Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:15 AM GMT

PDB ID	:	3DX9
Title	:	Crystal Structure of the DM1 TCR at 2.75A
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

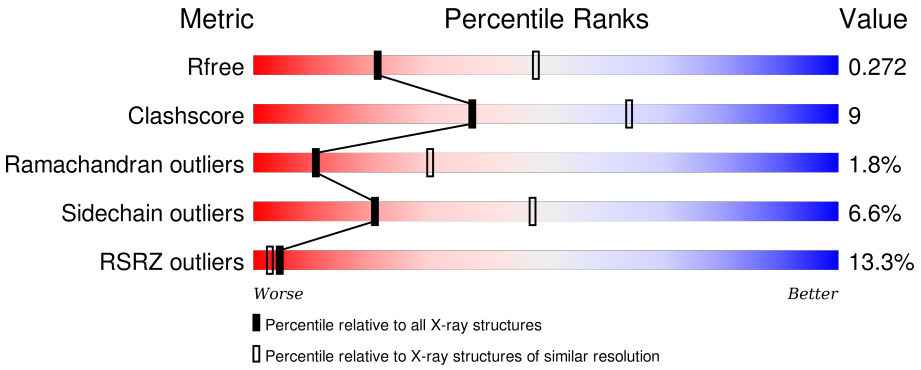
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	21% 72% 22% 6%
1	C	198	21% 73% 22% 6%
2	B	244	7% 80% 14% 5% •
2	D	244	8% 79% 17% •

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.

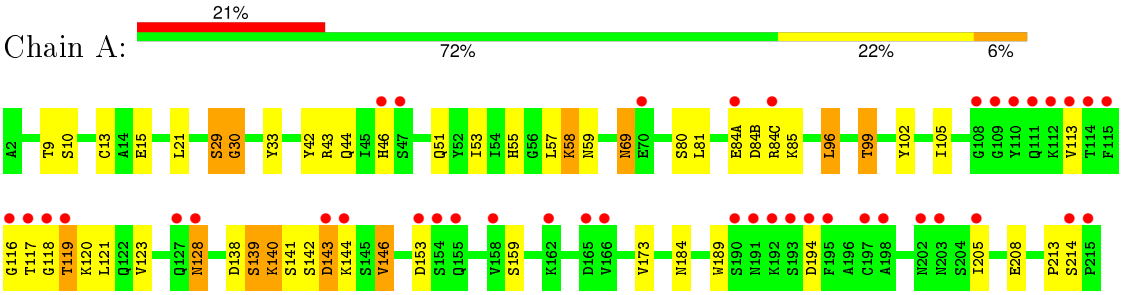
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	53	Total	O	0	0
			53	53		
3	C	31	Total	O	0	0
			31	31		
3	D	54	Total	O	0	0
			54	54		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

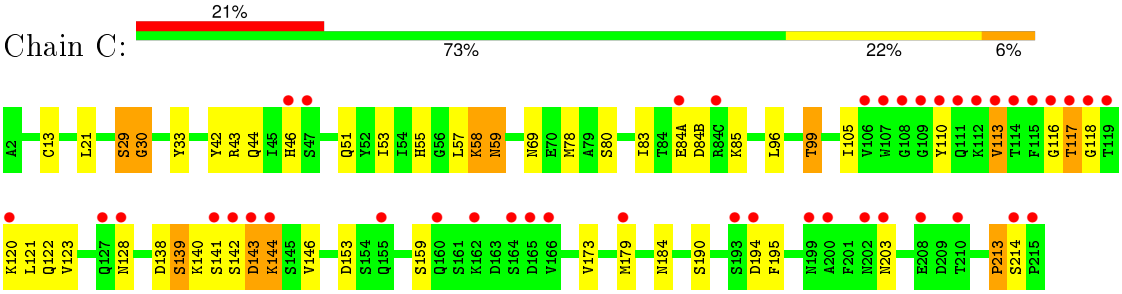
- Molecule 1: DM1 T cell receptor alpha chain

Chain A:



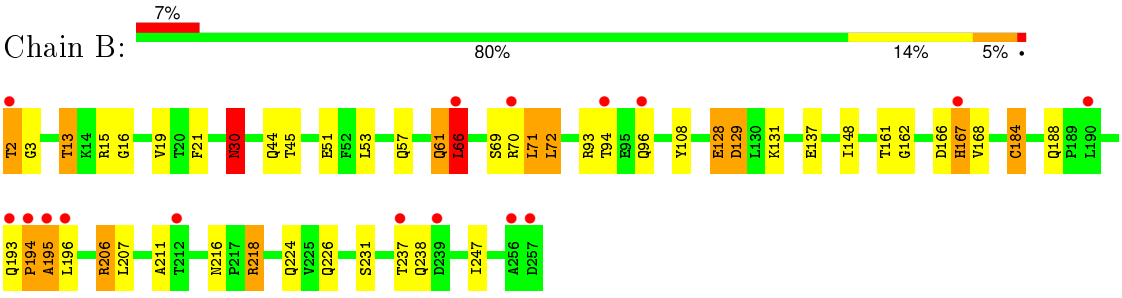
- Molecule 1: DM1 T cell receptor alpha chain

Chain C:



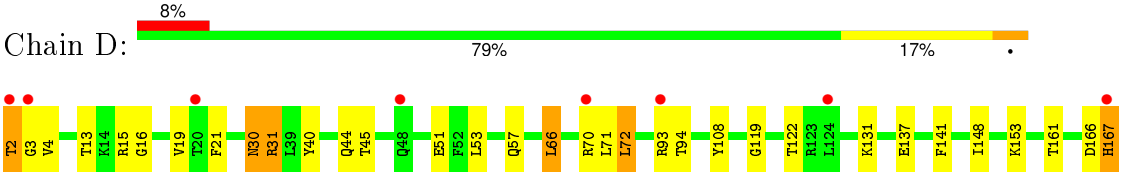
- Molecule 2: DM1 T cell receptor beta chain

Chain B:



- Molecule 2: DM1 T cell receptor beta chain

Chain D:




V168
C184
Q188
Q193
P194
A195
L196
N197
D198
R206
L207
A211
N216
P217
R218
Q226
S231
E232
N233
T237
Q238
D239
R255
A256
D257

4 Data and refinement statistics (i)

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 52.07 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.2 (154.30-2.75) 96.2 (52.07-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.204 , 0.263 0.228 , 0.272	Depositor DCC
R_{free} test set	1159 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 57.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 22660 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7257	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.59	1/1596 (0.1%)	0.75	2/2170 (0.1%)
1	C	0.57	1/1595 (0.1%)	0.76	3/2171 (0.1%)
2	B	0.62	2/2049 (0.1%)	1.18	4/2782 (0.1%)
2	D	0.55	0/2050	0.74	3/2782 (0.1%)
All	All	0.58	4/7290 (0.1%)	0.89	12/9905 (0.1%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	61	GLN	C-N	9.75	1.56	1.34
1	A	113	VAL	CB-CG1	-7.69	1.36	1.52
1	C	113	VAL	CB-CG2	-7.69	1.36	1.52
2	B	184	CYS	CB-SG	-5.77	1.72	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	61	GLN	O-C-N	-41.52	56.28	122.70
2	B	61	GLN	CA-C-N	25.34	172.94	117.20
2	B	194	PRO	N-CA-C	6.37	128.67	112.10
1	A	30	GLY	N-CA-C	-6.35	97.23	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	194	PRO	N-CA-C	6.26	128.38	112.10
1	C	113	VAL	CG1-CB-CG2	-6.20	100.97	110.90
1	C	30	GLY	N-CA-C	-6.18	97.65	113.10
2	D	31	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	113	VAL	CG1-CB-CG2	-5.89	101.48	110.90
1	C	117	THR	N-CA-C	-5.72	95.55	111.00
2	D	31	ARG	NE-CZ-NH1	5.65	123.13	120.30
2	B	162	GLY	N-CA-C	-5.12	100.29	113.10

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1557	0	1492	36	1
1	C	1556	0	1485	32	0
2	B	1992	0	1886	38	0
2	D	1993	0	1886	33	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	129	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 9.

All (129) 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	1.15
2:D:193:GLN:C	2:D:195:ALA:HB3	1.67	1.13
2:B:129:ASP:OD2	2:B:131:LYS:HG2	1.52	1.09
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:129:ASP:CG	2:B:131:LYS:HG2	2.09	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LEU:HD13	2:B:66:LEU:N	2.05	0.71
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:96:LEU:O	1:C:99:THR:HG23	1.93	0.68
1:C:13:CYS:SG	1:C:121:LEU:HD11	2.33	0.68
1:A:57:LEU:O	1:A:58:LYS:HG3	1.93	0.68
1:A:173:VAL:HG22	1:A:184:ASN:OD1	1.94	0.67
2:B:128:GLU:CD	2:B:128:GLU:H	1.98	0.66
1:A:13:CYS:SG	1:A:121:LEU:HD11	2.36	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
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
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: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
1:C:29:SER:HB3	1:C:30:GLY:HA3	1.88	0.56
2:B:2:THR:HB	2:B:3:GLY:HA2	1.88	0.56
1:A:117:THR:CG2	1:A:118:GLY:HA2	2.36	0.55
2:D:193:GLN:C	2:D:195:ALA:CB	2.60	0.53
2:B:193:GLN:C	2:B:195:ALA:CB	2.59	0.53
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
2:D:2:THR:HB	2:D:3:GLY:HA2	1.91	0.52
1:C:143:ASP:HA	1:C:144:LYS:O	2.10	0.52
1:A:13:CYS:HB2	3:A:233:HOH:O	2.10	0.52
2:B:57:GLN:CB	2:B:66:LEU:HD21	2.41	0.50
1:C:141:SER:CB	1:C:142:SER:HA	2.34	0.50
1:C:179:MET:CE	2:D:153:LYS:HE3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:SER:HB3	1:A:30:GLY:HA3	1.92	0.50
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:148:ILE:HG23	2:D:211:ALA:HB1	1.96	0.48
2:B:206:ARG:N	2:B:206:ARG:HD3	2.29	0.48
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
1:C:117:THR:HG23	1:C:118:GLY:N	2.31	0.46
2:B:168:VAL:HA	2:B:226:GLN:O	2.16	0.46
1:C:53:ILE:HG12	1:C:78:MET:HE1	1.98	0.45
1:A:43:ARG:HH21	1:A:51:GLN:NE2	2.14	0.45
1:C:179:MET:HE1	2:D:153:LYS:HE3	1.98	0.45
2:B:71:LEU:O	2:B:72:LEU:C	2.55	0.45
1:A:99:THR:HG22	1:A:123:VAL:H	1.82	0.45
2:B:129:ASP:OD2	2:B:131:LYS:NZ	2.38	0.45
1:C:142:SER:O	1:C:143:ASP:HB3	2.17	0.45
1:A:21:LEU:HD11	1:A:121:LEU:HD22	1.97	0.45
2:B:13:THR:HG21	2:B:19:VAL:HG23	1.99	0.45
2:B:57:GLN:HB2	2:B:66:LEU:HD21	1.98	0.45
1:A:42:TYR:CE2	1:A:105:ILE:HD11	2.52	0.45
2:B:224:GLN:HG3	2:B:247:ILE:CG2	2.47	0.45
2:D:19:VAL:CG1	2:D:21:PHE:CE1	3.00	0.44
2:D:15:ARG:O	2:D:94:THR:O	2.35	0.44
1:C:59:ASN:OD1	1:C:83:ILE:HD12	2.18	0.44
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
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
2:D:166:ASP:O	2:D:166:ASP:CG	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:237:THR:HG23	2:D:238:GLN:HG2	2.01	0.43
2:B:166:ASP:O	2:B:166:ASP:CG	2.58	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:C:146:VAL:HG13	2:D:141:PHE:CE1	2.55	0.42
1:A:205:ILE:HG22	1:A:205:ILE:O	2.18	0.42
1:C:117:THR:CG2	1:C:118:GLY:N	2.82	0.42
1:C:43:ARG:HH21	1:C:51:GLN:NE2	2.17	0.42
2:B:129:ASP:OD1	2:B:131:LYS:HG2	2.20	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
2:B:69:SER:C	2:B:71:LEU:N	2.74	0.41
1:A:146:VAL:HG22	1:A:189:TRP:HB3	2.01	0.41
1:A:84(B):ASP:HB3	1:A:85:LYS:H	1.86	0.41
1:A:69:ASN:C	1:A:69:ASN:HD22	2.23	0.41
1:A:143:ASP:N	1:A:143:ASP:OD1	2.54	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: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
2:D:256:ALA:O	2:D:257:ASP:C	2.60	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%)	7 21
1	C	197/198 (100%)	180 (91%)	13 (7%)	4 (2%)	9 27
2	B	243/244 (100%)	226 (93%)	12 (5%)	5 (2%)	9 25
2	D	243/244 (100%)	228 (94%)	12 (5%)	3 (1%)	16 43
All	All	880/884 (100%)	810 (92%)	53 (6%)	17 (2%)	11 28

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 (i)

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%)	166 (93%)	12 (7%)	20 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	178/177 (101%)	168 (94%)	10 (6%)	26 56
2	B	217/216 (100%)	200 (92%)	17 (8%)	16 38
2	D	217/216 (100%)	202 (93%)	15 (7%)	19 45
All	All	790/786 (100%)	736 (93%)	54 (7%)	21 46

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	69	ASN
1	A	80	SER
1	A	81	LEU
1	A	84(A)	GLU
1	A	96	LEU
1	A	99	THR
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	30	ASN
2	B	45	THR
2	B	51	GLU
2	B	66	LEU
2	B	70	ARG
2	B	128	GLU
2	B	129	ASP
2	B	167[A]	HIS
2	B	167[B]	HIS
2	B	184	CYS
2	B	188	GLN
2	B	196	LEU
2	B	206	ARG
2	B	207	LEU
2	B	218	ARG
2	B	231	SER
1	C	46	HIS
1	C	69	ASN
1	C	80	SER
1	C	84(A)	GLU

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Mol	Chain	Res	Type
1	C	99	THR
1	C	113	VAL
1	C	139	SER
1	C	153	ASP
1	C	159	SER
1	C	203	ASN
2	D	13	THR
2	D	30	ASN
2	D	45	THR
2	D	51	GLU
2	D	66	LEU
2	D	70	ARG
2	D	131	LYS
2	D	167[A]	HIS
2	D	167[B]	HIS
2	D	184	CYS
2	D	188	GLN
2	D	206	ARG
2	D	207	LEU
2	D	218	ARG
2	D	231	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	24	ASN
1	A	44	GLN
1	A	46	HIS
1	A	51	GLN
1	A	69	ASN
1	A	111	GLN
1	A	203	ASN
2	B	30	ASN
2	B	219	ASN
1	C	20	ASN
1	C	24	ASN
1	C	44	GLN
1	C	51	GLN
1	C	69	ASN
1	C	111	GLN
1	C	122	GLN

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Mol	Chain	Res	Type
2	D	30	ASN
2	D	132	ASN
2	D	219	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates 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, 95^{th} 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%)	1.36	41 (20%)	1	1	40, 42, 43, 45	10 (5%)
1	C	198/198 (100%)	1.26	42 (21%)	1	1	23, 42, 43, 44	14 (7%)
2	B	244/244 (100%)	0.63	16 (6%)	22	16	22, 42, 43, 45	18 (7%)
2	D	244/244 (100%)	0.70	19 (7%)	16	11	37, 42, 43, 45	12 (4%)
All	All	884/884 (100%)	0.95	118 (13%)	4	3	22, 42, 43, 45	54 (6%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	TYR	7.8
1	C	108	GLY	7.1
1	C	110	TYR	6.8
1	A	108	GLY	6.6
1	A	111	GLN	5.7
1	A	113	VAL	5.6
1	A	109	GLY	5.6
1	A	114	THR	5.4
1	A	215	PRO	5.4
1	C	109	GLY	5.4
2	D	237	THR	5.3
1	C	107	TRP	5.2
1	A	198	ALA	5.0
1	A	112	LYS	4.9
1	A	143	ASP	4.9
2	D	197	ASN	4.9
1	C	47	SER	4.9
2	B	2	THR	4.8
1	C	111	GLN	4.8
1	C	106	VAL	4.8
1	A	116	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	115	PHE	4.5
1	A	202	ASN	4.4
1	A	166	VAL	4.4
1	C	203	ASN	4.3
1	C	143	ASP	4.2
2	D	257	ASP	4.2
2	D	256	ALA	4.1
1	A	84(A)	GLU	4.1
1	C	202	ASN	4.0
1	C	112	LYS	3.9
1	C	113	VAL	3.9
1	C	84(A)	GLU	3.9
1	C	114	THR	3.8
2	D	233	ASN	3.8
1	C	200	ALA	3.8
1	A	203	ASN	3.7
1	C	141	SER	3.7
2	D	2	THR	3.7
1	A	117	THR	3.7
1	A	118	GLY	3.6
2	B	70	ARG	3.5
1	C	116	GLY	3.4
1	C	215	PRO	3.4
2	B	194	PRO	3.4
1	A	193	SER	3.3
1	A	214	SER	3.3
1	A	128	ASN	3.3
1	C	199	ASN	3.3
2	B	212	THR	3.3
1	C	115	PHE	3.2
1	A	153	ASP	3.2
1	A	192	LYS	3.2
1	C	117	THR	3.2
1	A	155	GLN	3.1
1	A	84(C)	ARG	3.1
1	C	118	GLY	3.1
1	A	194	ASP	3.1
1	A	119	THR	3.1
2	D	196	LEU	3.1
1	C	164	SER	3.0
1	C	155	GLN	3.0
2	D	193	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	70	GLU	2.9
2	D	167[A]	HIS	2.9
1	C	208	GLU	2.9
1	C	214	SER	2.9
2	D	198	ASP	2.9
2	B	256	ALA	2.9
1	C	166	VAL	2.8
2	B	195	ALA	2.8
1	A	197	CYS	2.8
1	A	195	PHE	2.8
1	C	210	THR	2.8
1	A	46	HIS	2.6
1	C	144	LYS	2.6
2	D	239	ASP	2.6
1	C	119	THR	2.6
1	C	194	ASP	2.6
1	A	165	ASP	2.6
2	D	255	ARG	2.6
1	A	162	LYS	2.6
2	D	195	ALA	2.5
2	B	257	ASP	2.5
2	D	124	LEU	2.5
1	C	160	GLN	2.5
2	D	93	ARG	2.5
1	A	144[A]	LYS	2.5
2	B	193	GLN	2.5
2	B	196	LEU	2.5
1	A	127	GLN	2.5
2	B	66	LEU	2.5
2	B	190	LEU	2.5
1	C	120	LYS	2.5
1	C	142	SER	2.4
2	D	3	GLY	2.4
1	C	165	ASP	2.4
1	C	128[A]	ASN	2.4
1	C	127	GLN	2.3
1	A	191	ASN	2.3
1	A	205	ILE	2.3
1	C	193	SER	2.3
1	A	158	VAL	2.3
2	B	96	GLN	2.3
1	C	46	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	237	THR	2.2
1	A	47	SER	2.2
1	A	190	SER	2.2
1	A	154	SER	2.2
2	B	167[A]	HIS	2.2
2	D	70	ARG	2.2
1	C	162	LYS	2.1
2	B	239	ASP	2.1
2	B	94	THR	2.0
1	C	179	MET	2.0
2	D	48	GLN	2.0
1	C	84(C)	ARG	2.0
2	D	20	THR	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.