



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:37 AM UTC

PDB ID : 3DX9 / pdb_00003dx9
Title : Crystal Structure of the DM1 TCR at 2.75Å
Authors : Archbold, J.K.; Macdonald, W.A.; Gras, S.; Rossjohn, J.
Deposited on : 2008-07-24
Resolution : 2.75 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

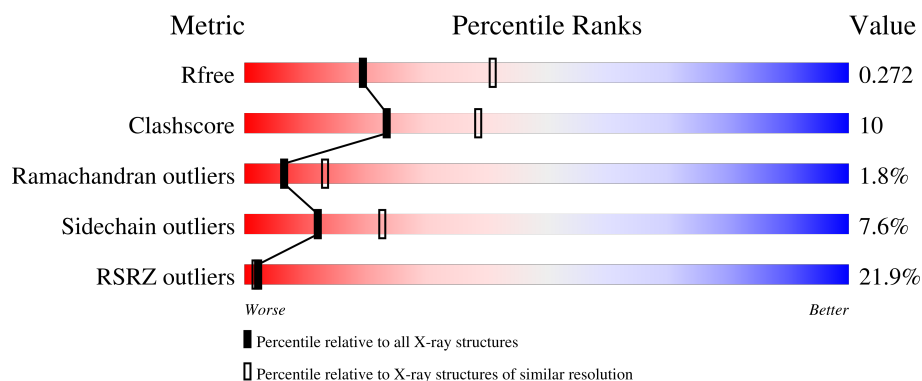
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	198	38% 67% 25% 7% .
1	C	198	33% 69% 25% 6% .
2	B	244	12% 78% 17% 5%
2	D	244	10% 77% 19% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7257 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 DM1 T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	1	0
			1557	975	262	310	10			
1	C	198	Total	C	N	O	S	0	1	0
			1556	973	262	311	10			

- Molecule 2 is a protein called DM1 T cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	1	0
			1992	1249	358	379	6			
2	D	244	Total	C	N	O	S	0	1	0
			1993	1249	358	380	6			

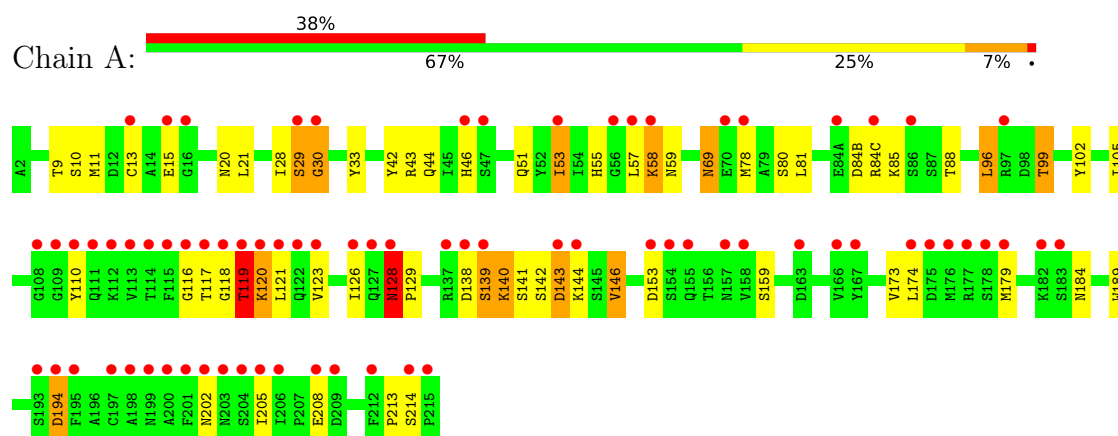
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	53	Total	O	0	0
			53	53		
3	C	31	Total	O	0	0
			31	31		
3	D	54	Total	O	0	0
			54	54		

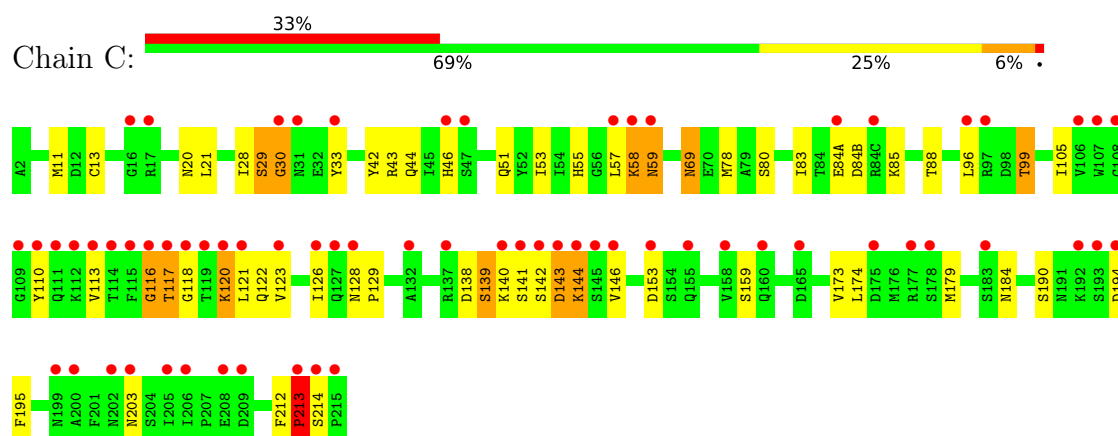
3 Residue-property plots [i](#)

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.

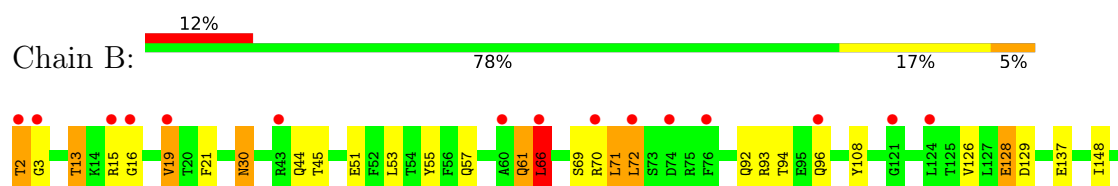
- Molecule 1: DM1 T cell receptor alpha chain

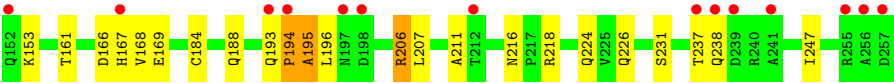


- Molecule 1: DM1 T cell receptor alpha chain

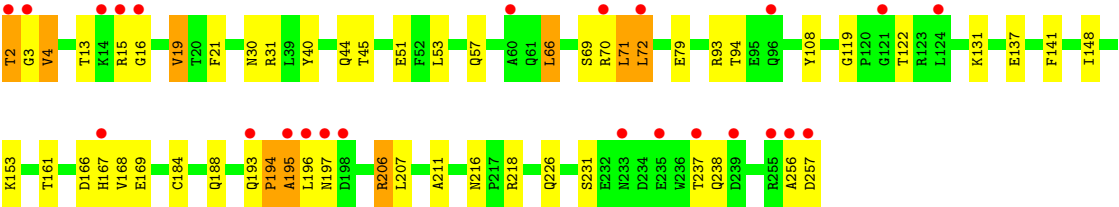
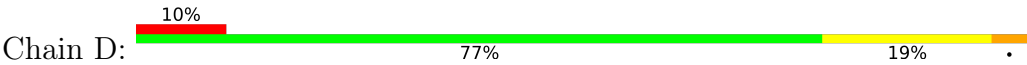


- Molecule 2: DM1 T cell receptor beta chain





● Molecule 2: DM1 T cell receptor beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.74Å 70.73Å 154.41Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	154.30 – 2.75 153.90 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.2 (154.30-2.75) 96.2 (153.90-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.77Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.204 , 0.263 0.229 , 0.272	Depositor DCC
R_{free} test set	1159 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtrriage
Anisotropy	0.073	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7257	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0090e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.76	1/1596 (0.1%)	0.95	6/2170 (0.3%)
1	C	0.71	0/1595	0.97	4/2171 (0.2%)
2	B	0.78	1/2049 (0.0%)	1.34	5/2782 (0.2%)
2	D	0.67	0/2050	0.84	3/2782 (0.1%)
All	All	0.73	2/7290 (0.0%)	1.05	18/9905 (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
1	A	0	9
1	C	0	9
2	B	1	2
2	D	0	1
All	All	1	21

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	61	GLN	C-N	16.52	1.56	1.33
1	A	128	ASN	CA-C	5.09	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	61	GLN	O-C-N	-54.09	56.28	122.81
1	C	117	THR	N-CA-C	-13.42	95.55	112.72
2	B	194	PRO	N-CA-C	11.46	128.67	114.35
2	D	194	PRO	N-CA-C	9.56	128.38	114.80
1	C	116	GLY	N-CA-C	-8.18	101.17	112.13
1	A	119	THR	CA-C-N	7.55	133.54	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	THR	C-N-CA	7.55	133.54	122.82
1	C	129	PRO	N-CA-C	7.07	122.31	111.57
1	A	120	LYS	N-CA-C	6.32	120.08	111.17
1	A	30	GLY	N-CA-C	-5.54	97.23	113.30
1	A	129	PRO	N-CA-C	5.49	119.92	111.57
2	B	194	PRO	CA-C-N	5.48	131.56	121.70
2	B	194	PRO	C-N-CA	5.48	131.56	121.70
2	D	194	PRO	CA-C-N	5.43	131.48	121.70
2	D	194	PRO	C-N-CA	5.43	131.48	121.70
1	C	30	GLY	N-CA-C	-5.40	97.65	113.30
2	B	61	GLN	N-CA-C	-5.34	103.09	110.35
1	A	53	ILE	CB-CA-C	-5.02	107.44	111.71

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	66	LEU	CA

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	GLY	Peptide
1	A	119	THR	Peptide
1	A	128	ASN	Peptide
1	A	140	LYS	Peptide
1	A	213	PRO	Peptide
1	A	214	SER	Peptide
1	A	29	SER	Peptide
1	A	55	HIS	Peptide
1	A	58	LYS	Peptide
2	B	2	THR	Peptide
2	B	61	GLN	Mainchain
1	C	116	GLY	Peptide
1	C	128[A]	ASN	Peptide
1	C	128[B]	ASN	Peptide
1	C	140	LYS	Peptide
1	C	213	PRO	Peptide
1	C	214	SER	Peptide
1	C	29	SER	Peptide
1	C	55	HIS	Peptide
1	C	58	LYS	Peptide
2	D	2	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	1557	0	1492	44	1
1	C	1556	0	1485	38	0
2	B	1992	0	1886	37	0
2	D	1993	0	1886	35	1
3	A	21	0	0	1	0
3	B	53	0	0	0	0
3	C	31	0	0	1	0
3	D	54	0	0	0	0
All	All	7257	0	6749	141	1

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 10.

All (141) 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:193:GLN:C	2:B:195:ALA:HB3	1.66	1.20
2:D:193:GLN:C	2:D:195:ALA:HB3	1.67	1.17
2:B:194:PRO:N	2:B:195:ALA:HB3	1.77	1.00
2:D:194:PRO:N	2:D:195:ALA:HB3	1.75	0.99
1:A:208:GLU:HG2	2:D:196:LEU:HD11	1.51	0.92
1:C:141:SER:HB3	1:C:142:SER:HA	1.55	0.89
1:A:44:GLN:HE22	2:B:44:GLN:HE22	1.20	0.89
1:A:208:GLU:HA	2:D:196:LEU:HD21	1.52	0.89
1:A:141:SER:HB3	1:A:142:SER:HA	1.52	0.89
1:C:99:THR:HG22	1:C:123:VAL:HG23	1.57	0.87
2:B:193:GLN:O	2:B:195:ALA:HB3	1.78	0.82
1:C:44:GLN:HE22	2:D:44:GLN:HE22	1.30	0.77
2:D:194:PRO:N	2:D:195:ALA:CB	2.48	0.75
2:D:193:GLN:O	2:D:195:ALA:HB3	1.87	0.74
1:C:99:THR:HG21	3:C:242:HOH:O	1.85	0.74
2:B:194:PRO:N	2:B:195:ALA:CB	2.50	0.73
1:C:57:LEU:O	1:C:58:LYS:HG3	1.88	0.73
2:B:128:GLU:H	2:B:128:GLU:CD	1.98	0.72
2:B:66:LEU:N	2:B:66:LEU:HD13	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:THR:HG22	1:C:123:VAL:CG2	2.20	0.70
2:B:53:LEU:HD22	2:B:72:LEU:HD23	1.73	0.69
1:A:96:LEU:O	1:A:99:THR:HG23	1.92	0.69
2:D:53:LEU:HD22	2:D:72:LEU:HD23	1.73	0.69
1:C:13:CYS:SG	1:C:121:LEU:HD11	2.33	0.68
1:C:96:LEU:O	1:C:99:THR:HG23	1.93	0.68
1:A:57:LEU:O	1:A:58:LYS:HG3	1.93	0.68
1:C:53:ILE:HG12	1:C:78:MET:HE2	1.75	0.67
1:A:173:VAL:HG22	1:A:184:ASN:OD1	1.94	0.67
1:A:13:CYS:SG	1:A:121:LEU:HD11	2.36	0.66
1:C:179:MET:HE1	2:D:153:LYS:HE3	1.77	0.66
1:C:173:VAL:HG22	1:C:184:ASN:OD1	1.96	0.66
1:A:208:GLU:HA	2:D:196:LEU:CD2	2.24	0.65
2:D:30:ASN:HB2	2:D:108:TYR:O	1.98	0.63
2:B:137:GLU:N	2:B:161:THR:O	2.26	0.62
2:D:137:GLU:N	2:D:161:THR:O	2.29	0.62
2:B:193:GLN:C	2:B:195:ALA:CB	2.59	0.62
1:A:179:MET:HE1	2:B:153:LYS:HE3	1.82	0.62
1:A:43:ARG:HB2	1:A:53:ILE:HD11	1.81	0.60
1:C:33:TYR:CE1	1:C:57:LEU:HD13	2.36	0.60
2:B:30:ASN:HB2	2:B:108:TYR:O	2.02	0.59
2:D:53:LEU:HD22	2:D:72:LEU:CD2	2.33	0.59
1:A:33:TYR:CE1	1:A:57:LEU:HD13	2.38	0.58
1:A:53:ILE:HG12	1:A:78:MET:HE2	1.85	0.57
2:D:4:VAL:HG22	2:D:119:GLY:CA	2.35	0.57
1:A:102:TYR:N	1:A:119:THR:O	2.32	0.57
2:B:66:LEU:N	2:B:66:LEU:CD1	2.67	0.57
2:D:193:GLN:C	2:D:195:ALA:CB	2.60	0.57
2:B:216:ASN:OD1	2:B:218:ARG:HG2	2.04	0.56
1:A:15:GLU:HB2	1:A:123:VAL:HG12	1.86	0.56
2:B:53:LEU:HD22	2:B:72:LEU:CD2	2.35	0.56
1:C:43:ARG:HB2	1:C:53:ILE:HD11	1.87	0.56
2:B:2:THR:HB	2:B:3:GLY:HA2	1.88	0.56
1:C:29:SER:HB3	1:C:30:GLY:HA3	1.88	0.56
1:A:117:THR:CG2	1:A:118:GLY:HA2	2.36	0.55
1:C:138:ASP:OD1	1:C:139:SER:N	2.41	0.53
1:A:117:THR:HG23	1:A:118:GLY:HA2	1.91	0.52
1:C:11:MET:HE1	1:C:20:ASN:O	2.09	0.52
2:D:2:THR:HB	2:D:3:GLY:HA2	1.91	0.52
1:A:13:CYS:HB2	3:A:233:HOH:O	2.10	0.52
1:C:143:ASP:HA	1:C:144:LYS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:NH2	1:A:78:MET:HE3	2.26	0.51
2:B:57:GLN:CB	2:B:66:LEU:HD21	2.41	0.50
2:B:71:LEU:O	2:B:72:LEU:C	2.55	0.50
1:C:141:SER:CB	1:C:142:SER:HA	2.34	0.50
1:A:29:SER:HB3	1:A:30:GLY:HA3	1.92	0.50
1:C:179:MET:CE	2:D:153:LYS:HE3	2.41	0.49
1:A:44:GLN:HE22	2:B:44:GLN:NE2	2.01	0.49
2:B:16:GLY:O	2:B:93:ARG:HA	2.13	0.49
1:A:99:THR:HG22	1:A:123:VAL:HG23	1.94	0.48
2:D:168:VAL:HA	2:D:226:GLN:O	2.13	0.48
2:B:237:THR:HG23	2:B:238:GLN:HG2	1.95	0.48
1:A:9:THR:O	1:A:120:LYS:HB2	2.13	0.48
2:D:166:ASP:O	2:D:166:ASP:CG	2.56	0.48
2:B:206:ARG:N	2:B:206:ARG:HD3	2.29	0.48
2:D:148:ILE:HG23	2:D:211:ALA:HB1	1.96	0.48
2:B:166:ASP:CG	2:B:166:ASP:O	2.58	0.47
2:D:31:ARG:HD3	2:D:40:TYR:OH	2.14	0.47
1:A:10:SER:CB	1:A:120:LYS:HB3	2.45	0.47
2:D:206:ARG:N	2:D:206:ARG:HD3	2.28	0.47
1:A:138:ASP:OD1	1:A:139:SER:N	2.48	0.47
1:A:141:SER:CB	1:A:142:SER:HA	2.33	0.46
1:C:21:LEU:HD11	1:C:121:LEU:HD22	1.97	0.46
2:D:16:GLY:O	2:D:93:ARG:HA	2.15	0.46
2:B:69:SER:C	2:B:71:LEU:N	2.74	0.46
1:C:117:THR:HG23	1:C:118:GLY:N	2.31	0.46
1:A:69:ASN:C	1:A:69:ASN:HD22	2.23	0.46
2:B:168:VAL:HA	2:B:226:GLN:O	2.16	0.46
1:A:43:ARG:HH21	1:A:51:GLN:NE2	2.14	0.45
1:A:99:THR:HG22	1:A:123:VAL:H	1.82	0.45
1:A:21:LEU:HD11	1:A:121:LEU:HD22	1.97	0.45
1:C:142:SER:O	1:C:143:ASP:HB3	2.17	0.45
2:B:13:THR:HG21	2:B:19:VAL:HG23	1.99	0.45
1:A:42:TYR:CE2	1:A:105:ILE:HD11	2.52	0.45
2:B:57:GLN:HB2	2:B:66:LEU:HD21	1.98	0.45
2:D:71:LEU:O	2:D:72:LEU:C	2.59	0.45
2:B:224:GLN:HG3	2:B:247:ILE:CG2	2.47	0.45
1:C:69:ASN:C	1:C:69:ASN:HD22	2.25	0.45
2:D:15:ARG:O	2:D:94:THR:O	2.35	0.44
2:D:19:VAL:CG1	2:D:21:PHE:CE1	3.00	0.44
1:A:202:ASN:CG	2:D:197:ASN:HB2	2.42	0.44
1:C:59:ASN:OD1	1:C:83:ILE:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:ARG:O	2:B:94:THR:O	2.35	0.44
2:B:148:ILE:HG23	2:B:211:ALA:HB1	1.98	0.44
2:B:53:LEU:HD23	2:B:71:LEU:HD23	1.99	0.44
2:D:256:ALA:O	2:D:257:ASP:C	2.60	0.44
1:A:11:MET:HE1	1:A:20:ASN:O	2.18	0.44
1:C:120:LYS:HE2	1:C:122:GLN:HE22	1.83	0.43
2:D:216:ASN:OD1	2:D:218:ARG:HG2	2.18	0.43
2:B:96:GLN:NE2	2:B:128:GLU:HG3	2.32	0.43
2:B:57:GLN:HB3	2:B:66:LEU:HD21	2.00	0.43
1:A:194:ASP:C	1:A:194:ASP:OD1	2.61	0.43
1:C:143:ASP:OD1	1:C:143:ASP:N	2.52	0.43
1:C:42:TYR:CE2	1:C:105:ILE:HD11	2.54	0.43
1:C:84(A):GLU:H	1:C:84(A):GLU:CD	2.27	0.43
2:D:237:THR:HG23	2:D:238:GLN:HG2	2.01	0.43
1:C:43:ARG:NH2	1:C:78:MET:HE3	2.35	0.42
1:C:110:TYR:HA	2:D:31:ARG:NH2	2.34	0.42
1:A:58:LYS:HE3	1:A:84(C):ARG:HD2	2.01	0.42
1:C:194:ASP:OD1	1:C:194:ASP:N	2.52	0.42
1:A:205:ILE:O	1:A:205:ILE:HG22	2.18	0.42
1:C:146:VAL:HG13	2:D:141:PHE:CE1	2.55	0.42
1:C:117:THR:CG2	1:C:118:GLY:N	2.82	0.42
2:D:69:SER:C	2:D:71:LEU:N	2.76	0.42
1:C:43:ARG:HH21	1:C:51:GLN:NE2	2.17	0.42
1:C:174:LEU:C	1:C:174:LEU:HD12	2.45	0.42
2:B:69:SER:C	2:B:71:LEU:H	2.28	0.41
2:B:92:GLN:O	2:B:93:ARG:C	2.63	0.41
1:C:212:PHE:O	1:C:213:PRO:C	2.63	0.41
1:A:174:LEU:HD12	1:A:174:LEU:C	2.45	0.41
1:C:190:SER:HB3	1:C:195:PHE:CG	2.55	0.41
2:B:19:VAL:CG1	2:B:21:PHE:CE1	3.04	0.41
2:D:21:PHE:CD1	2:D:122:THR:HG21	2.56	0.41
1:A:84(B):ASP:HB3	1:A:85:LYS:H	1.86	0.41
1:A:146:VAL:HG22	1:A:189:TRP:HB3	2.01	0.41
2:D:57:GLN:HB2	2:D:66:LEU:CD2	2.51	0.41
1:A:140:LYS:HB2	1:A:141:SER:HA	2.03	0.41
1:A:143:ASP:OD1	1:A:143:ASP:N	2.54	0.41
1:A:110:TYR:O	2:B:55:TYR:OH	2.37	0.40
1:A:142:SER:O	1:A:143:ASP:HB3	2.21	0.40
1:C:84(B):ASP:HB3	1:C:85:LYS:H	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASP:O	2:D:237:THR:OG1[1_455]	2.17	0.03

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	197/198 (100%)	176 (89%)	16 (8%)	5 (2%)	4	8
1	C	197/198 (100%)	180 (91%)	13 (7%)	4 (2%)	6	11
2	B	243/244 (100%)	226 (93%)	12 (5%)	5 (2%)	5	11
2	D	243/244 (100%)	228 (94%)	12 (5%)	3 (1%)	10	20
All	All	880/884 (100%)	810 (92%)	53 (6%)	17 (2%)	6	12

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	143	ASP
1	A	144[A]	LYS
1	A	144[B]	LYS
2	B	66	LEU
1	C	59	ASN
1	C	143	ASP
2	D	71	LEU
2	B	71	LEU
1	C	144	LYS
2	D	195	ALA
1	A	194	ASP
2	B	72	LEU
2	B	195	ALA
2	D	72	LEU
2	B	30	ASN
1	C	213	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	178/177 (101%)	164 (92%)	14 (8%)	11	21
1	C	178/177 (101%)	165 (93%)	13 (7%)	13	24
2	B	217/216 (100%)	199 (92%)	18 (8%)	10	19
2	D	217/216 (100%)	200 (92%)	17 (8%)	11	21
All	All	790/786 (100%)	728 (92%)	62 (8%)	12	21

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	46	HIS
1	A	69	ASN
1	A	80	SER
1	A	81	LEU
1	A	88	THR
1	A	96	LEU
1	A	99	THR
1	A	126	ILE
1	A	128	ASN
1	A	139	SER
1	A	146	VAL
1	A	153	ASP
1	A	159	SER
2	B	13	THR
2	B	19	VAL
2	B	45	THR
2	B	51	GLU
2	B	66	LEU
2	B	70	ARG
2	B	126	VAL
2	B	128	GLU
2	B	129	ASP
2	B	167[A]	HIS

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Mol	Chain	Res	Type
2	B	167[B]	HIS
2	B	169	GLU
2	B	184	CYS
2	B	188	GLN
2	B	196	LEU
2	B	206	ARG
2	B	207	LEU
2	B	231	SER
1	C	28	ILE
1	C	46	HIS
1	C	69	ASN
1	C	80	SER
1	C	88	THR
1	C	99	THR
1	C	113	VAL
1	C	120	LYS
1	C	126	ILE
1	C	139	SER
1	C	153	ASP
1	C	159	SER
1	C	203	ASN
2	D	4	VAL
2	D	13	THR
2	D	19	VAL
2	D	45	THR
2	D	51	GLU
2	D	66	LEU
2	D	70	ARG
2	D	79	GLU
2	D	131	LYS
2	D	167[A]	HIS
2	D	167[B]	HIS
2	D	169	GLU
2	D	184	CYS
2	D	188	GLN
2	D	206	ARG
2	D	207	LEU
2	D	231	SER

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	24	ASN
1	A	44	GLN
1	A	46	HIS
1	A	51	GLN
1	A	69	ASN
1	A	93	HIS
1	A	111	GLN
1	A	127	GLN
1	A	128	ASN
1	A	203	ASN
2	B	57	GLN
2	B	114	ASN
2	B	219	ASN
2	B	246	GLN
1	C	20	ASN
1	C	24	ASN
1	C	44	GLN
1	C	51	GLN
1	C	69	ASN
1	C	93	HIS
1	C	111	GLN
1	C	122	GLN
1	C	127	GLN
2	D	57	GLN
2	D	193	GLN
2	D	219	ASN
2	D	246	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

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

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	198/198 (100%)	2.34	75 (37%) 1 0	22, 42, 43, 45	11 (5%)
1	C	198/198 (100%)	2.05	66 (33%) 1 0	21, 42, 43, 44	15 (7%)
2	B	244/244 (100%)	1.07	29 (11%) 9 7	21, 41, 43, 45	18 (7%)
2	D	244/244 (100%)	1.10	24 (9%) 13 12	21, 42, 43, 45	12 (4%)
All	All	884/884 (100%)	1.58	194 (21%) 2 2	21, 42, 43, 45	56 (6%)

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	TYR	13.9
1	A	108	GLY	13.1
1	C	108	GLY	11.3
1	A	116	GLY	11.3
1	A	111	GLN	11.1
1	A	112	LYS	10.3
1	A	114	THR	10.1
1	C	110	TYR	9.9
1	A	113	VAL	9.5
1	A	109	GLY	9.4
1	C	109	GLY	9.1
1	C	111	GLN	9.1
1	A	115	PHE	8.4
1	C	107	TRP	8.0
1	C	116	GLY	8.0
1	A	117	THR	7.7
1	A	118	GLY	7.7
1	C	106	VAL	7.1
1	A	119	THR	6.8
1	C	113	VAL	6.7
1	C	114	THR	6.5

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Mol	Chain	Res	Type	RSRZ
1	C	155	GLN	6.5
1	A	215	PRO	6.4
1	C	112	LYS	6.2
2	D	256	ALA	6.0
1	A	203	ASN	5.9
1	A	204	SER	5.6
1	A	214	SER	5.5
1	A	127	GLN	5.5
1	A	143	ASP	5.4
1	A	46	HIS	5.3
1	A	120	LYS	5.1
2	D	193	GLN	5.1
1	C	118	GLY	5.0
2	D	257	ASP	4.9
1	A	177	ARG	4.8
1	A	202	ASN	4.8
1	C	46	HIS	4.7
1	A	198	ALA	4.7
1	C	47	SER	4.6
1	C	115	PHE	4.6
1	C	213	PRO	4.5
2	D	237	THR	4.5
2	D	197	ASN	4.5
2	D	235	GLU	4.4
1	C	143	ASP	4.4
1	C	202	ASN	4.4
2	B	152	GLN	4.3
1	C	203	ASN	4.3
2	B	167[A]	HIS	4.3
2	B	256	ALA	4.2
1	C	208	GLU	4.2
1	C	214	SER	4.2
1	C	215	PRO	4.1
1	C	119	THR	4.1
1	A	84(A)	GLU	4.0
1	C	126	ILE	3.9
2	B	66	LEU	3.9
1	A	155	GLN	3.9
1	A	121	LEU	3.9
1	C	117	THR	3.8
2	D	196	LEU	3.7
1	A	126	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	160	GLN	3.7
1	C	57	LEU	3.7
2	D	239	ASP	3.7
1	C	84(A)	GLU	3.6
2	D	72	LEU	3.6
2	D	167[A]	HIS	3.6
1	A	197	CYS	3.6
1	A	58	LYS	3.6
1	C	194	ASP	3.5
1	A	47	SER	3.5
1	A	205	ILE	3.5
2	B	257	ASP	3.5
1	C	141	SER	3.4
1	A	128	ASN	3.4
2	B	70	ARG	3.4
1	A	144[A]	LYS	3.4
2	D	255	ARG	3.4
1	A	153	ASP	3.3
1	C	84(C)	ARG	3.3
2	D	233	ASN	3.3
1	C	144	LYS	3.3
1	A	123	VAL	3.3
1	C	59	ASN	3.3
2	B	15	ARG	3.3
2	B	239	ASP	3.3
2	B	212	THR	3.2
1	A	70	GLU	3.2
1	A	206	ILE	3.2
1	A	175	ASP	3.1
2	B	2	THR	3.1
1	C	128[A]	ASN	3.1
1	A	209	ASP	3.1
2	B	255	ARG	3.1
2	B	72	LEU	3.1
1	A	56	GLY	3.1
2	D	195	ALA	3.1
1	A	84(C)	ARG	3.1
1	C	127	GLN	3.0
1	C	58	LYS	3.0
2	B	194	PRO	3.0
2	B	121	GLY	3.0
1	A	15	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	163	ASP	3.0
1	C	121	LEU	3.0
2	B	96	GLN	3.0
2	B	198	ASP	3.0
1	A	30	GLY	3.0
1	A	195	PHE	3.0
1	A	199	ASN	2.9
2	B	3	GLY	2.9
2	D	3	GLY	2.9
1	A	167	TYR	2.8
1	C	33	TYR	2.8
1	A	97	ARG	2.8
1	A	139	SER	2.8
2	D	121	GLY	2.8
1	C	97	ARG	2.8
2	D	96	GLN	2.7
1	A	157	ASN	2.7
1	C	17	ARG	2.7
1	C	177	ARG	2.7
1	C	120	LYS	2.7
2	D	2	THR	2.7
1	A	178	SER	2.7
1	A	201	PHE	2.7
1	A	194	ASP	2.7
1	A	154	SER	2.6
1	C	178	SER	2.6
1	C	205	ILE	2.6
1	C	96	LEU	2.6
1	A	16	GLY	2.6
2	D	14	LYS	2.6
1	C	206	ILE	2.6
1	C	193	SER	2.6
1	C	140	LYS	2.6
1	A	176	MET	2.5
1	A	208	GLU	2.5
2	B	16	GLY	2.5
2	B	60	ALA	2.5
1	A	182	LYS	2.5
1	C	137	ARG	2.5
2	D	124	LEU	2.5
1	C	132	ALA	2.5
1	C	145	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	153	ASP	2.4
1	C	30	GLY	2.4
1	C	192	LYS	2.4
1	A	158	VAL	2.4
1	C	158	VAL	2.4
2	D	70	ARG	2.4
2	B	19	VAL	2.4
1	A	137	ARG	2.4
1	C	31	ASN	2.3
1	C	16	GLY	2.3
1	A	13	CYS	2.3
2	B	76	PHE	2.3
1	A	200	ALA	2.3
1	C	209	ASP	2.3
2	D	198	ASP	2.3
2	D	16	GLY	2.3
1	A	57	LEU	2.3
1	C	142	SER	2.3
1	A	166	VAL	2.3
2	B	237	THR	2.2
2	B	193	GLN	2.2
1	C	146	VAL	2.2
2	B	197	ASN	2.2
2	B	238	GLN	2.2
2	B	124	LEU	2.2
1	A	53	ILE	2.2
1	A	122	GLN	2.2
2	D	60	ALA	2.1
1	C	165	ASP	2.1
1	C	175	ASP	2.1
1	A	183	SER	2.1
1	A	174	LEU	2.1
1	A	138	ASP	2.1
1	A	212	PHE	2.1
1	C	183	SER	2.1
1	C	199	ASN	2.1
1	C	123	VAL	2.1
1	A	193	SER	2.1
1	C	200	ALA	2.1
2	B	43	ARG	2.1
2	B	241	ALA	2.1
2	D	15	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	179	MET	2.1
2	B	74	ASP	2.0
1	A	86	SER	2.0
1	A	78	MET	2.0
1	A	29	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.