



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:17 AM UTC

PDB ID : 9DH2 / pdb_00009dh2
Title : Structure of Fab in complex with NKG2D extracellular domain
Authors : Fallon, D.; Huang, C.S.
Deposited on : 2024-09-03
Resolution : 2.98 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

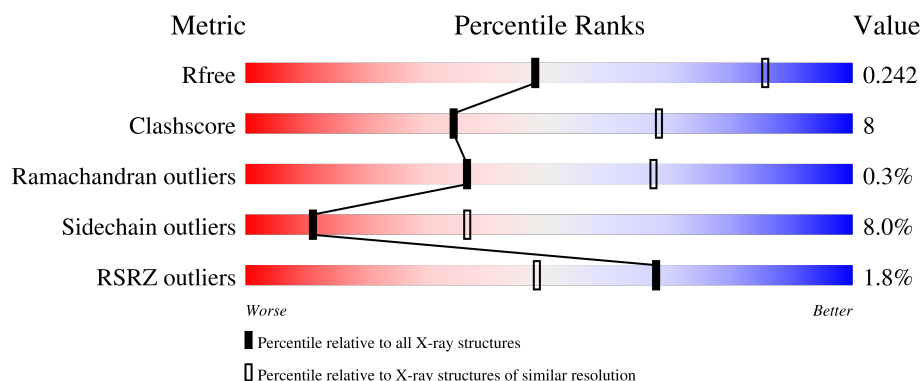
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	220	0% 80% 17% ..
1	G	220	2% 80% 15% ..
1	K	220	4% 76% 20% ..
1	P	220	3% 80% 17% ..
2	D	212	77% 21% .

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Mol	Chain	Length	Quality of chain
2	H	212	80%16%•
2	L	212	81%17%•
2	Q	212	78%20%•
3	M	137	3% 64%22%•10%
3	R	137	66%20%••9%
3	S	137	7% 60%25%5%10%
3	T	137	% 69%20%•9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17120 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 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1646	1043	270	326	7			
1	G	217	Total	C	N	O	S	0	0	0
			1646	1043	270	326	7			
1	K	217	Total	C	N	O	S	0	0	0
			1646	1043	270	326	7			
1	P	217	Total	C	N	O	S	0	0	0
			1646	1043	270	326	7			

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	211	Total	C	N	O	S	0	0	0
			1634	1029	271	329	5			
2	H	211	Total	C	N	O	S	0	0	0
			1634	1029	271	329	5			
2	L	211	Total	C	N	O	S	0	0	0
			1634	1029	271	329	5			
2	Q	211	Total	C	N	O	S	0	0	0
			1634	1029	271	329	5			

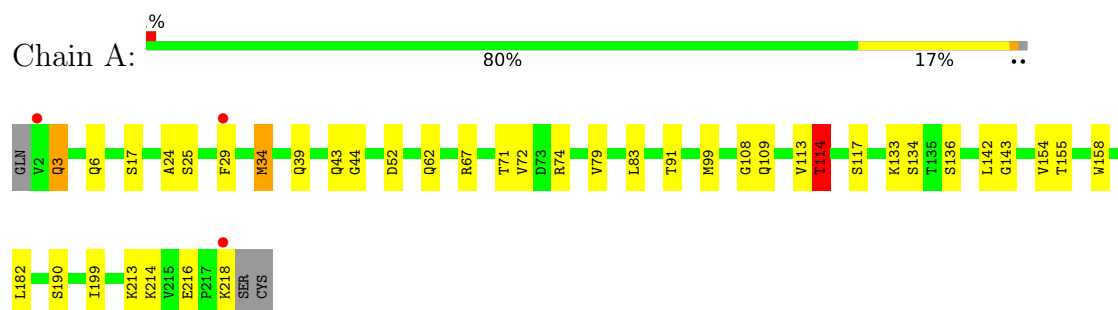
- Molecule 3 is a protein called NKG2-D type II integral membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	123	Total	C	N	O	S	0	0	0
			996	633	160	191	12			
3	R	124	Total	C	N	O	S	0	0	0
			1004	638	161	193	12			
3	S	123	Total	C	N	O	S	0	0	0
			996	633	160	191	12			
3	T	124	Total	C	N	O	S	0	0	0
			1004	638	161	193	12			

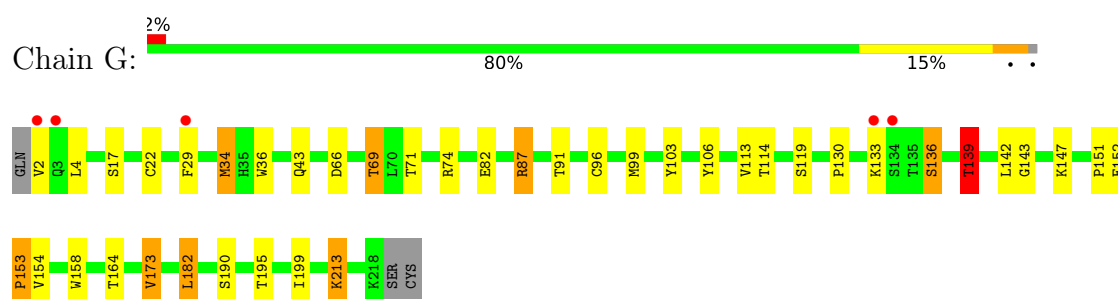
3 Residue-property plots [i](#)

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.

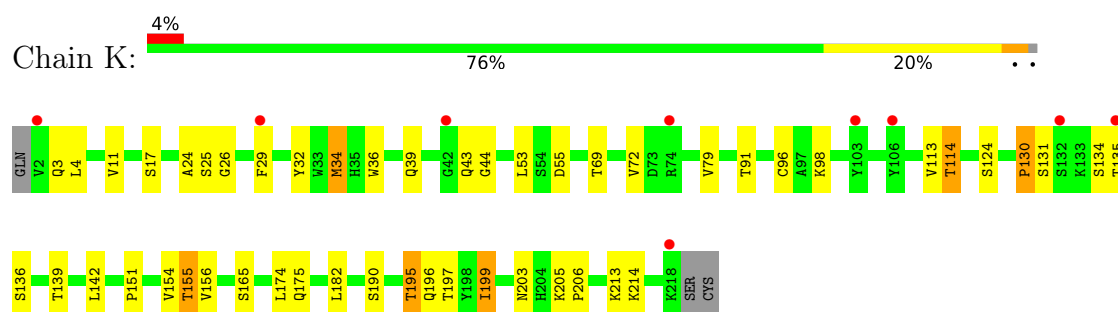
- Molecule 1: Fab heavy chain



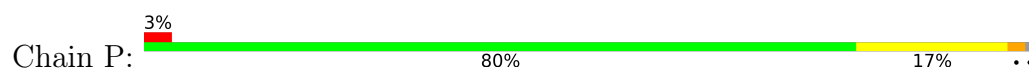
- Molecule 1: Fab heavy chain

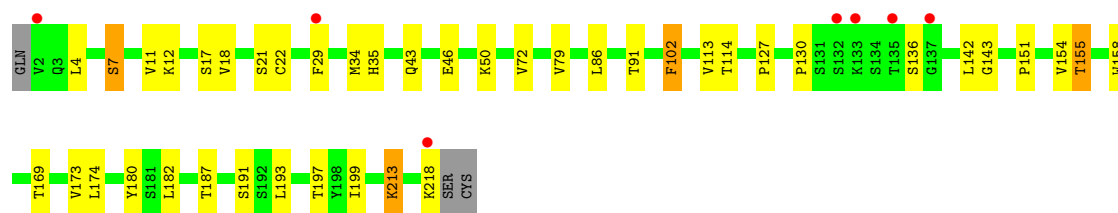


- Molecule 1: Fab heavy chain



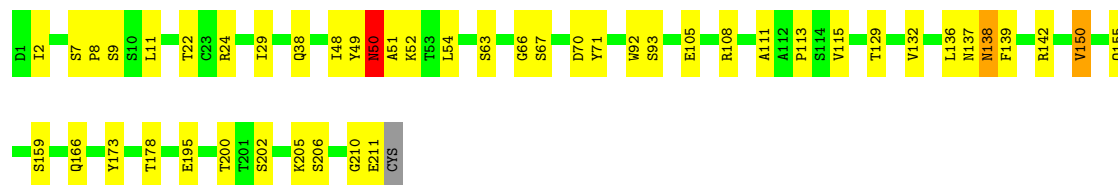
- Molecule 1: Fab heavy chain





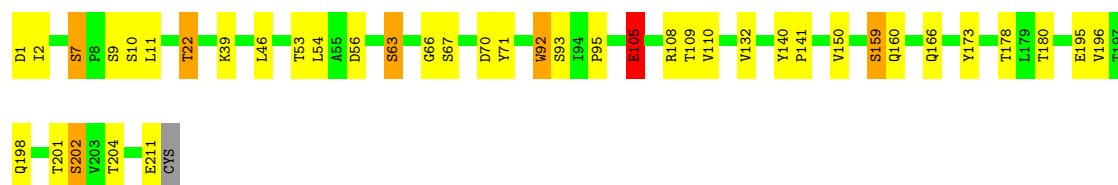
• Molecule 2: Fab light chain

Chain D: 77% 21% .



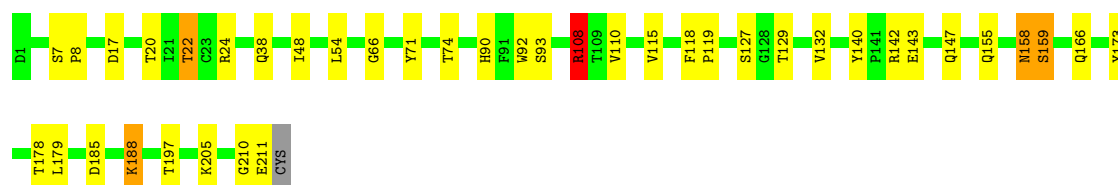
• Molecule 2: Fab light chain

Chain H: 80% 16% .



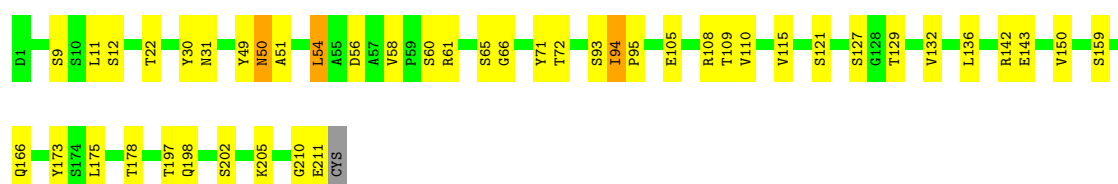
• Molecule 2: Fab light chain

Chain L: 81% 17% .

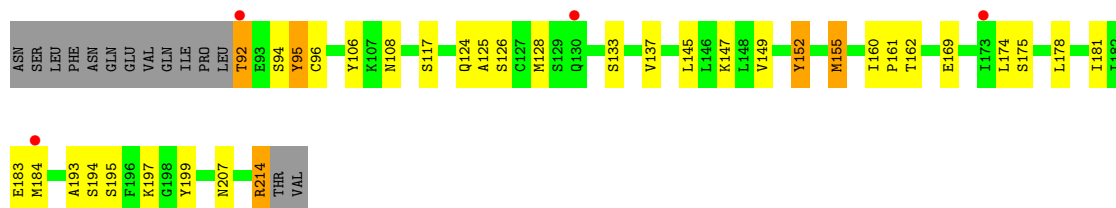


• Molecule 2: Fab light chain

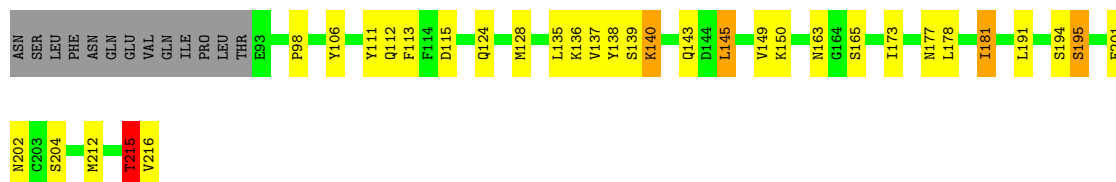
Chain Q: 78% 20% .



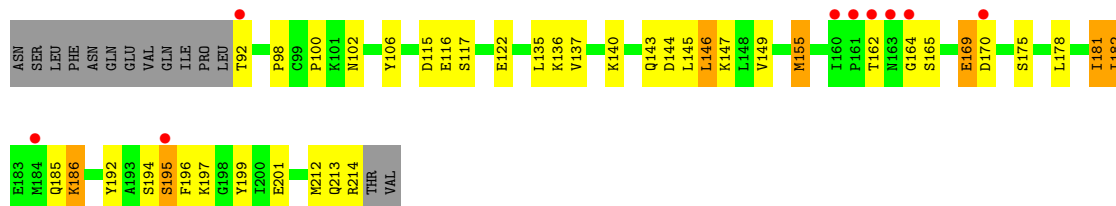
• Molecule 3: NKG2-D type II integral membrane protein



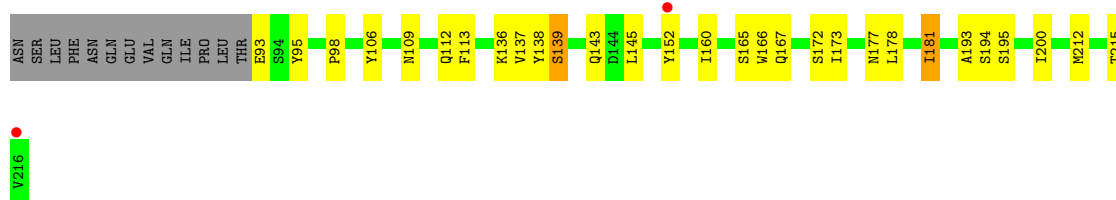
- Molecule 3: NKG2-D type II integral membrane protein



- Molecule 3: NKG2-D type II integral membrane protein



- Molecule 3: NKG2-D type II integral membrane protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.06Å 224.43Å 136.30Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	136.64 – 2.98 136.27 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.3 (136.64-2.98) 97.3 (136.27-2.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.197 , 0.243 0.198 , 0.242	Depositor DCC
R_{free} test set	2758 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17120	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.36% 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	0.70	1/1688 (0.1%)	1.20	3/2298 (0.1%)
1	G	0.65	0/1688	1.31	12/2298 (0.5%)
1	K	0.65	1/1688 (0.1%)	1.20	7/2298 (0.3%)
1	P	0.66	0/1688	1.18	5/2298 (0.2%)
2	D	0.75	2/1672 (0.1%)	1.18	4/2274 (0.2%)
2	H	0.67	0/1672	1.24	11/2274 (0.5%)
2	L	0.62	0/1672	1.19	5/2274 (0.2%)
2	Q	0.63	0/1672	1.14	3/2274 (0.1%)
3	M	0.61	0/1024	1.16	3/1388 (0.2%)
3	R	0.62	0/1032	1.18	4/1398 (0.3%)
3	S	0.61	0/1024	1.19	5/1388 (0.4%)
3	T	0.65	0/1032	1.14	0/1398
All	All	0.66	4/17552 (0.0%)	1.20	62/23860 (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	2
1	G	0	2
1	K	0	1
1	P	0	1
3	M	0	2
3	T	0	1
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	142	ARG	CD-NE	-12.51	1.28	1.46
1	A	136	SER	CA-CB	-8.30	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	142	ARG	CG-CD	5.75	1.69	1.52
1	K	165	SER	CA-CB	-5.70	1.45	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	147	LYS	CA-C-N	-12.14	104.54	123.24
1	G	147	LYS	C-N-CA	-12.14	104.54	123.24
1	G	153	PRO	CB-CA-C	11.17	121.25	111.87
1	A	62	GLN	CB-CG-CD	9.64	128.98	112.60
2	L	158	ASN	CB-CA-C	-9.63	90.01	109.55
2	L	108	ARG	CG-CD-NE	8.64	131.00	112.00
1	G	69	THR	CA-CB-OG1	-8.56	96.77	109.60
2	Q	22	THR	CA-CB-OG1	-8.38	97.03	109.60
3	S	122	GLU	CB-CG-CD	8.30	126.71	112.60
1	K	114	THR	CB-CA-C	8.26	124.24	109.38
1	P	29	PHE	CA-CB-CG	7.43	121.23	113.80
2	D	22	THR	CA-CB-OG1	-7.26	98.71	109.60
1	G	164	THR	CA-CB-OG1	-7.25	98.72	109.60
1	G	66	ASP	CB-CA-C	-7.24	96.78	110.67
2	H	22	THR	CA-CB-OG1	-7.23	98.76	109.60
3	M	183	GLU	CB-CG-CD	7.17	124.78	112.60
3	M	92	THR	CB-CA-C	6.94	124.36	109.10
2	H	211	GLU	CB-CA-C	6.82	123.06	110.10
1	P	169	THR	CB-CA-C	6.72	121.75	110.79
3	M	152	TYR	CB-CA-C	6.54	120.32	109.53
3	R	215	THR	CA-CB-OG1	-6.26	100.22	109.60
2	H	63	SER	CA-C-N	-6.15	117.84	122.33
2	H	63	SER	C-N-CA	-6.15	117.84	122.33
1	P	102	PHE	CA-CB-CG	6.07	119.86	113.80
1	K	29	PHE	CA-CB-CG	6.04	119.84	113.80
2	H	53	THR	CB-CA-C	5.95	119.54	109.84
1	G	74	ARG	CB-CG-CD	5.94	124.96	111.30
2	H	92	TRP	CA-C-N	5.82	129.53	120.75
2	H	92	TRP	C-N-CA	5.82	129.53	120.75
2	D	200	THR	CB-CA-C	5.70	121.21	111.46
3	S	155	MET	N-CA-CB	-5.69	101.65	111.55
1	K	114	THR	CA-CB-OG1	5.65	118.08	109.60
1	P	155	THR	CA-CB-OG1	-5.62	101.17	109.60
2	H	180	THR	CA-CB-OG1	-5.54	101.30	109.60
2	D	50	ASN	CA-C-N	-5.50	111.53	120.72
2	D	50	ASN	C-N-CA	-5.50	111.53	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	170	ASP	CB-CA-C	-5.49	100.48	110.63
2	H	105	GLU	CB-CG-CD	5.44	121.86	112.60
1	A	29	PHE	CB-CA-C	5.42	119.72	111.80
1	P	12	LYS	CG-CD-CE	5.39	123.70	111.30
3	S	169	GLU	CA-C-N	5.38	128.03	120.28
3	S	169	GLU	C-N-CA	5.38	128.03	120.28
3	R	215	THR	CA-C-N	5.32	131.28	121.70
3	R	215	THR	C-N-CA	5.32	131.28	121.70
2	H	105	GLU	N-CA-CB	-5.29	102.70	110.85
2	Q	143	GLU	CB-CG-CD	5.29	121.59	112.60
2	L	17	ASP	CA-C-N	5.26	128.32	120.95
2	L	17	ASP	C-N-CA	5.26	128.32	120.95
1	G	139	THR	CB-CA-C	5.25	118.30	109.48
1	A	114	THR	OG1-CB-CG2	5.24	119.79	109.30
1	G	195	THR	CB-CA-C	-5.24	104.29	112.31
1	G	29	PHE	CA-CB-CG	5.21	119.02	113.80
1	K	124	SER	CB-CA-C	5.19	118.20	109.48
1	K	155	THR	CA-C-N	-5.16	116.44	123.10
1	K	155	THR	C-N-CA	-5.16	116.44	123.10
1	G	87	ARG	CB-CG-CD	5.10	123.02	111.30
1	K	195	THR	CB-CA-C	5.07	118.84	110.83
1	G	195	THR	CA-CB-OG1	-5.05	102.03	109.60
3	R	115	ASP	CB-CA-C	-5.03	99.47	109.99
2	Q	108	ARG	CG-CD-NE	-5.03	100.93	112.00
2	H	180	THR	CB-CA-C	5.01	118.41	110.19
2	L	147	GLN	CB-CG-CD	-5.00	104.10	112.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	ALA	Peptide
1	A	83	LEU	Peptide
1	G	151	PRO	Peptide
1	G	43	GLN	Peptide
1	K	130	PRO	Peptide
3	M	193	ALA	Peptide
3	M	95	TYR	Peptide
1	P	43	GLN	Peptide
3	T	193	ALA	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	1646	0	1601	20	0
1	G	1646	0	1601	26	0
1	K	1646	0	1601	27	0
1	P	1646	0	1601	17	0
2	D	1634	0	1584	23	0
2	H	1634	0	1584	18	0
2	L	1634	0	1584	22	0
2	Q	1634	0	1584	18	0
3	M	996	0	933	22	0
3	R	1004	0	942	29	0
3	S	996	0	933	36	0
3	T	1004	0	942	21	0
All	All	17120	0	16490	255	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 (255) 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)
3:S:155:MET:HE3	3:S:192:TYR:HB2	1.34	1.05
3:S:155:MET:HE3	3:S:192:TYR:CB	1.91	0.99
3:R:135:LEU:HD12	3:R:212:MET:HE3	1.48	0.94
1:G:152:GLU:O	1:G:152:GLU:HG2	1.67	0.94
1:A:39:GLN:HE22	2:D:38:GLN:HE22	1.12	0.92
1:A:6:GLN:HE21	1:A:108:GLY:HA3	1.35	0.91
3:S:155:MET:HE3	3:S:192:TYR:CA	2.03	0.87
3:R:135:LEU:HD12	3:R:212:MET:CE	2.05	0.86
3:S:155:MET:CE	3:S:192:TYR:HB2	2.07	0.84
3:R:149:VAL:O	3:R:194:SER:HB2	1.79	0.81
2:Q:93:SER:HA	3:S:181:ILE:HG22	1.62	0.81
3:R:136:LYS:O	3:R:212:MET:HE1	1.81	0.80
2:L:90:HIS:HD2	2:L:92:TRP:H	1.30	0.77
3:T:138:TYR:H	3:T:143:GLN:NE2	1.83	0.77
3:M:152:TYR:HE1	3:M:207:ASN:ND2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:105:GLU:HG2	2:H:166:GLN:OE1	1.84	0.76
1:K:91:THR:HG23	1:K:114:THR:HG22	1.67	0.75
2:Q:105:GLU:OE2	2:Q:142:ARG:NH2	2.20	0.74
2:L:155:GLN:HB3	2:L:158:ASN:HD22	1.52	0.74
2:L:155:GLN:HB3	2:L:158:ASN:ND2	2.02	0.74
3:M:152:TYR:HE1	3:M:207:ASN:HD21	1.32	0.73
3:M:124:GLN:HG3	3:M:169:GLU:OE1	1.88	0.72
1:K:203:ASN:HD21	1:K:205:LYS:HD2	1.53	0.72
3:R:138:TYR:H	3:R:143:GLN:NE2	1.88	0.71
1:A:39:GLN:NE2	2:D:38:GLN:HE22	1.88	0.70
3:R:112:GLN:HE21	3:R:113:PHE:H	1.40	0.69
3:S:155:MET:HE2	3:S:192:TYR:HD1	1.56	0.69
1:K:203:ASN:ND2	1:K:205:LYS:HD2	2.07	0.69
1:G:103:TYR:CD2	2:H:46:LEU:HD22	2.29	0.69
1:K:39:GLN:HE22	2:L:38:GLN:HE22	1.41	0.68
2:L:20:THR:HG22	2:L:74:THR:OG1	1.94	0.68
3:S:149:VAL:O	3:S:194:SER:HB2	1.95	0.67
3:T:138:TYR:H	3:T:143:GLN:HE22	1.43	0.67
3:R:201:GLU:HG2	3:R:202:ASN:H	1.59	0.67
3:M:194:SER:HB3	3:M:197:LYS:HG3	1.78	0.65
3:S:135:LEU:HD21	3:S:146:LEU:HD21	1.79	0.65
1:A:99:MET:HG2	3:R:177:ASN:HD22	1.63	0.63
3:S:155:MET:HE3	3:S:192:TYR:HA	1.81	0.63
2:L:90:HIS:CD2	2:L:92:TRP:H	2.16	0.63
3:R:106:TYR:CD2	3:R:145:LEU:HD23	2.34	0.63
3:S:100:PRO:HA	3:T:93:GLU:HG2	1.79	0.63
3:T:160:ILE:HD12	3:T:167:GLN:CD	2.24	0.63
1:G:4:LEU:HD23	1:G:96:CYS:SG	2.38	0.63
3:R:194:SER:O	3:R:195:SER:HB2	1.99	0.63
3:T:112:GLN:HE21	3:T:113:PHE:H	1.47	0.63
1:G:182:LEU:C	1:G:182:LEU:HD23	2.24	0.62
1:K:34:MET:HE1	1:K:96:CYS:HB2	1.82	0.62
3:R:124:GLN:NE2	3:R:128:MET:HE2	2.13	0.62
1:K:182:LEU:C	1:K:182:LEU:HD12	2.25	0.62
1:A:52:ASP:OD2	3:R:140:LYS:HE2	1.99	0.61
2:L:185:ASP:HA	2:L:188:LYS:HD3	1.83	0.61
2:H:105:GLU:HG3	2:H:173:TYR:OH	1.99	0.61
1:P:72:VAL:HG22	1:P:79:VAL:HG22	1.81	0.61
3:S:185:GLN:OE1	3:S:201:GLU:OE1	2.19	0.61
2:Q:31:ASN:HD21	3:S:164:GLY:HA3	1.64	0.61
1:A:6:GLN:NE2	1:A:108:GLY:HA3	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:152:TYR:CE1	3:M:207:ASN:ND2	2.66	0.60
1:G:34:MET:HE3	1:G:96:CYS:HB2	1.83	0.60
3:S:182:ILE:HG13	3:S:199:TYR:CE1	2.37	0.60
1:A:182:LEU:C	1:A:182:LEU:HD12	2.27	0.60
3:S:155:MET:HE2	3:S:192:TYR:CD1	2.37	0.58
3:S:155:MET:CE	3:S:192:TYR:CB	2.71	0.58
3:M:108:ASN:O	3:M:214:ARG:HD3	2.03	0.58
2:H:140:TYR:CG	2:H:141:PRO:HA	2.39	0.57
2:H:198:GLN:HB2	2:H:201:THR:O	2.04	0.57
2:L:158:ASN:HB3	2:L:179:LEU:HD12	1.86	0.57
3:M:96:CYS:SG	3:M:96:CYS:O	2.63	0.57
3:S:155:MET:CE	3:S:192:TYR:HA	2.35	0.56
1:P:182:LEU:C	1:P:182:LEU:HD12	2.31	0.56
2:Q:30:TYR:HB3	3:S:165:SER:HA	1.86	0.56
3:R:124:GLN:HE21	3:R:128:MET:HE2	1.70	0.56
3:R:112:GLN:HE21	3:R:113:PHE:N	2.03	0.56
3:R:191:LEU:HD11	3:R:201:GLU:OE1	2.05	0.56
1:P:174:LEU:HD13	1:P:180:TYR:CE2	2.40	0.56
2:Q:65:SER:HB3	2:Q:72:THR:HG22	1.88	0.56
1:A:72:VAL:HG22	1:A:79:VAL:HG22	1.88	0.56
2:Q:166:GLN:HG3	2:Q:173:TYR:CE1	2.40	0.55
3:R:201:GLU:HG2	3:R:202:ASN:N	2.21	0.55
3:T:112:GLN:NE2	3:T:113:PHE:H	2.04	0.55
1:G:34:MET:CE	1:G:36:TRP:NE1	2.69	0.55
2:Q:54:LEU:HD21	2:Q:58:VAL:O	2.06	0.55
1:P:11:VAL:HG21	1:P:151:PRO:HG3	1.87	0.55
2:D:48:ILE:HD13	2:D:54:LEU:HD12	1.88	0.55
3:R:106:TYR:HD2	3:R:145:LEU:HD23	1.72	0.54
1:A:99:MET:HG2	3:R:177:ASN:ND2	2.22	0.54
3:T:98:PRO:HD2	3:T:215:THR:HG23	1.89	0.54
3:R:163:ASN:HB3	3:R:165:SER:OG	2.06	0.54
1:K:55:ASP:OD2	3:M:147:LYS:HE2	2.07	0.54
2:Q:49:TYR:C	2:Q:50:ASN:O	2.50	0.54
2:L:108:ARG:HG2	2:L:140:TYR:CG	2.41	0.54
3:R:137:VAL:HA	3:R:143:GLN:HE22	1.71	0.54
2:D:49:TYR:C	2:D:50:ASN:O	2.50	0.54
1:K:142:LEU:HD12	1:K:142:LEU:C	2.34	0.53
1:K:43:GLN:HG3	1:K:44:GLY:O	2.09	0.53
2:Q:65:SER:HB3	2:Q:72:THR:CG2	2.39	0.52
3:S:182:ILE:HB	3:S:199:TYR:HD1	1.73	0.52
2:L:166:GLN:HG3	2:L:173:TYR:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:93:SER:HA	3:T:181:ILE:HG22	1.92	0.52
1:K:24:ALA:O	1:K:25:SER:HB3	2.09	0.52
3:M:184:MET:SD	3:M:199:TYR:HD2	2.33	0.52
1:A:142:LEU:HD12	1:A:142:LEU:C	2.35	0.52
3:M:160:ILE:O	3:M:162:THR:N	2.44	0.51
2:D:115:VAL:O	2:D:205:LYS:HE3	2.10	0.51
1:G:136:SER:HB2	1:G:139:THR:O	2.10	0.51
2:L:48:ILE:CD1	2:L:54:LEU:HD12	2.41	0.51
3:M:137:VAL:HG23	3:M:155:MET:CE	2.40	0.51
2:Q:93:SER:CA	3:S:181:ILE:HG22	2.38	0.51
3:M:174:LEU:HD21	3:M:181:ILE:HD11	1.93	0.51
2:D:2:ILE:HD13	2:D:29:ILE:HG22	1.93	0.50
1:P:142:LEU:C	1:P:142:LEU:HD12	2.36	0.50
2:D:108:ARG:NH2	2:D:111:ALA:HB2	2.26	0.50
1:G:142:LEU:C	1:G:142:LEU:HD12	2.36	0.50
2:H:1:ASP:HB3	2:H:95:PRO:HD2	1.92	0.50
3:M:95:TYR:CZ	3:R:98:PRO:HG3	2.47	0.50
3:M:194:SER:OG	3:M:195:SER:N	2.45	0.50
2:Q:115:VAL:O	2:Q:205:LYS:HE3	2.12	0.50
1:G:69:THR:HG22	1:G:82:GLU:HB3	1.94	0.49
2:L:48:ILE:HD13	2:L:54:LEU:HD12	1.92	0.49
1:K:11:VAL:HG21	1:K:151:PRO:HG3	1.94	0.49
3:S:182:ILE:HB	3:S:199:TYR:CD1	2.47	0.49
3:M:133:SER:HB2	3:M:169:GLU:OE2	2.13	0.49
2:D:93:SER:HA	3:R:181:ILE:HG22	1.94	0.49
1:G:143:GLY:HA2	1:G:158:TRP:CH2	2.48	0.49
1:K:197:THR:HG23	1:K:214:LYS:HD2	1.95	0.48
3:T:137:VAL:HA	3:T:143:GLN:HE22	1.78	0.48
2:D:150:VAL:HG13	2:D:155:GLN:CG	2.43	0.48
2:D:166:GLN:HG3	2:D:173:TYR:CE1	2.49	0.48
3:T:194:SER:OG	3:T:195:SER:N	2.46	0.48
3:T:112:GLN:HE21	3:T:113:PHE:N	2.09	0.47
1:G:34:MET:HB3	1:G:34:MET:HE2	1.65	0.47
3:R:112:GLN:NE2	3:R:113:PHE:H	2.09	0.47
1:A:199:ILE:HA	1:A:213:LYS:O	2.15	0.47
2:L:115:VAL:O	2:L:205:LYS:HE3	2.14	0.47
3:S:155:MET:CE	3:S:192:TYR:HD1	2.24	0.47
2:Q:94:ILE:HD12	2:Q:95:PRO:HA	1.96	0.47
1:G:34:MET:HE1	1:G:36:TRP:NE1	2.30	0.47
1:P:127:PRO:HD2	2:Q:121:SER:HB3	1.95	0.47
1:A:143:GLY:HA2	1:A:158:TRP:CH2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:143:GLY:HA2	1:P:158:TRP:CH2	2.50	0.47
3:S:98:PRO:HD3	3:T:95:TYR:CE2	2.49	0.47
2:Q:66:GLY:HA3	2:Q:71:TYR:HA	1.97	0.47
3:T:139:SER:H	3:T:143:GLN:HE21	1.62	0.47
1:A:43:GLN:HG2	1:A:44:GLY:O	2.15	0.46
3:M:214:ARG:HA	3:M:214:ARG:HD2	1.56	0.46
2:D:48:ILE:CD1	2:D:54:LEU:HD12	2.45	0.46
3:T:166:TRP:CH2	3:T:200:ILE:HD12	2.50	0.46
1:G:199:ILE:HA	1:G:213:LYS:O	2.15	0.46
2:L:210:GLY:O	2:L:211:GLU:C	2.58	0.46
3:S:194:SER:O	3:S:195:SER:OG	2.23	0.46
2:L:22:THR:HG22	2:L:71:TYR:O	2.16	0.46
3:S:144:ASP:O	3:S:147:LYS:HB2	2.16	0.46
1:A:99:MET:CG	3:R:177:ASN:ND2	2.79	0.46
1:A:3:GLN:NE2	1:A:109:GLN:HG2	2.31	0.45
1:G:173:VAL:CG2	2:H:160:GLN:NE2	2.79	0.45
1:G:130:PRO:HD3	1:G:142:LEU:CB	2.47	0.45
1:P:199:ILE:HA	1:P:213:LYS:O	2.16	0.45
2:Q:159:SER:HA	2:Q:178:THR:O	2.16	0.45
3:S:213:GLN:HG2	3:S:214:ARG:N	2.31	0.45
1:K:130:PRO:HD3	1:K:142:LEU:HB3	1.98	0.45
3:S:213:GLN:HG2	3:S:214:ARG:H	1.82	0.45
3:R:111:TYR:HE2	3:R:212:MET:HE2	1.81	0.45
1:G:2:VAL:HA	1:G:106:TYR:CE2	2.51	0.45
2:D:137:ASN:O	2:D:138:ASN:CB	2.62	0.45
1:G:4:LEU:HD23	1:G:22:CYS:SG	2.57	0.45
1:P:7:SER:HG	1:P:21:SER:H	1.61	0.45
3:M:137:VAL:CG2	3:M:155:MET:CE	2.95	0.44
1:K:199:ILE:HA	1:K:213:LYS:O	2.18	0.44
2:L:66:GLY:HA3	2:L:71:TYR:HA	1.99	0.44
3:T:136:LYS:HB3	3:T:212:MET:HE1	1.99	0.44
2:D:137:ASN:O	2:D:138:ASN:CG	2.61	0.44
2:L:159:SER:HA	2:L:178:THR:O	2.18	0.44
1:P:4:LEU:HD22	1:P:22:CYS:SG	2.56	0.44
2:D:50:ASN:O	2:D:51:ALA:C	2.58	0.44
1:G:91:THR:HG23	1:G:114:THR:HA	1.99	0.44
1:K:130:PRO:HD3	1:K:142:LEU:CB	2.47	0.44
1:G:130:PRO:HD3	1:G:142:LEU:HB3	1.98	0.44
1:K:72:VAL:HG23	1:K:79:VAL:HG22	1.98	0.44
1:P:35:HIS:CE1	1:P:50:LYS:HD2	2.53	0.44
3:S:155:MET:CE	3:S:192:TYR:CD1	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:TYR:CG	2:H:46:LEU:HD22	2.53	0.44
1:G:152:GLU:O	1:G:152:GLU:CG	2.49	0.44
2:H:159:SER:HA	2:H:178:THR:O	2.18	0.44
1:K:39:GLN:HE22	2:L:38:GLN:NE2	2.14	0.44
1:A:34:MET:HE3	1:A:34:MET:HB2	1.78	0.44
2:D:113:PRO:HB3	2:D:139:PHE:HB3	1.99	0.44
1:K:53:LEU:HG	1:K:72:VAL:HG21	2.00	0.44
2:H:108:ARG:HG2	2:H:109:THR:N	2.33	0.43
2:H:92:TRP:CG	2:H:93:SER:H	2.37	0.43
1:K:24:ALA:C	1:K:26:GLY:H	2.26	0.43
3:S:102:ASN:HD22	3:S:102:ASN:N	2.15	0.43
1:A:39:GLN:HE22	2:D:38:GLN:NE2	1.96	0.43
3:R:216:VAL:HG22	3:R:216:VAL:O	2.18	0.43
2:L:7:SER:HA	2:L:8:PRO:HA	1.86	0.43
2:Q:210:GLY:O	2:Q:211:GLU:C	2.62	0.43
3:R:98:PRO:HD2	3:R:215:THR:HG23	2.01	0.43
2:H:196:VAL:O	2:H:202:SER:HA	2.19	0.43
2:H:66:GLY:HA3	2:H:71:TYR:HA	1.99	0.43
3:S:136:LYS:HB3	3:S:212:MET:HE1	2.00	0.43
3:S:143:GLN:HB3	3:S:146:LEU:HD13	2.00	0.43
2:D:159:SER:HA	2:D:178:THR:O	2.18	0.42
1:G:34:MET:CE	1:G:36:TRP:HE1	2.31	0.42
3:T:166:TRP:CZ2	3:T:200:ILE:HD12	2.54	0.42
1:A:91:THR:HG23	1:A:114:THR:HA	1.99	0.42
1:K:205:LYS:N	1:K:206:PRO:CD	2.82	0.42
2:D:166:GLN:HG3	2:D:173:TYR:CZ	2.54	0.42
1:A:91:THR:HA	1:A:113:VAL:O	2.19	0.42
3:T:138:TYR:N	3:T:143:GLN:HE22	2.12	0.42
2:D:92:TRP:CG	2:D:93:SER:N	2.88	0.42
2:H:195:GLU:HG3	2:H:204:THR:OG1	2.19	0.42
1:P:18:VAL:HG12	1:P:86:LEU:HD21	2.02	0.42
3:S:137:VAL:O	3:S:178:LEU:HD21	2.19	0.42
3:S:155:MET:CE	3:S:192:TYR:CA	2.84	0.42
1:G:34:MET:HE1	1:G:36:TRP:CE2	2.54	0.42
2:H:7:SER:OG	2:H:22:THR:HB	2.20	0.42
3:M:137:VAL:HG21	3:M:155:MET:HE1	2.02	0.42
1:P:91:THR:HA	1:P:113:VAL:O	2.20	0.42
2:Q:136:LEU:HB2	2:Q:175:LEU:HB3	2.02	0.42
2:D:210:GLY:O	2:D:211:GLU:HG3	2.19	0.42
1:G:91:THR:HA	1:G:113:VAL:O	2.20	0.42
3:S:106:TYR:CD2	3:S:145:LEU:HD22	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:50:ASN:O	2:Q:51:ALA:C	2.61	0.41
3:S:194:SER:O	3:S:197:LYS:HE2	2.20	0.41
3:T:152:TYR:N	3:T:152:TYR:CD1	2.88	0.41
1:K:34:MET:HB3	1:K:34:MET:HE3	1.66	0.41
1:K:36:TRP:HE1	1:K:79:VAL:HG11	1.85	0.41
2:L:158:ASN:CB	2:L:179:LEU:HD12	2.49	0.41
2:D:7:SER:HA	2:D:8:PRO:HA	1.76	0.41
2:D:66:GLY:HA3	2:D:71:TYR:HA	2.03	0.41
2:D:210:GLY:O	2:D:211:GLU:CG	2.69	0.41
1:K:91:THR:HA	1:K:113:VAL:O	2.20	0.41
3:R:178:LEU:HD12	3:R:178:LEU:HA	1.88	0.41
3:S:186:LYS:HD2	3:S:186:LYS:HA	1.74	0.41
1:G:152:GLU:N	1:G:153:PRO:CD	2.84	0.41
3:M:106:TYR:CD2	3:M:145:LEU:HD22	2.56	0.41
3:M:160:ILE:C	3:M:162:THR:H	2.29	0.41
1:P:130:PRO:HD3	1:P:142:LEU:HB3	2.03	0.41
1:K:32:TYR:CD1	1:K:53:LEU:HD13	2.55	0.41
3:M:125:ALA:HA	3:M:128:MET:HE3	2.03	0.41
1:P:91:THR:HG23	1:P:114:THR:HA	2.02	0.41
1:A:214:LYS:HE2	1:A:216:GLU:OE2	2.21	0.41
1:K:174:LEU:HD23	1:K:175:GLN:O	2.19	0.41
3:R:138:TYR:H	3:R:143:GLN:HE22	1.62	0.41
1:G:99:MET:HG2	3:T:177:ASN:HD22	1.86	0.41
1:P:130:PRO:HD3	1:P:142:LEU:CB	2.51	0.41
3:T:178:LEU:HD12	3:T:178:LEU:HA	1.87	0.41
3:M:137:VAL:CG2	3:M:155:MET:HE1	2.51	0.41
3:T:106:TYR:CD2	3:T:145:LEU:HD22	2.56	0.40
3:S:140:LYS:HA	3:S:196:PHE:CZ	2.56	0.40
1:K:182:LEU:C	1:K:182:LEU:CD1	2.94	0.40
2:L:92:TRP:CG	2:L:93:SER:N	2.89	0.40
2:L:118:PHE:HA	2:L:119:PRO:HD3	1.96	0.40
2:H:1:ASP:CB	2:H:95:PRO:HD2	2.52	0.40
2:H:140:TYR:CD1	2:H:141:PRO:HA	2.57	0.40
1:K:43:GLN:HG3	1:K:44:GLY:N	2.37	0.40
1:P:34:MET:HB2	1:P:34:MET:HE3	1.78	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	215/220 (98%)	205 (95%)	10 (5%)	0	100	100
1	G	215/220 (98%)	205 (95%)	10 (5%)	0	100	100
1	K	215/220 (98%)	208 (97%)	7 (3%)	0	100	100
1	P	215/220 (98%)	206 (96%)	9 (4%)	0	100	100
2	D	209/212 (99%)	199 (95%)	8 (4%)	2 (1%)	12	42
2	H	209/212 (99%)	197 (94%)	12 (6%)	0	100	100
2	L	209/212 (99%)	201 (96%)	8 (4%)	0	100	100
2	Q	209/212 (99%)	200 (96%)	8 (4%)	1 (0%)	24	58
3	M	121/137 (88%)	113 (93%)	7 (6%)	1 (1%)	16	47
3	R	122/137 (89%)	115 (94%)	6 (5%)	1 (1%)	16	47
3	S	121/137 (88%)	111 (92%)	9 (7%)	1 (1%)	16	47
3	T	122/137 (89%)	114 (93%)	8 (7%)	0	100	100
All	All	2182/2276 (96%)	2074 (95%)	102 (5%)	6 (0%)	36	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	R	195	SER
3	S	195	SER
2	Q	50	ASN
2	D	50	ASN
2	D	138	ASN
3	M	161	PRO

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	186/189 (98%)	171 (92%)	15 (8%)	11	36
1	G	186/189 (98%)	173 (93%)	13 (7%)	14	42
1	K	186/189 (98%)	168 (90%)	18 (10%)	8	29
1	P	186/189 (98%)	172 (92%)	14 (8%)	12	39
2	D	184/185 (100%)	169 (92%)	15 (8%)	10	35
2	H	184/185 (100%)	167 (91%)	17 (9%)	8	31
2	L	184/185 (100%)	172 (94%)	12 (6%)	15	45
2	Q	184/185 (100%)	167 (91%)	17 (9%)	8	31
3	M	113/127 (89%)	104 (92%)	9 (8%)	11	36
3	R	114/127 (90%)	106 (93%)	8 (7%)	14	42
3	S	113/127 (89%)	102 (90%)	11 (10%)	8	29
3	T	114/127 (90%)	108 (95%)	6 (5%)	20	52
All	All	1934/2004 (96%)	1779 (92%)	155 (8%)	11	36

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	17	SER
1	A	25	SER
1	A	34	MET
1	A	67	ARG
1	A	71	THR
1	A	74	ARG
1	A	114	THR
1	A	117	SER
1	A	133	LYS
1	A	134	SER
1	A	154	VAL
1	A	155	THR
1	A	190	SER
1	A	218	LYS
2	D	9	SER
2	D	11	LEU
2	D	24	ARG

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Mol	Chain	Res	Type
2	D	52	LYS
2	D	63	SER
2	D	67	SER
2	D	70	ASP
2	D	105	GLU
2	D	129	THR
2	D	132	VAL
2	D	136	LEU
2	D	150	VAL
2	D	195	GLU
2	D	202	SER
2	D	206	SER
1	G	17	SER
1	G	34	MET
1	G	71	THR
1	G	87	ARG
1	G	119	SER
1	G	133	LYS
1	G	136	SER
1	G	139	THR
1	G	154	VAL
1	G	173	VAL
1	G	182	LEU
1	G	190	SER
1	G	213	LYS
2	H	2	ILE
2	H	7	SER
2	H	9	SER
2	H	10	SER
2	H	11	LEU
2	H	39	LYS
2	H	54	LEU
2	H	56	ASP
2	H	63	SER
2	H	67	SER
2	H	70	ASP
2	H	105	GLU
2	H	110	VAL
2	H	132	VAL
2	H	150	VAL
2	H	159	SER
2	H	202	SER

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Mol	Chain	Res	Type
1	K	3	GLN
1	K	4	LEU
1	K	17	SER
1	K	34	MET
1	K	69	THR
1	K	98	LYS
1	K	131	SER
1	K	134	SER
1	K	135	THR
1	K	136	SER
1	K	139	THR
1	K	154	VAL
1	K	155	THR
1	K	156	VAL
1	K	190	SER
1	K	195	THR
1	K	196	GLN
1	K	199	ILE
2	L	22	THR
2	L	24	ARG
2	L	108	ARG
2	L	110	VAL
2	L	127	SER
2	L	129	THR
2	L	132	VAL
2	L	142	ARG
2	L	143	GLU
2	L	159	SER
2	L	188	LYS
2	L	197	THR
3	M	92	THR
3	M	94	SER
3	M	117	SER
3	M	126	SER
3	M	149	VAL
3	M	155	MET
3	M	175	SER
3	M	178	LEU
3	M	214	ARG
1	P	7	SER
1	P	17	SER
1	P	46	GLU

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Mol	Chain	Res	Type
1	P	102	PHE
1	P	136	SER
1	P	154	VAL
1	P	155	THR
1	P	173	VAL
1	P	187	THR
1	P	191	SER
1	P	193	LEU
1	P	197	THR
1	P	213	LYS
1	P	218	LYS
2	Q	9	SER
2	Q	11	LEU
2	Q	12	SER
2	Q	54	LEU
2	Q	56	ASP
2	Q	60	SER
2	Q	61	ARG
2	Q	94	ILE
2	Q	109	THR
2	Q	110	VAL
2	Q	127	SER
2	Q	129	THR
2	Q	132	VAL
2	Q	150	VAL
2	Q	197	THR
2	Q	198	GLN
2	Q	202	SER
3	R	139	SER
3	R	140	LYS
3	R	145	LEU
3	R	150	LYS
3	R	173	ILE
3	R	181	ILE
3	R	204	SER
3	R	215	THR
3	S	92	THR
3	S	115	ASP
3	S	116	GLU
3	S	117	SER
3	S	146	LEU
3	S	162	THR

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Mol	Chain	Res	Type
3	S	169	GLU
3	S	175	SER
3	S	181	ILE
3	S	182	ILE
3	S	186	LYS
3	T	109	ASN
3	T	139	SER
3	T	165	SER
3	T	172	SER
3	T	173	ILE
3	T	181	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	6	GLN
1	A	39	GLN
1	A	62	GLN
2	D	189	HIS
2	D	198	GLN
2	H	37	GLN
2	H	160	GLN
2	H	189	HIS
2	H	198	GLN
1	K	39	GLN
1	K	196	GLN
1	K	203	ASN
2	L	79	GLN
2	L	90	HIS
2	L	158	ASN
2	L	189	HIS
3	M	102	ASN
3	M	109	ASN
3	M	153	HIS
3	M	167	GLN
3	M	185	GLN
3	M	207	ASN
1	P	168	HIS
1	P	196	GLN
2	Q	31	ASN
2	Q	50	ASN

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Mol	Chain	Res	Type
2	Q	138	ASN
2	Q	160	GLN
3	R	112	GLN
3	R	143	GLN
3	R	177	ASN
3	R	207	ASN
3	R	213	GLN
3	S	102	ASN
3	S	130	GLN
3	S	213	GLN
3	T	112	GLN
3	T	130	GLN
3	T	143	GLN
3	T	177	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	217/220 (98%)	-0.42	3 (1%) 73 55	29, 41, 61, 99	0
1	G	217/220 (98%)	-0.30	5 (2%) 61 42	30, 44, 73, 94	0
1	K	217/220 (98%)	-0.15	9 (4%) 41 25	28, 46, 80, 144	0
1	P	217/220 (98%)	-0.21	7 (3%) 50 33	29, 46, 81, 140	0
2	D	211/212 (99%)	-0.35	0 100 100	31, 47, 65, 80	0
2	H	211/212 (99%)	-0.51	0 100 100	26, 38, 53, 69	0
2	L	211/212 (99%)	-0.40	0 100 100	30, 46, 65, 79	0
2	Q	211/212 (99%)	-0.27	0 100 100	29, 51, 75, 90	0
3	M	123/137 (89%)	0.27	4 (3%) 49 32	46, 65, 95, 130	0
3	R	124/137 (90%)	-0.25	0 100 100	36, 51, 79, 104	0
3	S	123/137 (89%)	0.41	9 (7%) 21 13	47, 69, 96, 111	0
3	T	124/137 (90%)	-0.07	2 (1%) 70 51	39, 55, 87, 104	0
All	All	2206/2276 (96%)	-0.23	39 (1%) 67 48	26, 47, 80, 144	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	2	VAL	5.7
1	P	135	THR	5.3
3	M	92	THR	4.2
1	G	2	VAL	4.0
3	S	92	THR	3.5
1	P	133	LYS	3.4
1	K	29	PHE	3.3
3	T	216	VAL	3.2
1	P	137	GLY	3.2
1	P	2	VAL	3.1
1	P	29	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	106	TYR	2.9
3	S	170	ASP	2.8
3	S	162	THR	2.8
3	S	195	SER	2.6
3	M	184	MET	2.5
1	P	132	SER	2.5
1	A	29	PHE	2.4
1	K	135	THR	2.4
3	M	173	ILE	2.4
3	S	160	ILE	2.4
3	T	152	TYR	2.4
3	S	161	PRO	2.3
3	S	163	ASN	2.3
1	G	29	PHE	2.3
1	K	74	ARG	2.3
1	K	103	TYR	2.2
1	G	133	LYS	2.2
1	A	2	VAL	2.2
1	K	132	SER	2.2
3	S	164	GLY	2.2
1	K	42	GLY	2.2
1	K	218	LYS	2.2
1	G	3	GLN	2.1
1	P	218	LYS	2.1
1	G	134	SER	2.1
3	M	130	GLN	2.1
1	A	218	LYS	2.0
3	S	184	MET	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.