



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:31 PM GMT

PDB ID : 4LU5
Title : Structure of murine IgG2a A20G2-Fab in complex with vaccinia antigen A33R
at the resolution of 2.9 Angstroms
Authors : Matho, M.H.; Schlossman, A.M.; Zajonc, D.M.
Deposited on : 2013-07-24
Resolution : 2.90 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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

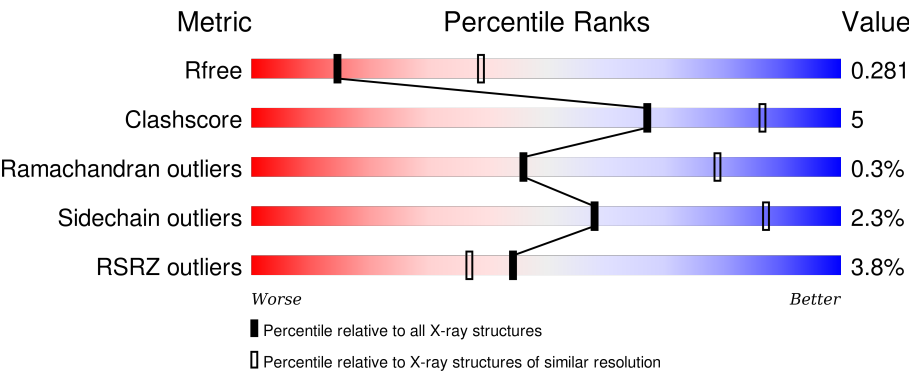
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	97	<div><div>5%</div><div><div></div><div>81%</div><div>7%</div><div>•</div><div>10%</div></div></div>
1	B	97	<div><div>4%</div><div><div></div><div>74%</div><div>14%</div><div>11%</div></div></div>
2	H	213	<div><div>2%</div><div><div></div><div>85%</div><div>14%</div><div>•</div></div></div>
2	I	213	<div><div>7%</div><div><div></div><div>82%</div><div>16%</div><div>•</div></div></div>
3	L	219	<div><div></div><div><div></div><div>84%</div><div>16%</div></div></div>

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Mol	Chain	Length	Quality of chain
3	M	219	 A horizontal bar chart showing the quality of chain M. The bar is divided into three segments: a red segment on the left labeled '5%', a green segment in the middle labeled '88%', and a yellow segment on the right labeled '11%'. The segments are separated by thin white lines.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8008 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 A33R.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	87	Total	C	N	O	S	0	0	0
			679	419	106	147	7			
1	B	86	Total	C	N	O	S	0	0	0
			671	415	105	144	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	MET	SER	ENGINEERED MUTATION	UNP Q71TT1
A	118	MET	LEU	ENGINEERED MUTATION	UNP Q71TT1
A	123	ALA	LYS	ENGINEERED MUTATION	UNP Q71TT1
A	140	MET	LEU	ENGINEERED MUTATION	UNP Q71TT1
B	89	MET	SER	ENGINEERED MUTATION	UNP Q71TT1
B	118	MET	LEU	ENGINEERED MUTATION	UNP Q71TT1
B	123	ALA	LYS	ENGINEERED MUTATION	UNP Q71TT1
B	140	MET	LEU	ENGINEERED MUTATION	UNP Q71TT1

- Molecule 2 is a protein called Murine IgG2a A20G2 Heavy chain Fab domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	209	Total	C	N	O	S	0	0	0
			1601	1020	262	312	7			
2	I	210	Total	C	N	O	S	0	0	0
			1602	1020	262	313	7			

- Molecule 3 is a protein called Murine IgG2a A20G2 Light chain Fab domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	219	Total	C	N	O	S	0	0	0
			1698	1064	285	342	7			
3	M	219	Total	C	N	O	S	0	0	0
			1698	1064	285	342	7			

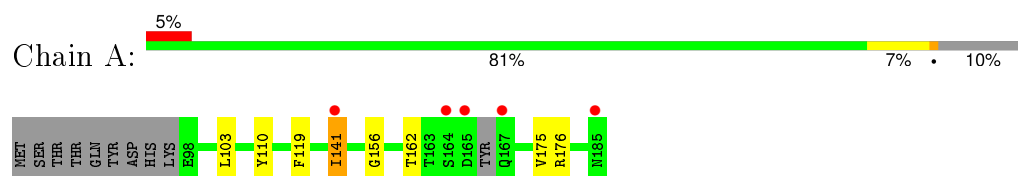
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total 6	O 6	0	0
4	B	6	Total 6	O 6	0	0
4	H	9	Total 9	O 9	0	0
4	I	5	Total 5	O 5	0	0
4	L	14	Total 14	O 14	0	0
4	M	19	Total 19	O 19	0	0

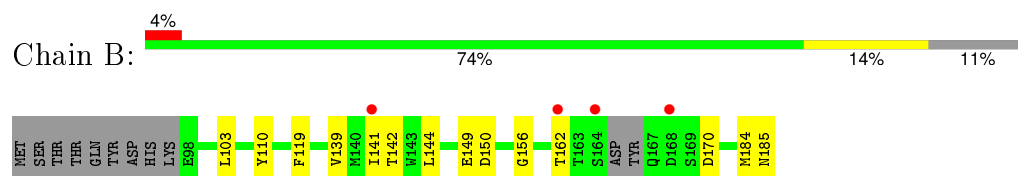
3 Residue-property plots [i](#)

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

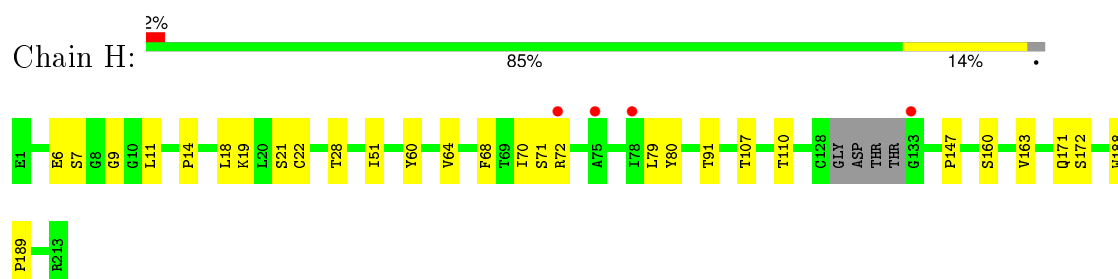
- Molecule 1: A33R



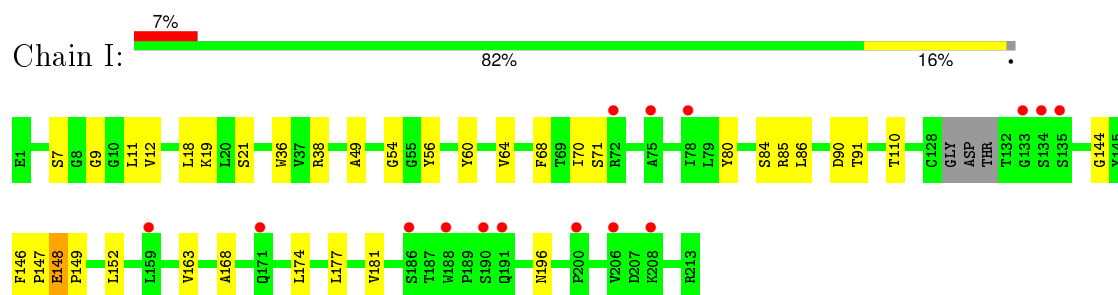
- Molecule 1: A33R



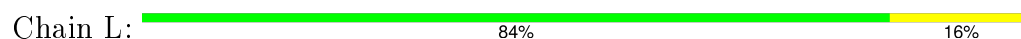
- Molecule 2: Murine IgG2a A20G2 Heavy chain Fab domain

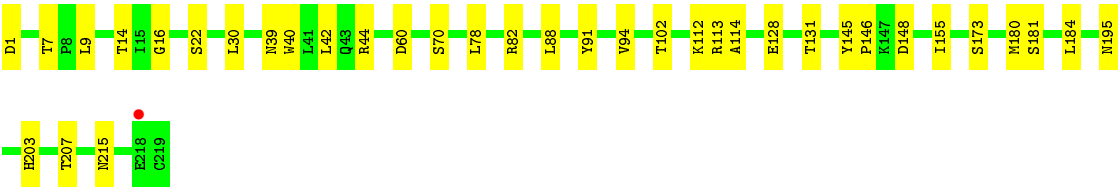


- Molecule 2: Murine IgG2a A20G2 Heavy chain Fab domain

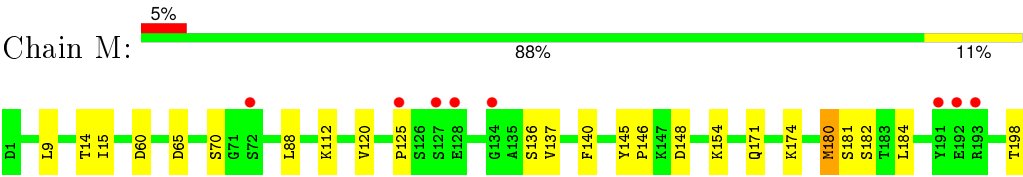


- Molecule 3: Murine IgG2a A20G2 Light chain Fab domain





● Molecule 3: Murine IgG2a A20G2 Light chain Fab domain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.90Å 157.26Å 175.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.94 – 2.90 54.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (54.94-2.90) 97.2 (54.94-2.90)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.234 , 0.282 0.234 , 0.281	Depositor DCC
R_{free} test set	1556 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	3 of 30843 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8008	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 30.40 % 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 1.3173e-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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.31	0/692	0.49	0/938
1	B	0.32	0/684	0.51	0/927
2	H	0.30	0/1642	0.51	0/2238
2	I	0.30	0/1643	0.49	0/2241
3	L	0.31	0/1735	0.51	0/2354
3	M	0.30	0/1735	0.51	0/2354
All	All	0.30	0/8131	0.51	0/11052

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	679	0	611	4	0
1	B	671	0	607	9	0
2	H	1601	0	1574	15	0
2	I	1602	0	1564	20	0
3	L	1698	0	1658	17	0
3	M	1698	0	1657	10	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	H	9	0	0	0	0
4	I	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	14	0	0	0	0
4	M	19	0	0	0	0
All	All	8008	0	7671	75	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (75) 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:B:184:MET:HG3	1:B:185:ASN:H	1.48	0.79
2:H:91:THR:HG23	2:H:110:THR:HA	1.65	0.78
1:B:139:VAL:O	1:B:142:THR:HG22	1.85	0.76
2:H:64:VAL:HG13	2:H:68:PHE:HB2	1.67	0.74
1:B:142:THR:HG23	1:B:144:LEU:H	1.57	0.69
2:I:91:THR:HG23	2:I:110:THR:HA	1.74	0.69
2:I:71:SER:HB2	2:I:80:TYR:HB2	1.75	0.69
2:I:7:SER:HB2	2:I:21:SER:HB2	1.77	0.65
2:H:9:GLY:HA2	2:H:18:LEU:HD21	1.77	0.65
2:I:11:LEU:HB2	2:I:147:PRO:HG3	1.79	0.64
2:H:7:SER:HB2	2:H:21:SER:HB2	1.79	0.64
2:H:71:SER:HB2	2:H:80:TYR:HB2	1.80	0.61
2:I:148:GLU:HG2	2:I:149:PRO:HA	1.82	0.61
2:I:168:ALA:HB2	2:I:177:LEU:HD12	1.84	0.60
2:H:11:LEU:HB2	2:H:147:PRO:HG3	1.86	0.57
2:I:12:VAL:HG21	2:I:86:LEU:HD13	1.85	0.57
1:B:184:MET:O	1:B:185:ASN:HB2	2.06	0.56
3:L:88:LEU:HD21	3:L:173:SER:HA	1.87	0.55
3:L:14:THR:HA	3:L:112:LYS:HB2	1.89	0.55
3:M:88:LEU:HD22	3:M:171:GLN:HB3	1.89	0.54
2:I:144:GLY:HA2	2:I:174:LEU:HB3	1.90	0.54
2:H:171:GLN:HG3	2:H:172:SER:H	1.73	0.53
2:I:84:SER:OG	2:I:85:ARG:NH1	2.43	0.52
3:M:14:THR:HA	3:M:112:LYS:HB2	1.92	0.52
1:B:103:LEU:HB2	1:B:110:TYR:HB2	1.91	0.52
2:I:60:TYR:OH	2:I:70:ILE:HG22	2.12	0.50
2:I:54:GLY:HA3	2:I:56:TYR:CE2	2.48	0.48
3:L:128:GLU:O	3:L:131:THR:HB	2.14	0.48
2:I:64:VAL:HG13	2:I:68:PHE:CG	2.48	0.47
3:M:154:LYS:HB2	3:M:198:THR:HB	1.95	0.47
2:H:171:GLN:HG3	2:H:172:SER:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:38:ARG:NH1	2:I:90:ASP:HA	2.31	0.46
2:H:60:TYR:OH	2:H:70:ILE:HG22	2.15	0.46
3:L:113:ARG:NH1	3:L:114:ALA:O	2.41	0.46
1:B:119:PHE:CD1	1:B:156:GLY:HA2	2.51	0.46
3:L:42:LEU:HD13	3:L:91:TYR:CZ	2.50	0.46
3:L:180:MET:HG2	3:L:181:SER:N	2.31	0.45
2:I:19:LYS:HE3	2:I:80:TYR:CD1	2.52	0.45
1:B:184:MET:O	1:B:185:ASN:CB	2.65	0.44
3:M:112:LYS:HA	3:M:145:TYR:OH	2.18	0.44
1:B:141:ILE:O	1:B:141:ILE:HG22	2.16	0.44
2:I:9:GLY:HA2	2:I:18:LEU:HD21	1.99	0.43
2:H:188:TRP:CG	2:H:189:PRO:HA	2.53	0.43
2:H:51:ILE:HD13	2:H:72:ARG:HD3	2.00	0.43
3:M:120:VAL:HA	3:M:140:PHE:O	2.19	0.43
2:H:22:CYS:HB3	2:H:79:LEU:HB3	1.99	0.43
1:A:175:VAL:O	1:A:176:ARG:HG3	2.18	0.43
1:A:103:LEU:HB2	1:A:110:TYR:HB2	2.00	0.43
1:A:119:PHE:CD1	1:A:156:GLY:HA2	2.54	0.42
3:L:155:ILE:HD11	3:L:184:LEU:HD21	2.01	0.42
3:L:16:GLY:HA2	3:L:82:ARG:HG2	2.02	0.42
2:H:19:LYS:HE3	2:H:80:TYR:HB3	2.02	0.42
3:L:7:THR:HG23	3:L:22:SER:HB2	2.02	0.42
3:L:40:TRP:CE2	3:L:78:LEU:HB2	2.54	0.42
2:H:160:SER:O	2:H:163:VAL:HG22	2.20	0.42
3:M:145:TYR:CG	3:M:146:PRO:HA	2.55	0.41
2:I:64:VAL:HG13	2:I:68:PHE:HB2	2.02	0.41
3:L:113:ARG:HG2	3:L:114:ALA:H	1.85	0.41
3:L:1:ASP:HB3	3:L:102:THR:HG21	2.02	0.41
2:I:152:LEU:HA	2:I:196:ASN:O	2.20	0.41
3:M:180:MET:HE2	3:M:182:SER:HB2	2.02	0.41
3:L:112:LYS:HA	3:L:145:TYR:OH	2.20	0.41
3:L:113:ARG:HG2	3:L:114:ALA:N	2.36	0.41
3:M:136:SER:HA	3:M:184:LEU:O	2.20	0.41
2:H:6:GLU:HB3	2:H:107:THR:HB	2.03	0.41
1:A:141:ILE:HG22	1:A:141:ILE:O	2.21	0.41
3:M:125:PRO:HD3	3:M:137:VAL:HG22	2.02	0.41
1:B:149:GLU:O	1:B:150:ASP:HB2	2.20	0.41
3:L:195:ASN:HB2	3:L:215:ASN:OD1	2.20	0.41
3:M:180:MET:HG2	3:M:181:SER:N	2.36	0.41
3:L:146:PRO:HD2	3:L:203:HIS:CE1	2.56	0.41
3:L:39:ASN:HB2	3:L:94:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:146:PHE:HA	2:I:147:PRO:HA	1.84	0.40
2:I:163:VAL:HG12	2:I:181:VAL:HG23	2.02	0.40
2:I:36:TRP:HB2	2:I:49:ALA:HB3	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	A	83/97 (86%)	78 (94%)	4 (5%)	1 (1%)	16	48
1	B	82/97 (84%)	76 (93%)	6 (7%)	0	100	100
2	H	205/213 (96%)	195 (95%)	9 (4%)	1 (0%)	34	71
2	I	206/213 (97%)	193 (94%)	13 (6%)	0	100	100
3	L	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
3	M	217/219 (99%)	209 (96%)	7 (3%)	1 (0%)	34	71
All	All	1010/1058 (96%)	962 (95%)	45 (4%)	3 (0%)	46	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	14	PRO
3	M	218	GLU
1	A	141	ILE

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	78/89 (88%)	77 (99%)	1 (1%)	76	94
1	B	77/89 (86%)	75 (97%)	2 (3%)	54	85
2	H	181/184 (98%)	180 (99%)	1 (1%)	90	97
2	I	180/184 (98%)	179 (99%)	1 (1%)	90	97
3	L	196/196 (100%)	189 (96%)	7 (4%)	42	78
3	M	196/196 (100%)	187 (95%)	9 (5%)	33	69
All	All	908/938 (97%)	887 (98%)	21 (2%)	58	87

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	THR
1	B	162	THR
1	B	170	ASP
2	H	28	THR
2	I	148	GLU
3	L	9	LEU
3	L	30	LEU
3	L	44	ARG
3	L	60	ASP
3	L	70	SER
3	L	148	ASP
3	L	207	THR
3	M	9	LEU
3	M	15	ILE
3	M	60	ASP
3	M	65	ASP
3	M	70	SER
3	M	148	ASP
3	M	174	LYS
3	M	180	MET
3	M	219	CYS

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

Mol	Chain	Res	Type
2	I	171	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	87/97 (89%)	0.48	5 (5%)	27	21	22, 34, 66, 91	0
1	B	86/97 (88%)	0.23	4 (4%)	35	29	20, 30, 59, 83	0
2	H	209/213 (98%)	0.28	4 (1%)	70	66	19, 37, 53, 63	0
2	I	210/213 (98%)	0.57	15 (7%)	19	13	22, 50, 80, 90	0
3	L	219/219 (100%)	-0.06	1 (0%)	91	90	17, 28, 45, 76	0
3	M	219/219 (100%)	0.22	10 (4%)	36	30	18, 35, 68, 93	0
All	All	1030/1058 (97%)	0.27	39 (3%)	44	37	17, 35, 72, 93	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	135	SER	4.1
1	B	168	ASP	3.9
3	M	219	CYS	3.7
3	M	127	SER	3.6
3	M	217	ASN	3.4
2	I	186	SER	3.3
3	M	134	GLY	3.1
2	I	206	VAL	2.9
2	I	72	ARG	2.8
1	A	185	ASN	2.7
3	M	125	PRO	2.7
2	I	208	LYS	2.7
2	H	78	ILE	2.6
2	H	72	ARG	2.6
1	A	165	ASP	2.5
2	I	171	GLN	2.5
3	L	218	GLU	2.4
1	A	167	GLN	2.4
2	H	75	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
3	M	72	SER	2.4
3	M	192	GLU	2.4
2	I	188	TRP	2.4
1	B	164	SER	2.4
2	I	133	GLY	2.3
3	M	128	GLU	2.3
1	B	162	THR	2.3
3	M	193	ARG	2.3
2	I	191	GLN	2.2
2	I	200	PRO	2.2
2	I	159	LEU	2.2
3	M	191	TYR	2.2
1	A	141	ILE	2.1
1	A	164	SER	2.1
2	I	78	ILE	2.1
2	I	190	SER	2.1
2	H	133	GLY	2.1
2	I	134	SER	2.1
1	B	141	ILE	2.0
2	I	75	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.