



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:24 PM UTC

PDB ID : 4ZS7 / pdb_00004zs7
Title : Structural mimicry of receptor interaction by antagonistic IL-6 antibodies
Authors : Blanchetot, C.; De Jonge, N.; Desmyter, A.; Ongenae, N.; Hofman, E.; Klarenbeek, A.; Sadi, A.; Hultberg, A.; Kretz-Rommel, A.; Spinelli, S.; Loris, R.; Cambillau, C.; de Haard, H.
Deposited on : 2015-05-13
Resolution : 2.93 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

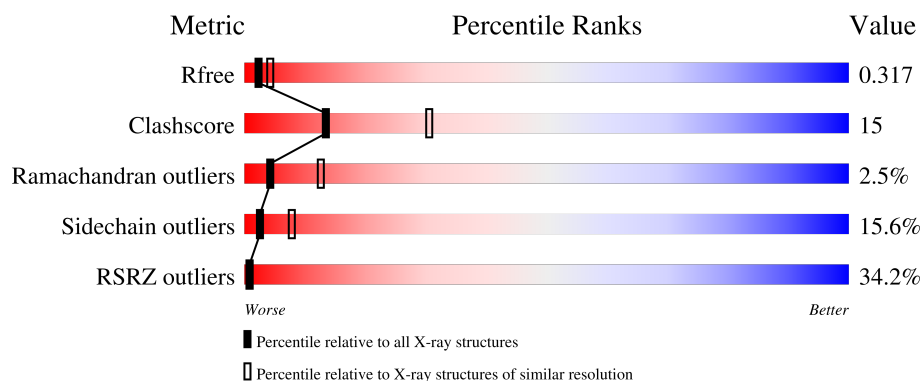
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	171	75% 37% 27% 12% 5% 19%
2	H	222	18% 67% 26% 6%
3	L	216	12% 69% 25% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4454 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 Interleukin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	1	0
			1124	712	193	211	8			

- Molecule 2 is a protein called Llama Fab fragment 68F2 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1678	1062	272	339	5			

- Molecule 3 is a protein called Llama Fab fragment 68F2 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1572	989	264	315	4			

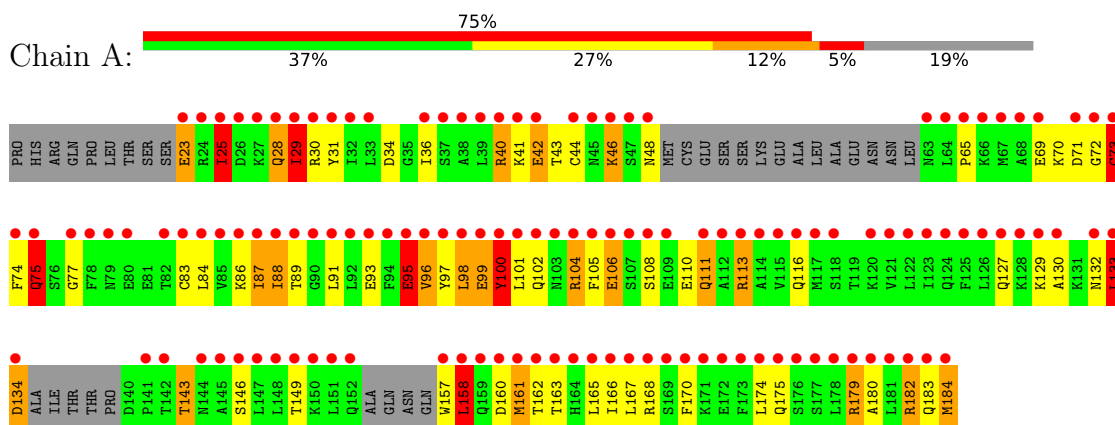
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	H	38	Total	O	0	0
			38	38		
4	L	26	Total	O	0	0
			26	26		

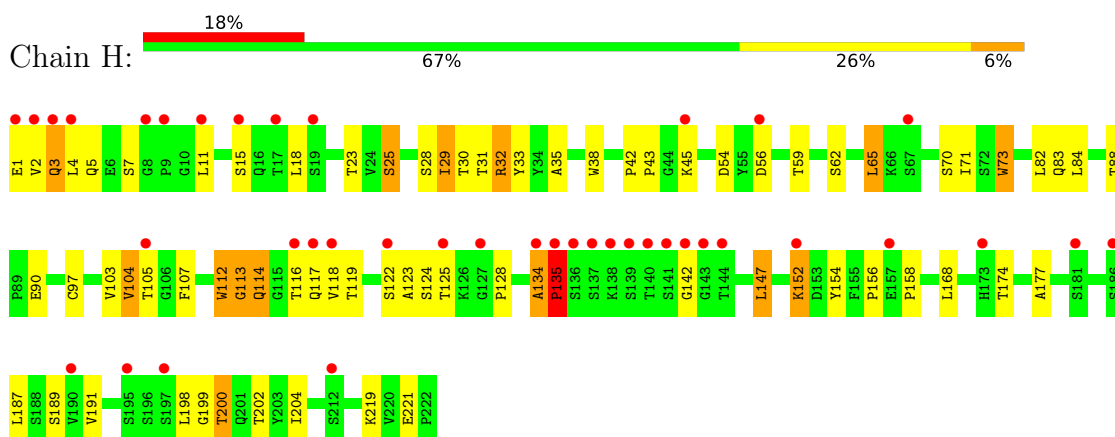
3 Residue-property plots [i](#)

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.

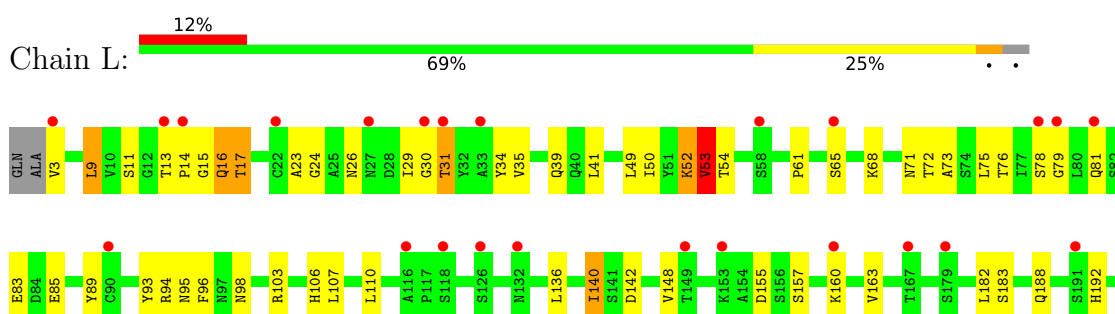
• Molecule 1: Interleukin-6

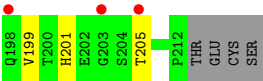


• Molecule 2: Llama Fab fragment 68F2 heavy chain



• Molecule 3: Llama Fab fragment 68F2 light chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	46.55Å 92.86Å 84.63Å 90.00° 103.93° 90.00°	Depositor
Resolution (Å)	44.35 – 2.93 44.35 – 2.93	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.35-2.93) 97.9 (44.35-2.93)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.95Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.261 , 0.293 0.284 , 0.317	Depositor DCC
R_{free} test set	1490 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	1.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	4454	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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	0.82	0/1139	1.69	18/1523 (1.2%)
2	H	0.73	0/1725	1.32	10/2363 (0.4%)
3	L	0.69	0/1611	1.19	6/2204 (0.3%)
All	All	0.74	0/4475	1.38	34/6090 (0.6%)

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
2	H	0	1

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	112	TRP	N-CA-C	-8.15	97.05	110.17
2	H	134	ALA	N-CA-C	7.67	120.63	110.36
1	A	134	ASP	CA-CB-CG	7.39	119.99	112.60
2	H	3	GLN	CA-C-N	7.19	135.03	121.87
2	H	3	GLN	C-N-CA	7.19	135.03	121.87
3	L	16	GLN	CA-C-N	7.13	134.53	121.70
3	L	16	GLN	C-N-CA	7.13	134.53	121.70
2	H	42	PRO	O-C-N	6.61	124.35	121.31
1	A	44	CYS	N-CA-C	-6.51	105.08	113.16
1	A	161	MET	N-CA-C	-6.28	104.44	111.28
3	L	61	PRO	CA-C-N	6.22	128.62	120.28
3	L	61	PRO	C-N-CA	6.22	128.62	120.28
1	A	99	GLU	CA-C-N	6.04	133.07	121.54
1	A	99	GLU	C-N-CA	6.04	133.07	121.54
2	H	113	GLY	N-CA-C	-6.03	95.82	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ILE	CB-CA-C	6.01	116.80	110.91
1	A	143	THR	N-CA-C	-6.00	104.65	111.07
1	A	158	LEU	N-CA-C	-5.96	105.84	113.23
1	A	160	ASP	CA-C-N	5.80	128.05	120.28
1	A	160	ASP	C-N-CA	5.80	128.05	120.28
1	A	111	GLN	N-CA-C	-5.79	104.97	111.28
1	A	96	VAL	CB-CA-C	5.61	116.15	110.65
1	A	77	GLY	N-CA-C	-5.60	107.27	115.72
3	L	31	THR	N-CA-C	5.59	119.58	112.87
2	H	152	LYS	N-CA-C	5.46	118.71	109.76
1	A	160	ASP	N-CA-C	-5.44	106.58	113.43
2	H	5	GLN	N-CA-C	5.38	118.26	109.59
2	H	4	LEU	N-CA-C	-5.37	98.47	107.32
3	L	98	ASN	CA-CB-CG	5.28	117.88	112.60
2	H	135	PRO	N-CA-C	5.16	123.10	112.47
1	A	149	THR	CA-C-N	5.12	127.86	120.38
1	A	149	THR	C-N-CA	5.12	127.86	120.38
1	A	100	TYR	N-CA-C	-5.09	99.97	110.80
1	A	106	GLU	CB-CG-CD	5.01	121.12	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	112	TRP	Peptide

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	1124	0	1138	61	0
2	H	1678	0	1621	46	0
3	L	1572	0	1534	34	0
4	A	16	0	0	1	0
4	H	38	0	0	2	0
4	L	26	0	0	0	0
All	All	4454	0	4293	127	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 15.

All (127) 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:105:PHE:HB3	1:A:106:GLU:HA	1.13	1.09
1:A:179:ARG:HH11	1:A:179:ARG:HG3	1.18	1.06
1:A:105:PHE:CB	1:A:106:GLU:HA	2.02	0.89
1:A:40:ARG:NH2	2:H:56:ASP:O	2.08	0.87
1:A:105:PHE:HB3	1:A:106:GLU:CA	2.04	0.84
1:A:98:LEU:O	1:A:102:GLN:HG2	1.79	0.83
2:H:28:SER:OG	2:H:31:THR:OG1	1.98	0.81
2:H:135:PRO:HD3	2:H:147:LEU:HB3	1.63	0.81
1:A:73:CYS:SG	1:A:180:ALA:HB1	2.20	0.81
2:H:200:THR:HA	4:H:301:HOH:O	1.81	0.79
3:L:11:SER:HB2	3:L:110:LEU:CD1	2.12	0.79
1:A:157:TRP:HD1	1:A:158:LEU:HD23	1.47	0.78
3:L:34:TYR:HE1	3:L:52:LYS:HE3	1.48	0.77
1:A:179:ARG:HG3	1:A:179:ARG:NH1	1.96	0.77
2:H:199:GLY:O	4:H:301:HOH:O	2.01	0.77
1:A:100:TYR:O	1:A:104:ARG:HB2	1.85	0.75
1:A:72:GLY:C	1:A:74:PHE:H	1.96	0.73
3:L:14:PRO:HD3	3:L:110:LEU:O	1.89	0.72
1:A:116:GLN:HG3	4:A:201:HOH:O	1.89	0.71
1:A:25:ILE:O	1:A:29:ILE:HG12	1.92	0.68
1:A:132:ASN:O	1:A:133:LEU:HB2	1.94	0.66
1:A:40:ARG:HH22	2:H:56:ASP:C	2.02	0.66
1:A:88:ILE:HG21	1:A:127:GLN:HG3	1.79	0.65
3:L:26:ASN:O	3:L:31:THR:HG23	1.96	0.65
2:H:219:LYS:HE2	2:H:221:GLU:OE1	1.95	0.65
1:A:175:GLN:HB3	1:A:179:ARG:HH12	1.62	0.65
2:H:113:GLY:C	2:H:114:GLN:HG2	2.24	0.63
1:A:100:TYR:CD2	1:A:101:LEU:HD23	2.34	0.62
1:A:98:LEU:HD12	1:A:116:GLN:HA	1.82	0.62
3:L:89:TYR:CE1	3:L:103:ARG:O	2.53	0.62
3:L:11:SER:HB2	3:L:110:LEU:HD11	1.80	0.61
1:A:91:LEU:O	1:A:95:GLU:HB2	2.00	0.61
1:A:74:PHE:HB3	3:L:31:THR:HG22	1.82	0.60
3:L:34:TYR:CE1	3:L:52:LYS:HE3	2.34	0.60
1:A:102:GLN:C	1:A:104:ARG:H	2.09	0.59
2:H:135:PRO:HD3	2:H:147:LEU:CB	2.33	0.59
2:H:105:THR:O	3:L:52:LYS:NZ	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HD22	1:A:163:THR:HG23	1.86	0.58
1:A:75:GLN:HB3	3:L:30:GLY:O	2.04	0.57
2:H:128:PRO:HB3	2:H:154:TYR:HB3	1.87	0.57
2:H:38:TRP:CD1	2:H:71:ILE:HD12	2.40	0.57
1:A:65:PRO:HG3	1:A:93:GLU:HB2	1.86	0.57
2:H:134:ALA:HB1	2:H:135:PRO:HD2	1.88	0.56
3:L:9:LEU:HD22	3:L:106:HIS:HB3	1.87	0.56
3:L:103:ARG:HD3	3:L:103:ARG:C	2.31	0.55
2:H:35:ALA:HA	2:H:54:ASP:HA	1.89	0.54
2:H:168:LEU:HD21	2:H:191:VAL:HG21	1.89	0.54
2:H:32:ARG:HB3	2:H:33:TYR:CD2	2.43	0.54
2:H:18:LEU:HD21	2:H:118:VAL:HG11	1.90	0.54
2:H:97:CYS:O	2:H:113:GLY:CA	2.56	0.53
1:A:23:GLU:C	1:A:25:ILE:H	2.17	0.53
2:H:105:THR:O	2:H:105:THR:HG22	2.09	0.53
3:L:39:GLN:HB2	3:L:49:LEU:HD11	1.91	0.53
1:A:71:ASP:O	1:A:83:CYS:HB2	2.09	0.53
1:A:98:LEU:O	1:A:102:GLN:CG	2.54	0.52
2:H:35:ALA:HB2	2:H:103:VAL:CG2	2.40	0.52
1:A:110:GLU:HA	1:A:113:ARG:HB2	1.92	0.51
2:H:97:CYS:O	2:H:113:GLY:HA3	2.12	0.50
3:L:16:GLN:HB3	3:L:79:GLY:HA2	1.94	0.50
2:H:29:ILE:HG23	2:H:73:TRP:CZ3	2.46	0.50
1:A:72:GLY:C	1:A:74:PHE:N	2.68	0.49
1:A:162:THR:HA	1:A:165:LEU:HD21	1.95	0.49
3:L:23:ALA:HA	3:L:72:THR:HG22	1.93	0.49
1:A:157:TRP:HD1	1:A:158:LEU:CD2	2.23	0.49
2:H:135:PRO:HG3	2:H:198:LEU:HD22	1.94	0.49
1:A:100:TYR:C	1:A:102:GLN:H	2.22	0.48
2:H:202:THR:HG23	2:H:219:LYS:HE3	1.95	0.48
3:L:35:VAL:HG11	3:L:73:ALA:HB3	1.95	0.48
1:A:42:GLU:OE2	1:A:46:LYS:HE3	2.13	0.47
2:H:38:TRP:HD1	2:H:71:ILE:HD12	1.78	0.47
1:A:97:TYR:O	1:A:101:LEU:HG	2.14	0.47
2:H:18:LEU:O	2:H:83:GLN:HA	2.14	0.47
2:H:113:GLY:O	2:H:114:GLN:HG2	2.13	0.47
3:L:13:THR:C	3:L:15:GLY:H	2.22	0.47
3:L:30:GLY:CA	3:L:71:ASN:OD1	2.62	0.47
1:A:157:TRP:O	1:A:161:MET:HB2	2.15	0.47
3:L:65:SER:HB3	3:L:76:THR:HB	1.97	0.47
2:H:107:PHE:CD1	3:L:93:TYR:HD1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:24:GLY:HA3	3:L:29:ILE:HD12	1.98	0.46
3:L:35:VAL:HG11	3:L:73:ALA:CB	2.45	0.46
2:H:35:ALA:HB2	2:H:103:VAL:HG23	1.97	0.46
1:A:28:GLN:O	1:A:31:TYR:N	2.49	0.46
2:H:107:PHE:CD1	3:L:93:TYR:CD1	3.04	0.46
1:A:161:MET:O	1:A:165:LEU:HD23	2.16	0.45
1:A:179:ARG:HD3	3:L:34:TYR:CE2	2.51	0.45
2:H:62:SER:HB3	2:H:65:LEU:HB2	1.97	0.45
3:L:188:GLN:O	3:L:192:HIS:HD2	1.98	0.45
2:H:117:GLN:HB3	2:H:158:PRO:HD3	1.99	0.45
1:A:100:TYR:HD2	1:A:101:LEU:HD23	1.78	0.45
2:H:105:THR:O	2:H:105:THR:CG2	2.65	0.45
2:H:177:ALA:HB2	2:H:187:LEU:HD23	1.99	0.45
1:A:34:ASP:CG	2:H:33:TYR:HH	2.23	0.45
2:H:11:LEU:HD23	2:H:156:PRO:HG3	1.99	0.44
2:H:2:VAL:HG23	2:H:25:SER:OG	2.17	0.44
1:A:30:ARG:HD3	2:H:33:TYR:CZ	2.52	0.44
1:A:162:THR:O	1:A:166:ILE:HG12	2.18	0.44
2:H:32:ARG:HB3	2:H:33:TYR:CE2	2.52	0.44
1:A:74:PHE:CG	3:L:31:THR:HB	2.52	0.44
1:A:34:ASP:OD1	2:H:33:TYR:OH	2.30	0.44
1:A:179:ARG:HH11	1:A:179:ARG:CG	2.05	0.43
2:H:174:THR:HA	2:H:189:SER:HA	2.00	0.43
3:L:95:ASN:HA	3:L:96:PHE:HA	1.75	0.43
1:A:158:LEU:O	1:A:162:THR:HB	2.19	0.43
2:H:177:ALA:HA	2:H:187:LEU:HB3	2.00	0.43
1:A:75:GLN:HE21	3:L:68:LYS:NZ	2.16	0.43
2:H:104:VAL:CG2	2:H:104:VAL:O	2.67	0.43
3:L:140:ILE:HG12	3:L:199:VAL:HG21	2.01	0.42
1:A:87:ILE:H	1:A:87:ILE:HG12	1.73	0.42
3:L:17:THR:HB	3:L:78:SER:HA	2.01	0.42
1:A:29:ILE:HG22	1:A:174:LEU:HB3	2.01	0.42
1:A:36:ILE:HG23	1:A:167:LEU:HB3	2.02	0.42
3:L:53:VAL:HG22	3:L:54:THR:HG23	2.00	0.41
3:L:85:GLU:HG3	3:L:107:LEU:O	2.20	0.41
1:A:182:ARG:HE	1:A:182:ARG:HB3	1.59	0.41
1:A:71:ASP:CG	1:A:86:LYS:HD3	2.46	0.41
1:A:23:GLU:C	1:A:25:ILE:N	2.78	0.41
1:A:28:GLN:O	1:A:29:ILE:C	2.64	0.41
1:A:84:LEU:HG	1:A:130:ALA:HB2	2.03	0.41
1:A:168:ARG:NH2	2:H:59:THR:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:204:ILE:HG12	2:H:219:LYS:HB2	2.02	0.41
1:A:36:ILE:HD11	1:A:170:PHE:CD2	2.56	0.41
2:H:38:TRP:CE2	2:H:82:LEU:HB2	2.56	0.40
1:A:29:ILE:HG22	1:A:174:LEU:HD22	2.02	0.40
3:L:163:VAL:HG22	3:L:182:LEU:HD13	2.03	0.40
1:A:73:CYS:SG	1:A:184:MET:CE	3.10	0.40
1:A:83:CYS:HA	1:A:86:LYS:HB3	2.03	0.40
3:L:148:VAL:HG12	3:L:201:HIS:HB2	2.04	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	132/171 (77%)	108 (82%)	16 (12%)	8 (6%)	1	2
2	H	220/222 (99%)	194 (88%)	22 (10%)	4 (2%)	6	19
3	L	208/216 (96%)	192 (92%)	14 (7%)	2 (1%)	12	31
All	All	560/609 (92%)	494 (88%)	52 (9%)	14 (2%)	4	12

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	LEU
2	H	43	PRO
1	A	43	THR
1	A	75	GLN
2	H	123	ALA
1	A	28	GLN
1	A	73	CYS
1	A	95	GLU
1	A	100	TYR

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Mol	Chain	Res	Type
3	L	53	VAL
3	L	155	ASP
1	A	29	ILE
2	H	135	PRO
2	H	142	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	125/156 (80%)	92 (74%)	33 (26%)	0	0
2	H	194/194 (100%)	168 (87%)	26 (13%)	4	10
3	L	175/180 (97%)	157 (90%)	18 (10%)	7	18
All	All	494/530 (93%)	417 (84%)	77 (16%)	2	8

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	25	ILE
1	A	29	ILE
1	A	40	ARG
1	A	41	LYS
1	A	42	GLU
1	A	46	LYS
1	A	48	ASN
1	A	69	GLU
1	A	70	LYS
1	A	73	CYS
1	A	75	GLN
1	A	87	ILE
1	A	88	ILE
1	A	89	THR
1	A	95	GLU
1	A	96	VAL

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Mol	Chain	Res	Type
1	A	98	LEU
1	A	99	GLU
1	A	104	ARG
1	A	108	SER
1	A	111	GLN
1	A	113	ARG
1	A	129	LYS
1	A	133	LEU
1	A	134	ASP
1	A	143	THR
1	A	146	SER
1	A	158	LEU
1	A	179	ARG
1	A	182	ARG
1	A	183	GLN
1	A	184	MET
2	H	1	GLU
2	H	3	GLN
2	H	7	SER
2	H	15	SER
2	H	23	THR
2	H	25	SER
2	H	29	ILE
2	H	30	THR
2	H	32	ARG
2	H	45	LYS
2	H	65	LEU
2	H	70	SER
2	H	73	TRP
2	H	84	LEU
2	H	88	THR
2	H	90	GLU
2	H	104	VAL
2	H	114	GLN
2	H	116	THR
2	H	119	THR
2	H	122	SER
2	H	124	SER
2	H	125	THR
2	H	147	LEU
2	H	152	LYS
2	H	200	THR

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Mol	Chain	Res	Type
3	L	3	VAL
3	L	9	LEU
3	L	17	THR
3	L	41	LEU
3	L	50	ILE
3	L	52	LYS
3	L	53	VAL
3	L	75	LEU
3	L	81	GLN
3	L	83	GLU
3	L	94	ARG
3	L	136	LEU
3	L	140	ILE
3	L	142	ASP
3	L	157	SER
3	L	160	LYS
3	L	183	SER
3	L	205	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	48	ASN
1	A	75	GLN
1	A	127	GLN
1	A	164	HIS
2	H	3	GLN
2	H	5	GLN
2	H	208	ASN
3	L	6	GLN
3	L	95	ASN
3	L	98	ASN
3	L	192	HIS

5.3.3 RNA ⓘ

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	139/171 (81%)	3.36	128 (92%)	0 0	47, 70, 78, 85	1 (0%)
2	H	222/222 (100%)	1.16	40 (18%)	3 3	3, 14, 37, 59	10 (4%)
3	L	210/216 (97%)	1.04	27 (12%)	7 7	3, 14, 29, 40	10 (4%)
All	All	571/609 (93%)	1.65	195 (34%)	1 1	3, 17, 75, 85	21 (3%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	181	SER	13.6
3	L	126	SER	8.8
3	L	167	THR	8.0
3	L	30	GLY	7.3
2	H	157	GLU	7.0
3	L	179	SER	6.9
2	H	190	VAL	6.8
3	L	22	CYS	6.7
1	A	101	LEU	6.6
2	H	2	VAL	6.5
3	L	65	SER	6.5
2	H	186	SER	6.4
1	A	105	PHE	6.4
3	L	149	THR	6.3
2	H	45	LYS	6.2
3	L	90	CYS	5.9
1	A	151	LEU	5.9
1	A	106	GLU	5.9
1	A	117[A]	MET	5.8
1	A	83	CYS	5.7
1	A	111	GLN	5.7
3	L	205	THR	5.6
3	L	132	ASN	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	125	PHE	5.5
1	A	48	ASN	5.5
2	H	140	THR	5.4
1	A	65	PRO	5.4
1	A	92	LEU	5.4
2	H	139	SER	5.3
2	H	135	PRO	5.3
1	A	37	SER	5.3
1	A	73	CYS	5.2
1	A	134	ASP	5.1
2	H	141	SER	5.1
1	A	63	ASN	5.1
2	H	136	SER	5.0
1	A	157	TRP	5.0
1	A	127	GLN	4.9
1	A	116	GLN	4.9
1	A	164	HIS	4.9
3	L	118	SER	4.8
1	A	66	LYS	4.8
2	H	11	LEU	4.7
1	A	47	SER	4.7
1	A	173	PHE	4.7
2	H	137	SER	4.7
1	A	171	LYS	4.7
2	H	134	ALA	4.6
1	A	99	GLU	4.6
1	A	141	PRO	4.5
1	A	84	LEU	4.5
1	A	87	ILE	4.4
1	A	152	GLN	4.4
1	A	126	LEU	4.4
1	A	118	SER	4.4
1	A	113	ARG	4.4
2	H	173	HIS	4.4
1	A	100	TYR	4.3
1	A	165	LEU	4.3
1	A	78	PHE	4.3
1	A	115	VAL	4.2
1	A	90	GLY	4.2
1	A	120	LYS	4.1
1	A	124	GLN	4.1
1	A	170	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
2	H	3	GLN	3.8
1	A	128	LYS	3.7
1	A	179	ARG	3.7
1	A	72	GLY	3.7
1	A	85	VAL	3.7
1	A	129	LYS	3.6
3	L	78	SER	3.6
1	A	133	LEU	3.6
2	H	67	SER	3.5
1	A	71	ASP	3.5
1	A	24	ARG	3.5
1	A	104	ARG	3.5
1	A	109	GLU	3.5
1	A	168	ARG	3.5
1	A	23	GLU	3.5
3	L	31	THR	3.5
2	H	142	GLY	3.4
1	A	80	GLU	3.4
1	A	142	THR	3.4
1	A	77	GLY	3.4
1	A	39	LEU	3.3
1	A	38	ALA	3.3
1	A	123	ILE	3.3
1	A	169	SER	3.3
1	A	88	ILE	3.3
1	A	27	LYS	3.3
1	A	183	GLN	3.3
1	A	94	PHE	3.2
1	A	97	TYR	3.2
1	A	64	LEU	3.2
1	A	40	ARG	3.2
1	A	176	SER	3.2
1	A	144	ASN	3.2
1	A	175	GLN	3.2
1	A	67	MET	3.2
1	A	86	LYS	3.1
2	H	15	SER	3.1
2	H	117	GLN	3.1
1	A	172	GLU	3.1
2	H	197	SER	3.1
3	L	203	GLY	3.1
1	A	69	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	184	MET	3.1
1	A	121	VAL	3.0
2	H	195	SER	3.0
1	A	158	LEU	3.0
1	A	178	LEU	3.0
3	L	160	LYS	3.0
1	A	159	GLN	3.0
1	A	150	LYS	3.0
1	A	25	ILE	3.0
2	H	138	LYS	3.0
1	A	122	LEU	3.0
2	H	4	LEU	3.0
1	A	96	VAL	3.0
1	A	93	GLU	3.0
1	A	182	ARG	2.9
1	A	98	LEU	2.9
1	A	103	ASN	2.9
3	L	14	PRO	2.9
1	A	36	ILE	2.9
1	A	75	GLN	2.9
2	H	116	THR	2.9
1	A	79	ASN	2.9
1	A	28	GLN	2.9
1	A	112	ALA	2.9
1	A	89	THR	2.9
2	H	8	GLY	2.8
1	A	29	ILE	2.8
1	A	91	LEU	2.8
3	L	81	GLN	2.8
1	A	148	LEU	2.8
1	A	82	THR	2.8
1	A	177	SER	2.7
3	L	79	GLY	2.7
1	A	32	ILE	2.7
2	H	56	ASP	2.7
2	H	19	SER	2.7
1	A	174	LEU	2.7
3	L	3	VAL	2.6
1	A	108	SER	2.6
1	A	30	ARG	2.6
1	A	161	MET	2.6
3	L	191	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	74	PHE	2.6
1	A	107	SER	2.5
1	A	166	ILE	2.5
1	A	132	ASN	2.5
1	A	147	LEU	2.5
1	A	42	GLU	2.5
1	A	102	GLN	2.5
3	L	198	GLN	2.5
1	A	46	LYS	2.5
1	A	163	THR	2.5
1	A	33	LEU	2.4
3	L	116	ALA	2.4
3	L	27	ASN	2.3
1	A	114	ALA	2.3
2	H	1	GLU	2.3
2	H	122	SER	2.3
1	A	149	THR	2.3
1	A	180	ALA	2.3
1	A	26	ASP	2.3
1	A	145	ALA	2.3
1	A	160	ASP	2.3
2	H	9	PRO	2.3
3	L	153	LYS	2.2
1	A	146	SER	2.2
1	A	162	THR	2.2
2	H	17	THR	2.2
2	H	125	THR	2.2
1	A	44	CYS	2.2
2	H	143	GLY	2.2
1	A	181	LEU	2.2
2	H	118	VAL	2.2
1	A	41	LYS	2.2
3	L	58	SER	2.2
3	L	33	ALA	2.2
1	A	68	ALA	2.1
1	A	167	LEU	2.1
1	A	95	GLU	2.1
2	H	212	SER	2.1
2	H	144	THR	2.1
3	L	13	THR	2.1
2	H	127	GLY	2.0
2	H	152	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	45	ASN	2.0
1	A	130	ALA	2.0
2	H	105	THR	2.0
1	A	31	TYR	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.