



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:17 AM UTC

PDB ID : 4QCI / pdb_00004qci
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

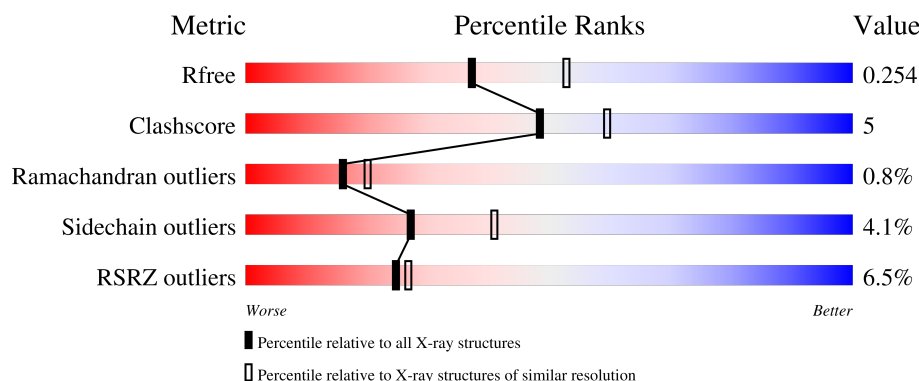
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

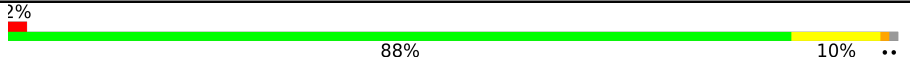
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of 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 $\leq 5\%$. 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	15% 65% 20% • 13%

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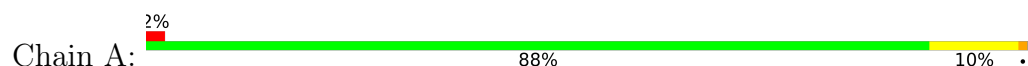
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	95	Total 95	O 95	0	0
4	C	16	Total 16	O 16	0	0
4	D	22	Total 22	O 22	0	0
4	H	63	Total 63	O 63	0	0
4	L	50	Total 50	O 50	0	0

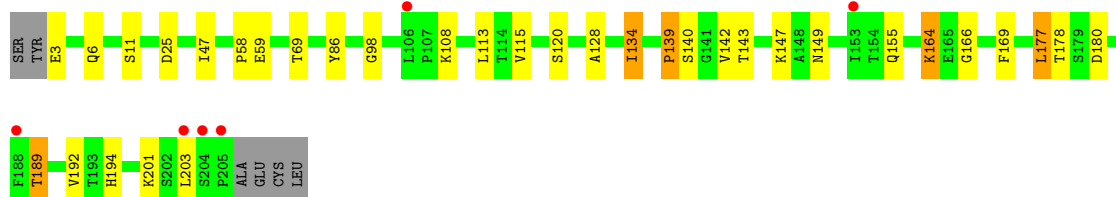
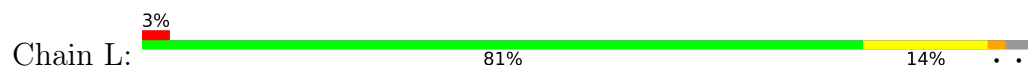
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

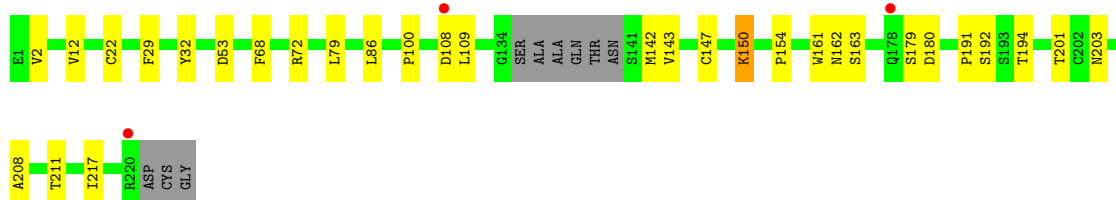
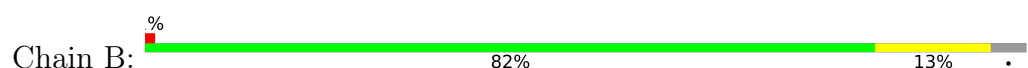
- Molecule 1: anti-PDGF-BB antibody - Light Chain



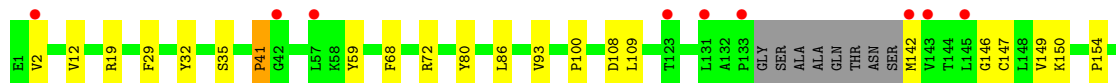
- Molecule 1: anti-PDGF-BB antibody - Light Chain

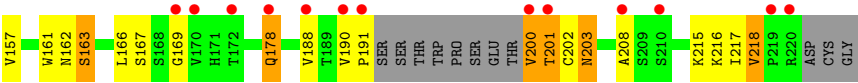


- Molecule 2: anti-PDGF-BB antibody - Heavy chain

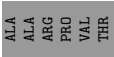
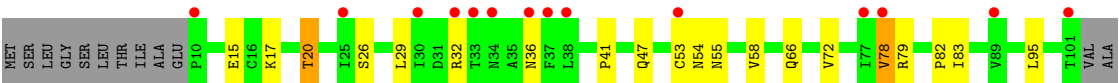


- Molecule 2: anti-PDGF-BB antibody - Heavy chain

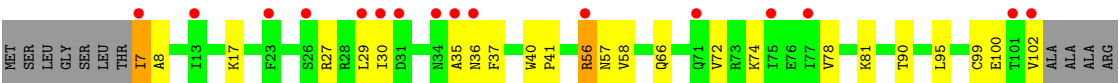




● Molecule 3: Platelet-derived growth factor subunit B



● 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 (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.9	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	0.74	0/1593	1.21	7/2176 (0.3%)
1	L	0.75	0/1566	1.26	9/2139 (0.4%)
2	B	0.72	0/1665	1.19	6/2275 (0.3%)
2	H	0.76	0/1589	1.18	8/2168 (0.4%)
3	C	0.76	0/751	1.21	2/1013 (0.2%)
3	D	0.77	0/780	1.35	8/1054 (0.8%)
All	All	0.75	0/7944	1.22	40/10825 (0.4%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	29	LEU	N-CA-C	7.74	119.36	111.07
2	B	180	ASP	N-CA-C	-7.72	103.20	114.39
1	A	68	ASN	CA-CB-CG	6.70	119.30	112.60
1	L	59	GLU	CA-C-N	6.64	129.48	120.38
1	L	59	GLU	C-N-CA	6.64	129.48	120.38
1	L	139	PRO	CA-C-N	6.34	128.77	120.28
1	L	139	PRO	C-N-CA	6.34	128.77	120.28
2	H	201	THR	N-CA-C	6.25	119.76	108.69
1	A	94	SER	N-CA-C	6.24	118.88	111.71
3	D	56	ARG	CA-C-N	6.00	128.61	120.38
3	D	56	ARG	C-N-CA	6.00	128.61	120.38
1	L	140	SER	N-CA-C	5.98	117.80	111.28
1	A	93	ASN	CA-CB-CG	5.97	118.57	112.60
3	D	7	ILE	CA-C-N	5.92	132.35	121.70
3	D	7	ILE	C-N-CA	5.92	132.35	121.70
2	H	68	PHE	CA-CB-CG	5.79	119.59	113.80
2	H	41	PRO	N-CA-C	5.77	124.36	112.47
2	B	68	PHE	CA-CB-CG	5.65	119.45	113.80
3	D	100	GLU	N-CA-C	5.61	118.62	109.59
2	H	218	VAL	CB-CA-C	5.60	116.47	110.53
1	L	58	PRO	CA-C-N	5.59	128.54	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	58	PRO	C-N-CA	5.59	128.54	120.38
2	H	146	GLY	N-CA-C	5.54	119.29	111.42
2	B	150	LYS	N-CA-C	5.50	117.86	108.90
1	A	140	SER	N-CA-C	5.38	119.10	112.54
3	D	57	ASN	CA-C-N	5.33	128.76	120.34
3	D	57	ASN	C-N-CA	5.33	128.76	120.34
1	A	184	SER	N-CA-C	5.23	116.98	111.28
1	L	69	THR	N-CA-C	5.19	117.54	108.76
2	B	211	THR	CB-CA-C	5.14	118.18	109.50
1	A	150	GLY	CA-C-N	5.11	127.52	120.67
1	A	150	GLY	C-N-CA	5.11	127.52	120.67
1	L	25	ASP	CA-CB-CG	5.11	117.70	112.60
2	H	32	TYR	N-CA-C	5.08	117.68	109.40
2	H	93	VAL	N-CA-C	-5.07	101.28	108.58
2	B	32	TYR	N-CA-C	5.05	117.63	109.40
3	C	32	ARG	CA-C-N	5.04	127.04	120.28
3	C	32	ARG	C-N-CA	5.04	127.04	120.28
2	B	53	ASP	CA-CB-CG	5.01	117.61	112.60
2	H	150	LYS	N-CA-C	5.00	117.64	109.59

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
3:D:7:ILE:HG22	3:D:8:ALA:C	2.25	0.61
2:H:201:THR:HG23	2:H:215:LYS:C	2.28	0.58
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:C:36:ASN:HB3	3:C:78:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:VAL:CG1	2:B:109:LEU:HD22	2.37	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:41:PRO:HD2	3:D:72:VAL:HG12	2.00	0.44
3:D:56:ARG:HG3	4:D:220:HOH:O	2.17	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:29:PHE:O	2:H:72:ARG:NH1	2.53	0.41
2:H:149:VAL:HG11	2:H:157:VAL:HG21	2.03	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%)	24	31
1	L	201/209 (96%)	195 (97%)	4 (2%)	2 (1%)	12	15
2	B	210/223 (94%)	206 (98%)	4 (2%)	0	100	100
2	H	198/223 (89%)	192 (97%)	4 (2%)	2 (1%)	12	15
3	C	90/110 (82%)	88 (98%)	1 (1%)	1 (1%)	11	13
3	D	94/110 (86%)	88 (94%)	4 (4%)	2 (2%)	5	4
All	All	997/1084 (92%)	964 (97%)	25 (2%)	8 (1%)	16	20

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%)	172 (97%)	6 (3%)	32	49
1	L	176/181 (97%)	167 (95%)	9 (5%)	21	32
2	B	182/188 (97%)	178 (98%)	4 (2%)	45	65
2	H	173/188 (92%)	163 (94%)	10 (6%)	18	26
3	C	86/99 (87%)	83 (96%)	3 (4%)	32	48
3	D	89/99 (90%)	85 (96%)	4 (4%)	24	37
All	All	884/936 (94%)	848 (96%)	36 (4%)	27	41

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	55	SER
1	A	143	THR
1	A	147	LYS
1	A	163	THR
1	A	184	SER
2	B	147	CYS
2	B	150	LYS
2	B	179	SER
2	B	194	THR
3	C	15	GLU

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Mol	Chain	Res	Type
3	C	17	LYS
3	C	20	THR
3	D	17	LYS
3	D	30	ILE
3	D	90	THR
3	D	102	VAL
2	H	35	SER
2	H	147	CYS
2	H	163	SER
2	H	167	SER
2	H	178	GLN
2	H	190	VAL
2	H	200	VAL
2	H	202	CYS
2	H	203	ASN
2	H	218	VAL
1	L	11	SER
1	L	47	ILE
1	L	120	SER
1	L	134	ILE
1	L	143	THR
1	L	155	GLN
1	L	164	LYS
1	L	177	LEU
1	L	189	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	41	GLN
1	A	68	ASN
1	A	136	ASN
1	A	191	GLN
2	B	3	GLN
2	B	112	GLN
2	B	162	ASN
2	B	171	HIS
2	B	203	ASN
3	C	47	GLN
3	C	54	ASN
3	D	34	ASN

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Mol	Chain	Res	Type
3	D	36	ASN
3	D	47	GLN
2	H	3	GLN
2	H	99	HIS
2	H	162	ASN
2	H	203	ASN
1	L	6	GLN
1	L	36	GLN
1	L	68	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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%)	0.22	5 (2%) 59 62	36, 53, 76, 108	0
1	L	203/209 (97%)	0.52	6 (2%) 52 54	36, 66, 104, 116	0
2	B	214/223 (95%)	0.24	3 (1%) 73 75	37, 52, 70, 136	0
2	H	204/223 (91%)	0.74	22 (10%) 11 12	36, 63, 110, 160	0
3	C	92/110 (83%)	1.06	14 (15%) 5 6	49, 73, 104, 117	0
3	D	96/110 (87%)	1.28	16 (16%) 4 5	59, 84, 128, 141	0
All	All	1015/1084 (93%)	0.56	66 (6%) 25 27	36, 60, 106, 160	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	30	ILE	4.9
3	D	29	LEU	4.7
3	D	35	ALA	4.1
1	A	2	TYR	3.9
3	C	10	PRO	3.6
3	C	101	THR	3.6
3	C	36	ASN	3.5
3	C	77	ILE	3.4
2	H	133	PRO	3.4
1	L	205	PRO	3.4
2	H	191	PRO	3.3
2	H	142	MET	3.2
3	D	71	GLN	3.2
3	D	102	VAL	3.0
3	C	37	PHE	3.0
1	L	153	ILE	3.0
2	H	201	THR	2.9
3	C	38	LEU	2.9
2	H	145	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	123	THR	2.8
1	L	106	LEU	2.8
2	H	208	ALA	2.8
3	D	77	ILE	2.7
2	B	220	ARG	2.7
3	D	31	ASP	2.7
3	D	101	THR	2.7
2	H	143	VAL	2.7
3	C	33	THR	2.6
2	H	200	VAL	2.5
2	B	178	GLN	2.5
2	H	219	PRO	2.5
2	H	210	SER	2.4
2	H	170	VAL	2.4
2	H	190	VAL	2.4
1	A	92	HIS	2.4
1	L	188	PHE	2.4
3	C	25	ILE	2.4
3	D	75	ILE	2.4
2	H	188	VAL	2.4
2	B	108	ASP	2.3
3	C	34	ASN	2.3
3	D	7	ILE	2.3
2	H	220	ARG	2.3
2	H	57	LEU	2.3
1	A	207	GLU	2.3
3	D	23	PHE	2.3
3	D	13	ILE	2.3
3	C	78	VAL	2.3
3	C	32	ARG	2.3
2	H	178	GLN	2.3
2	H	131	LEU	2.2
2	H	42	GLY	2.2
3	D	56	ARG	2.2
1	A	102	LYS	2.1
2	H	172	THR	2.1
3	D	26	SER	2.1
2	H	169	GLY	2.1
3	C	30	ILE	2.1
2	H	2	VAL	2.1
3	C	89	VAL	2.1
3	C	53	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	107	PRO	2.1
1	L	203	LEU	2.0
3	D	34	ASN	2.0
1	L	204	SER	2.0
3	D	36	ASN	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 oligosaccharides 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.