)	52	36
2	H	185/191 (97%)	179 (97%)	6 (3%)	46	29
All	All	1510/1540 (98%)	1471 (97%)	39 (3%)	55	37

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	163	SER
1	E	106	ILE
2	H	115	LYS
2	D	175	ASP
2	D	179	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	82(B)	ASN
1	E	91	ASN
1	G	157	ASN
1	E	27(D)	HIS
1	E	190	ASN

### 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 ⓘ

44 carbohydrates 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$
3	RAM	B	301	3	10,10,11	0.54	0	14,14,16	1.34	3 (21%)
3	RAM	B	302	3	10,10,11	0.47	0	14,14,16	1.49	3 (21%)
3	RAM	B	303	3	10,10,11	0.63	0	14,14,16	1.18	2 (14%)
3	GLC	B	304	3	11,11,12	0.68	0	14,15,17	1.33	2 (14%)
3	NAG	B	305	3	14,14,15	0.61	0	15,19,21	1.29	2 (13%)
3	RAM	B	306	3	10,10,11	0.69	0	14,14,16	1.58	4 (28%)
3	RAM	B	307	3	10,10,11	0.60	0	14,14,16	1.11	2 (14%)
3	RAM	B	308	3	10,10,11	0.57	0	14,14,16	0.96	1 (7%)
3	GLC	B	309	3	11,11,12	0.49	0	14,15,17	0.82	1 (7%)
3	NAG	B	310	3	14,14,15	0.60	0	15,19,21	1.27	2 (13%)
3	RAM	B	311	3	10,10,11	0.58	0	14,14,16	1.89	3 (21%)
3	RAM	D	301	3	10,10,11	0.72	0	14,14,16	1.48	1 (7%)
3	RAM	D	302	3	10,10,11	0.79	0	14,14,16	1.79	4 (28%)
3	RAM	D	303	3	10,10,11	0.74	0	14,14,16	1.40	3 (21%)
3	GLC	D	304	3	11,11,12	0.88	0	14,15,17	1.80	4 (28%)
3	NAG	D	305	3	14,14,15	0.54	0	15,19,21	1.10	1 (6%)
3	RAM	D	306	3	10,10,11	0.91	0	14,14,16	1.97	4 (28%)
3	RAM	D	307	3	10,10,11	0.59	0	14,14,16	0.86	0
3	RAM	D	308	3	10,10,11	0.68	0	14,14,16	0.91	0
3	GLC	D	309	3	11,11,12	0.63	0	14,15,17	1.15	1 (7%)
3	NAG	D	310	3	14,14,15	0.47	0	15,19,21	0.84	0
3	RAM	D	311	3	10,10,11	0.54	0	14,14,16	1.61	5 (35%)
3	RAM	F	301	3	10,10,11	0.44	0	14,14,16	1.67	4 (28%)
3	RAM	F	302	3	10,10,11	0.58	0	14,14,16	1.21	2 (14%)
3	RAM	F	303	3	10,10,11	0.61	0	14,14,16	1.22	2 (14%)
3	GLC	F	304	3	11,11,12	1.09	1 (9%)	14,15,17	1.27	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	F	305	3	14,14,15	0.79	1 (7%)	15,19,21	0.89	0
3	RAM	F	306	3	10,10,11	0.82	0	14,14,16	1.20	1 (7%)
3	RAM	F	307	3	10,10,11	0.76	1 (10%)	14,14,16	1.16	2 (14%)
3	RAM	F	308	3	10,10,11	0.84	1 (10%)	14,14,16	0.99	1 (7%)
3	GLC	F	309	3	11,11,12	0.61	0	14,15,17	0.99	1 (7%)
3	NAG	F	310	3	14,14,15	0.60	0	15,19,21	1.14	2 (13%)
3	RAM	F	311	3	10,10,11	0.45	0	14,14,16	0.94	0
3	RAM	H	301	3	10,10,11	0.49	0	14,14,16	1.29	2 (14%)
3	RAM	H	302	3	10,10,11	0.64	0	14,14,16	1.17	2 (14%)
3	RAM	H	303	3	10,10,11	0.54	0	14,14,16	1.42	3 (21%)
3	GLC	H	304	3	11,11,12	0.75	0	14,15,17	1.48	2 (14%)
3	NAG	H	305	3	14,14,15	0.80	1 (7%)	15,19,21	0.88	0
3	RAM	H	306	3	10,10,11	0.83	0	14,14,16	1.39	3 (21%)
3	RAM	H	307	3	10,10,11	0.83	1 (10%)	14,14,16	1.29	3 (21%)
3	RAM	H	308	3	10,10,11	0.83	1 (10%)	14,14,16	0.88	0
3	GLC	H	309	3	11,11,12	0.70	0	14,15,17	1.34	1 (7%)
3	NAG	H	310	3	14,14,15	0.45	0	15,19,21	1.00	0
3	RAM	H	311	3	10,10,11	0.55	0	14,14,16	1.13	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
3	RAM	B	301	3	-	0/0/17/20	0/1/1/1
3	RAM	B	302	3	-	0/0/17/20	0/1/1/1
3	RAM	B	303	3	-	0/0/17/20	0/1/1/1
3	GLC	B	304	3	-	0/2/19/22	0/1/1/1
3	NAG	B	305	3	-	0/6/23/26	0/1/1/1
3	RAM	B	306	3	-	0/0/17/20	0/1/1/1
3	RAM	B	307	3	-	0/0/17/20	0/1/1/1
3	RAM	B	308	3	-	0/0/17/20	0/1/1/1
3	GLC	B	309	3	-	0/2/19/22	0/1/1/1
3	NAG	B	310	3	-	0/6/23/26	0/1/1/1
3	RAM	B	311	3	-	0/0/17/20	0/1/1/1
3	RAM	D	301	3	-	0/0/17/20	0/1/1/1
3	RAM	D	302	3	-	0/0/17/20	0/1/1/1
3	RAM	D	303	3	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	D	304	3	-	0/2/19/22	0/1/1/1
3	NAG	D	305	3	-	0/6/23/26	0/1/1/1
3	RAM	D	306	3	-	0/0/17/20	0/1/1/1
3	RAM	D	307	3	-	0/0/17/20	0/1/1/1
3	RAM	D	308	3	-	0/0/17/20	0/1/1/1
3	GLC	D	309	3	-	0/2/19/22	0/1/1/1
3	NAG	D	310	3	-	0/6/23/26	0/1/1/1
3	RAM	D	311	3	-	0/0/17/20	0/1/1/1
3	RAM	F	301	3	-	0/0/17/20	0/1/1/1
3	RAM	F	302	3	-	0/0/17/20	0/1/1/1
3	RAM	F	303	3	-	0/0/17/20	0/1/1/1
3	GLC	F	304	3	-	0/2/19/22	0/1/1/1
3	NAG	F	305	3	-	0/6/23/26	0/1/1/1
3	RAM	F	306	3	-	0/0/17/20	0/1/1/1
3	RAM	F	307	3	-	0/0/17/20	0/1/1/1
3	RAM	F	308	3	-	0/0/17/20	0/1/1/1
3	GLC	F	309	3	-	0/2/19/22	0/1/1/1
3	NAG	F	310	3	-	0/6/23/26	0/1/1/1
3	RAM	F	311	3	-	0/0/17/20	0/1/1/1
3	RAM	H	301	3	-	0/0/17/20	0/1/1/1
3	RAM	H	302	3	-	0/0/17/20	0/1/1/1
3	RAM	H	303	3	-	0/0/17/20	0/1/1/1
3	GLC	H	304	3	-	0/2/19/22	0/1/1/1
3	NAG	H	305	3	-	0/6/23/26	0/1/1/1
3	RAM	H	306	3	-	0/0/17/20	0/1/1/1
3	RAM	H	307	3	-	0/0/17/20	0/1/1/1
3	RAM	H	308	3	-	0/0/17/20	0/1/1/1
3	GLC	H	309	3	-	0/2/19/22	0/1/1/1
3	NAG	H	310	3	-	0/6/23/26	0/1/1/1
3	RAM	H	311	3	-	0/0/17/20	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	304	GLC	O5-C1	-3.25	1.38	1.43
3	F	305	NAG	O5-C1	-2.25	1.40	1.43
3	F	308	RAM	O5-C1	-2.20	1.40	1.43
3	H	307	RAM	O2-C2	-2.11	1.38	1.43
3	F	307	RAM	O2-C2	-2.11	1.38	1.43

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	304	GLC	O5-C1-C2	-3.46	105.25	110.86
3	D	305	NAG	O3-C3-C4	-3.09	103.38	110.34
3	D	311	RAM	C1-C2-C3	-2.87	106.15	109.54
3	H	303	RAM	O5-C1-C2	-2.84	106.25	110.86
3	B	311	RAM	C1-C2-C3	-2.81	106.21	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	305	NAG	1	0
3	D	306	RAM	1	0
3	F	305	NAG	1	0
3	F	306	RAM	2	0
3	H	305	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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<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	216/219 (98%)	-0.35	0 100 100	11, 21, 31, 42	0
1	C	218/219 (99%)	-0.29	0 100 100	10, 21, 34, 41	0
1	E	216/219 (98%)	-0.29	1 (0%) 91 90	10, 19, 30, 41	0
1	G	216/219 (98%)	-0.25	1 (0%) 91 90	9, 21, 34, 45	0
2	B	209/217 (96%)	-0.26	1 (0%) 91 90	14, 22, 35, 40	0
2	D	209/217 (96%)	-0.31	0 100 100	10, 19, 34, 40	0
2	F	209/217 (96%)	-0.36	0 100 100	8, 18, 32, 36	0
2	H	209/217 (96%)	-0.31	1 (0%) 91 90	8, 19, 32, 44	0
All	All	1702/1744 (97%)	-0.30	4 (0%) 95 93	8, 20, 33, 45	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	193	GLU	2.8
1	E	11	ASN	2.4
1	G	13	VAL	2.3
2	B	189	THR	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 ⓘ

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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	F	305	14/15	0.96	0.08	1.49	12,14,17,19	0
3	RAM	F	303	10/11	0.96	0.08	1.20	12,14,18,22	0
3	RAM	H	303	10/11	0.93	0.09	0.86	14,18,22,27	0
3	NAG	D	305	14/15	0.95	0.10	0.48	18,20,24,26	0
3	GLC	D	304	11/12	0.95	0.09	0.14	16,17,19,19	0
3	NAG	H	305	14/15	0.95	0.08	-0.21	15,17,20,21	0
3	GLC	H	304	11/12	0.96	0.08	-0.50	17,19,21,22	0
3	RAM	B	303	10/11	0.94	0.07	-0.52	19,20,23,25	0
3	GLC	F	304	11/12	0.97	0.07	-0.53	13,15,16,18	0
3	NAG	B	305	14/15	0.96	0.07	-0.57	17,18,21,22	0
3	RAM	D	303	10/11	0.96	0.07	-0.93	19,21,23,25	0
3	GLC	B	304	11/12	0.98	0.06	-2.98	15,16,18,18	0
3	RAM	H	301	10/11	0.86	0.20	-	43,45,47,49	0
3	GLC	D	309	11/12	0.91	0.10	-	30,32,34,35	0
3	NAG	H	310	14/15	0.80	0.26	-	37,45,47,47	0
3	RAM	D	307	10/11	0.90	0.10	-	29,33,35,35	0
3	RAM	B	307	10/11	0.91	0.10	-	22,25,25,26	0
3	RAM	F	308	10/11	0.90	0.10	-	26,30,32,34	0
3	RAM	B	308	10/11	0.93	0.11	-	26,32,34,36	0
3	RAM	F	311	10/11	0.75	0.15	-	44,46,46,47	0
3	NAG	F	310	14/15	0.81	0.17	-	37,41,45,46	0
3	RAM	D	308	10/11	0.85	0.17	-	36,39,40,41	0
3	RAM	B	311	10/11	0.55	0.30	-	55,59,59,60	0
3	RAM	H	302	10/11	0.87	0.16	-	32,37,41,41	0
3	RAM	D	301	10/11	0.80	0.17	-	37,38,39,39	0
3	RAM	H	306	10/11	0.93	0.14	-	19,23,25,26	0
3	RAM	F	301	10/11	0.81	0.18	-	34,36,40,41	0
3	RAM	H	308	10/11	0.93	0.13	-	23,30,32,33	0
3	RAM	F	302	10/11	0.92	0.11	-	24,27,30,31	0
3	RAM	D	311	10/11	0.77	0.21	-	50,53,53,54	0
3	RAM	F	306	10/11	0.95	0.08	-	16,20,22,23	0
3	GLC	H	309	11/12	0.95	0.08	-	17,19,23,23	0
3	NAG	D	310	14/15	0.82	0.20	-	43,47,48,48	0
3	RAM	D	302	10/11	0.86	0.14	-	29,32,34,34	0
3	GLC	B	309	11/12	0.94	0.08	-	21,23,25,25	0
3	RAM	H	307	10/11	0.93	0.08	-	22,24,25,26	0
3	RAM	B	301	10/11	0.77	0.18	-	37,39,41,42	0
3	NAG	B	310	14/15	0.83	0.27	-	42,50,52,52	0
3	RAM	F	307	10/11	0.94	0.09	-	17,20,23,24	0
3	RAM	B	306	10/11	0.94	0.11	-	19,23,26,26	0
3	RAM	D	306	10/11	0.84	0.17	-	24,31,32,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GLC	F	309	11/12	0.96	0.07	-	19,22,23,24	0
3	RAM	B	302	10/11	0.90	0.15	-	29,31,32,34	0
3	RAM	H	311	10/11	0.82	0.23	-	51,54,54,54	0

## 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<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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PD	A	215	1/1	1.00	0.02	-3.90	26,26,26,26	0

## 6.5 Other polymers

There are no such residues in this entry.