



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:04 PM UTC

PDB ID : 8Z8M / pdb_00008z8m
Title : Crystal structure of human TNF alpha in complex with TNF30(VHH) domain of ozoralizumab
Authors : Mima, M.; Mishima-Tsumagari, C.
Deposited on : 2024-04-22
Resolution : 2.59 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

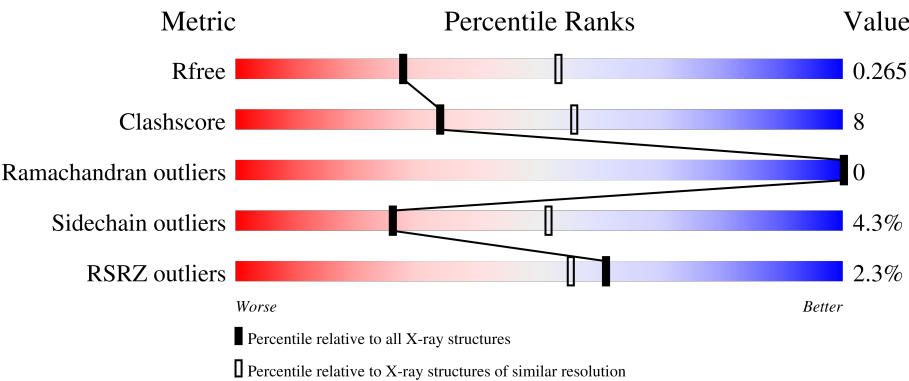
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	157	66%22%9%
1	C	157	74%17%10%
1	E	157	67%22%8%
1	G	157	76%13%10%
1	I	157	75%14%11%

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Mol	Chain	Length	Quality of chain
1	K	157	4% 80% 13% • 5%
2	B	123	% 77% 15% • 5%
2	D	123	67% 24% • 7%
2	F	123	% 76% 17% • 7%
2	H	123	12% 78% 14% • 7%
2	J	123	% 71% 20% • 7%
2	L	123	% 72% 20% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12130 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 Tumor necrosis factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	0	0
			1125	720	195	208	2			
1	C	142	Total	C	N	O	S	0	0	0
			1110	713	191	204	2			
1	E	145	Total	C	N	O	S	0	0	0
			1139	728	197	212	2			
1	G	141	Total	C	N	O	S	0	0	0
			1103	708	190	203	2			
1	I	140	Total	C	N	O	S	0	0	0
			1091	702	188	199	2			
1	K	149	Total	C	N	O	S	0	0	0
			1164	743	201	218	2			

- Molecule 2 is a protein called TNF30:VHH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total	C	N	O	S	0	0	0
			907	570	160	173	4			
2	D	115	Total	C	N	O	S	0	0	0
			887	558	154	171	4			
2	F	115	Total	C	N	O	S	0	0	0
			887	558	154	171	4			
2	H	115	Total	C	N	O	S	0	0	0
			887	558	154	171	4			
2	J	115	Total	C	N	O	S	0	0	0
			887	558	154	171	4			
2	L	116	Total	C	N	O	S	0	0	0
			897	564	157	172	4			

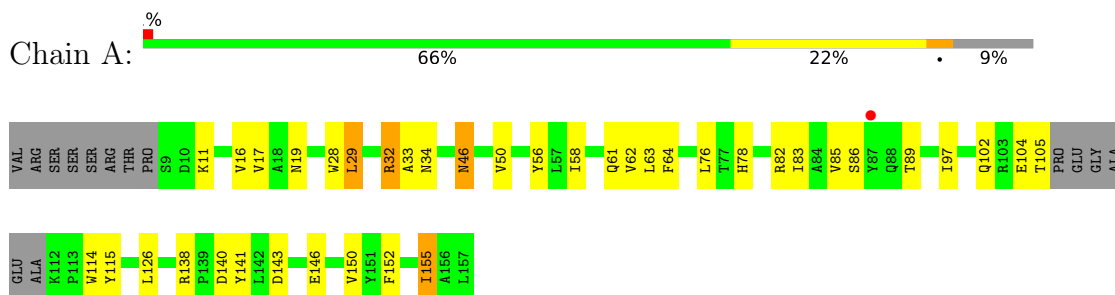
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	4	Total O 4 4	0	0
3	C	3	Total O 3 3	0	0
3	D	5	Total O 5 5	0	0
3	E	12	Total O 12 12	0	0
3	F	4	Total O 4 4	0	0
3	G	2	Total O 2 2	0	0
3	I	2	Total O 2 2	0	0
3	K	4	Total O 4 4	0	0
3	L	2	Total O 2 2	0	0

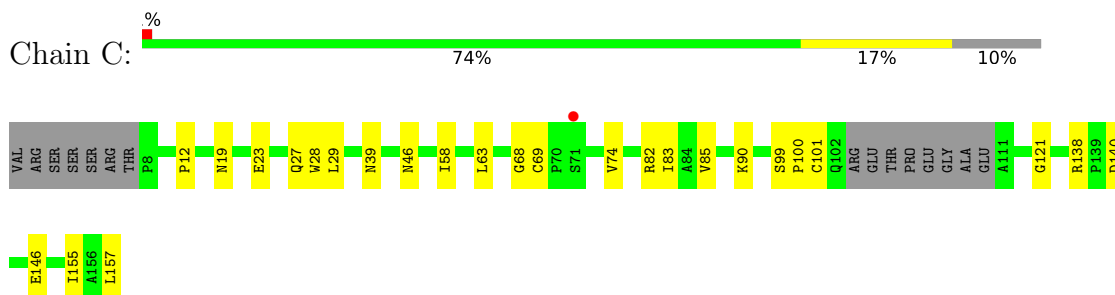
3 Residue-property plots [i](#)

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.

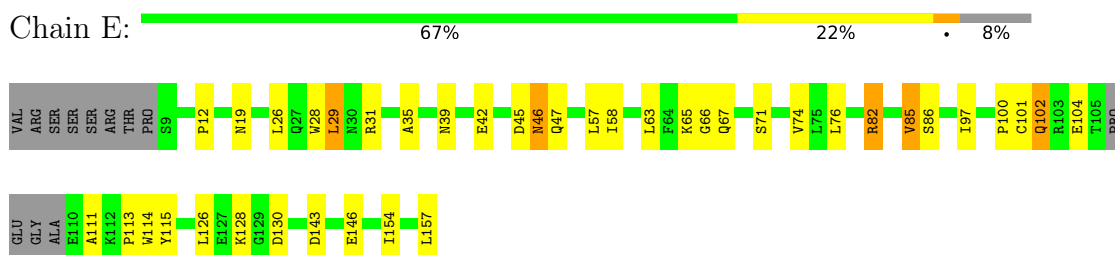
- Molecule 1: Tumor necrosis factor



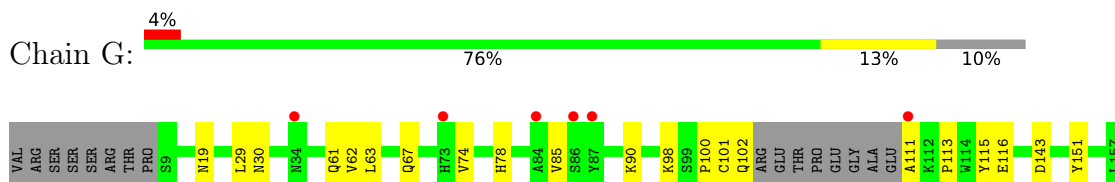
- Molecule 1: Tumor necrosis factor



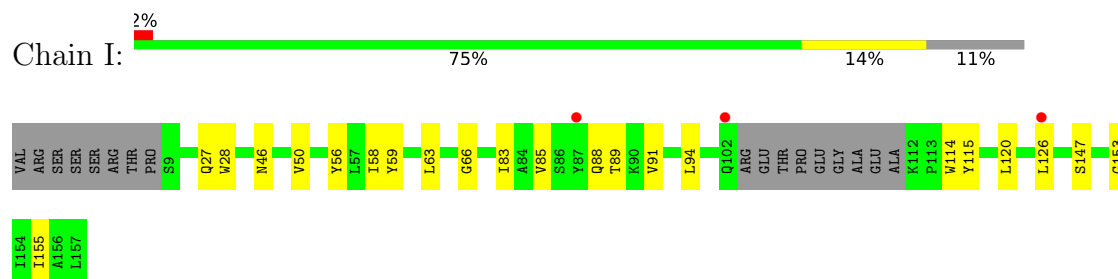
- Molecule 1: Tumor necrosis factor



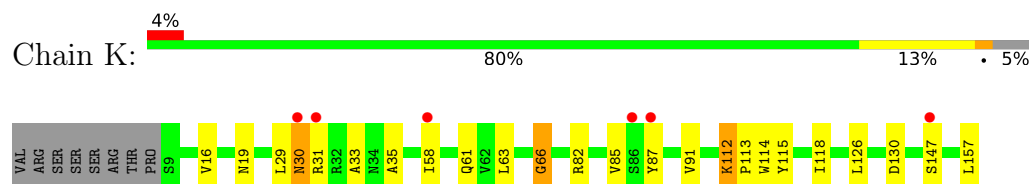
- Molecule 1: Tumor necrosis factor



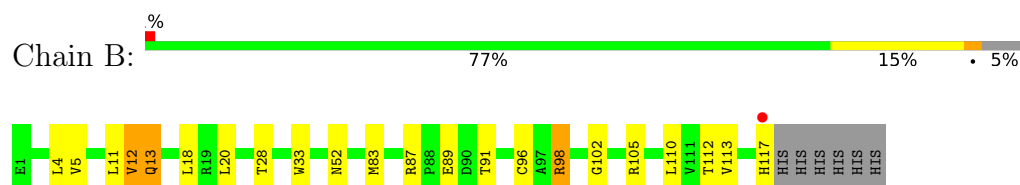
- Molecule 1: Tumor necrosis factor



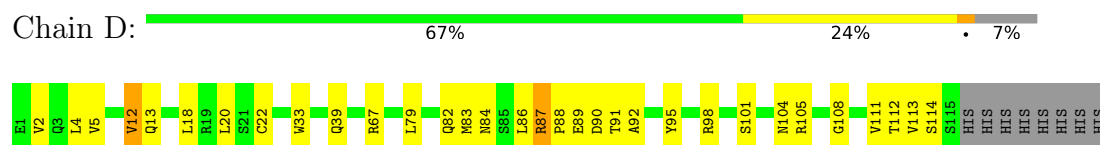
- Molecule 1: Tumor necrosis factor



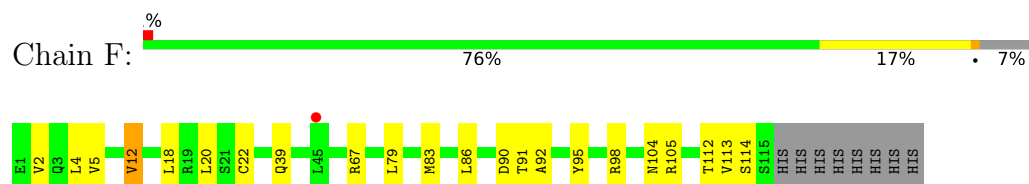
- Molecule 2: TNF30:VHH



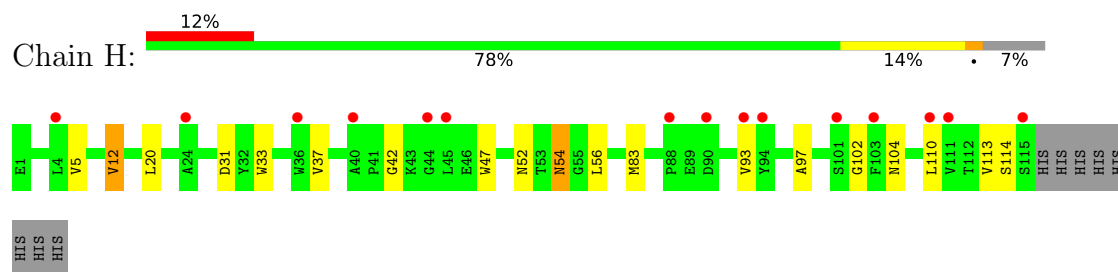
- Molecule 2: TNF30:VHH



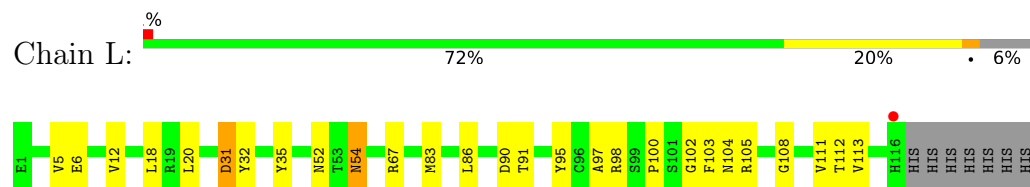
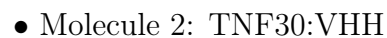
- Molecule 2: TNF30:VHH



- Molecule 2: TNF30:VHH



- Molecule 2: TNF30:VHH



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.03Å 121.16Å 123.61Å 90.00° 94.58° 90.00°	Depositor
Resolution (Å)	45.79 – 2.59 45.79 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.79-2.59) 99.3 (45.79-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.269 0.212 , 0.265	Depositor DCC
R_{free} test set	2381 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12130	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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	1.01	0/1149	1.30	0/1562
1	C	1.03	0/1135	1.27	2/1544 (0.1%)
1	E	1.05	0/1163	1.31	2/1581 (0.1%)
1	G	1.03	0/1127	1.29	0/1533
1	I	1.06	0/1115	1.32	0/1517
1	K	1.10	0/1190	1.31	1/1620 (0.1%)
2	B	1.06	0/929	1.33	3/1260 (0.2%)
2	D	1.07	0/907	1.33	1/1230 (0.1%)
2	F	1.10	0/907	1.30	0/1230
2	H	1.11	0/907	1.33	1/1230 (0.1%)
2	J	1.06	0/907	1.31	1/1230 (0.1%)
2	L	1.05	0/918	1.30	2/1245 (0.2%)
All	All	1.06	0/12354	1.31	13/16782 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	GLN	CB-CA-C	7.14	119.84	108.91
2	L	31	ASP	CA-CB-CG	6.47	119.07	112.60
2	D	108	GLY	CA-C-O	-5.92	117.84	122.52
2	L	108	GLY	CA-C-O	-5.85	118.19	122.23
1	K	66	GLY	CA-C-O	-5.56	116.73	121.57
1	C	146	GLU	CA-C-N	5.42	129.38	121.31
1	C	146	GLU	C-N-CA	5.42	129.38	121.31
2	J	13	GLN	CB-CA-C	5.31	116.50	108.86
2	H	104	ASN	CB-CA-C	5.08	119.11	111.89
1	E	85	VAL	CA-C-N	5.03	127.27	120.38
1	E	85	VAL	C-N-CA	5.03	127.27	120.38
2	B	28	THR	CA-C-N	5.01	127.24	120.38
2	B	28	THR	C-N-CA	5.01	127.24	120.38

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	1125	0	1125	22	0
1	C	1110	0	1112	16	0
1	E	1139	0	1136	27	0
1	G	1103	0	1104	12	0
1	I	1091	0	1091	14	0
1	K	1164	0	1158	17	0
2	B	907	0	876	11	0
2	D	887	0	862	18	0
2	F	887	0	862	14	0
2	H	887	0	862	13	0
2	J	887	0	862	19	0
2	L	897	0	869	22	0
3	A	8	0	0	2	0
3	B	4	0	0	0	0
3	C	3	0	0	0	0
3	D	5	0	0	1	0
3	E	12	0	0	3	0
3	F	4	0	0	0	0
3	G	2	0	0	0	0
3	I	2	0	0	0	0
3	K	4	0	0	0	0
3	L	2	0	0	0	0
All	All	12130	0	11919	185	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 8.

All (185) 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:E:146:GLU:HG3	3:E:206:HOH:O	1.61	1.00
2:D:87:ARG:NH1	3:D:201:HOH:O	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:93:VAL:HG22	2:J:110:LEU:HG	1.63	0.79
1:A:28:TRP:H	1:A:46:ASN:HD21	1.35	0.73
1:I:155:ILE:HD13	1:K:157:LEU:HD13	1.73	0.71
2:L:52:ASN:HD21	2:L:54:ASN:ND2	1.88	0.71
2:J:2:VAL:HG11	2:J:104:ASN:HD22	1.58	0.69
1:E:42:GLU:HA	3:E:210:HOH:O	1.91	0.68
2:F:83:MET:HB3	2:F:86:LEU:HD21	1.77	0.66
2:F:2:VAL:HG11	2:F:104:ASN:ND2	2.10	0.66
2:D:83:MET:HE1	2:D:111:VAL:HG21	1.77	0.65
1:C:19:ASN:HB2	1:C:29:LEU:HD13	1.79	0.65
2:H:93:VAL:HG22	2:H:110:LEU:HD23	1.78	0.65
2:L:91:THR:HG23	2:L:112:THR:HA	1.79	0.64
1:A:155:ILE:HD13	1:C:157:LEU:HD13	1.80	0.63
2:B:91:THR:HG23	2:B:112:THR:HA	1.81	0.63
2:L:83:MET:HB3	2:L:86:LEU:HD21	1.81	0.62
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.30	0.61
2:F:91:THR:HG23	2:F:112:THR:HA	1.82	0.61
2:D:91:THR:HG23	2:D:112:THR:HA	1.82	0.61
2:F:67:ARG:NH2	2:F:90:ASP:OD2	2.32	0.61
1:K:19:ASN:HB2	1:K:29:LEU:HD13	1.82	0.60
2:F:20:LEU:HG	2:F:83:MET:HE2	1.84	0.59
1:A:17:VAL:HG23	3:A:206:HOH:O	2.02	0.59
1:I:155:ILE:HD13	1:K:157:LEU:CD1	2.32	0.59
1:K:112:LYS:O	1:K:112:LYS:HD2	2.03	0.59
1:I:28:TRP:H	1:I:46:ASN:HD21	1.50	0.58
1:E:28:TRP:H	1:E:46:ASN:HD21	1.51	0.58
2:B:102:GLY:O	2:B:105:ARG:HB3	2.03	0.58
2:J:83:MET:HB3	2:J:86:LEU:HD21	1.86	0.58
1:A:34:ASN:HD21	1:C:82:ARG:HH21	1.50	0.57
1:E:63:LEU:HD11	1:E:115:TYR:HD2	1.68	0.57
2:F:98:ARG:HH11	2:F:104:ASN:ND2	2.02	0.57
1:E:31:ARG:O	1:E:35:ALA:HB3	2.05	0.56
1:G:19:ASN:HB2	1:G:29:LEU:HD13	1.85	0.56
1:K:31:ARG:O	1:K:35:ALA:HB3	2.05	0.56
2:J:95:TYR:HB3	2:J:105:ARG:HB2	1.88	0.56
2:B:87:ARG:HD3	2:B:89:GLU:OE2	2.06	0.56
1:C:28:TRP:H	1:C:46:ASN:HD21	1.53	0.55
2:L:18:LEU:HB3	2:L:83:MET:HE3	1.88	0.55
2:L:83:MET:HE1	2:L:111:VAL:HG21	1.89	0.55
1:C:12:PRO:HA	1:C:39:ASN:HB2	1.87	0.55
1:E:82:ARG:NH1	1:E:130:ASP:OD2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:LEU:HG	2:B:83:MET:HE2	1.89	0.55
1:G:61:GLN:HE22	1:I:120:LEU:HD23	1.71	0.55
1:K:63:LEU:HD11	1:K:115:TYR:HD2	1.72	0.54
2:F:18:LEU:HB3	2:F:83:MET:HE3	1.90	0.54
1:K:91:VAL:HG12	2:L:32:TYR:CE2	2.43	0.54
2:H:52:ASN:HD21	2:H:54:ASN:ND2	2.06	0.54
1:E:28:TRP:N	1:E:46:ASN:HD21	2.07	0.53
1:K:91:VAL:CG1	2:L:32:TYR:CE2	2.91	0.53
2:L:97:ALA:CB	2:L:102:GLY:HA2	2.39	0.53
1:C:101:CYS:HB2	1:E:102:GLN:HG2	1.90	0.53
1:G:63:LEU:HD12	1:G:143:ASP:HB3	1.88	0.53
1:I:88:GLN:HB3	2:J:99:SER:HB2	1.90	0.53
1:A:104:GLU:HG2	1:A:105:THR:HG23	1.91	0.52
1:G:98:LYS:HD3	1:G:116:GLU:HB3	1.91	0.52
2:L:67:ARG:NH2	2:L:90:ASP:OD2	2.39	0.52
1:E:19:ASN:HA	1:E:29:LEU:HD22	1.92	0.52
1:G:74:VAL:O	1:G:100:PRO:HD2	2.09	0.52
1:A:19:ASN:HB2	1:A:29:LEU:HD13	1.92	0.51
2:J:12:VAL:O	2:J:113:VAL:HA	2.10	0.51
2:J:89:GLU:H	2:J:89:GLU:CD	2.17	0.51
1:A:63:LEU:HD12	1:A:143:ASP:HB3	1.92	0.51
2:D:98:ARG:NH1	2:D:104:ASN:OD1	2.43	0.51
1:A:58:ILE:HD11	1:A:126:LEU:HD11	1.92	0.51
1:G:151:TYR:CZ	1:I:94:LEU:HD22	2.46	0.51
2:F:22:CYS:HB3	2:F:79:LEU:HB3	1.93	0.51
1:G:111:ALA:O	1:G:113:PRO:HD3	2.11	0.51
1:A:138:ARG:NH1	1:A:140:ASP:OD2	2.44	0.51
1:C:68:GLY:O	1:C:69:CYS:C	2.53	0.51
2:L:12:VAL:O	2:L:113:VAL:HA	2.11	0.50
1:A:102:GLN:HG2	3:A:208:HOH:O	2.11	0.50
2:B:18:LEU:HB3	2:B:83:MET:HE3	1.93	0.50
2:J:9:GLY:HA3	2:J:109:THR:OG1	2.11	0.50
2:D:4:LEU:HD12	2:D:104:ASN:O	2.12	0.50
2:H:97:ALA:HB1	2:H:102:GLY:HA2	1.94	0.50
1:I:63:LEU:HD11	1:I:115:TYR:HD1	1.77	0.50
1:K:66:GLY:O	1:K:113:PRO:HA	2.12	0.49
1:C:74:VAL:O	1:C:100:PRO:HD2	2.12	0.49
2:L:91:THR:HA	2:L:111:VAL:O	2.12	0.49
2:H:37:VAL:HG12	2:H:47:TRP:HA	1.95	0.48
2:J:103:PHE:CD2	2:J:104:ASN:OD1	2.66	0.48
2:J:4:LEU:HD12	2:J:104:ASN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ILE:O	1:C:121:GLY:HA2	2.13	0.48
2:D:39:GLN:O	2:D:92:ALA:HB1	2.12	0.48
2:H:97:ALA:CB	2:H:102:GLY:HA2	2.43	0.48
1:E:71:SER:HA	1:E:104:GLU:CD	2.39	0.48
2:J:52:ASN:HD21	2:J:54:ASN:ND2	2.12	0.48
1:E:45:ASP:O	1:E:47:GLN:HG3	2.14	0.48
2:B:12:VAL:O	2:B:113:VAL:HA	2.14	0.47
2:D:2:VAL:HG11	2:D:104:ASN:OD1	2.14	0.47
2:D:20:LEU:HG	2:D:83:MET:HE2	1.97	0.47
1:E:66:GLY:HA3	1:E:114:TRP:NE1	2.30	0.47
2:J:67:ARG:HH21	2:J:86:LEU:HA	1.80	0.46
1:A:76:LEU:O	1:A:97:ILE:HA	2.15	0.46
2:F:12:VAL:O	2:F:113:VAL:HA	2.15	0.46
2:D:82:GLN:HE21	2:D:84:ASN:HD21	1.64	0.46
1:E:74:VAL:O	1:E:100:PRO:HD2	2.16	0.46
2:H:93:VAL:HG22	2:H:110:LEU:CD2	2.44	0.46
2:F:95:TYR:HB3	2:F:105:ARG:HB2	1.98	0.46
1:C:83:ILE:HG13	1:C:90:LYS:HG3	1.97	0.46
1:I:147:SER:HB3	2:L:31:ASP:OD1	2.16	0.46
2:J:6:GLU:CD	2:J:108:GLY:HA2	2.40	0.46
1:K:16:VAL:HG12	1:K:30:ASN:HD22	1.81	0.45
1:E:12:PRO:HA	1:E:39:ASN:HB2	1.98	0.45
1:E:66:GLY:HA3	1:E:114:TRP:CE2	2.50	0.45
1:I:58:ILE:HD11	1:I:126:LEU:HD11	1.97	0.45
2:J:67:ARG:NH2	2:J:87:ARG:HG3	2.32	0.45
2:L:35:TYR:CE2	2:L:100:PRO:HG3	2.52	0.45
2:L:52:ASN:HD21	2:L:54:ASN:HD21	1.60	0.45
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.98	0.45
2:H:12:VAL:O	2:H:113:VAL:HA	2.17	0.45
1:A:16:VAL:HG22	1:A:152:PHE:O	2.16	0.45
2:B:4:LEU:HB3	2:B:96:CYS:SG	2.57	0.45
1:I:66:GLY:HA3	1:I:114:TRP:NE1	2.32	0.45
1:A:114:TRP:HA	1:C:99:SER:OG	2.17	0.44
2:D:95:TYR:HB3	2:D:105:ARG:HB2	1.99	0.44
1:A:63:LEU:HD11	1:A:115:TYR:HD2	1.82	0.44
2:B:11:LEU:HG	2:B:117:HIS:CE1	2.52	0.44
2:L:95:TYR:HB3	2:L:105:ARG:HB2	1.98	0.44
2:F:98:ARG:NH1	2:F:104:ASN:ND2	2.65	0.44
1:E:58:ILE:HD11	1:E:126:LEU:HD11	1.99	0.44
1:G:90:LYS:HB3	2:H:33:TRP:HB2	1.99	0.44
1:A:61:GLN:O	1:A:150:VAL:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:HD3	1:A:126:LEU:CD2	2.48	0.44
1:E:19:ASN:HB2	1:E:29:LEU:HD13	2.00	0.44
2:F:2:VAL:HG11	2:F:104:ASN:HD22	1.80	0.43
2:L:18:LEU:HA	2:L:18:LEU:HD12	1.74	0.43
2:L:98:ARG:HD3	2:L:104:ASN:OD1	2.17	0.43
1:A:64:PHE:HA	1:A:141:TYR:O	2.17	0.43
2:H:31:ASP:OD1	1:K:147:SER:HB3	2.17	0.43
1:A:89:THR:HG22	2:B:98:ARG:HB3	2.01	0.43
1:G:74:VAL:HG12	1:G:100:PRO:HG3	1.99	0.43
1:A:32:ARG:HD2	1:A:33:ALA:N	2.34	0.43
2:D:13:GLN:HB2	2:H:42:GLY:HA2	1.99	0.43
2:F:39:GLN:O	2:F:92:ALA:HB1	2.19	0.43
1:A:83:ILE:HA	1:A:89:THR:O	2.19	0.43
1:I:88:GLN:CB	2:J:99:SER:HB2	2.49	0.43
2:J:54:ASN:C	2:J:54:ASN:HD22	2.26	0.43
1:G:62:VAL:HG13	1:G:78:HIS:CE1	2.54	0.43
2:D:12:VAL:O	2:D:113:VAL:HA	2.19	0.42
1:E:26:LEU:HD21	1:E:28:TRP:CZ2	2.54	0.42
1:A:62:VAL:HG13	1:A:78:HIS:CE1	2.55	0.42
1:E:46:ASN:HD22	1:E:46:ASN:HA	1.58	0.42
2:F:4:LEU:HD12	2:F:104:ASN:O	2.20	0.42
1:C:138:ARG:NH1	1:C:140:ASP:OD2	2.53	0.42
2:J:91:THR:HA	2:J:111:VAL:O	2.19	0.42
1:I:83:ILE:HA	1:I:89:THR:O	2.19	0.42
2:J:18:LEU:HD12	2:J:18:LEU:HA	1.87	0.42
1:K:82:ARG:NH1	1:K:130:ASP:OD2	2.46	0.42
1:E:57:LEU:O	1:E:154:ILE:HA	2.19	0.42
1:E:63:LEU:HD12	1:E:143:ASP:HB3	2.02	0.42
2:L:97:ALA:HB2	2:L:102:GLY:HA2	2.01	0.42
1:A:50:VAL:HG13	1:A:56:TYR:CZ	2.54	0.42
1:I:50:VAL:HG13	1:I:56:TYR:CZ	2.55	0.42
1:E:65:LYS:HA	1:E:114:TRP:O	2.20	0.42
1:E:67:GLN:HE22	1:E:113:PRO:HG3	1.85	0.42
1:K:31:ARG:C	1:K:33:ALA:H	2.27	0.42
1:K:87:TYR:HB3	2:L:103:PHE:CE2	2.55	0.42
2:H:52:ASN:HD21	2:H:54:ASN:HD21	1.68	0.41
2:D:91:THR:HA	2:D:111:VAL:O	2.20	0.41
1:K:58:ILE:HD11	1:K:126:LEU:HD11	2.02	0.41
1:K:61:GLN:HA	1:K:118:ILE:O	2.19	0.41
2:D:22:CYS:HB3	2:D:79:LEU:HB3	2.03	0.41
2:H:20:LEU:HG	2:H:83:MET:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:TRP:CD2	2:B:52:ASN:HA	2.55	0.41
2:J:93:VAL:CG1	2:J:95:TYR:CZ	3.04	0.41
2:B:13:GLN:HG3	2:B:117:HIS:CE1	2.56	0.41
1:E:101:CYS:O	3:E:201:HOH:O	2.22	0.41
1:K:66:GLY:HA3	1:K:114:TRP:CE2	2.56	0.41
1:E:76:LEU:O	1:E:97:ILE:HA	2.21	0.41
2:L:102:GLY:HA3	2:L:105:ARG:HH11	1.85	0.41
1:C:155:ILE:HD13	1:E:157:LEU:HD13	2.02	0.40
1:E:67:GLN:O	1:E:111:ALA:HB1	2.21	0.40
1:G:63:LEU:HD11	1:G:115:TYR:HD2	1.85	0.40
2:L:6:GLU:HG2	2:L:95:TYR:HA	2.02	0.40
1:C:74:VAL:HB	1:C:100:PRO:HG2	2.02	0.40
1:C:90:LYS:HD3	2:D:33:TRP:CD2	2.56	0.40
2:D:88:PRO:HA	2:D:113:VAL:HB	2.02	0.40
1:I:59:TYR:CZ	1:I:153:GLY:HA3	2.55	0.40
2:L:20:LEU:HG	2:L:83:MET:HE2	2.03	0.40
1:G:19:ASN:HA	1:G:29:LEU:HD22	2.03	0.40
1:C:28:TRP:O	1:C:29:LEU:HD12	2.21	0.40
2:H:54:ASN:HD22	2:H:56:LEU:H	1.69	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	139/157 (88%)	136 (98%)	3 (2%)	0	100	100
1	C	138/157 (88%)	132 (96%)	6 (4%)	0	100	100
1	E	141/157 (90%)	133 (94%)	8 (6%)	0	100	100
1	G	137/157 (87%)	129 (94%)	8 (6%)	0	100	100
1	I	136/157 (87%)	134 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	147/157 (94%)	145 (99%)	2 (1%)	0	100	100
2	B	115/123 (94%)	114 (99%)	1 (1%)	0	100	100
2	D	113/123 (92%)	110 (97%)	3 (3%)	0	100	100
2	F	113/123 (92%)	111 (98%)	2 (2%)	0	100	100
2	H	113/123 (92%)	112 (99%)	1 (1%)	0	100	100
2	J	113/123 (92%)	111 (98%)	2 (2%)	0	100	100
2	L	114/123 (93%)	111 (97%)	3 (3%)	0	100	100
All	All	1519/1680 (90%)	1478 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	122/133 (92%)	114 (93%)	8 (7%)	15	34
1	C	120/133 (90%)	116 (97%)	4 (3%)	33	61
1	E	123/133 (92%)	116 (94%)	7 (6%)	18	40
1	G	119/133 (90%)	114 (96%)	5 (4%)	26	52
1	I	117/133 (88%)	114 (97%)	3 (3%)	40	68
1	K	125/133 (94%)	122 (98%)	3 (2%)	43	70
2	B	98/104 (94%)	94 (96%)	4 (4%)	27	54
2	D	96/104 (92%)	89 (93%)	7 (7%)	13	29
2	F	96/104 (92%)	93 (97%)	3 (3%)	35	63
2	H	96/104 (92%)	92 (96%)	4 (4%)	26	52
2	J	96/104 (92%)	90 (94%)	6 (6%)	16	36
2	L	97/104 (93%)	95 (98%)	2 (2%)	47	73
All	All	1305/1422 (92%)	1249 (96%)	56 (4%)	26	51

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	29	LEU
1	A	32	ARG
1	A	46	ASN
1	A	85	VAL
1	A	86	SER
1	A	146	GLU
1	A	155	ILE
2	B	5	VAL
2	B	12	VAL
2	B	98	ARG
2	B	110	LEU
1	C	23	GLU
1	C	27	GLN
1	C	63	LEU
1	C	85	VAL
2	D	5	VAL
2	D	12	VAL
2	D	18	LEU
2	D	87	ARG
2	D	89	GLU
2	D	101	SER
2	D	114	SER
1	E	29	LEU
1	E	46	ASN
1	E	82	ARG
1	E	85	VAL
1	E	86	SER
1	E	102	GLN
1	E	128	LYS
2	F	5	VAL
2	F	12	VAL
2	F	114	SER
1	G	30	ASN
1	G	67	GLN
1	G	85	VAL
1	G	101	CYS
1	G	102	GLN
2	H	5	VAL
2	H	12	VAL
2	H	54	ASN
2	H	114	SER

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Mol	Chain	Res	Type
1	I	27	GLN
1	I	85	VAL
1	I	91	VAL
2	J	5	VAL
2	J	12	VAL
2	J	18	LEU
2	J	54	ASN
2	J	89	GLU
2	J	114	SER
1	K	30	ASN
1	K	85	VAL
1	K	112	LYS
2	L	5	VAL
2	L	54	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	30	ASN
1	A	34	ASN
1	A	46	ASN
1	A	67	GLN
1	A	78	HIS
2	B	39	GLN
2	B	116	HIS
2	B	117	HIS
1	C	46	ASN
1	C	61	GLN
1	C	67	GLN
1	C	73	HIS
1	C	102	GLN
2	D	84	ASN
1	E	25	GLN
1	E	30	ASN
1	E	34	ASN
1	E	46	ASN
1	E	67	GLN
1	E	78	HIS
1	E	102	GLN
2	F	82	GLN
2	F	84	ASN

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Mol	Chain	Res	Type
2	F	104	ASN
1	G	30	ASN
1	G	61	GLN
1	G	78	HIS
1	G	102	GLN
1	G	149	GLN
2	H	39	GLN
2	H	54	ASN
2	H	77	ASN
1	I	27	GLN
1	I	34	ASN
1	I	39	ASN
1	I	46	ASN
1	I	61	GLN
1	I	67	GLN
1	I	149	GLN
2	J	39	GLN
2	J	54	ASN
2	J	107	GLN
1	K	27	GLN
1	K	30	ASN
1	K	39	ASN
1	K	61	GLN
1	K	73	HIS
1	K	78	HIS
1	K	102	GLN
1	K	125	GLN
2	L	54	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	143/157 (91%)	-0.28	1 (0%) 84 82	39, 57, 106, 131	0
1	C	142/157 (90%)	-0.20	1 (0%) 84 82	40, 60, 103, 129	0
1	E	145/157 (92%)	-0.17	0 100 100	38, 58, 113, 147	0
1	G	141/157 (89%)	0.46	6 (4%) 40 34	58, 89, 131, 148	0
1	I	140/157 (89%)	0.21	3 (2%) 63 58	52, 80, 117, 149	0
1	K	149/157 (94%)	0.17	6 (4%) 42 37	47, 74, 116, 168	0
2	B	117/123 (95%)	-0.09	1 (0%) 81 78	44, 74, 107, 145	0
2	D	115/123 (93%)	-0.20	0 100 100	44, 61, 101, 124	0
2	F	115/123 (93%)	-0.07	1 (0%) 81 78	47, 74, 103, 130	0
2	H	115/123 (93%)	0.98	15 (13%) 7 5	84, 147, 205, 252	0
2	J	115/123 (93%)	0.54	1 (0%) 81 78	63, 115, 169, 194	0
2	L	116/123 (94%)	-0.13	1 (0%) 81 78	42, 62, 108, 126	0
All	All	1553/1680 (92%)	0.09	36 (2%) 61 55	38, 75, 147, 252	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	103	PHE	4.7
1	G	87	TYR	4.3
2	H	45	LEU	3.7
1	K	87	TYR	3.5
2	H	101	SER	3.0
2	H	40	ALA	2.8
2	H	94	TYR	2.8
1	G	86	SER	2.7
1	K	147	SER	2.7
1	I	102	GLN	2.5
2	L	116	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	111	ALA	2.5
2	H	115	SER	2.4
2	H	90	ASP	2.4
1	G	34	ASN	2.3
2	H	88	PRO	2.3
2	H	44	GLY	2.3
2	H	111	VAL	2.3
1	K	31	ARG	2.2
1	K	30	ASN	2.2
1	I	126	LEU	2.1
1	G	73	HIS	2.1
2	H	93	VAL	2.1
2	H	4	LEU	2.1
2	F	45	LEU	2.1
1	K	58	ILE	2.1
1	I	87	TYR	2.1
1	K	86	SER	2.1
2	H	24	ALA	2.1
1	G	84	ALA	2.0
2	H	36	TRP	2.0
2	J	42	GLY	2.0
1	C	71	SER	2.0
2	B	117	HIS	2.0
2	H	110	LEU	2.0
1	A	87	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.