



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:32 AM UTC

PDB ID : 1QRN / pdb_00001qrn
Title : CRYSTAL STRUCTURE OF HUMAN A6 TCR COMPLEXED WITH HLA-A2 BOUND TO ALTERED HTLV-1 TAX PEPTIDE P6A
Authors : Ding, Y.H.; Baker, B.M.; Garboczi, D.N.; Biddison, W.E.; Wiley, D.C.
Deposited on : 1999-06-14
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

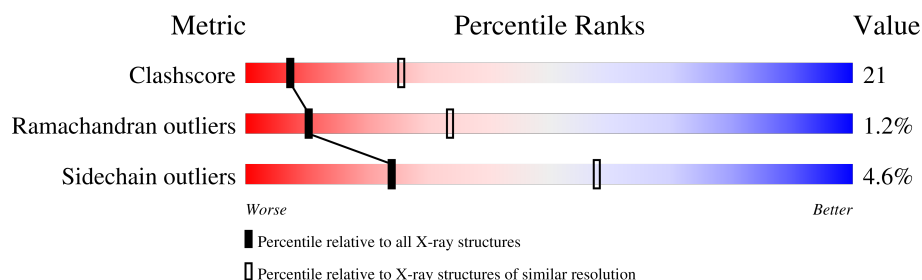
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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	274	 67% 31% •
2	B	100	 73% 25% •
3	C	9	 44% 44% 11%
4	D	200	 61% 34% 6%
5	E	243	 55% 40% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6576 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, A-2 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	16	0	0
			2238	1398	408	423	9			

- 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
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called TAX PEPTIDE P6A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			75	54	9	12			

- Molecule 4 is a protein called T-CELL RECEPTOR, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	200	Total	C	N	O	S	0	0	0
			1504	943	247	308	6			

- Molecule 5 is a protein called T-CELL RECEPTOR, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1871	1177	329	357	8			

- Molecule 6 is water.

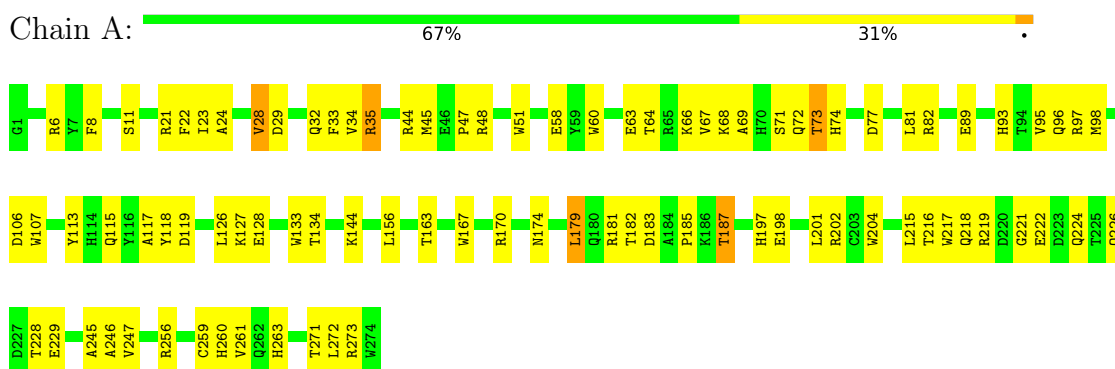
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total 18	O 18	0	0
6	B	16	Total 16	O 16	0	0
6	C	2	Total 2	O 2	0	0
6	D	6	Total 6	O 6	0	0
6	E	9	Total 9	O 9	0	0

3 Residue-property plots

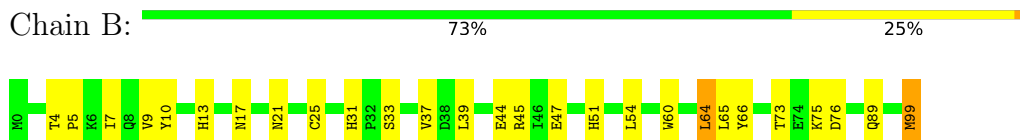
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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, A-2 ALPHA CHAIN



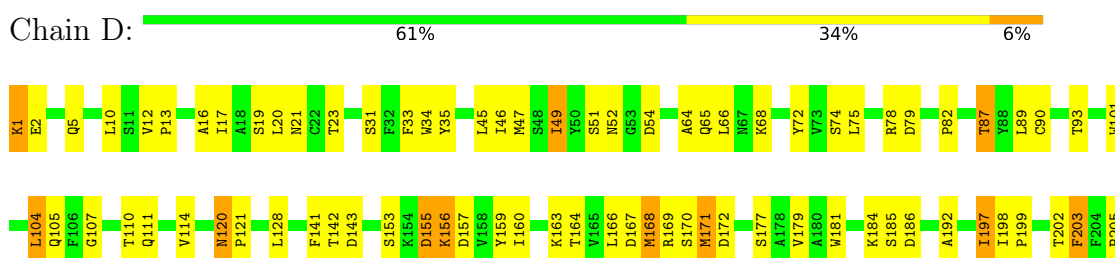
- Molecule 2: BETA-2 MICROGLOBULIN



- Molecule 3: TAX PEPTIDE P6A

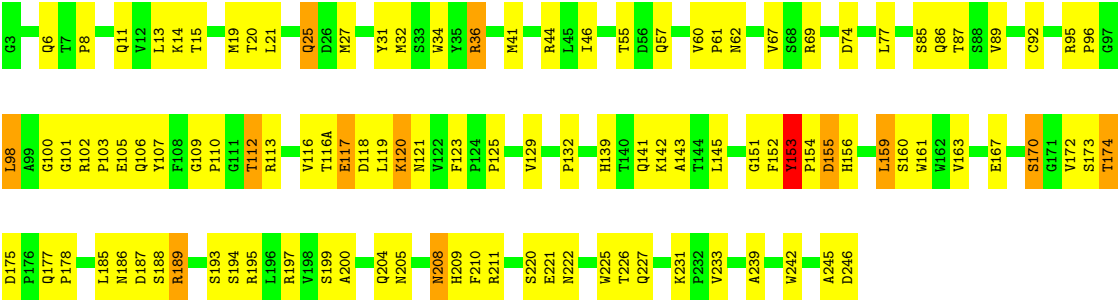


- Molecule 4: T-CELL RECEPTOR, ALPHA CHAIN



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• Molecule 5: T-CELL RECEPTOR, BETA CHAIN



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	226.95Å 48.76Å 95.55Å 90.00° 90.79° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6576	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

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	0.42	0/2303	0.86	4/3125 (0.1%)
2	B	0.46	0/860	0.89	3/1162 (0.3%)
3	C	0.50	0/77	1.10	0/103
4	D	0.43	0/1537	0.90	2/2094 (0.1%)
5	E	0.41	0/1924	0.90	6/2628 (0.2%)
All	All	0.43	0/6701	0.89	15/9112 (0.2%)

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
3	C	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	LEU	N-CA-C	6.47	118.42	111.36
2	B	33	SER	N-CA-C	6.42	118.36	111.36
4	D	185	SER	N-CA-C	-6.40	105.46	113.20
5	E	153	TYR	CA-C-N	-6.37	111.88	119.84
5	E	153	TYR	C-N-CA	-6.37	111.88	119.84
2	B	7	ILE	N-CA-C	5.89	116.34	107.80
2	B	47	GLU	N-CA-C	5.75	117.36	111.14
1	A	28	VAL	N-CA-C	-5.75	97.24	107.18
5	E	186	ASN	N-CA-C	-5.55	106.34	114.39
5	E	187	ASP	N-CA-C	-5.42	103.94	110.44
4	D	128	LEU	N-CA-C	-5.37	103.60	110.53
5	E	62	ASN	N-CA-C	5.27	117.34	109.59
1	A	187	THR	N-CA-C	5.10	117.11	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ASP	CB-CA-C	-5.03	110.79	116.63
5	E	208	ASN	N-CA-C	5.01	116.93	108.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	5	TYR	Sidechain

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	2238	0	2090	80	0
2	B	837	0	803	20	0
3	C	75	0	77	9	0
4	D	1504	0	1375	62	0
5	E	1871	0	1740	109	0
6	A	18	0	0	0	0
6	B	16	0	0	2	0
6	C	2	0	0	0	0
6	D	6	0	0	1	0
6	E	9	0	0	2	0
All	All	6576	0	6085	258	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 21.

All (258) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:MET:H	1:A:64:THR:HG22	1.13	1.09
5:E:159:LEU:HD12	5:E:160:SER:N	1.83	0.94
5:E:116(A):THR:HG22	5:E:118:ASP:H	1.33	0.92
1:A:219:ARG:HB2	1:A:222:GLU:HB2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.59	0.84
5:E:6:GLN:HG2	5:E:110:PRO:HD2	1.61	0.80
4:D:168:MET:HE2	5:E:197:ARG:HD3	1.64	0.79
1:A:45:MET:N	1:A:64:THR:HG22	1.96	0.78
5:E:13:LEU:HD11	5:E:19:MET:HB2	1.64	0.78
1:A:21:ARG:CZ	1:A:23:ILE:HD11	2.13	0.77
1:A:96:GLN:HE22	2:B:31:HIS:HE1	1.33	0.74
1:A:202:ARG:HG2	1:A:246:ALA:HB2	1.68	0.74
4:D:5:GLN:HE21	4:D:107:GLY:HA3	1.52	0.74
4:D:1:LYS:HB3	4:D:1:LYS:NZ	2.02	0.74
2:B:13:HIS:HB2	2:B:21:ASN:HD21	1.53	0.73
1:A:44:ARG:HB3	1:A:64:THR:HG21	1.69	0.73
4:D:31:SER:HB2	4:D:93:THR:HG22	1.71	0.73
1:A:96:GLN:NE2	2:B:31:HIS:HE1	1.87	0.71
1:A:77:ASP:OD1	3:C:9:VAL:HG22	1.90	0.70
5:E:119:LEU:C	5:E:121:ASN:H	1.99	0.70
1:A:167:TRP:NE1	3:C:1:LEU:HD22	2.06	0.70
5:E:205:ASN:HB3	5:E:208:ASN:ND2	2.06	0.70
5:E:118:ASP:OD1	5:E:120:LYS:HD3	1.92	0.69
4:D:52:ASN:HA	4:D:66:LEU:HB3	1.73	0.68
5:E:118:ASP:CG	5:E:120:LYS:HD3	2.18	0.68
5:E:36:ARG:HD2	5:E:44:ARG:HH21	1.59	0.67
1:A:202:ARG:CZ	2:B:99:MET:HG3	2.25	0.67
5:E:25:GLN:HB3	5:E:32:MET:HE3	1.76	0.66
4:D:198:ILE:HD12	4:D:202:THR:HG21	1.77	0.65
1:A:74:HIS:CE1	1:A:97:ARG:HH21	2.15	0.65
1:A:93:HIS:HD2	1:A:119:ASP:OD1	1.78	0.64
4:D:5:GLN:NE2	4:D:90:CYS:H	1.96	0.64
1:A:69:ALA:O	1:A:73:THR:HG22	1.98	0.64
2:B:13:HIS:HB2	2:B:21:ASN:ND2	2.12	0.64
5:E:25:GLN:HE21	5:E:32:MET:HE3	1.61	0.64
1:A:197:HIS:ND1	1:A:198:GLU:HG3	2.12	0.64
4:D:163:LYS:HA	4:D:177:SER:O	1.99	0.63
5:E:116(A):THR:HG22	5:E:117:GLU:N	2.13	0.63
4:D:12:VAL:HG13	4:D:16:ALA:HB3	1.81	0.63
1:A:181:ARG:HG2	1:A:182:THR:N	2.13	0.62
5:E:132:PRO:HD3	5:E:145:LEU:HG	1.80	0.62
5:E:209:HIS:HB2	5:E:242:TRP:CZ3	2.35	0.62
5:E:163:VAL:HG12	5:E:210:PHE:HD1	1.65	0.61
1:A:82:ARG:CZ	1:A:89:GLU:HG2	2.31	0.61
4:D:45:LEU:HD21	5:E:105:GLU:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:21:LEU:HD22	5:E:77:LEU:HD23	1.81	0.60
5:E:159:LEU:HD12	5:E:159:LEU:C	2.26	0.60
5:E:225:TRP:NE1	5:E:227:GLN:HB2	2.16	0.60
5:E:21:LEU:HD12	5:E:21:LEU:N	2.17	0.60
1:A:218:GLN:HE21	1:A:221:GLY:N	1.99	0.59
4:D:93:THR:HB	4:D:104:LEU:HD22	1.83	0.59
4:D:1:LYS:HB3	4:D:1:LYS:HZ3	1.66	0.59
5:E:153:TYR:O	5:E:154:PRO:C	2.44	0.59
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.84	0.58
1:A:127:LYS:HE2	1:A:134:THR:OG1	2.03	0.58
1:A:187:THR:HA	1:A:204:TRP:O	2.03	0.58
4:D:203:PHE:O	4:D:205:PRO:HD3	2.04	0.58
5:E:6:GLN:HE22	5:E:92:CYS:H	1.52	0.57
1:A:256:ARG:HH11	1:A:256:ARG:HB3	1.69	0.57
5:E:101:GLY:O	5:E:103:PRO:HD3	2.04	0.57
5:E:117:GLU:CD	5:E:117:GLU:H	2.10	0.57
5:E:175:ASP:OD2	5:E:193:SER:HB3	2.04	0.57
5:E:177:GLN:HG3	5:E:178:PRO:HD2	1.86	0.57
5:E:132:PRO:HG3	5:E:143:ALA:HB1	1.87	0.56
1:A:217:TRP:HD1	1:A:228:THR:HG23	1.70	0.56
5:E:13:LEU:HD11	5:E:19:MET:CB	2.35	0.56
2:B:45:ARG:HD3	6:B:106:HOH:O	2.05	0.56
4:D:31:SER:HB2	4:D:93:THR:CG2	2.35	0.56
1:A:32:GLN:HE21	1:A:48:ARG:HG3	1.71	0.56
4:D:45:LEU:CD2	5:E:105:GLU:HG2	2.37	0.55
5:E:96:PRO:HG2	5:E:102:ARG:O	2.07	0.55
3:C:5:TYR:CE2	5:E:103:PRO:HB3	2.41	0.55
5:E:55:THR:HG22	6:E:248:HOH:O	2.05	0.55
5:E:154:PRO:O	5:E:156:HIS:N	2.33	0.55
5:E:155:ASP:HB2	5:E:178:PRO:HG2	1.88	0.55
5:E:185:LEU:HB2	5:E:188:SER:HB2	1.89	0.55
1:A:44:ARG:HB3	1:A:64:THR:CG2	2.35	0.55
5:E:200:ALA:O	5:E:204:GLN:HG3	2.06	0.55
5:E:205:ASN:HB3	5:E:208:ASN:HD22	1.70	0.55
1:A:156:LEU:HG	3:C:3:PHE:CZ	2.42	0.54
4:D:34:TRP:HB2	4:D:47:MET:HB2	1.90	0.54
5:E:25:GLN:HB3	5:E:32:MET:CE	2.38	0.54
1:A:217:TRP:CD1	1:A:247:VAL:HG13	2.43	0.54
1:A:229:GLU:O	1:A:245:ALA:HA	2.07	0.54
4:D:52:ASN:HB2	4:D:66:LEU:O	2.08	0.54
5:E:226:THR:O	5:E:227:GLN:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HD22	1:A:261:VAL:HG22	1.90	0.54
4:D:5:GLN:HE22	4:D:90:CYS:H	1.56	0.54
5:E:119:LEU:C	5:E:121:ASN:N	2.64	0.53
4:D:19:SER:O	4:D:20:LEU:HD23	2.08	0.53
5:E:153:TYR:CD2	5:E:154:PRO:HD3	2.44	0.53
5:E:159:LEU:CD1	5:E:160:SER:N	2.67	0.53
5:E:154:PRO:C	5:E:156:HIS:H	2.17	0.53
5:E:209:HIS:HB2	5:E:242:TRP:CH2	2.44	0.53
5:E:31:TYR:HB3	5:E:95:ARG:HB2	1.90	0.53
1:A:187:THR:HB	1:A:272:LEU:HD11	1.91	0.53
5:E:60:VAL:O	5:E:60:VAL:HG23	2.08	0.53
4:D:166:LEU:C	4:D:166:LEU:HD23	2.34	0.52
4:D:49:ILE:HD11	4:D:64:ALA:HB1	1.92	0.52
4:D:82:PRO:HA	4:D:114:VAL:HB	1.91	0.52
1:A:11:SER:HB3	1:A:95:VAL:HB	1.91	0.52
5:E:13:LEU:HB2	5:E:116:VAL:HG22	1.91	0.52
5:E:221:GLU:C	5:E:231:LYS:HZ1	2.18	0.52
1:A:45:MET:CE	3:C:2:LEU:HD11	2.38	0.52
5:E:120:LYS:C	5:E:121:ASN:HD22	2.17	0.52
1:A:106:ASP:O	1:A:107:TRP:HB2	2.11	0.51
5:E:6:GLN:HE21	5:E:109:GLY:HA3	1.75	0.51
4:D:155:ASP:O	4:D:157:ASP:N	2.43	0.51
5:E:141:GLN:NE2	5:E:141:GLN:HA	2.25	0.51
5:E:195:ARG:HD3	5:E:195:ARG:N	2.25	0.51
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.45	0.51
4:D:101:TRP:CE2	5:E:98:LEU:HD21	2.45	0.51
4:D:168:MET:CE	5:E:142:LYS:HD3	2.41	0.51
5:E:161:TRP:O	5:E:167:GLU:HA	2.11	0.51
5:E:11:GLN:HG2	5:E:19:MET:SD	2.51	0.50
5:E:25:GLN:HG2	5:E:27:MET:H	1.75	0.50
4:D:12:VAL:O	4:D:114:VAL:HA	2.12	0.50
1:A:45:MET:H	1:A:64:THR:CG2	2.04	0.50
5:E:163:VAL:HG12	5:E:210:PHE:CD1	2.45	0.50
5:E:245:ALA:O	5:E:246:ASP:C	2.54	0.50
1:A:24:ALA:O	1:A:35:ARG:HA	2.12	0.49
1:A:47:PRO:O	1:A:48:ARG:HD2	2.12	0.49
5:E:231:LYS:HE2	5:E:233:VAL:HG12	1.93	0.49
5:E:145:LEU:HD12	5:E:145:LEU:N	2.27	0.49
5:E:221:GLU:C	5:E:231:LYS:NZ	2.71	0.49
4:D:153:SER:HB3	4:D:160:ILE:HD12	1.94	0.49
4:D:142:THR:OG1	4:D:143:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HE3	3:C:2:LEU:HB2	1.95	0.49
4:D:51:SER:HA	6:D:212:HOH:O	2.11	0.49
1:A:69:ALA:O	1:A:73:THR:CG2	2.59	0.49
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.47	0.49
5:E:125:PRO:HB3	5:E:152:PHE:HB3	1.94	0.49
5:E:153:TYR:HB3	5:E:154:PRO:CD	2.43	0.48
5:E:121:ASN:N	5:E:121:ASN:HD22	2.11	0.48
4:D:13:PRO:HG2	4:D:16:ALA:HB2	1.95	0.48
1:A:33:PHE:O	1:A:48:ARG:N	2.45	0.48
4:D:164:THR:OG1	5:E:195:ARG:NH2	2.46	0.48
5:E:172:VAL:HG12	5:E:173:SER:N	2.29	0.48
4:D:52:ASN:HA	4:D:66:LEU:CB	2.43	0.48
1:A:185:PRO:HD3	1:A:263:HIS:CD2	2.49	0.48
5:E:6:GLN:NE2	5:E:92:CYS:H	2.12	0.48
5:E:95:ARG:HG2	5:E:106:GLN:HB2	1.96	0.47
5:E:116(A):THR:CG2	5:E:117:GLU:N	2.76	0.47
5:E:119:LEU:O	5:E:121:ASN:N	2.47	0.47
5:E:117:GLU:N	5:E:117:GLU:CD	2.71	0.47
1:A:21:ARG:NH1	1:A:23:ILE:HD11	2.30	0.47
1:A:82:ARG:NH1	1:A:89:GLU:HG2	2.30	0.47
1:A:167:TRP:CE2	3:C:1:LEU:HD22	2.48	0.47
1:A:8:PHE:N	1:A:8:PHE:CD1	2.83	0.47
1:A:22:PHE:HE1	1:A:74:HIS:HD2	1.61	0.47
1:A:22:PHE:HE1	1:A:74:HIS:CD2	2.31	0.47
1:A:126:LEU:HD13	1:A:133:TRP:CH2	2.49	0.47
1:A:228:THR:HA	1:A:247:VAL:HG12	1.95	0.47
4:D:35:TYR:HB2	4:D:89:LEU:HB2	1.97	0.47
1:A:170:ARG:HG2	1:A:174:ASN:ND2	2.29	0.47
1:A:45:MET:HE2	3:C:2:LEU:HD11	1.96	0.47
1:A:218:GLN:HE21	1:A:221:GLY:H	1.60	0.47
1:A:228:THR:HA	1:A:246:ALA:O	2.15	0.47
1:A:181:ARG:HD2	1:A:183:ASP:OD2	2.15	0.47
2:B:17:ASN:HD22	2:B:73:THR:C	2.22	0.47
4:D:87:THR:HA	4:D:111:GLN:HA	1.96	0.47
1:A:64:THR:O	1:A:67:VAL:HG12	2.15	0.46
2:B:10:TYR:CD1	2:B:10:TYR:N	2.83	0.46
5:E:14:LYS:O	5:E:15:THR:C	2.57	0.46
5:E:27:MET:HE1	5:E:107:TYR:CE2	2.50	0.46
5:E:100:GLY:HA3	6:E:255:HOH:O	2.15	0.46
5:E:174:THR:HG22	5:E:194:SER:OG	2.15	0.46
5:E:154:PRO:C	5:E:156:HIS:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:MET:SD	1:A:98:MET:C	2.98	0.46
1:A:218:GLN:HE21	1:A:221:GLY:CA	2.29	0.46
5:E:141:GLN:HA	5:E:141:GLN:HE21	1.81	0.46
1:A:115:GLN:HB3	2:B:60:TRP:CH2	2.51	0.46
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.98	0.46
5:E:151:GLY:O	5:E:189:ARG:HB3	2.15	0.46
5:E:36:ARG:HB3	5:E:46:ILE:HD11	1.97	0.46
1:A:201:LEU:O	1:A:246:ALA:HA	2.16	0.46
4:D:166:LEU:HD23	4:D:167:ASP:N	2.31	0.46
1:A:256:ARG:HH11	1:A:256:ARG:CB	2.29	0.45
1:A:163:THR:OG1	4:D:68:LYS:NZ	2.50	0.45
2:B:54:LEU:HA	2:B:64:LEU:HD13	1.99	0.45
1:A:259:CYS:O	1:A:271:THR:HA	2.16	0.45
4:D:78:ARG:HG2	4:D:79:ASP:H	1.81	0.45
5:E:8:PRO:O	5:E:112:THR:HB	2.17	0.45
5:E:20:THR:HG23	5:E:20:THR:O	2.17	0.45
1:A:51:TRP:NE1	1:A:179:LEU:HD21	2.32	0.45
2:B:17:ASN:ND2	2:B:73:THR:C	2.75	0.45
5:E:194:SER:C	5:E:195:ARG:HD3	2.42	0.45
5:E:199:SER:O	5:E:200:ALA:C	2.60	0.45
4:D:78:ARG:O	4:D:79:ASP:C	2.60	0.45
1:A:6:ARG:HB3	1:A:8:PHE:CE1	2.52	0.44
4:D:49:ILE:CD1	4:D:64:ALA:HB1	2.47	0.44
4:D:171:MET:O	4:D:172:ASP:C	2.59	0.44
5:E:34:TRP:CE2	5:E:77:LEU:HB2	2.53	0.44
5:E:211:ARG:HB3	5:E:211:ARG:NH1	2.33	0.44
5:E:89:VAL:HG22	5:E:113:ARG:HG3	1.98	0.44
5:E:118:ASP:OD2	5:E:120:LYS:HD3	2.18	0.44
4:D:21:ASN:ND2	4:D:72:TYR:HE2	2.16	0.44
5:E:69:ARG:HD2	5:E:74:ASP:O	2.18	0.44
5:E:172:VAL:HA	5:E:195:ARG:O	2.17	0.44
2:B:25:CYS:HB2	2:B:39:LEU:HD21	2.00	0.43
2:B:51:HIS:HA	2:B:65:LEU:O	2.18	0.43
4:D:153:SER:HB3	4:D:160:ILE:CD1	2.48	0.43
4:D:197:ILE:HD13	4:D:197:ILE:N	2.33	0.43
4:D:203:PHE:CD2	5:E:139:HIS:HD2	2.36	0.43
5:E:211:ARG:HB3	5:E:211:ARG:HH11	1.82	0.43
4:D:52:ASN:HA	4:D:66:LEU:CG	2.48	0.43
4:D:184:LYS:C	4:D:186:ASP:H	2.25	0.43
5:E:36:ARG:NH2	5:E:86:GLN:HA	2.34	0.43
1:A:93:HIS:CD2	1:A:119:ASP:OD1	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:VAL:HG13	4:D:13:PRO:HD2	1.99	0.43
5:E:123:PHE:O	5:E:152:PHE:HA	2.18	0.43
2:B:9:VAL:HG13	2:B:9:VAL:O	2.18	0.43
1:A:224:GLN:C	1:A:226:GLN:H	2.26	0.43
4:D:20:LEU:O	4:D:74:SER:HA	2.18	0.43
4:D:120:ASN:HD22	4:D:120:ASN:HA	1.61	0.43
1:A:58:GLU:H	1:A:58:GLU:CD	2.26	0.42
1:A:182:THR:HG23	1:A:182:THR:O	2.20	0.42
1:A:256:ARG:CB	1:A:256:ARG:NH1	2.82	0.42
5:E:174:THR:HA	5:E:194:SER:HA	2.01	0.42
4:D:20:LEU:HB2	4:D:75:LEU:HB3	2.01	0.42
5:E:21:LEU:N	5:E:21:LEU:CD1	2.81	0.42
1:A:60:TRP:O	1:A:64:THR:HG23	2.20	0.42
2:B:4:THR:HG23	2:B:5:PRO:HD2	2.01	0.42
5:E:13:LEU:O	5:E:116:VAL:HA	2.19	0.42
5:E:143:ALA:O	5:E:197:ARG:HA	2.19	0.42
4:D:159:TYR:HD1	4:D:181:TRP:NE1	2.18	0.42
4:D:199:PRO:O	4:D:202:THR:HG23	2.18	0.42
1:A:216:THR:HB	1:A:260:HIS:HB2	2.01	0.42
5:E:153:TYR:CB	5:E:154:PRO:CD	2.98	0.42
5:E:153:TYR:CG	5:E:154:PRO:N	2.85	0.42
1:A:224:GLN:C	1:A:226:GLN:N	2.78	0.42
5:E:85:SER:C	5:E:87:THR:H	2.27	0.42
5:E:220:SER:C	5:E:222:ASN:N	2.77	0.42
1:A:35:ARG:O	1:A:35:ARG:HG3	2.19	0.42
4:D:12:VAL:CG1	4:D:16:ALA:HB3	2.49	0.42
5:E:129:VAL:HG23	5:E:239:ALA:HB3	2.01	0.42
5:E:121:ASN:N	5:E:121:ASN:ND2	2.68	0.41
5:E:57:GLN:HB2	5:E:61:PRO:HG3	2.02	0.41
1:A:63:GLU:OE2	3:C:1:LEU:HD12	2.20	0.41
1:A:68:LYS:O	1:A:71:SER:HB3	2.20	0.41
2:B:31:HIS:HD2	6:B:115:HOH:O	2.04	0.41
4:D:170:SER:C	4:D:172:ASP:H	2.29	0.41
5:E:170:SER:C	5:E:172:VAL:H	2.29	0.41
5:E:113:ARG:HD3	5:E:156:HIS:CD2	2.56	0.41
1:A:170:ARG:HG2	1:A:174:ASN:HD21	1.86	0.41
4:D:46:ILE:O	4:D:47:MET:HG2	2.21	0.41
4:D:155:ASP:O	4:D:156:LYS:C	2.64	0.41
4:D:54:ASP:OD1	4:D:65:GLN:HG2	2.21	0.41
2:B:39:LEU:HA	2:B:39:LEU:HD23	1.82	0.40
4:D:2:GLU:OE1	4:D:105:GLN:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1:LYS:HB3	4:D:1:LYS:HZ2	1.81	0.40
4:D:31:SER:HB3	4:D:33:PHE:CZ	2.55	0.40
4:D:141:PHE:O	4:D:177:SER:HA	2.21	0.40
4:D:167:ASP:OD2	4:D:169:ARG:HG3	2.22	0.40
2:B:37:VAL:HB	2:B:66:TYR:CZ	2.56	0.40
2:B:75:LYS:HG3	2:B:76:ASP:N	2.36	0.40
1:A:6:ARG:NE	1:A:113:TYR:OH	2.55	0.40
5:E:116(A):THR:HG22	5:E:118:ASP:N	2.16	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	272/274 (99%)	248 (91%)	24 (9%)	0	100	100
2	B	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	198/200 (99%)	172 (87%)	20 (10%)	6 (3%)	3	12
5	E	241/243 (99%)	218 (90%)	19 (8%)	4 (2%)	7	25
All	All	816/826 (99%)	737 (90%)	69 (8%)	10 (1%)	10	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	156	LYS
5	E	170	SER
4	D	155	ASP
5	E	120	LYS
5	E	153	TYR
4	D	171	MET

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Mol	Chain	Res	Type
4	D	192	ALA
5	E	155	ASP
4	D	203	PHE
4	D	121	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	230/230 (100%)	224 (97%)	6 (3%)	40	75
2	B	95/95 (100%)	91 (96%)	4 (4%)	26	61
3	C	7/7 (100%)	7 (100%)	0	100	100
4	D	161/178 (90%)	149 (92%)	12 (8%)	12	37
5	E	196/208 (94%)	186 (95%)	10 (5%)	21	54
All	All	689/718 (96%)	657 (95%)	32 (5%)	24	58

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	35	ARG
1	A	72	GLN
1	A	73	THR
1	A	128	GLU
1	A	273	ARG
2	B	44	GLU
2	B	64	LEU
2	B	89	GLN
2	B	99	MET
4	D	1	LYS
4	D	10	LEU
4	D	17	ILE
4	D	23	THR
4	D	49	ILE

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Mol	Chain	Res	Type
4	D	87	THR
4	D	104	LEU
4	D	110	THR
4	D	120	ASN
4	D	168	MET
4	D	179	VAL
4	D	197	ILE
5	E	25	GLN
5	E	36	ARG
5	E	41	MET
5	E	67	VAL
5	E	98	LEU
5	E	112	THR
5	E	117	GLU
5	E	159	LEU
5	E	174	THR
5	E	189	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	43	GLN
1	A	74	HIS
1	A	86	ASN
1	A	93	HIS
1	A	96	GLN
1	A	141	GLN
1	A	151	HIS
1	A	174	ASN
1	A	218	GLN
2	B	31	HIS
2	B	83	ASN
4	D	5	GLN
4	D	37	GLN
4	D	65	GLN
4	D	71	GLN
4	D	111	GLN
4	D	120	ASN
4	D	127	GLN
4	D	149	ASN
4	D	183	ASN

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Mol	Chain	Res	Type
5	E	6	GLN
5	E	37	GLN
5	E	121	ASN
5	E	141	GLN
5	E	156	HIS

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

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.