Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:55 pm BST

PDB ID	:	6BIT
Title	:	SIRPalpha antibody complex
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Deposited on	:	2017-11-03
Resolution	:	2.19 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:

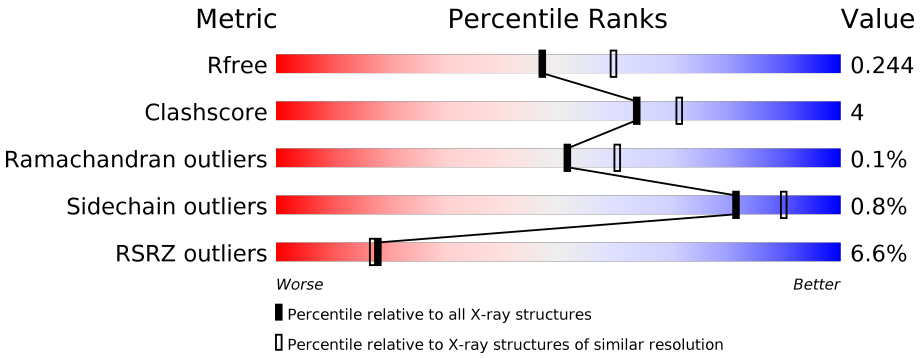
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	I	213	8% 88% 12%
1	J	213	8% 88% 9%
2	K	212	5% 89% 10%
2	L	212	12% 80% 19%
3	G	117	2% 91% 7%
3	H	117	93% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8398 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 KWAR23 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	213	Total	C	N	O	S	0	0	0
			1600	1014	265	316	5			
1	J	207	Total	C	N	O	S	0	0	0
			1559	992	253	309	5			

- Molecule 2 is a protein called KWAR23 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	212	Total	C	N	O	S	0	0	0
			1618	1013	267	331	7			
2	L	211	Total	C	N	O	S	0	0	0
			1608	1008	263	330	7			

- Molecule 3 is a protein called Tyrosine-protein phosphatase non-receptor type substrate 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	115	Total	C	N	O	S	0	1	0
			884	556	157	168	3			
3	G	115	Total	C	N	O	S	0	1	0
			884	555	156	170	3			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	9	Total	O	0	0
			9	9		
4	K	17	Total	O	0	0
			17	17		
4	H	55	Total	O	0	0
			55	55		
4	J	60	Total	O	0	0
			60	60		

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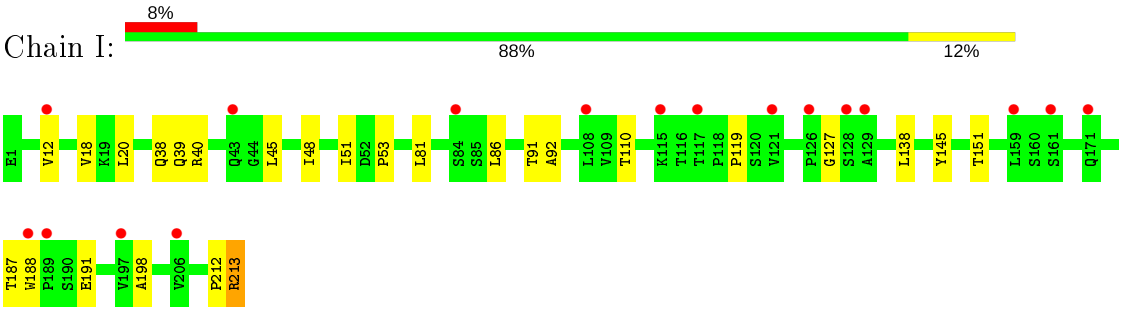
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	36	Total O 36 36	0	0
4	G	68	Total O 68 68	0	0

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.

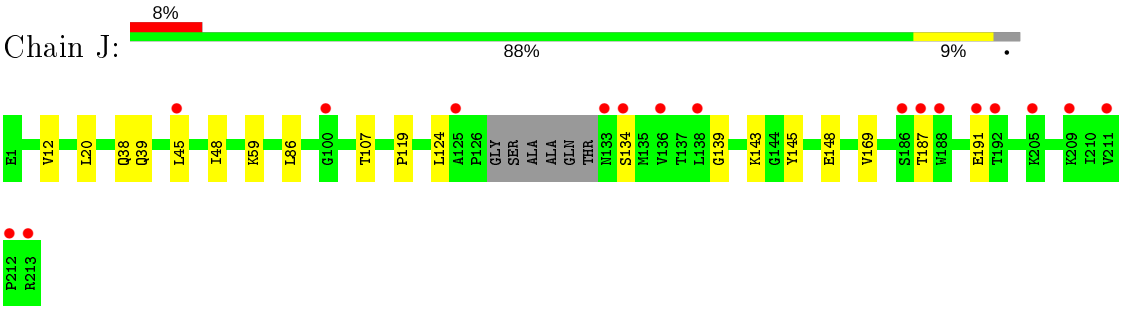
- Molecule 1: KWAR23 Fab heavy chain

Chain I:



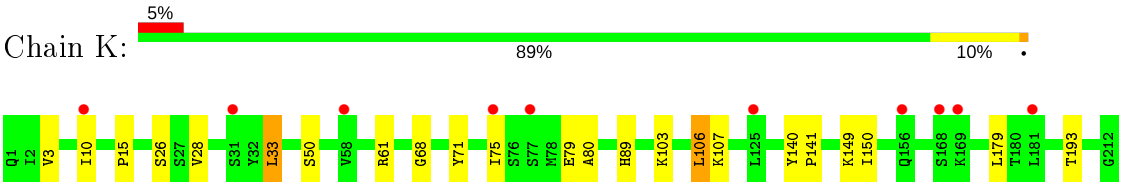
- Molecule 1: KWAR23 Fab heavy chain

Chain J:



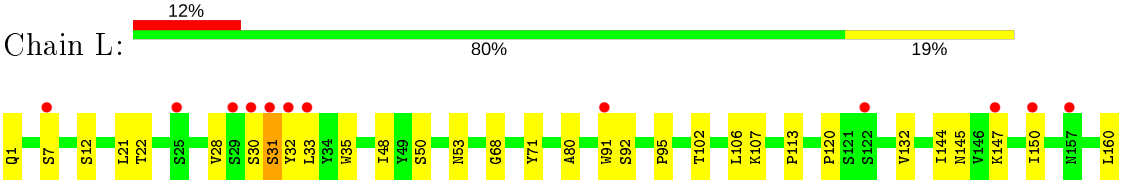
- Molecule 2: KWAR23 Fab light chain

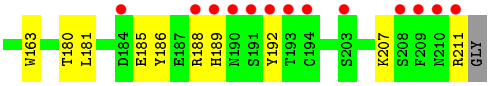
Chain K:



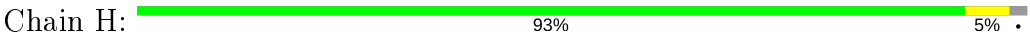
- Molecule 2: KWAR23 Fab light chain

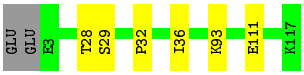
Chain L:



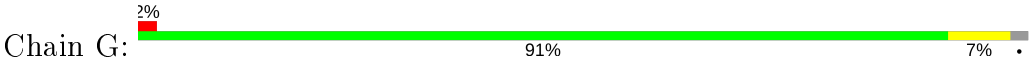


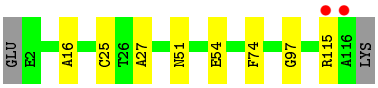
• Molecule 3: Tyrosine-protein phosphatase non-receptor type substrate 1





• Molecule 3: Tyrosine-protein phosphatase non-receptor type substrate 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	164.97Å 164.97Å 96.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.62 – 2.19 47.62 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.62-2.19) 98.8 (47.62-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.210 , 0.240 0.213 , 0.244	Depositor DCC
R_{free} test set	3856 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8398	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	I	0.25	0/1643	0.46	0/2254
1	J	0.46	2/1601 (0.1%)	0.49	0/2196
2	K	0.44	1/1652 (0.1%)	0.46	0/2248
2	L	0.25	0/1642	0.47	0/2236
3	G	0.25	0/904	0.45	0/1225
3	H	0.35	1/904 (0.1%)	0.57	3/1224 (0.2%)
All	All	0.35	4/8346 (0.0%)	0.48	3/11383 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	29	SER	C-N	-7.11	1.17	1.34
1	J	148	GLU	CD-OE1	-6.10	1.19	1.25
1	J	148	GLU	CD-OE2	-5.82	1.19	1.25
2	K	50	SER	CB-OG	-5.53	1.35	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	29	SER	O-C-N	-7.65	110.46	122.70
3	H	28	THR	O-C-N	-5.13	114.49	122.70
3	H	29	SER	CA-C-N	5.04	128.28	117.20

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	I	1600	0	1552	15	0
1	J	1559	0	1505	10	0
2	K	1618	0	1542	13	0
2	L	1608	0	1528	25	0
3	G	884	0	881	6	0
3	H	884	0	887	3	0
4	G	68	0	0	0	0
4	H	55	0	0	1	0
4	I	9	0	0	0	0
4	J	60	0	0	0	0
4	K	17	0	0	0	0
4	L	36	0	0	0	0
All	All	8398	0	7895	68	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 (68) 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:H:111:GLU:OE1	4:H:201:HOH:O	2.15	0.65
2:K:149:LYS:HB2	2:K:193:THR:HB	1.79	0.63
2:L:28:VAL:HG13	2:L:68:GLY:HA2	1.81	0.62
1:J:119:PRO:HB3	1:J:145:TYR:HB3	1.83	0.61
1:J:143:LYS:HE3	2:L:180:THR:HG21	1.84	0.59
2:L:189:HIS:O	2:L:211:ARG:NH1	2.37	0.58
2:L:21:LEU:HD22	2:L:102:THR:HG21	1.86	0.57
2:L:113:PRO:HG3	2:L:144:ILE:HD11	1.86	0.56
2:L:32:TYR:HD2	2:L:91:TRP:CD2	2.23	0.56
2:L:7:SER:HB3	2:L:22:THR:HB	1.87	0.55
3:G:16:ALA:HA	3:G:115:ARG:HG3	1.89	0.55
1:J:59:LYS:NZ	3:G:97:GLY:O	2.40	0.55
3:H:32:PRO:O	3:H:93:LYS:NZ	2.38	0.55
1:I:40:ARG:HG2	1:I:92:ALA:HB2	1.89	0.54
2:K:15:PRO:HG3	2:K:106:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:12:VAL:HG11	1:I:86:LEU:HD12	1.90	0.52
2:K:28:VAL:HG13	2:K:68:GLY:HA2	1.91	0.52
1:J:39:GLN:HB2	1:J:45:LEU:HD23	1.93	0.51
1:J:187:THR:O	1:J:191:GLU:N	2.38	0.51
2:K:80:ALA:HA	2:K:106:LEU:HD13	1.91	0.51
1:I:38:GLN:HB3	1:I:48:ILE:HD11	1.92	0.51
1:J:38:GLN:HB2	1:J:48:ILE:HD11	1.92	0.51
1:I:39:GLN:HB2	1:I:45:LEU:HD23	1.94	0.50
2:L:188:ARG:HG3	2:L:189:HIS:CD2	2.47	0.49
2:L:80:ALA:HA	2:L:106:LEU:HG	1.94	0.49
1:I:119:PRO:HB3	1:I:145:TYR:HB3	1.95	0.49
2:L:50:SER:OG	2:L:53:ASN:ND2	2.43	0.48
2:L:1:PCA:HB3	2:L:95:PRO:HD2	1.94	0.48
1:I:91:THR:HG23	1:I:110:THR:HA	1.96	0.47
1:I:127:GLY:HA2	1:I:213:ARG:N	2.30	0.47
2:L:32:TYR:HB3	2:L:91:TRP:H	1.81	0.46
1:J:12:VAL:HG11	1:J:86:LEU:HD12	1.97	0.45
1:I:213:ARG:HH21	2:L:145:ASN:HB2	1.80	0.45
2:K:33:LEU:HA	2:K:89:HIS:O	2.16	0.45
2:L:186:TYR:O	2:L:192:TYR:OH	2.34	0.45
2:L:33:LEU:HG	2:L:71:TYR:CG	2.50	0.45
3:G:25:CYS:SG	3:G:74:PHE:HB2	2.57	0.44
2:L:32:TYR:HD2	2:L:91:TRP:CE2	2.35	0.44
1:I:212:PRO:O	1:I:213:ARG:HB2	2.17	0.44
2:K:150:ILE:HD11	2:K:179:LEU:HD21	2.00	0.44
2:L:144:ILE:HG22	2:L:163:TRP:CH2	2.53	0.44
3:G:16:ALA:HB2	3:G:115:ARG:HE	1.82	0.43
2:K:3:VAL:HB	2:K:26:SER:HB3	2.00	0.43
2:L:181:LEU:HB3	2:L:185:GLU:HG3	2.01	0.43
1:J:20:LEU:HD22	1:J:107:THR:HG21	2.00	0.43
3:H:36:ILE:HD13	3:H:93:LYS:HA	1.99	0.43
3:G:27:ALA:HB2	3:G:74:PHE:CE2	2.54	0.43
1:I:18:VAL:HG12	1:I:86:LEU:HD11	2.00	0.43
2:K:61:ARG:HG3	2:K:75:ILE:HG23	2.01	0.43
2:L:150:ILE:HD11	2:L:189:HIS:CD2	2.53	0.43
2:L:30:SER:HB3	2:L:32:TYR:HD1	1.83	0.43
2:L:32:TYR:CD1	2:L:92:SER:HB3	2.53	0.42
1:J:124:LEU:HB2	1:J:139:GLY:HA3	2.01	0.42
2:K:33:LEU:HD22	2:K:71:TYR:CD2	2.54	0.42
2:L:12:SER:OG	2:L:107:LYS:HB2	2.18	0.42
1:J:169:VAL:HG11	2:L:160:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:140:TYR:CG	2:K:141:PRO:HA	2.54	0.42
1:I:51:ILE:O	1:I:53:PRO:HD3	2.20	0.42
1:I:187:THR:O	1:I:191:GLU:N	2.51	0.41
2:L:35:TRP:HB2	2:L:48:ILE:HB	2.03	0.41
1:I:138:LEU:HD11	1:I:188:TRP:CD1	2.56	0.41
1:I:20:LEU:HD12	1:I:81:LEU:HD23	2.02	0.41
2:K:107:LYS:HA	2:K:140:TYR:OH	2.21	0.41
1:I:151:THR:HB	1:I:198:ALA:HB3	2.02	0.40
3:G:51:ASN:HB3	3:G:54:GLU:O	2.20	0.40
2:K:10:ILE:HD12	2:K:103:LYS:O	2.22	0.40
2:K:61:ARG:CZ	2:K:79:GLU:HG3	2.52	0.40
2:L:120:PRO:HD3	2:L:132:VAL:HG22	2.03	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	I	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
1	J	203/213 (95%)	198 (98%)	5 (2%)	0	100	100
2	K	210/212 (99%)	200 (95%)	10 (5%)	0	100	100
2	L	209/212 (99%)	195 (93%)	13 (6%)	1 (0%)	29	31
3	G	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
3	H	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
All	All	1061/1084 (98%)	1020 (96%)	40 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	31	SER

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	I	177/181 (98%)	176 (99%)	1 (1%)	86 93
1	J	173/181 (96%)	172 (99%)	1 (1%)	86 93
2	K	183/184 (100%)	181 (99%)	2 (1%)	73 85
2	L	182/184 (99%)	179 (98%)	3 (2%)	62 76
3	G	96/97 (99%)	96 (100%)	0	100 100
3	H	96/97 (99%)	96 (100%)	0	100 100
All	All	907/924 (98%)	900 (99%)	7 (1%)	81 90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	213	ARG
2	K	33	LEU
2	K	106	LEU
1	J	134	SER
2	L	31	SER
2	L	147	LYS
2	L	207	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	53	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
2	PCA	K	1	2	7,8,9	1.80	1 (14%)	9,10,12	2.13	5 (55%)
2	PCA	L	1	2	7,8,9	1.81	1 (14%)	9,10,12	2.14	5 (55%)

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
2	PCA	K	1	2	-	0/0/11/13	0/1/1/1
2	PCA	L	1	2	-	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)
2	L	1	PCA	CD-N	4.68	1.46	1.34
2	K	1	PCA	CD-N	4.64	1.46	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	PCA	OE-CD-CG	-3.16	121.25	126.76
2	L	1	PCA	OE-CD-CG	-3.11	121.33	126.76
2	L	1	PCA	CA-N-CD	-2.87	103.74	113.58
2	K	1	PCA	CA-N-CD	-2.78	104.05	113.58
2	L	1	PCA	CB-CA-N	2.62	110.82	103.30
2	K	1	PCA	CB-CA-N	2.58	110.70	103.30
2	K	1	PCA	CB-CA-C	-2.53	109.23	112.70
2	K	1	PCA	CG-CD-N	2.50	114.85	108.39
2	L	1	PCA	CB-CA-C	-2.48	109.30	112.70
2	L	1	PCA	CG-CD-N	2.44	114.72	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	PCA	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	29:SER	C	30:LEU	N	1.17

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	I	213/213 (100%)	0.52	17 (7%) 12 11	46, 70, 87, 98	0
1	J	207/213 (97%)	0.58	17 (8%) 11 10	28, 48, 93, 109	0
2	K	211/212 (99%)	0.45	10 (4%) 31 30	43, 60, 89, 95	0
2	L	210/212 (99%)	0.84	25 (11%) 4 4	32, 55, 97, 110	0
3	G	115/117 (98%)	0.14	2 (1%) 70 68	30, 38, 57, 76	0
3	H	115/117 (98%)	0.18	0 100 100	33, 42, 57, 81	0
All	All	1071/1084 (98%)	0.50	71 (6%) 18 17	28, 56, 90, 110	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	209	PHE	6.9
2	L	7	SER	5.1
2	L	150	ILE	5.1
2	L	32	TYR	5.0
2	L	31	SER	4.6
1	J	133	ASN	4.6
2	L	91	TRP	4.5
2	L	203	SER	4.1
1	I	129	ALA	4.0
3	G	116	ALA	3.8
1	J	100	GLY	3.7
1	I	206	VAL	3.7
2	L	188	ARG	3.6
2	L	211	ARG	3.5
2	K	77	SER	3.5
2	L	30	SER	3.5
1	I	189	PRO	3.3
1	I	188	TRP	3.3
1	J	138	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	190	ASN	3.2
2	L	192	TYR	3.2
1	I	197	VAL	3.1
3	G	115	ARG	3.1
2	L	157	ASN	3.0
1	J	187	THR	3.0
2	L	210	ASN	3.0
1	J	212	PRO	3.0
2	L	191	SER	3.0
1	I	12	VAL	2.9
2	K	58	VAL	2.9
1	J	188	TRP	2.9
2	K	31	SER	2.8
2	L	208	SER	2.8
1	J	125	ALA	2.8
2	L	33	LEU	2.7
1	I	117	THR	2.7
1	J	45	LEU	2.7
1	J	192	THR	2.6
1	J	186	SER	2.6
1	J	191	GLU	2.6
2	L	29	SER	2.6
1	J	205	LYS	2.6
1	I	43	GLN	2.5
1	I	121	VAL	2.5
1	J	136	VAL	2.4
2	K	156	GLN	2.3
2	K	168	SER	2.3
2	L	189	HIS	2.3
1	I	128	SER	2.3
2	L	25	SER	2.3
1	J	213	ARG	2.3
1	I	115	LYS	2.3
2	L	122	SER	2.3
2	K	181	LEU	2.2
1	I	126	PRO	2.2
2	K	169	LYS	2.2
2	K	125	LEU	2.2
1	I	161	SER	2.2
1	I	171	GLN	2.2
1	J	211	VAL	2.1
2	L	147	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	108	LEU	2.1
1	I	84	SER	2.1
2	L	194	CYS	2.1
1	I	159	LEU	2.1
1	J	134	SER	2.1
2	L	184	ASP	2.1
2	K	75	ILE	2.0
2	K	10	ILE	2.0
2	L	193	THR	2.0
1	J	209	LYS	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
2	PCA	K	1	8/9	0.93	0.15	57,64,70,77	0
2	PCA	L	1	8/9	0.95	0.11	40,48,54,63	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.