



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:30 PM UTC

PDB ID : 2BNR / pdb_00002bnr
Title : Structural and kinetic basis for heightened immunogenicity of T cell vaccines
Authors : Chen, J.-L.; Stewart-Jones, G.; Bossi, G.; Lissin, N.M.; Wooldridge, L.; Choi, E.M.L.; Held, G.; Dunbar, P.R.; Esnouf, R.M.; Sami, M.; Boulter, J.M.; Rizkallah, P.J.; Renner, C.; Sewell, A.; van der Merwe, P.A.; Jackobsen, B.K.; Griffiths, G.; Jones, E.Y.; Cerundolo, V.
Deposited on : 2005-03-31
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

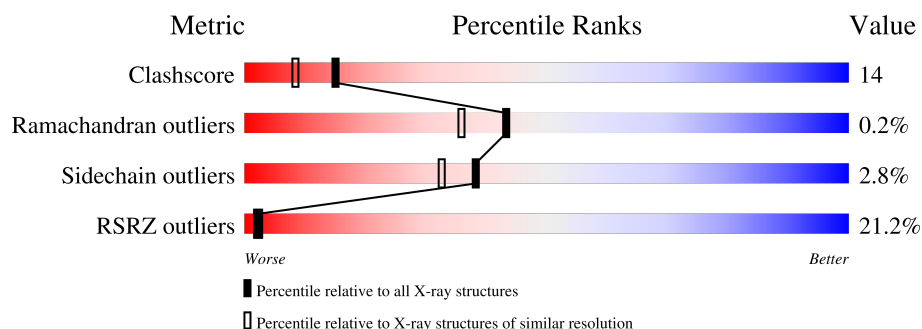
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	
2	B	100	
3	C	9	
4	D	203	
5	E	241	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7145 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	1	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 SYNTHETIC PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			75	49	11	13	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	203	Total	C	N	O	S	0	0	0
			1557	968	262	320	7			

- 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	0
			1902	1196	327	370	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	116	LYS	ASN	conflict	UNP P01850
E	117	ASN	LYS	conflict	UNP P01850

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Chain	Residue	Modelled	Actual	Comment	Reference
E	149	TYR	PHE	conflict	UNP P01850
E	169	CYS	SER	conflict	UNP P01850
E	187	ALA	CYS	conflict	UNP P01850
E	201	ASP	ASN	conflict	UNP P01850

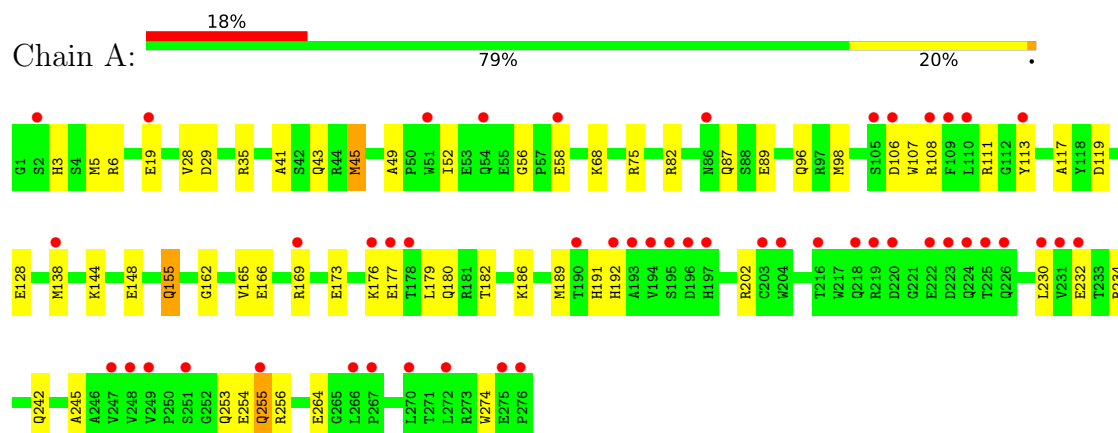
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	158	Total 158	O 158	0	0
6	B	37	Total 37	O 37	0	0
6	C	6	Total 6	O 6	0	0
6	D	138	Total 138	O 138	0	0
6	E	181	Total 181	O 181	0	0

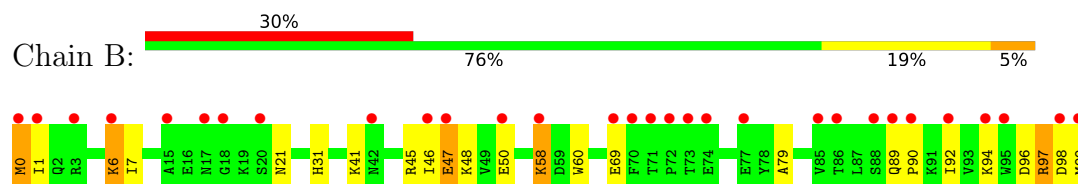
3 Residue-property plots

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.

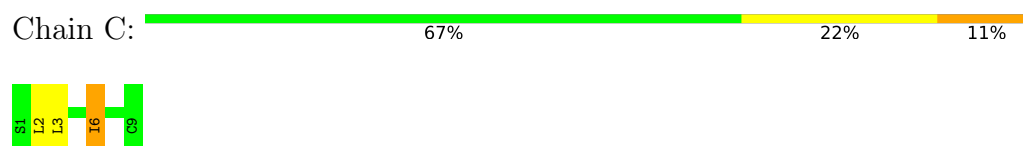
• Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN



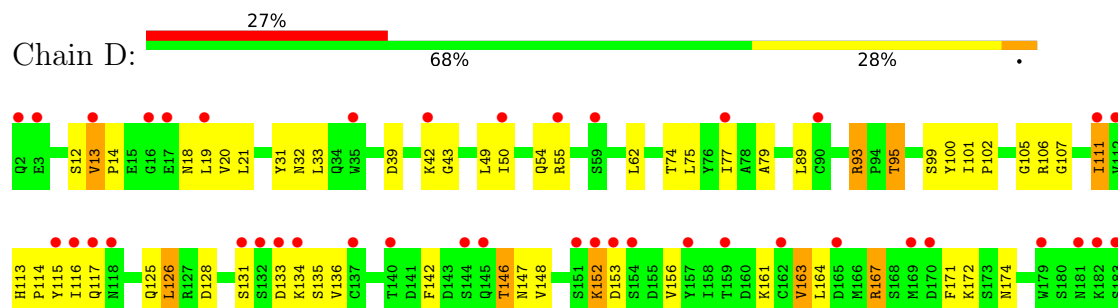
• Molecule 2: BETA-2-MICROGLOBULIN

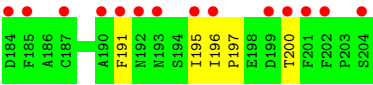


• Molecule 3: SYNTHETIC PEPTIDE

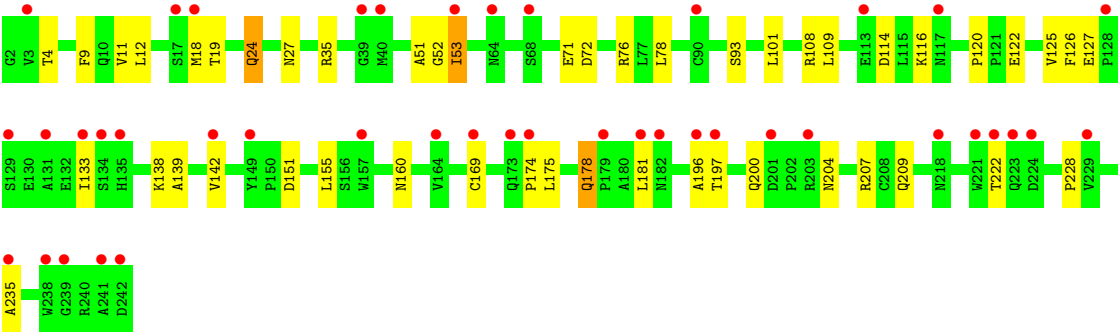
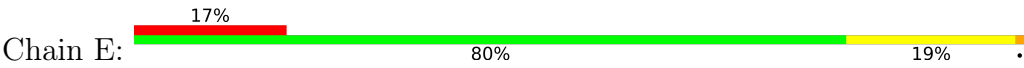


• Molecule 4: T-CELL RECEPTOR ALPHA CHAIN V REGION





● 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	72.56Å 62.49Å 116.95Å 90.00° 105.34° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-1.90) 93.7 (20.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7145	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/2320	0.89	7/3149 (0.2%)
2	B	0.34	0/860	0.85	1/1162 (0.1%)
3	C	0.46	0/76	1.15	1/101 (1.0%)
4	D	0.38	0/1589	0.90	5/2159 (0.2%)
5	E	0.38	0/1953	0.90	6/2659 (0.2%)
All	All	0.38	0/6798	0.89	20/9230 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	122	GLU	N-CA-C	-7.28	97.88	109.59
2	B	6	LYS	N-CA-C	-7.02	99.16	110.32
1	A	28	VAL	N-CA-C	-6.96	97.59	107.75
1	A	41	ALA	N-CA-C	6.96	118.87	111.28
5	E	71	GLU	N-CA-C	6.93	119.86	111.82
4	D	167	ARG	N-CA-C	6.69	119.14	111.11
5	E	178	GLN	CA-C-N	6.62	128.11	119.84
5	E	178	GLN	C-N-CA	6.62	128.11	119.84
1	A	56	GLY	CA-C-N	6.52	126.28	119.05
1	A	56	GLY	C-N-CA	6.52	126.28	119.05
4	D	13	VAL	N-CA-C	6.23	114.30	109.19
3	C	3	LEU	N-CA-C	-6.11	101.89	110.50
1	A	45	MET	N-CA-C	-5.84	101.63	110.28
1	A	179	LEU	N-CA-C	5.62	117.49	111.36
4	D	105	GLY	N-CA-C	-5.60	104.04	112.89
5	E	35	ARG	N-CA-C	-5.56	99.95	109.24
4	D	101	ILE	N-CA-C	5.53	114.37	108.95
1	A	186	LYS	N-CA-C	-5.36	100.00	108.73
4	D	156	VAL	N-CA-C	-5.17	100.20	107.75
5	E	72	ASP	N-CA-C	5.02	117.67	109.59

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	51	0
2	B	837	0	803	25	0
3	C	75	0	79	4	0
4	D	1557	0	1489	69	0
5	E	1902	0	1796	46	0
6	A	158	0	0	4	0
6	B	37	0	0	0	0
6	C	6	0	0	0	0
6	D	138	0	0	3	0
6	E	181	0	0	3	0
All	All	7145	0	6270	177	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 14.

All (177) 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:47:GLU:HG3	2:B:48:LYS:H	1.25	0.99
1:A:68:LYS:HD3	5:E:53:ILE:HG12	1.42	0.97
1:A:176:LYS:HG2	1:A:180:GLN:NE2	1.92	0.85
2:B:79:ALA:HB2	2:B:94:LYS:HD3	1.58	0.83
2:B:41:LYS:HB2	2:B:46:ILE:HD11	1.57	0.83
4:D:93:ARG:HD3	4:D:102:PRO:HG3	1.60	0.82
1:A:68:LYS:CD	5:E:53:ILE:HG12	2.12	0.80
4:D:42:LYS:HG2	4:D:43:GLY:H	1.48	0.78
5:E:126:PHE:HB2	5:E:142:VAL:CG2	2.15	0.77
4:D:136:VAL:HG21	5:E:142:VAL:HG21	1.69	0.75
2:B:41:LYS:CB	2:B:46:ILE:HD11	2.17	0.75
5:E:133:ILE:HD11	5:E:139:ALA:HB2	1.68	0.74
1:A:173:GLU:O	1:A:176:LYS:HG3	1.86	0.74
4:D:12:SER:HA	4:D:111:ILE:HG23	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLN:O	1:A:68:LYS:HE3	1.89	0.72
5:E:178:GLN:HB3	5:E:181:LEU:HD13	1.75	0.69
5:E:151:ASP:OD1	5:E:174:PRO:HG2	1.95	0.67
4:D:131:SER:C	4:D:133:ASP:H	2.01	0.67
5:E:133:ILE:CD1	5:E:139:ALA:HB2	2.24	0.67
5:E:181:LEU:HD12	5:E:181:LEU:N	2.10	0.66
1:A:3:HIS:HD2	1:A:29:ASP:OD2	1.80	0.64
1:A:6:ARG:NH2	1:A:113:TYR:CD1	2.64	0.64
4:D:128:ASP:HB2	4:D:134:LYS:HG3	1.79	0.64
4:D:142:PHE:HB2	4:D:146:THR:HG21	1.81	0.63
4:D:196:ILE:HG23	4:D:197:PRO:HD2	1.80	0.63
2:B:6:LYS:C	2:B:7:ILE:HD12	2.24	0.62
2:B:47:GLU:HG3	2:B:48:LYS:N	2.06	0.62
1:A:111:ARG:NH2	1:A:128:GLU:HG2	2.15	0.61
5:E:18:MET:HE1	5:E:109:LEU:HD22	1.83	0.61
1:A:232:GLU:OE2	2:B:6:LYS:HE3	2.00	0.61
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.47	0.60
4:D:116:ILE:HD12	4:D:116:ILE:N	2.15	0.60
1:A:155:GLN:HG3	4:D:31:TYR:CE2	2.37	0.60
1:A:176:LYS:HE2	1:A:180:GLN:HE22	1.67	0.60
4:D:42:LYS:HG2	4:D:43:GLY:N	2.16	0.60
2:B:58:LYS:NZ	2:B:58:LYS:HB3	2.17	0.60
4:D:42:LYS:HD3	4:D:43:GLY:O	2.02	0.59
1:A:234:ARG:HE	1:A:242:GLN:NE2	2.01	0.59
2:B:7:ILE:HD12	2:B:7:ILE:N	2.18	0.58
2:B:97:ARG:HG3	2:B:97:ARG:HH11	1.68	0.58
1:A:45:MET:CE	3:C:2:LEU:HD11	2.33	0.58
3:C:6:ILE:HD12	3:C:6:ILE:H	1.69	0.58
4:D:21:LEU:HD12	4:D:75:LEU:HD23	1.85	0.58
2:B:92:ILE:HD12	2:B:92:ILE:N	2.19	0.58
1:A:253:GLN:NE2	1:A:256:ARG:HH12	2.02	0.57
5:E:9:PHE:HE1	5:E:108:ARG:HD3	1.69	0.57
5:E:126:PHE:HB2	5:E:142:VAL:HG22	1.86	0.57
1:A:6:ARG:HH22	1:A:113:TYR:HD1	1.48	0.57
4:D:114:PRO:HG2	4:D:163:VAL:HG11	1.87	0.56
4:D:146:THR:HG22	6:D:2104:HOH:O	2.05	0.56
4:D:146:THR:HB	6:D:2131:HOH:O	2.04	0.56
1:A:108:ARG:HA	1:A:169:ARG:HH21	1.70	0.56
4:D:126:LEU:HB3	5:E:127:GLU:O	2.05	0.56
4:D:131:SER:C	4:D:133:ASP:N	2.63	0.56
5:E:9:PHE:CE1	5:E:108:ARG:HD3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:LEU:HD12	5:E:109:LEU:HD11	1.87	0.56
5:E:125:VAL:HG23	5:E:235:ALA:HB3	1.89	0.55
1:A:119:ASP:HB3	2:B:0:MET:HG3	1.89	0.55
1:A:6:ARG:HG3	6:A:2018:HOH:O	2.06	0.55
1:A:82:ARG:CZ	1:A:89:GLU:HG2	2.37	0.55
5:E:52:GLY:C	5:E:53:ILE:HG13	2.32	0.54
1:A:176:LYS:HG2	1:A:180:GLN:HE21	1.68	0.54
4:D:114:PRO:HB3	4:D:172:LYS:HD3	1.89	0.54
1:A:162:GLY:O	1:A:166:GLU:HG3	2.08	0.53
5:E:196:ALA:O	5:E:200:GLN:HG3	2.08	0.53
2:B:0:MET:HG2	2:B:1:ILE:H	1.72	0.53
4:D:115:TYR:HE1	4:D:117:GLN:HG2	1.72	0.53
5:E:126:PHE:HB2	5:E:142:VAL:HG23	1.86	0.53
2:B:0:MET:HG2	2:B:1:ILE:N	2.24	0.53
4:D:18:ASN:HD22	4:D:79:ALA:H	1.57	0.53
5:E:175:LEU:C	5:E:175:LEU:HD12	2.33	0.53
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.73	0.52
5:E:12:LEU:HD11	5:E:18:MET:SD	2.50	0.52
1:A:49:ALA:O	1:A:52:ILE:HG22	2.10	0.52
1:A:255:GLN:HB2	6:A:2147:HOH:O	2.09	0.52
5:E:24:GLN:OE1	5:E:27:ASN:N	2.43	0.52
4:D:163:VAL:HG12	4:D:174:ASN:OD1	2.10	0.52
4:D:195:ILE:O	4:D:195:ILE:HG23	2.09	0.52
1:A:128:GLU:HG3	6:A:2094:HOH:O	2.09	0.51
5:E:133:ILE:HD11	5:E:139:ALA:CB	2.39	0.51
5:E:76:ARG:HE	5:E:78:LEU:HD23	1.76	0.51
1:A:253:GLN:CD	1:A:256:ARG:HH12	2.18	0.51
1:A:155:GLN:HG3	4:D:31:TYR:HE2	1.74	0.51
1:A:106:ASP:OD2	1:A:108:ARG:NH1	2.44	0.51
1:A:189:MET:SD	1:A:274:TRP:HB2	2.51	0.51
1:A:230:LEU:HD12	1:A:245:ALA:HB2	1.92	0.51
2:B:96:ASP:OD1	2:B:98:ASP:HB3	2.10	0.51
2:B:97:ARG:HG3	2:B:97:ARG:NH1	2.26	0.50
4:D:33:LEU:HB3	4:D:50:ILE:CG2	2.40	0.50
4:D:39:ASP:HB2	4:D:42:LYS:HD2	1.93	0.50
4:D:42:LYS:HG2	6:D:2040:HOH:O	2.11	0.50
5:E:18:MET:HG2	5:E:19:THR:N	2.26	0.49
4:D:126:LEU:O	4:D:135:SER:HB2	2.12	0.49
1:A:144:LYS:O	1:A:148:GLU:HG3	2.13	0.49
4:D:62:LEU:HG	4:D:77:ILE:CD1	2.42	0.49
4:D:191:PHE:CB	4:D:196:ILE:HD11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:128:ASP:HB3	4:D:131:SER:O	2.12	0.48
4:D:89:LEU:HD23	4:D:107:GLY:HA3	1.96	0.48
4:D:93:ARG:NH2	5:E:93:SER:OG	2.34	0.48
4:D:18:ASN:ND2	4:D:79:ALA:H	2.12	0.48
5:E:197:THR:HG23	6:E:2155:HOH:O	2.14	0.48
4:D:31:TYR:HA	4:D:95:THR:HG23	1.95	0.48
5:E:114:ASP:OD2	5:E:116:LYS:HD2	2.15	0.47
1:A:82:ARG:HG3	1:A:87:GLN:HB2	1.95	0.47
2:B:45:ARG:HG2	2:B:45:ARG:HH11	1.80	0.47
2:B:89:GLN:HG3	2:B:90:PRO:HD2	1.96	0.47
4:D:42:LYS:CG	4:D:43:GLY:N	2.78	0.47
4:D:126:LEU:HD23	4:D:126:LEU:N	2.30	0.47
5:E:4:THR:HG23	6:E:2002:HOH:O	2.14	0.47
1:A:192:HIS:CD2	1:A:202:ARG:HH12	2.32	0.47
4:D:20:VAL:HG13	4:D:74:THR:CG2	2.44	0.47
1:A:232:GLU:CD	2:B:6:LYS:HE3	2.41	0.46
1:A:106:ASP:OD1	1:A:108:ARG:HG2	2.15	0.46
4:D:49:LEU:C	4:D:49:LEU:HD13	2.41	0.46
4:D:126:LEU:HD12	5:E:142:VAL:HG22	1.97	0.46
5:E:11:VAL:HG23	6:E:2114:HOH:O	2.15	0.46
4:D:125:GLN:C	4:D:126:LEU:HD23	2.40	0.46
4:D:147:ASN:HA	4:D:161:LYS:HE2	1.98	0.46
1:A:98:MET:SD	1:A:98:MET:C	2.99	0.45
4:D:148:VAL:H	4:D:161:LYS:HZ1	1.64	0.45
5:E:51:ALA:O	5:E:53:ILE:HD12	2.17	0.45
1:A:255:GLN:HE21	1:A:255:GLN:CA	2.30	0.45
4:D:50:ILE:HG23	4:D:50:ILE:O	2.15	0.45
4:D:19:LEU:HD12	4:D:19:LEU:C	2.41	0.45
4:D:152:LYS:NZ	4:D:153:ASP:OD1	2.49	0.45
5:E:181:LEU:N	5:E:181:LEU:CD1	2.76	0.45
4:D:89:LEU:HD23	4:D:107:GLY:CA	2.47	0.45
5:E:160:ASN:HD21	5:E:204:ASN:HD22	1.63	0.45
1:A:162:GLY:O	1:A:165:VAL:HG22	2.16	0.45
4:D:146:THR:O	4:D:161:LYS:HE2	2.17	0.45
4:D:39:ASP:O	4:D:42:LYS:HB3	2.18	0.44
4:D:191:PHE:HB2	4:D:196:ILE:HD11	1.97	0.44
1:A:5:MET:C	1:A:6:ARG:HG2	2.43	0.44
1:A:255:GLN:HE21	1:A:255:GLN:N	2.16	0.44
1:A:191:HIS:HE1	1:A:254:GLU:OE2	2.01	0.44
4:D:99:SER:O	4:D:100:TYR:HB2	2.18	0.44
5:E:114:ASP:CG	5:E:116:LYS:HD2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:151:ASP:CG	5:E:151:ASP:O	2.60	0.44
1:A:111:ARG:HD3	1:A:113:TYR:OH	2.16	0.43
4:D:131:SER:OG	4:D:134:LYS:HG2	2.18	0.43
4:D:196:ILE:HG22	4:D:200:THR:OG1	2.18	0.43
1:A:19:GLU:N	1:A:19:GLU:OE1	2.52	0.43
1:A:43:GLN:O	1:A:68:LYS:CE	2.65	0.43
4:D:171:PHE:CD2	5:E:138:LYS:HE2	2.54	0.43
5:E:207:ARG:NH1	5:E:209:GLN:HB2	2.33	0.43
1:A:96:GLN:OE1	2:B:31:HIS:HE1	2.01	0.43
1:A:75:ARG:HD3	6:A:2058:HOH:O	2.17	0.43
4:D:115:TYR:CE1	4:D:117:GLN:HG2	2.51	0.43
4:D:164:LEU:C	4:D:164:LEU:HD12	2.43	0.43
5:E:160:ASN:HD21	5:E:204:ASN:ND2	2.17	0.43
4:D:196:ILE:CG2	4:D:197:PRO:HD2	2.49	0.43
4:D:55:ARG:HG3	4:D:55:ARG:HH11	1.83	0.43
4:D:32:ASN:OD1	4:D:32:ASN:C	2.61	0.42
4:D:113:HIS:HA	4:D:114:PRO:HD3	1.89	0.42
4:D:102:PRO:HG2	5:E:101:LEU:HD11	2.01	0.42
5:E:19:THR:HG22	5:E:76:ARG:HB2	2.01	0.42
2:B:96:ASP:O	2:B:99:MET:HG2	2.20	0.42
5:E:52:GLY:O	5:E:53:ILE:HG13	2.20	0.42
2:B:0:MET:CG	2:B:1:ILE:H	2.30	0.42
4:D:152:LYS:HD3	4:D:152:LYS:C	2.45	0.41
4:D:167:ARG:HD3	4:D:167:ARG:HA	1.90	0.41
1:A:45:MET:HE1	3:C:2:LEU:HD11	2.03	0.41
2:B:21:ASN:O	2:B:69:GLU:HG3	2.20	0.41
2:B:58:LYS:HB3	2:B:58:LYS:HZ2	1.83	0.41
5:E:133:ILE:HD13	5:E:138:LYS:O	2.20	0.41
4:D:106:ARG:HA	4:D:106:ARG:HD2	1.91	0.41
4:D:13:VAL:HA	4:D:14:PRO:HD3	1.93	0.41
5:E:120:PRO:HD3	5:E:228:PRO:HB3	2.03	0.41
4:D:152:LYS:HD3	4:D:153:ASP:N	2.36	0.41
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.55	0.41
4:D:164:LEU:HB3	5:E:169:CYS:HB2	2.03	0.41
3:C:6:ILE:HD12	3:C:6:ILE:N	2.34	0.41
4:D:142:PHE:HB2	4:D:146:THR:CG2	2.49	0.41
1:A:106:ASP:O	1:A:107:TRP:HB2	2.21	0.40
5:E:155:LEU:C	5:E:155:LEU:HD23	2.46	0.40
4:D:50:ILE:HD11	4:D:54:GLN:C	2.47	0.40
1:A:182:THR:HG22	1:A:264:GLU:OE2	2.21	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	274/276 (99%)	266 (97%)	8 (3%)	0	100	100
2	B	98/100 (98%)	94 (96%)	3 (3%)	1 (1%)	12	5
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	201/203 (99%)	196 (98%)	5 (2%)	0	100	100
5	E	239/241 (99%)	230 (96%)	8 (3%)	1 (0%)	30	22
All	All	819/829 (99%)	793 (97%)	24 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	47	GLU
5	E	222	THR

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%)	226 (97%)	6 (3%)	40	35
2	B	95/95 (100%)	91 (96%)	4 (4%)	26	19
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	2
4	D	179/179 (100%)	172 (96%)	7 (4%)	28	21
5	E	208/208 (100%)	206 (99%)	2 (1%)	68	70
All	All	723/723 (100%)	703 (97%)	20 (3%)	38	32

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	58	GLU
1	A	138	MET
1	A	155	GLN
1	A	177	GLU
1	A	255	GLN
2	B	0	MET
2	B	50	GLU
2	B	58	LYS
2	B	97	ARG
3	C	6	ILE
4	D	93	ARG
4	D	95	THR
4	D	111	ILE
4	D	126	LEU
4	D	146	THR
4	D	152	LYS
4	D	163	VAL
5	E	24	GLN
5	E	53	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	54	GLN
1	A	141	GLN
1	A	155	GLN
1	A	174	ASN
1	A	180	GLN
1	A	191	HIS
1	A	218	GLN
1	A	242	GLN
1	A	253	GLN
1	A	255	GLN
2	B	13	HIS
2	B	31	HIS
2	B	51	HIS
2	B	83	ASN
3	C	8	GLN
4	D	18	ASN

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Mol	Chain	Res	Type
4	D	38	GLN
4	D	63	ASN
4	D	117	GLN
4	D	125	GLN
4	D	192	ASN
5	E	36	GLN
5	E	56	GLN
5	E	61	ASN
5	E	152	HIS
5	E	204	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 [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%)	0.98	49 (17%)  	17, 29, 50, 63	1 (0%)
2	B	100/100 (100%)	1.58	30 (30%)  	21, 40, 60, 66	0
3	C	9/9 (100%)	0.60	0  	21, 22, 27, 28	0
4	D	203/203 (100%)	1.55	55 (27%)  	20, 33, 45, 53	0
5	E	241/241 (100%)	1.23	42 (17%)  	19, 28, 43, 60	0
All	All	829/829 (100%)	1.26	176 (21%)  	17, 30, 51, 66	1 (0%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	18	GLY	6.0
2	B	1	ILE	5.8
2	B	71	THR	4.7
5	E	222	THR	4.7
4	D	42	LYS	4.5
5	E	221	TRP	4.4
1	A	194	VAL	4.3
1	A	275	GLU	4.2
4	D	13	VAL	4.2
5	E	182	ASN	4.2
2	B	70	PHE	4.1
4	D	204	SER	3.9
1	A	193	ALA	3.9
5	E	90	CYS	3.9
4	D	196	ILE	3.9
5	E	224	ASP	3.9
5	E	242	ASP	3.9
5	E	181	LEU	3.8
2	B	46	ILE	3.8
2	B	85	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
5	E	197	THR	3.8
2	B	72	PRO	3.7
4	D	131	SER	3.7
5	E	53	ILE	3.7
1	A	138	MET	3.7
2	B	50	GLU	3.6
1	A	192	HIS	3.6
1	A	197	HIS	3.6
4	D	195	ILE	3.6
4	D	170	ASP	3.5
2	B	47	GLU	3.5
1	A	177	GLU	3.5
1	A	222	GLU	3.5
4	D	133	ASP	3.4
4	D	182	LYS	3.4
1	A	251	SER	3.4
4	D	181	ASN	3.4
1	A	247	VAL	3.4
4	D	132	SER	3.4
1	A	225	THR	3.4
2	B	0	MET	3.3
2	B	73	THR	3.3
5	E	174	PRO	3.3
1	A	248	VAL	3.3
2	B	89	GLN	3.3
1	A	196	ASP	3.3
1	A	219	ARG	3.3
4	D	187	CYS	3.3
4	D	111	ILE	3.2
4	D	144	SER	3.2
4	D	169	MET	3.2
5	E	169	CYS	3.2
4	D	116	ILE	3.2
2	B	98	ASP	3.2
1	A	105	SER	3.2
4	D	162	CYS	3.2
2	B	99	MET	3.1
1	A	276	PRO	3.0
1	A	108	ARG	3.0
1	A	113	TYR	3.0
4	D	115	TYR	2.9
1	A	226	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	110	LEU	2.9
4	D	152	LYS	2.9
1	A	230	LEU	2.9
5	E	218	ASN	2.9
5	E	223	GLN	2.9
4	D	184	ASP	2.9
4	D	157	TYR	2.8
4	D	145	GLN	2.8
1	A	195	SER	2.8
5	E	157	TRP	2.8
5	E	142	VAL	2.8
4	D	137	CYS	2.8
1	A	255	GLN	2.8
4	D	117	GLN	2.8
4	D	55	ARG	2.7
2	B	77	GLU	2.7
2	B	17	ASN	2.7
5	E	229	VAL	2.7
2	B	69	GLU	2.7
2	B	94	LYS	2.7
5	E	238	TRP	2.6
5	E	64	ASN	2.6
4	D	153	ASP	2.6
2	B	86	THR	2.6
1	A	231	VAL	2.6
5	E	17	SER	2.6
4	D	165	ASP	2.6
4	D	159	THR	2.6
1	A	54	GLN	2.5
5	E	39	GLY	2.5
1	A	58	GLU	2.5
1	A	270	LEU	2.5
2	B	95	TRP	2.5
1	A	86	ASN	2.5
5	E	196	ALA	2.5
1	A	106	ASP	2.5
5	E	201	ASP	2.5
1	A	169	ARG	2.4
4	D	118	ASN	2.4
1	A	178	THR	2.4
4	D	140	THR	2.4
1	A	223	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	249	VAL	2.4
5	E	149	TYR	2.4
1	A	190	THR	2.4
4	D	16	GLY	2.4
2	B	88	SER	2.4
5	E	68	SER	2.4
5	E	134	SER	2.4
1	A	224	GLN	2.4
5	E	40	MET	2.4
4	D	179	TRP	2.4
1	A	203	CYS	2.4
4	D	191	PHE	2.3
4	D	202	PHE	2.3
5	E	133	ILE	2.3
5	E	135	HIS	2.3
5	E	239	GLY	2.3
2	B	6	LYS	2.3
1	A	266	LEU	2.3
2	B	3	ARG	2.3
5	E	117	ASN	2.3
2	B	58	LYS	2.3
1	A	267	PRO	2.3
2	B	15	ALA	2.3
4	D	190	ALA	2.3
2	B	92	ILE	2.3
5	E	129	SER	2.3
1	A	220	ASP	2.3
4	D	90	CYS	2.3
4	D	134	LYS	2.3
1	A	51	TRP	2.2
1	A	2	SER	2.2
4	D	151	SER	2.2
4	D	183	SER	2.2
1	A	176	LYS	2.2
2	B	42	ASN	2.2
5	E	18	MET	2.2
5	E	203	ARG	2.2
4	D	19	LEU	2.2
5	E	173	GLN	2.2
4	D	199	ASP	2.2
2	B	90	PRO	2.2
1	A	109	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	192	ASN	2.1
2	B	74	GLU	2.1
4	D	201	PHE	2.1
5	E	113	GLU	2.1
4	D	35	TRP	2.1
1	A	216	THR	2.1
4	D	200	THR	2.1
2	B	20	SER	2.1
4	D	59	SER	2.1
5	E	3	VAL	2.1
1	A	19	GLU	2.1
4	D	3	GLU	2.1
4	D	17	GLU	2.1
1	A	272	LEU	2.1
5	E	128	PRO	2.1
5	E	241	ALA	2.1
4	D	50	ILE	2.1
1	A	232	GLU	2.1
4	D	112	VAL	2.1
5	E	164	VAL	2.1
5	E	179	PRO	2.1
5	E	131	ALA	2.1
4	D	185	PHE	2.0
1	A	218	GLN	2.0
4	D	2	GLN	2.0
1	A	204	TRP	2.0
5	E	235	ALA	2.0
4	D	154	SER	2.0
4	D	77	ILE	2.0
4	D	193	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

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.