



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:46 PM UTC

PDB ID : 2IAM / pdb_00002iam
Title : Structural basis for recognition of mutant self by a tumor-specific, MHC class II-restricted TCR
Authors : Deng, L.; Langley, R.J.; Mariuzza, R.A.
Deposited on : 2006-09-08
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)	:	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

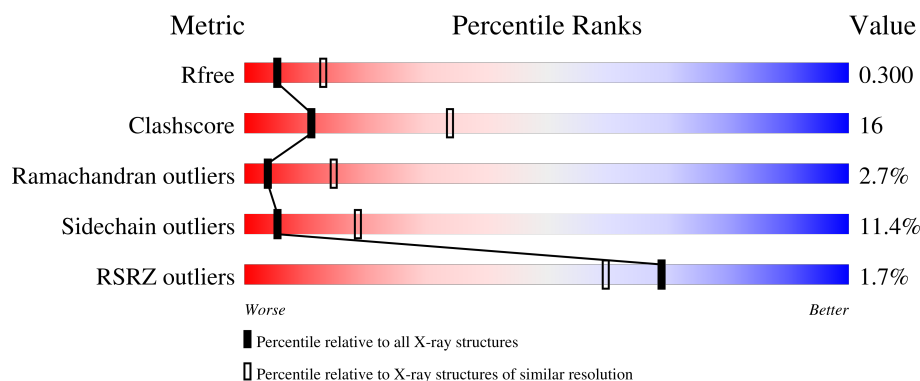
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	4% 53% 37% 6% ..
2	B	190	% 60% 28% ..
3	P	15	53% 33% 7% 7%
4	C	202	% 60% 30% 7% ..
5	D	240	% 61% 31% 7% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6551 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 II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1473	954	239	275	5			

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	182	Total	C	N	O	S	0	0	0
			1487	936	264	281	6			

- Molecule 3 is a protein called 15-mer peptide from Triosephosphate isomerase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	15	Total	C	N	O	0	0	0
			104	66	17	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	28	ILE	THR	engineered mutation	UNP P60174

- Molecule 4 is a protein called CD4+ T cell receptor E8 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	198	Total	C	N	O	S	0	0	0
			1546	967	260	312	7			

- Molecule 5 is a protein called CD4+ T cell receptor E8 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	239	Total	C	N	O	S	0	0	0
			1901	1206	324	362	9			

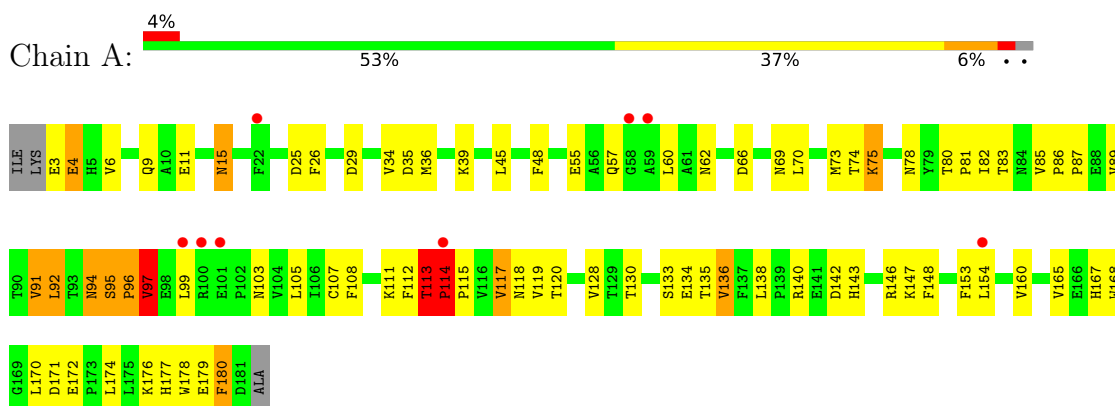
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total 17	O 17	0	0
6	B	7	Total 7	O 7	0	0
6	P	1	Total 1	O 1	0	0
6	C	6	Total 6	O 6	0	0
6	D	9	Total 9	O 9	0	0

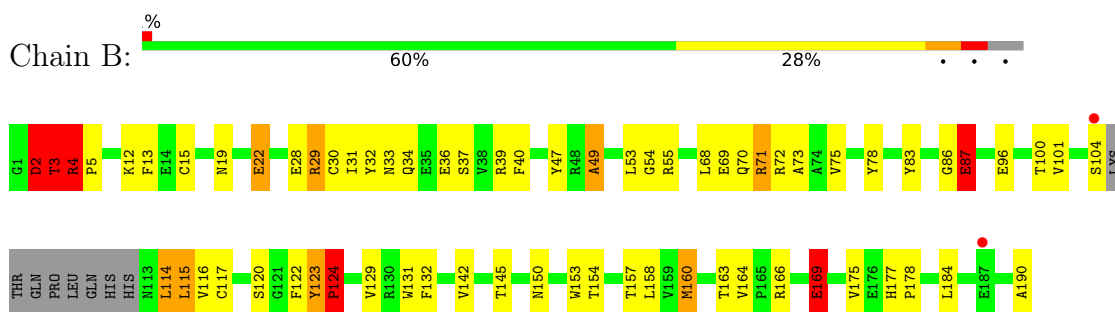
3 Residue-property plots

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 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: HLA class II histocompatibility antigen, DR alpha chain



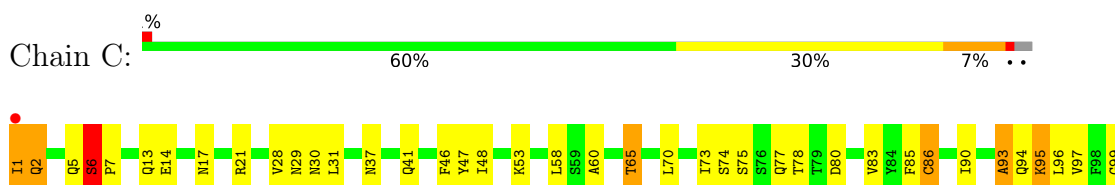
- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

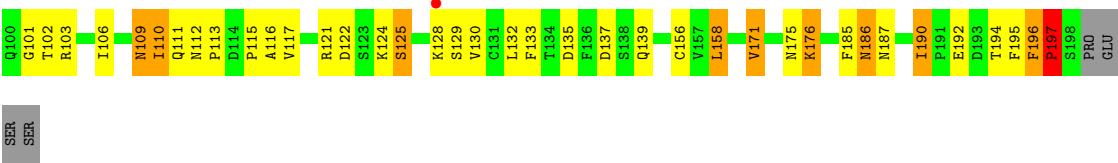


- Molecule 3: 15-mer peptide from Triosephosphate isomerase

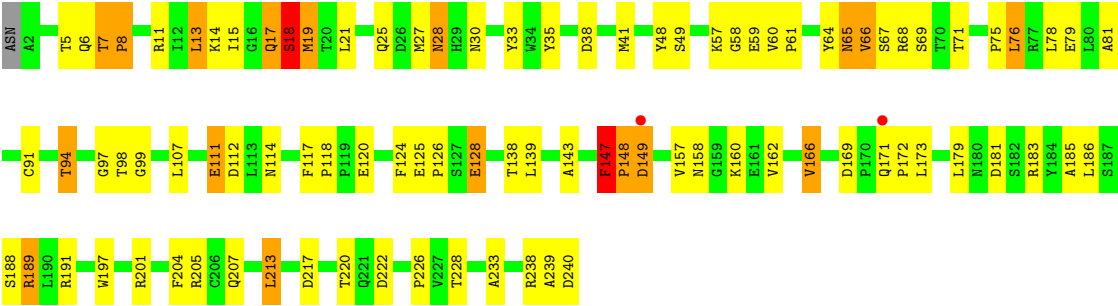


- Molecule 4: CD4+ T cell receptor E8 alpha chain





● Molecule 5: CD4+ T cell receptor E8 beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.39Å 270.54Å 97.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.91 – 2.80 41.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (41.91-2.80) 92.1 (41.91-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.279 0.242 , 0.300	Depositor DCC
R_{free} test set	1329 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 9.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6551	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.07	3/1518 (0.2%)	1.42	9/2070 (0.4%)
2	B	1.21	3/1523 (0.2%)	1.30	14/2067 (0.7%)
3	P	1.41	1/104 (1.0%)	1.52	1/139 (0.7%)
4	C	1.09	3/1579 (0.2%)	1.30	12/2148 (0.6%)
5	D	1.10	1/1956 (0.1%)	1.35	15/2666 (0.6%)
All	All	1.12	11/6680 (0.2%)	1.35	51/9090 (0.6%)

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	1
2	B	0	3
4	C	0	2
5	D	0	3
All	All	0	9

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	169	GLU	CD-OE2	21.29	1.65	1.25
2	B	190	ALA	C-O	6.66	1.36	1.23
1	A	179	GLU	C-N	6.22	1.42	1.33
4	C	190	ILE	CA-C	6.14	1.58	1.52
4	C	190	ILE	CA-CB	6.03	1.62	1.54
5	D	64	TYR	CA-C	-5.83	1.45	1.52
1	A	179	GLU	C-O	5.78	1.31	1.23
2	B	169	GLU	CD-OE1	5.74	1.36	1.25
1	A	180	PHE	C-O	5.63	1.30	1.23
4	C	46	PHE	CA-C	-5.63	1.45	1.52
3	P	30	ASN	CA-C	-5.05	1.46	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	THR	CA-C-N	23.36	144.44	120.38
1	A	113	THR	C-N-CA	23.36	144.44	120.38
5	D	147	PHE	CA-C-N	15.64	139.39	119.84
5	D	147	PHE	C-N-CA	15.64	139.39	119.84
5	D	7	THR	CA-C-N	12.71	135.73	119.84
5	D	7	THR	C-N-CA	12.71	135.73	119.84
2	B	123	TYR	CA-C-N	12.01	134.85	119.84
2	B	123	TYR	C-N-CA	12.01	134.85	119.84
5	D	30	ASN	N-CA-C	-9.33	102.03	113.41
4	C	196	PHE	CA-C-N	9.15	131.28	119.84
4	C	196	PHE	C-N-CA	9.15	131.28	119.84
4	C	2	GLN	N-CA-C	8.79	123.14	109.52
4	C	93	ALA	CA-C-N	-8.03	106.20	121.54
4	C	93	ALA	C-N-CA	-8.03	106.20	121.54
1	A	114	PRO	CA-C-N	7.88	129.69	119.84
1	A	114	PRO	C-N-CA	7.88	129.69	119.84
1	A	15	ASN	O-C-N	7.70	126.46	120.38
1	A	15	ASN	N-CA-C	7.64	122.87	112.55
4	C	47	TYR	N-CA-C	-6.80	98.54	109.96
5	D	222	ASP	N-CA-C	6.47	118.03	110.97
5	D	111	GLU	N-CA-C	-6.42	104.20	111.14
2	B	190	ALA	CA-C-O	-6.25	110.18	120.80
4	C	129	SER	N-CA-C	6.00	117.97	108.79
5	D	94	THR	CB-CA-C	-5.87	99.99	112.78
4	C	80	ASP	N-CA-C	-5.80	105.97	113.16
2	B	124	PRO	N-CA-C	-5.71	100.70	112.47
5	D	228	THR	N-CA-C	-5.62	101.73	110.10
4	C	110	ILE	N-CA-C	5.60	116.47	107.73
2	B	83	TYR	N-CA-C	-5.52	105.16	111.07
2	B	122	PHE	N-CA-C	5.51	118.56	109.85
5	D	18	SER	N-CA-C	5.51	116.34	108.74
2	B	132	PHE	N-CA-C	5.50	118.06	108.76
5	D	166	VAL	N-CA-C	5.50	116.67	109.58
2	B	96	GLU	N-CA-C	5.43	116.49	109.65
2	B	120	SER	N-CA-C	5.37	117.14	109.14
5	D	128	GLU	N-CA-C	-5.34	105.45	111.28
1	A	176	LYS	N-CA-C	5.24	117.06	108.52
1	A	133	SER	N-CA-C	-5.21	101.56	108.74
4	C	93	ALA	O-C-N	-5.18	116.65	122.97
2	B	4	ARG	CA-C-N	5.17	125.46	119.93
2	B	4	ARG	C-N-CA	5.17	125.46	119.93
2	B	73	ALA	N-CA-C	-5.14	107.04	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	28	ILE	CB-CA-C	-5.10	104.21	111.19
4	C	95	LYS	CA-CB-CG	5.05	124.20	114.10
2	B	115	LEU	N-CA-C	5.05	117.67	109.24
5	D	233	ALA	N-CA-C	-5.04	101.40	109.07
4	C	86	CYS	N-CA-CB	5.04	118.48	110.16
1	A	113	THR	C-N-CD	-5.04	104.34	125.00
5	D	8	PRO	CA-N-CD	-5.03	104.96	112.00
2	B	49	ALA	N-CA-C	-5.03	102.61	110.10
5	D	28	ASN	N-CA-C	5.00	118.69	112.58

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	THR	Peptide
2	B	123	TYR	Peptide
2	B	169	GLU	Sidechain
2	B	3	THR	Peptide
4	C	1	ILE	Peptide
4	C	6	SER	Peptide
5	D	147	PHE	Peptide
5	D	18	SER	Peptide
5	D	7	THR	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	1473	0	1407	51	0
2	B	1487	0	1419	48	0
3	P	104	0	109	7	0
4	C	1546	0	1474	55	0
5	D	1901	0	1800	61	0
6	A	17	0	0	2	0
6	B	7	0	0	0	0
6	C	6	0	0	0	0
6	D	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	1	0	0	0	0
All	All	6551	0	6209	208	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 16.

All (208) 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)
2:B:169:GLU:OE2	2:B:169:GLU:CD	1.65	1.35
2:B:19:ASN:HD22	2:B:22:GLU:HG2	1.11	1.16
2:B:2:ASP:O	2:B:3:THR:HB	1.49	1.11
5:D:94:THR:HG22	5:D:99:GLY:HA2	1.34	1.04
1:A:82:ILE:HD13	1:A:114:PRO:HD3	1.48	0.93
5:D:13:LEU:HD13	5:D:81:ALA:HB2	1.58	0.83
5:D:149:ASP:OD1	5:D:172:PRO:HG3	1.79	0.82
2:B:4:ARG:HB2	2:B:5:PRO:HD2	1.61	0.82
5:D:11:ARG:HG2	5:D:19:MET:HE3	1.66	0.78
5:D:117:PHE:CD1	5:D:183:ARG:HD3	2.17	0.78
2:B:69:GLU:OE2	4:C:53:LYS:HD2	1.83	0.77
5:D:169:ASP:OD1	5:D:189:ARG:NH2	2.20	0.74
1:A:69:ASN:OD1	3:P:34:VAL:HG22	1.86	0.74
5:D:6:GLN:HE22	5:D:91:CYS:H	1.36	0.74
1:A:3:GLU:HG2	1:A:4:GLU:H	1.52	0.72
4:C:65:THR:CG2	4:C:65:THR:O	2.38	0.72
5:D:94:THR:CG2	5:D:99:GLY:HA2	2.17	0.72
2:B:19:ASN:ND2	2:B:22:GLU:HG2	1.96	0.71
1:A:94:ASN:HB3	1:A:103:ASN:OD1	1.91	0.71
4:C:117:VAL:HA	4:C:132:LEU:O	1.90	0.71
4:C:6:SER:HB3	4:C:21:ARG:HB3	1.74	0.70
2:B:2:ASP:O	2:B:3:THR:CB	2.32	0.69
5:D:38:ASP:O	5:D:41:MET:HB2	1.92	0.69
1:A:105:LEU:HG	1:A:153:PHE:CE1	2.26	0.69
1:A:15:ASN:HB2	1:A:70:LEU:HD21	1.74	0.69
5:D:6:GLN:NE2	5:D:91:CYS:H	1.90	0.68
1:A:92:LEU:HG	1:A:108:PHE:CE1	2.28	0.68
1:A:35:ASP:O	1:A:39:LYS:N	2.28	0.67
2:B:115:LEU:O	2:B:160:MET:HA	1.95	0.67
2:B:157:THR:C	2:B:158:LEU:HD12	2.20	0.66
5:D:33:TYR:HD2	5:D:48:TYR:HB2	1.63	0.64
5:D:58:GLY:O	5:D:61:PRO:HD3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:30:ASN:HD22	3:P:30:ASN:H	1.46	0.64
1:A:92:LEU:HG	1:A:108:PHE:HE1	1.62	0.64
4:C:90:ILE:HD12	4:C:95:LYS:HB2	1.80	0.64
5:D:13:LEU:HD13	5:D:81:ALA:CB	2.28	0.62
1:A:95:SER:CB	1:A:96:PRO:HD2	2.30	0.61
4:C:29:ASN:OD1	4:C:30:ASN:N	2.30	0.61
5:D:205:ARG:NH1	5:D:207:GLN:OE1	2.28	0.61
5:D:33:TYR:CD2	5:D:48:TYR:HB2	2.36	0.61
5:D:238:ARG:HB3	5:D:238:ARG:HH11	1.66	0.60
2:B:129:VAL:HG22	2:B:175:VAL:HG13	1.82	0.60
1:A:97:VAL:HG11	1:A:178:TRP:HH2	1.66	0.60
4:C:117:VAL:O	4:C:197:PRO:HG2	2.02	0.60
1:A:113:THR:HG23	1:A:114:PRO:HD2	1.83	0.59
1:A:142:ASP:O	1:A:143:HIS:HB2	2.03	0.59
4:C:65:THR:O	4:C:65:THR:HG22	2.03	0.59
5:D:11:ARG:HG2	5:D:19:MET:CE	2.32	0.59
4:C:5:GLN:NE2	4:C:86:CYS:H	2.00	0.58
3:P:30:ASN:H	3:P:30:ASN:ND2	2.01	0.58
2:B:33:ASN:O	2:B:34:GLN:CB	2.49	0.58
1:A:82:ILE:HD13	1:A:114:PRO:CD	2.29	0.57
2:B:101:VAL:HA	2:B:116:VAL:O	2.05	0.57
5:D:18:SER:HB3	5:D:79:GLU:O	2.04	0.57
1:A:99:LEU:HD21	1:A:180:PHE:CE2	2.40	0.56
5:D:57:LYS:HB3	5:D:61:PRO:HG3	1.87	0.56
5:D:205:ARG:HH11	5:D:205:ARG:HG2	1.70	0.56
2:B:124:PRO:HD2	2:B:177:HIS:NE2	2.21	0.56
2:B:145:THR:HG23	2:B:160:MET:HE1	1.86	0.56
5:D:65:ASN:HD22	5:D:66:VAL:H	1.55	0.55
4:C:158:LEU:HD23	4:C:158:LEU:O	2.06	0.55
1:A:3:GLU:CG	1:A:4:GLU:H	2.19	0.55
5:D:15:ILE:HD12	5:D:111:GLU:HA	1.88	0.55
4:C:1:ILE:HD12	4:C:2:GLN:OE1	2.07	0.54
4:C:133:PHE:HB2	4:C:185:PHE:CE2	2.41	0.54
2:B:49:ALA:HB2	2:B:55:ARG:HA	1.87	0.54
5:D:125:GLU:OE1	5:D:238:ARG:HD2	2.07	0.54
1:A:57:GLN:OE1	1:A:57:GLN:N	2.38	0.53
5:D:169:ASP:HB2	5:D:186:LEU:HD12	1.90	0.53
2:B:78:TYR:CD2	3:P:29:LEU:HD22	2.43	0.53
1:A:85:VAL:HB	1:A:113:THR:HG22	1.91	0.53
2:B:124:PRO:CD	2:B:177:HIS:CE1	2.92	0.53
4:C:158:LEU:HD23	4:C:158:LEU:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HD12	1:A:48:PHE:CZ	2.44	0.52
1:A:55:GLU:HG2	4:C:93:ALA:HB2	1.91	0.52
2:B:124:PRO:HD3	2:B:177:HIS:CE1	2.44	0.52
4:C:185:PHE:C	4:C:187:ASN:H	2.16	0.52
5:D:213:LEU:HB3	5:D:217:ASP:OD2	2.10	0.52
1:A:97:VAL:HG11	1:A:178:TRP:CH2	2.44	0.52
4:C:96:LEU:HB3	5:D:35:TYR:OH	2.09	0.52
5:D:126:PRO:HD3	5:D:139:LEU:HG	1.91	0.51
4:C:48:ILE:HG23	4:C:48:ILE:O	2.11	0.51
2:B:150:ASN:HB2	2:B:154:THR:O	2.10	0.51
4:C:158:LEU:HD11	5:D:191:ARG:HB2	1.92	0.51
5:D:118:PRO:HD3	5:D:226:PRO:HB3	1.92	0.50
1:A:111:LYS:HE2	1:A:140:ARG:HH22	1.76	0.50
4:C:5:GLN:HG3	4:C:101:GLY:H	1.76	0.50
4:C:31:LEU:C	4:C:31:LEU:HD23	2.36	0.50
2:B:39:ARG:O	2:B:47:TYR:HA	2.12	0.50
2:B:31:ILE:HD12	2:B:31:ILE:N	2.27	0.49
4:C:7:PRO:O	4:C:102:THR:HG23	2.13	0.49
4:C:83:VAL:HG22	4:C:103:ARG:HG3	1.94	0.49
4:C:113:PRO:HG3	4:C:137:ASP:HB3	1.95	0.49
1:A:11:GLU:OE1	1:A:66:ASP:OD2	2.30	0.49
5:D:166:VAL:HA	5:D:189:ARG:O	2.12	0.49
1:A:135:THR:O	1:A:147:LYS:HE2	2.13	0.49
1:A:142:ASP:O	1:A:143:HIS:CB	2.62	0.48
5:D:157:VAL:O	5:D:158:ASN:C	2.56	0.48
4:C:37:ASN:OD1	4:C:37:ASN:C	2.56	0.48
4:C:185:PHE:C	4:C:187:ASN:N	2.72	0.48
4:C:90:ILE:O	4:C:93:ALA:O	2.30	0.48
4:C:60:ALA:HA	4:C:70:LEU:O	2.14	0.48
1:A:25:ASP:OD1	1:A:26:PHE:N	2.47	0.47
2:B:86:GLY:O	2:B:87:GLU:C	2.57	0.47
5:D:143:ALA:O	5:D:185:ALA:HA	2.14	0.47
5:D:197:TRP:CZ2	5:D:238:ARG:HG3	2.49	0.47
2:B:19:ASN:HD22	2:B:22:GLU:CG	2.03	0.47
5:D:238:ARG:NH1	5:D:240:ASP:OD1	2.47	0.47
1:A:119:VAL:HG22	1:A:165:VAL:HG22	1.97	0.47
4:C:28:VAL:HG12	4:C:90:ILE:HA	1.95	0.47
4:C:78:THR:HA	4:C:106:ILE:HB	1.95	0.47
4:C:121:ARG:O	5:D:124:PHE:HA	2.13	0.47
2:B:70:GLN:O	2:B:71:ARG:C	2.56	0.47
4:C:122:ASP:HB2	4:C:128:LYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:138:THR:OG1	5:D:191:ARG:HG3	2.15	0.47
4:C:74:SER:O	4:C:75:SER:C	2.57	0.46
4:C:94:GLN:HE21	4:C:94:GLN:HA	1.80	0.46
1:A:9:GLN:O	2:B:12:LYS:HA	2.16	0.46
4:C:109:ASN:HD22	4:C:109:ASN:C	2.23	0.46
4:C:112:ASN:O	4:C:113:PRO:C	2.58	0.46
1:A:114:PRO:HA	1:A:115:PRO:HD2	1.54	0.46
2:B:4:ARG:HB2	2:B:5:PRO:CD	2.38	0.46
4:C:137:ASP:C	4:C:137:ASP:OD1	2.59	0.46
1:A:87:PRO:HB3	1:A:112:PHE:HB3	1.97	0.46
2:B:33:ASN:O	2:B:34:GLN:HB2	2.15	0.46
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.50	0.46
4:C:186:ASN:OD1	4:C:186:ASN:N	2.49	0.46
1:A:73:MET:HB3	2:B:32:TYR:CD1	2.51	0.46
5:D:149:ASP:CG	5:D:172:PRO:HG3	2.41	0.45
5:D:124:PHE:CD1	5:D:124:PHE:N	2.84	0.45
1:A:73:MET:O	1:A:74:THR:C	2.57	0.45
2:B:13:PHE:CE1	2:B:28:GLU:HG3	2.51	0.45
2:B:169:GLU:OE2	2:B:169:GLU:CG	2.57	0.45
4:C:111:GLN:HA	4:C:111:GLN:OE1	2.16	0.45
5:D:204:PHE:CD1	5:D:204:PHE:N	2.83	0.45
4:C:6:SER:CB	4:C:21:ARG:HB3	2.44	0.45
2:B:40:PHE:CE2	2:B:71:ARG:HB3	2.51	0.45
5:D:13:LEU:CD1	5:D:81:ALA:HB2	2.38	0.45
5:D:238:ARG:C	5:D:240:ASP:H	2.25	0.45
2:B:124:PRO:HD2	2:B:177:HIS:CE1	2.52	0.45
4:C:196:PHE:HA	4:C:197:PRO:HD2	1.72	0.45
1:A:82:ILE:HG12	1:A:83:THR:N	2.32	0.45
2:B:166:ARG:N	2:B:169:GLU:OE2	2.32	0.45
5:D:94:THR:HG22	5:D:98:THR:O	2.17	0.45
1:A:135:THR:CG2	1:A:148:PHE:HB2	2.46	0.44
1:A:167:HIS:ND1	1:A:168:TRP:N	2.65	0.44
4:C:5:GLN:NE2	4:C:85:PHE:HA	2.32	0.44
4:C:175:ASN:C	4:C:176:LYS:O	2.59	0.44
4:C:110:ILE:O	4:C:113:PRO:HD3	2.17	0.44
5:D:18:SER:HB2	5:D:78:LEU:O	2.17	0.44
2:B:4:ARG:CB	2:B:5:PRO:HD2	2.33	0.44
4:C:116:ALA:HB2	4:C:195:PHE:HB3	1.99	0.44
5:D:41:MET:HE3	5:D:41:MET:HB3	1.85	0.44
5:D:60:VAL:N	5:D:61:PRO:CD	2.81	0.44
4:C:5:GLN:C	4:C:6:SER:O	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:11:ARG:CG	5:D:19:MET:HE3	2.41	0.44
5:D:205:ARG:NH1	5:D:205:ARG:HG2	2.32	0.44
2:B:29:ARG:HD3	2:B:36:GLU:OE2	2.18	0.44
1:A:80:THR:HA	1:A:81:PRO:HD3	1.70	0.43
4:C:130:VAL:HG23	5:D:124:PHE:CD2	2.53	0.43
4:C:194:THR:HB	4:C:196:PHE:CE2	2.53	0.43
1:A:6:VAL:HA	2:B:15:CYS:O	2.18	0.43
1:A:99:LEU:H	1:A:99:LEU:HG	1.66	0.43
3:P:30:ASN:HD22	3:P:30:ASN:N	2.10	0.43
4:C:48:ILE:HD13	4:C:53:LYS:HD3	2.00	0.43
5:D:13:LEU:CD2	5:D:17:GLN:HB3	2.49	0.43
2:B:124:PRO:HD3	2:B:177:HIS:HE1	1.84	0.43
5:D:112:ASP:OD2	5:D:114:ASN:HB3	2.19	0.43
1:A:26:PHE:CD2	1:A:26:PHE:C	2.97	0.42
2:B:30:CYS:O	2:B:36:GLU:HA	2.19	0.42
5:D:67:SER:O	5:D:75:PRO:HD2	2.19	0.42
5:D:173:LEU:C	5:D:173:LEU:HD12	2.44	0.42
5:D:49:SER:OG	5:D:68:ARG:NH1	2.46	0.42
5:D:21:LEU:HD12	5:D:76:LEU:HD23	2.00	0.42
1:A:39:LYS:NZ	6:A:199:HOH:O	2.49	0.42
1:A:95:SER:HB2	1:A:96:PRO:HD2	2.02	0.42
1:A:136:VAL:N	6:A:185:HOH:O	2.46	0.42
4:C:95:LYS:HG2	5:D:48:TYR:CE1	2.54	0.42
4:C:109:ASN:C	4:C:109:ASN:ND2	2.77	0.42
1:A:117:VAL:O	1:A:117:VAL:HG23	2.20	0.42
5:D:27:MET:O	5:D:28:ASN:HB2	2.19	0.42
2:B:177:HIS:CG	2:B:178:PRO:HD2	2.55	0.41
4:C:130:VAL:CG1	4:C:171:VAL:HG12	2.50	0.41
2:B:114:LEU:HD11	2:B:160:MET:HB3	2.01	0.41
2:B:177:HIS:CD2	2:B:178:PRO:HD2	2.55	0.41
1:A:11:GLU:OE1	1:A:62:ASN:HB3	2.20	0.41
4:C:65:THR:O	4:C:65:THR:HG23	2.18	0.41
5:D:169:ASP:O	5:D:186:LEU:HD11	2.21	0.41
1:A:29:ASP:HB3	2:B:153:TRP:CE2	2.56	0.41
5:D:14:LYS:HB2	6:D:243:HOH:O	2.21	0.41
1:A:3:GLU:CG	1:A:4:GLU:N	2.84	0.41
2:B:28:GLU:HB3	2:B:40:PHE:HB3	2.03	0.41
1:A:85:VAL:HA	1:A:86:PRO:HD3	1.91	0.41
1:A:91:VAL:HG22	1:A:107:CYS:HA	2.03	0.41
1:A:113:THR:HG23	1:A:114:PRO:CD	2.49	0.41
3:P:34:VAL:HB	3:P:35:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:115:PRO:O	4:C:194:THR:HA	2.21	0.41
5:D:147:PHE:CD2	5:D:148:PRO:CD	3.04	0.41
5:D:238:ARG:HB3	5:D:238:ARG:NH1	2.33	0.41
4:C:124:LYS:O	4:C:125:SER:CB	2.69	0.40
1:A:34:VAL:HB	1:A:36:MET:HE2	2.03	0.40
2:B:68:LEU:O	2:B:72:ARG:HG3	2.21	0.40
1:A:75:LYS:NZ	3:P:37:ASP:OD1	2.47	0.40
2:B:37:SER:O	2:B:54:GLY:HA3	2.21	0.40
2:B:54:GLY:O	2:B:55:ARG:C	2.65	0.40
2:B:124:PRO:HD2	2:B:177:HIS:HE2	1.85	0.40
4:C:17:ASN:HA	4:C:73:ILE:O	2.22	0.40
5:D:188:SER:C	5:D:189:ARG:HG3	2.46	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	177/182 (97%)	157 (89%)	15 (8%)	5 (3%)	4	14
2	B	178/190 (94%)	161 (90%)	12 (7%)	5 (3%)	4	14
3	P	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
4	C	196/202 (97%)	173 (88%)	17 (9%)	6 (3%)	3	12
5	D	237/240 (99%)	218 (92%)	13 (6%)	6 (2%)	4	16
All	All	801/829 (97%)	721 (90%)	58 (7%)	22 (3%)	4	15

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
2	B	2	ASP

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Mol	Chain	Res	Type
2	B	87	GLU
2	B	169	GLU
4	C	6	SER
4	C	192	GLU
4	C	197	PRO
5	D	8	PRO
5	D	148	PRO
5	D	149	ASP
4	C	99	GLY
5	D	71	THR
1	A	4	GLU
1	A	97	VAL
2	B	3	THR
2	B	124	PRO
4	C	176	LYS
1	A	96	PRO
4	C	186	ASN
5	D	239	ALA
5	D	97	GLY
1	A	136	VAL

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	164/166 (99%)	140 (85%)	24 (15%)	3	11
2	B	163/171 (95%)	146 (90%)	17 (10%)	7	22
3	P	10/10 (100%)	7 (70%)	3 (30%)	0	1
4	C	178/182 (98%)	162 (91%)	16 (9%)	9	28
5	D	206/207 (100%)	184 (89%)	22 (11%)	6	21
All	All	721/736 (98%)	639 (89%)	82 (11%)	5	19

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	75	LYS
1	A	78	ASN
1	A	89	VAL
1	A	91	VAL
1	A	92	LEU
1	A	94	ASN
1	A	95	SER
1	A	97	VAL
1	A	117	VAL
1	A	118	ASN
1	A	120	THR
1	A	128	VAL
1	A	130	THR
1	A	134	GLU
1	A	138	LEU
1	A	146	ARG
1	A	154	LEU
1	A	160	VAL
1	A	170	LEU
1	A	171	ASP
1	A	172	GLU
1	A	174	LEU
1	A	177	HIS
2	B	2	ASP
2	B	3	THR
2	B	4	ARG
2	B	22	GLU
2	B	29	ARG
2	B	53	LEU
2	B	71	ARG
2	B	75	VAL
2	B	87	GLU
2	B	100	THR
2	B	104	SER
2	B	114	LEU
2	B	142	VAL
2	B	160	MET
2	B	163	THR
2	B	164	VAL
2	B	184	LEU
3	P	25	LEU
3	P	29	LEU

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Mol	Chain	Res	Type
3	P	30	ASN
4	C	13	GLN
4	C	14	GLU
4	C	41	GLN
4	C	58	LEU
4	C	65	THR
4	C	77	GLN
4	C	97	VAL
4	C	109	ASN
4	C	125	SER
4	C	135	ASP
4	C	139	GLN
4	C	156	CYS
4	C	158	LEU
4	C	171	VAL
4	C	190	ILE
4	C	197	PRO
5	D	5	THR
5	D	13	LEU
5	D	17	GLN
5	D	19	MET
5	D	25	GLN
5	D	59	GLU
5	D	65	ASN
5	D	66	VAL
5	D	69	SER
5	D	76	LEU
5	D	107	LEU
5	D	120	GLU
5	D	128	GLU
5	D	160	LYS
5	D	162	VAL
5	D	171	GLN
5	D	179	LEU
5	D	181	ASP
5	D	189	ARG
5	D	201	ARG
5	D	213	LEU
5	D	220	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	149	HIS
2	B	19	ASN
2	B	33	ASN
2	B	92	GLN
2	B	113	ASN
2	B	134	ASN
2	B	150	ASN
2	B	156	GLN
3	P	30	ASN
4	C	5	GLN
4	C	30	ASN
4	C	44	ASN
4	C	94	GLN
4	C	141	ASN
4	C	168	ASN
4	C	187	ASN
5	D	6	GLN
5	D	22	GLN
5	D	65	ASN
5	D	96	HIS
5	D	199	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

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(Å ²)	Q<0.9
1	A	179/182 (98%)	0.50	8 (4%) 38 30	53, 68, 76, 79	0
2	B	182/190 (95%)	0.42	2 (1%) 78 70	53, 66, 72, 75	0
3	P	15/15 (100%)	0.47	0 100 100	45, 52, 69, 76	0
4	C	198/202 (98%)	0.21	2 (1%) 79 72	43, 60, 84, 88	0
5	D	239/240 (99%)	-0.03	2 (0%) 82 75	45, 57, 71, 83	0
All	All	813/829 (98%)	0.26	14 (1%) 69 60	43, 64, 77, 88	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	ARG	4.4
4	C	1	ILE	3.8
5	D	171	GLN	3.5
2	B	187	GLU	3.2
1	A	114	PRO	3.0
1	A	154	LEU	2.7
1	A	22	PHE	2.6
1	A	99	LEU	2.4
1	A	101	GLU	2.3
5	D	149	ASP	2.2
1	A	58	GLY	2.1
2	B	104	SER	2.1
4	C	128	LYS	2.1
1	A	59	ALA	2.1

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.