



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:44 AM GMT

PDB ID : 3BZ4
Title : Crystal structure of Fab F22-4 in complex with a Shigella flexneri 2a O-Ag deca-saccharide
Authors : Saul, F.A.; Vulliez-le-Normand, B.; Bentley, G.A.
Deposited on : 2008-01-17
Resolution : 1.80 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 (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

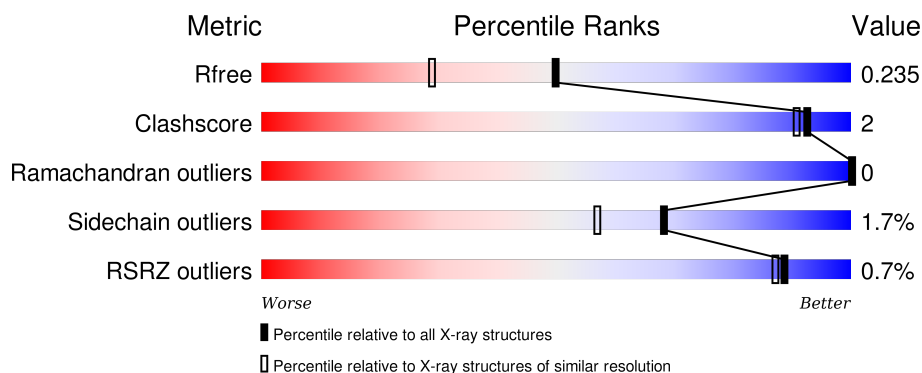
1 Overall quality at a glance

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 ≥ 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>94%</div> <div>5% .</div> </div>
1	C	219	<div> <div>%</div> <div>95%</div> <div>.</div> </div>
1	E	219	<div> <div>94%</div> <div>5% .</div> </div>
1	G	219	<div> <div>%</div> <div>92%</div> <div>6% .</div> </div>
2	B	217	<div> <div>92%</div> <div>5% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	217	<div><div></div><div>88%</div><div>6% . .</div></div>
2	F	217	<div>%<div><div></div><div>91%</div><div>5% .</div></div></div>
2	H	217	<div>%<div><div></div><div>91%</div><div>5% . .</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16117 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	4	0
			1710	1067	295	342	6			
1	E	216	Total	C	N	O	S	0	3	0
			1686	1054	289	337	6			
1	G	216	Total	C	N	O	S	0	1	0
			1680	1051	288	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	1	0
			1605	1022	260	314	9			
2	D	209	Total	C	N	O	S	0	1	0
			1609	1025	261	314	9			
2	F	209	Total	C	N	O	S	0	3	0
			1619	1030	261	319	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 (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	10	Total	C	N	O	0	0
			112	65	2	45		
3	D	10	Total	C	N	O	0	0
			112	65	2	45		
3	F	10	Total	C	N	O	0	0
			112	65	2	45		
3	H	10	Total	C	N	O	0	0
			112	65	2	45		

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	362	Total	O	0	0
			362	362		
5	B	338	Total	O	0	0
			338	338		
5	C	282	Total	O	0	0
			282	282		
5	D	338	Total	O	0	0
			338	338		
5	E	311	Total	O	0	0
			311	311		
5	E	1	Total	O	0	0
			1	1		
5	F	287	Total	O	0	0
			287	287		
5	G	255	Total	O	0	0
			255	255		
5	H	301	Total	O	0	0
			301	301		

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:  94% 5% .



- Molecule 1: Fab F22-4 light chain

Chain C:  95% .

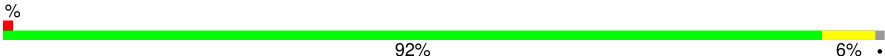


- Molecule 1: Fab F22-4 light chain

Chain E:  94% 5% .



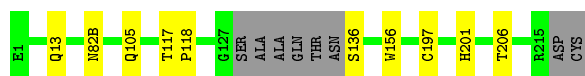
- Molecule 1: Fab F22-4 light chain

Chain G:  92% 6% .




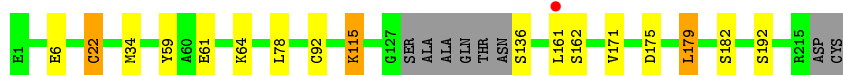
- Molecule 2: Fab F22-4 heavy chain

Chain B:  92% 5% .

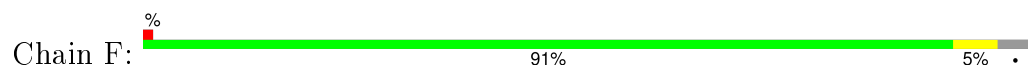


- Molecule 2: Fab F22-4 heavy chain

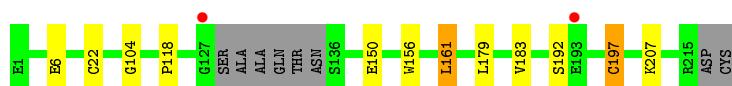
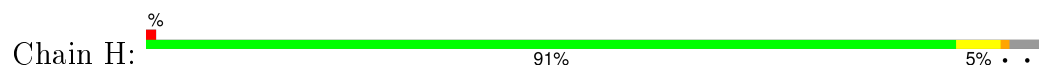
Chain D:  88% 6% . .



- Molecule 2: Fab F22-4 heavy chain



- Molecule 2: Fab F22-4 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.06Å 137.60Å 109.80Å 90.00° 95.15° 90.00°	Depositor
Resolution (Å)	47.92 – 1.80 47.92 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.92-1.80) 99.2 (47.92-1.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.176 , 0.230 0.185 , 0.235	Depositor DCC
R_{free} test set	2708 reflections (1.51%)	DCC
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 197475 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16117	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.95 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.4798e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: RAM, GLC, NAG, EAG, 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	0.58	0/1723	0.72	0/2340
1	C	0.56	0/1765	0.68	1/2397 (0.0%)
1	E	0.59	0/1737	0.74	2/2359 (0.1%)
1	G	0.53	0/1723	0.69	0/2340
2	B	0.64	0/1651	0.72	0/2252
2	D	0.67	1/1655 (0.1%)	0.75	1/2256 (0.0%)
2	F	0.56	0/1672	0.66	0/2280
2	H	0.61	2/1646 (0.1%)	0.70	0/2245
All	All	0.59	3/13572 (0.0%)	0.71	4/18469 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	22	CYS	CB-SG	-6.53	1.71	1.82
2	H	197	CYS	CB-SG	-6.39	1.71	1.82
2	H	150	GLU	CD-OE2	5.07	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1	ASP	CB-CG-OD1	6.74	124.37	118.30
1	C	24	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	E	47	LEU	CA-CB-CG	5.27	127.41	115.30
2	D	179	LEU	CA-CB-CG	5.03	126.87	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	1680	0	1625	4	0
1	C	1710	0	1649	5	0
1	E	1686	0	1628	6	0
1	G	1680	0	1625	11	0
2	B	1605	0	1572	9	1
2	D	1609	0	1583	10	0
2	F	1619	0	1584	4	0
2	H	1604	0	1574	6	0
3	B	112	0	98	0	0
3	D	112	0	98	0	0
3	F	112	0	98	0	0
3	H	112	0	98	1	0
4	E	1	0	0	0	0
5	A	362	0	0	2	0
5	B	338	0	0	5	1
5	C	282	0	0	0	1
5	D	338	0	0	5	1
5	E	312	0	0	2	0
5	F	287	0	0	0	0
5	G	255	0	0	3	0
5	H	301	0	0	3	0
All	All	16117	0	13232	54	2

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 2.

All (54) 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:D:92:CYS:HB3	5:D:648:HOH:O	1.16	1.30
1:E:211:ARG:C	5:E:405:HOH:O	1.88	1.11
2:D:92:CYS:CB	5:D:648:HOH:O	1.93	0.76
2:B:136:SER:N	5:B:440:HOH:O	2.28	0.66
1:G:81:GLU:OE2	5:G:467:HOH:O	2.12	0.66
2:B:201:HIS:HB3	2:B:206:THR:OG1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:TRP:CD1	1:A:175:MET:HG3	2.39	0.58
1:G:163:TRP:CD2	1:G:175:MET:HG3	2.39	0.57
2:B:206:THR:HG22	5:H:390:HOH:O	2.06	0.56
1:A:74[B]:ARG:NH1	5:A:496:HOH:O	2.38	0.55
1:C:160:LEU:HD21	2:D:171:VAL:HB	1.89	0.55
1:G:126:THR:HB	5:G:299:HOH:O	2.06	0.54
1:G:142:LYS:NZ	5:G:328:HOH:O	2.42	0.53
1:E:136:LEU:HD12	1:E:136:LEU:N	2.24	0.53
1:G:186:TYR:O	1:G:192:TYR:OH	2.26	0.52
1:G:157:ASN:N	1:G:157:ASN:HD22	2.06	0.52
2:D:92:CYS:SG	5:D:648:HOH:O	2.55	0.52
1:E:145[B]:ASN:ND2	5:E:322:HOH:O	2.43	0.52
2:F:6:GLU:HG3	2:F:22:CYS:HB3	1.93	0.51
1:G:124:GLN:O	1:G:127:SER:OG	2.18	0.50
2:D:136:SER:N	5:D:584:HOH:O	2.46	0.49
2:D:59:TYR:O	2:D:64:LYS:HE2	2.12	0.48
1:E:15:LEU:HD23	1:E:106:ILE:HD12	1.93	0.48
2:F:24:VAL:HG11	2:F:27:LEU:HD11	1.96	0.47
2:B:13:GLN:NE2	5:B:640:HOH:O	2.30	0.47
2:F:93:PHE:O	2:F:95:PRO:HD3	2.17	0.45
5:B:645:HOH:O	2:H:118:PRO:HD2	2.17	0.45
1:C:50:HIS:HB2	1:C:53:ASN:HD22	1.81	0.45
1:E:161:ASN:ND2	1:E:177:SER:OG	2.50	0.44
2:H:156:TRP:CZ3	2:H:197:CYS:HB3	2.52	0.44
2:H:6:GLU:OE2	2:H:104:GLY:HA3	2.18	0.44
2:B:118:PRO:HB3	2:B:206:THR:HG21	2.00	0.44
2:B:156:TRP:CZ3	2:B:197:CYS:HB3	2.53	0.44
5:B:484:HOH:O	1:G:183:LYS:HD3	2.18	0.44
2:H:161:LEU:HD13	2:H:183:VAL:HG21	2.01	0.43
1:C:190:ASN:O	1:C:210:ASN:HA	2.19	0.43
1:G:186:TYR:HA	1:G:192:TYR:OH	2.19	0.42
2:D:6:GLU:HG3	2:D:22:CYS:HB3	2.01	0.42
2:H:6:GLU:HG3	2:H:22:CYS:HB3	2.02	0.42
2:F:95:PRO:HA	2:F:96:MET:HA	1.80	0.42
2:B:117:THR:CG2	5:B:645:HOH:O	2.67	0.41
2:H:179:LEU:HD12	2:H:179:LEU:C	2.40	0.41
1:A:161:ASN:HD22	1:A:177:SER:HA	1.85	0.41
1:G:157:ASN:N	1:G:157:ASN:ND2	2.68	0.41
1:C:135:PHE:CE2	2:D:182:SER:CB	3.03	0.41
2:D:34:MET:HB3	2:D:78:LEU:HD22	2.02	0.41
3:H:310:EAG:H8B	5:H:491:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:LEU:HD12	1:G:136:LEU:N	2.36	0.41
5:A:302:HOH:O	1:E:27:LYS:HG2	2.21	0.41
1:A:27(D):HIS:HB3	1:A:28:ASP:OD1	2.21	0.41
2:B:206:THR:CG2	5:H:390:HOH:O	2.68	0.40
2:B:82(B):ASN:O	2:B:82(B):ASN:CG	2.59	0.40
2:D:115[A]:LYS:HD2	5:D:419:HOH:O	2.22	0.40

All (2) 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:B:136:SER:N	5:C:262:HOH:O[2_645]	1.97	0.23
5:B:389:HOH:O	5:D:388:HOH:O[2_645]	2.05	0.15

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%)	211 (98%)	4 (2%)	0	100	100
1	C	220/219 (100%)	217 (99%)	3 (1%)	0	100	100
1	E	217/219 (99%)	212 (98%)	5 (2%)	0	100	100
1	G	215/219 (98%)	209 (97%)	6 (3%)	0	100	100
2	B	206/217 (95%)	201 (98%)	5 (2%)	0	100	100
2	D	206/217 (95%)	204 (99%)	2 (1%)	0	100	100
2	F	208/217 (96%)	205 (99%)	3 (1%)	0	100	100
2	H	205/217 (94%)	203 (99%)	2 (1%)	0	100	100
All	All	1692/1744 (97%)	1662 (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	197/194 (102%)	195 (99%)	2 (1%)	82	77
1	E	194/194 (100%)	193 (100%)	1 (0%)	92	91
1	G	192/194 (99%)	188 (98%)	4 (2%)	61	47
2	B	185/191 (97%)	184 (100%)	1 (0%)	92	91
2	D	186/191 (97%)	178 (96%)	8 (4%)	35	17
2	F	188/191 (98%)	184 (98%)	4 (2%)	61	47
2	H	185/191 (97%)	182 (98%)	3 (2%)	70	59
All	All	1519/1540 (99%)	1493 (98%)	26 (2%)	68	57

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	ASP
1	A	169	LYS
1	A	191	SER
2	B	105	GLN
1	C	175	MET
1	C	190	ASN
2	D	61	GLU
2	D	115[A]	LYS
2	D	115[B]	LYS
2	D	161	LEU
2	D	162	SER
2	D	175	ASP
2	D	179	LEU
2	D	192	SER
1	E	71	PHE
2	F	18	MET
2	F	83	ARG
2	F	115	LYS
2	F	198	ASN

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Mol	Chain	Res	Type
1	G	81	GLU
1	G	122	SER
1	G	143	ASP
1	G	184	ASP
2	H	161	LEU
2	H	192	SER
2	H	207	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	157	ASN
1	A	161	ASN
2	B	31	ASN
2	B	54	ASN
2	B	82(A)	ASN
1	C	53	ASN
1	C	145	ASN
1	C	157	ASN
1	C	161	ASN
1	C	190	ASN
1	C	212	ASN
2	D	31	ASN
1	E	161	ASN
2	F	31	ASN
1	G	156	GLN
1	G	157	ASN
1	G	161	ASN
2	H	31	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 ⓘ

40 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	0.52	0	14,14,16	1.35	1 (7%)
3	RAM	B	302	3	10,10,11	0.68	0	14,14,16	1.18	1 (7%)
3	RAM	B	303	3	10,10,11	0.65	0	14,14,16	1.37	2 (14%)
3	GLC	B	304	3	11,11,12	0.69	0	14,15,17	1.09	1 (7%)
3	NAG	B	305	3	14,14,15	0.57	0	15,19,21	1.09	1 (6%)
3	RAM	B	306	3	10,10,11	0.70	0	14,14,16	0.89	0
3	RAM	B	307	3	10,10,11	0.50	0	14,14,16	1.12	1 (7%)
3	RAM	B	308	3	10,10,11	0.62	0	14,14,16	1.01	0
3	GLC	B	309	3	11,11,12	0.55	0	14,15,17	1.17	1 (7%)
3	EAG	B	310	3	16,16,18	0.54	0	21,22,24	1.38	1 (4%)
3	RAM	D	301	3	10,10,11	0.52	0	14,14,16	1.52	2 (14%)
3	RAM	D	302	3	10,10,11	0.42	0	14,14,16	1.14	1 (7%)
3	RAM	D	303	3	10,10,11	0.67	0	14,14,16	0.89	0
3	GLC	D	304	3	11,11,12	0.64	0	14,15,17	1.26	1 (7%)
3	NAG	D	305	3	14,14,15	0.66	0	15,19,21	1.07	2 (13%)
3	RAM	D	306	3	10,10,11	0.85	1 (10%)	14,14,16	1.17	1 (7%)
3	RAM	D	307	3	10,10,11	0.57	0	14,14,16	0.92	1 (7%)
3	RAM	D	308	3	10,10,11	0.54	0	14,14,16	1.03	1 (7%)
3	GLC	D	309	3	11,11,12	0.62	0	14,15,17	1.32	2 (14%)
3	EAG	D	310	3	16,16,18	0.51	0	21,22,24	1.26	1 (4%)
3	RAM	F	301	3	10,10,11	0.56	0	14,14,16	1.43	2 (14%)
3	RAM	F	302	3	10,10,11	0.64	0	14,14,16	1.17	1 (7%)
3	RAM	F	303	3	10,10,11	0.56	0	14,14,16	0.89	0
3	GLC	F	304	3	11,11,12	0.75	0	14,15,17	1.09	1 (7%)
3	NAG	F	305	3	14,14,15	0.62	0	15,19,21	1.08	1 (6%)
3	RAM	F	306	3	10,10,11	0.63	0	14,14,16	1.17	1 (7%)
3	RAM	F	307	3	10,10,11	0.54	0	14,14,16	1.09	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	RAM	F	308	3	10,10,11	0.60	0	14,14,16	1.16	1 (7%)
3	GLC	F	309	3	11,11,12	0.65	0	14,15,17	1.43	3 (21%)
3	EAG	F	310	3	16,16,18	0.49	0	21,22,24	1.38	1 (4%)
3	RAM	H	301	3	10,10,11	0.52	0	14,14,16	1.01	0
3	RAM	H	302	3	10,10,11	0.57	0	14,14,16	1.03	1 (7%)
3	RAM	H	303	3	10,10,11	0.94	1 (10%)	14,14,16	0.91	0
3	GLC	H	304	3	11,11,12	0.59	0	14,15,17	1.37	1 (7%)
3	NAG	H	305	3	14,14,15	0.43	0	15,19,21	0.55	0
3	RAM	H	306	3	10,10,11	0.73	0	14,14,16	0.92	0
3	RAM	H	307	3	10,10,11	0.65	0	14,14,16	0.97	1 (7%)
3	RAM	H	308	3	10,10,11	0.75	0	14,14,16	1.13	0
3	GLC	H	309	3	11,11,12	0.68	0	14,15,17	1.19	1 (7%)
3	EAG	H	310	3	16,16,18	0.43	0	21,22,24	1.30	1 (4%)

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	EAG	B	310	3	-	0/8/28/30	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
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	EAG	D	310	3	-	0/8/28/30	0/1/1/1
3	RAM	F	301	3	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	EAG	F	310	3	-	0/8/28/30	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	EAG	H	310	3	-	0/8/28/30	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	306	RAM	O5-C1	-2.15	1.40	1.43
3	H	303	RAM	O5-C1	-2.11	1.40	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	306	RAM	O5-C1-C2	-2.87	106.20	110.86
3	B	302	RAM	C1-C2-C3	-2.50	106.59	109.54
3	F	306	RAM	O5-C1-C2	-2.49	106.81	110.86
3	F	308	RAM	O4-C4-C3	-2.46	104.81	110.34
3	D	309	GLC	O5-C5-C6	-2.29	102.38	107.35
3	D	305	NAG	O3-C3-C4	-2.24	105.30	110.34
3	F	307	RAM	O2-C2-C3	-2.23	105.64	110.12
3	D	305	NAG	O7-C7-C8	-2.14	118.13	122.06
3	D	308	RAM	O4-C4-C3	-2.13	105.53	110.34
3	F	309	GLC	O4-C4-C3	-2.08	105.65	110.34
3	D	301	RAM	O5-C1-C2	-2.05	107.53	110.86
3	F	309	GLC	O3-C3-C4	-2.04	105.73	110.34
3	D	307	RAM	O2-C2-C3	-2.04	106.02	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	305	NAG	O7-C7-C8	-2.01	118.38	122.06
3	H	302	RAM	O5-C5-C6	2.10	109.60	106.13
3	B	307	RAM	O3-C3-C2	2.14	113.86	110.00
3	F	304	GLC	C1-O5-C5	2.21	115.05	112.25
3	H	307	RAM	O5-C5-C6	2.26	109.86	106.13
3	F	301	RAM	C1-O5-C5	2.44	116.15	112.38
3	B	303	RAM	C1-O5-C5	2.52	116.27	112.38
3	F	309	GLC	C1-O5-C5	2.60	115.54	112.25
3	D	302	RAM	O5-C5-C6	2.65	110.51	106.13
3	D	304	GLC	C1-O5-C5	2.73	115.71	112.25
3	B	301	RAM	O5-C5-C6	2.76	110.69	106.13
3	B	309	GLC	C1-O5-C5	2.77	115.76	112.25
3	F	302	RAM	O5-C5-C6	2.81	110.77	106.13
3	H	304	GLC	C1-O5-C5	3.03	116.09	112.25
3	B	304	GLC	O2-C2-C1	3.11	115.45	109.21
3	F	301	RAM	C1-C2-C3	3.22	113.35	109.54
3	F	305	NAG	C1-O5-C5	3.28	116.41	112.25
3	B	303	RAM	O5-C5-C6	3.61	112.11	106.13
3	D	309	GLC	C1-O5-C5	3.65	116.88	112.25
3	H	309	GLC	C1-O5-C5	3.70	116.94	112.25
3	D	301	RAM	C1-O5-C5	3.83	118.29	112.38
3	D	310	EAG	C9-O1-C1	4.78	121.12	113.29
3	H	310	EAG	C9-O1-C1	4.85	121.24	113.29
3	B	310	EAG	C9-O1-C1	5.53	122.35	113.29
3	F	310	EAG	C9-O1-C1	5.56	122.39	113.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	310	EAG	1	0

5.6 Ligand geometry

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

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, 95th 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	216/219 (98%)	-0.35	1 (0%) 91 90	9, 18, 30, 41	0
1	C	218/219 (99%)	-0.20	3 (1%) 78 74	11, 23, 39, 47	0
1	E	216/219 (98%)	-0.25	0 100 100	11, 21, 33, 41	0
1	G	216/219 (98%)	-0.10	2 (0%) 85 83	14, 25, 45, 55	0
2	B	209/217 (96%)	-0.30	0 100 100	12, 20, 32, 38	0
2	D	209/217 (96%)	-0.17	1 (0%) 91 90	9, 18, 41, 46	0
2	F	209/217 (96%)	-0.08	3 (1%) 78 74	14, 24, 40, 46	0
2	H	209/217 (96%)	-0.15	2 (0%) 84 82	10, 20, 35, 50	0
All	All	1702/1744 (97%)	-0.20	12 (0%) 89 87	9, 21, 38, 55	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	193	GLU	3.5
1	C	202	THR	3.2
1	G	188	ARG	3.1
1	C	157	ASN	2.9
2	D	161	LEU	2.9
2	F	189	THR	2.7
2	F	161	LEU	2.4
1	A	11	ASN	2.2
1	G	186	TYR	2.2
2	F	163	SER	2.2
1	C	109	ALA	2.0
2	H	127	GLY	2.0

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, 95th 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	NAG	H	305	14/15	0.96	0.10	0.41	15,17,20,21	0
3	NAG	B	305	14/15	0.96	0.07	-0.08	13,14,18,20	0
3	NAG	F	305	14/15	0.97	0.07	-0.34	18,19,21,22	0
3	RAM	H	303	10/11	0.96	0.08	-0.35	15,17,18,20	0
3	GLC	F	304	11/12	0.94	0.08	-0.55	18,22,22,22	0
3	RAM	D	303	10/11	0.98	0.06	-0.58	12,13,15,18	0
3	NAG	D	305	14/15	0.98	0.06	-0.93	11,13,16,17	0
3	GLC	H	304	11/12	0.97	0.07	-0.97	16,17,20,21	0
3	RAM	F	303	10/11	0.96	0.07	-1.12	16,18,20,23	0
3	GLC	D	304	11/12	0.98	0.06	-1.16	12,14,16,16	0
3	GLC	B	304	11/12	0.96	0.06	-1.60	17,18,19,19	0
3	RAM	B	303	10/11	0.98	0.06	-1.64	13,15,18,24	0
3	EAG	B	310	16/18	0.88	0.17	-	32,37,43,43	0
3	EAG	D	310	16/18	0.88	0.18	-	31,37,41,44	0
3	RAM	F	306	10/11	0.94	0.10	-	19,24,28,28	0
3	RAM	H	301	10/11	0.92	0.17	-	32,34,36,38	0
3	RAM	D	301	10/11	0.87	0.20	-	27,30,30,33	0
3	RAM	B	306	10/11	0.96	0.08	-	14,19,22,23	0
3	RAM	F	307	10/11	0.95	0.08	-	24,26,26,27	0
3	RAM	B	301	10/11	0.84	0.22	-	35,37,39,39	0
3	GLC	H	309	11/12	0.96	0.09	-	21,23,25,25	0
3	RAM	H	302	10/11	0.91	0.12	-	25,27,29,29	0
3	GLC	D	309	11/12	0.95	0.10	-	19,21,23,24	0
3	EAG	H	310	16/18	0.82	0.18	-	38,45,47,48	0
3	RAM	B	307	10/11	0.97	0.06	-	18,20,21,23	0
3	RAM	H	307	10/11	0.93	0.08	-	22,25,27,28	0
3	EAG	F	310	16/18	0.86	0.17	-	35,41,43,44	0
3	GLC	B	309	11/12	0.97	0.07	-	18,19,21,22	0
3	RAM	B	302	10/11	0.86	0.11	-	29,33,34,35	0
3	RAM	D	302	10/11	0.92	0.10	-	20,24,26,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	RAM	F	301	10/11	0.93	0.16	-	34,36,38,38	0
3	RAM	D	308	10/11	0.93	0.09	-	22,26,28,29	0
3	RAM	F	308	10/11	0.93	0.12	-	26,30,33,33	0
3	RAM	B	308	10/11	0.95	0.07	-	20,24,27,28	0
3	RAM	H	308	10/11	0.93	0.13	-	27,30,33,34	0
3	RAM	H	306	10/11	0.95	0.13	-	21,24,26,26	0
3	GLC	F	309	11/12	0.96	0.06	-	21,25,27,30	0
3	RAM	D	306	10/11	0.95	0.10	-	15,19,21,22	0
3	RAM	D	307	10/11	0.96	0.07	-	18,20,22,25	0
3	RAM	F	302	10/11	0.92	0.08	-	27,29,32,32	0

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. 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, 95th 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(\AA^2)	Q<0.9
4	PD	E	215	1/1	1.00	0.02	-5.04	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.