



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2018 – 09:51 PM EST

PDB ID : 4QCI
Title : PDGF-B blocking antibody bound to PDGF-BB
Authors : Kuai, J.; Mosyak, L.; Tam, M.; LaVallie, E.; Pullen, N.; Carven, G.
Deposited on : 2014-05-12
Resolution : 2.30 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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

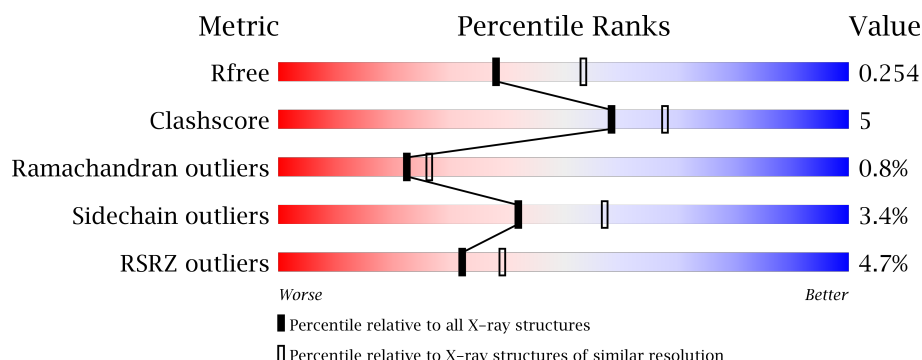
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	209	
1	L	209	
2	B	223	
2	H	223	
3	C	110	

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Mol	Chain	Length	Quality of chain
3	D	110	<div><div></div><div>14%</div><div>69%</div><div>18%</div><div>13%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8086 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 anti-PDGF-BB antibody - Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1553	968	259	321	5			
1	L	203	Total	C	N	O	S	0	0	0
			1527	951	256	315	5			

- Molecule 2 is a protein called anti-PDGF-BB antibody - Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1621	1031	268	315	7			
2	H	204	Total	C	N	O	S	0	0	0
			1549	988	257	297	7			

- Molecule 3 is a protein called Platelet-derived growth factor subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	92	Total	C	N	O	S	0	0	0
			740	460	142	129	9			
3	D	96	Total	C	N	O	S	0	0	0
			769	479	146	135	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	EXPRESSION TAG	UNP P01127
D	0	MET	-	EXPRESSION TAG	UNP P01127

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		

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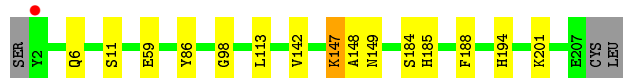
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	95	Total 95	O 95	0	0
4	C	16	Total 16	O 16	0	0
4	D	22	Total 22	O 22	0	0
4	H	63	Total 63	O 63	0	0
4	L	50	Total 50	O 50	0	0

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.

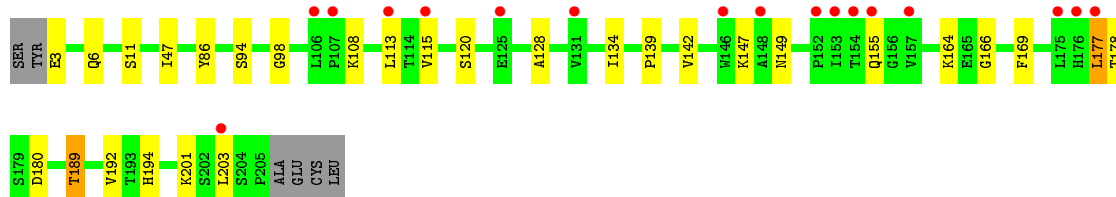
- Molecule 1: anti-PDGF-BB antibody - Light Chain

Chain A: 




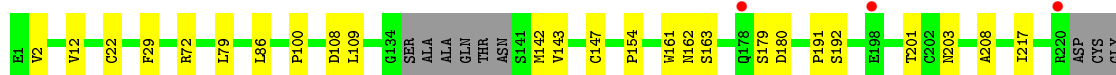
- Molecule 1: anti-PDGF-BB antibody - Light Chain

Chain L: 




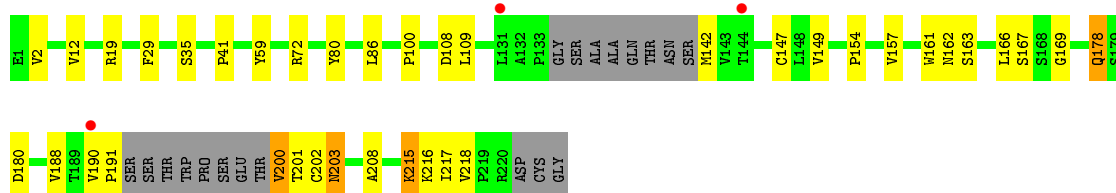
- Molecule 2: anti-PDGF-BB antibody - Heavy chain

Chain B: 



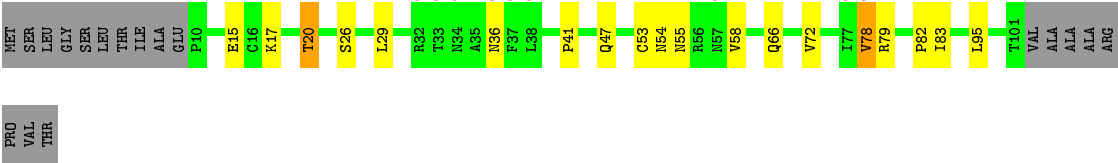
- Molecule 2: anti-PDGF-BB antibody - Heavy chain

Chain H: 



- Molecule 3: Platelet-derived growth factor subunit B

Chain C: 



● Molecule 3: Platelet-derived growth factor subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.15Å 68.47Å 95.25Å 90.00° 97.56° 90.00°	Depositor
Resolution (Å)	69.64 – 2.30 69.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (69.64-2.30) 99.4 (69.64-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.211 , 0.247 0.224 , 0.254	Depositor DCC
R_{free} test set	2612 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8086	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.44	0/1593	0.69	0/2176
1	L	0.44	0/1566	0.69	0/2139
2	B	0.43	0/1665	0.72	0/2275
2	H	0.45	0/1589	0.74	0/2168
3	C	0.43	0/751	0.68	0/1013
3	D	0.44	0/780	0.77	0/1054
All	All	0.44	0/7944	0.71	0/10825

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	1553	0	1469	7	0
1	L	1527	0	1449	12	0
2	B	1621	0	1578	15	0
2	H	1549	0	1520	24	0
3	C	740	0	766	18	0
3	D	769	0	796	12	0
4	A	81	0	0	1	0
4	B	95	0	0	0	0
4	C	16	0	0	0	0
4	D	22	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	63	0	0	0	0
4	L	50	0	0	1	0
All	All	8086	0	7578	84	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 (84) 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:L:147:LYS:HB2	1:L:189:THR:HG22	1.58	0.86
2:H:200:VAL:HG12	2:H:217:ILE:HD13	1.57	0.84
2:H:200:VAL:O	2:H:217:ILE:N	2.15	0.77
2:H:163:SER:H	2:H:203:ASN:HD21	1.30	0.77
2:H:200:VAL:HG12	2:H:217:ILE:CD1	2.17	0.75
3:C:26:SER:HB3	3:C:29:LEU:HD13	1.67	0.74
3:C:54:ASN:OD1	3:D:40:TRP:HH2	1.72	0.73
2:H:201:THR:OG1	2:H:216:LYS:HG2	1.92	0.69
2:H:100:PRO:HD3	2:H:108:ASP:HB2	1.75	0.69
2:B:162:ASN:ND2	2:B:201:THR:H	1.91	0.68
1:L:115:VAL:HG12	1:L:203:LEU:HD11	1.76	0.68
2:B:163:SER:H	2:B:203:ASN:HD21	1.43	0.67
3:C:53:CYS:HB3	3:C:58:VAL:HG23	1.75	0.67
1:L:164:LYS:HG2	1:L:169:PHE:CE1	2.29	0.67
2:B:100:PRO:HD3	2:B:108:ASP:HB2	1.77	0.66
2:H:162:ASN:HB2	2:H:166:LEU:CD1	2.26	0.66
1:L:113:LEU:HB2	1:L:201:LYS:HG3	1.78	0.65
1:A:113:LEU:HB2	1:A:201:LYS:HG3	1.77	0.65
1:L:3:GLU:HG3	4:L:335:HOH:O	1.96	0.65
2:H:2:VAL:HG22	2:H:109:LEU:HD22	1.79	0.64
2:H:200:VAL:O	2:H:216:LYS:HA	1.98	0.63
3:C:66:GLN:HB2	3:C:95:LEU:HD11	1.82	0.61
2:H:200:VAL:CG1	2:H:217:ILE:HD13	2.30	0.61
2:B:162:ASN:HD21	2:B:201:THR:H	1.51	0.58
2:B:163:SER:H	2:B:203:ASN:ND2	2.02	0.57
3:C:20:THR:CG2	3:C:47:GLN:HE22	2.17	0.57
3:D:58:VAL:HG11	3:D:99:CYS:HB3	1.87	0.56
3:C:20:THR:HG23	3:C:47:GLN:HE22	1.70	0.56
3:D:7:ILE:HG22	3:D:8:ALA:C	2.25	0.55
3:C:36:ASN:HB3	3:C:78:VAL:HG22	1.89	0.55
2:B:2:VAL:CG1	2:B:109:LEU:HD22	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:201:THR:HG23	2:H:215:LYS:C	2.28	0.54
3:C:79:ARG:HD2	3:C:83:ILE:HD12	1.90	0.53
3:D:66:GLN:HB2	3:D:95:LEU:HD11	1.91	0.52
1:L:108:LYS:HG2	1:L:139:PRO:HD3	1.92	0.51
3:D:27:ARG:HD3	3:D:35:ALA:HB1	1.93	0.51
2:H:142:MET:SD	2:H:191:PRO:HB3	2.51	0.51
2:H:166:LEU:HD12	2:H:166:LEU:N	2.25	0.50
1:L:134:ILE:HG12	1:L:192:VAL:HG21	1.92	0.50
2:H:154:PRO:HD2	2:H:208:ALA:CB	2.43	0.49
3:C:66:GLN:HB2	3:C:95:LEU:CD1	2.43	0.48
1:L:178:THR:HG22	1:L:180:ASP:H	1.79	0.48
1:L:142:VAL:HG12	1:L:194:HIS:HB2	1.95	0.48
1:A:147:LYS:O	1:A:188:PHE:HA	2.13	0.48
3:D:7:ILE:HB	3:D:8:ALA:HA	1.96	0.47
2:B:154:PRO:HD2	2:B:208:ALA:CB	2.43	0.47
1:A:6:GLN:HE21	1:A:98:GLY:HA3	1.79	0.47
1:L:128:ALA:HB3	1:L:177:LEU:HD12	1.95	0.47
1:A:148:ALA:HB1	1:A:185:HIS:CD2	2.50	0.47
2:H:163:SER:H	2:H:203:ASN:ND2	2.07	0.47
2:B:143:VAL:HG23	2:B:192:SER:HA	1.96	0.47
1:A:59:GLU:HG2	4:A:379:HOH:O	2.16	0.46
2:B:161:TRP:HZ3	2:B:217:ILE:HD13	1.81	0.46
1:A:142:VAL:HG12	1:A:194:HIS:HB2	1.97	0.46
3:C:82:PRO:HD3	2:H:59:TYR:CD1	2.50	0.46
1:L:6:GLN:HE21	1:L:98:GLY:HA3	1.80	0.46
2:H:12:VAL:HG11	2:H:86:LEU:HD13	1.99	0.45
2:B:22:CYS:HB3	2:B:79:LEU:HB3	1.99	0.44
2:H:19:ARG:NH1	2:H:80:TYR:CD2	2.86	0.44
3:D:56:ARG:HG3	4:D:220:HOH:O	2.17	0.44
3:D:41:PRO:HD2	3:D:72:VAL:HG12	2.00	0.44
2:B:142:MET:HG2	2:B:191:PRO:HA	1.99	0.44
2:B:161:TRP:HZ3	2:B:217:ILE:CD1	2.31	0.44
1:A:6:GLN:HE22	1:A:86:TYR:HA	1.83	0.44
3:D:37:PHE:CD1	3:D:74:LYS:HG3	2.53	0.43
3:C:36:ASN:HB3	3:C:78:VAL:CG2	2.48	0.43
1:L:6:GLN:HE22	1:L:86:TYR:HA	1.83	0.43
3:C:53:CYS:HB3	3:C:58:VAL:CG2	2.48	0.42
3:C:54:ASN:OD1	3:D:40:TRP:CH2	2.62	0.42
3:C:53:CYS:CB	3:C:58:VAL:HG23	2.45	0.42
2:B:12:VAL:HG11	2:B:86:LEU:HD13	2.02	0.42
2:B:2:VAL:HG12	2:B:109:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:ASN:HB2	3:C:58:VAL:HG22	2.02	0.42
2:H:162:ASN:HB2	2:H:166:LEU:HD11	2.02	0.42
3:C:41:PRO:HD2	3:C:72:VAL:HG12	2.02	0.41
3:C:54:ASN:HA	3:D:40:TRP:CZ3	2.55	0.41
2:H:161:TRP:HZ3	2:H:217:ILE:HD13	1.85	0.41
3:D:81:LYS:NZ	4:D:203:HOH:O	2.53	0.41
2:H:149:VAL:HG11	2:H:157:VAL:HG21	2.03	0.41
2:H:29:PHE:O	2:H:72:ARG:NH1	2.53	0.41
3:C:26:SER:O	3:C:29:LEU:HB2	2.20	0.41
2:H:169:GLY:O	2:H:188:VAL:HA	2.21	0.41
2:H:200:VAL:HG12	2:H:217:ILE:HB	2.04	0.40
2:B:29:PHE:O	2:B:72:ARG:NH1	2.54	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	204/209 (98%)	195 (96%)	8 (4%)	1 (0%)	32	39
1	L	201/209 (96%)	195 (97%)	4 (2%)	2 (1%)	18	20
2	B	210/223 (94%)	206 (98%)	4 (2%)	0	100	100
2	H	198/223 (89%)	192 (97%)	4 (2%)	2 (1%)	18	20
3	C	90/110 (82%)	88 (98%)	1 (1%)	1 (1%)	17	18
3	D	94/110 (86%)	88 (94%)	4 (4%)	2 (2%)	8	6
All	All	997/1084 (92%)	964 (97%)	25 (2%)	8 (1%)	22	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	178	GLN

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Mol	Chain	Res	Type
3	C	78	VAL
3	D	36	ASN
3	D	78	VAL
2	H	41	PRO
1	A	149	ASN
1	L	149	ASN
1	L	166	GLY

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	178/181 (98%)	175 (98%)	3 (2%)	66	81
1	L	176/181 (97%)	169 (96%)	7 (4%)	36	50
2	B	182/188 (97%)	179 (98%)	3 (2%)	68	82
2	H	173/188 (92%)	162 (94%)	11 (6%)	20	27
3	C	86/99 (87%)	83 (96%)	3 (4%)	41	56
3	D	89/99 (90%)	86 (97%)	3 (3%)	42	57
All	All	884/936 (94%)	854 (97%)	30 (3%)	42	57

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	147	LYS
1	A	184	SER
2	B	147	CYS
2	B	179	SER
2	B	180	ASP
3	C	15	GLU
3	C	17	LYS
3	C	20	THR
3	D	17	LYS
3	D	30	ILE

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Mol	Chain	Res	Type
3	D	90	THR
2	H	35	SER
2	H	147	CYS
2	H	167	SER
2	H	178	GLN
2	H	180	ASP
2	H	190	VAL
2	H	200	VAL
2	H	202	CYS
2	H	203	ASN
2	H	215	LYS
2	H	218	VAL
1	L	11	SER
1	L	47	ILE
1	L	94	SER
1	L	120	SER
1	L	155	GLN
1	L	177	LEU
1	L	189	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
2	B	3	GLN
2	B	162	ASN
2	B	203	ASN
3	C	47	GLN
2	H	3	GLN
2	H	99	HIS
2	H	203	ASN
1	L	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	206/209 (98%)	0.14	1 (0%) 90 93	36, 53, 76, 108	0
1	L	203/209 (97%)	0.59	17 (8%) 12 16	36, 66, 104, 116	0
2	B	214/223 (95%)	0.16	3 (1%) 75 80	37, 52, 70, 136	0
2	H	204/223 (91%)	0.39	3 (1%) 74 78	36, 63, 110, 160	0
3	C	92/110 (83%)	0.59	9 (9%) 8 11	49, 73, 104, 117	0
3	D	96/110 (87%)	1.02	15 (15%) 2 3	59, 84, 128, 141	0
All	All	1015/1084 (93%)	0.41	48 (4%) 32 39	36, 60, 106, 160	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	29	LEU	10.2
3	D	30	ILE	9.3
3	D	35	ALA	9.2
1	L	153	ILE	6.6
3	D	32	ARG	4.5
3	D	31	ASP	4.5
1	A	2	TYR	4.3
2	B	220	ARG	4.2
1	L	155	GLN	4.2
3	C	32	ARG	4.1
1	L	154	THR	4.0
1	L	148	ALA	3.9
3	D	77	ILE	3.7
3	D	34	ASN	3.7
1	L	152	PRO	3.6
1	L	146	TRP	3.5
1	L	125	GLU	3.5
3	C	57	ASN	3.4
1	L	106	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
3	D	102	VAL	3.2
3	D	36	ASN	3.2
2	H	190	VAL	3.1
2	H	131	LEU	3.0
3	D	71	GLN	3.0
3	C	77	ILE	3.0
3	C	34	ASN	2.9
3	C	37	PHE	2.8
1	L	175	LEU	2.8
1	L	157	VAL	2.8
3	C	36	ASN	2.7
2	B	178	GLN	2.7
1	L	177	LEU	2.6
1	L	115	VAL	2.6
3	D	28	ARG	2.5
2	H	144	THR	2.5
3	D	66	GLN	2.5
1	L	107	PRO	2.5
1	L	176	HIS	2.5
3	D	23	PHE	2.4
1	L	113	LEU	2.3
2	B	198	GLU	2.3
1	L	131	VAL	2.3
3	C	33	THR	2.3
3	D	75	ILE	2.2
1	L	203	LEU	2.2
3	C	38	LEU	2.1
3	C	78	VAL	2.0
3	D	27	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.