



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2016 – 03:08 PM EDT

PDB ID : 5F3H
Title : Structure of myostatin in complex with humanized RK35 antibody
Authors : Parris, K.D.; Mosyak, L.
Deposited on : 2015-12-02
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

A user guide is available at

<http://wwpdb.org/validation/2016/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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

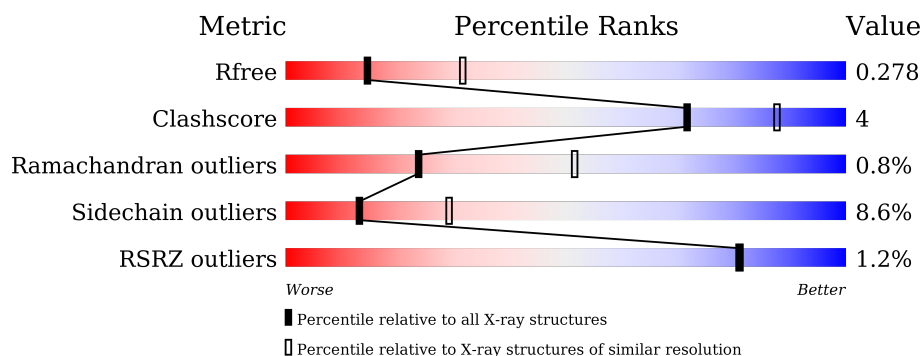
1 Overall quality at a glance

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	221	<div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
1	C	221	<div> <div>82%</div> <div>13%</div> <div>5%</div> </div>
1	E	221	<div> <div>79%</div> <div>15%</div> <div>• 5%</div> </div>
1	G	221	<div> <div>%</div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
2	B	214	<div> <div>86%</div> <div>11%</div> <div>••</div> </div>
2	D	214	<div> <div>85%</div> <div>12%</div> <div>••</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	214	<div><div></div><div>79%18%..</div></div>
2	H	214	<div><div></div><div>83%14%..</div></div>
3	I	108	<div><div>12%</div><div></div><div>71%19%6%. </div></div>
3	J	108	<div><div>4%</div><div></div><div>70%20%6%. </div></div>
3	K	108	<div><div>%</div><div></div><div>81%16%.. </div></div>
3	L	108	<div><div>4%</div><div></div><div>75%16%5%.. </div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15926 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 humanized RK35 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1535	969	254	305	7			
1	C	211	Total	C	N	O	S	0	0	0
			1564	986	259	312	7			
1	E	211	Total	C	N	O	S	0	1	0
			1579	995	264	313	7			
1	G	208	Total	C	N	O	S	0	0	0
			1547	975	257	308	7			

- Molecule 2 is a protein called humanized RK35 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1620	1016	270	329	5			
2	D	211	Total	C	N	O	S	0	0	0
			1619	1015	270	329	5			
2	F	211	Total	C	N	O	S	0	0	0
			1619	1015	270	329	5			
2	H	211	Total	C	N	O	S	0	0	0
			1613	1009	271	328	5			

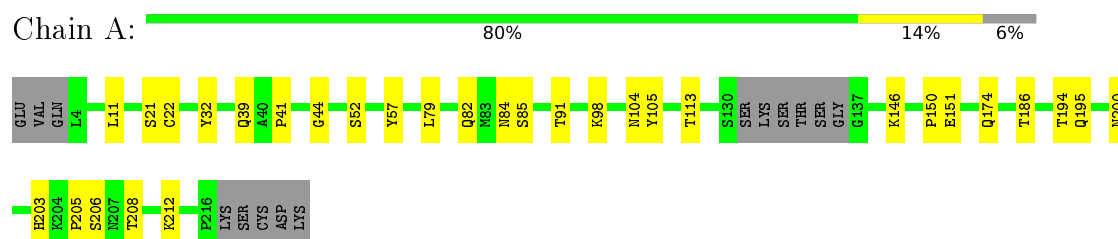
- Molecule 3 is a protein called Growth/differentiation factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	104	Total	C	N	O	S	0	0	0
			802	511	134	145	12			
3	J	104	Total	C	N	O	S	0	0	0
			805	514	135	144	12			
3	K	105	Total	C	N	O	S	0	0	0
			821	524	136	149	12			
3	L	104	Total	C	N	O	S	0	0	0
			802	511	134	145	12			

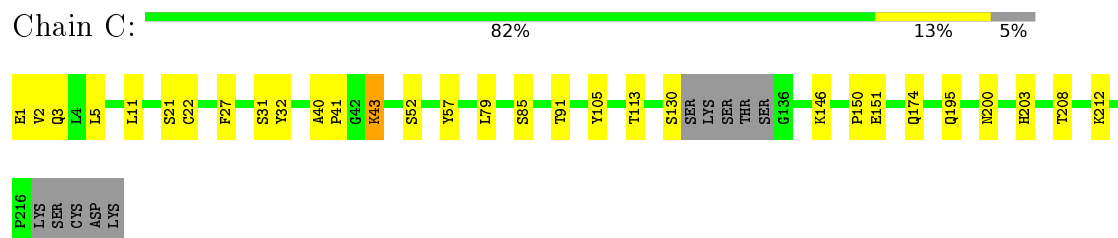
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

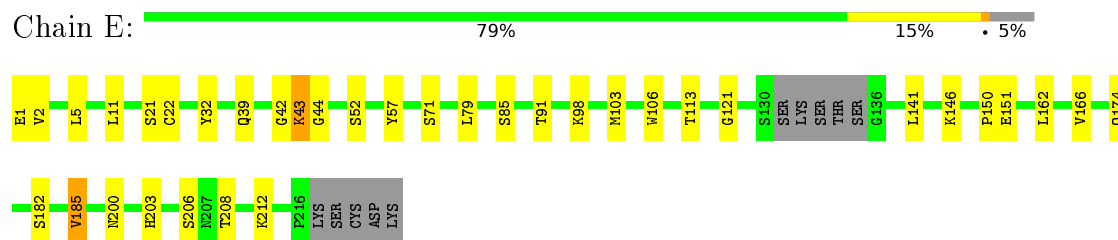
- Molecule 1: humanized RK35 antibody heavy chain



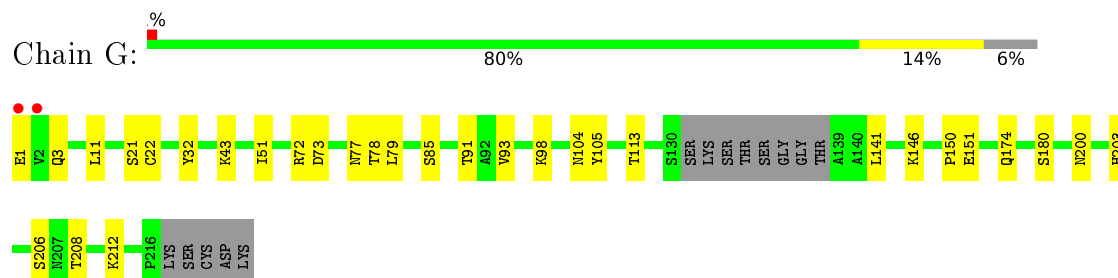
- Molecule 1: humanized RK35 antibody heavy chain




- Molecule 1: humanized RK35 antibody heavy chain

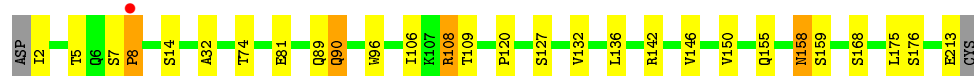


- Molecule 1: humanized RK35 antibody heavy chain




- Molecule 2: humanized RK35 antibody light chain

Chain B:  86% 11% ..




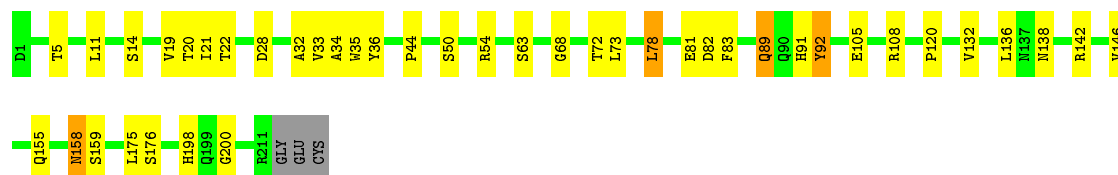
- Molecule 2: humanized RK35 antibody light chain

Chain D:  85% 12% ..




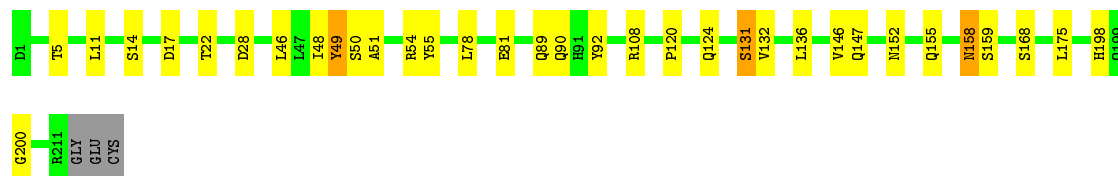
- Molecule 2: humanized RK35 antibody light chain

Chain F:  79% 18% ..



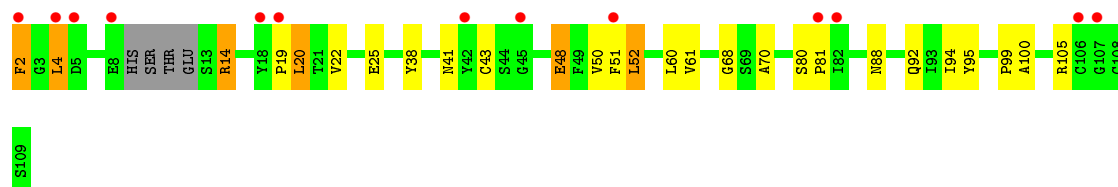
- Molecule 2: humanized RK35 antibody light chain

Chain H:  83% 14% ..



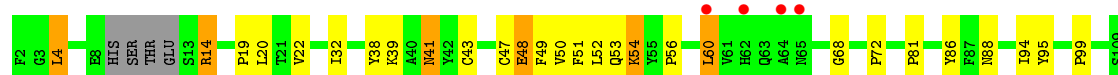
- Molecule 3: Growth/differentiation factor 8

Chain I:  12% 71% 19% 6% .

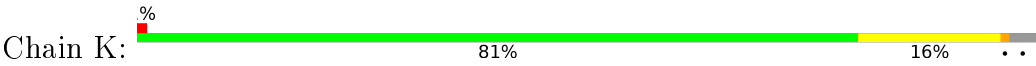


- Molecule 3: Growth/differentiation factor 8

Chain J:  4% 70% 20% 6% .



● Molecule 3: Growth/differentiation factor 8



● Molecule 3: Growth/differentiation factor 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.14Å 80.92Å 101.40Å 88.33° 103.78° 92.40°	Depositor
Resolution (Å)	19.99 – 2.70 19.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	63.5 (19.99-2.70) 63.5 (19.87-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.71Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.218 , 0.270 0.229 , 0.278	Depositor DCC
R_{free} test set	2044 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 7.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.082 for -h,k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15926	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 20.62 % 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 8.3619e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.42	0/1572	0.71	0/2143
1	C	0.41	0/1601	0.71	0/2182
1	E	0.43	0/1616	0.76	0/2200
1	G	0.41	0/1583	0.73	0/2157
2	B	0.45	0/1658	0.76	2/2255 (0.1%)
2	D	0.42	0/1657	0.69	0/2254
2	F	0.46	0/1657	0.69	0/2254
2	H	0.44	0/1650	0.69	0/2243
3	I	0.48	0/826	0.70	0/1122
3	J	0.48	0/829	0.79	1/1124 (0.1%)
3	K	0.51	0/846	0.67	0/1148
3	L	0.47	0/826	0.75	0/1122
All	All	0.44	0/16321	0.72	3/22204 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	51	PHE	C-N-CA	7.08	139.40	121.70
2	B	127	SER	C-N-CA	5.88	134.65	122.30
2	B	127	SER	CA-C-N	5.64	127.49	116.20

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	1535	0	1490	12	0
1	C	1564	0	1519	8	0
1	E	1579	0	1542	15	0
1	G	1547	0	1510	8	0
2	B	1620	0	1554	10	0
2	D	1619	0	1558	8	0
2	F	1619	0	1558	25	0
2	H	1613	0	1553	13	0
3	I	802	0	734	14	0
3	J	805	0	745	13	0
3	K	821	0	753	9	0
3	L	802	0	734	13	0
All	All	15926	0	15250	134	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 (134) 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)
2:H:46:LEU:HD23	2:H:55:TYR:CB	1.96	0.96
2:F:50:SER:H	2:F:91:HIS:HE1	1.15	0.88
2:F:32:ALA:HB1	2:F:91:HIS:HB2	1.62	0.81
3:L:76:PRO:HB3	3:L:103:VAL:HG13	1.68	0.75
2:H:124:GLN:HE22	2:H:131:SER:HB2	1.53	0.71
2:F:19:VAL:HG11	2:F:78:LEU:HD12	1.72	0.71
2:F:50:SER:H	2:F:91:HIS:CE1	2.05	0.70
2:F:36:TYR:HE2	2:F:89:GLN:HG2	1.57	0.67
1:C:146:LYS:HE2	1:C:174:GLN:HE22	1.64	0.63
1:A:146:LYS:HE2	1:A:174:GLN:HE22	1.63	0.63
3:J:49:PHE:HB3	3:J:50:VAL:HA	1.80	0.62
1:E:162:LEU:HD21	1:E:185:VAL:HG11	1.83	0.61
3:I:2:PHE:HA	3:I:105:ARG:HD3	1.82	0.61
3:L:88:ASN:HB3	3:L:94:ILE:HD11	1.84	0.59
2:H:198:HIS:CD2	2:H:200:GLY:H	2.21	0.59
1:G:146:LYS:HE2	1:G:174:GLN:HE22	1.66	0.58
2:D:198:HIS:CD2	2:D:200:GLY:H	2.21	0.58
2:F:20:THR:CG2	2:F:72:THR:CG2	2.82	0.58
2:F:19:VAL:CG1	2:F:78:LEU:HD12	2.34	0.58
3:K:2:PHE:HA	3:K:105:ARG:HD3	1.86	0.57
3:K:31:TRP:HE1	3:L:52:LEU:HD23	1.70	0.57
2:F:78:LEU:HD23	2:F:82:ASP:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:ILE:HD13	1:G:72:ARG:HG2	1.87	0.56
3:L:4:LEU:HD21	3:L:14:ARG:HH11	1.70	0.56
2:F:198:HIS:CD2	2:F:200:GLY:H	2.23	0.56
2:F:19:VAL:HG11	2:F:78:LEU:CD1	2.35	0.56
1:E:146:LYS:HE2	1:E:174:GLN:HE22	1.69	0.56
3:I:4:LEU:HD21	3:I:14:ARG:HH11	1.72	0.55
1:A:203:HIS:HB3	1:A:208:THR:HG23	1.89	0.54
1:C:203:HIS:HB3	1:C:208:THR:HG23	1.89	0.54
3:L:19:PRO:HA	3:L:41:ASN:HD22	1.74	0.53
1:C:40:ALA:HB3	1:C:43:LYS:HB2	1.91	0.53
2:B:155:GLN:HB3	2:B:158:ASN:HD21	1.74	0.53
2:F:155:GLN:HB3	2:F:158:ASN:HD21	1.73	0.53
2:H:155:GLN:HB3	2:H:158:ASN:HD21	1.73	0.53
1:C:11:LEU:HB2	1:C:150:PRO:HG3	1.91	0.52
2:D:78:LEU:HD13	2:D:82:ASP:HB2	1.91	0.52
1:E:39:GLN:HE21	1:E:44:GLY:H	1.57	0.52
2:F:36:TYR:HE2	2:F:89:GLN:CG	2.23	0.51
2:D:32:ALA:HB2	3:I:95:TYR:CD2	2.45	0.51
1:G:203:HIS:HB3	1:G:208:THR:HG23	1.91	0.51
1:A:98:LYS:HB2	1:A:104:ASN:O	2.12	0.50
2:F:36:TYR:CE2	2:F:89:GLN:HG2	2.44	0.50
3:K:61:VAL:HG21	3:K:70:ALA:HB2	1.93	0.50
2:D:90:GLN:HE22	2:D:93:SER:H	1.59	0.50
2:B:89:GLN:HG2	2:B:90:GLN:H	1.76	0.49
3:J:81:PRO:HB3	3:J:99:PRO:HA	1.94	0.49
3:J:48:GLU:HG2	3:J:72:PRO:HG2	1.94	0.49
2:H:49:TYR:O	2:H:50:SER:C	2.51	0.49
2:H:89:GLN:HG2	2:H:90:GLN:N	2.28	0.49
3:I:19:PRO:HA	3:I:41:ASN:HD22	1.77	0.49
3:L:24:PHE:CD1	3:L:32:ILE:HD13	2.48	0.49
3:L:81:PRO:HB3	3:L:99:PRO:HA	1.95	0.49
1:G:22:CYS:HB3	1:G:79:LEU:HB3	1.95	0.48
3:J:22:VAL:HB	3:J:38:TYR:CE1	2.48	0.48
1:A:11:LEU:HB2	1:A:150:PRO:HG3	1.96	0.48
1:E:2:VAL:HG11	1:E:98:LYS:HE2	1.95	0.48
2:H:49:TYR:O	2:H:51:ALA:N	2.47	0.48
3:K:22:VAL:O	3:K:37:ARG:HA	2.13	0.48
3:I:81:PRO:HB3	3:I:99:PRO:HA	1.95	0.48
1:C:22:CYS:HB3	1:C:79:LEU:HB3	1.96	0.48
3:I:43:CYS:O	3:J:68:GLY:HA2	2.14	0.47
1:A:22:CYS:HB3	1:A:79:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:32:ALA:HB2	3:L:95:TYR:CD2	2.49	0.47
3:I:100:ALA:O	3:J:54:LYS:HE3	2.15	0.47
1:E:11:LEU:HB2	1:E:150:PRO:HG3	1.97	0.47
1:G:11:LEU:HB2	1:G:150:PRO:HG3	1.96	0.47
3:J:32:ILE:HA	3:J:86:TYR:HB3	1.96	0.46
3:K:81:PRO:HB3	3:K:99:PRO:HA	1.97	0.46
1:A:39:GLN:HG3	1:A:44:GLY:HA3	1.96	0.46
1:A:82:GLN:HE21	1:A:84:ASN:HD21	1.62	0.46
2:B:7:SER:O	2:B:8:PRO:C	2.53	0.46
3:I:48:GLU:HA	3:I:50:VAL:HG22	1.97	0.46
3:J:19:PRO:HA	3:J:41:ASN:HD22	1.80	0.46
1:G:91:THR:HG23	1:G:113:THR:HA	1.98	0.46
1:C:91:THR:HG23	1:C:113:THR:HA	1.97	0.46
1:C:2:VAL:HG22	1:C:27:PHE:HB3	1.98	0.46
2:D:198:HIS:HD2	2:D:200:GLY:H	1.64	0.45
1:G:98:LYS:HB2	1:G:104:ASN:O	2.16	0.45
3:I:68:GLY:HA2	3:J:43:CYS:O	2.16	0.45
3:K:68:GLY:HA2	3:L:43:CYS:O	2.16	0.45
3:J:4:LEU:HD11	3:J:14:ARG:HB2	1.99	0.44
1:E:91:THR:HG23	1:E:113:THR:HA	1.99	0.44
2:F:78:LEU:HD22	2:F:83:PHE:CZ	2.53	0.44
1:E:106:TRP:CE3	2:F:44:PRO:HD2	2.52	0.44
1:A:203:HIS:ND1	1:A:206:SER:HB3	2.32	0.44
2:H:198:HIS:HD2	2:H:200:GLY:H	1.65	0.44
3:K:73:CYS:HB2	3:L:75:THR:HB	2.00	0.44
1:E:52:SER:HB3	1:E:57:TYR:HB2	2.00	0.44
2:F:20:THR:HG23	2:F:72:THR:CG2	2.47	0.44
2:F:34:ALA:HB2	2:F:91:HIS:NE2	2.33	0.44
1:E:98:LYS:O	1:E:103:MET:HA	2.17	0.43
1:A:52:SER:HB3	1:A:57:TYR:HB2	2.00	0.43
2:B:89:GLN:HE21	2:B:96:TRP:HB3	1.82	0.43
1:A:91:THR:HG23	1:A:113:THR:HA	2.00	0.43
1:E:166:VAL:HG22	1:E:185:VAL:HG13	2.00	0.43
2:F:19:VAL:HG23	2:F:21:ILE:CD1	2.49	0.43
1:G:203:HIS:ND1	1:G:206:SER:HB3	2.34	0.43
3:I:50:VAL:HA	3:I:51:PHE:HA	1.77	0.43
3:J:53:GLN:O	3:J:56:PRO:HD2	2.19	0.43
2:H:92:TYR:HA	3:K:95:TYR:HB3	2.00	0.43
1:E:121:GLY:HA3	1:E:208:THR:HG21	2.00	0.43
2:D:11:LEU:HD23	2:D:104:VAL:HG13	2.00	0.42
2:H:120:PRO:HD3	2:H:132:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:LEU:HD13	2:B:175:LEU:HD22	2.01	0.42
2:H:17:ASP:HB2	2:H:78:LEU:HD12	2.01	0.42
2:B:120:PRO:HD3	2:B:132:VAL:HG22	2.02	0.42
1:A:82:GLN:HE21	1:A:84:ASN:ND2	2.17	0.42
2:B:89:GLN:HG2	2:B:90:GLN:N	2.34	0.42
2:F:120:PRO:HD3	2:F:132:VAL:HG22	2.02	0.42
2:H:46:LEU:CD2	2:H:55:TYR:CB	2.84	0.42
2:D:120:PRO:HD3	2:D:132:VAL:HG22	2.01	0.42
1:E:42:GLY:O	1:E:43:LYS:O	2.38	0.41
2:F:35:TRP:CE2	2:F:73:LEU:HB2	2.56	0.41
3:I:61:VAL:HG21	3:I:70:ALA:HB2	2.01	0.41
2:B:32:ALA:HB2	3:J:95:TYR:CD2	2.55	0.41
1:C:52:SER:HB3	1:C:57:TYR:HB2	2.01	0.41
1:E:203:HIS:ND1	1:E:206:SER:OG	2.44	0.41
1:E:206:SER:OG	1:E:208:THR:HG22	2.20	0.41
1:E:22:CYS:HB3	1:E:79:LEU:HB3	2.02	0.41
2:F:28:ASP:OD1	2:F:68:GLY:HA2	2.20	0.41
3:L:17:ARG:HG3	3:L:106:CYS:SG	2.61	0.41
2:F:92:TYR:HA	3:L:95:TYR:HB3	2.03	0.41
1:A:150:PRO:HD2	1:A:205:PRO:HB2	2.03	0.41
3:I:22:VAL:HB	3:I:38:TYR:CE1	2.55	0.41
3:I:20:LEU:HD21	3:J:60:LEU:HB3	2.03	0.41
2:F:136:LEU:HB2	2:F:175:LEU:HB3	2.02	0.41
2:H:136:LEU:HB2	2:H:175:LEU:HB3	2.03	0.40
3:K:20:LEU:HD21	3:L:60:LEU:HB3	2.04	0.40
2:B:136:LEU:HB2	2:B:175:LEU:HB3	2.02	0.40
3:I:51:PHE:O	3:I:52:LEU:HB2	2.22	0.40
2:B:108:ARG:HD3	2:B:109:THR:O	2.22	0.40
2:D:136:LEU:HB2	2:D:175:LEU:HB3	2.02	0.40
2:F:20:THR:HG22	2:F:72:THR:HG23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	203/221 (92%)	194 (96%)	7 (3%)	2 (1%)	19	45
1	C	207/221 (94%)	199 (96%)	6 (3%)	2 (1%)	19	45
1	E	208/221 (94%)	198 (95%)	9 (4%)	1 (0%)	34	63
1	G	204/221 (92%)	189 (93%)	12 (6%)	3 (2%)	13	32
2	B	210/214 (98%)	192 (91%)	17 (8%)	1 (0%)	34	63
2	D	209/214 (98%)	198 (95%)	11 (5%)	0	100	100
2	F	209/214 (98%)	197 (94%)	10 (5%)	2 (1%)	19	45
2	H	209/214 (98%)	198 (95%)	11 (5%)	0	100	100
3	I	100/108 (93%)	91 (91%)	8 (8%)	1 (1%)	19	45
3	J	100/108 (93%)	90 (90%)	9 (9%)	1 (1%)	19	45
3	K	101/108 (94%)	95 (94%)	5 (5%)	1 (1%)	19	45
3	L	100/108 (93%)	91 (91%)	7 (7%)	2 (2%)	9	24
All	All	2060/2172 (95%)	1932 (94%)	112 (5%)	16 (1%)	24	51

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	PRO
1	E	43	LYS
1	G	43	LYS
1	G	77	ASN
3	J	52	LEU
2	F	92	TYR
3	I	52	LEU
3	K	15	CYS
1	C	41	PRO
1	C	105	TYR
1	G	105	TYR
1	A	41	PRO
1	A	105	TYR
2	F	138	ASN
3	L	41	ASN
3	L	53	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/186 (92%)	163 (95%)	9 (5%)	29	58
1	C	175/186 (94%)	162 (93%)	13 (7%)	17	39
1	E	177/186 (95%)	165 (93%)	12 (7%)	20	43
1	G	174/186 (94%)	161 (92%)	13 (8%)	17	38
2	B	183/187 (98%)	167 (91%)	16 (9%)	13	29
2	D	184/187 (98%)	165 (90%)	19 (10%)	9	20
2	F	184/187 (98%)	167 (91%)	17 (9%)	11	25
2	H	183/187 (98%)	166 (91%)	17 (9%)	11	25
3	I	85/94 (90%)	74 (87%)	11 (13%)	5	12
3	J	86/94 (92%)	75 (87%)	11 (13%)	5	12
3	K	88/94 (94%)	83 (94%)	5 (6%)	25	53
3	L	85/94 (90%)	76 (89%)	9 (11%)	8	19
All	All	1776/1868 (95%)	1624 (91%)	152 (9%)	13	29

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	32	TYR
1	A	85	SER
1	A	151	GLU
1	A	186	THR
1	A	194	THR
1	A	195	GLN
1	A	200	ASN
1	A	212	LYS
2	B	2	ILE
2	B	5	THR
2	B	14	SER
2	B	74	THR
2	B	81	GLU

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Mol	Chain	Res	Type
2	B	90	GLN
2	B	106	ILE
2	B	108	ARG
2	B	142	ARG
2	B	146	VAL
2	B	150	VAL
2	B	158	ASN
2	B	159	SER
2	B	168	SER
2	B	176	SER
2	B	213	GLU
1	C	1	GLU
1	C	3	GLN
1	C	5	LEU
1	C	21	SER
1	C	31	SER
1	C	32	TYR
1	C	43	LYS
1	C	85	SER
1	C	130	SER
1	C	151	GLU
1	C	195	GLN
1	C	200	ASN
1	C	212	LYS
2	D	1	ASP
2	D	2	ILE
2	D	5	THR
2	D	10	SER
2	D	11	LEU
2	D	12	SER
2	D	14	SER
2	D	19	VAL
2	D	48	ILE
2	D	54	ARG
2	D	78	LEU
2	D	81	GLU
2	D	90	GLN
2	D	108	ARG
2	D	146	VAL
2	D	155	GLN
2	D	156	SER
2	D	158	ASN

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Mol	Chain	Res	Type
2	D	159	SER
1	E	1	GLU
1	E	5	LEU
1	E	21	SER
1	E	32	TYR
1	E	71	SER
1	E	85	SER
1	E	141	LEU
1	E	151	GLU
1	E	182	SER
1	E	185	VAL
1	E	200	ASN
1	E	212	LYS
2	F	5	THR
2	F	11	LEU
2	F	14	SER
2	F	22	THR
2	F	33	VAL
2	F	54	ARG
2	F	63	SER
2	F	78	LEU
2	F	81	GLU
2	F	89	GLN
2	F	105	GLU
2	F	108	ARG
2	F	142	ARG
2	F	146	VAL
2	F	158	ASN
2	F	159	SER
2	F	176	SER
1	G	1	GLU
1	G	3	GLN
1	G	21	SER
1	G	32	TYR
1	G	73	ASP
1	G	78	THR
1	G	85	SER
1	G	93	VAL
1	G	141	LEU
1	G	151	GLU
1	G	180	SER
1	G	200	ASN

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Mol	Chain	Res	Type
1	G	212	LYS
2	H	5	THR
2	H	11	LEU
2	H	14	SER
2	H	22	THR
2	H	28	ASP
2	H	48	ILE
2	H	49	TYR
2	H	54	ARG
2	H	81	GLU
2	H	108	ARG
2	H	131	SER
2	H	146	VAL
2	H	147	GLN
2	H	152	ASN
2	H	158	ASN
2	H	159	SER
2	H	168	SER
3	I	2	PHE
3	I	4	LEU
3	I	14	ARG
3	I	20	LEU
3	I	25	GLU
3	I	48	GLU
3	I	60	LEU
3	I	80	SER
3	I	88	ASN
3	I	92	GLN
3	I	94	ILE
3	J	4	LEU
3	J	14	ARG
3	J	20	LEU
3	J	39	LYS
3	J	41	ASN
3	J	47	CYS
3	J	48	GLU
3	J	54	LYS
3	J	60	LEU
3	J	88	ASN
3	J	94	ILE
3	K	20	LEU
3	K	41	ASN

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Mol	Chain	Res	Type
3	K	57	HIS
3	K	75	THR
3	K	94	ILE
3	L	4	LEU
3	L	14	ARG
3	L	25	GLU
3	L	41	ASN
3	L	50	VAL
3	L	60	LEU
3	L	88	ASN
3	L	92	GLN
3	L	94	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	207	ASN
2	B	6	GLN
2	B	155	GLN
2	B	158	ASN
1	C	99	GLN
1	C	104	ASN
1	C	174	GLN
1	C	195	GLN
1	C	207	ASN
2	D	3	GLN
2	D	90	GLN
2	D	138	ASN
2	D	147	GLN
2	D	152	ASN
2	D	158	ASN
1	E	174	GLN
2	F	91	HIS
2	F	155	GLN
2	F	158	ASN
2	F	198	HIS
1	G	174	GLN
1	G	207	ASN
2	H	124	GLN
2	H	138	ASN
2	H	155	GLN

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Mol	Chain	Res	Type
2	H	158	ASN
2	H	198	HIS
2	H	199	GLN
3	I	41	ASN
3	I	92	GLN
3	J	41	ASN
3	J	57	HIS
3	K	41	ASN
3	K	57	HIS
3	L	41	ASN
3	L	92	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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](#)

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, 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	207/221 (93%)	-0.47	0 100 100	12, 28, 43, 69	0
1	C	211/221 (95%)	-0.48	0 100 100	15, 29, 45, 55	0
1	E	211/221 (95%)	-0.48	0 100 100	15, 29, 44, 91	0
1	G	208/221 (94%)	-0.27	2 (0%) 84 85	22, 41, 61, 78	0
2	B	212/214 (99%)	-0.50	1 (0%) 91 93	14, 31, 47, 60	0
2	D	211/214 (98%)	-0.47	0 100 100	19, 34, 48, 60	0
2	F	211/214 (98%)	-0.46	0 100 100	14, 33, 45, 60	0
2	H	211/214 (98%)	-0.36	0 100 100	23, 40, 56, 63	0
3	I	104/108 (96%)	0.60	13 (12%) 5 4	38, 67, 102, 114	0
3	J	104/108 (96%)	0.09	4 (3%) 44 44	22, 51, 88, 99	0
3	K	105/108 (97%)	-0.06	1 (0%) 84 85	35, 58, 72, 92	0
3	L	104/108 (96%)	0.09	4 (3%) 44 44	26, 55, 81, 87	0
All	All	2099/2172 (96%)	-0.31	25 (1%) 81 81	12, 36, 69, 114	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	4	LEU	4.6
3	L	51	PHE	4.5
3	I	2	PHE	4.3
3	L	52	LEU	4.2
3	I	5	ASP	3.7
3	L	64	ALA	3.4
3	I	42	TYR	3.3
3	I	51	PHE	3.1
3	I	18	TYR	3.0
3	I	19	PRO	2.9
3	J	65	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
3	J	64	ALA	2.7
3	I	107	GLY	2.6
3	J	62	HIS	2.6
1	G	1	GLU	2.5
3	J	60	LEU	2.4
3	I	81	PRO	2.4
3	I	82	ILE	2.4
3	I	45	GLY	2.4
3	K	89	GLY	2.4
3	I	8	GLU	2.2
1	G	2	VAL	2.2
3	I	106	CYS	2.2
2	B	8	PRO	2.1
3	L	60	LEU	2.1

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 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.