



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:20 AM BST

PDB ID : 6CPR  
Title : Crystal structure of 4-1BBL/4-1BB complex in C2 space group  
Authors : Aruna, B.; Zajonc, D.M.  
Deposited on : 2018-03-14  
Resolution : 2.70 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

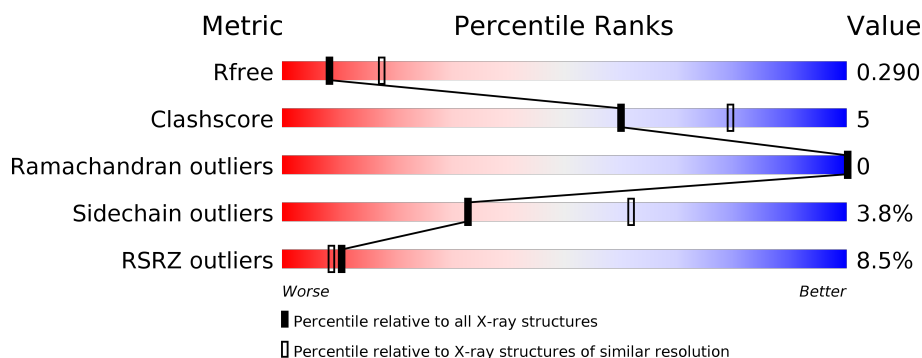
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	165	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>8%</div> </div> </div>
1	B	165	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>8%</div> </div> </div>
1	C	165	<div> <div>8%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>10%</div> </div> </div>
2	D	138	<div> <div>8%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>.</div> </div> </div>
2	E	138	<div> <div>10%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>.</div> </div> </div>
2	F	138	<div> <div>13%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>.</div> </div> </div>

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	GOL	A	601	-	-	-	X
5	SO4	C	302	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6257 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 Tumor necrosis factor ligand superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1101	707	197	196	1			
1	B	151	Total	C	N	O	S	0	0	0
			1116	717	200	198	1			
1	C	148	Total	C	N	O	S	0	0	0
			1101	706	196	198	1			

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	132	Total	C	N	O	S	0	0	0
			898	526	161	189	22			
2	F	132	Total	C	N	O	S	0	0	0
			895	525	163	185	22			
2	E	133	Total	C	N	O	S	0	0	0
			911	538	166	186	21			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		
4	A	2	Total	Cl	0	0
			2	2		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Na	0	0
			1	1		
7	E	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	24	Total	O	0	0
			24	24		
8	B	32	Total	O	0	0
			32	32		
8	C	23	Total	O	0	0
			23	23		
8	D	18	Total	O	0	0
			18	18		

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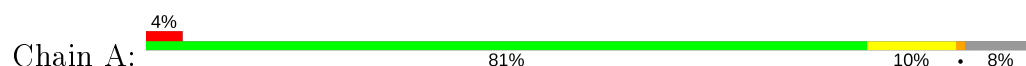
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	26	Total	O	0	0
			26	26		
8	E	25	Total	O	0	0
			25	25		



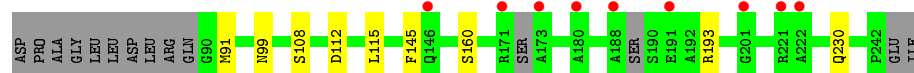
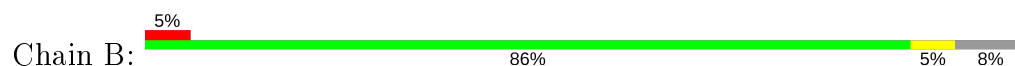
### 3 Residue-property plots [i](#)

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.

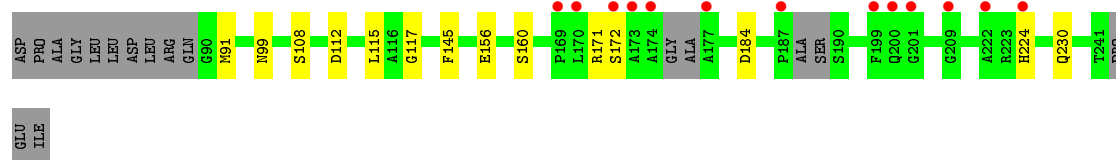
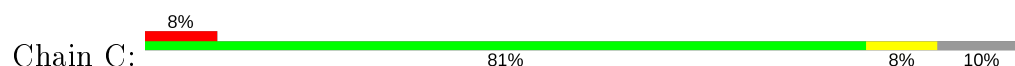
- Molecule 1: Tumor necrosis factor ligand superfamily member 9



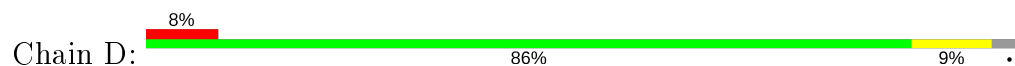
- Molecule 1: Tumor necrosis factor ligand superfamily member 9



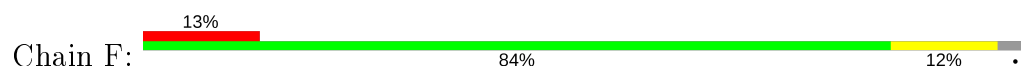
- Molecule 1: Tumor necrosis factor ligand superfamily member 9



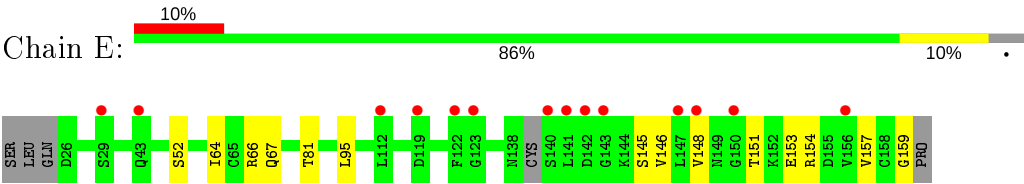
- Molecule 2: Tumor necrosis factor receptor superfamily member 9



- Molecule 2: Tumor necrosis factor receptor superfamily member 9



● Molecule 2: Tumor necrosis factor receptor superfamily member 9



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.28Å 66.50Å 129.36Å 90.00° 103.09° 90.00°	Depositor
Resolution (Å)	38.00 – 2.70 37.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (38.00-2.70) 97.6 (37.87-2.70)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.249 , 0.280 0.255 , 0.290	Depositor DCC
$R_{free}$ test set	1321 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.4	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6257	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.44% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, NAG, NA, CL

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	0.50	0/1124	0.73	0/1532
1	B	0.47	0/1138	0.69	0/1546
1	C	0.49	0/1122	0.72	0/1524
2	D	0.55	0/912	0.67	0/1237
2	E	0.52	0/925	0.66	0/1251
2	F	0.52	0/909	0.67	0/1233
All	All	0.51	0/6130	0.69	0/8323

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	1101	0	1092	21	0
1	B	1116	0	1125	11	0
1	C	1101	0	1103	13	0
2	D	898	0	717	8	0
2	E	911	0	762	8	0
2	F	895	0	720	9	0
3	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	2	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	10	0	0	1	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
6	D	14	0	13	0	0
6	E	14	0	13	0	0
6	F	14	0	13	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	A	24	0	0	1	0
8	B	32	0	0	0	0
8	C	23	0	0	0	0
8	D	18	0	0	0	0
8	E	25	0	0	0	0
8	F	26	0	0	0	0
All	All	6257	0	5566	54	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 (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)
1:A:221:ARG:HG2	8:A:713:HOH:O	1.65	0.94
1:A:221:ARG:NE	1:A:221:ARG:HA	1.82	0.92
1:A:173:ALA:H	2:F:59:GLN:NE2	1.76	0.83
2:D:73:ARG:NH2	2:D:90:PRO:HD3	2.04	0.72
5:A:604:SO4:O3	1:C:117:GLY:N	2.24	0.69
1:B:193:ARG:HD3	1:C:184:ASP:CG	2.15	0.67
1:A:99:ASN:HD21	1:A:108:SER:H	1.44	0.66
1:B:99:ASN:HD21	1:B:108:SER:H	1.45	0.64
1:C:99:ASN:HD21	1:C:108:SER:H	1.45	0.64
2:F:145:SER:O	2:F:158:CYS:SG	2.57	0.62
2:D:73:ARG:HH21	2:D:90:PRO:HD3	1.66	0.59
1:A:215:HIS:HB2	4:A:602:CL:CL	2.43	0.56
1:A:158:SER:OG	1:A:221:ARG:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:148:VAL:CB	2:E:157:VAL:HB	2.36	0.54
1:A:230:GLN:HE22	2:E:67:GLN:H	1.55	0.54
1:A:173:ALA:N	2:F:59:GLN:NE2	2.52	0.54
2:F:123:GLY:HA2	2:F:136:TRP:CE3	2.43	0.53
1:A:112:ASP:HB3	1:A:115:LEU:CD2	2.39	0.53
2:E:151:THR:HG23	2:E:153:GLU:H	1.74	0.53
1:C:112:ASP:HB3	1:C:115:LEU:CD2	2.39	0.53
1:A:171:ARG:HH11	1:A:171:ARG:CG	2.21	0.52
1:A:171:ARG:HG3	1:A:171:ARG:HH11	1.75	0.52
1:C:172:SER:O	1:C:172:SER:OG	2.22	0.52
1:B:230:GLN:HE22	2:D:67:GLN:H	1.59	0.51
1:C:230:GLN:HE22	2:F:67:GLN:H	1.59	0.51
1:B:112:ASP:HB3	1:B:115:LEU:CD2	2.41	0.50
1:C:99:ASN:HD22	1:C:99:ASN:H	1.59	0.49
2:E:151:THR:HG22	2:E:154:ARG:CB	2.42	0.49
1:A:221:ARG:HE	1:A:221:ARG:HA	1.75	0.49
1:A:157:GLY:HA2	1:A:222:ALA:HB3	1.95	0.49
1:B:99:ASN:HD22	1:B:99:ASN:H	1.62	0.48
2:E:145:SER:O	2:E:159:GLY:N	2.44	0.48
2:D:151:THR:HG23	2:D:154:ARG:H	1.78	0.47
1:A:99:ASN:HD21	1:A:108:SER:N	2.12	0.47
1:B:193:ARG:HD3	1:C:184:ASP:OD1	2.13	0.47
1:A:171:ARG:CG	1:A:171:ARG:NH1	2.77	0.46
1:A:99:ASN:HD22	1:A:99:ASN:H	1.61	0.46
1:C:230:GLN:HE22	2:F:66:ARG:HA	1.81	0.45
1:B:230:GLN:HE22	2:D:66:ARG:HA	1.80	0.45
1:A:230:GLN:HE22	2:E:66:ARG:HA	1.82	0.44
1:B:193:ARG:NE	1:C:184:ASP:HB3	2.33	0.43
1:B:115:LEU:HD11	2:D:52:SER:HB3	2.00	0.43
1:A:115:LEU:HD12	2:E:64:ILE:HD13	2.00	0.43
1:A:188:ALA:O	1:A:190:SER:N	2.52	0.43
1:B:99:ASN:HD21	1:B:108:SER:N	2.13	0.43
2:F:53:PHE:CZ	2:F:83:ASN:HB2	2.54	0.43
2:D:151:THR:HG23	2:D:153:GLU:H	1.84	0.42
1:A:205:HIS:HB2	4:A:603:CL:CL	2.56	0.42
1:A:115:LEU:HD11	2:E:52:SER:HB3	2.01	0.42
1:C:99:ASN:HD21	1:C:108:SER:N	2.13	0.41
1:C:156:GLU:OE1	1:C:224:HIS:NE2	2.54	0.41
1:B:115:LEU:HD12	2:D:64:ILE:HD13	2.02	0.41
2:F:28:CYS:O	2:F:58:GLY:HA2	2.21	0.40
1:C:115:LEU:HD12	2:F:64:ILE:HD13	2.04	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	148/165 (90%)	147 (99%)	1 (1%)	0	100	100
1	B	145/165 (88%)	141 (97%)	4 (3%)	0	100	100
1	C	142/165 (86%)	135 (95%)	7 (5%)	0	100	100
2	D	128/138 (93%)	125 (98%)	3 (2%)	0	100	100
2	E	129/138 (94%)	127 (98%)	2 (2%)	0	100	100
2	F	128/138 (93%)	126 (98%)	2 (2%)	0	100	100
All	All	820/909 (90%)	801 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	106/125 (85%)	101 (95%)	5 (5%)	26	54
1	B	110/125 (88%)	107 (97%)	3 (3%)	44	74
1	C	110/125 (88%)	106 (96%)	4 (4%)	35	64
2	D	94/120 (78%)	90 (96%)	4 (4%)	29	57
2	E	96/120 (80%)	93 (97%)	3 (3%)	40	69
2	F	93/120 (78%)	89 (96%)	4 (4%)	29	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	609/735 (83%)	586 (96%)	23 (4%)	33	62

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	MET
1	A	145	PHE
1	A	160	SER
1	A	171	ARG
1	A	221	ARG
1	B	91	MET
1	B	145	PHE
1	B	160	SER
1	C	91	MET
1	C	145	PHE
1	C	160	SER
1	C	171	ARG
2	D	81	THR
2	D	95	LEU
2	D	145	SER
2	D	146	VAL
2	F	81	THR
2	F	95	LEU
2	F	121	CYS
2	F	146	VAL
2	E	81	THR
2	E	95	LEU
2	E	146	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	210	GLN
1	A	230	GLN
1	B	99	ASN
1	B	230	GLN
1	C	99	ASN
1	C	230	GLN
2	F	59	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 ⓘ

Of 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 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	SO4	C	302	-	4,4,4	0.36	0	6,6,6	0.09	0
6	NAG	E	201	-	14,14,15	0.65	0	17,19,21	0.93	1 (5%)
3	GOL	A	601	-	5,5,5	0.56	0	5,5,5	0.54	0
6	NAG	F	501	2	14,14,15	0.34	0	17,19,21	0.84	0
6	NAG	D	201	2	14,14,15	0.39	0	17,19,21	1.68	4 (23%)
5	SO4	D	204	-	4,4,4	0.32	0	6,6,6	0.10	0
5	SO4	B	303	-	4,4,4	0.44	0	6,6,6	0.51	0
5	SO4	D	203	-	4,4,4	0.46	0	6,6,6	0.62	0
5	SO4	A	605	-	4,4,4	0.40	0	6,6,6	0.19	0
5	SO4	A	604	-	4,4,4	0.36	0	6,6,6	0.49	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
6	NAG	E	201	-	-	0/6/23/26	0/1/1/1
6	NAG	F	501	2	-	0/6/23/26	0/1/1/1
6	NAG	D	201	2	-	0/6/23/26	0/1/1/1
3	GOL	A	601	-	-	4/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	201	NAG	C4-C3-C2	3.96	116.82	111.02
6	D	201	NAG	C3-C4-C5	3.48	116.44	110.24
6	D	201	NAG	C1-C2-N2	-2.45	106.31	110.49
6	D	201	NAG	O4-C4-C3	-2.25	105.15	110.35
6	E	201	NAG	C4-C3-C2	2.17	114.20	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	GOL	C1-C2-C3-O3
3	A	601	GOL	O1-C1-C2-C3
3	A	601	GOL	O2-C2-C3-O3
3	A	601	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	SO4	1	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, 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	152/165 (92%)	0.58	7 (4%) 32 31	30, 54, 93, 134	0
1	B	151/165 (91%)	0.56	9 (5%) 21 20	36, 55, 107, 135	0
1	C	148/165 (89%)	0.60	13 (8%) 10 8	32, 55, 104, 126	0
2	D	132/138 (95%)	0.51	11 (8%) 11 9	31, 66, 105, 116	0
2	E	133/138 (96%)	0.58	14 (10%) 6 4	36, 70, 111, 137	0
2	F	132/138 (95%)	0.63	18 (13%) 3 2	29, 70, 97, 115	0
All	All	848/909 (93%)	0.58	72 (8%) 10 9	29, 59, 105, 137	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	173	ALA	4.8
2	F	122	PHE	4.5
2	E	141	LEU	4.2
2	E	122	PHE	4.1
2	F	136	TRP	4.0
1	A	175	GLY	3.9
2	E	123	GLY	3.9
2	D	150	GLY	3.9
1	A	129	ASP	3.8
2	F	147	LEU	3.7
2	F	40	ASN	3.7
2	E	150	GLY	3.7
1	C	172	SER	3.7
1	B	173	ALA	3.6
1	C	174	ALA	3.5
1	A	172	SER	3.5
2	F	29	SER	3.5
2	E	112	LEU	3.5
2	F	146	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	43	GLN	3.4
1	C	170	LEU	3.4
1	A	222	ALA	3.3
1	B	171	ARG	3.3
1	B	188	ALA	3.2
2	F	123	GLY	3.2
2	E	156	VAL	3.1
1	B	201	GLY	3.1
2	D	122	PHE	3.1
2	F	156	VAL	3.1
2	F	42	ASN	3.0
2	D	140	SER	3.0
2	E	147	LEU	3.0
1	C	187	PRO	2.9
2	D	123	GLY	2.9
2	F	139	CYS	2.8
2	F	158	CYS	2.8
2	E	140	SER	2.8
1	B	180	ALA	2.7
2	D	70	GLY	2.6
2	E	148	VAL	2.6
2	D	25	GLN	2.6
2	E	142	ASP	2.6
1	C	169	PRO	2.6
1	C	209	GLY	2.5
2	D	136	TRP	2.5
1	A	201	GLY	2.5
2	F	150	GLY	2.5
2	D	42	ASN	2.4
1	C	177	ALA	2.4
2	F	119	ASP	2.4
2	E	29	SER	2.3
1	C	200	GLN	2.3
2	E	119	ASP	2.3
2	D	120	CYS	2.3
1	C	201	GLY	2.2
1	B	146	GLN	2.2
2	D	112	LEU	2.2
1	A	174	ALA	2.2
1	B	191	GLU	2.2
1	C	222	ALA	2.2
1	B	221	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	157	VAL	2.2
1	C	224	HIS	2.1
1	B	222	ALA	2.1
2	F	142	ASP	2.1
2	F	141	LEU	2.1
1	C	199	PHE	2.1
2	D	40	ASN	2.1
2	F	108	GLN	2.0
2	E	143	GLY	2.0
2	F	26	ASP	2.0
1	A	145	PHE	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(Å <sup>2</sup> )	Q<0.9
5	SO4	D	204	5/5	0.49	0.40	160,168,170,177	0
5	SO4	C	302	5/5	0.54	0.43	148,153,159,163	0
6	NAG	E	201	14/15	0.60	0.40	119,124,132,132	0
7	NA	E	203	1/1	0.68	0.34	70,70,70,70	0
3	GOL	A	601	6/6	0.70	0.71	67,78,79,80	0
7	NA	D	205	1/1	0.75	0.29	74,74,74,74	0
6	NAG	D	201	14/15	0.76	0.26	83,94,103,105	0
5	SO4	A	605	5/5	0.83	0.23	99,103,115,117	0
6	NAG	F	501	14/15	0.85	0.25	89,99,105,107	0
5	SO4	A	604	5/5	0.86	0.21	69,76,78,85	0
4	CL	A	602	1/1	0.90	0.21	89,89,89,89	0
4	CL	D	202	1/1	0.91	0.10	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	301	1/1	0.92	0.33	55,55,55,55	0
5	SO4	B	303	5/5	0.92	0.14	70,75,79,81	0
5	SO4	D	203	5/5	0.93	0.18	64,66,69,69	0
4	CL	A	603	1/1	0.94	0.13	76,76,76,76	0
4	CL	B	302	1/1	0.95	0.06	83,83,83,83	0
4	CL	C	301	1/1	0.96	0.12	60,60,60,60	0
4	CL	E	202	1/1	0.97	0.11	61,61,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.