



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:01 PM UTC

PDB ID : 6IAP / pdb_00006iap
Title : structure of human NKp46 in complex with antibody NKp46-1 and NKp46-4
Authors : Roussel, A.; Amigues, B.
Deposited on : 2018-11-27
Resolution : 2.90 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

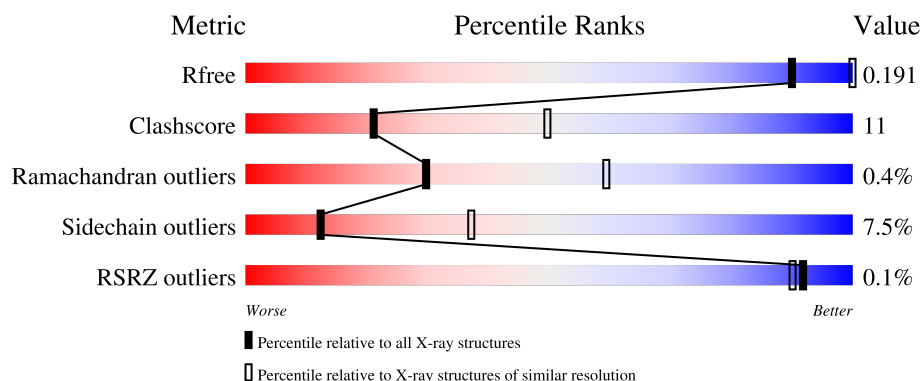
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	182	
2	D	211	
3	E	217	
4	H	220	
5	L	211	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8138 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 Natural cytotoxicity triggering receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1444	929	241	264	10			

- Molecule 2 is a protein called Fab NKp46-4 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	211	Total	C	N	O	S	0	0	0
			1622	1017	274	326	5			

- Molecule 3 is a protein called Fab NKp46-4 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	217	Total	C	N	O	S	7	0	0
			1625	1025	270	324	6			

- Molecule 4 is a protein called Fab NKp46-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	220	Total	C	N	O	S	0	0	0
			1653	1042	275	329	7			

- Molecule 5 is a protein called Fab NKp46-1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	211	Total	C	N	O	S	0	0	0
			1635	1023	279	328	5			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	30	Total	O	0	0
			30	30		

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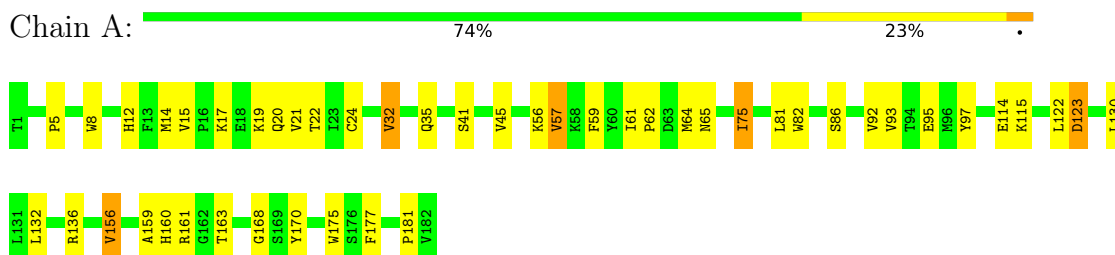
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	27	Total 27	O 27	0	0
6	E	44	Total 44	O 44	0	0
6	H	30	Total 30	O 30	0	0
6	L	28	Total 28	O 28	0	0

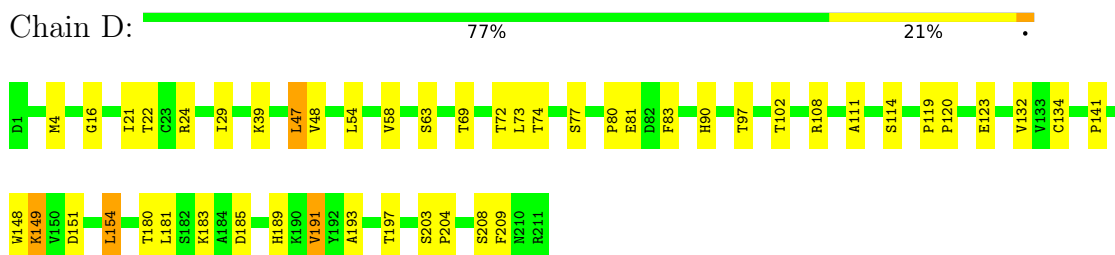
3 Residue-property plots

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.

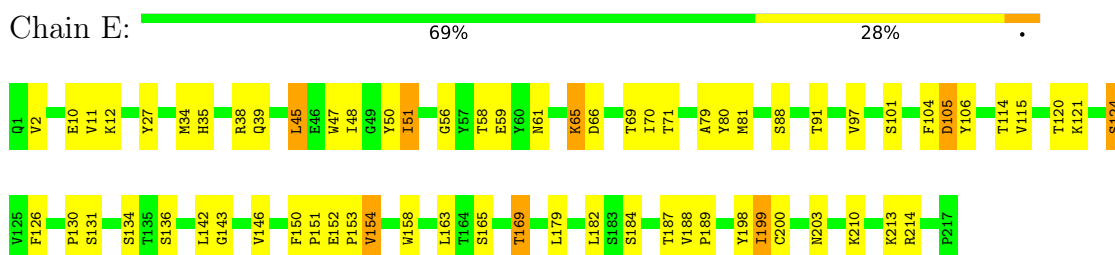
- Molecule 1: Natural cytotoxicity triggering receptor 1



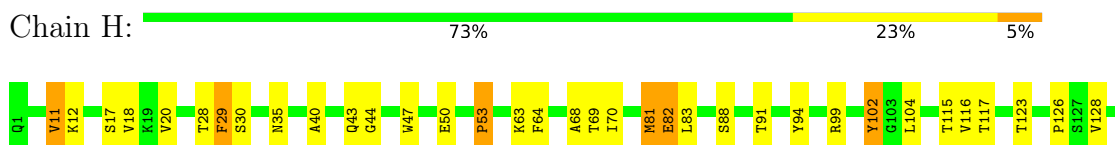
- Molecule 2: Fab NKp46-4 light chain



- Molecule 3: Fab NKp46-4 heavy chain

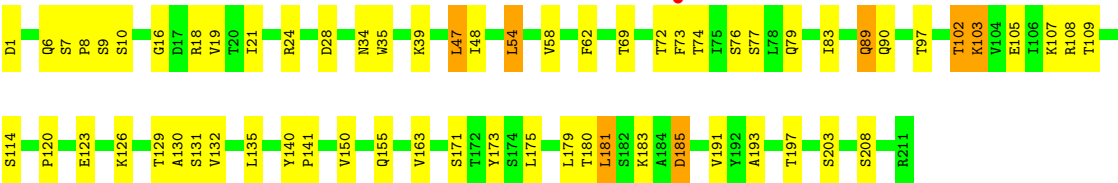


- Molecule 4: Fab NKp46-1 heavy chain





● Molecule 5: Fab NKp46-1 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.86Å 73.83Å 128.52Å 90.00° 90.57° 90.00°	Depositor
Resolution (Å)	48.47 – 2.90 48.47 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.47-2.90) 99.5 (48.47-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.187 , 0.263 0.195 , 0.191	Depositor DCC
R_{free} test set	1439 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 91.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8138	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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	0/1491	1.26	11/2031 (0.5%)
2	D	0.84	0/1659	1.27	6/2255 (0.3%)
3	E	0.92	0/1665	1.32	4/2269 (0.2%)
4	H	0.85	1/1693 (0.1%)	1.31	8/2305 (0.3%)
5	L	0.78	0/1672	1.26	10/2270 (0.4%)
All	All	0.84	1/8180 (0.0%)	1.29	39/11130 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	208	LYS	CA-C	5.26	1.58	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	65	LYS	CA-C-N	9.43	132.69	120.44
3	E	65	LYS	C-N-CA	9.43	132.69	120.44
2	D	29	ILE	N-CA-C	-6.91	98.50	108.17
4	H	29	PHE	CA-CB-CG	6.34	120.14	113.80
4	H	191	VAL	N-CA-CB	-5.97	105.25	111.64
5	L	28	ASP	CA-CB-CG	5.92	118.52	112.60
4	H	11	VAL	N-CA-CB	5.80	117.95	110.99
5	L	1	ASP	CA-C-N	5.74	128.26	120.63
5	L	1	ASP	C-N-CA	5.74	128.26	120.63
3	E	61	ASN	CA-CB-CG	5.70	118.30	112.60
1	A	168	GLY	N-CA-C	-5.67	102.81	112.51
4	H	53	PRO	CA-C-N	5.62	126.32	120.03
4	H	53	PRO	C-N-CA	5.62	126.32	120.03
1	A	123	ASP	N-CA-C	-5.61	103.30	110.53
1	A	59	PHE	CA-C-N	-5.56	113.72	122.73
1	A	59	PHE	C-N-CA	-5.56	113.72	122.73
3	E	56	GLY	N-CA-C	-5.49	108.08	115.21
5	L	90	GLN	CB-CG-CD	5.46	121.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	VAL	N-CA-C	5.38	116.15	110.72
2	D	183	LYS	CA-C-N	5.33	127.38	120.44
2	D	183	LYS	C-N-CA	5.33	127.38	120.44
5	L	114	SER	N-CA-C	-5.33	100.49	108.96
2	D	114	SER	N-CA-C	-5.28	100.57	108.96
4	H	207	HIS	CA-C-N	5.27	128.77	120.97
4	H	207	HIS	C-N-CA	5.27	128.77	120.97
4	H	102	TYR	N-CA-C	-5.20	99.81	108.34
5	L	185	ASP	CA-CB-CG	5.19	117.79	112.60
5	L	141	PRO	CA-C-N	5.14	127.17	120.28
5	L	141	PRO	C-N-CA	5.14	127.17	120.28
1	A	17	LYS	CA-C-N	5.12	129.60	122.08
1	A	17	LYS	C-N-CA	5.12	129.60	122.08
5	L	183	LYS	CA-C-N	5.09	127.10	120.28
5	L	183	LYS	C-N-CA	5.09	127.10	120.28
1	A	181	PRO	N-CA-C	5.06	119.19	111.34
2	D	141	PRO	CA-C-N	5.05	127.04	120.28
2	D	141	PRO	C-N-CA	5.05	127.04	120.28
1	A	163	THR	CB-CA-C	5.04	118.35	110.19
1	A	170	TYR	CA-C-N	5.01	133.71	122.19
1	A	170	TYR	C-N-CA	5.01	133.71	122.19

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	1444	0	1382	24	0
2	D	1622	0	1573	27	0
3	E	1625	0	1586	59	0
4	H	1653	0	1617	35	0
5	L	1635	0	1588	34	0
6	A	30	0	0	0	0
6	D	27	0	0	0	0
6	E	44	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	30	0	0	1	0
6	L	28	0	0	0	0
All	All	8138	0	7746	173	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 11.

All (173) 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)
5:L:105:GLU:OE2	5:L:173:TYR:OH	1.60	1.19
3:E:51:ILE:HD11	3:E:70:ILE:C	1.74	1.12
3:E:51:ILE:HD11	3:E:70:ILE:HG22	1.25	1.10
3:E:51:ILE:CD1	3:E:70:ILE:C	2.25	1.09
3:E:91:THR:HG22	3:E:115:VAL:H	1.11	1.06
3:E:51:ILE:CD1	3:E:70:ILE:HG22	1.85	1.05
5:L:8:PRO:O	5:L:102:THR:HB	1.58	1.03
3:E:51:ILE:HD11	3:E:70:ILE:CG2	1.90	1.01
4:H:188:VAL:HG21	5:L:135:LEU:HD22	1.53	0.91
3:E:51:ILE:HD11	3:E:70:ILE:CB	2.06	0.84
3:E:51:ILE:CG1	3:E:70:ILE:HG22	2.09	0.82
3:E:91:THR:HG22	3:E:115:VAL:N	1.93	0.79
3:E:51:ILE:HD11	3:E:70:ILE:CA	2.16	0.76
3:E:51:ILE:HG23	3:E:58:THR:HG22	1.67	0.75
3:E:71:THR:HG23	3:E:80:TYR:HB2	1.73	0.71
4:H:133:PRO:HG3	4:H:145:LEU:HB3	1.73	0.70
3:E:51:ILE:HD13	3:E:70:ILE:O	1.92	0.69
3:E:91:THR:CG2	3:E:115:VAL:H	1.99	0.69
3:E:51:ILE:CD1	3:E:71:THR:N	2.57	0.68
4:H:18:VAL:HG12	4:H:83:LEU:HB2	1.78	0.66
4:H:11:VAL:HG22	4:H:154:PRO:HG3	1.78	0.65
3:E:88:SER:O	3:E:91:THR:HG23	1.96	0.65
3:E:152:GLU:HG2	3:E:153:PRO:HA	1.78	0.65
2:D:151:ASP:HA	2:D:191:VAL:HG13	1.80	0.64
4:H:40:ALA:HB3	4:H:43:GLN:HB2	1.80	0.63
2:D:134:CYS:HB2	2:D:148:TRP:CZ2	2.34	0.63
3:E:51:ILE:CD1	3:E:70:ILE:O	2.46	0.63
2:D:193:ALA:HB2	2:D:208:SER:HB3	1.80	0.62
3:E:105:ASP:HB3	3:E:106:TYR:CD2	2.34	0.62
3:E:51:ILE:HD13	3:E:70:ILE:C	2.22	0.61
5:L:181:LEU:HD23	5:L:185:ASP:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:193:ALA:HB2	5:L:208:SER:HB3	1.81	0.61
2:D:151:ASP:OD1	2:D:191:VAL:N	2.29	0.60
3:E:51:ILE:CG1	3:E:70:ILE:CG2	2.79	0.60
3:E:50:TYR:CE2	3:E:59:GLU:HB2	2.38	0.59
3:E:51:ILE:CD1	3:E:70:ILE:CG2	2.66	0.59
1:A:64:MET:HG3	1:A:93:VAL:HG23	1.84	0.59
4:H:134:SER:H	4:H:137:SER:HB3	1.66	0.59
3:E:51:ILE:HG13	3:E:70:ILE:HG22	1.84	0.58
4:H:11:VAL:HG21	4:H:123:THR:OG1	2.05	0.57
1:A:65:ASN:HD22	4:H:28:THR:HG21	1.69	0.57
3:E:131:SER:H	3:E:134:SER:HB3	1.70	0.57
4:H:102:TYR:C	4:H:104:LEU:H	2.13	0.56
3:E:51:ILE:HD11	3:E:71:THR:N	2.18	0.55
4:H:30:SER:HA	4:H:53:PRO:HB2	1.89	0.55
1:A:21:VAL:CG1	1:A:61:ILE:HB	2.36	0.55
1:A:14:MET:HE1	1:A:132:LEU:CD1	2.37	0.55
2:D:108:ARG:HH22	2:D:111:ALA:HB2	1.72	0.55
3:E:121:LYS:HD3	3:E:179:LEU:HD21	1.89	0.55
3:E:188:VAL:HG11	3:E:198:TYR:OH	2.06	0.54
5:L:21:ILE:HD12	5:L:73:PHE:HD2	1.73	0.54
1:A:12:HIS:NE2	1:A:14:MET:HE3	2.23	0.54
2:D:151:ASP:OD1	2:D:191:VAL:HG13	2.08	0.54
2:D:123:GLU:HG2	3:E:213:LYS:HZ3	1.73	0.54
4:H:69:THR:HB	4:H:82:GLU:HB3	1.90	0.54
5:L:9:SER:O	5:L:102:THR:HA	2.09	0.53
1:A:21:VAL:HG12	1:A:61:ILE:HB	1.91	0.53
2:D:123:GLU:HG2	3:E:213:LYS:NZ	2.22	0.52
5:L:62:PHE:HD2	5:L:73:PHE:CZ	2.27	0.52
4:H:91:THR:HG23	4:H:117:THR:HA	1.90	0.52
3:E:27:TYR:OH	3:E:34:MET:HE1	2.10	0.52
5:L:35:TRP:CE2	5:L:73:PHE:HB2	2.44	0.52
4:H:161:TRP:CH2	4:H:203:CYS:HB3	2.45	0.51
5:L:108:ARG:HD2	5:L:171:SER:HB2	1.91	0.51
3:E:50:TYR:C	3:E:50:TYR:CD1	2.89	0.51
3:E:130:PRO:HG3	3:E:142:LEU:HB3	1.93	0.50
4:H:149:VAL:HG11	4:H:157:VAL:HG21	1.92	0.50
1:A:56:LYS:HG2	1:A:57:VAL:N	2.26	0.50
2:D:181:LEU:HD23	2:D:185:ASP:HB3	1.92	0.50
3:E:169:THR:HG22	3:E:184:SER:OG	2.10	0.50
2:D:4:MET:HG2	2:D:97:THR:HG22	1.93	0.50
5:L:6:GLN:NE2	5:L:102:THR:HG23	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:146:GLY:HA2	4:H:161:TRP:CH2	2.47	0.50
3:E:120:THR:HA	3:E:150:PHE:O	2.12	0.50
4:H:148:LEU:HD21	4:H:150:LYS:HD2	1.94	0.50
2:D:47:LEU:HA	2:D:58:VAL:HG21	1.93	0.50
4:H:70:ILE:HG12	4:H:81:MET:HE3	1.94	0.50
4:H:35:ASN:HD21	4:H:99:ARG:HB2	1.76	0.49
4:H:11:VAL:HG22	4:H:154:PRO:HD3	1.93	0.49
5:L:47:LEU:HA	5:L:58:VAL:HG21	1.92	0.49
3:E:210:LYS:HE2	6:E:312:HOH:O	2.13	0.49
4:H:123:THR:HG22	4:H:210:SER:HB3	1.95	0.49
1:A:20:GLN:HG2	1:A:62:PRO:HA	1.95	0.48
3:E:188:VAL:HG13	3:E:189:PRO:HD2	1.95	0.48
2:D:149:LYS:HG2	2:D:154:LEU:HA	1.93	0.48
2:D:151:ASP:OD2	2:D:189:HIS:HB3	2.14	0.48
3:E:34:MET:HG2	3:E:79:ALA:CB	2.44	0.48
1:A:14:MET:HE1	1:A:132:LEU:HD11	1.95	0.48
5:L:123:GLU:O	5:L:126:LYS:HB2	2.13	0.48
5:L:48:ILE:CD1	5:L:54:LEU:HD12	2.44	0.48
3:E:39:GLN:HB2	3:E:45:LEU:HD23	1.96	0.47
3:E:199:ILE:HG12	3:E:214:ARG:HG2	1.95	0.47
1:A:12:HIS:CD2	1:A:14:MET:HB2	2.50	0.47
1:A:75:ILE:CG2	1:A:82:TRP:CE3	2.98	0.47
5:L:107:LYS:HA	5:L:140:TYR:OH	2.15	0.46
1:A:35:GLN:HG2	1:A:45:VAL:HG22	1.97	0.46
2:D:108:ARG:HH22	2:D:111:ALA:CB	2.28	0.46
3:E:188:VAL:CG1	3:E:189:PRO:HD2	2.46	0.46
2:D:119:PRO:HB3	2:D:209:PHE:CE2	2.51	0.46
5:L:24:ARG:HA	5:L:69:THR:O	2.15	0.46
5:L:62:PHE:HD2	5:L:73:PHE:HZ	1.62	0.46
1:A:92:VAL:HG11	1:A:175:TRP:CD2	2.50	0.46
2:D:90:HIS:CE1	2:D:97:THR:H	2.34	0.46
3:E:121:LYS:HD3	3:E:179:LEU:CD2	2.45	0.46
5:L:83:ILE:HD12	5:L:83:ILE:O	2.16	0.45
5:L:150:VAL:CG2	5:L:155:GLN:HG3	2.45	0.45
3:E:146:VAL:HG11	3:E:154:VAL:HG11	1.98	0.45
5:L:18:ARG:HG3	5:L:76:SER:O	2.17	0.45
1:A:130:LEU:HD13	1:A:175:TRP:CE2	2.52	0.45
4:H:161:TRP:CZ3	4:H:203:CYS:HB3	2.51	0.45
1:A:81:LEU:HD22	3:E:101:SER:HB3	1.99	0.45
1:A:93:VAL:O	1:A:93:VAL:HG13	2.16	0.44
4:H:94:TYR:CE1	4:H:116:VAL:HG12	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:123:GLU:HA	5:L:126:LYS:HD2	2.00	0.44
4:H:68:ALA:HB1	4:H:81:MET:HE2	1.99	0.44
2:D:90:HIS:CE1	2:D:97:THR:HB	2.53	0.44
3:E:35:HIS:HB2	3:E:97:VAL:HG13	1.99	0.44
3:E:38:ARG:HB3	3:E:48:ILE:HD11	2.00	0.44
3:E:97:VAL:CG2	3:E:104:PHE:HB3	2.48	0.44
3:E:2:VAL:HG22	3:E:27:TYR:HB3	1.99	0.44
3:E:51:ILE:HD12	3:E:71:THR:N	2.30	0.44
3:E:143:GLY:HA2	3:E:158:TRP:CZ2	2.53	0.44
3:E:158:TRP:CH2	3:E:200:CYS:HB3	2.52	0.44
4:H:206:ASN:HB3	4:H:213:LYS:HG2	2.00	0.44
4:H:35:ASN:ND2	4:H:99:ARG:HB2	2.33	0.43
4:H:126:PRO:HB3	4:H:152:TYR:HB3	2.01	0.43
3:E:97:VAL:HG21	3:E:104:PHE:HB3	2.00	0.43
5:L:10:SER:HA	5:L:103:LYS:O	2.19	0.43
3:E:51:ILE:HD12	3:E:71:THR:CA	2.48	0.43
4:H:11:VAL:CG2	4:H:154:PRO:HD3	2.48	0.43
5:L:16:GLY:HA2	5:L:77:SER:HB2	2.00	0.43
5:L:179:LEU:HG	5:L:181:LEU:HD12	2.01	0.43
4:H:128:VAL:O	4:H:216:LYS:HE2	2.19	0.42
5:L:47:LEU:HD23	5:L:73:PHE:CZ	2.54	0.42
2:D:21:ILE:HD12	2:D:73:LEU:HD23	2.01	0.42
5:L:19:VAL:O	5:L:74:THR:HA	2.18	0.42
2:D:120:PRO:HD3	2:D:132:VAL:HG22	2.01	0.42
5:L:120:PRO:HD3	5:L:132:VAL:HG22	2.02	0.42
1:A:97:TYR:OH	4:H:30:SER:O	2.33	0.42
3:E:12:LYS:O	3:E:115:VAL:HA	2.19	0.42
5:L:131:SER:OG	5:L:180:THR:HG22	2.20	0.42
1:A:130:LEU:HD13	1:A:175:TRP:CD2	2.55	0.42
5:L:34:ASN:HB2	5:L:89:GLN:HG2	2.02	0.42
2:D:24:ARG:HA	2:D:69:THR:O	2.19	0.42
4:H:47:TRP:HZ2	4:H:50:GLU:HG2	1.85	0.42
5:L:120:PRO:HG2	5:L:130:ALA:HB1	2.02	0.42
4:H:17:SER:HA	4:H:83:LEU:O	2.20	0.41
1:A:15:VAL:O	1:A:93:VAL:HA	2.19	0.41
3:E:154:VAL:HG12	3:E:182:LEU:HD21	2.01	0.41
3:E:51:ILE:CD1	3:E:70:ILE:CB	2.90	0.41
5:L:163:VAL:HB	5:L:175:LEU:HD12	2.02	0.41
2:D:48:VAL:HG22	2:D:54:LEU:HD23	2.01	0.41
2:D:16:GLY:HA2	2:D:77:SER:HB2	2.02	0.41
1:A:5:PRO:HG2	1:A:86:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:63:LYS:HD2	4:H:64:PHE:CE2	2.56	0.41
1:A:95:GLU:HA	1:A:177:PHE:HA	2.01	0.41
2:D:197:THR:HG23	2:D:204:PRO:HB3	2.03	0.41
4:H:11:VAL:HG22	4:H:154:PRO:CG	2.47	0.41
2:D:151:ASP:OD1	2:D:191:VAL:CG1	2.67	0.41
4:H:207:HIS:CD2	4:H:209:PRO:HD2	2.56	0.41
1:A:156:VAL:HG12	1:A:160:HIS:HB2	2.03	0.41
4:H:44:GLY:HA2	6:H:304:HOH:O	2.21	0.41
5:L:21:ILE:HD12	5:L:73:PHE:CD2	2.55	0.41
2:D:193:ALA:HB2	2:D:208:SER:CB	2.47	0.40
3:E:124:SER:HB2	3:E:126:PHE:CZ	2.57	0.40
5:L:150:VAL:HG23	5:L:155:GLN:HG3	2.03	0.40
1:A:159:ALA:C	1:A:161:ARG:H	2.29	0.40
3:E:47:TRP:HZ2	3:E:50:TYR:HD2	1.68	0.40
2:D:80:PRO:O	2:D:83:PHE:HD2	2.05	0.40
5:L:62:PHE:CD2	5:L:73:PHE:HZ	2.38	0.40
1:A:8:TRP:CE2	1:A:24:CYS:HB2	2.56	0.40
2:D:21:ILE:HG12	2:D:102:THR:HG21	2.03	0.40
3:E:11:VAL:CG2	3:E:151:PRO:HG3	2.51	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	180/182 (99%)	160 (89%)	18 (10%)	2 (1%)	11	36
2	D	209/211 (99%)	199 (95%)	10 (5%)	0	100	100
3	E	215/217 (99%)	202 (94%)	12 (6%)	1 (0%)	24	54
4	H	218/220 (99%)	203 (93%)	14 (6%)	1 (0%)	24	54
5	L	209/211 (99%)	195 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1031/1041 (99%)	959 (93%)	68 (7%)	4 (0%)	30	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	65	LYS
1	A	122	LEU
1	A	136	ARG
4	H	29	PHE

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	158/161 (98%)	148 (94%)	10 (6%)	16	45
2	D	183/183 (100%)	171 (93%)	12 (7%)	15	43
3	E	184/185 (100%)	167 (91%)	17 (9%)	8	27
4	H	184/184 (100%)	172 (94%)	12 (6%)	15	44
5	L	187/187 (100%)	171 (91%)	16 (9%)	10	30
All	All	896/900 (100%)	829 (92%)	67 (8%)	12	37

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	22	THR
1	A	32	VAL
1	A	41	SER
1	A	57	VAL
1	A	75	ILE
1	A	114	GLU
1	A	115	LYS
1	A	123	ASP
1	A	156	VAL

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Mol	Chain	Res	Type
2	D	22	THR
2	D	39	LYS
2	D	47	LEU
2	D	63	SER
2	D	72	THR
2	D	74	THR
2	D	81	GLU
2	D	149	LYS
2	D	154	LEU
2	D	180	THR
2	D	191	VAL
2	D	203	SER
3	E	10	GLU
3	E	45	LEU
3	E	51	ILE
3	E	66	ASP
3	E	69	THR
3	E	81	MET
3	E	105	ASP
3	E	114	THR
3	E	124	SER
3	E	136	SER
3	E	154	VAL
3	E	163	LEU
3	E	165	SER
3	E	169	THR
3	E	187	THR
3	E	199	ILE
3	E	203	ASN
4	H	12	LYS
4	H	20	VAL
4	H	81	MET
4	H	82	GLU
4	H	88	SER
4	H	115	THR
4	H	145	LEU
4	H	150	LYS
4	H	155	GLU
4	H	185	LEU
4	H	191	VAL
4	H	212	THR
5	L	7	SER

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Mol	Chain	Res	Type
5	L	39	LYS
5	L	47	LEU
5	L	54	LEU
5	L	72	THR
5	L	79	GLN
5	L	89	GLN
5	L	97	THR
5	L	102	THR
5	L	103	LYS
5	L	109	THR
5	L	129	THR
5	L	181	LEU
5	L	191	VAL
5	L	197	THR
5	L	203	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	172	ASN
2	D	137	ASN
3	E	168	HIS
4	H	206	ASN
5	L	89	GLN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9	
1	A	182/182 (100%)	-0.10	0	100	100	66, 94, 132, 154	0
2	D	211/211 (100%)	-0.36	0	100	100	62, 87, 111, 127	0
3	E	217/217 (100%)	-0.28	0	100	100	32, 88, 124, 140	1 (0%)
4	H	220/220 (100%)	-0.33	0	100	100	68, 89, 115, 125	0
5	L	211/211 (100%)	-0.24	1 (0%)	87	83	66, 93, 119, 152	0
All	All	1041/1041 (100%)	-0.26	1 (0%)	92	90	32, 90, 122, 154	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	73	PHE	2.2

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.