



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 06:45 AM BST

PDB ID : 4R4B
Title : Crystal structure of the anti-hiv-1 antibody 2.2c
Authors : McLellan, J.S.; Acharya, P.; Huang, C.-C.; Robinson, J.; Kwong, P.D.
Deposited on : 2014-08-19
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

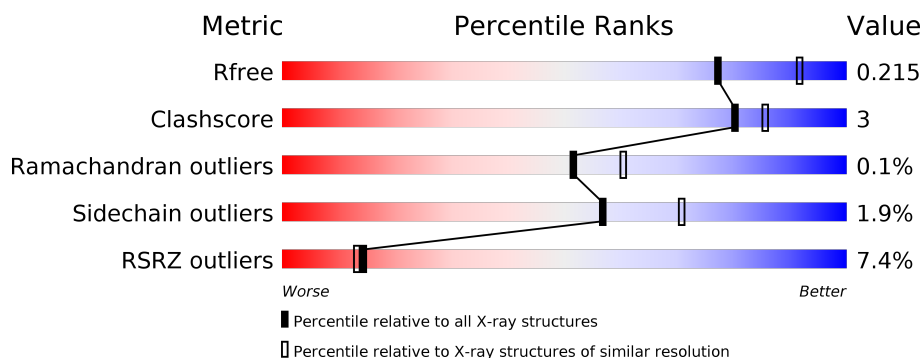
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



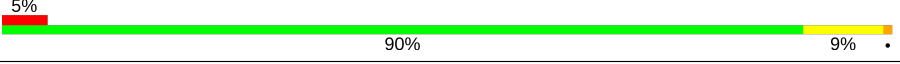
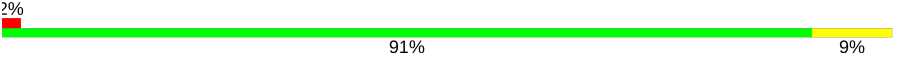
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	210	<div> <div style="width: 94%;"></div> <div style="width: 5%;"></div> </div>
1	C	210	<div> <div style="width: 20%;"></div> <div style="width: 88%;"></div> <div style="width: 9%;"></div> <div style="width: 3%;"></div> </div>
1	E	210	<div> <div style="width: 24%;"></div> <div style="width: 87%;"></div> <div style="width: 10%;"></div> <div style="width: 1%;"></div> </div>
1	L	210	<div> <div style="width: 95%;"></div> <div style="width: 5%;"></div> </div>
2	B	220	<div> <div style="width: 5%;"></div> <div style="width: 95%;"></div> <div style="width: 5%;"></div> </div>
2	D	220	<div> <div style="width: 4%;"></div> <div style="width: 92%;"></div> <div style="width: 8%;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	F	220	
2	H	220	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	F	303	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14523 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 2.2C LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	210	Total	C	N	O	S	0	0	0
			1612	1012	272	323	5			
1	A	210	Total	C	N	O	S	0	0	0
			1612	1012	272	323	5			
1	C	204	Total	C	N	O	S	0	0	0
			1573	989	265	314	5			
1	E	204	Total	C	N	O	S	0	0	0
			1573	989	265	314	5			

- Molecule 2 is a protein called FAB 2.2C HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1671	1064	283	319	5			
2	B	220	Total	C	N	O	S	0	0	0
			1671	1064	283	319	5			
2	D	220	Total	C	N	O	S	0	0	0
			1671	1064	283	319	5			
2	F	220	Total	C	N	O	S	0	0	0
			1671	1064	283	319	5			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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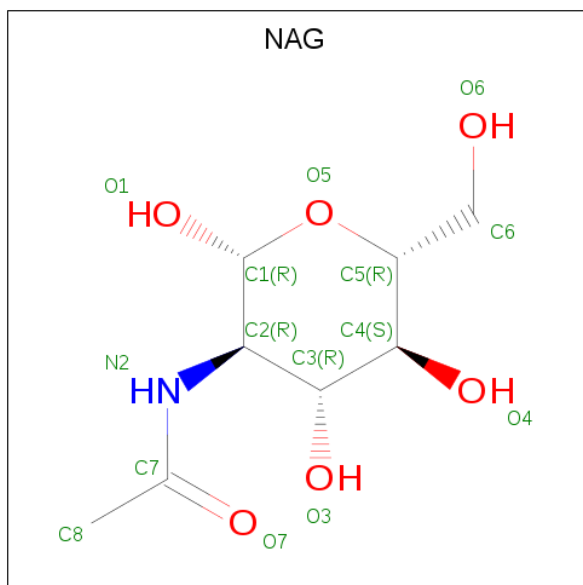
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	214	Total	O	0	0
			214	214		
5	H	189	Total	O	0	0
			189	189		
5	A	186	Total	O	0	0
			186	186		
5	B	152	Total	O	0	0
			152	152		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	101	Total 101	O 101	0	0
5	D	164	Total 164	O 164	0	0
5	E	66	Total 66	O 66	0	0
5	F	161	Total 161	O 161	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: FAB 2.2C LIGHT CHAIN

Chain L: 




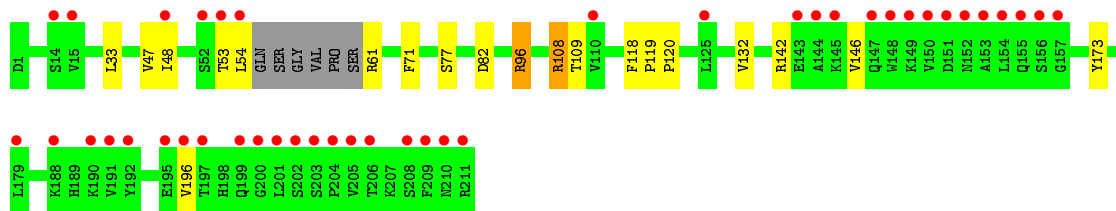
- Molecule 1: FAB 2.2C LIGHT CHAIN

Chain A: 




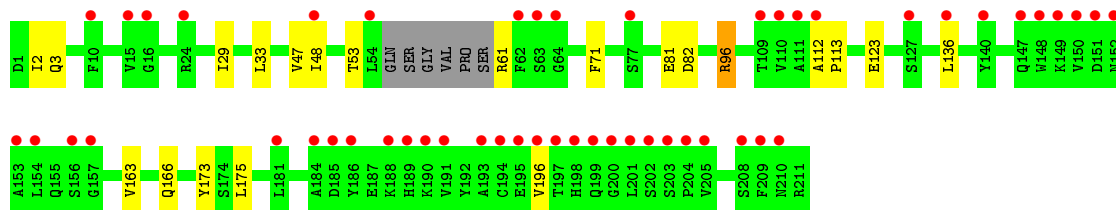
- Molecule 1: FAB 2.2C LIGHT CHAIN

Chain C: 




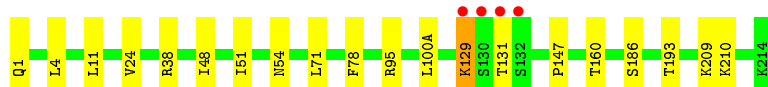
- Molecule 1: FAB 2.2C LIGHT CHAIN

Chain E: 



- Molecule 2: FAB 2.2C HEAVY CHAIN

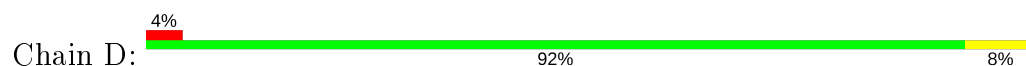
Chain H: 



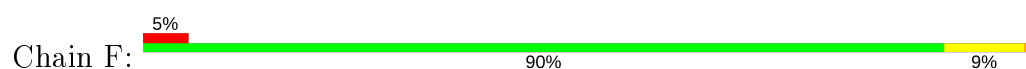
• Molecule 2: FAB 2.2C HEAVY CHAIN



• Molecule 2: FAB 2.2C HEAVY CHAIN



• Molecule 2: FAB 2.2C HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.01Å 133.56Å 90.77Å 90.00° 91.36° 90.00°	Depositor
Resolution (Å)	48.66 – 2.20 48.66 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.2 (48.66-2.20) 88.2 (48.66-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.166 , 0.214 0.168 , 0.215	Depositor DCC
R_{free} test set	5223 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14523	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NAG, SO4

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	0.27	0/1646	0.46	0/2231
1	C	0.25	0/1605	0.43	0/2173
1	E	0.24	0/1605	0.43	0/2173
1	L	0.29	0/1646	0.47	0/2231
2	B	0.27	0/1720	0.49	0/2352
2	D	0.26	0/1720	0.45	0/2352
2	F	0.27	0/1720	0.48	0/2352
2	H	0.27	0/1720	0.49	0/2352
All	All	0.27	0/13382	0.46	0/18216

There are no bond length outliers.

There are no bond angle outliers.

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	1612	0	1583	6	0
1	C	1573	0	1545	12	0
1	E	1573	0	1545	10	0
1	L	1612	0	1583	4	0
2	B	1671	0	1647	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1671	0	1647	15	0
2	F	1671	0	1647	17	0
2	H	1671	0	1647	9	0
3	A	25	0	0	0	0
3	B	40	0	0	0	0
3	C	15	0	0	0	0
3	D	5	0	0	0	0
3	E	10	0	0	0	0
3	F	30	0	0	2	0
3	H	25	0	0	0	0
3	L	30	0	0	0	0
4	B	14	0	13	0	0
4	D	14	0	13	0	0
4	F	14	0	13	0	0
4	H	14	0	13	0	0
5	A	186	0	0	0	0
5	B	152	0	0	2	0
5	C	101	0	0	1	0
5	D	164	0	0	0	0
5	E	66	0	0	0	0
5	F	161	0	0	2	0
5	H	189	0	0	0	0
5	L	214	0	0	0	0
All	All	14523	0	12896	71	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 3.

All (71) 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)
3:F:303:SO4:S	5:F:405:HOH:O	2.49	0.70
1:A:22:THR:HG22	1:A:72:THR:HG22	1.76	0.65
3:F:303:SO4:O3	5:F:405:HOH:O	2.14	0.64
1:E:47:VAL:HG12	1:E:48:ILE:HG13	1.82	0.62
1:E:61:ARG:NH1	1:E:82:ASP:OD2	2.33	0.62
1:L:166:GLN:HG3	1:L:173:TYR:CZ	2.35	0.61
2:H:1:GLN:HB2	2:F:100:TYR:CE1	2.35	0.61
1:A:47:VAL:HG12	1:A:48:ILE:HG13	1.83	0.60
2:F:143:LYS:HA	2:F:177:SER:HB2	1.84	0.60
2:F:129:LYS:HD3	2:F:129:LYS:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:66:ARG:NH2	2:F:86:ASP:OD2	2.36	0.57
1:E:136:LEU:HD21	1:E:196:VAL:HG21	1.86	0.57
2:F:18:LEU:HB3	2:F:82:LEU:HB3	1.87	0.56
1:C:47:VAL:HG12	1:C:48:ILE:HG13	1.88	0.56
2:H:4:LEU:HD22	2:H:24:VAL:HG22	1.88	0.55
2:D:4:LEU:HD22	2:D:24:VAL:HG22	1.88	0.54
2:H:193:THR:HG23	2:H:210:LYS:HE3	1.90	0.54
2:D:94:ARG:NH1	2:F:1:GLN:HG3	2.23	0.53
1:C:96:ARG:HD2	2:D:47:TRP:CE2	2.44	0.53
2:B:117:LYS:NZ	5:B:426:HOH:O	2.42	0.52
2:D:94:ARG:HH12	2:F:1:GLN:HG3	1.75	0.52
1:E:166:GLN:HG3	1:E:173:TYR:CZ	2.46	0.51
1:C:61:ARG:N	5:C:480:HOH:O	2.42	0.51
1:A:108:ARG:HD3	1:A:109:THR:O	2.10	0.51
2:H:71:LEU:HD23	2:H:78:PHE:HB3	1.92	0.51
2:F:71:LEU:HD23	2:F:78:PHE:HB3	1.91	0.51
1:C:61:ARG:NH1	1:C:82:ASP:OD2	2.43	0.51
1:L:21:ILE:HD11	1:L:73:LEU:HD23	1.94	0.50
1:E:96:ARG:HD2	2:F:47:TRP:CE2	2.48	0.49
1:C:48:ILE:HG12	1:C:54:LEU:HD23	1.94	0.49
2:D:142:VAL:HB	2:D:178:LEU:HD23	1.95	0.49
1:L:10:PHE:CZ	1:L:105:GLU:HG2	2.48	0.48
2:B:43:LYS:NZ	5:B:524:HOH:O	2.45	0.48
1:C:33:LEU:HD22	1:C:71:PHE:CG	2.48	0.48
2:D:33:TYR:CZ	2:D:52:LYS:HD2	2.48	0.48
2:D:38:ARG:HB3	2:D:48:ILE:HD11	1.96	0.48
1:E:33:LEU:HD22	1:E:71:PHE:CG	2.50	0.47
2:B:1:GLN:HG2	2:D:100:TYR:CE1	2.50	0.47
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.96	0.47
2:B:129:LYS:HD3	2:B:129:LYS:H	1.79	0.47
2:F:142:VAL:HB	2:F:178:LEU:HD23	1.97	0.46
2:H:131:THR:HG23	2:H:186:SER:OG	2.15	0.46
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.98	0.46
2:F:29:LEU:HD13	2:F:71:LEU:HD22	1.98	0.46
2:H:11:LEU:HD22	2:H:147:PRO:HG3	1.98	0.46
2:D:97:ASN:H	2:F:1:GLN:HE22	1.63	0.45
1:C:61:ARG:HD2	1:C:77:SER:O	2.17	0.45
2:D:33:TYR:CE1	2:D:52:LYS:HD2	2.52	0.44
1:E:2:ILE:HD13	1:E:29:ILE:HG22	1.99	0.44
1:E:112:ALA:HA	1:E:113:PRO:HD3	1.85	0.44
1:A:48:ILE:HG12	1:A:54:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:LEU:HD22	2:F:24:VAL:HG22	1.98	0.43
2:D:1:GLN:OE1	2:F:32:HIS:NE2	2.35	0.43
2:H:51:ILE:HD11	2:H:54:ASN:HA	2.01	0.43
1:C:118:PHE:HA	1:C:119:PRO:HD3	1.92	0.43
1:E:166:GLN:HG3	1:E:173:TYR:CE1	2.52	0.43
1:E:163:VAL:HG22	1:E:175:LEU:HD12	2.01	0.42
1:A:123:GLU:HA	1:A:126:LYS:HD3	2.00	0.42
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.88	0.42
2:F:101:ASP:HA	2:F:102:PRO:HA	1.89	0.42
2:D:97:ASN:H	2:F:1:GLN:NE2	2.17	0.42
1:C:108:ARG:HD3	1:C:109:THR:O	2.19	0.41
2:B:60:HIS:HA	2:B:61:PRO:HD3	1.93	0.41
2:H:129:LYS:HD3	2:H:129:LYS:H	1.85	0.41
1:C:120:PRO:HD3	1:C:132:VAL:HG22	2.03	0.41
1:C:146:VAL:HG22	1:C:196:VAL:HG22	2.03	0.41
1:L:75:ILE:HG21	1:L:78:LEU:HD23	2.03	0.41
2:D:101:ASP:HA	2:D:102:PRO:HA	1.91	0.40
1:C:142:ARG:HB2	1:C:173:TYR:CE2	2.55	0.40
2:F:66:ARG:HH22	2:F:86:ASP:CG	2.24	0.40
2:D:129:LYS:H	2:D:129:LYS:HD3	1.86	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	208/210 (99%)	202 (97%)	6 (3%)	0	100	100
1	C	200/210 (95%)	191 (96%)	9 (4%)	0	100	100
1	E	200/210 (95%)	188 (94%)	12 (6%)	0	100	100
1	L	208/210 (99%)	200 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
2	D	218/220 (99%)	212 (97%)	6 (3%)	0	100	100
2	F	218/220 (99%)	213 (98%)	5 (2%)	0	100	100
2	H	218/220 (99%)	211 (97%)	6 (3%)	1 (0%)	29	31
All	All	1688/1720 (98%)	1627 (96%)	60 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	100(A)	LEU

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	183/183 (100%)	181 (99%)	2 (1%)	73	85
1	C	178/183 (97%)	175 (98%)	3 (2%)	60	74
1	E	178/183 (97%)	173 (97%)	5 (3%)	43	56
1	L	183/183 (100%)	180 (98%)	3 (2%)	62	76
2	B	191/191 (100%)	186 (97%)	5 (3%)	46	58
2	D	191/191 (100%)	190 (100%)	1 (0%)	88	94
2	F	191/191 (100%)	186 (97%)	5 (3%)	46	58
2	H	191/191 (100%)	187 (98%)	4 (2%)	53	67
All	All	1486/1496 (99%)	1458 (98%)	28 (2%)	57	71

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	72	THR
1	L	105	GLU
1	L	108	ARG

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Mol	Chain	Res	Type
2	H	95	ARG
2	H	129	LYS
2	H	160	THR
2	H	209	LYS
1	A	33	LEU
1	A	108	ARG
2	B	28	SER
2	B	95	ARG
2	B	115	SER
2	B	129	LYS
2	B	209	LYS
1	C	53	THR
1	C	96	ARG
1	C	108	ARG
2	D	129	LYS
1	E	3	GLN
1	E	53	THR
1	E	81	GLU
1	E	96	ARG
1	E	123	GLU
2	F	52	LYS
2	F	129	LYS
2	F	177	SER
2	F	178	LEU
2	F	193	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

40 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	$\# Z > 2$
3	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	L	306	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	A	305	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	A	302	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	L	302	-	4,4,4	0.14	0	6,6,6	0.10	0
4	NAG	H	301	2	14,14,15	0.48	0	17,19,21	0.66	0
3	SO4	B	306	-	4,4,4	0.13	0	6,6,6	0.11	0
3	SO4	D	302	-	4,4,4	0.12	0	6,6,6	0.08	0
3	SO4	A	304	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	H	304	-	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	H	303	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	H	305	-	4,4,4	0.15	0	6,6,6	0.05	0
3	SO4	H	302	-	4,4,4	0.15	0	6,6,6	0.05	0
3	SO4	H	306	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	L	303	-	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	F	305	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	C	302	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	B	304	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	F	306	-	4,4,4	0.13	0	6,6,6	0.05	0
3	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.05	0
4	NAG	F	301	2	14,14,15	0.36	0	17,19,21	0.61	0
3	SO4	A	303	-	4,4,4	0.15	0	6,6,6	0.10	0
3	SO4	F	307	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	B	309	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	F	303	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	E	302	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	F	304	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	L	305	-	4,4,4	0.14	0	6,6,6	0.05	0
4	NAG	B	301	2	14,14,15	0.50	0	17,19,21	0.55	0
3	SO4	B	305	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	308	-	4,4,4	0.15	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	E	301	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	302	-	4,4,4	0.16	0	6,6,6	0.06	0
4	NAG	D	301	2	14,14,15	0.31	0	17,19,21	0.51	0
3	SO4	C	301	-	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	F	302	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	L	304	-	4,4,4	0.19	0	6,6,6	0.16	0
3	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	B	307	-	4,4,4	0.14	0	6,6,6	0.06	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
4	NAG	H	301	2	-	3/6/23/26	0/1/1/1
4	NAG	B	301	2	-	3/6/23/26	0/1/1/1
4	NAG	D	301	2	-	3/6/23/26	0/1/1/1
4	NAG	F	301	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	NAG	C4-C5-C6-O6
4	H	301	NAG	O5-C5-C6-O6
4	H	301	NAG	C4-C5-C6-O6
4	B	301	NAG	O5-C5-C6-O6
4	D	301	NAG	C4-C5-C6-O6
4	D	301	NAG	O5-C5-C6-O6
4	H	301	NAG	C3-C2-N2-C7
4	B	301	NAG	C3-C2-N2-C7
4	D	301	NAG	C3-C2-N2-C7
4	F	301	NAG	C3-C2-N2-C7
4	F	301	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	303	SO4	2	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 ⓘ

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	210/210 (100%)	-0.20	0 100 100	19, 29, 49, 83	0
1	C	204/210 (97%)	0.90	42 (20%) 1 1	22, 53, 87, 116	0
1	E	204/210 (97%)	1.00	51 (25%) 0 0	22, 58, 101, 127	0
1	L	210/210 (100%)	-0.21	0 100 100	18, 27, 44, 70	0
2	B	220/220 (100%)	0.25	10 (4%) 33 32	20, 33, 89, 227	0
2	D	220/220 (100%)	-0.02	8 (3%) 42 41	20, 34, 66, 165	0
2	F	220/220 (100%)	0.09	11 (5%) 28 27	19, 35, 77, 187	0
2	H	220/220 (100%)	-0.15	4 (1%) 68 66	19, 31, 72, 134	0
All	All	1708/1720 (99%)	0.20	126 (7%) 14 13	18, 34, 85, 227	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	130	SER	23.0
2	B	129	LYS	14.4
2	B	131	THR	10.4
2	F	129	LYS	9.7
2	D	129	LYS	7.2
2	D	130	SER	6.9
2	H	129	LYS	6.6
2	F	131	THR	6.6
1	E	154	LEU	6.3
2	B	133	GLY	6.1
2	B	128	SER	6.0
2	B	132	SER	5.9
1	C	152	ASN	5.6
1	C	154	LEU	5.5
1	C	205	VAL	5.5
1	C	206	THR	5.4

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Mol	Chain	Res	Type	RSRZ
2	F	133	GLY	5.4
2	D	128	SER	5.3
1	C	191	VAL	5.1
1	C	201	LEU	5.0
2	F	132	SER	4.9
1	E	112	ALA	4.9
1	E	201	LEU	4.8
2	D	131	THR	4.8
1	C	149	LYS	4.8
1	C	150	VAL	4.5
1	E	151	ASP	4.5
1	E	199	GLN	4.4
1	C	203	SER	4.4
1	C	210	ASN	4.2
2	F	130	SER	4.2
2	F	128	SER	4.1
1	C	52	SER	4.0
1	E	152	ASN	4.0
1	E	205	VAL	4.0
1	C	202	SER	4.0
1	E	202	SER	3.8
1	E	62	PHE	3.5
1	E	209	PHE	3.5
1	C	54	LEU	3.5
1	E	153	ALA	3.4
2	B	55	GLY	3.4
1	C	190	LYS	3.3
2	F	127	SER	3.3
2	D	132	SER	3.3
1	E	196	VAL	3.3
1	E	148	TRP	3.3
1	E	191	VAL	3.3
1	E	188	LYS	3.2
1	E	203	SER	3.2
1	C	156	SER	3.2
1	C	153	ALA	3.2
1	E	197	THR	3.1
1	C	155	GLN	3.1
2	H	132	SER	3.0
2	D	127	SER	3.0
2	H	130	SER	3.0
1	E	189	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	214	LYS	2.9
1	C	209	PHE	2.9
1	C	199	GLN	2.9
1	E	54	LEU	2.9
1	E	208	SER	2.9
1	E	111	ALA	2.9
1	C	148	TRP	2.8
1	C	15	VAL	2.8
1	E	150	VAL	2.8
1	C	151	ASP	2.8
1	E	204	PRO	2.8
2	H	131	THR	2.8
1	C	208	SER	2.8
2	F	135	THR	2.8
1	E	200	GLY	2.8
1	E	77	SER	2.7
1	E	190	LYS	2.7
1	C	204	PRO	2.7
2	F	134	GLY	2.6
1	E	181	LEU	2.6
1	C	200	GLY	2.6
1	E	147	GLN	2.6
2	D	133	GLY	2.6
1	C	188	LYS	2.5
1	C	144	ALA	2.5
1	C	196	VAL	2.5
1	C	110	VAL	2.5
1	C	147	GLN	2.5
1	C	195	GLU	2.5
1	E	194	CYS	2.4
1	C	192	TYR	2.4
1	C	48	ILE	2.4
1	E	63	SER	2.4
1	C	125	LEU	2.4
1	C	197	THR	2.4
1	E	109	THR	2.4
1	E	127	SER	2.4
1	E	185	ASP	2.4
1	E	210	ASN	2.3
1	E	64	GLY	2.3
1	E	193	ALA	2.3
2	B	127	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	53	THR	2.3
2	F	1	GLN	2.3
1	E	157	GLY	2.3
2	B	1	GLN	2.3
1	E	149	LYS	2.2
1	C	14	SER	2.2
1	C	143	GLU	2.2
1	E	24	ARG	2.2
1	C	145	LYS	2.2
1	E	184	ALA	2.2
1	E	136	LEU	2.2
1	E	48	ILE	2.2
1	E	110	VAL	2.2
1	E	140	TYR	2.1
2	B	214	LYS	2.1
1	C	211	ARG	2.1
1	E	195	GLU	2.1
1	C	157	GLY	2.1
2	D	1	GLN	2.1
1	E	156	SER	2.1
1	E	198	HIS	2.1
1	E	10	PHE	2.0
1	E	186	TYR	2.0
1	E	15	VAL	2.0
1	C	179	LEU	2.0
1	E	16	GLY	2.0

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 monosaccharides 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, 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	B-factors(\AA^2)	Q<0.9
4	NAG	F	301	14/15	0.72	0.29	94,117,126,128	0
4	NAG	H	301	14/15	0.77	0.33	95,118,126,131	0
4	NAG	B	301	14/15	0.79	0.33	102,130,138,139	0
4	NAG	D	301	14/15	0.84	0.32	77,97,102,105	0
3	SO4	L	306	5/5	0.85	0.21	96,104,109,110	0
3	SO4	E	302	5/5	0.87	0.18	76,83,85,94	0
3	SO4	L	305	5/5	0.87	0.18	97,102,103,104	0
3	SO4	B	306	5/5	0.88	0.21	86,91,93,94	0
3	SO4	A	305	5/5	0.89	0.39	100,102,105,105	0
3	SO4	F	306	5/5	0.90	0.21	94,96,99,104	0
3	SO4	H	305	5/5	0.91	0.19	84,89,92,97	0
3	SO4	B	307	5/5	0.91	0.18	85,87,89,94	0
3	SO4	F	303	5/5	0.92	0.24	71,81,87,90	0
3	SO4	C	302	5/5	0.92	0.17	86,88,92,93	0
3	SO4	B	305	5/5	0.93	0.15	78,84,89,93	0
3	SO4	C	303	5/5	0.94	0.22	111,111,113,115	0
3	SO4	B	308	5/5	0.94	0.18	89,91,92,94	0
3	SO4	A	304	5/5	0.95	0.15	62,69,71,75	0
3	SO4	B	309	5/5	0.95	0.14	83,86,87,89	0
3	SO4	B	303	5/5	0.95	0.13	74,80,81,88	0
3	SO4	F	304	5/5	0.95	0.20	74,75,78,82	0
3	SO4	F	307	5/5	0.96	0.11	80,81,84,85	0
3	SO4	L	303	5/5	0.96	0.23	72,76,80,86	0
3	SO4	A	303	5/5	0.96	0.09	43,48,62,67	0
3	SO4	F	305	5/5	0.97	0.18	72,73,75,81	0
3	SO4	H	306	5/5	0.97	0.24	83,83,83,89	0
3	SO4	B	304	5/5	0.97	0.13	59,60,68,74	0
3	SO4	A	301	5/5	0.97	0.12	59,62,67,68	0
3	SO4	A	302	5/5	0.97	0.13	44,50,59,68	0
3	SO4	L	302	5/5	0.98	0.13	50,57,63,69	0
3	SO4	B	302	5/5	0.98	0.09	42,45,47,48	0
3	SO4	H	302	5/5	0.98	0.14	39,47,50,55	0
3	SO4	C	301	5/5	0.98	0.12	38,39,42,43	0
3	SO4	L	304	5/5	0.98	0.15	64,66,67,68	5
3	SO4	L	301	5/5	0.98	0.13	50,51,58,58	0
3	SO4	H	304	5/5	0.98	0.11	50,51,56,59	0
3	SO4	F	302	5/5	0.99	0.12	32,33,36,36	0
3	SO4	H	303	5/5	0.99	0.11	47,50,55,58	0
3	SO4	D	302	5/5	0.99	0.14	35,37,42,45	0
3	SO4	E	301	5/5	0.99	0.10	42,46,49,51	0

6.5 Other polymers

There are no such residues in this entry.