W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 23, 2020 – 12:56 am BST

PDB ID	:	5N2K
Title	:	Structure of unbound Briakinumab FAb
Authors	:	Bloch, Y.; Savvides, S.N.
Deposited on	:	2017-02-07
Resolution	:	2.22 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.11
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)	:	2.11

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 2.22 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.
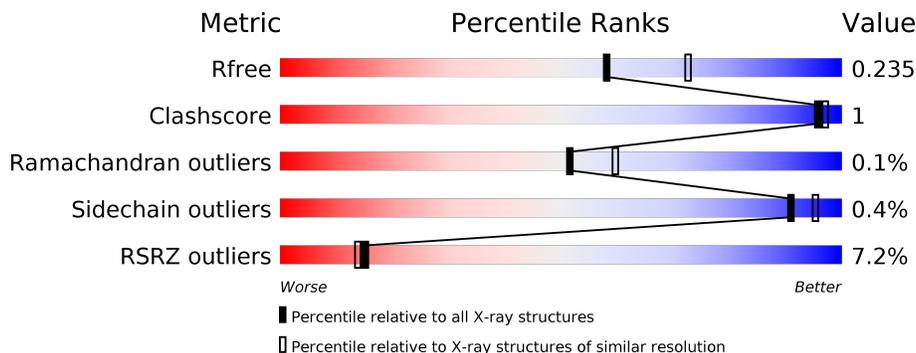
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 <=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	245	
1	C	245	
1	E	245	
1	I	245	
1	K	245	
1	M	245	

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Mol	Chain	Length	Quality of chain
1	O	245	9% 83% 14%
2	B	289	% 71% 27%
2	D	289	7% 74% 23%
2	F	289	2% 71% 27%
2	H	289	17% 64% 33%
2	L	289	5% 70% 28%
2	N	289	4% 70% 28%
2	P	289	6% 68% 28%
3	G	245	10% 83% 13%
4	J	289	6% 70% 27%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 50584 atoms, of which 24272 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 Briakinumab FAb light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	216	Total 3271	C 1043	H 1605	N 280	O 338	S 5	0	7	0
1	C	215	Total 3106	C 997	H 1521	N 262	O 321	S 5	0	0	0
1	E	214	Total 3153	C 1001	H 1554	N 270	O 324	S 4	0	0	0
1	I	214	Total 3299	C 1050	H 1624	N 284	O 337	S 4	0	10	0
1	K	214	Total 3082	C 989	H 1509	N 262	O 318	S 4	0	0	0
1	M	212	Total 3035	C 977	H 1477	N 259	O 318	S 4	0	0	0
1	O	210	Total 3026	C 974	H 1476	N 255	O 317	S 4	0	0	0

- Molecule 2 is a protein called Briakinumab FAb heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	212	Total 3138	C 1007	H 1539	N 274	O 308	S 10	0	5	0
2	D	223	Total 3253	C 1044	H 1594	N 282	O 323	S 10	0	3	0
2	F	210	Total 3101	C 995	H 1524	N 270	O 303	S 9	0	3	0
2	H	193	Total 2731	C 897	H 1309	N 248	O 269	S 8	0	2	0
2	L	209	Total 3096	C 993	H 1524	N 268	O 303	S 8	0	2	0
2	N	209	Total 3076	C 987	H 1510	N 270	O 301	S 8	0	2	0
2	P	207	Total 3048	C 981	H 1490	N 268	O 301	S 8	0	2	0

- Molecule 3 is a protein called Briakinumab FAb light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	213	Total 3061	C 982	H 1496	N 259	O 319	S 5	0	2	0

- Molecule 4 is a protein called Briakinumab FAb heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	J	211	Total 3093	C 994	H 1514	N 270	O 307	S 8	0	2	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
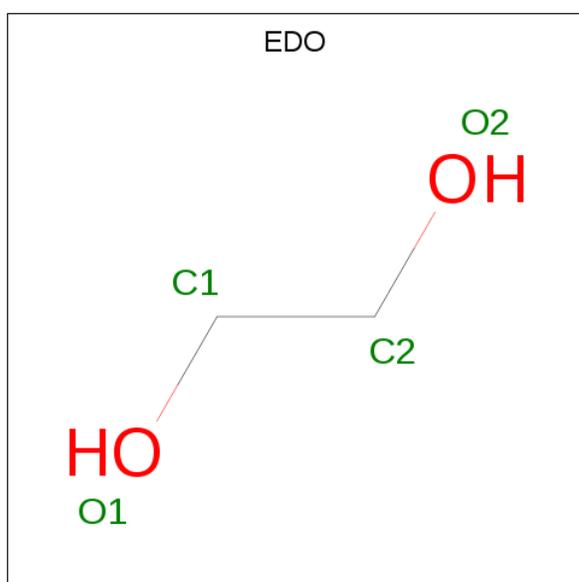
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	I	1	Total 10	C 2	H 6	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	138	Total 138	O 138	0	0
6	B	84	Total 84	O 84	0	0
6	C	59	Total 59	O 59	0	0
6	D	44	Total 44	O 44	0	0

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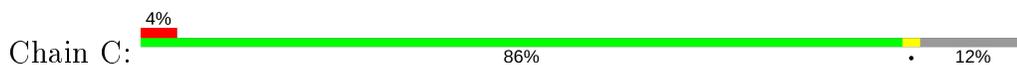| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	72	Total 72	O 72	0	0
6	F	60	Total 60	O 60	0	0
6	G	67	Total 67	O 67	0	0
6	H	35	Total 35	O 35	0	0
6	I	103	Total 103	O 103	0	0
6	J	36	Total 36	O 36	0	0
6	K	28	Total 28	O 28	0	0
6	L	56	Total 56	O 56	0	0
6	M	37	Total 37	O 37	0	0
6	N	56	Total 56	O 56	0	0
6	P	63	Total 63	O 63	0	0
6	O	67	Total 67	O 67	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Briakinumab FAb light chain

- Molecule 1: Briakinumab FAb light chain

- Molecule 1: Briakinumab FAb light chain
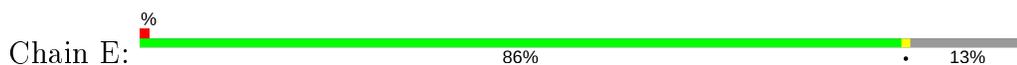

- Molecule 1: Briakinumab FAb light chain

- Molecule 1: Briakinumab FAb light chain

• Molecule 1: Briakinumab FAb light chain

Chain M:

• Molecule 1: Briakinumab FAb light chain

Chain O:

• Molecule 2: Briakinumab FAb heavy chain

Chain B:

• Molecule 2: Briakinumab FAb heavy chain

Chain D:

• Molecule 2: Briakinumab FAb heavy chain

Chain F:

ASP LYS GLY THR SER GLY LEU VAL PRO ARG GLY SER GLY SER GLY SER GLY LEU LEU ASN ASP ILE PHE GLU ALA GLN LYS ILE GLU TRP HIS GLU GLY ARG THR LYS HIS HIS HIS HIS HIS

• Molecule 2: Briakinumab FAb heavy chain

Chain H:

• Molecule 2: Briakinumab FAb heavy chain

Chain L:

• Molecule 2: Briakinumab FAb heavy chain

Chain N:

• Molecule 2: Briakinumab FAb heavy chain

Chain P:

E150 P151 W156 L161 H166 P169 V184 T185 V186 P187 S188 SER SER L191 G192 T193 Q194 T195 Y196 K216 SER CYS ASP GLY LYS GLY THR SER GLY LEU VAL PRO ARG GLY SER GLY SER GLY SER GLY SER GLY SER LEU LEU ASN ASP ILE PHE GLU ALA GLN LYS ILE GLU TRP

HIS GLU GLY ARG THR LYS HIS HIS HIS HIS HIS HIS

- **Molecule 3: Briakinumab FAb light chain**

Chain G:

MET GLY ILE LEU PRO SER PRO GLY MET PRO ALA LEU LEU SER LEU VAL SER LEU LEU SER VAL LEU MET GLY CYS VAL ALA Q1 S27 N28 I29 K35 D93 L101 V120 F123 P124 P125 S126 S127 E128 E129 L130 K134 A135 T136 L137 V138 C139 L140 S158

P159 V160 L185 T186 P187 E188 Q189 W190 K191 S192 S195 Y196 S197 E208 K209 T210 V211 A212 P213 THR GLU CYS SER
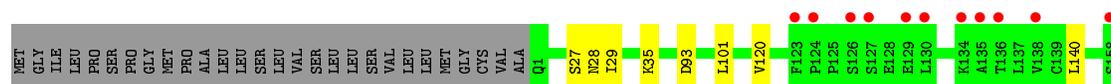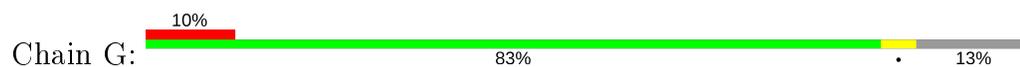
- **Molecule 4: Briakinumab FAb heavy chain**

Chain J:

MET GLY ILE LEU PRO SER PRO GLY MET PRO ALA LEU LEU SER LEU VAL SER LEU LEU SER VAL LEU MET GLY CYS VAL ALA Q1 V12 Q13 P14 G15 G66 R67 D90 G100 S115 A116 S117 T118 P128 SER SER LYS SER THR SER G135 F148 P149 E150

S155 T162 Q173 V186 L191 N201 H202 K203 N206 V209 S217 CYS ASP LYS GLY THR SER GLY LEU VAL PRO ARG GLY SER GLY SER GLY SER GLY SER GLY SER LEU LEU ASN ASP ILE PHE GLU ALA GLN LYS ILE GLU TRP HIS GLU GLY ARG THR LYS HIS HIS HIS

HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.25Å 172.54Å 138.16Å 90.00° 106.16° 90.00°	Depositor
Resolution (Å)	81.88 – 2.22 81.88 – 2.22	Depositor EDS
% Data completeness (in resolution range)	94.5 (81.88-2.22) 94.5 (81.88-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.22Å)	Xtriage
Refinement program	PHENIX (dev_2614: ???)	Depositor
R, R_{free}	0.204 , 0.234 0.204 , 0.235	Depositor DCC
R_{free} test set	2154 reflections (1.21%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.5	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	50584	wwPDB-VP
Average B, all atoms (Å^2)	70.0	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 31.57 % 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 1.0840e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PCA, EDO

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	0/1714	0.47	0/2345
1	C	0.25	0/1625	0.45	0/2226
1	E	0.25	0/1639	0.46	0/2242
1	I	0.27	0/1735	0.48	0/2373
1	K	0.26	0/1613	0.46	0/2211
1	M	0.26	0/1598	0.46	0/2192
1	O	0.26	0/1589	0.46	0/2178
2	B	0.27	0/1658	0.48	0/2256
2	D	0.26	0/1711	0.47	0/2328
2	F	0.26	0/1627	0.47	0/2215
2	H	0.26	0/1465	0.48	0/1993
2	L	0.28	0/1620	0.49	0/2203
2	N	0.26	0/1614	0.47	0/2196
2	P	0.26	0/1605	0.48	0/2183
3	G	0.26	0/1606	0.46	0/2203
4	J	0.26	0/1620	0.48	0/2207
All	All	0.26	0/26039	0.47	0/35551

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	1666	1605	1599	5	0
1	C	1585	1521	1514	3	0
1	E	1599	1554	1552	2	0
1	I	1675	1624	1607	7	0
1	K	1573	1509	1505	7	0
1	M	1558	1477	1475	1	0
1	O	1550	1476	1475	5	0
2	B	1599	1539	1517	3	1
2	D	1659	1594	1576	4	1
2	F	1577	1524	1508	3	1
2	H	1422	1309	1294	3	1
2	L	1572	1524	1508	4	1
2	N	1566	1510	1496	3	0
2	P	1558	1490	1470	6	1
3	G	1565	1496	1479	6	0
4	J	1579	1514	1496	5	0
5	I	4	6	6	0	0
6	A	138	0	0	0	0
6	B	84	0	0	0	0
6	C	59	0	0	0	0
6	D	44	0	0	0	0
6	E	72	0	0	0	0
6	F	60	0	0	0	0
6	G	67	0	0	0	0
6	H	35	0	0	0	1
6	I	103	0	0	0	0
6	J	36	0	0	1	0
6	K	28	0	0	0	0
6	L	56	0	0	0	1
6	M	37	0	0	0	0
6	N	56	0	0	0	0
6	O	67	0	0	1	0
6	P	63	0	0	0	0
All	All	26312	24272	24077	54	4

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 1.

The worst 5 of 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:I:133:ASN:ND2	2:L:72:ARG:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:67:ARG:NH2	2:F:90:ASP:OD2	2.35	0.57
4:J:67:ARG:NH2	4:J:90:ASP:OD2	2.33	0.57
4:J:173:GLN:NE2	6:J:302:HOH:O	2.39	0.55
2:F:197:ILE:HD13	2:F:212:LYS:HA	1.89	0.53

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:TYR:OH	2:P:59:TYR:OH[2_445]	1.91	0.29
2:B:59:TYR:OH	2:F:59:TYR:OH[2_454]	1.92	0.28
2:H:59:TYR:OH	2:L:59:TYR:OH[2_445]	1.95	0.25
6:H:329:HOH:O	6:L:330:HOH:O[2_445]	2.12	0.08

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	221/245 (90%)	210 (95%)	9 (4%)	2 (1%)	17	15
1	C	213/245 (87%)	205 (96%)	8 (4%)	0	100	100
1	E	212/245 (86%)	204 (96%)	8 (4%)	0	100	100
1	I	222/245 (91%)	212 (96%)	10 (4%)	0	100	100
1	K	212/245 (86%)	205 (97%)	7 (3%)	0	100	100
1	M	210/245 (86%)	202 (96%)	8 (4%)	0	100	100
1	O	206/245 (84%)	199 (97%)	7 (3%)	0	100	100
2	B	213/289 (74%)	210 (99%)	3 (1%)	0	100	100
2	D	222/289 (77%)	218 (98%)	3 (1%)	1 (0%)	29	30
2	F	209/289 (72%)	206 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	187/289 (65%)	183 (98%)	4 (2%)	0	100	100
2	L	207/289 (72%)	204 (99%)	3 (1%)	0	100	100
2	N	207/289 (72%)	204 (99%)	3 (1%)	0	100	100
2	P	203/289 (70%)	200 (98%)	3 (2%)	0	100	100
3	G	213/245 (87%)	206 (97%)	7 (3%)	0	100	100
4	J	209/289 (72%)	205 (98%)	4 (2%)	0	100	100
All	All	3366/4272 (79%)	3273 (97%)	90 (3%)	3 (0%)	51	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	222	THR
1	A	97[A]	HIS
1	A	97[B]	HIS

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	186/207 (90%)	186 (100%)	0	100	100
1	C	173/207 (84%)	173 (100%)	0	100	100
1	E	179/207 (86%)	179 (100%)	0	100	100
1	I	189/207 (91%)	189 (100%)	0	100	100
1	K	172/207 (83%)	172 (100%)	0	100	100
1	M	170/207 (82%)	170 (100%)	0	100	100
1	O	171/207 (83%)	171 (100%)	0	100	100
2	B	179/240 (75%)	178 (99%)	1 (1%)	86	92
2	D	183/240 (76%)	179 (98%)	4 (2%)	52	64
2	F	174/240 (72%)	173 (99%)	1 (1%)	86	92
2	H	146/240 (61%)	145 (99%)	1 (1%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	174/240 (72%)	172 (99%)	2 (1%)	73	84
2	N	173/240 (72%)	170 (98%)	3 (2%)	60	73
2	P	170/240 (71%)	169 (99%)	1 (1%)	86	92
3	G	171/206 (83%)	171 (100%)	0	100	100
4	J	173/239 (72%)	173 (100%)	0	100	100
All	All	2783/3574 (78%)	2770 (100%)	13 (0%)	91	94

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	166	HIS
2	H	1	GLN
2	N	201	ASN
2	D	198[B]	CYS
2	N	198	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	201	ASN
1	K	199	GLN
2	L	173	GLN
2	L	206	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
4	PCA	J	1	4	7,8,9	1.77	1 (14%)	9,10,12	1.63	3 (33%)
3	PCA	G	1	3	7,8,9	1.77	1 (14%)	9,10,12	1.70	4 (44%)

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	PCA	J	1	4	-	0/0/11/13	0/1/1/1
3	PCA	G	1	3	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	PCA	CD-N	4.55	1.46	1.34
4	J	1	PCA	CD-N	4.54	1.46	1.34

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	PCA	OE-CD-CG	-2.58	122.26	126.76
4	J	1	PCA	OE-CD-CG	-2.49	122.43	126.76
3	G	1	PCA	CB-CA-N	2.20	109.61	103.30
3	G	1	PCA	CB-CA-C	-2.16	109.73	112.70
4	J	1	PCA	CB-CA-N	2.14	109.44	103.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	#$|Z| > 2$
5	EDO	I	301	-	3,3,3	0.47	0	2,2,2	0.25	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
5	EDO	I	301	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	216/245 (88%)	0.46	7 (3%)	47	45	26, 41, 71, 139	0
1	C	215/245 (87%)	0.53	10 (4%)	31	29	28, 60, 114, 144	0
1	E	214/245 (87%)	0.37	3 (1%)	75	73	30, 50, 86, 111	0
1	I	214/245 (87%)	0.41	5 (2%)	60	58	28, 42, 65, 121	0
1	K	214/245 (87%)	0.83	26 (12%)	4	3	35, 71, 132, 152	0
1	M	212/245 (86%)	0.54	10 (4%)	31	29	31, 65, 125, 157	0
1	O	210/245 (85%)	0.76	23 (10%)	5	4	30, 58, 144, 170	0
2	B	212/289 (73%)	0.50	3 (1%)	75	73	27, 50, 101, 152	0
2	D	223/289 (77%)	0.67	19 (8%)	10	9	35, 70, 105, 143	0
2	F	210/289 (72%)	0.48	5 (2%)	59	57	32, 57, 108, 134	0
2	H	193/289 (66%)	1.34	48 (24%)	0	0	33, 70, 162, 191	0
2	L	209/289 (72%)	0.61	15 (7%)	15	14	30, 64, 110, 138	0
2	N	209/289 (72%)	0.61	12 (5%)	23	22	32, 65, 117, 131	0
2	P	207/289 (71%)	0.81	18 (8%)	10	8	28, 57, 135, 158	0
3	G	212/245 (86%)	0.91	25 (11%)	4	3	29, 55, 136, 162	0
4	J	210/289 (72%)	0.71	16 (7%)	13	12	37, 63, 107, 148	0
All	All	3380/4272 (79%)	0.65	245 (7%)	15	14	26, 57, 125, 191	0

The worst 5 of 245 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	170	ALA	9.3
1	O	196	TYR	8.6
2	H	169	PRO	7.3
2	P	195	THR	7.2
2	H	142	CYS	7.2

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
3	PCA	G	1	8/9	0.80	0.30	116,124,146,149	0
4	PCA	J	1	8/9	0.87	0.17	68,77,92,92	0

6.3 Carbohydrates (i)

There are no carbohydrates 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(Å^2)	Q<0.9
5	EDO	I	301	4/4	0.90	0.18	44,59,65,71	0

6.5 Other polymers (i)

There are no such residues in this entry.