



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:55 PM BST

PDB ID : 6A3W  
Title : Complex structure of 4-1BB and utomilumab  
Authors : Li, Y.; Tan, S.; Zhang, C.; Chai, Y.; Qi, J.; Tien, P.; Gao, S.; Gao, G.F.  
Deposited on : 2018-06-17  
Resolution : 2.00 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.

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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 : 1.8.5 (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

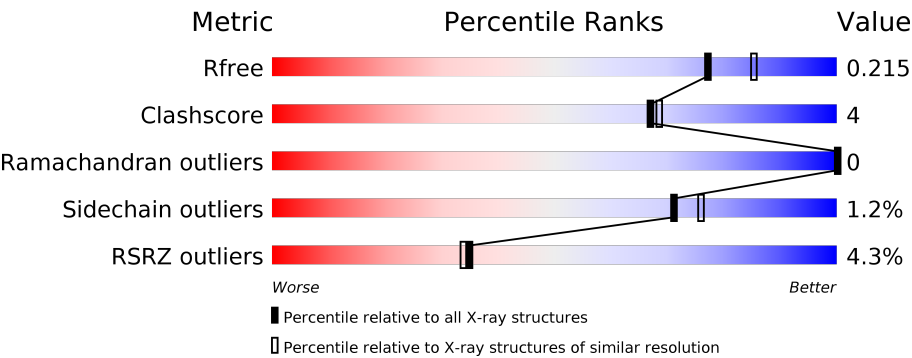
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	116	<div><div></div><div>98%</div><div></div></div>
1	D	116	<div><div>3%</div><div>98%</div><div></div></div>
1	G	116	<div><div></div><div>98%</div><div></div></div>
1	J	116	<div><div>%</div><div>94%</div><div>5%</div></div>
2	B	109	<div><div></div><div>94%</div><div></div></div>
2	E	109	<div><div>%</div><div>91%</div><div>7%</div></div>

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Mol	Chain	Length	Quality of chain
2	H	109	<div><div></div><div>90%</div><div>8%</div><div></div></div>
2	K	109	<div><div>2%</div><div></div><div>91%</div><div>7%</div><div></div></div>
3	C	163	<div><div>4%</div><div></div><div>64%</div><div>17%</div><div></div><div>17%</div></div>
3	F	163	<div><div>7%</div><div></div><div>48%</div><div>9%</div><div></div><div>43%</div></div>
3	I	163	<div><div>12%</div><div></div><div>63%</div><div>15%</div><div></div><div>21%</div></div>
3	L	163	<div><div>9%</div><div></div><div>63%</div><div>10%</div><div></div><div>26%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11536 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 utomilumab VH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	0	0
			906	581	145	175	5			
1	D	116	Total	C	N	O	S	0	0	0
			906	581	145	175	5			
1	G	116	Total	C	N	O	S	0	0	0
			906	581	145	175	5			
1	J	116	Total	C	N	O	S	0	0	0
			906	581	145	175	5			

- Molecule 2 is a protein called utomilumab VL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	106	Total	C	N	O	S	0	1	0
			787	490	130	164	3			
2	E	107	Total	C	N	O	S	0	0	0
			796	497	131	165	3			
2	H	107	Total	C	N	O	S	0	0	0
			796	497	131	165	3			
2	K	107	Total	C	N	O	S	0	1	0
			799	499	131	166	3			

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	135	Total	C	N	O	S	0	0	0
			997	589	187	199	22			
3	F	93	Total	C	N	O	S	0	0	0
			702	419	132	135	16			
3	I	128	Total	C	N	O	S	0	0	0
			938	557	173	186	22			
3	L	120	Total	C	N	O	S	0	0	0
			887	528	165	174	20			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	181	HIS	-	expression tag	UNP Q07011
C	182	HIS	-	expression tag	UNP Q07011
C	183	HIS	-	expression tag	UNP Q07011
C	184	HIS	-	expression tag	UNP Q07011
C	185	HIS	-	expression tag	UNP Q07011
C	186	HIS	-	expression tag	UNP Q07011
F	181	HIS	-	expression tag	UNP Q07011
F	182	HIS	-	expression tag	UNP Q07011
F	183	HIS	-	expression tag	UNP Q07011
F	184	HIS	-	expression tag	UNP Q07011
F	185	HIS	-	expression tag	UNP Q07011
F	186	HIS	-	expression tag	UNP Q07011
I	181	HIS	-	expression tag	UNP Q07011
I	182	HIS	-	expression tag	UNP Q07011
I	183	HIS	-	expression tag	UNP Q07011
I	184	HIS	-	expression tag	UNP Q07011
I	185	HIS	-	expression tag	UNP Q07011
I	186	HIS	-	expression tag	UNP Q07011
L	181	HIS	-	expression tag	UNP Q07011
L	182	HIS	-	expression tag	UNP Q07011
L	183	HIS	-	expression tag	UNP Q07011
L	184	HIS	-	expression tag	UNP Q07011
L	185	HIS	-	expression tag	UNP Q07011
L	186	HIS	-	expression tag	UNP Q07011

- 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	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total	O	0	0
			131	131		
5	B	114	Total	O	0	0
			114	114		
5	C	105	Total	O	0	0
			105	105		
5	D	92	Total	O	0	0
			92	92		
5	E	73	Total	O	0	0
			73	73		
5	F	49	Total	O	0	0
			49	49		
5	G	122	Total	O	0	0
			122	122		
5	H	123	Total	O	0	0
			123	123		
5	I	104	Total	O	0	0
			104	104		
5	J	100	Total	O	0	0
			100	100		
5	K	94	Total	O	0	0
			94	94		

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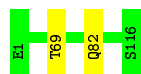
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	89	Total	O	0	0
			89	89		

### 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.

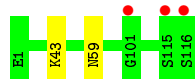
- Molecule 1: utomilumab VH

Chain A:  98% .



- Molecule 1: utomilumab VH

Chain D:  98% .



- Molecule 1: utomilumab VH

Chain G:  98% .



- Molecule 1: utomilumab VH

Chain J:  94% 5% .



- Molecule 2: utomilumab VL

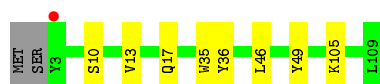
Chain B:  94% .



- Molecule 2: utomilumab VL

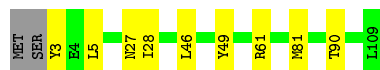
Chain E:  91% 7% .





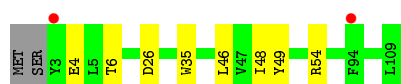
- Molecule 2: utomilumab VL

Chain H: 90% 8%



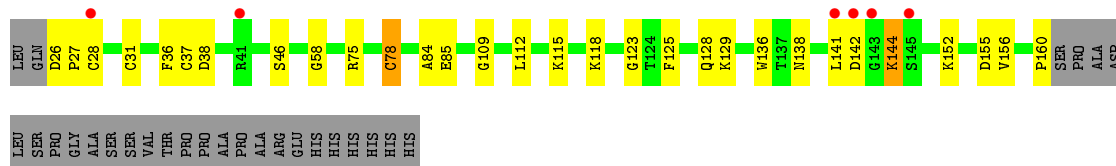
- Molecule 2: utomilumab VL

Chain K: 2% 91% 7%



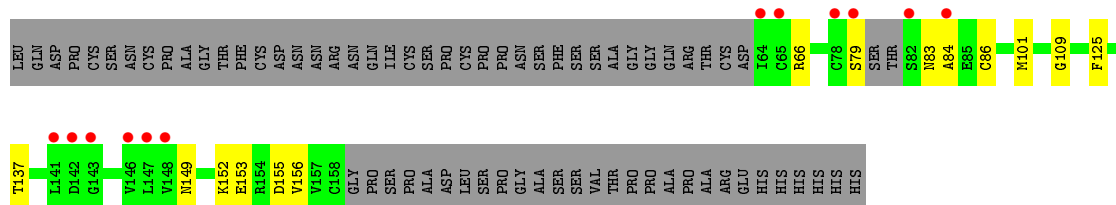
- Molecule 3: Tumor necrosis factor receptor superfamily member 9

Chain C: 4% 64% 17% 17%



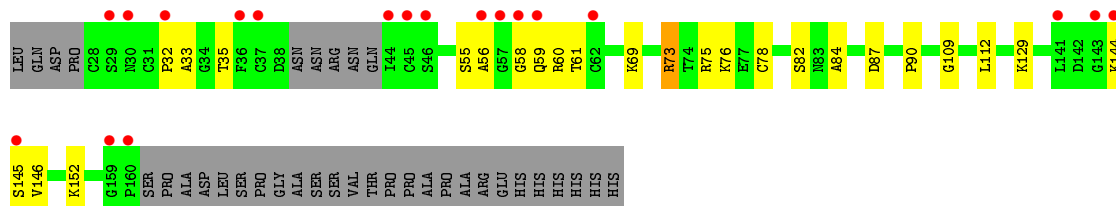
- Molecule 3: Tumor necrosis factor receptor superfamily member 9

Chain F: 7% 48% 9% 43%

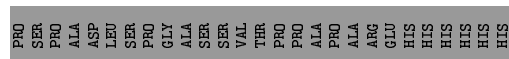
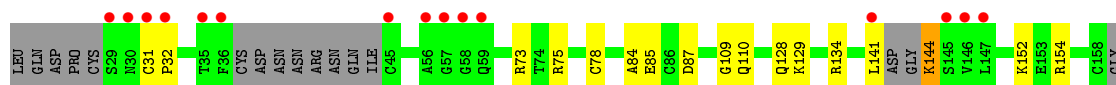


- Molecule 3: Tumor necrosis factor receptor superfamily member 9

Chain I: 12% 63% 15% 21%



- Molecule 3: Tumor necrosis factor receptor superfamily member 9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.73Å 184.60Å 90.20Å 90.00° 104.04° 90.00°	Depositor
Resolution (Å)	39.54 – 2.00 39.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (39.54-2.00) 95.0 (39.54-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.184 , 0.215 0.184 , 0.215	Depositor DCC
$R_{free}$ test set	5047 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11536	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NAG

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	0.25	0/932	0.48	0/1263
1	D	0.25	0/932	0.45	0/1263
1	G	0.25	0/932	0.47	0/1263
1	J	0.25	0/932	0.47	0/1263
2	B	0.26	0/808	0.49	0/1102
2	E	0.26	0/815	0.46	0/1112
2	H	0.25	0/815	0.46	0/1112
2	K	0.25	0/821	0.46	0/1120
3	C	0.31	0/1013	0.48	0/1361
3	F	0.24	0/709	0.48	0/943
3	I	0.25	0/952	0.51	0/1276
3	L	0.25	0/899	0.50	0/1202
All	All	0.26	0/10560	0.47	0/14280

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	55	SER	Peptide

## 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	906	0	867	1	0
1	D	906	0	867	1	0
1	G	906	0	867	1	0
1	J	906	0	867	5	0
2	B	787	0	745	2	0
2	E	796	0	749	7	0
2	H	796	0	749	5	0
2	K	799	0	754	6	0
3	C	997	0	918	18	0
3	F	702	0	665	9	0
3	I	938	0	866	14	0
3	L	887	0	826	15	0
4	I	14	0	13	0	0
5	A	131	0	0	0	0
5	B	114	0	0	0	0
5	C	105	0	0	3	0
5	D	92	0	0	0	0
5	E	73	0	0	2	0
5	F	49	0	0	2	0
5	G	122	0	0	0	0
5	H	123	0	0	1	0
5	I	104	0	0	1	0
5	J	100	0	0	1	0
5	K	94	0	0	3	0
5	L	89	0	0	3	0
All	All	11536	0	9753	79	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 4.

All (79) 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:C:115:LYS:NZ	5:C:201:HOH:O	2.06	0.89
1:J:31:THR:HB	3:L:128:GLN:HE22	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:54:ARG:NH2	5:K:202:HOH:O	2.24	0.68
3:C:128:GLN:NE2	5:C:204:HOH:O	2.25	0.67
3:L:73:ARG:NH1	3:L:87:ASP:OD1	2.21	0.66
2:E:105:LYS:NZ	5:E:202:HOH:O	2.25	0.64
3:C:138:ASN:HB3	3:C:141:LEU:HD12	1.78	0.64
2:H:27:ASN:OD1	5:H:201:HOH:O	2.15	0.64
1:J:1:GLU:O	5:J:201:HOH:O	2.16	0.63
2:K:4:GLU:OE1	5:K:201:HOH:O	2.16	0.62
3:I:76:LYS:NZ	3:I:82:SER:OG	2.31	0.61
1:G:13:LYS:HG3	1:G:14:PRO:HD2	1.84	0.58
3:I:129:LYS:NZ	5:I:301:HOH:O	2.12	0.57
2:K:6:THR:OG1	5:K:201:HOH:O	2.17	0.57
2:E:13:VAL:HG22	2:E:17:GLN:HB2	1.87	0.57
3:F:149:ASN:ND2	5:F:202:HOH:O	2.24	0.54
3:C:75:ARG:HH11	3:C:75:ARG:HG2	1.73	0.53
3:F:153:GLU:OE2	5:F:201:HOH:O	2.18	0.53
1:D:43:LYS:NZ	2:K:26:ASP:OD1	2.41	0.53
3:L:75:ARG:NH1	3:L:85:GLU:OE1	2.43	0.51
3:C:78:CYS:HB3	3:C:84:ALA:HB2	1.93	0.51
2:E:10:SER:OG	5:E:201:HOH:O	2.19	0.50
3:L:78:CYS:HB3	3:L:84:ALA:HB2	1.93	0.50
3:C:75:ARG:NH1	3:C:75:ARG:HG2	2.26	0.49
3:I:75:ARG:HG2	3:I:75:ARG:HH21	1.76	0.49
3:L:129:LYS:NZ	5:L:206:HOH:O	2.45	0.48
3:F:109:GLY:HA2	3:F:152:LYS:O	2.14	0.48
3:I:58:GLY:O	3:I:60:ARG:NH2	2.45	0.48
3:L:152:LYS:NZ	5:L:203:HOH:O	2.41	0.48
1:J:13:LYS:HG2	1:J:16:GLU:HG3	1.94	0.48
3:L:141:LEU:HD22	3:L:144:LYS:HZ1	1.78	0.48
1:J:31:THR:HB	3:L:128:GLN:NE2	2.24	0.48
3:C:109:GLY:HA2	3:C:152:LYS:O	2.14	0.47
3:L:109:GLY:HA2	3:L:152:LYS:O	2.14	0.47
3:C:38:ASP:OD1	3:C:38:ASP:N	2.41	0.47
2:K:35:TRP:HB2	2:K:48:ILE:HB	1.97	0.47
3:L:154:ARG:HH11	3:L:154:ARG:HG2	1.78	0.47
3:I:59:GLN:HG2	3:I:61:THR:O	2.14	0.47
3:C:31:CYS:SG	3:C:37:CYS:HB2	2.54	0.47
3:I:69:LYS:HE3	3:I:69:LYS:HB2	1.78	0.46
3:C:123:GLY:HA2	3:C:136:TRP:CE3	2.50	0.46
3:C:85:GLU:HG3	5:C:217:HOH:O	2.15	0.46
3:I:109:GLY:HA2	3:I:152:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:32:PRO:O	3:I:35:THR:HG22	2.15	0.46
3:I:145:SER:OG	3:I:146:VAL:N	2.49	0.46
2:B:54:ARG:HG3	2:B:58:ILE:HB	1.98	0.46
2:E:46:LEU:HD21	2:E:49:TYR:HB3	1.98	0.45
3:I:144:LYS:HB3	3:I:144:LYS:HZ2	1.80	0.45
2:K:46:LEU:HD21	2:K:49:TYR:HB3	1.99	0.45
2:E:36:TYR:CE2	2:E:46:LEU:HD13	2.52	0.45
3:I:33:ALA:HB2	3:I:56:ALA:HA	1.99	0.45
3:C:36:PHE:CE1	3:C:46:SER:HB2	2.51	0.45
1:J:55:ASP:OD2	3:L:134:ARG:NH2	2.50	0.45
3:L:129:LYS:HE3	3:L:129:LYS:HB3	1.58	0.45
3:F:83:ASN:OD1	3:F:84:ALA:N	2.50	0.44
3:L:31:CYS:HA	3:L:32:PRO:HD3	1.74	0.44
3:I:73:ARG:HG3	3:I:87:ASP:OD2	2.17	0.44
1:A:69:THR:HB	1:A:82:GLN:HG2	1.99	0.43
2:E:35:TRP:O	2:E:46:LEU:HD12	2.19	0.43
3:F:66:ARG:NE	3:F:86:CYS:SG	2.91	0.43
3:C:125:PHE:CZ	3:C:155:ASP:HB2	2.54	0.43
2:H:46:LEU:HD21	2:H:49:TYR:HB3	2.00	0.43
3:C:28:CYS:O	3:C:58:GLY:HA2	2.18	0.43
3:C:144:LYS:HE2	3:C:160:PRO:HA	2.00	0.42
2:H:61:ARG:NH1	2:H:81:MET:SD	2.92	0.42
2:E:46:LEU:HD23	3:F:101:MET:SD	2.59	0.42
3:F:137:THR:HG23	3:F:155:ASP:OD2	2.20	0.42
3:L:154:ARG:NH1	3:L:154:ARG:HG2	2.34	0.42
2:H:5:LEU:HD11	2:H:90:THR:HG22	2.02	0.42
3:F:155:ASP:OD1	3:F:156:VAL:N	2.53	0.41
3:I:73:ARG:NH2	3:I:90:PRO:HD3	2.35	0.41
3:I:78:CYS:HB2	3:I:84:ALA:HB2	2.02	0.41
3:F:125:PHE:CZ	3:F:155:ASP:HB2	2.56	0.41
3:L:110:GLN:NE2	5:L:208:HOH:O	2.52	0.40
3:C:129:LYS:HB2	3:C:129:LYS:HE3	1.84	0.40
3:C:155:ASP:OD1	3:C:156:VAL:N	2.54	0.40
2:H:5:LEU:HD22	2:H:28:ILE:HD12	2.03	0.40
3:C:26:ASP:HA	3:C:27:PRO:HD2	1.97	0.40
2:B:36:TYR:CE2	2:B:46:LEU:HD13	2.56	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	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
1	D	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
1	G	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
1	J	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
2	B	105/109 (96%)	103 (98%)	2 (2%)	0	100	100
2	E	105/109 (96%)	103 (98%)	2 (2%)	0	100	100
2	H	105/109 (96%)	103 (98%)	2 (2%)	0	100	100
2	K	106/109 (97%)	103 (97%)	3 (3%)	0	100	100
3	C	133/163 (82%)	133 (100%)	0	0	100	100
3	F	89/163 (55%)	87 (98%)	2 (2%)	0	100	100
3	I	124/163 (76%)	121 (98%)	3 (2%)	0	100	100
3	L	114/163 (70%)	110 (96%)	4 (4%)	0	100	100
All	All	1337/1552 (86%)	1315 (98%)	22 (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	97/97 (100%)	97 (100%)	0	100	100
1	D	97/97 (100%)	96 (99%)	1 (1%)	76	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	97/97 (100%)	97 (100%)	0	100	100
1	J	97/97 (100%)	94 (97%)	3 (3%)	40	40
2	B	87/89 (98%)	87 (100%)	0	100	100
2	E	87/89 (98%)	87 (100%)	0	100	100
2	H	87/89 (98%)	86 (99%)	1 (1%)	73	78
2	K	88/89 (99%)	88 (100%)	0	100	100
3	C	117/140 (84%)	112 (96%)	5 (4%)	29	26
3	F	81/140 (58%)	80 (99%)	1 (1%)	71	76
3	I	110/140 (79%)	108 (98%)	2 (2%)	59	63
3	L	104/140 (74%)	103 (99%)	1 (1%)	76	81
All	All	1149/1304 (88%)	1135 (99%)	14 (1%)	71	76

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	78	CYS
3	C	112	LEU
3	C	118	LYS
3	C	142	ASP
3	C	144	LYS
1	D	59	ASN
3	F	79	SER
2	H	3	TYR
3	I	73	ARG
3	I	112	LEU
1	J	1	GLU
1	J	115	SER
1	J	116	SER
3	L	144	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	I	59	GLN
3	I	67	GLN
3	L	128	GLN

### 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 ⓘ

1 ligand is 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	$\# Z  > 2$
4	NAG	I	201	3	14,14,15	0.31	0	17,19,21	0.58	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	I	201	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	201	NAG	O5-C5-C6-O6

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	116/116 (100%)	-0.23	0 100 100	13, 20, 29, 72	0
1	D	116/116 (100%)	-0.12	3 (2%) 56 54	22, 31, 43, 67	0
1	G	116/116 (100%)	-0.32	0 100 100	13, 21, 32, 68	0
1	J	116/116 (100%)	-0.48	1 (0%) 84 83	14, 23, 35, 69	0
2	B	106/109 (97%)	-0.40	0 100 100	14, 22, 33, 56	0
2	E	107/109 (98%)	-0.23	1 (0%) 84 83	22, 30, 41, 69	0
2	H	107/109 (98%)	-0.28	0 100 100	15, 22, 35, 60	0
2	K	107/109 (98%)	-0.32	2 (1%) 66 65	17, 24, 40, 89	0
3	C	135/163 (82%)	0.15	6 (4%) 34 33	19, 33, 68, 86	0
3	F	93/163 (57%)	0.59	12 (12%) 3 3	28, 43, 92, 111	0
3	I	128/163 (78%)	0.47	19 (14%) 2 2	20, 33, 82, 102	0
3	L	120/163 (73%)	0.31	15 (12%) 3 3	21, 35, 74, 101	0
All	All	1367/1552 (88%)	-0.07	59 (4%) 35 34	13, 27, 64, 111	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	141	LEU	6.0
3	I	30	ASN	5.9
3	I	160	PRO	5.6
3	I	143	GLY	5.0
3	I	56	ALA	4.7
3	I	37	CYS	4.7
3	L	30	ASN	4.0
3	C	141	LEU	3.9
3	I	159	GLY	3.7
3	F	64	ILE	3.7
3	I	45	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
3	L	29	SER	3.5
1	D	116	SER	3.5
2	K	3	TYR	3.5
3	F	65	CYS	3.4
3	L	57	GLY	3.4
3	F	82	SER	3.4
3	I	36	PHE	3.3
3	I	57	GLY	3.3
3	F	84	ALA	3.3
3	L	31	CYS	3.3
3	L	45	CYS	3.3
3	C	145	SER	3.2
3	L	56	ALA	3.2
3	C	41	ARG	3.1
3	L	32	PRO	3.1
1	J	116	SER	3.1
3	F	143	GLY	3.0
3	F	141	LEU	3.0
3	I	145	SER	3.0
3	F	78	CYS	2.9
3	F	146	VAL	2.9
3	C	142	ASP	2.9
3	I	44	ILE	2.8
3	I	144	LYS	2.8
3	I	29	SER	2.8
3	L	35	THR	2.7
3	C	143	GLY	2.6
3	F	142	ASP	2.6
3	I	32	PRO	2.6
3	I	58	GLY	2.6
3	I	46	SER	2.5
3	I	141	LEU	2.5
3	L	36	PHE	2.5
2	E	3	TYR	2.5
3	L	145	SER	2.5
3	L	58	GLY	2.5
1	D	115	SER	2.4
2	K	94	PHE	2.3
3	F	79	SER	2.3
3	L	147	LEU	2.3
3	F	148	VAL	2.2
3	L	59	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
3	I	59	GLN	2.1
1	D	101	GLY	2.1
3	C	28	CYS	2.1
3	L	146	VAL	2.0
3	F	147	LEU	2.0
3	I	62	CYS	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
4	NAG	I	201	14/15	0.59	0.23	54,66,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.