



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2024 – 02:41 PM EDT

PDB ID : 1IM9
Title : Crystal structure of the human natural killer cell inhibitory receptor KIR2DL1 bound to its MHC ligand HLA-Cw4
Authors : Fan, Q.R.; Long, E.O.; Wiley, D.C.
Deposited on : 2001-05-10
Resolution : 2.80 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	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

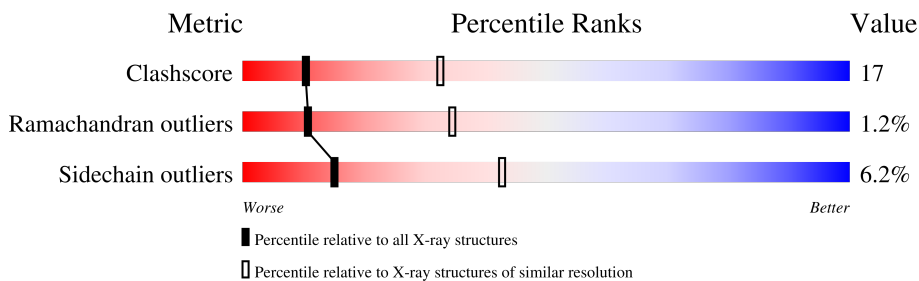
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	276	69% 27% .
1	E	276	66% 32% .
2	B	100	73% 25% .
2	F	100	65% 32% .
3	C	9	33% 56% 11%
3	G	9	33% 56% 11%
4	D	225	48% 35% . 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8096 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 HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, CW-4 CW*0401 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2262	1410	414	432	6			
1	E	275	Total	C	N	O	S	0	0	0
			2262	1410	414	432	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	cloning artifact	UNP P30504
E	0	MET	-	cloning artifact	UNP P30504

- Molecule 2 is a protein called Beta-2 microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			832	529	140	159	4			
2	F	100	Total	C	N	O	S	0	0	0
			832	529	140	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	cloning artifact	UNP P61769
F	0	MET	-	cloning artifact	UNP P61769

- Molecule 3 is a protein called HLA-Cw4-specific peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			79	51	11	17			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	9	Total	C	N	O	0	0	0
			79	51	11	17			

- Molecule 4 is a protein called KILLER CELL IMMUNOGLOBULIN-LIKE RECEPTOR 2DL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	195	Total	C	N	O	S	0	0	0
			1512	953	262	289	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	cloning artifact	UNP P43626

- Molecule 5 is water.

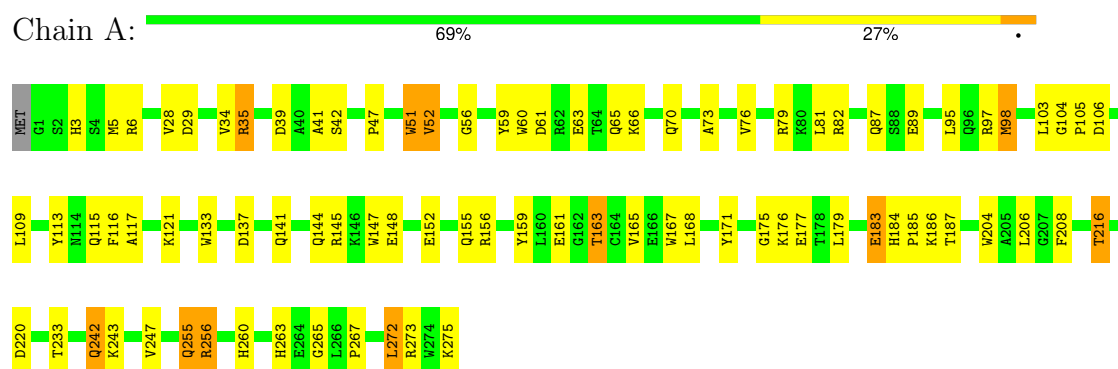
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total	O	0	0
			76	76		
5	B	36	Total	O	0	0
			36	36		
5	C	1	Total	O	0	0
			1	1		
5	D	30	Total	O	0	0
			30	30		
5	E	64	Total	O	0	0
			64	64		
5	F	26	Total	O	0	0
			26	26		
5	G	5	Total	O	0	0
			5	5		

3 Residue-property plots

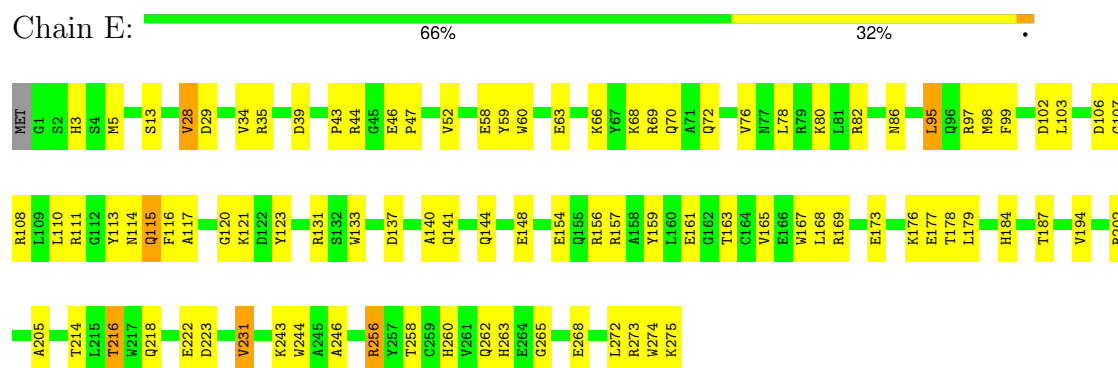
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

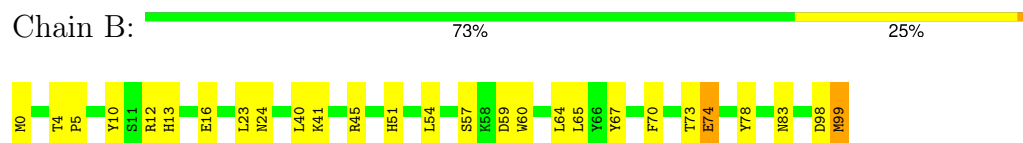
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, CW-4 CW*0401 ALPHA CHAIN



- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, CW-4 CW*0401 ALPHA CHAIN



- Molecule 2: Beta-2 microglobulin



- Molecule 2: Beta-2 microglobulin

Chain F:  65% 32% .




- Molecule 3: HLA-Cw4-specific peptide

Chain C:  33% 56% 11%



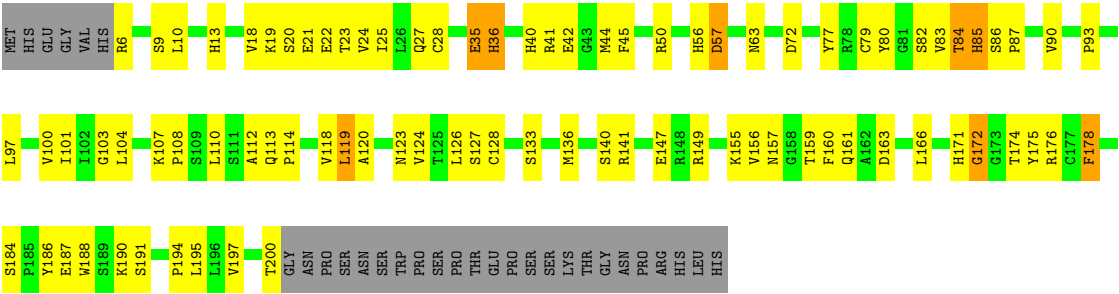
- Molecule 3: HLA-Cw4-specific peptide

Chain G:  33% 56% 11%



- Molecule 4: KILLER CELL IMMUNOGLOBULIN-LIKE RECEPTOR 2DL1

Chain D:  48% 35% 13%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	213.63Å 75.87Å 125.75Å 90.00° 120.96° 90.00°	Depositor
Resolution (Å)	29.21 – 2.80	Depositor
% Data completeness (in resolution range)	97.8 (29.21-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.213 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8096	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.40	0/2327	0.63	0/3159
1	E	0.39	0/2327	0.62	1/3159 (0.0%)
2	B	0.41	0/855	0.68	1/1156 (0.1%)
2	F	0.42	0/855	0.63	0/1156
3	C	0.50	0/80	0.66	0/106
3	G	0.48	0/80	0.54	0/106
4	D	0.38	0/1556	0.67	1/2116 (0.0%)
All	All	0.40	0/8080	0.64	3/10958 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	200	THR	N-CA-C	6.31	128.03	111.00
2	B	99	MET	N-CA-C	-6.22	94.20	111.00
1	E	28	VAL	N-CA-C	-5.56	95.99	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2262	0	2105	66	0
1	E	2262	0	2105	73	0
2	B	832	0	791	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	832	0	791	29	0
3	C	79	0	74	11	0
3	G	79	0	74	11	0
4	D	1512	0	1446	77	0
5	A	76	0	0	2	0
5	B	36	0	0	2	0
5	C	1	0	0	0	0
5	D	30	0	0	1	0
5	E	64	0	0	3	0
5	F	26	0	0	0	0
5	G	5	0	0	0	0
All	All	8096	0	7386	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 17.

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)
1:E:256:ARG:HB3	1:E:256:ARG:HH11	1.23	0.98
4:D:19:LYS:HB2	4:D:22:GLU:HG3	1.43	0.98
1:A:183:GLU:OE1	1:A:183:GLU:HA	1.67	0.94
1:A:275:LYS:OXT	3:G:6:VAL:HG11	1.70	0.90
4:D:83:VAL:HG12	4:D:84:THR:H	1.39	0.86
1:A:70:GLN:HE22	3:C:6:VAL:HA	1.41	0.85
4:D:112:ALA:HB2	4:D:195:LEU:HD21	1.58	0.85
2:F:83:ASN:HD22	2:F:84:HIS:H	1.24	0.84
2:F:83:ASN:HD22	2:F:84:HIS:N	1.77	0.82
1:A:79:ARG:HG3	1:A:79:ARG:HH11	1.47	0.79
2:F:24:ASN:HB3	2:F:65:LEU:HD11	1.68	0.75
1:A:61:ASP:O	1:A:65:GLN:HG2	1.87	0.75
1:E:13:SER:HB3	1:E:78:LEU:HD13	1.68	0.75
4:D:35:GLU:HG2	4:D:85:HIS:HB2	1.68	0.74
1:A:155:GLN:HE21	3:C:5:ALA:HB2	1.53	0.74
1:E:121:LYS:HE3	2:F:1:ILE:HG21	1.69	0.74
1:E:59:TYR:OH	3:G:1:GLN:HG2	1.88	0.73
1:E:274:TRP:O	1:E:275:LYS:HB3	1.89	0.72
4:D:19:LYS:CB	4:D:22:GLU:HG3	2.17	0.72
1:E:102:ASP:OD2	1:E:113:TYR:HE2	1.73	0.71
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.73	0.71
1:E:167:TRP:CG	3:G:1:GLN:HG3	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TRP:HB2	1:A:144:GLN:HE21	1.55	0.70
1:A:155:GLN:NE2	3:C:5:ALA:HB2	2.06	0.70
1:E:202:ARG:HG3	1:E:246:ALA:HB2	1.75	0.69
1:E:133:TRP:HB2	1:E:144:GLN:HE21	1.58	0.69
1:E:117:ALA:HB2	2:F:60:TRP:CE2	2.27	0.68
1:A:73:ALA:O	1:A:76:VAL:HG22	1.93	0.68
1:A:206:LEU:HD23	1:A:242:GLN:HB3	1.75	0.67
2:F:27:VAL:HG12	2:F:30:PHE:CE1	2.30	0.66
1:E:256:ARG:HB3	1:E:256:ARG:NH1	2.04	0.66
4:D:27:GLN:HG3	4:D:63:ASN:OD1	1.96	0.66
1:A:103:LEU:HD11	1:A:165:VAL:HG13	1.77	0.65
2:B:73:THR:O	2:B:74:GLU:HG2	1.97	0.65
2:F:27:VAL:HG11	2:F:35:ILE:HD13	1.76	0.65
1:A:145:ARG:HD2	4:D:133:SER:OG	1.96	0.65
1:E:111:ARG:HA	5:E:286:HOH:O	1.95	0.65
4:D:56:HIS:O	4:D:57:ASP:HB2	1.96	0.64
1:A:70:GLN:NE2	3:C:6:VAL:HA	2.11	0.64
4:D:83:VAL:HG12	4:D:84:THR:N	2.12	0.64
4:D:176:ARG:HD3	4:D:191:SER:OG	1.98	0.64
1:E:106:ASP:OD2	1:E:108:ARG:HG2	1.98	0.64
1:E:120:GLY:O	1:E:121:LYS:HE2	1.98	0.64
2:F:73:THR:O	2:F:74:GLU:HB3	1.98	0.64
4:D:36:HIS:CE1	4:D:50:ARG:HE	2.16	0.64
1:E:216:THR:HG23	5:E:277:HOH:O	1.97	0.63
4:D:155:LYS:HB2	4:D:159:THR:O	1.99	0.62
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.34	0.62
4:D:100:VAL:HG13	4:D:186:TYR:O	1.99	0.62
1:E:256:ARG:HH11	1:E:256:ARG:CB	2.07	0.61
1:A:79:ARG:HG3	1:A:79:ARG:NH1	2.12	0.61
1:A:47:PRO:HB3	1:A:60:TRP:CZ2	2.35	0.61
1:E:121:LYS:HE2	1:E:121:LYS:HA	1.82	0.61
1:A:144:GLN:O	1:A:148:GLU:HG3	2.02	0.60
1:E:28:VAL:HG11	1:E:179:LEU:HD13	1.83	0.60
2:F:17:ASN:CG	2:F:97:ARG:HH22	2.05	0.60
4:D:172:GLY:HA3	4:D:197:VAL:O	2.02	0.59
1:A:63:GLU:OE1	1:A:66:LYS:NZ	2.36	0.59
4:D:80:TYR:CZ	4:D:93:PRO:HB3	2.37	0.59
4:D:82:SER:HB2	4:D:90:VAL:HG12	1.84	0.59
1:A:56:GLY:O	1:A:59:TYR:HB3	2.03	0.59
1:A:155:GLN:NE2	3:C:5:ALA:CB	2.65	0.59
1:E:70:GLN:HE22	3:G:7:TYR:H	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:GLU:HG2	4:D:85:HIS:CB	2.32	0.58
4:D:84:THR:HG22	4:D:86:SER:OG	2.04	0.58
4:D:119:LEU:HD23	4:D:120:ALA:H	1.68	0.58
1:E:258:THR:HG22	1:E:273:ARG:HB2	1.85	0.57
4:D:171:HIS:O	4:D:172:GLY:O	2.23	0.57
2:F:59:ASP:O	2:F:60:TRP:HB2	2.04	0.57
1:A:155:GLN:HE21	3:C:5:ALA:CB	2.17	0.56
1:A:263:HIS:CD2	1:A:265:GLY:H	2.22	0.56
1:E:274:TRP:O	1:E:275:LYS:CB	2.53	0.56
1:A:6:ARG:NH1	1:A:113:TYR:CE1	2.72	0.56
2:B:51:HIS:HA	2:B:65:LEU:O	2.06	0.56
4:D:10:LEU:HD13	4:D:79:CYS:HB2	1.86	0.56
4:D:128:CYS:O	4:D:161:GLN:HB2	2.04	0.56
4:D:80:TYR:CE2	4:D:93:PRO:HB3	2.39	0.56
1:E:167:TRP:CD1	3:G:1:GLN:HG3	2.41	0.55
2:F:25:CYS:HB2	2:F:39:LEU:HD21	1.87	0.55
1:E:97:ARG:HG3	1:E:116:PHE:CE2	2.42	0.55
1:A:185:PRO:HB3	1:A:208:PHE:HB3	1.87	0.55
1:E:187:THR:HG22	1:E:205:ALA:HA	1.89	0.55
1:A:3:HIS:HD2	1:A:29:ASP:OD2	1.89	0.55
1:E:159:TYR:CE1	3:G:3:ASP:HB2	2.42	0.54
4:D:18:VAL:HG21	4:D:24:VAL:HG11	1.89	0.54
1:A:51:TRP:CZ3	1:A:171:TYR:HB3	2.41	0.54
1:E:131:ARG:HG3	1:E:131:ARG:HH11	1.72	0.54
1:E:157:ARG:HG2	1:E:161:GLU:OE1	2.07	0.54
1:E:137:ASP:O	1:E:141:GLN:HG3	2.08	0.54
2:F:23:LEU:O	2:F:67:TYR:HA	2.07	0.54
4:D:118:VAL:HG11	4:D:124:VAL:CG1	2.38	0.53
2:F:73:THR:O	2:F:74:GLU:CB	2.57	0.53
1:E:103:LEU:HD11	1:E:165:VAL:HG13	1.90	0.53
4:D:141:ARG:HD2	4:D:175:TYR:CZ	2.43	0.52
4:D:178:PHE:CD1	4:D:178:PHE:N	2.78	0.52
1:E:102:ASP:OD2	1:E:113:TYR:CE2	2.61	0.52
1:E:69:ARG:HH11	1:E:72:GLN:HE21	1.58	0.52
4:D:178:PHE:CE2	4:D:191:SER:HB2	2.45	0.51
1:A:184:HIS:HB3	1:A:265:GLY:O	2.11	0.51
1:A:104:GLY:C	1:A:106:ASP:H	2.13	0.51
4:D:6:ARG:HH11	4:D:6:ARG:HG2	1.75	0.51
1:E:231:VAL:O	1:E:243:LYS:HE3	2.11	0.51
4:D:35:GLU:HG2	4:D:85:HIS:CA	2.41	0.51
1:E:78:LEU:HD21	1:E:95:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:101:ILE:HG23	4:D:101:ILE:O	2.10	0.51
1:E:121:LYS:CE	2:F:1:ILE:HG21	2.40	0.51
1:A:6:ARG:HH12	1:A:113:TYR:HE1	1.55	0.51
4:D:176:ARG:CZ	4:D:194:PRO:HG3	2.41	0.51
4:D:40:HIS:HE1	4:D:42:GLU:OE1	1.93	0.50
2:B:4:THR:HG23	2:B:5:PRO:HD2	1.92	0.50
1:E:263:HIS:CD2	1:E:265:GLY:H	2.29	0.50
1:E:154:GLU:HG2	1:E:157:ARG:HH22	1.76	0.50
1:E:159:TYR:CZ	3:G:3:ASP:HB2	2.47	0.50
1:A:51:TRP:CE3	1:A:52:VAL:HG13	2.46	0.50
2:F:27:VAL:HG11	2:F:35:ILE:CD1	2.42	0.50
1:E:121:LYS:HE3	2:F:1:ILE:CG2	2.39	0.49
1:A:109:LEU:HD22	1:A:161:GLU:HA	1.93	0.49
1:A:76:VAL:HG12	4:D:72:ASP:HB3	1.94	0.49
1:A:66:LYS:HD3	3:C:4:ASP:HA	1.93	0.49
2:B:54:LEU:HA	2:B:64:LEU:HD21	1.95	0.49
1:A:175:GLY:O	1:A:177:GLU:N	2.45	0.49
1:E:133:TRP:HB2	1:E:144:GLN:NE2	2.25	0.49
1:A:34:VAL:HG22	1:A:35:ARG:N	2.28	0.49
1:E:47:PRO:HG3	1:E:60:TRP:CE2	2.48	0.49
1:A:76:VAL:CG1	4:D:72:ASP:HB3	2.42	0.48
1:A:6:ARG:NH1	1:A:113:TYR:CD1	2.81	0.48
1:A:187:THR:OG1	1:A:272:LEU:HD21	2.13	0.48
4:D:126:LEU:HD22	4:D:195:LEU:HD23	1.95	0.48
1:A:82:ARG:HG2	1:A:87:GLN:HB2	1.95	0.48
2:B:73:THR:O	2:B:74:GLU:CG	2.62	0.48
4:D:24:VAL:HG22	4:D:25:ILE:N	2.28	0.48
1:E:76:VAL:HG23	1:E:80:LYS:HE2	1.96	0.48
1:A:97:ARG:HD2	3:C:7:TYR:CE2	2.48	0.48
4:D:110:LEU:HD13	4:D:128:CYS:SG	2.54	0.48
1:A:220:ASP:OD2	1:A:256:ARG:NH1	2.47	0.47
4:D:9:SER:O	4:D:28:CYS:HA	2.13	0.47
4:D:136:MET:CE	4:D:149:ARG:HE	2.27	0.47
1:A:159:TYR:HA	1:A:163:THR:HG23	1.95	0.47
4:D:35:GLU:CG	4:D:85:HIS:HB2	2.40	0.47
4:D:6:ARG:HG2	4:D:6:ARG:NH1	2.29	0.47
4:D:100:VAL:HG11	4:D:188:TRP:CD2	2.50	0.47
1:A:216:THR:HG23	1:A:260:HIS:HB2	1.97	0.47
2:B:73:THR:O	2:B:74:GLU:CB	2.63	0.47
1:E:218:GLN:HG2	1:E:223:ASP:HA	1.97	0.47
1:A:104:GLY:O	1:A:106:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:48:LYS:HE3	2:F:50:GLU:HG3	1.96	0.47
2:F:24:ASN:HA	2:F:66:TYR:O	2.14	0.47
2:B:59:ASP:O	2:B:60:TRP:HB2	2.15	0.46
1:E:106:ASP:OD2	1:E:108:ARG:CG	2.63	0.46
1:E:194:VAL:HG12	1:E:194:VAL:O	2.15	0.46
4:D:44:MET:HG3	4:D:45:PHE:CD2	2.50	0.46
2:F:11:SER:HA	2:F:22:PHE:O	2.15	0.46
1:A:187:THR:CB	1:A:272:LEU:HD21	2.46	0.46
2:B:10:TYR:CD1	2:B:10:TYR:N	2.83	0.46
4:D:160:PHE:N	4:D:160:PHE:CD1	2.84	0.46
1:E:167:TRP:CD2	3:G:1:GLN:HG3	2.50	0.46
2:F:67:TYR:CD1	2:F:67:TYR:N	2.84	0.46
1:A:156:ARG:NH1	3:C:3:ASP:OD2	2.50	0.45
4:D:36:HIS:ND1	4:D:50:ARG:NE	2.64	0.45
4:D:174:THR:CG2	4:D:194:PRO:HB3	2.46	0.45
1:E:231:VAL:HG13	1:E:244:TRP:CZ2	2.52	0.45
2:F:59:ASP:O	2:F:60:TRP:CB	2.64	0.45
4:D:119:LEU:HD23	4:D:120:ALA:N	2.30	0.45
1:E:97:ARG:HD2	3:G:7:TYR:CE2	2.51	0.45
1:A:116:PHE:N	1:A:116:PHE:CD1	2.84	0.45
1:E:214:THR:HB	1:E:262:GLN:HE21	1.82	0.45
4:D:124:VAL:HG23	4:D:166:LEU:HD12	1.98	0.45
4:D:140:SER:CB	4:D:147:GLU:HG3	2.46	0.45
1:E:184:HIS:HB3	1:E:265:GLY:O	2.17	0.45
4:D:184:SER:HB2	5:D:227:HOH:O	2.15	0.45
1:E:115:GLN:HE21	1:E:115:GLN:HB3	1.55	0.45
1:A:147:TRP:HB3	1:A:152:GLU:HB3	1.99	0.44
2:B:98:ASP:OD1	2:B:98:ASP:O	2.34	0.44
1:A:167:TRP:CD2	3:C:1:GLN:HG3	2.52	0.44
1:E:95:LEU:HD11	3:G:9:LEU:HD11	2.00	0.44
1:E:97:ARG:CZ	1:E:99:PHE:CD2	3.01	0.44
1:A:167:TRP:CE2	3:C:1:GLN:HG3	2.53	0.44
2:F:39:LEU:CD1	2:F:68:THR:HG22	2.47	0.44
5:A:299:HOH:O	4:D:44:MET:HB2	2.17	0.44
1:E:69:ARG:HA	1:E:69:ARG:HD2	1.81	0.44
1:A:137:ASP:O	1:A:141:GLN:HG3	2.17	0.44
1:E:43:PRO:HB2	1:E:68:LYS:HE2	2.00	0.44
1:A:273:ARG:HD3	5:A:322:HOH:O	2.17	0.44
2:F:89:GLN:O	2:F:90:PRO:C	2.57	0.43
1:A:5:MET:HB2	1:A:168:LEU:HD13	2.00	0.43
2:B:57:SER:HB3	5:B:111:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:124:VAL:HG23	4:D:166:LEU:HB2	2.00	0.43
1:E:44:ARG:O	1:E:46:GLU:HG3	2.18	0.43
2:F:89:GLN:O	2:F:89:GLN:HG3	2.18	0.43
1:A:121:LYS:HE3	5:B:118:HOH:O	2.18	0.43
1:A:187:THR:HB	1:A:272:LEU:HD21	2.01	0.43
4:D:114:PRO:HD2	4:D:124:VAL:HG12	1.99	0.43
2:F:48:LYS:HD2	2:F:48:LYS:HA	1.74	0.43
3:G:5:ALA:O	3:G:6:VAL:C	2.55	0.43
1:A:104:GLY:C	1:A:106:ASP:N	2.72	0.43
1:A:204:TRP:HZ2	2:B:99:MET:HB2	1.83	0.43
4:D:56:HIS:O	4:D:57:ASP:CB	2.66	0.43
4:D:84:THR:O	4:D:85:HIS:HB3	2.18	0.43
4:D:156:VAL:HG23	4:D:157:ASN:N	2.34	0.43
2:B:23:LEU:O	2:B:67:TYR:HA	2.19	0.43
1:E:28:VAL:O	1:E:29:ASP:HB2	2.19	0.43
1:E:176:LYS:HE3	1:E:177:GLU:OE2	2.18	0.43
1:A:103:LEU:HD13	1:A:168:LEU:HD23	2.01	0.43
2:B:12:ARG:HG2	2:B:13:HIS:CE1	2.53	0.43
1:A:82:ARG:NH1	1:A:89:GLU:HG2	2.34	0.43
2:B:40:LEU:HD23	2:B:45:ARG:HA	2.01	0.43
4:D:124:VAL:CG2	4:D:166:LEU:HD12	2.49	0.43
4:D:126:LEU:HD22	4:D:195:LEU:CD2	2.49	0.43
1:A:233:THR:OG1	1:A:243:LYS:HD2	2.18	0.42
1:A:255:GLN:H	1:A:255:GLN:NE2	2.16	0.42
4:D:41:ARG:HB2	4:D:77:TYR:CE2	2.54	0.42
4:D:83:VAL:O	4:D:85:HIS:N	2.49	0.42
4:D:41:ARG:HD3	4:D:77:TYR:OH	2.19	0.42
4:D:104:LEU:HD12	4:D:187:GLU:HB3	2.01	0.42
1:E:34:VAL:HG22	1:E:35:ARG:N	2.35	0.42
2:F:48:LYS:NZ	2:F:50:GLU:HG2	2.34	0.42
4:D:83:VAL:CG1	4:D:84:THR:H	2.21	0.42
1:E:63:GLU:HA	1:E:66:LYS:HD2	2.01	0.42
4:D:84:THR:C	4:D:86:SER:H	2.22	0.42
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.02	0.42
1:A:97:ARG:HG2	1:A:98:MET:N	2.34	0.42
4:D:56:HIS:ND1	4:D:57:ASP:OD2	2.52	0.42
1:E:97:ARG:HH21	1:E:114:ASN:ND2	2.18	0.42
4:D:113:GLN:HA	4:D:114:PRO:C	2.40	0.41
1:E:5:MET:HB2	1:E:168:LEU:HD13	2.02	0.41
4:D:41:ARG:HD3	4:D:77:TYR:CZ	2.55	0.41
4:D:176:ARG:NE	4:D:194:PRO:HG3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:39:LEU:HD12	2:F:68:THR:HG22	2.03	0.41
2:F:70:PHE:CE2	2:F:72:PRO:HG3	2.56	0.41
1:E:3:HIS:HD2	1:E:29:ASP:OD2	2.04	0.41
1:E:107:GLY:O	1:E:169:ARG:NH1	2.47	0.41
2:B:67:TYR:CD1	2:B:67:TYR:N	2.89	0.41
4:D:86:SER:HA	4:D:87:PRO:HD3	1.92	0.41
1:E:218:GLN:HA	1:E:222:GLU:O	2.21	0.41
2:B:41:LYS:HG3	2:B:78:TYR:CE2	2.56	0.41
4:D:10:LEU:HD23	4:D:97:LEU:HB3	2.03	0.41
4:D:13:HIS:O	4:D:24:VAL:HG23	2.20	0.41
1:E:123:TYR:CZ	1:E:140:ALA:HA	2.56	0.41
1:E:202:ARG:NE	2:F:99:MET:O	2.54	0.41
1:A:220:ASP:CG	1:A:256:ARG:NH1	2.74	0.41
1:E:69:ARG:HH11	1:E:72:GLN:NE2	2.18	0.41
1:E:218:GLN:NE2	1:E:260:HIS:NE2	2.69	0.41
1:E:60:TRP:HA	1:E:60:TRP:CE3	2.57	0.40
1:E:82:ARG:HD2	5:E:324:HOH:O	2.20	0.40
4:D:103:GLY:HA2	4:D:190:LYS:HA	2.03	0.40
1:A:115:GLN:HE21	1:A:115:GLN:HB3	1.62	0.40
2:B:16:GLU:OE2	1:E:148:GLU:HB3	2.20	0.40
4:D:107:LYS:HA	4:D:108:PRO:HD3	1.79	0.40
2:B:54:LEU:HA	2:B:64:LEU:CD2	2.51	0.40
4:D:20:SER:O	4:D:21:GLU:HB2	2.21	0.40
1:E:110:LEU:HD23	1:E:110:LEU:O	2.21	0.40
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.97	0.40
4:D:20:SER:O	4:D:21:GLU:CB	2.69	0.40
4:D:35:GLU:HG2	4:D:85:HIS:HA	2.02	0.40
1:E:108:ARG:HG2	1:E:108:ARG:HH11	1.85	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	273/276 (99%)	243 (89%)	25 (9%)	5 (2%)	7	24
1	E	273/276 (99%)	248 (91%)	25 (9%)	0	100	100
2	B	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	13	39
2	F	98/100 (98%)	89 (91%)	7 (7%)	2 (2%)	6	21
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	G	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
4	D	193/225 (86%)	169 (88%)	21 (11%)	3 (2%)	8	27
All	All	949/995 (95%)	851 (90%)	87 (9%)	11 (1%)	11	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	LYS
4	D	172	GLY
4	D	57	ASP
1	A	51	TRP
2	F	74	GLU
1	A	41	ALA
1	A	267	PRO
2	B	74	GLU
4	D	84	THR
2	F	52	SER
1	A	105	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	232/233 (100%)	217 (94%)	15 (6%)	14	40
1	E	232/233 (100%)	216 (93%)	16 (7%)	13	37
2	B	94/95 (99%)	91 (97%)	3 (3%)	34	68
2	F	94/95 (99%)	87 (93%)	7 (7%)	11	33
3	C	8/8 (100%)	7 (88%)	1 (12%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	8/8 (100%)	7 (88%)	1 (12%)	3	12
4	D	169/196 (86%)	160 (95%)	9 (5%)	19	49
All	All	837/868 (96%)	785 (94%)	52 (6%)	15	43

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	39	ASP
1	A	42	SER
1	A	52	VAL
1	A	95	LEU
1	A	98	MET
1	A	163	THR
1	A	183	GLU
1	A	186	LYS
1	A	216	THR
1	A	242	GLN
1	A	247	VAL
1	A	255	GLN
1	A	256	ARG
1	A	272	LEU
2	B	0	MET
2	B	70	PHE
2	B	83	ASN
3	C	1	GLN
4	D	23	THR
4	D	35	GLU
4	D	36	HIS
4	D	85	HIS
4	D	119	LEU
4	D	123	ASN
4	D	127	SER
4	D	163	ASP
4	D	178	PHE
1	E	39	ASP
1	E	52	VAL
1	E	58	GLU
1	E	86	ASN
1	E	95	LEU
1	E	98	MET

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Mol	Chain	Res	Type
1	E	115	GLN
1	E	156	ARG
1	E	163	THR
1	E	173	GLU
1	E	178	THR
1	E	216	THR
1	E	231	VAL
1	E	256	ARG
1	E	268	GLU
1	E	272	LEU
2	F	0	MET
2	F	4	THR
2	F	20	SER
2	F	82	VAL
2	F	83	ASN
2	F	98	ASP
2	F	99	MET
3	G	1	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	70	GLN
1	A	86	ASN
1	A	114	ASN
1	A	115	GLN
1	A	127	ASN
1	A	141	GLN
1	A	144	GLN
1	A	155	GLN
1	A	218	GLN
1	A	224	GLN
1	A	260	HIS
1	A	263	HIS
2	B	2	GLN
2	B	13	HIS
2	B	83	ASN
4	D	40	HIS
4	D	71	GLN
1	E	3	HIS
1	E	70	GLN

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Mol	Chain	Res	Type
1	E	72	GLN
1	E	86	ASN
1	E	87	GLN
1	E	93	HIS
1	E	114	ASN
1	E	115	GLN
1	E	127	ASN
1	E	141	GLN
1	E	144	GLN
1	E	197	HIS
1	E	218	GLN
1	E	262	GLN
1	E	263	HIS
2	F	2	GLN
2	F	42	ASN
2	F	83	ASN
3	G	1	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.