



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:38 PM UTC

PDB ID : 1OGA / pdb_00001oga
Title : A structural basis for immunodominant human T-cell receptor recognition.
Authors : Stewart-Jones, G.B.E.; McMichael, A.J.; Bell, J.I.; Stuart, D.I.; Jones, E.Y.
Deposited on : 2003-04-28
Resolution : 1.40 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

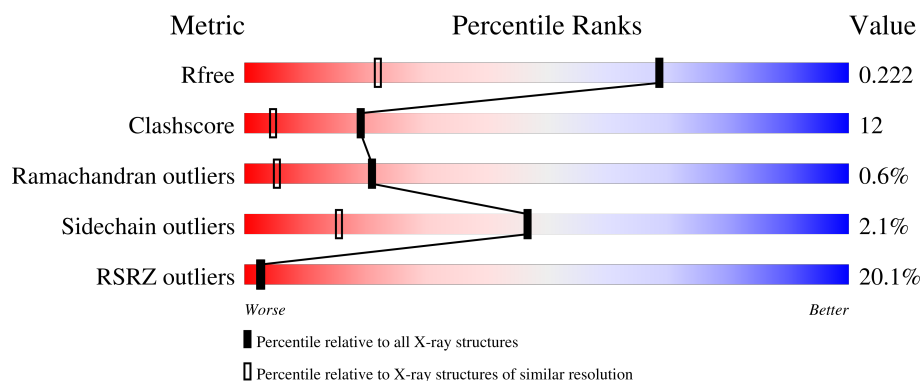
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	276	15% 80% 19% .
2	B	100	12% 82% 17% .
3	C	9	11% 89% 11% .
4	D	215	28% 73% 18% 7% .
5	E	252	21% 70% 23% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7192 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	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			

- Molecule 3 is a protein called GILGFVFTL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			69	49	9	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	200	Total	C	N	O	S	0	0	1
			1531	959	256	310	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	0	0	1
			1933	1218	335	375	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	118	LYS	ASN	conflict	UNP P01850
E	119	ASN	LYS	conflict	UNP P01850

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Chain	Residue	Modelled	Actual	Comment	Reference
E	151	TYR	PHE	conflict	UNP P01850
E	189	SER	CYS	conflict	UNP P01850

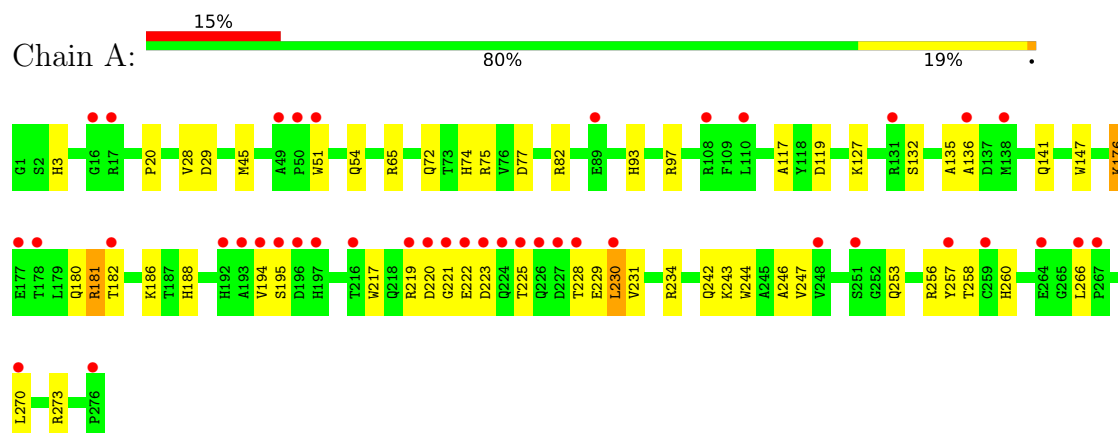
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	192	Total	O	0	0
			192	192		
6	B	105	Total	O	0	0
			105	105		
6	C	7	Total	O	0	0
			7	7		
6	D	108	Total	O	0	0
			108	108		
6	E	156	Total	O	0	0
			156	156		

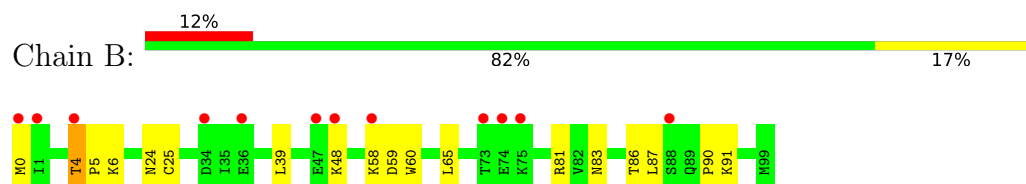
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

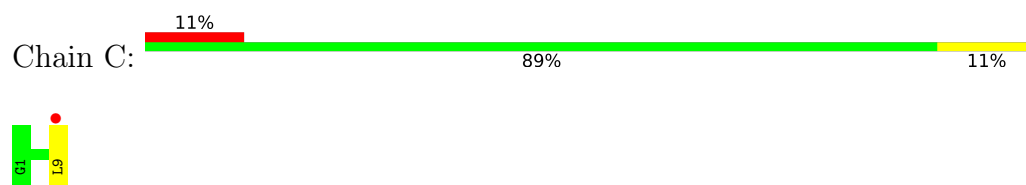
• Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN



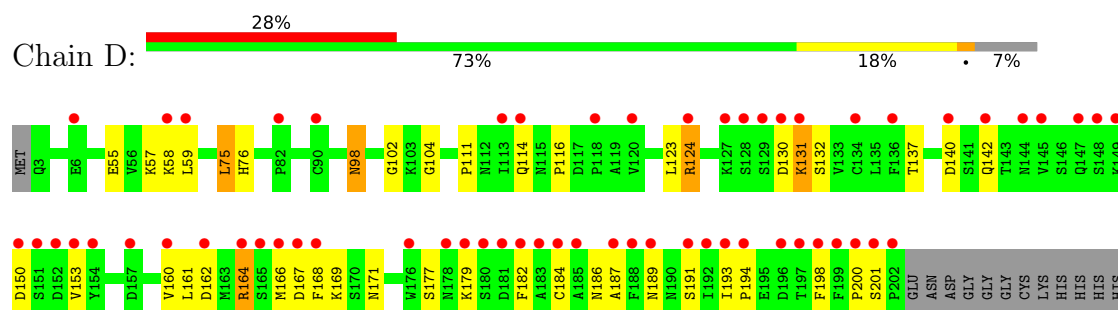
• Molecule 2: BETA-2-MICROGLOBULIN



• Molecule 3: GILGFVFTL



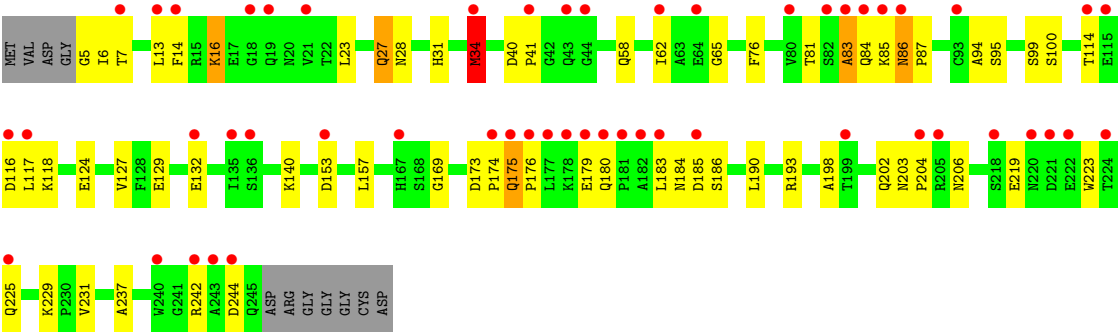
• Molecule 4: T-CELL RECEPTOR ALPHA CHAIN V REGION



HIS

HIS

● Molecule 5: T-CELL RECEPTOR BETA CHAIN C REGION



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.02Å 108.84Å 77.74Å 90.00° 112.46° 90.00°	Depositor
Resolution (Å)	29.98 – 1.40 29.98 – 1.40	Depositor EDS
% Data completeness (in resolution range)	93.0 (29.98-1.40) 93.0 (29.98-1.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.231 0.209 , 0.222	Depositor DCC
R_{free} test set	9914 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7192	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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 [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	0.43	0/2320	0.87	6/3149 (0.2%)
2	B	0.49	0/860	0.88	1/1162 (0.1%)
3	C	0.65	0/70	0.82	0/92
4	D	0.42	1/1561 (0.1%)	0.86	3/2115 (0.1%)
5	E	0.49	3/1986 (0.2%)	0.88	1/2702 (0.0%)
All	All	0.46	4/6797 (0.1%)	0.87	11/9220 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	34	MET	SD-CE	-7.98	1.59	1.79
4	D	201	SER	C-N	-5.78	1.25	1.34
5	E	244	ASP	C-N	-5.67	1.25	1.33
5	E	34	MET	CG-SD	-5.45	1.67	1.80

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	124	GLU	N-CA-C	-7.57	97.35	109.76
2	B	6	LYS	N-CA-C	-7.39	98.56	110.32
1	A	45	MET	N-CA-C	-6.53	100.16	109.96
1	A	28	VAL	N-CA-C	-6.47	98.30	107.75
1	A	222	GLU	N-CA-C	6.16	116.41	108.34
1	A	186	LYS	N-CA-C	-6.12	99.30	109.46
4	D	104	GLY	N-CA-C	5.58	119.71	112.68
1	A	257	TYR	N-CA-C	5.50	118.77	109.76
1	A	136	ALA	N-CA-C	5.47	118.17	111.82
4	D	102	GLY	N-CA-C	-5.35	104.24	112.85
4	D	137	THR	N-CA-C	5.11	116.75	109.14

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	2254	0	2103	47	0
2	B	837	0	803	11	0
3	C	69	0	75	2	0
4	D	1531	0	1480	41	0
5	E	1933	0	1829	58	0
6	A	192	0	0	5	0
6	B	105	0	0	0	0
6	C	7	0	0	0	0
6	D	108	0	0	0	0
6	E	156	0	0	3	0
All	All	7192	0	6290	151	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 12.

All (151) 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:E:34:MET:SD	5:E:94:ALA:O	2.19	1.00
4:D:111:PRO:HG2	4:D:160:VAL:HG11	1.55	0.88
4:D:164:ARG:HG2	4:D:164:ARG:HH11	1.36	0.88
1:A:266:LEU:HD13	1:A:270:LEU:HD23	1.61	0.82
5:E:229:LYS:HG3	5:E:231:VAL:HG13	1.62	0.82
5:E:84:GLN:O	5:E:87:PRO:HD3	1.89	0.73
1:A:219:ARG:O	1:A:221:GLY:N	2.19	0.71
5:E:116:ASP:OD1	5:E:118:LYS:HG2	1.91	0.71
5:E:34:MET:CE	5:E:95:SER:HB3	2.20	0.71
5:E:183:LEU:HG	5:E:185:ASP:H	1.56	0.70
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.37	0.70
1:A:229:GLU:HG3	1:A:244:TRP:HZ3	1.56	0.70
1:A:72:GLN:HE22	1:A:75:ARG:HH11	1.40	0.69
4:D:111:PRO:HG2	4:D:160:VAL:CG1	2.23	0.68
4:D:164:ARG:HG2	4:D:164:ARG:NH1	2.01	0.67
5:E:34:MET:HE1	5:E:95:SER:HB3	1.75	0.67
1:A:147:TRP:CZ2	3:C:9:LEU:HD23	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:LEU:HD22	2:B:91:LYS:HE3	1.77	0.67
4:D:123:LEU:O	4:D:132:SER:HB2	1.95	0.67
2:B:81:ARG:HH12	2:B:90:PRO:HG2	1.60	0.66
5:E:153:ASP:OD2	5:E:176:PRO:HG2	1.96	0.66
1:A:230:LEU:C	1:A:230:LEU:HD23	2.21	0.66
1:A:3:HIS:HD2	1:A:29:ASP:OD2	1.79	0.65
5:E:84:GLN:HG3	5:E:85:LYS:H	1.62	0.64
4:D:124:ARG:HD3	4:D:124:ARG:H	1.63	0.63
1:A:230:LEU:HD21	1:A:243:LYS:HE3	1.82	0.61
4:D:124:ARG:H	4:D:124:ARG:CD	2.13	0.61
4:D:193:ILE:HG23	4:D:194:PRO:HD2	1.83	0.60
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.82	0.60
4:D:111:PRO:CG	4:D:160:VAL:HG11	2.31	0.60
1:A:188:HIS:HD2	6:A:2158:HOH:O	1.85	0.59
4:D:179:LYS:HA	4:D:179:LYS:HE2	1.84	0.59
4:D:124:ARG:HH12	5:E:129:GLU:CD	2.11	0.58
1:A:20:PRO:HG2	6:A:2017:HOH:O	2.03	0.57
4:D:75:LEU:HD22	4:D:76:HIS:N	2.19	0.57
1:A:74:HIS:HD2	1:A:77:ASP:OD2	1.87	0.57
5:E:86:ASN:H	5:E:87:PRO:CD	2.18	0.57
4:D:124:ARG:HH11	4:D:124:ARG:HG2	1.70	0.56
5:E:27:GLN:HG2	5:E:34:MET:HE2	1.86	0.56
4:D:162:ASP:OD1	4:D:164:ARG:HD3	2.05	0.56
1:A:65:ARG:HG3	6:E:2046:HOH:O	2.04	0.56
5:E:242:ARG:HG3	5:E:242:ARG:HH11	1.69	0.56
4:D:186:ASN:HA	4:D:189:ASN:OD1	2.06	0.56
1:A:82:ARG:HH11	1:A:82:ARG:HG2	1.70	0.55
5:E:198:ALA:O	5:E:202:GLN:HG3	2.07	0.55
5:E:27:GLN:HE22	5:E:31:HIS:H	1.54	0.55
1:A:93:HIS:HE1	6:A:2081:HOH:O	1.89	0.55
1:A:234:ARG:HE	1:A:242:GLN:NE2	2.03	0.55
4:D:191:SER:HB2	4:D:193:ILE:HD11	1.89	0.54
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.43	0.54
4:D:59:LEU:N	4:D:59:LEU:HD22	2.21	0.54
5:E:6:ILE:N	5:E:6:ILE:HD12	2.22	0.54
1:A:230:LEU:HD21	1:A:243:LYS:CE	2.38	0.53
2:B:4:THR:HG23	2:B:86:THR:OG1	2.09	0.53
4:D:98:ASN:HD22	4:D:98:ASN:C	2.15	0.53
4:D:130:ASP:O	4:D:131:LYS:O	2.27	0.53
2:B:48:LYS:NZ	2:B:48:LYS:HB3	2.24	0.52
1:A:229:GLU:HG3	1:A:244:TRP:CZ3	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:LYS:HD3	2:B:59:ASP:N	2.24	0.52
5:E:127:VAL:HG23	5:E:237:ALA:HB3	1.92	0.52
1:A:51:TRP:O	1:A:54:GLN:HG2	2.09	0.52
1:A:217:TRP:CD1	1:A:247:VAL:HG13	2.44	0.52
4:D:184:CYS:HA	4:D:187:ALA:HB2	1.93	0.51
4:D:164:ARG:HD3	4:D:164:ARG:N	2.25	0.51
6:A:2079:HOH:O	2:B:0:MET:HB2	2.10	0.51
5:E:118:LYS:HD2	5:E:225:GLN:CG	2.41	0.51
4:D:150:ASP:HB2	4:D:153:VAL:HG23	1.91	0.51
4:D:160:VAL:HG22	4:D:171:ASN:OD1	2.10	0.51
1:A:230:LEU:C	1:A:230:LEU:CD2	2.84	0.50
1:A:147:TRP:CH2	3:C:9:LEU:HD23	2.46	0.50
4:D:124:ARG:NH1	5:E:129:GLU:CD	2.70	0.50
5:E:86:ASN:N	5:E:87:PRO:CD	2.74	0.50
5:E:62:ILE:HG13	5:E:62:ILE:O	2.11	0.49
2:B:4:THR:HG22	2:B:5:PRO:HD2	1.94	0.49
5:E:183:LEU:HD12	5:E:184:ASN:H	1.78	0.49
4:D:168:PHE:CD2	5:E:140:LYS:HE2	2.47	0.49
5:E:183:LEU:HG	5:E:185:ASP:N	2.25	0.49
2:B:58:LYS:HD3	2:B:58:LYS:C	2.37	0.49
1:A:225:THR:HG22	1:A:225:THR:O	2.12	0.49
5:E:132:GLU:H	5:E:132:GLU:CD	2.20	0.49
4:D:55:GLU:OE1	4:D:57:LYS:HE3	2.13	0.48
1:A:3:HIS:HE1	6:A:2093:HOH:O	1.95	0.48
1:A:266:LEU:HD22	1:A:270:LEU:HD21	1.95	0.48
5:E:7:THR:HG23	6:E:2002:HOH:O	2.12	0.48
1:A:228:THR:OG1	1:A:247:VAL:HG12	2.14	0.48
4:D:191:SER:HB2	4:D:193:ILE:CD1	2.44	0.48
5:E:153:ASP:CG	5:E:176:PRO:HG2	2.39	0.47
1:A:74:HIS:HE1	1:A:97:ARG:HH11	1.62	0.47
1:A:181:ARG:HG2	1:A:182:THR:N	2.29	0.47
1:A:127:LYS:HD2	1:A:132:SER:OG	2.15	0.47
1:A:230:LEU:HD23	1:A:231:VAL:O	2.15	0.47
5:E:174:PRO:HD2	6:E:2124:HOH:O	2.14	0.46
5:E:65:GLY:HA3	5:E:83:ALA:HA	1.97	0.46
1:A:253:GLN:NE2	1:A:256:ARG:HH11	2.13	0.46
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.97	0.46
1:A:258:THR:OG1	1:A:260:HIS:HE1	1.99	0.46
4:D:114:GLN:C	4:D:116:PRO:HD3	2.41	0.46
5:E:173:ASP:HB2	5:E:190:LEU:HD12	1.98	0.46
5:E:180:GLN:O	5:E:186:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:140:ASP:OD2	4:D:140:ASP:C	2.58	0.45
5:E:132:GLU:CD	5:E:132:GLU:N	2.74	0.45
5:E:40:ASP:HB3	5:E:41:PRO:HD2	1.97	0.45
4:D:161:LEU:C	4:D:161:LEU:HD23	2.42	0.45
4:D:193:ILE:HD12	4:D:193:ILE:N	2.31	0.45
5:E:13:LEU:CD1	5:E:23:LEU:HD22	2.47	0.45
1:A:74:HIS:CE1	1:A:97:ARG:HH11	2.35	0.45
1:A:230:LEU:CD2	1:A:243:LYS:HE3	2.46	0.45
1:A:229:GLU:HG2	1:A:246:ALA:HB3	1.97	0.45
4:D:164:ARG:HH12	5:E:169:GLY:H	1.64	0.44
4:D:98:ASN:C	4:D:98:ASN:ND2	2.74	0.44
4:D:179:LYS:HA	4:D:179:LYS:CE	2.47	0.44
1:A:266:LEU:HD22	1:A:270:LEU:CD2	2.48	0.43
4:D:58:LYS:C	4:D:59:LEU:HD22	2.43	0.43
5:E:179:GLU:O	5:E:180:GLN:NE2	2.50	0.43
5:E:129:GLU:OE1	5:E:242:ARG:CZ	2.67	0.43
5:E:62:ILE:O	5:E:62:ILE:HG23	2.19	0.43
1:A:82:ARG:HG2	1:A:82:ARG:NH1	2.33	0.43
5:E:86:ASN:H	5:E:87:PRO:HD3	1.84	0.43
1:A:266:LEU:CD1	1:A:270:LEU:HD23	2.43	0.43
1:A:135:ALA:HB3	1:A:141:GLN:NE2	2.33	0.43
5:E:202:GLN:O	5:E:204:PRO:HD3	2.19	0.43
1:A:219:ARG:C	1:A:221:GLY:N	2.75	0.42
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.01	0.42
5:E:173:ASP:HB2	5:E:190:LEU:CD1	2.50	0.42
4:D:164:ARG:HH11	4:D:164:ARG:H	1.65	0.42
5:E:81:THR:O	5:E:83:ALA:N	2.43	0.42
5:E:203:ASN:HB3	5:E:206:ASN:ND2	2.34	0.42
1:A:176:LYS:HG3	1:A:180:GLN:NE2	2.35	0.42
4:D:177:SER:HB3	4:D:182:PHE:CG	2.55	0.42
5:E:5:GLY:N	5:E:28:ASN:OD1	2.52	0.42
5:E:16:LYS:HZ2	5:E:16:LYS:HB2	1.85	0.42
1:A:176:LYS:NZ	1:A:176:LYS:CB	2.83	0.42
4:D:198:PHE:CE2	4:D:200:PRO:HG3	2.54	0.42
5:E:99:SER:O	5:E:100:SER:HB2	2.20	0.42
5:E:175:GLN:HE21	5:E:175:GLN:HB2	1.62	0.41
4:D:162:ASP:OD2	4:D:169:LYS:HE2	2.20	0.41
5:E:16:LYS:NZ	5:E:117:LEU:HD11	2.35	0.41
5:E:219:GLU:OE1	5:E:219:GLU:HA	2.20	0.41
5:E:34:MET:HG3	5:E:76:PHE:HD2	1.86	0.41
5:E:157:LEU:C	5:E:157:LEU:HD23	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:173:ASP:OD1	5:E:193:ARG:NH2	2.52	0.41
5:E:223:TRP:CZ2	5:E:225:GLN:HB2	2.56	0.41
1:A:176:LYS:HB2	1:A:176:LYS:HZ2	1.86	0.40
4:D:124:ARG:CD	4:D:124:ARG:N	2.83	0.40
5:E:183:LEU:HD12	5:E:184:ASN:N	2.36	0.40
1:A:65:ARG:HD2	5:E:58:GLN:NE2	2.37	0.40
5:E:14:PHE:HZ	5:E:114:THR:HG21	1.85	0.40
5:E:34:MET:HG3	5:E:76:PHE:CD2	2.56	0.40
4:D:166:MET:O	4:D:167:ASP:C	2.63	0.40
1:A:194:VAL:O	1:A:195:SER:HB3	2.20	0.40
5:E:16:LYS:NZ	5:E:16:LYS:CB	2.85	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	274/276 (99%)	263 (96%)	9 (3%)	2 (1%)	18	4
2	B	98/100 (98%)	98 (100%)	0	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	198/215 (92%)	188 (95%)	9 (4%)	1 (0%)	24	7
5	E	239/252 (95%)	226 (95%)	11 (5%)	2 (1%)	16	3
All	All	816/852 (96%)	781 (96%)	30 (4%)	5 (1%)	21	5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
4	D	131	LYS
5	E	83	ALA

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Mol	Chain	Res	Type
5	E	86	ASN
1	A	220	ASP

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	232/232 (100%)	228 (98%)	4 (2%)	53	21
2	B	95/95 (100%)	93 (98%)	2 (2%)	47	15
3	C	7/7 (100%)	7 (100%)	0	100	100
4	D	175/188 (93%)	170 (97%)	5 (3%)	37	9
5	E	212/220 (96%)	208 (98%)	4 (2%)	50	18
All	All	721/742 (97%)	706 (98%)	15 (2%)	47	15

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	LYS
1	A	181	ARG
1	A	230	LEU
1	A	273	ARG
2	B	4	THR
2	B	83	ASN
4	D	75	LEU
4	D	98	ASN
4	D	124	ARG
4	D	142	GLN
4	D	164	ARG
5	E	16	LYS
5	E	27	GLN
5	E	34	MET
5	E	175	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	72	GLN
1	A	74	HIS
1	A	93	HIS
1	A	115	GLN
1	A	141	GLN
1	A	180	GLN
1	A	188	HIS
1	A	242	GLN
1	A	253	GLN
1	A	260	HIS
1	A	262	GLN
2	B	2	GLN
2	B	13	HIS
2	B	51	HIS
2	B	83	ASN
2	B	89	GLN
4	D	15	GLN
4	D	98	ASN
4	D	114	GLN
5	E	27	GLN
5	E	43	GLN
5	E	175	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	276/276 (100%)	0.86	41 (14%)	5 6	16, 26, 50, 72	0
2	B	100/100 (100%)	0.53	12 (12%)	9 9	17, 22, 38, 61	0
3	C	9/9 (100%)	0.18	1 (11%)	10 10	17, 17, 19, 25	0
4	D	200/215 (93%)	1.35	60 (30%)	1 1	17, 33, 71, 75	0
5	E	241/252 (95%)	1.24	52 (21%)	2 2	15, 30, 56, 64	0
All	All	826/852 (96%)	1.04	166 (20%)	3 2	15, 28, 61, 75	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	83	ALA	7.0
1	A	227	ASP	6.9
5	E	34	MET	6.3
5	E	177	LEU	5.8
2	B	0	MET	5.5
1	A	220	ASP	5.4
4	D	193	ILE	5.3
5	E	84	GLN	5.2
4	D	198	PHE	5.1
4	D	184	CYS	5.0
4	D	192	ILE	4.9
5	E	85	LYS	4.9
5	E	183	LEU	4.7
5	E	82	SER	4.6
1	A	136	ALA	4.5
5	E	243	ALA	4.5
4	D	129	SER	4.5
1	A	228	THR	4.4
2	B	1	ILE	4.4
4	D	199	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
4	D	145	VAL	4.3
1	A	178	THR	4.3
2	B	48	LYS	4.3
4	D	188	PHE	4.3
4	D	164	ARG	4.2
5	E	86	ASN	4.1
5	E	62	ILE	4.1
5	E	176	PRO	4.1
1	A	226	GLN	4.1
4	D	202	PRO	4.0
1	A	194	VAL	3.9
4	D	194	PRO	3.9
1	A	221	GLY	3.9
1	A	224	GLN	3.9
4	D	130	ASP	3.9
4	D	152	ASP	3.8
4	D	182	PHE	3.8
4	D	167	ASP	3.8
1	A	223	ASP	3.7
1	A	225	THR	3.6
5	E	222	GLU	3.5
5	E	41	PRO	3.5
1	A	270	LEU	3.5
4	D	153	VAL	3.5
4	D	183	ALA	3.5
5	E	180	GLN	3.5
4	D	178	ASN	3.4
5	E	19	GLN	3.4
1	A	197	HIS	3.3
3	C	9	LEU	3.3
1	A	196	ASP	3.3
5	E	224	THR	3.3
5	E	175	GLN	3.3
4	D	114	GLN	3.2
5	E	181	PRO	3.2
5	E	242	ARG	3.2
1	A	230	LEU	3.2
5	E	135	ILE	3.1
4	D	200	PRO	3.1
5	E	199	THR	3.0
4	D	201	SER	3.0
1	A	17	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
5	E	44	GLY	3.0
5	E	220	ASN	3.0
4	D	142	GLN	3.0
4	D	185	ALA	3.0
4	D	187	ALA	3.0
1	A	16	GLY	3.0
4	D	59	LEU	3.0
5	E	64	GLU	2.9
5	E	182	ALA	2.9
4	D	165	SER	2.9
4	D	124	ARG	2.9
4	D	131	LYS	2.9
4	D	149	LYS	2.9
5	E	185	ASP	2.8
1	A	267	PRO	2.8
5	E	174	PRO	2.8
1	A	251	SER	2.8
4	D	160	VAL	2.8
4	D	189	ASN	2.8
4	D	180	SER	2.8
4	D	154	TYR	2.8
1	A	50	PRO	2.8
1	A	276	PRO	2.8
1	A	192	HIS	2.8
4	D	127	LYS	2.8
4	D	181	ASP	2.7
4	D	196	ASP	2.7
1	A	182	THR	2.7
2	B	58	LYS	2.7
4	D	58	LYS	2.7
1	A	222	GLU	2.7
1	A	193	ALA	2.7
5	E	132	GLU	2.7
1	A	257	TYR	2.6
4	D	166	MET	2.6
4	D	82	PRO	2.6
4	D	147	GLN	2.6
1	A	216	THR	2.6
5	E	116	ASP	2.6
4	D	148	SER	2.6
4	D	150	ASP	2.6
2	B	73	THR	2.6

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Mol	Chain	Res	Type	RSRZ
4	D	168	PHE	2.6
1	A	89	GLU	2.6
4	D	128	SER	2.6
5	E	115	GLU	2.5
4	D	136	PHE	2.5
5	E	14	PHE	2.5
1	A	138	MET	2.5
5	E	221	ASP	2.5
4	D	118	PRO	2.5
5	E	7	THR	2.5
4	D	6	GLU	2.5
1	A	49	ALA	2.4
2	B	75	LYS	2.4
4	D	179	LYS	2.4
5	E	117	LEU	2.4
5	E	204	PRO	2.4
4	D	90	CYS	2.4
2	B	34	ASP	2.4
5	E	205	ARG	2.4
2	B	74	GLU	2.4
5	E	114	THR	2.3
4	D	134	CYS	2.3
4	D	151	SER	2.3
4	D	176	TRP	2.3
5	E	153	ASP	2.3
5	E	179	GLU	2.3
5	E	21	VAL	2.3
4	D	140	ASP	2.3
5	E	18	GLY	2.3
5	E	178	LYS	2.3
1	A	266	LEU	2.2
5	E	13	LEU	2.2
4	D	144	ASN	2.2
5	E	244	ASP	2.2
5	E	93	CYS	2.2
1	A	264	GLU	2.2
2	B	47	GLU	2.2
5	E	167	HIS	2.2
5	E	218	SER	2.2
1	A	108	ARG	2.2
2	B	88	SER	2.2
1	A	219	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	43	GLN	2.2
5	E	80	VAL	2.2
1	A	110	LEU	2.1
4	D	197	THR	2.1
4	D	157	ASP	2.1
4	D	162	ASP	2.1
4	D	120	VAL	2.1
5	E	136	SER	2.1
5	E	225	GLN	2.1
1	A	259	CYS	2.1
4	D	113	ILE	2.1
1	A	51	TRP	2.1
1	A	195	SER	2.1
1	A	248	VAL	2.1
2	B	4	THR	2.0
1	A	131	ARG	2.0
1	A	177	GLU	2.0
2	B	36	GLU	2.0
5	E	240	TRP	2.0
4	D	191	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.