



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 05:29 PM EDT

PDB ID : 4AEI  
Title : Crystal structure of the AaHII-Fab4C1 complex  
Authors : Fabrichny, I.P.; Mondielli, G.; Conrod, S.; Martin-Eauculaire, M.F.; Bourne, Y.; Marchot, P.  
Deposited on : 2012-01-10  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

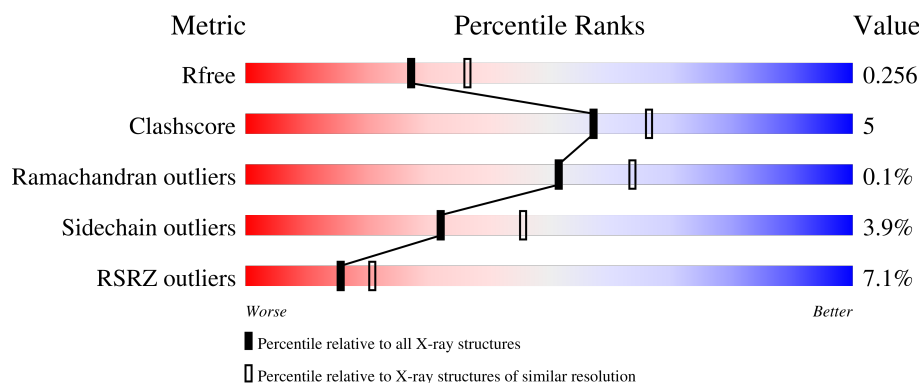
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	65	<div> <div>95%</div> <div>5%</div> </div>
1	B	65	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	C	65	<div> <div>85%</div> <div>15%</div> </div>
2	H	229	<div> <div>4%</div> <div>83%</div> <div>12%</div> <div>.</div> <div>.</div> </div>
2	I	229	<div> <div>7%</div> <div>79%</div> <div>11%</div> <div>.</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	229	<div><div></div><div>10%</div><div>81%</div><div>8%</div><div>9%</div></div>
3	L	219	<div><div></div><div>3%</div><div>81%</div><div>17%</div></div>
3	M	219	<div><div></div><div>9%</div><div>84%</div><div>15%</div></div>
3	N	219	<div><div></div><div>15%</div><div>89%</div><div>10%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11864 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 ALPHA-MAMMAL TOXIN AAH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	65	Total	C	N	O	S	0	2	1
			524	324	96	96	8			
1	B	65	Total	C	N	O	S	0	2	1
			527	325	97	97	8			
1	C	65	Total	C	N	O	S	0	3	1
			536	331	99	98	8			

- Molecule 2 is a protein called FAB ANTIBODY HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	2	0
			1697	1075	277	337	8			
2	I	210	Total	C	N	O	S	0	0	0
			1604	1025	258	314	7			
2	J	208	Total	C	N	O	S	0	1	0
			1596	1018	257	314	7			

- Molecule 3 is a protein called FAB ANTIBODY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	218	Total	C	N	O	S	0	4	0
			1727	1076	296	348	7			
3	M	217	Total	C	N	O	S	0	2	0
			1694	1059	288	341	6			
3	N	217	Total	C	N	O	S	0	2	0
			1698	1059	290	343	6			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

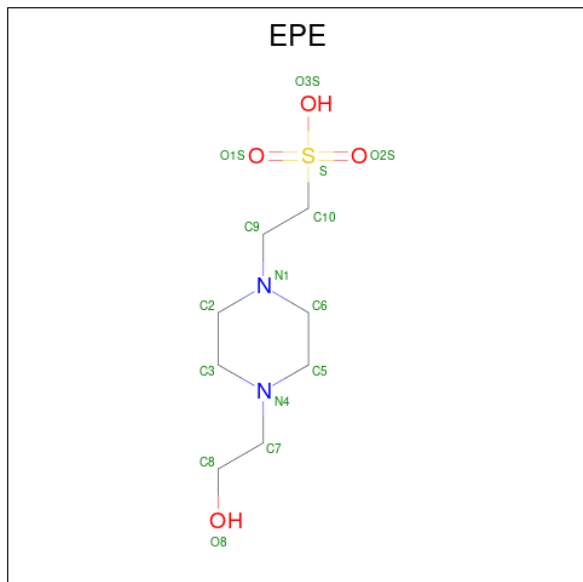
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		
4	I	1	Total	Cl	0	0
			1	1		
4	J	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	21	Total	O	0	0
			21	21		

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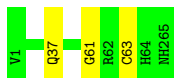
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	18	Total 18	O 18	0	0
6	C	22	Total 22	O 22	0	0
6	H	46	Total 46	O 46	0	0
6	I	27	Total 27	O 27	0	0
6	J	14	Total 14	O 14	0	0
6	L	31	Total 31	O 31	0	0
6	M	25	Total 25	O 25	0	0
6	N	6	Total 6	O 6	0	0

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


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.

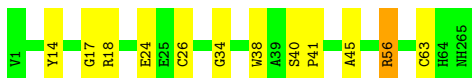
- Molecule 1: ALPHA-MAMMAL TOXIN AAH2

Chain A: 




- Molecule 1: ALPHA-MAMMAL TOXIN AAH2

Chain B: 




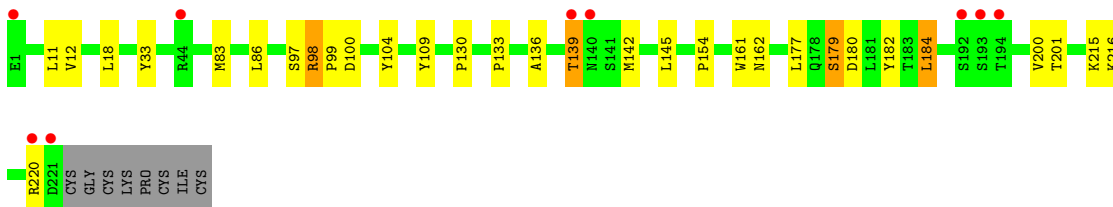
- Molecule 1: ALPHA-MAMMAL TOXIN AAH2

Chain C: 




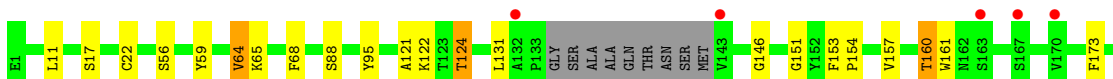
- Molecule 2: FAB ANTIBODY HEAVY CHAIN

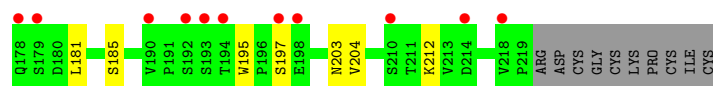
Chain H: 



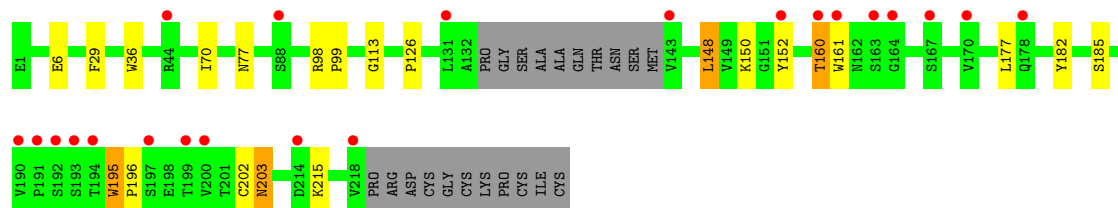
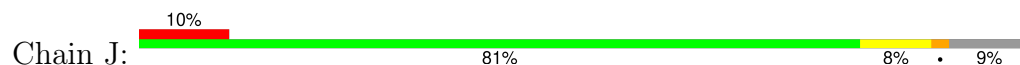
- Molecule 2: FAB ANTIBODY HEAVY CHAIN

Chain I: 

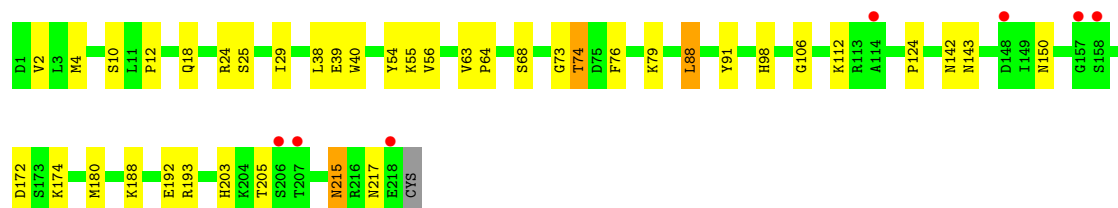
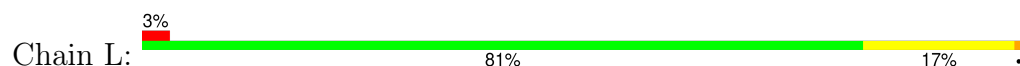




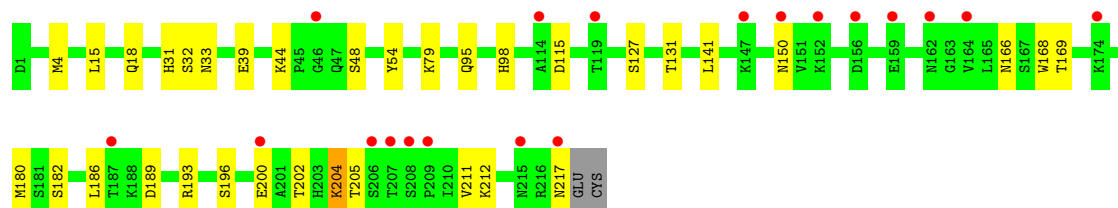
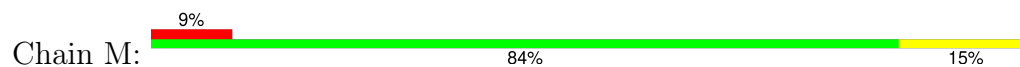
• Molecule 2: FAB ANTIBODY HEAVY CHAIN



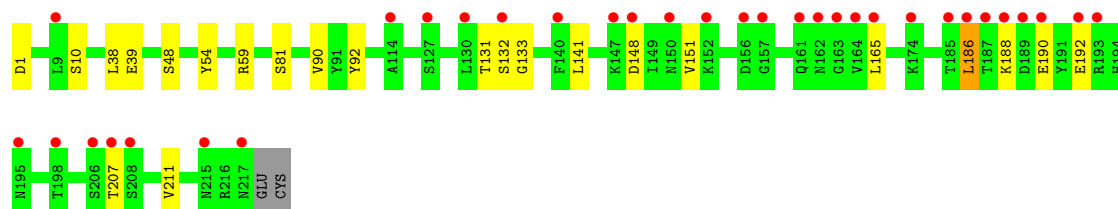
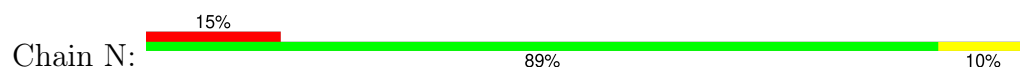
• Molecule 3: FAB ANTIBODY LIGHT CHAIN



• Molecule 3: FAB ANTIBODY LIGHT CHAIN



• Molecule 3: FAB ANTIBODY LIGHT CHAIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.94Å 38.74Å 154.07Å 90.00° 91.36° 90.00°	Depositor
Resolution (Å)	12.97 – 2.30 12.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (12.97-2.30) 99.9 (12.97-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.199 , 0.254 0.200 , 0.256	Depositor DCC
$R_{free}$ test set	3298 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	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 66.19 % 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 6.2882e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, CL, NH2

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	0.69	0/540	0.71	0/728
1	B	0.71	1/540 (0.2%)	0.70	0/728
1	C	0.66	1/549 (0.2%)	0.65	0/739
2	H	0.65	1/1745 (0.1%)	0.69	1/2385 (0.0%)
2	I	0.64	2/1651 (0.1%)	0.68	0/2257
2	J	0.59	2/1641 (0.1%)	0.62	0/2241
3	L	0.59	1/1765 (0.1%)	0.72	1/2393 (0.0%)
3	M	0.55	1/1735 (0.1%)	0.67	0/2354
3	N	0.50	0/1736	0.63	1/2356 (0.0%)
All	All	0.60	9/11902 (0.1%)	0.67	3/16181 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	168	TRP	CD2-CE2	5.61	1.48	1.41
1	C	38	TRP	CD2-CE2	5.58	1.48	1.41
3	L	40	TRP	CD2-CE2	5.34	1.47	1.41
2	H	161	TRP	CD2-CE2	5.26	1.47	1.41
2	I	195	TRP	CD2-CE2	5.26	1.47	1.41
2	J	161	TRP	CD2-CE2	5.25	1.47	1.41
2	I	161	TRP	CD2-CE2	5.15	1.47	1.41
1	B	38	TRP	CD2-CE2	5.14	1.47	1.41
2	J	195	TRP	CD2-CE2	5.03	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	88	LEU	CA-CB-CG	8.58	135.04	115.30
2	H	184	LEU	CA-CB-CG	5.18	127.22	115.30
3	N	186	LEU	CA-CB-CG	5.05	126.91	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	524	0	482	2	0
1	B	527	0	481	5	0
1	C	536	0	493	4	0
2	H	1697	0	1626	19	0
2	I	1604	0	1547	14	0
2	J	1596	0	1537	12	0
3	L	1727	0	1663	27	0
3	M	1694	0	1640	27	0
3	N	1698	0	1635	9	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	A	15	0	18	0	0
5	B	15	0	18	0	0
5	C	15	0	18	0	0
6	A	21	0	0	0	0
6	B	18	0	0	0	0
6	C	22	0	0	1	0
6	H	46	0	0	1	0
6	I	27	0	0	0	0
6	J	14	0	0	0	0
6	L	31	0	0	0	0
6	M	25	0	0	1	0
6	N	6	0	0	0	0
All	All	11864	0	11158	112	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 5.

All (112) 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:M:204[A]:LYS:HE3	3:M:204[A]:LYS:HA	1.41	1.02
3:M:204[A]:LYS:O	3:M:204[A]:LYS:HD3	1.60	1.01
2:I:160:THR:HG22	2:I:203:ASN:HB2	1.47	0.96
3:M:95:GLN:HE22	3:M:98:HIS:H	1.16	0.92
3:L:18:GLN:NE2	3:L:79:LYS:HD2	1.91	0.85
3:M:200:GLU:HG2	3:M:211:VAL:HG12	1.59	0.84
3:M:31:HIS:HD2	3:M:33:ASN:H	1.25	0.83
3:N:132:SER:HB3	3:N:133:GLY:HA2	1.64	0.78
2:I:64:VAL:HG13	2:I:68:PHE:HB2	1.65	0.77
3:M:95:GLN:HE22	3:M:98:HIS:N	1.88	0.70
3:L:215:ASN:HD22	3:L:217:ASN:H	1.38	0.69
3:M:95:GLN:NE2	3:M:98:HIS:H	1.90	0.69
3:M:31:HIS:CD2	3:M:33:ASN:H	2.11	0.68
3:N:132:SER:CB	3:N:133:GLY:HA2	2.23	0.68
3:M:44:LYS:NZ	6:M:2012:HOH:O	2.26	0.67
3:L:142:ASN:HB3	3:L:143:ASN:HD22	1.60	0.66
3:M:166:ASN:OD1	3:M:182:SER:HB2	1.97	0.65
2:H:136:ALA:O	2:H:139:THR:HB	1.97	0.65
2:I:11:LEU:HB2	2:I:154:PRO:HG3	1.79	0.64
3:L:18:GLN:HE22	3:L:79:LYS:HD2	1.62	0.64
3:M:204[A]:LYS:HA	3:M:204[A]:LYS:CE	2.21	0.64
3:L:18:GLN:HE22	3:L:79:LYS:HB3	1.62	0.63
3:L:142:ASN:HB3	3:L:143:ASN:ND2	2.17	0.59
1:B:40:SER:HB2	1:B:41:PRO:HD2	1.83	0.59
2:J:160:THR:HG23	2:J:203:ASN:HB2	1.85	0.58
3:L:172:ASP:OD1	3:L:174:LYS:HG2	2.04	0.58
2:J:36:TRP:HD1	2:J:70:ILE:HD12	1.68	0.57
2:H:130:PRO:HD3	2:H:215:LYS:NZ	2.20	0.56
2:H:220:ARG:CZ	3:L:124:PRO:HG2	2.35	0.56
3:M:31:HIS:HD2	3:M:33:ASN:N	2.00	0.56
3:M:127:SER:O	3:M:131:THR:HG23	2.06	0.56
2:I:160:THR:CG2	2:I:203:ASN:HB2	2.27	0.56
3:M:204[A]:LYS:HE3	3:M:204[A]:LYS:CA	2.18	0.55
3:L:2:VAL:HG12	3:L:4:MET:CE	2.36	0.55
2:H:11:LEU:HB2	2:H:154:PRO:HG3	1.89	0.55
2:J:177:LEU:HB2	2:J:182:TYR:CE1	2.43	0.54
3:M:204[A]:LYS:O	3:M:204[A]:LYS:CD	2.45	0.53
6:C:2021:HOH:O	2:J:99:PRO:HB3	2.09	0.53
3:M:39:GLU:HG2	3:M:54:TYR:HA	1.89	0.52
1:C:26:CYS:SG	1:C:34:GLY:HA3	2.50	0.52
2:I:131:LEU:HB2	2:I:146:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:18:GLN:NE2	3:L:79:LYS:HB3	2.24	0.52
3:N:141:LEU:HD21	3:N:151:VAL:HG22	1.91	0.52
3:M:18[A]:GLN:NE2	3:M:79:LYS:HD2	2.26	0.51
1:B:26:CYS:SG	1:B:34:GLY:HA3	2.50	0.51
3:N:188:LYS:O	3:N:192:GLU:HG2	2.11	0.50
2:H:100:ASP:O	2:H:104:TYR:HA	2.12	0.50
2:H:98:ARG:HG2	2:H:99:PRO:HD2	1.93	0.50
3:M:150:ASN:HB2	3:M:202:THR:HB	1.94	0.49
1:A:37:GLN:OE1	1:C:53:ASP:HB2	2.13	0.49
3:L:24[B]:ARG:HH21	3:L:74:THR:HG22	1.77	0.49
3:L:4:MET:HE2	3:L:25:SER:CB	2.43	0.48
3:L:2:VAL:HG21	3:L:98:HIS:ND1	2.29	0.47
1:C:10:VAL:HB	1:C:64:HIS:HB2	1.94	0.47
2:J:148:LEU:HD21	2:J:150:LYS:HD3	1.95	0.47
3:L:203:HIS:HD2	3:L:205:THR:OG1	1.96	0.47
2:H:12:VAL:HG11	2:H:86:LEU:HD13	1.96	0.47
3:L:4:MET:CE	3:L:25:SER:HB3	2.44	0.47
3:N:39:GLU:HG2	3:N:54:TYR:HA	1.96	0.47
2:J:126:PRO:HB3	2:J:152:TYR:HB3	1.97	0.46
2:J:215:LYS:HA	2:J:215:LYS:HD2	1.66	0.46
2:H:162:ASN:ND2	2:H:201:THR:H	2.13	0.46
2:I:122:LYS:O	2:I:124:THR:HG22	2.16	0.46
3:M:115:ASP:HB3	3:M:205:THR:HG22	1.96	0.46
3:L:2:VAL:HG12	3:L:4:MET:HE3	1.98	0.46
2:H:18:LEU:HB3	2:H:83:MET:HE3	1.96	0.46
2:I:173:PHE:CD1	3:M:169:THR:HG23	2.51	0.46
2:H:97:SER:HA	2:H:109:TYR:O	2.16	0.45
3:L:39:GLU:HG2	3:L:54:TYR:HA	1.97	0.45
3:L:12:PRO:HB2	3:L:112:LYS:HE3	1.99	0.45
2:H:18:LEU:HB3	2:H:83:MET:CE	2.46	0.45
3:L:55:LYS:O	3:L:56:VAL:HB	2.17	0.45
1:C:14:TYR:O	1:C:45:ALA:HA	2.17	0.45
3:N:90:VAL:HG23	3:N:92:TYR:CE1	2.51	0.45
2:H:133:PRO:HD3	2:H:145:LEU:HD23	1.99	0.44
2:H:162:ASN:HD21	2:H:200:VAL:HA	1.82	0.44
2:J:203:ASN:N	2:J:203:ASN:OD1	2.51	0.44
2:I:151:GLY:HA2	2:I:181:LEU:HB3	2.00	0.44
3:L:188:LYS:O	3:L:192:GLU:HG3	2.17	0.44
2:H:179:SER:O	2:H:180:ASP:HB2	2.17	0.44
2:H:216:LYS:HB2	2:H:216:LYS:HE3	1.90	0.44
3:L:18:GLN:HE21	3:L:79:LYS:HD2	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:180:MET:HE1	3:M:182:SER:HB3	1.99	0.44
2:I:121:ALA:HB3	2:I:153:PHE:CE2	2.53	0.44
2:I:131:LEU:HB2	2:I:146:GLY:CA	2.48	0.43
3:M:189:ASP:O	3:M:193:ARG:HG3	2.18	0.43
3:N:186:LEU:HB3	3:N:190:GLU:HB2	2.00	0.43
2:I:204:VAL:O	2:I:212:LYS:HA	2.18	0.43
1:A:61:GLY:HA3	2:H:33:TYR:CG	2.54	0.43
3:L:63:VAL:HA	3:L:64:PRO:HD3	1.88	0.43
2:I:65:LYS:HB3	2:I:65:LYS:HE2	1.76	0.42
2:J:29:PHE:CD2	2:J:77:ASN:HA	2.55	0.42
3:M:31:HIS:CD2	3:M:32:SER:N	2.87	0.42
2:H:220:ARG:NE	3:L:124:PRO:HG2	2.33	0.42
3:L:29:ILE:HD11	3:L:76:PHE:CE1	2.54	0.42
2:H:220:ARG:NH2	6:H:2035:HOH:O	2.27	0.42
3:M:211:VAL:O	3:M:212:LYS:HD2	2.20	0.42
3:N:148[B]:ASP:OD1	3:N:148[B]:ASP:N	2.37	0.42
2:H:177:LEU:HB2	2:H:182:TYR:CE1	2.55	0.41
3:L:4:MET:CE	3:L:25:SER:CB	2.97	0.41
3:L:193[B]:ARG:HA	3:L:193[B]:ARG:HD3	1.76	0.41
2:J:195:TRP:CG	2:J:196:PRO:HA	2.55	0.41
1:B:14:TYR:O	1:B:45:ALA:HA	2.21	0.41
3:L:91:TYR:O	3:L:106:GLY:HA2	2.19	0.41
2:J:6:GLU:CD	2:J:113:GLY:H	2.23	0.41
2:J:195:TRP:CD1	2:J:196:PRO:HA	2.55	0.41
3:M:4:MET:SD	3:M:95:GLN:HB2	2.61	0.41
2:I:95:TYR:CE1	3:M:48:SER:HB3	2.56	0.40
3:M:204[A]:LYS:CE	3:M:204[A]:LYS:CA	2.87	0.40
1:B:17:GLY:C	1:B:18[B]:ARG:HG2	2.40	0.40
3:N:59:ARG:HG3	3:N:59:ARG:HH11	1.86	0.40
1:B:56[A]:ARG:NH2	2:I:59:TYR:OH	2.54	0.40

There are no symmetry-related clashes.

## 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	65/65 (100%)	63 (97%)	2 (3%)	0	100	100
1	B	65/65 (100%)	64 (98%)	1 (2%)	0	100	100
1	C	66/65 (102%)	64 (97%)	2 (3%)	0	100	100
2	H	221/229 (96%)	218 (99%)	3 (1%)	0	100	100
2	I	206/229 (90%)	200 (97%)	6 (3%)	0	100	100
2	J	205/229 (90%)	199 (97%)	6 (3%)	0	100	100
3	L	220/219 (100%)	217 (99%)	2 (1%)	1 (0%)	29	35
3	M	217/219 (99%)	213 (98%)	4 (2%)	0	100	100
3	N	217/219 (99%)	210 (97%)	7 (3%)	0	100	100
All	All	1482/1539 (96%)	1448 (98%)	33 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	73	GLY

### 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	56/54 (104%)	55 (98%)	1 (2%)	59	75
1	B	56/54 (104%)	52 (93%)	4 (7%)	14	19
1	C	57/54 (106%)	55 (96%)	2 (4%)	36	50
2	H	191/196 (97%)	186 (97%)	5 (3%)	46	63
2	I	181/196 (92%)	171 (94%)	10 (6%)	21	30
2	J	180/196 (92%)	174 (97%)	6 (3%)	38	53
3	L	199/196 (102%)	190 (96%)	9 (4%)	27	39
3	M	196/196 (100%)	189 (96%)	7 (4%)	35	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	196/196 (100%)	187 (95%)	9 (5%)	27	38
All	All	1312/1338 (98%)	1259 (96%)	53 (4%)	32	44

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	CYS
1	B	24	GLU
1	B	56[A]	ARG
1	B	56[B]	ARG
1	B	63	CYS
1	C	24	GLU
1	C	63	CYS
2	H	98	ARG
2	H	139	THR
2	H	142	MET
2	H	179	SER
2	H	184	LEU
2	I	17	SER
2	I	22	CYS
2	I	56	SER
2	I	64	VAL
2	I	88	SER
2	I	124	THR
2	I	157	VAL
2	I	160	THR
2	I	185	SER
2	I	197	SER
2	J	98	ARG
2	J	148	LEU
2	J	160	THR
2	J	185	SER
2	J	202	CYS
2	J	203	ASN
3	L	10	SER
3	L	38	LEU
3	L	68	SER
3	L	74	THR
3	L	88	LEU
3	L	150	ASN
3	L	180[A]	MET
3	L	180[B]	MET

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Mol	Chain	Res	Type
3	L	215	ASN
3	M	15	LEU
3	M	141	LEU
3	M	186	LEU
3	M	196	SER
3	M	204[A]	LYS
3	M	204[B]	LYS
3	M	217	ASN
3	N	1	ASP
3	N	10	SER
3	N	38	LEU
3	N	48	SER
3	N	81	SER
3	N	131	THR
3	N	165	LEU
3	N	207	THR
3	N	211	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	162	ASN
2	H	171	HIS
2	I	77	ASN
2	J	77	ASN
2	J	78	ASN
3	L	18	GLN
3	L	58	ASN
3	L	129	GLN
3	L	143	ASN
3	L	203	HIS
3	L	215	ASN
3	M	31	HIS
3	M	35	ASN
3	M	95	GLN
3	M	217	ASN
3	N	143	ASN
3	N	161	GLN
3	N	203	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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$
5	EPE	B	1066	-	15,15,15	2.23	2 (13%)	19,20,20	1.33	3 (15%)
5	EPE	C	1066	-	15,15,15	2.21	2 (13%)	19,20,20	1.16	2 (10%)
5	EPE	A	1066	-	15,15,15	2.30	2 (13%)	19,20,20	1.37	3 (15%)

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
5	EPE	B	1066	-	-	5/9/19/19	0/1/1/1
5	EPE	C	1066	-	-	3/9/19/19	0/1/1/1
5	EPE	A	1066	-	-	1/9/19/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1066	EPE	C10-S	-7.36	1.67	1.77
5	C	1066	EPE	C10-S	-7.21	1.67	1.77
5	B	1066	EPE	C10-S	-7.18	1.67	1.77
5	A	1066	EPE	O3S-S	4.60	1.64	1.47
5	B	1066	EPE	O3S-S	4.46	1.64	1.47
5	C	1066	EPE	O3S-S	4.33	1.63	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1066	EPE	O1S-S-C10	3.61	112.19	106.73
5	A	1066	EPE	C6-C5-N4	-2.64	105.33	110.65
5	A	1066	EPE	O1S-S-C10	2.38	110.32	106.73
5	B	1066	EPE	O2S-S-O1S	-2.20	106.66	113.82
5	B	1066	EPE	O2S-S-C10	2.07	109.86	106.73
5	C	1066	EPE	O1S-S-C10	2.05	109.83	106.73
5	C	1066	EPE	C5-N4-C3	2.02	113.19	108.84
5	A	1066	EPE	O2S-S-C10	2.02	109.78	106.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1066	EPE	C10-C9-N1-C2
5	B	1066	EPE	C9-C10-S-O2S
5	B	1066	EPE	C9-C10-S-O3S
5	A	1066	EPE	N4-C7-C8-O8
5	B	1066	EPE	N4-C7-C8-O8
5	C	1066	EPE	N4-C7-C8-O8
5	C	1066	EPE	C8-C7-N4-C5
5	C	1066	EPE	C8-C7-N4-C3
5	B	1066	EPE	C9-C10-S-O1S

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, 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(Å²)	Q<0.9	
1	A	64/65 (98%)	-0.27	0	100	100	17, 26, 36, 49	0
1	B	64/65 (98%)	-0.30	0	100	100	21, 27, 37, 43	0
1	C	64/65 (98%)	-0.36	0	100	100	20, 27, 35, 44	0
2	H	221/229 (96%)	-0.01	9 (4%)	37	44	21, 34, 52, 81	0
2	I	210/229 (91%)	0.30	16 (7%)	13	18	22, 45, 71, 91	0
2	J	208/229 (90%)	0.61	22 (10%)	6	8	28, 57, 94, 114	0
3	L	218/219 (99%)	0.04	7 (3%)	47	54	20, 37, 58, 73	0
3	M	217/219 (99%)	0.41	19 (8%)	10	13	22, 50, 84, 90	0
3	N	217/219 (99%)	0.71	33 (15%)	2	3	28, 62, 110, 121	0
All	All	1483/1539 (96%)	0.26	106 (7%)	16	21	17, 41, 88, 121	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	194	THR	9.5
2	J	192	SER	6.2
2	J	164	GLY	6.2
2	J	193	SER	5.7
3	N	206	SER	5.5
2	I	190	VAL	5.3
3	L	207	THR	5.1
2	H	221	ASP	5.1
2	J	218	VAL	5.0
3	N	207	THR	5.0
2	J	214	ASP	4.8
3	N	217	ASN	4.8
3	N	132	SER	4.7
2	H	140[A]	ASN	4.5
3	M	206	SER	4.5

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Mol	Chain	Res	Type	RSRZ
3	N	215	ASN	4.5
3	M	208	SER	4.4
2	J	199	THR	4.4
2	J	88	SER	4.3
3	N	208	SER	4.2
3	M	217	ASN	4.1
2	J	191	PRO	4.1
2	I	179	SER	3.9
3	N	195	ASN	3.7
3	M	207	THR	3.7
3	M	187	THR	3.6
3	N	164	VAL	3.6
2	I	167	SER	3.6
3	M	159	GLU	3.5
2	I	197	SER	3.5
3	N	187	THR	3.5
3	N	162	ASN	3.4
2	I	163	SER	3.3
3	N	156	ASP	3.2
3	N	157	GLY	3.1
2	I	218	VAL	3.1
3	N	163	GLY	3.1
3	M	174	LYS	3.1
3	N	188	LYS	3.1
2	J	160	THR	3.1
3	L	157	GLY	3.1
3	L	206	SER	3.1
3	N	161	GLN	3.0
2	H	139	THR	3.0
2	I	210	SER	3.0
3	M	162	ASN	2.9
3	N	193	ARG	2.9
3	N	189	ASP	2.9
2	J	170	VAL	2.9
3	M	46	GLY	2.8
3	N	9	LEU	2.8
3	N	114	ALA	2.8
2	H	1	GLU	2.8
3	M	114	ALA	2.7
2	H	194	THR	2.7
3	N	192	GLU	2.7
2	J	131	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	J	190	VAL	2.7
3	N	190	GLU	2.6
3	N	152	LYS	2.6
3	M	156	ASP	2.6
2	I	178	GLN	2.5
3	L	218	GLU	2.5
2	I	192	SER	2.5
2	I	170	VAL	2.4
2	J	161	TRP	2.4
2	I	132	ALA	2.4
3	N	174	LYS	2.4
3	N	185	THR	2.4
3	L	158	SER	2.4
3	M	215	ASN	2.4
3	M	150	ASN	2.3
2	I	198	GLU	2.3
2	H	192	SER	2.3
2	H	193	SER	2.3
3	M	200	GLU	2.3
3	M	209	PRO	2.3
3	N	165	LEU	2.2
3	N	198	THR	2.2
2	H	220	ARG	2.2
2	J	200	VAL	2.2
2	J	167	SER	2.2
3	N	130	LEU	2.2
2	I	214	ASP	2.2
3	M	147	LYS	2.2
2	J	163	SER	2.2
2	H	44	ARG	2.2
2	J	44	ARG	2.2
3	N	127	SER	2.2
3	N	148[A]	ASP	2.2
3	M	164	VAL	2.2
2	J	197	SER	2.2
2	I	143	VAL	2.1
2	J	143	VAL	2.1
2	I	194	THR	2.1
2	J	152	TYR	2.1
2	J	178	GLN	2.1
3	L	148	ASP	2.1
3	L	114	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	M	119	THR	2.1
2	I	193	SER	2.1
3	N	186	LEU	2.0
3	N	150	ASN	2.0
3	N	140	PHE	2.0
3	N	147	LYS	2.0
3	M	152	LYS	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EPE	A	1066	15/15	0.94	0.12	46,52,63,63	0
5	EPE	B	1066	15/15	0.94	0.15	44,47,65,66	0
5	EPE	C	1066	15/15	0.94	0.15	47,50,60,64	0
4	CL	I	1220	1/1	0.95	0.08	46,46,46,46	0
4	CL	B	1065	1/1	0.95	0.30	48,48,48,48	0
4	CL	J	1219	1/1	0.97	0.06	47,47,47,47	0
4	CL	C	1065	1/1	0.97	0.20	42,42,42,42	0
4	CL	H	1222	1/1	0.97	0.06	43,43,43,43	0
4	CL	A	1065	1/1	0.97	0.23	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.