Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:28 am BST

PDB ID	:	5YXN
Title	:	A T cell receptor in complex with HLA-A0201 restricted Hepatitis C virus NS3 peptide (KLVALGINAV)
Authors	:	Hui, F.
Deposited on	:	2017-12-06
Resolution	:	2.03 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 following versions of software and data (see references ⓘ) were used in the production of this report:

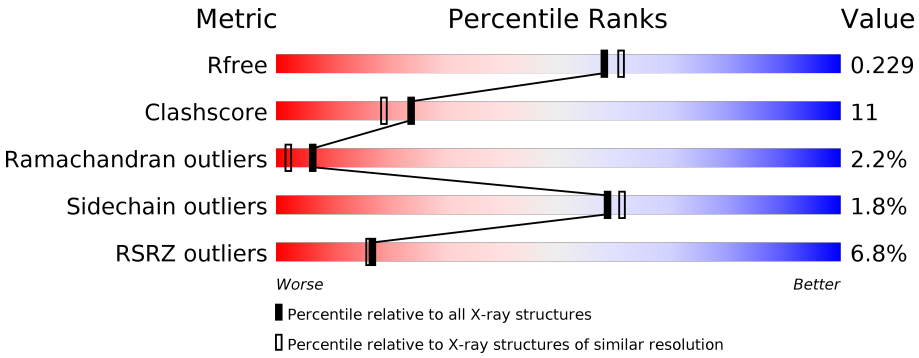
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.03 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}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 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 <=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	192	14% 76% 15% 8%
2	B	241	3% 84% 15%
3	C	275	7% 88% 11%
4	D	100	3% 86% 13%
5	I	10	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7158 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 T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1523	949	253	311	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1934	1217	336	373	8			

- Molecule 3 is a protein called HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	275	Total	C	N	O	S	0	0	0
			2232	1394	405	424	9			

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	100	Total	C	N	O	S	0	0	0
			815	518	139	155	3			

- Molecule 5 is a protein called NS3 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	10	Total	C	N	O	0	0	0
			69	46	12	11			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	111	Total	O	0	0
			111	111		

Continued on next page...

Continued from previous page...

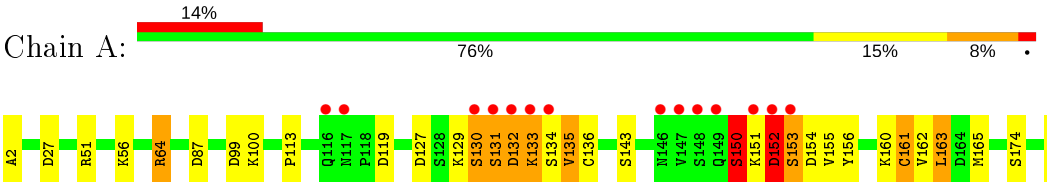
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	175	Total O 175 175	0	0
6	C	198	Total O 198 198	0	0
6	D	93	Total O 93 93	0	0
6	I	8	Total O 8 8	0	0

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 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.

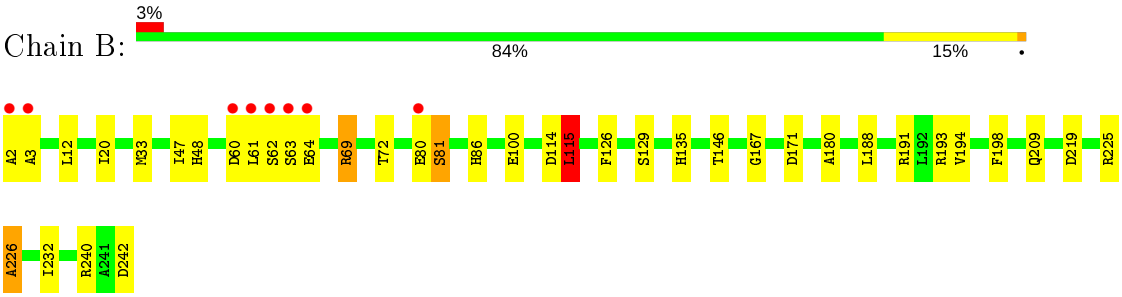
- Molecule 1: T cell receptor alpha chain

Chain A:



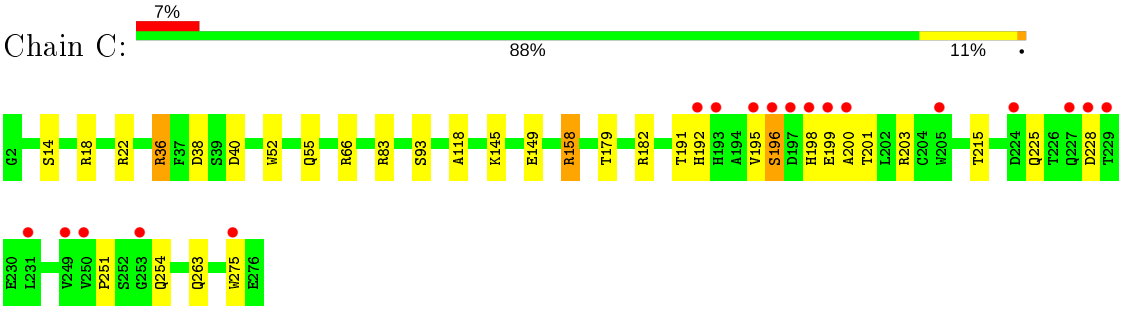
- Molecule 2: T cell receptor beta chain

Chain B:



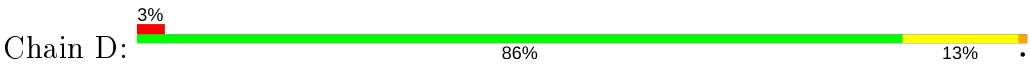
- Molecule 3: HLA class I histocompatibility antigen, A-2 alpha chain

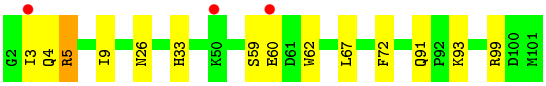
Chain C:



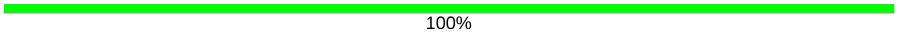
- Molecule 4: Beta-2-microglobulin

Chain D:





- Molecule 5: NS3 peptide

Chain I: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	79.99Å 53.65Å 224.98Å 90.00° 95.27° 90.00°	Depositor
Resolution (Å)	20.00 – 2.03 77.32 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.03) 99.2 (77.32-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.25 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.193 , 0.223 0.197 , 0.229	Depositor DCC
R_{free} test set	3065 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7158	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.54	1/1553 (0.1%)	0.74	4/2100 (0.2%)
2	B	0.52	0/1989	0.61	2/2709 (0.1%)
3	C	0.49	0/2297	0.63	2/3119 (0.1%)
4	D	0.61	0/838	0.65	1/1134 (0.1%)
5	I	0.46	0/68	0.82	0/91
All	All	0.53	1/6745 (0.0%)	0.66	9/9153 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	CYS	CB-SG	-5.53	1.72	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	LEU	CB-CG-CD1	-8.07	97.28	111.00
3	C	158	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	64	ARG	NE-CZ-NH2	-6.80	116.90	120.30
4	D	5	ARG	NE-CZ-NH2	-6.70	116.95	120.30
2	B	61	LEU	CA-CB-CG	5.80	128.63	115.30
1	A	64	ARG	NE-CZ-NH1	5.37	122.99	120.30
2	B	69	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	A	99	ASP	CB-CG-OD1	5.16	122.94	118.30
3	C	158	ARG	NE-CZ-NH1	5.01	122.80	120.30

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	1523	0	1441	78	0
2	B	1934	0	1831	34	0
3	C	2232	0	2066	25	0
4	D	815	0	763	15	0
5	I	69	0	85	0	0
6	A	111	0	0	10	3
6	B	175	0	0	5	0
6	C	198	0	0	8	3
6	D	93	0	0	2	0
6	I	8	0	0	0	0
All	All	7158	0	6186	141	3

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 11.

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)
1:A:188:ASN:HB2	1:A:192:ASN:ND2	1.25	1.44
1:A:188:ASN:CB	1:A:192:ASN:HD21	1.32	1.43
1:A:188:ASN:CB	1:A:192:ASN:ND2	1.83	1.35
1:A:154:ASP:O	1:A:179:SER:OG	1.56	1.19
1:A:188:ASN:CA	1:A:192:ASN:ND2	2.08	1.16
1:A:188:ASN:O	1:A:190:PHE:N	1.83	1.11
1:A:165:MET:SD	6:B:454:HOH:O	2.16	1.03
1:A:181:LYS:HG2	1:A:182:SER:H	1.24	0.97
1:A:188:ASN:HA	1:A:192:ASN:ND2	1.83	0.91
1:A:188:ASN:CA	1:A:192:ASN:HD21	1.73	0.90
2:B:33:MET:SD	2:B:69:ARG:NH1	2.48	0.87
1:A:131:SER:OG	1:A:132:ASP:N	2.08	0.87
1:A:188:ASN:HB2	1:A:192:ASN:HD21	0.77	0.84
1:A:188:ASN:CB	1:A:192:ASN:HD22	1.85	0.83
1:A:56:LYS:NZ	6:A:204:HOH:O	2.11	0.82
1:A:179:SER:OG	1:A:181:LYS:NZ	2.12	0.81
1:A:190:PHE:N	6:A:201:HOH:O	2.08	0.80
1:A:181:LYS:HG2	1:A:182:SER:N	1.97	0.78
2:B:60:ASP:O	6:B:301:HOH:O	2.02	0.78
3:C:22:ARG:NH1	3:C:38:ASP:OD1	2.18	0.77
3:C:195:VAL:O	3:C:196:SER:OG	2.02	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:SER:OG	6:A:202:HOH:O	2.03	0.76
1:A:155:VAL:HA	1:A:179:SER:HB2	1.69	0.74
2:B:69:ARG:NH1	2:B:72:THR:O	2.20	0.74
3:C:83:ARG:NH2	6:C:303:HOH:O	2.17	0.74
1:A:188:ASN:ND2	1:A:189:ALA:H	1.87	0.72
2:B:240:ARG:NH1	2:B:242:ASP:OD2	2.23	0.72
4:D:3:ILE:HG13	4:D:4:GLN:H	1.53	0.71
2:B:225:ARG:O	2:B:226:ALA:HB3	1.91	0.71
4:D:3:ILE:HG13	4:D:4:GLN:N	2.07	0.70
1:A:153:SER:O	6:A:203:HOH:O	2.10	0.69
1:A:154:ASP:HB3	1:A:181:LYS:HD2	1.74	0.69
1:A:178:TRP:O	1:A:179:SER:HB2	1.92	0.68
1:A:190:PHE:O	1:A:192:ASN:N	2.27	0.67
4:D:60:GLU:OE1	4:D:60:GLU:N	2.28	0.67
3:C:203:ARG:HD2	6:D:207:HOH:O	1.94	0.67
2:B:47:ILE:HG22	2:B:48:HIS:CD2	2.30	0.66
1:A:184:PHE:HE2	1:A:186:CYS:SG	2.17	0.66
3:C:18:ARG:NE	6:C:307:HOH:O	2.28	0.66
1:A:180:ASN:N	1:A:181:LYS:HE2	2.11	0.66
1:A:152:ASP:O	1:A:154:ASP:N	2.26	0.65
3:C:22:ARG:NH1	3:C:40:ASP:HB2	2.12	0.65
4:D:3:ILE:HD12	4:D:5:ARG:NH1	2.12	0.64
1:A:64:ARG:NH2	1:A:87:ASP:OD2	2.25	0.64
3:C:158:ARG:NH2	6:C:305:HOH:O	2.22	0.64
1:A:129:LYS:O	1:A:130:SER:OG	2.15	0.63
1:A:127:ASP:OD2	1:A:131:SER:HB3	1.97	0.63
1:A:180:ASN:C	1:A:181:LYS:HD3	2.19	0.63
2:B:62:SER:O	2:B:64:GLU:HA	1.99	0.62
1:A:100:LYS:HE3	6:A:207:HOH:O	2.00	0.62
1:A:179:SER:C	1:A:181:LYS:HE2	2.21	0.61
3:C:195:VAL:O	3:C:195:VAL:HG12	2.01	0.61
1:A:177:ALA:HB2	1:A:190:PHE:CZ	2.36	0.60
2:B:194:VAL:HG13	2:B:198:PHE:HB3	1.83	0.60
4:D:3:ILE:O	4:D:4:GLN:HB2	2.00	0.60
2:B:180:ALA:N	6:B:302:HOH:O	2.09	0.60
1:A:51:ARG:HD3	2:B:100:GLU:OE1	2.03	0.59
1:A:190:PHE:CA	6:A:201:HOH:O	2.49	0.59
1:A:191:ASN:O	1:A:192:ASN:HB3	2.02	0.59
4:D:3:ILE:CD1	4:D:5:ARG:NH1	2.67	0.58
2:B:47:ILE:HG23	2:B:62:SER:HB2	1.86	0.58
1:A:163:LEU:HD11	2:B:167:GLY:C	2.25	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:SER:O	2:B:86:HIS:NE2	2.37	0.58
4:D:59:SER:HB3	4:D:60:GLU:OE1	2.03	0.58
3:C:198:HIS:ND1	3:C:199:GLU:HG3	2.19	0.57
1:A:143:SER:O	1:A:160:LYS:NZ	2.37	0.57
1:A:152:ASP:N	1:A:152:ASP:OD1	2.37	0.57
1:A:174:SER:OG	2:B:191:ARG:HD2	2.05	0.55
1:A:165:MET:CE	2:B:193:ARG:HD3	2.37	0.55
2:B:225:ARG:O	2:B:226:ALA:CB	2.55	0.55
4:D:3:ILE:CG1	4:D:4:GLN:H	2.19	0.55
1:A:181:LYS:CG	1:A:182:SER:H	2.10	0.55
2:B:2:ALA:O	2:B:3:ALA:HB3	2.05	0.55
4:D:3:ILE:HD12	4:D:5:ARG:CZ	2.37	0.55
3:C:66:ARG:HD2	6:C:364:HOH:O	2.06	0.54
3:C:228:ASP:OD1	6:C:304:HOH:O	2.19	0.54
1:A:188:ASN:C	1:A:192:ASN:HD21	2.12	0.54
1:A:183:ASP:O	1:A:184:PHE:HB2	2.06	0.53
4:D:91:GLN:NE2	6:D:205:HOH:O	2.32	0.53
3:C:251:PRO:O	3:C:254:GLN:HB2	2.09	0.52
2:B:219:ASP:OD1	6:B:303:HOH:O	2.18	0.52
2:B:80:GLU:O	2:B:81:SER:HB3	2.09	0.52
1:A:163:LEU:HD11	2:B:167:GLY:O	2.09	0.52
1:A:151:LYS:O	1:A:153:SER:N	2.43	0.51
3:C:179:THR:O	3:C:182:ARG:NH1	2.42	0.51
1:A:133:LYS:HA	1:A:180:ASN:ND2	2.26	0.51
2:B:114:ASP:O	2:B:115:LEU:HB2	2.10	0.51
1:A:165:MET:HE1	2:B:193:ARG:HD3	1.92	0.50
4:D:3:ILE:CG1	4:D:4:GLN:N	2.73	0.50
3:C:192:HIS:CD2	3:C:200:ALA:HB1	2.45	0.50
3:C:192:HIS:HB3	3:C:275:TRP:CZ2	2.47	0.50
1:A:191:ASN:N	6:A:201:HOH:O	2.45	0.50
1:A:134:SER:HA	2:B:126:PHE:CE2	2.46	0.50
3:C:36:ARG:NH2	6:C:310:HOH:O	2.45	0.50
1:A:150:SER:OG	1:A:151:LYS:N	2.44	0.50
3:C:118:ALA:HB2	4:D:62:TRP:CE2	2.47	0.49
4:D:9:ILE:HD12	4:D:93:LYS:HD2	1.93	0.49
1:A:119:ASP:OD2	2:B:135:HIS:NE2	2.45	0.49
1:A:163:LEU:HB2	6:A:216:HOH:O	2.13	0.49
1:A:190:PHE:HB2	6:A:201:HOH:O	2.13	0.49
1:A:188:ASN:C	1:A:190:PHE:N	2.63	0.48
2:B:12:LEU:HD21	2:B:20:ILE:HG12	1.94	0.48
1:A:188:ASN:CG	1:A:189:ALA:H	2.11	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:182:ARG:NH1	6:C:312:HOH:O	2.47	0.47
3:C:215:THR:HG23	3:C:263:GLN:HB2	1.95	0.47
1:A:129:LYS:HE2	6:A:294:HOH:O	2.14	0.47
3:C:52:TRP:O	3:C:55:GLN:HG2	2.14	0.47
1:A:180:ASN:O	1:A:181:LYS:HB3	2.14	0.47
1:A:184:PHE:CE2	1:A:186:CYS:SG	3.04	0.47
4:D:26:ASN:HB3	4:D:67:LEU:HD11	1.97	0.47
2:B:225:ARG:O	6:B:304:HOH:O	2.20	0.47
1:A:184:PHE:CE1	1:A:189:ALA:HB2	2.50	0.46
2:B:171:ASP:OD1	2:B:191:ARG:NH2	2.47	0.46
4:D:4:GLN:HA	4:D:33:HIS:O	2.15	0.46
2:B:63:SER:O	2:B:86:HIS:CE1	2.69	0.46
1:A:2:ALA:N	1:A:27:ASP:OD2	2.48	0.45
1:A:188:ASN:C	1:A:192:ASN:ND2	2.65	0.45
2:B:209:GLN:HG3	2:B:232:ILE:HG23	1.99	0.45
1:A:181:LYS:N	1:A:181:LYS:CE	2.80	0.45
1:A:180:ASN:C	1:A:181:LYS:CD	2.86	0.44
1:A:134:SER:HA	2:B:126:PHE:HE2	1.82	0.44
3:C:191:THR:HG22	6:C:388:HOH:O	2.17	0.44
3:C:215:THR:CG2	3:C:263:GLN:HB2	2.47	0.44
1:A:177:ALA:CB	1:A:190:PHE:CZ	3.00	0.44
1:A:180:ASN:O	1:A:181:LYS:HD3	2.18	0.44
1:A:155:VAL:HA	1:A:179:SER:CB	2.46	0.43
1:A:136:CYS:SG	1:A:184:PHE:CZ	3.12	0.43
2:B:171:ASP:HB2	2:B:188:LEU:HD12	2.01	0.43
3:C:192:HIS:HA	3:C:201:THR:O	2.19	0.43
1:A:154:ASP:O	1:A:179:SER:CB	2.60	0.43
1:A:113:PRO:HG3	1:A:162:VAL:HG22	2.00	0.43
1:A:180:ASN:CA	1:A:181:LYS:HE2	2.49	0.42
2:B:115:LEU:HD12	2:B:115:LEU:HA	1.79	0.42
3:C:14:SER:O	3:C:93:SER:OG	2.26	0.41
1:A:136:CYS:SG	1:A:184:PHE:HZ	2.44	0.41
1:A:156:TYR:O	1:A:177:ALA:HA	2.20	0.41
1:A:135:VAL:HG22	1:A:178:TRP:HB3	2.03	0.41
2:B:63:SER:HA	2:B:64:GLU:HG3	2.03	0.41
3:C:145:LYS:HE2	3:C:149:GLU:OE2	2.21	0.40
1:A:181:LYS:N	1:A:181:LYS:HE3	2.36	0.40
1:A:165:MET:HE2	2:B:193:ARG:HD3	2.03	0.40

All (3) 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)
6:A:311:HOH:O	6:C:488:HOH:O[3_445]	1.93	0.27
6:A:294:HOH:O	6:C:478:HOH:O[3_445]	2.04	0.16
6:A:306:HOH:O	6:C:478:HOH:O[3_445]	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	190/192 (99%)	164 (86%)	13 (7%)	13 (7%)	1 0
2	B	239/241 (99%)	224 (94%)	12 (5%)	3 (1%)	12 5
3	C	273/275 (99%)	267 (98%)	5 (2%)	1 (0%)	34 28
4	D	98/100 (98%)	94 (96%)	3 (3%)	1 (1%)	15 9
5	I	8/10 (80%)	8 (100%)	0	0	100 100
All	All	808/818 (99%)	757 (94%)	33 (4%)	18 (2%)	6 2

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	SER
1	A	133	LYS
1	A	150	SER
1	A	152	ASP
1	A	181	LYS
1	A	189	ALA
1	A	191	ASN
1	A	192	ASN
2	B	115	LEU
3	C	196	SER
1	A	131	SER
1	A	179	SER
1	A	153	SER
1	A	184	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	132	ASP
2	B	226	ALA
2	B	81	SER
4	D	99	ARG

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	173/173 (100%)	166 (96%)	7 (4%)	31 28
2	B	212/212 (100%)	209 (99%)	3 (1%)	67 70
3	C	228/231 (99%)	226 (99%)	2 (1%)	78 82
4	D	90/94 (96%)	89 (99%)	1 (1%)	73 77
5	I	7/7 (100%)	7 (100%)	0	100 100
All	All	710/717 (99%)	697 (98%)	13 (2%)	59 61

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	150	SER
1	A	152	ASP
1	A	161	CYS
1	A	180	ASN
1	A	181	LYS
1	A	182	SER
2	B	115	LEU
2	B	129	SER
2	B	146	THR
3	C	36	ARG
3	C	225	GLN
4	D	72	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	192	ASN
3	C	192	HIS

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	192/192 (100%)	0.64	27 (14%) 2 2	13, 27, 70, 88	0
2	B	241/241 (100%)	-0.02	8 (3%) 46 46	10, 22, 42, 62	0
3	C	275/275 (100%)	0.01	18 (6%) 18 18	10, 21, 60, 81	0
4	D	100/100 (100%)	-0.17	3 (3%) 50 50	14, 22, 35, 57	0
5	I	10/10 (100%)	-0.51	0 100 100	10, 12, 15, 16	0
All	All	818/818 (100%)	0.12	56 (6%) 17 16	10, 22, 57, 88	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	SER	17.3
1	A	130	SER	9.6
1	A	181	LYS	9.3
1	A	183	ASP	8.7
1	A	192	ASN	8.5
2	B	63	SER	8.2
1	A	131	SER	7.5
3	C	253	GLY	6.9
4	D	3	ILE	6.0
1	A	191	ASN	5.5
2	B	2	ALA	5.5
1	A	152	ASP	5.0
2	B	61	LEU	4.8
2	B	3	ALA	4.7
1	A	116	GLN	4.6
1	A	132	ASP	4.6
1	A	148	SER	4.6
3	C	196	SER	4.5
1	A	190	PHE	4.2
1	A	180	ASN	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	134	SER	4.2
1	A	146	ASN	4.1
1	A	184	PHE	3.9
1	A	133	LYS	3.9
1	A	188	ASN	3.8
3	C	200	ALA	3.6
3	C	227	GLN	3.6
3	C	198	HIS	3.3
1	A	151	LYS	3.3
1	A	117	ASN	3.3
3	C	250	VAL	3.3
3	C	275	TRP	3.2
1	A	149	GLN	3.0
2	B	80	GLU	2.9
3	C	192	HIS	2.9
1	A	178	TRP	2.9
2	B	62	SER	2.8
2	B	64	GLU	2.7
3	C	193	HIS	2.7
3	C	224	ASP	2.7
2	B	60	ASP	2.6
3	C	195	VAL	2.5
1	A	189	ALA	2.5
3	C	199	GLU	2.5
3	C	228	ASP	2.4
1	A	193	SER	2.4
3	C	231	LEU	2.4
3	C	249	VAL	2.3
1	A	153	SER	2.2
3	C	205	TRP	2.2
3	C	197	ASP	2.2
4	D	50	LYS	2.2
1	A	147	VAL	2.1
4	D	60	GLU	2.1
1	A	187	ALA	2.0
3	C	229	THR	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

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.