



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:33 AM UTC

PDB ID : 8YX1 / pdb_00008yx1
Title : CD40 in complex with Bleselumab Fab
Authors : Caaveiro, J.M.M.; Fernandez-Perez, J.; Tsumoto, K.
Deposited on : 2024-04-01
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

<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

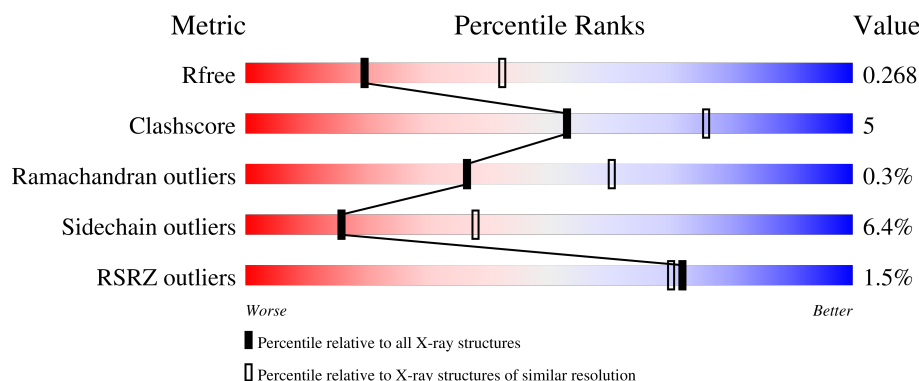
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

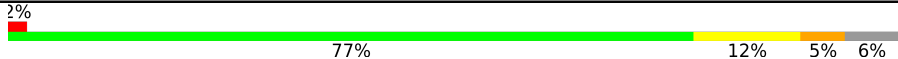
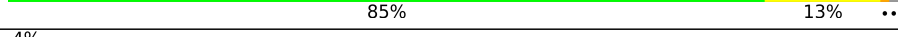
The reported resolution of this entry is 2.70 Å.

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	229	 2% 77% 12% 5% 6%
1	H	229	 79% 14% 6%
2	B	213	 83% 15% 2% 2%
2	L	213	 85% 13% 2% 2%
3	C	179	 4% 68% 19% 1% 11%

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Mol	Chain	Length	Quality of chain
3	R	179	% 64% 20% • 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8837 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 Bleselumab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	216	Total	C	N	O	S	0	0	0
			1612	1029	265	314	4			
1	A	216	Total	C	N	O	S	0	0	0
			1612	1029	265	314	4			

- Molecule 2 is a protein called Bleselumab, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1609	1007	270	328	4			
2	B	211	Total	C	N	O	S	0	0	0
			1609	1007	270	328	4			

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	150	Total	C	N	O	S	0	0	0
			1147	697	197	234	19			
3	C	160	Total	C	N	O	S	0	0	0
			1223	745	209	249	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	174	HIS	-	expression tag	UNP P25942
R	175	HIS	-	expression tag	UNP P25942
R	176	HIS	-	expression tag	UNP P25942
R	177	HIS	-	expression tag	UNP P25942
R	178	HIS	-	expression tag	UNP P25942
R	179	HIS	-	expression tag	UNP P25942
C	174	HIS	-	expression tag	UNP P25942
C	175	HIS	-	expression tag	UNP P25942

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Chain	Residue	Modelled	Actual	Comment	Reference
C	176	HIS	-	expression tag	UNP P25942
C	177	HIS	-	expression tag	UNP P25942
C	178	HIS	-	expression tag	UNP P25942
C	179	HIS	-	expression tag	UNP P25942

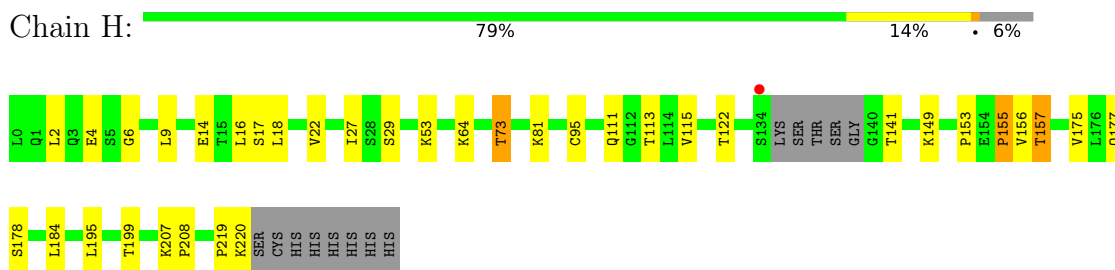
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	11	Total 11	O 11	0	0
4	L	3	Total 3	O 3	0	0
4	R	2	Total 2	O 2	0	0
4	A	4	Total 4	O 4	0	0
4	B	3	Total 3	O 3	0	0
4	C	2	Total 2	O 2	0	0

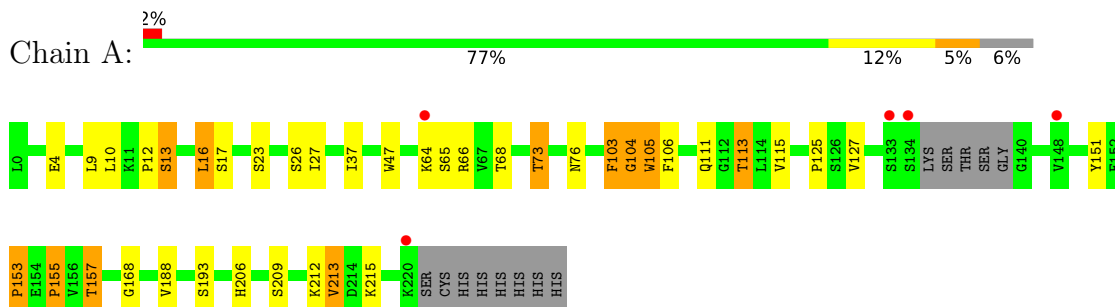
3 Residue-property plots

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.

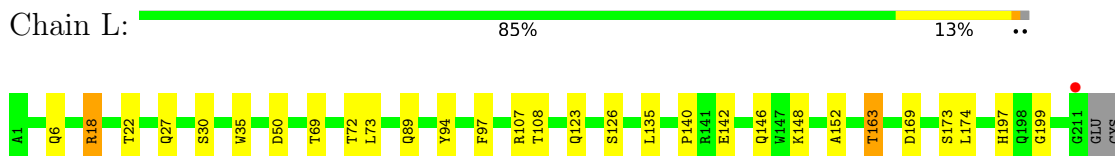
- Molecule 1: Bleselumab, heavy chain



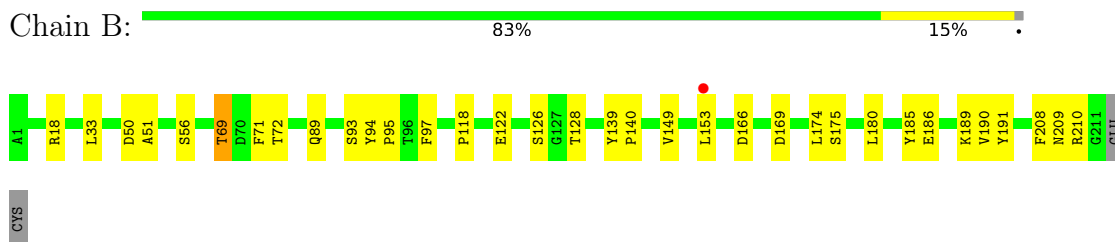
- Molecule 1: Bleselumab, heavy chain



- Molecule 2: Bleselumab, light chain

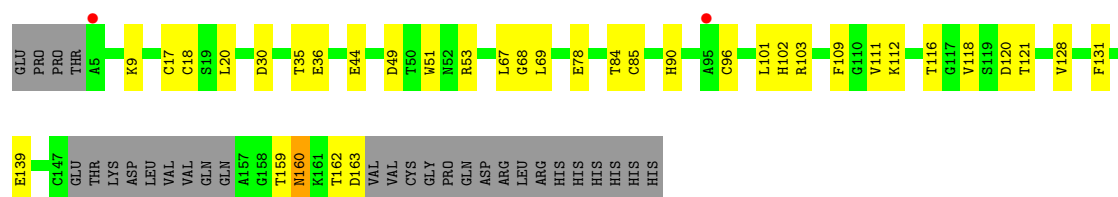


- Molecule 2: Bleselumab, light chain



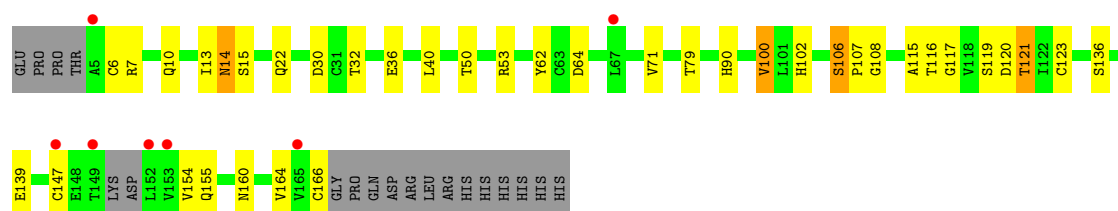
- Molecule 3: Tumor necrosis factor receptor superfamily member 5

Chain R:  %



- Molecule 3: Tumor necrosis factor receptor superfamily member 5

Chain C:  %



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.56Å 116.00Å 121.65Å 90.00° 91.71° 90.00°	Depositor
Resolution (Å)	45.56 – 2.70 45.56 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.56-2.70) 99.9 (45.56-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.204 , 0.265 0.209 , 0.268	Depositor DCC
R_{free} test set	1858 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.016 for -h,-l,-k 0.037 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8837	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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	0.59	0/1656	1.11	7/2263 (0.3%)
1	H	0.61	0/1656	1.11	4/2263 (0.2%)
2	B	0.56	0/1643	1.09	2/2231 (0.1%)
2	L	0.59	0/1643	1.10	6/2231 (0.3%)
3	C	0.53	0/1248	1.08	5/1693 (0.3%)
3	R	0.57	0/1172	1.17	10/1588 (0.6%)
All	All	0.58	0/9018	1.11	34/12269 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	1
2	L	0	2
All	All	0	6

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	157	THR	CA-CB-OG1	-8.84	96.34	109.60
1	H	73	THR	CA-CB-OG1	-7.11	98.94	109.60
1	A	212	LYS	CB-CA-C	-7.08	101.88	110.94
3	R	163	ASP	CA-CB-CG	6.93	119.53	112.60
2	L	27	GLN	CB-CA-C	-6.92	95.58	110.45
3	R	35	THR	CA-CB-OG1	-6.92	99.23	109.60
1	A	157	THR	CA-CB-OG1	-6.40	100.00	109.60
2	L	94	TYR	CB-CA-C	6.24	119.41	109.62
3	R	109	PHE	CA-CB-CG	5.98	119.78	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	128	THR	CA-CB-OG1	-5.85	100.82	109.60
1	H	155	PRO	N-CA-CB	-5.79	96.22	102.60
2	B	69	THR	CA-CB-OG1	-5.79	100.91	109.60
2	L	142	GLU	CB-CG-CD	5.65	122.21	112.60
1	A	155	PRO	N-CA-CB	-5.54	96.50	102.60
3	R	120	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	73	THR	CA-CB-OG1	-5.46	101.41	109.60
3	R	17	CYS	CB-CA-C	5.46	120.58	111.30
3	C	121	THR	CA-CB-OG1	-5.41	101.49	109.60
3	C	6	CYS	CB-CA-C	5.37	119.99	110.16
1	A	106	PHE	N-CA-CB	-5.35	102.14	110.55
2	L	146	GLN	CB-CA-C	5.34	118.87	109.80
3	C	30	ASP	CA-CB-CG	5.30	117.90	112.60
3	R	30	ASP	CA-CB-CG	5.28	117.88	112.60
3	C	22	GLN	CB-CA-C	-5.25	99.81	109.51
3	R	18	CYS	CB-CA-C	-5.18	100.75	109.50
1	A	4	GLU	CB-CA-C	5.17	118.27	109.53
3	R	49	ASP	CA-CB-CG	5.15	117.75	112.60
2	L	169	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	113	THR	CA-CB-OG1	-5.10	101.95	109.60
1	H	141	THR	CA-CB-OG1	-5.09	101.96	109.60
3	C	32	THR	CA-CB-OG1	-5.09	101.96	109.60
2	L	72	THR	CA-CB-OG1	-5.06	102.02	109.60
3	R	36	GLU	CB-CG-CD	5.05	121.18	112.60
3	R	116	THR	CA-CB-OG1	5.01	117.11	109.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	PHE	Peptide
1	A	104	GLY	Peptide
1	A	66	ARG	Sidechain
2	B	18	ARG	Sidechain
2	L	107	ARG	Sidechain
2	L	18	ARG	Sidechain

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	1612	0	1601	15	0
1	H	1612	0	1601	15	0
2	B	1609	0	1567	19	0
2	L	1609	0	1567	12	0
3	C	1223	0	1117	20	0
3	R	1147	0	1038	11	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	H	11	0	0	0	0
4	L	3	0	0	0	0
4	R	2	0	0	0	0
All	All	8837	0	8491	86	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 (86) 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:A:47:TRP:CE3	2:B:95:PRO:HD2	2.22	0.74
2:B:185:TYR:O	2:B:191:TYR:OH	2.13	0.67
1:A:16:LEU:HD12	1:A:115:VAL:HG11	1.77	0.65
3:C:155:GLN:H	3:C:166:CYS:HA	1.63	0.62
3:C:164:VAL:HG12	3:C:166:CYS:HB3	1.83	0.61
1:A:103:PHE:HB3	2:B:95:PRO:HG3	1.85	0.59
1:H:2:LEU:CD2	1:H:22:VAL:HG22	2.33	0.58
3:R:9:LYS:HD2	3:R:51:TRP:CE2	2.38	0.57
2:L:140:PRO:O	2:L:197:HIS:HE1	1.87	0.57
3:C:90:HIS:HA	3:C:117:GLY:HA2	1.86	0.57
2:B:50:ASP:O	2:B:51:ALA:HB3	2.03	0.57
3:R:9:LYS:HD2	3:R:51:TRP:CD2	2.39	0.56
1:A:9:LEU:HB2	1:A:153:PRO:HG3	1.89	0.54
3:R:9:LYS:HA	3:R:20:LEU:HD12	1.91	0.53
1:H:184:LEU:HD12	1:H:184:LEU:C	2.35	0.52
2:B:118:PRO:HB3	2:B:208:PHE:CZ	2.45	0.52
1:A:37:ILE:HD13	1:A:47:TRP:HA	1.92	0.50
3:C:90:HIS:CD2	3:C:100:VAL:O	2.64	0.50
3:C:108:GLY:HA2	3:C:160:ASN:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:GLN:HB3	2:B:97:PHE:CD2	2.47	0.49
3:C:14:ASN:ND2	3:C:15:SER:H	2.09	0.49
2:L:148:LYS:HA	2:L:152:ALA:O	2.12	0.49
2:B:174:LEU:HD23	2:B:175:SER:N	2.28	0.49
2:L:135:LEU:HB2	2:L:174:LEU:HB3	1.95	0.49
3:C:13:ILE:O	3:C:14:ASN:HB3	2.13	0.48
2:L:6:GLN:HA	2:L:22:THR:O	2.14	0.48
3:R:160:ASN:OD1	3:R:160:ASN:N	2.45	0.48
1:A:12:PRO:O	1:A:13:SER:HB3	2.14	0.48
3:C:14:ASN:HD22	3:C:15:SER:H	1.63	0.47
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.50	0.47
2:L:50:ASP:OD1	3:R:53:ARG:NH2	2.40	0.46
3:C:62:TYR:CD2	3:C:64:ASP:HB2	2.51	0.46
1:H:207:LYS:N	1:H:208:PRO:CD	2.78	0.46
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.51	0.46
3:C:90:HIS:CD2	3:C:102:HIS:CD2	3.04	0.46
2:L:123:GLN:O	2:L:126:SER:OG	2.27	0.45
1:A:27:ILE:HD12	1:A:76:ASN:HA	1.98	0.45
1:A:104:GLY:O	1:A:105:TRP:O	2.33	0.45
1:H:27:ILE:O	1:H:27:ILE:HG22	2.15	0.45
2:L:163:THR:HG22	2:L:173:SER:H	1.82	0.45
3:C:102:HIS:CD2	3:C:115:ALA:HB1	2.51	0.45
3:R:67:LEU:HB2	3:R:69:LEU:CD2	2.47	0.45
1:A:10:LEU:HD11	1:A:16:LEU:HA	1.98	0.45
2:B:93:SER:O	2:B:94:TYR:C	2.60	0.45
3:C:7:ARG:H	3:C:10:GLN:HE21	1.65	0.45
1:H:4:GLU:HG3	1:H:95:CYS:SG	2.57	0.44
2:L:197:HIS:CD2	2:L:199:GLY:H	2.35	0.44
1:H:195:LEU:HD23	1:H:195:LEU:HA	1.88	0.44
3:R:111:VAL:HG23	3:R:139:GLU:O	2.18	0.44
2:B:50:ASP:CG	3:C:53:ARG:HH22	2.25	0.44
3:C:106:SER:HB2	3:C:107:PRO:HD2	1.99	0.44
1:H:18:LEU:HD22	1:H:113:THR:HG21	2.00	0.44
2:B:166:ASP:HB3	2:B:169:ASP:OD1	2.17	0.44
3:C:136:SER:HB3	3:C:139:GLU:HB2	1.99	0.44
1:A:12:PRO:O	1:A:13:SER:CB	2.65	0.44
2:B:118:PRO:HB3	2:B:208:PHE:CE2	2.53	0.43
1:H:149:LYS:HE3	1:H:177:GLN:HE22	1.83	0.43
1:H:9:LEU:HB2	1:H:153:PRO:HG3	2.01	0.43
3:R:67:LEU:HB2	3:R:69:LEU:HD23	1.99	0.43
3:C:90:HIS:CE1	3:C:100:VAL:HG13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:HIS:CD2	3:C:115:ALA:CB	3.02	0.43
2:B:190:VAL:HG22	2:B:209:ASN:OD1	2.18	0.43
2:L:89:GLN:HB3	2:L:97:PHE:CD2	2.54	0.43
1:A:125:PRO:HB3	1:A:151:TYR:HB3	2.01	0.43
1:A:215:LYS:NZ	2:B:122:GLU:OE1	2.53	0.42
2:B:50:ASP:OD1	3:C:53:ARG:NH2	2.50	0.42
1:A:127:VAL:HG21	1:A:213:VAL:HG22	2.00	0.42
1:H:156:VAL:HG23	1:H:184:LEU:HD21	2.02	0.42
3:R:68:GLY:O	3:R:85:CYS:HA	2.18	0.42
2:L:135:LEU:N	2:L:135:LEU:HD12	2.34	0.42
2:B:139:TYR:CG	2:B:140:PRO:HA	2.55	0.42
1:H:16:LEU:O	1:H:81:LYS:HA	2.20	0.42
2:B:149:VAL:HG13	2:B:191:TYR:CE1	2.55	0.42
3:C:90:HIS:CD2	3:C:102:HIS:HD2	2.38	0.42
1:H:219:PRO:O	1:H:220:LYS:C	2.62	0.41
1:H:6:GLY:HA3	1:H:18:LEU:HD23	2.01	0.41
1:H:16:LEU:HD21	1:H:18:LEU:CD1	2.50	0.41
2:B:50:ASP:O	2:B:51:ALA:CB	2.67	0.41
3:R:131:PHE:HA	3:R:160:ASN:O	2.21	0.41
3:C:90:HIS:CE1	3:C:120:ASP:CG	2.98	0.41
1:H:16:LEU:HD12	1:H:115:VAL:HG11	2.02	0.41
2:L:174:LEU:C	2:L:174:LEU:HD23	2.45	0.41
2:B:186:GLU:O	2:B:210:ARG:NH2	2.54	0.41
1:A:206:HIS:ND1	1:A:209:SER:HB3	2.36	0.40
3:R:90:HIS:ND1	3:R:102:HIS:HD2	2.19	0.40
1:A:168:GLY:O	1:A:188:VAL:HA	2.22	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	212/229 (93%)	202 (95%)	8 (4%)	2 (1%)	14	35
1	H	212/229 (93%)	200 (94%)	12 (6%)	0	100	100
2	B	209/213 (98%)	198 (95%)	11 (5%)	0	100	100
2	L	209/213 (98%)	199 (95%)	10 (5%)	0	100	100
3	C	156/179 (87%)	148 (95%)	7 (4%)	1 (1%)	21	44
3	R	146/179 (82%)	140 (96%)	5 (3%)	1 (1%)	18	41
All	All	1144/1242 (92%)	1087 (95%)	53 (5%)	4 (0%)	36	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	TRP
3	R	96	CYS
1	A	13	SER
3	C	14	ASN

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	186/198 (94%)	171 (92%)	15 (8%)	11	27
1	H	186/198 (94%)	173 (93%)	13 (7%)	14	34
2	B	183/185 (99%)	176 (96%)	7 (4%)	29	58
2	L	183/185 (99%)	178 (97%)	5 (3%)	39	69
3	C	145/163 (89%)	132 (91%)	13 (9%)	9	23
3	R	135/163 (83%)	123 (91%)	12 (9%)	9	23
All	All	1018/1092 (93%)	953 (94%)	65 (6%)	16	38

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	14	GLU

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Mol	Chain	Res	Type
1	H	17	SER
1	H	29	SER
1	H	53	LYS
1	H	64	LYS
1	H	73	THR
1	H	111	GLN
1	H	122	THR
1	H	155	PRO
1	H	157	THR
1	H	175	VAL
1	H	178	SER
1	H	199	THR
2	L	18	ARG
2	L	30	SER
2	L	69	THR
2	L	108	THR
2	L	163	THR
3	R	44	GLU
3	R	78	GLU
3	R	84	THR
3	R	101	LEU
3	R	103	ARG
3	R	112	LYS
3	R	118	VAL
3	R	121	THR
3	R	128	VAL
3	R	159	THR
3	R	160	ASN
3	R	162	THR
1	A	16	LEU
1	A	17	SER
1	A	23	SER
1	A	26	SER
1	A	64	LYS
1	A	65	SER
1	A	68	THR
1	A	73	THR
1	A	111	GLN
1	A	113	THR
1	A	153	PRO
1	A	155	PRO
1	A	157	THR

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Mol	Chain	Res	Type
1	A	193	SER
1	A	213	VAL
2	B	56	SER
2	B	69	THR
2	B	72	THR
2	B	126	SER
2	B	153	LEU
2	B	180	LEU
2	B	189	LYS
3	C	36	GLU
3	C	40	LEU
3	C	50	THR
3	C	71	VAL
3	C	79	THR
3	C	100	VAL
3	C	106	SER
3	C	116	THR
3	C	119	SER
3	C	121	THR
3	C	123	CYS
3	C	147	CYS
3	C	154	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	111	GLN
1	H	177	GLN
2	L	123	GLN
2	L	159	GLN
2	L	197	HIS
2	L	198	GLN
3	R	102	HIS
1	A	177	GLN
2	B	27	GLN
2	B	198	GLN
3	C	10	GLN
3	C	14	ASN
3	C	16	GLN
3	C	25	GLN
3	C	102	HIS

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Mol	Chain	Res	Type
3	C	155	GLN
3	C	156	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 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	216/229 (94%)	0.06	5 (2%) 61 58	32, 50, 80, 112	0
1	H	216/229 (94%)	-0.32	1 (0%) 87 86	27, 42, 61, 102	0
2	B	211/213 (99%)	-0.14	1 (0%) 87 86	32, 48, 84, 101	0
2	L	211/213 (99%)	-0.25	1 (0%) 87 86	28, 44, 67, 80	0
3	C	160/179 (89%)	0.48	7 (4%) 39 35	41, 67, 98, 114	0
3	R	150/179 (83%)	0.16	2 (1%) 75 73	37, 59, 82, 106	0
All	All	1164/1242 (93%)	-0.03	17 (1%) 72 70	27, 49, 83, 114	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	152	LEU	4.0
1	A	134	SER	3.8
3	C	153	VAL	3.7
3	R	5	ALA	3.5
3	C	149	THR	3.5
2	B	153	LEU	3.1
3	C	67	LEU	2.9
2	L	211	GLY	2.9
3	C	5	ALA	2.9
3	C	147	CYS	2.7
1	A	220	LYS	2.5
3	R	95	ALA	2.3
1	A	64	LYS	2.2
3	C	165	VAL	2.2
1	A	133	SER	2.1
1	H	134	SER	2.0
1	A	148	VAL	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.