Full wwPDB X-ray Structure Validation Report ⓘ

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)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

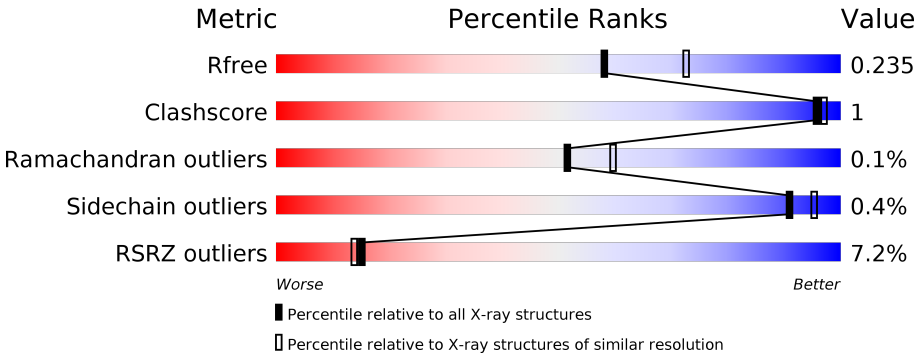
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	3% 86% 12%
1	C	245	4% 86% 12%
1	E	245	% 86% 13%
1	I	245	2% 84% 13%
1	K	245	11% 82% 5% 13%
1	M	245	4% 86% 13%

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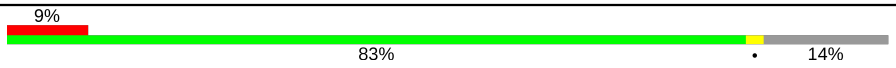
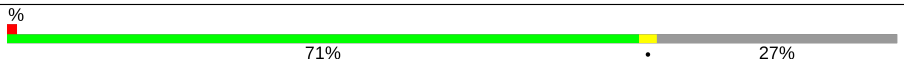
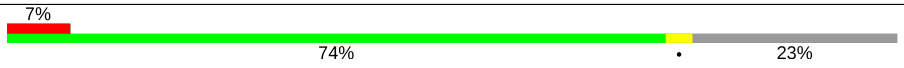
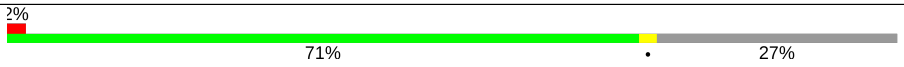
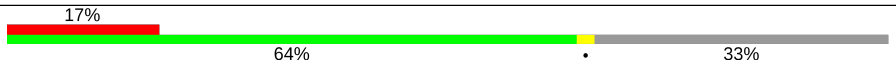
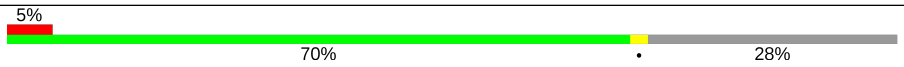
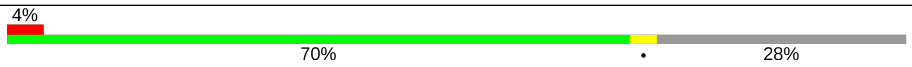
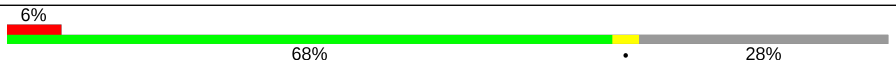
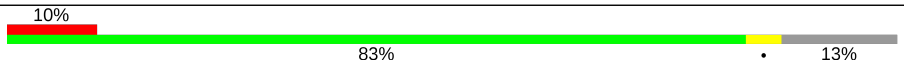
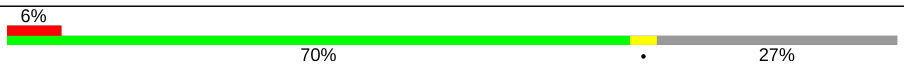
Mol	Chain	Length	Quality of chain
1	O	245	
2	B	289	
2	D	289	
2	F	289	
2	H	289	
2	L	289	
2	N	289	
2	P	289	
3	G	245	
4	J	289	

2 Entry composition

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

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

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

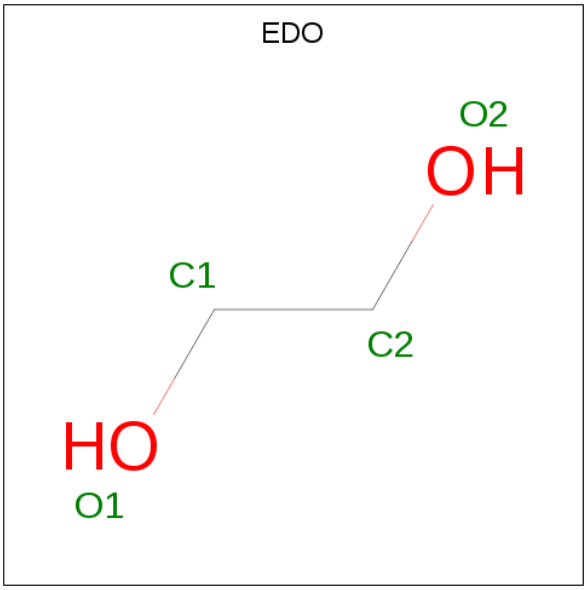
- Molecule 3 is a protein called Briakinumab FAb light chain.

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

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

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

- 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	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is water.

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

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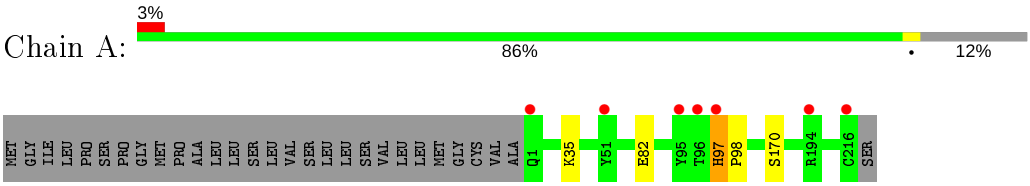
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	72	Total O 72 72	0	0
6	F	60	Total O 60 60	0	0
6	G	67	Total O 67 67	0	0
6	H	35	Total O 35 35	0	0
6	I	103	Total O 103 103	0	0
6	J	36	Total O 36 36	0	0
6	K	28	Total O 28 28	0	0
6	L	56	Total O 56 56	0	0
6	M	37	Total O 37 37	0	0
6	N	56	Total O 56 56	0	0
6	P	63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

3 Residue-property plots (i)

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.

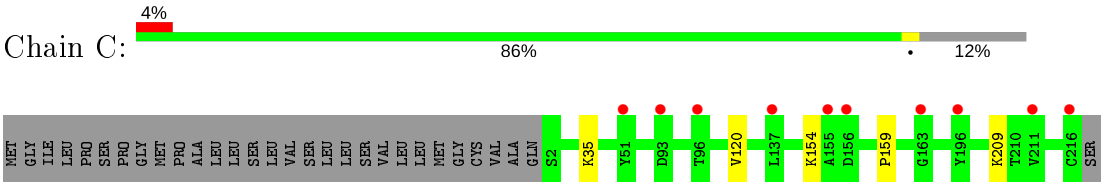
- Molecule 1: Briakinumab FAb light chain

Chain A:



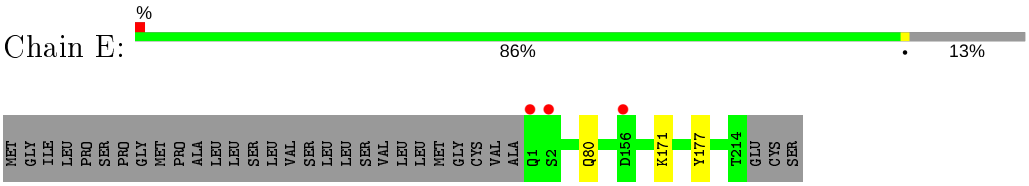
- Molecule 1: Briakinumab FAb light chain

Chain C:



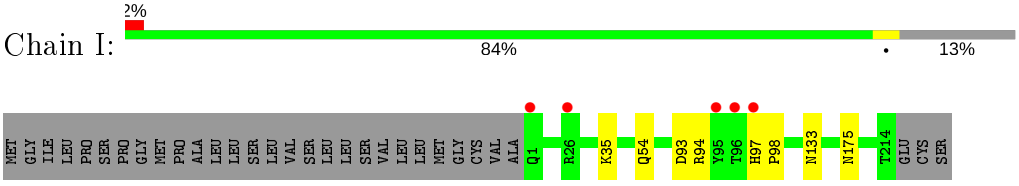
- Molecule 1: Briakinumab FAb light chain

Chain E:



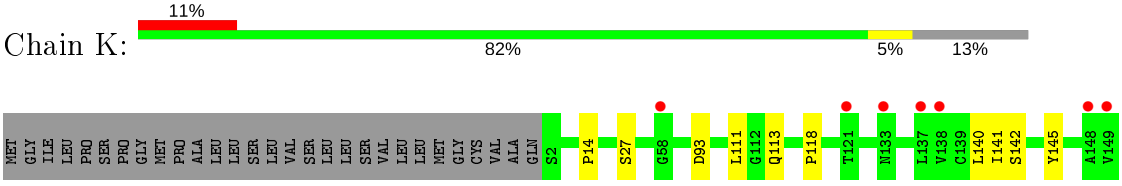
- Molecule 1: Briakinumab FAb light chain

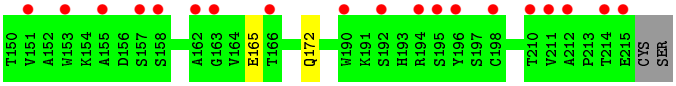
Chain I:



- Molecule 1: Briakinumab FAb light chain

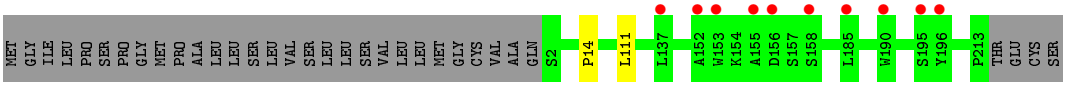
Chain K:





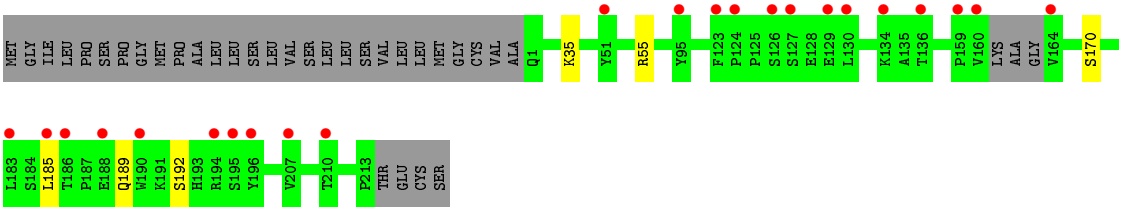
- Molecule 1: Briakinumab FAb light chain

Chain M:



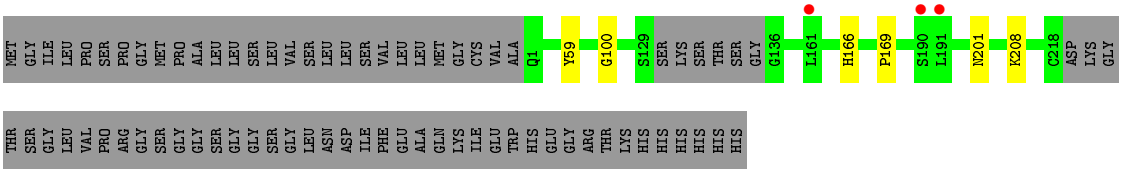
- Molecule 1: Briakinumab FAb light chain

Chain O:



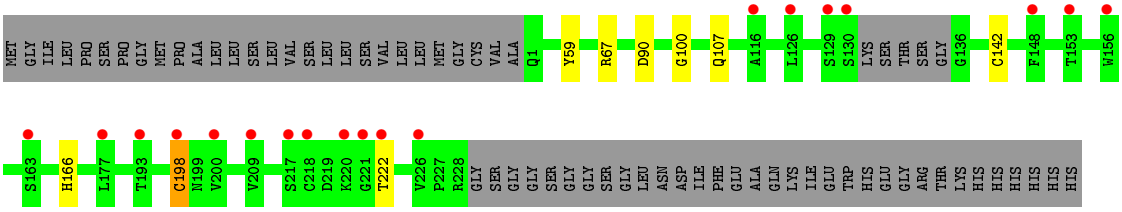
- Molecule 2: Briakinumab FAb heavy chain

Chain B:



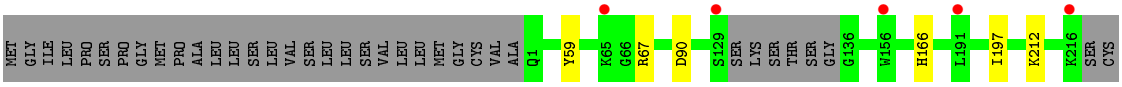
- Molecule 2: Briakinumab FAb heavy chain

Chain D:



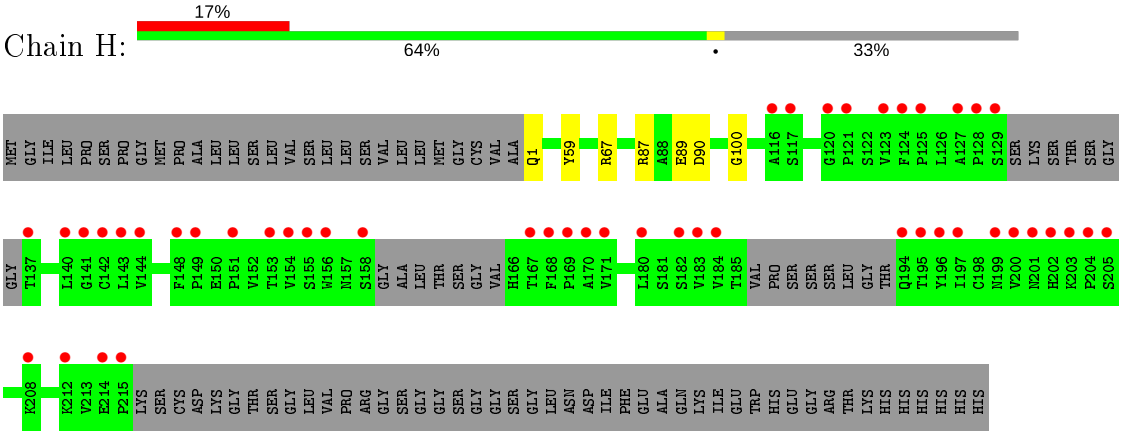
- Molecule 2: Briakinumab FAb heavy chain

Chain F:



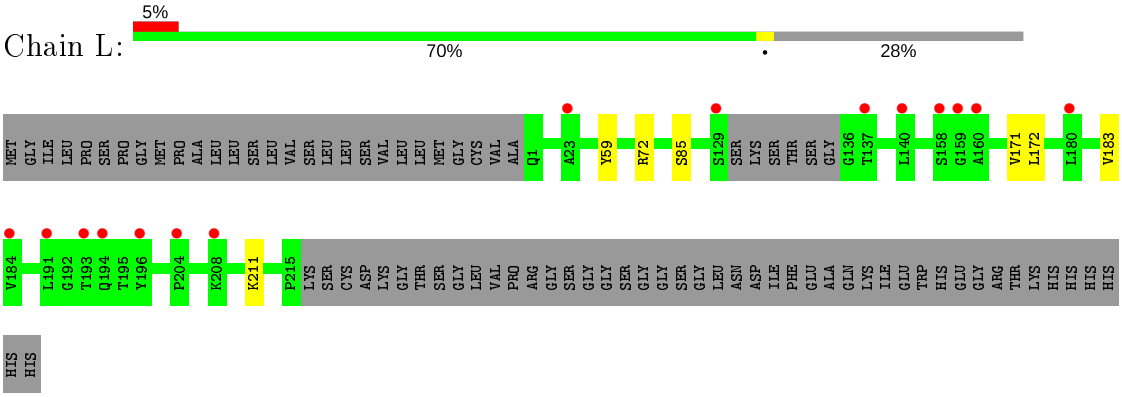
- Molecule 2: Briakinumab FAb heavy chain

Chain H:



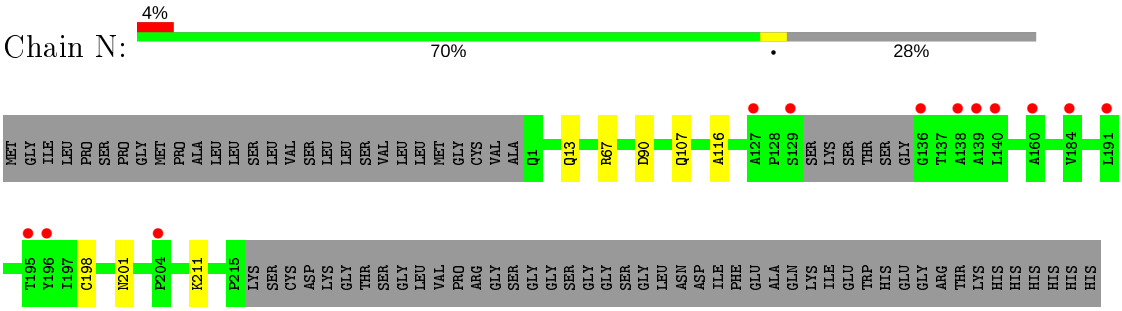
- Molecule 2: Briakinumab FAb heavy chain

Chain L:



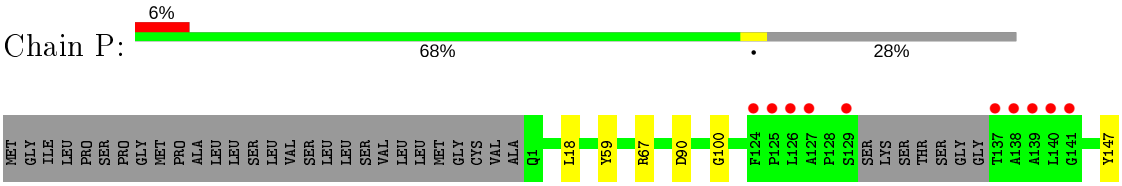
- Molecule 2: Briakinumab FAb heavy chain

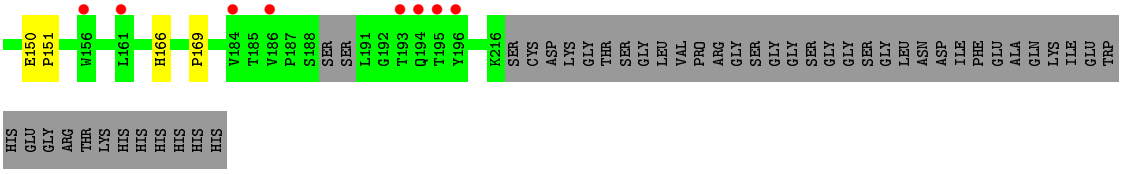
Chain N:



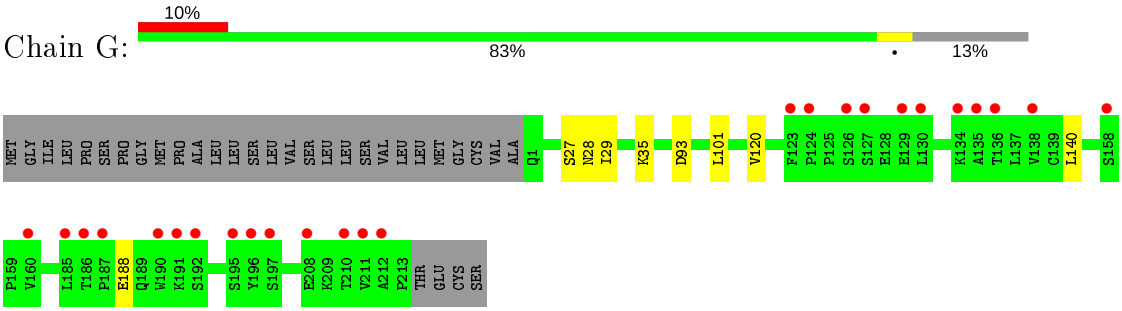
- Molecule 2: Briakinumab FAb heavy chain

Chain P:

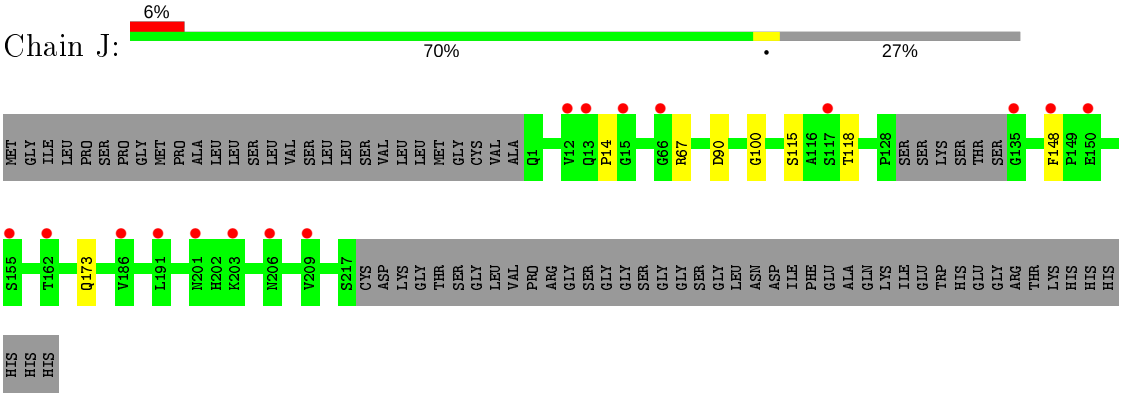




• Molecule 3: Briakinumab FAb light chain



• Molecule 4: Briakinumab FAb heavy chain



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.*

[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

5.1 Standard geometry

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

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.

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: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
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.36	0.53
1:I:97[A]:HIS:HB3	1:I:98[A]:PRO:CD	2.39	0.53
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.40	0.52
3:G:188:GLU:N	3:G:188:GLU:OE1	2.39	0.52
1:K:140:LEU:CD1	2:L:183:VAL:HG11	2.40	0.52
2:N:67:ARG:NH2	2:N:90:ASP:OD2	2.39	0.51
1:E:80:GLN:NE2	1:I:54:GLN:OE1	2.42	0.51
2:P:100:GLY:O	1:O:35:LYS:NZ	2.43	0.51
1:C:35:LYS:NZ	2:D:100:GLY:O	2.44	0.51
2:L:85:SER:HB2	2:P:18:LEU:HD11	1.93	0.51
1:I:93[A]:ASP:OD1	1:I:94[A]:ARG:N	2.44	0.50
1:A:82:GLU:OE1	1:I:175:ASN:ND2	2.38	0.50
2:H:87:ARG:HD2	2:H:89:GLU:OE2	2.12	0.50
1:C:154:LYS:HD3	1:C:159:PRO:HA	1.93	0.50
1:I:97[A]:HIS:HB3	1:I:98[A]:PRO:HD3	1.94	0.49
3:G:35:LYS:NZ	2:H:100:GLY:O	2.43	0.49
2:P:67:ARG:NH2	2:P:90:ASP:OD2	2.39	0.48
2:N:107:GLN:OE1	2:N:107:GLN:N	2.45	0.46
1:K:27:SER:O	1:K:93:ASP:O	2.33	0.46
1:A:35:LYS:NZ	2:B:100:GLY:O	2.46	0.46
2:D:142:CYS:SG	2:D:198[B]:CYS:HB2	2.56	0.45
1:I:35:LYS:NZ	4:J:100:GLY:O	2.46	0.45
1:C:120:VAL:O	1:C:209:LYS:NZ	2.41	0.45
2:P:147:TYR:OH	2:P:150:GLU:OE2	2.17	0.45
1:A:97[B]:HIS:HB3	1:A:98[B]:PRO:CD	2.47	0.44
2:N:13:GLN:NE2	2:N:116:ALA:O	2.50	0.44
1:K:118:PRO:HB2	1:K:141:ILE:HG23	1.98	0.44
2:F:197:ILE:CD1	2:F:212:LYS:HA	2.48	0.44
1:A:97[B]:HIS:HB3	1:A:98[B]:PRO:HD3	2.00	0.43
1:O:185:LEU:HB3	1:O:189:GLN:HG3	2.00	0.43
1:M:14:PRO:HD3	1:M:111:LEU:O	2.18	0.43
1:K:14:PRO:HD3	1:K:111:LEU:O	2.19	0.43
1:K:142:SER:HB2	1:K:172:GLN:OE1	2.19	0.43
1:O:189:GLN:HA	1:O:192:SER:HB3	2.01	0.42
3:G:28:ASN:OD1	3:G:29:ILE:N	2.42	0.42
1:E:171:LYS:HE2	1:E:177:TYR:OH	2.19	0.42
3:G:120:VAL:HA	3:G:140:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:27:SER:O	3:G:93:ASP:O	2.38	0.42
4:J:118:THR:HA	4:J:148:PHE:O	2.20	0.42
2:D:142:CYS:HB3	2:D:198[B]:CYS:SG	2.61	0.41
4:J:14:PRO:HD2	4:J:115:SER:HB3	2.02	0.41
2:P:169:PRO:HG2	1:O:170:SER:OG	2.20	0.41
1:K:165:GLU:HB3	2:L:171:VAL:HG21	2.02	0.41
1:A:170:SER:OG	2:B:169:PRO:HG2	2.21	0.41
2:B:201:ASN:CG	2:B:208:LYS:HE2	2.42	0.41
1:K:113:GLN:HG3	1:K:145:TYR:CD2	2.56	0.41
1:O:55:ARG:NH2	6:O:306:HOH:O	2.49	0.40
2:P:150:GLU:OE1	2:P:151:PRO:HA	2.22	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	166	HIS
2	D	107	GLN
2	D	166	HIS
2	D	198[A]	CYS
2	D	198[B]	CYS
2	F	166	HIS
2	H	1	GLN
2	L	172	LEU
2	L	211	LYS
2	N	198	CYS
2	N	201	ASN
2	N	211	LYS
2	P	166	HIS

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

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	PCA	CA-N-CD	-2.08	106.46	113.58
4	J	1	PCA	CA-N-CD	-2.05	106.57	113.58

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

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^{th} 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

All (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

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Mol	Chain	Res	Type	RSRZ
3	G	196	TYR	7.1
2	D	129	SER	6.5
2	P	196	TYR	6.4
2	H	127	ALA	6.2
2	H	125	PRO	6.1
2	H	153	THR	5.9
4	J	15	GLY	5.9
2	H	167	THR	5.8
3	G	123	PHE	5.7
3	G	190	TRP	5.7
2	L	160	ALA	5.4
3	G	187	PRO	5.2
3	G	129	GLU	5.2
2	H	183	VAL	5.0
4	J	191	LEU	5.0
1	K	194	ARG	4.9
2	P	127	ALA	4.9
1	K	212	ALA	4.8
2	L	196	TYR	4.8
3	G	191	LYS	4.8
2	H	149	PRO	4.7
2	H	123	VAL	4.6
2	H	194	GLN	4.5
3	G	130	LEU	4.5
3	G	211	VAL	4.5
2	P	184	VAL	4.5
3	G	124	PRO	4.4
1	K	162	ALA	4.4
2	P	138	ALA	4.3
2	H	180	LEU	4.3
2	H	199	ASN	4.3
2	D	130	SER	4.3
2	H	120	GLY	4.2
2	H	156	TRP	4.2
2	H	196	TYR	4.2
1	O	194	ARG	4.1
1	K	211	VAL	4.1
3	G	136	THR	4.1
2	P	140	LEU	4.1
1	O	183	LEU	4.1
1	O	159	PRO	4.0
1	O	190	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
1	K	137	LEU	4.0
2	N	129	SER	4.0
2	B	191	LEU	4.0
1	M	137	LEU	4.0
2	H	128	PRO	4.0
2	H	182	SER	3.9
1	K	149	VAL	3.8
1	O	185	LEU	3.8
2	D	209	VAL	3.8
1	O	160	VAL	3.8
2	P	125	PRO	3.8
2	H	144	VAL	3.7
3	G	186	THR	3.7
4	J	135	GLY	3.7
1	K	166	THR	3.7
1	E	1	GLN	3.6
1	O	195	SER	3.6
2	H	124	PHE	3.6
3	G	135	ALA	3.6
1	A	194	ARG	3.6
2	H	154	VAL	3.6
1	K	214	THR	3.6
1	M	185	LEU	3.5
2	D	200	VAL	3.5
2	H	116	ALA	3.5
2	H	214	GLU	3.5
1	O	186	THR	3.5
2	L	191	LEU	3.5
1	O	129	GLU	3.5
2	H	151	PRO	3.4
1	O	124	PRO	3.4
2	P	126	LEU	3.4
1	M	156	ASP	3.4
2	H	158	SER	3.4
2	P	129	SER	3.4
3	G	126	SER	3.4
3	G	127	SER	3.4
2	H	140	LEU	3.4
2	H	141	GLY	3.3
2	H	215	PRO	3.3
2	N	204	PRO	3.3
1	C	93	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	O	130	LEU	3.3
2	N	195	THR	3.3
1	M	155	ALA	3.3
1	K	157	SER	3.3
2	L	129	SER	3.3
2	D	220	LYS	3.2
4	J	206	ASN	3.2
2	L	204	PRO	3.2
1	M	158	SER	3.2
3	G	197	SER	3.2
3	G	134	LYS	3.2
3	G	160	VAL	3.2
2	D	221	GLY	3.2
1	K	58	GLY	3.1
2	N	136	GLY	3.1
2	L	194	GLN	3.1
2	H	168	PHE	3.1
3	G	212	ALA	3.1
1	K	153	TRP	3.1
2	F	191	LEU	3.1
2	P	139	ALA	3.0
1	A	95[A]	TYR	3.0
1	O	126	SER	3.0
2	N	160	ALA	3.0
4	J	148	PHE	3.0
1	C	155	ALA	2.9
1	O	134	LYS	2.9
1	A	96[A]	THR	2.9
2	P	137	THR	2.9
2	H	117	SER	2.9
1	M	196	TYR	2.9
1	K	158	SER	2.9
1	K	163	GLY	2.9
2	D	222	THR	2.9
2	H	212	LYS	2.9
2	L	159	GLY	2.8
2	N	127	ALA	2.8
2	P	161	LEU	2.8
1	A	51	TYR	2.8
2	D	148	PHE	2.8
1	K	148	ALA	2.8
1	O	51	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	184	VAL	2.8
2	L	140	LEU	2.8
1	K	192	SER	2.8
3	G	192	SER	2.8
1	K	215	GLU	2.8
2	L	158	SER	2.8
2	H	203	LYS	2.8
1	M	190	TRP	2.8
1	E	2	SER	2.8
1	C	96	THR	2.7
4	J	150	GLU	2.7
1	M	195	SER	2.7
2	D	193	THR	2.7
2	L	180	LEU	2.7
2	F	129	SER	2.7
1	O	188	GLU	2.7
2	L	193	THR	2.7
2	B	190	SER	2.7
1	K	196	TYR	2.7
1	O	207	VAL	2.7
2	P	124	PHE	2.7
2	H	129	SER	2.6
1	K	155	ALA	2.6
2	H	204	PRO	2.6
2	N	139	ALA	2.6
1	I	95[A]	TYR	2.6
2	H	148	PHE	2.6
2	L	208	LYS	2.6
1	I	97[A]	HIS	2.6
1	I	96[A]	THR	2.6
1	K	138	VAL	2.6
2	H	171	VAL	2.6
4	J	12	VAL	2.6
2	F	216	LYS	2.6
1	O	164	VAL	2.6
2	H	201	ASN	2.5
2	H	197	ILE	2.5
2	P	193	THR	2.5
1	A	1	GLN	2.5
2	D	226	VAL	2.5
2	P	186	VAL	2.5
1	K	190	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	137	LEU	2.5
2	L	137	THR	2.4
4	J	203	LYS	2.4
1	A	216	CYS	2.4
1	C	216	CYS	2.4
2	H	143	LEU	2.4
1	C	211	VAL	2.4
2	H	200	VAL	2.4
2	D	163	SER	2.4
1	M	152	ALA	2.4
2	D	198[A]	CYS	2.4
2	N	138	ALA	2.3
4	J	66	GLY	2.3
2	N	196	TYR	2.3
3	G	210	THR	2.3
3	G	158	SER	2.3
2	D	218	CYS	2.3
4	J	13	GLN	2.3
1	K	151	VAL	2.3
1	C	163	GLY	2.3
1	K	198	CYS	2.3
3	G	208	GLU	2.3
2	N	191	LEU	2.3
2	P	194	GLN	2.3
1	A	97[A]	HIS	2.3
1	K	133	ASN	2.3
2	D	126	LEU	2.3
2	D	217	SER	2.3
2	L	23	ALA	2.3
2	P	141	GLY	2.2
2	H	155	SER	2.2
2	H	195	THR	2.2
1	K	210	THR	2.2
2	F	65	LYS	2.2
2	N	184	VAL	2.2
4	J	209	VAL	2.2
2	H	202	HIS	2.2
2	B	161	LEU	2.2
2	N	140	LEU	2.2
3	G	185	LEU	2.2
2	H	205	SER	2.2
4	J	117	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	184	VAL	2.1
1	C	196	TYR	2.1
4	J	162	THR	2.1
1	K	195	SER	2.1
2	H	121	PRO	2.1
4	J	201	ASN	2.1
2	D	153	THR	2.1
2	H	137	THR	2.1
3	G	138	VAL	2.1
1	I	1	GLN	2.1
2	D	177	LEU	2.1
1	O	95	TYR	2.1
1	I	26	ARG	2.1
2	H	208	LYS	2.1
1	K	121	THR	2.1
2	P	156	TRP	2.1
4	J	186	VAL	2.1
1	O	123	PHE	2.1
1	E	156	ASP	2.0
1	O	136	THR	2.0
1	O	127	SER	2.0
1	M	153	TRP	2.0
1	C	51	TYR	2.0
4	J	155	SER	2.0
2	D	156	TRP	2.0
2	F	156	TRP	2.0
1	C	156	ASP	2.0
1	O	210	THR	2.0
3	G	195	SER	2.0
2	D	116	ALA	2.0

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, 95^{th} 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, 95^{th} 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.