Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 03:54 PM EDT

PDB ID	:	6MNN
Title	:	6236 TCR bound to I-Ab Padi4
Authors	:	Blevins, S.J.; Stadinski, B.D.; Huseby, E.S.
Deposited on	:	2018-10-02
Resolution	:	2.83 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 (i) 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 (1)) were used in the production of this report:

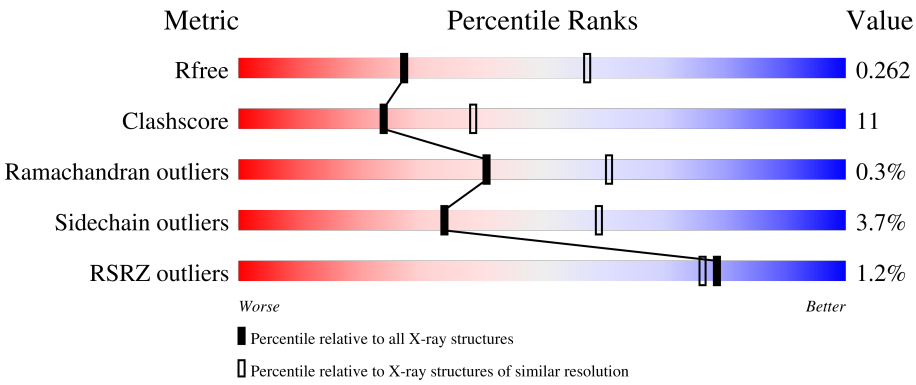
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.83 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 <=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	C	179	3%, 76%, 20%, • •
2	D	217	67%, 21%, •, 11%
3	A	208	73%, 20%, •, 6%
4	B	239	%, 72%, 27%, •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6102 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 H-2 class II histocompatibility antigen, A-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	174	1304	847	208	246	3	0	0	0

- Molecule 2 is a protein called Padi4 (92-105) peptide and MHC Class II I-Ab beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	194	1538	973	268	290	7	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	GLY	-	linker	UNP Q9Z183
D	-11	GLY	-	linker	UNP Q9Z183
D	-10	GLY	-	linker	UNP Q9Z183
D	-9	GLY	-	linker	UNP Q9Z183
D	-8	SER	-	linker	UNP Q9Z183
D	-7	LEU	-	linker	UNP Q9Z183
D	-6	VAL	-	linker	UNP Q9Z183
D	-5	PRO	-	linker	UNP Q9Z183
D	-4	ARG	-	linker	UNP Q9Z183
D	-3	GLY	-	linker	UNP Q9Z183
D	-2	SER	-	linker	UNP Q9Z183
D	-1	GLY	-	linker	UNP Q9Z183
D	0	GLY	-	linker	UNP Q9Z183
D	1	GLY	-	linker	UNP Q9Z183
D	2	GLY	-	linker	UNP Q9Z183

- Molecule 3 is a protein called 6236 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	196	1454	929	237	282	6	0	0	0

- Molecule 4 is a protein called 6236 TCR beta chain.

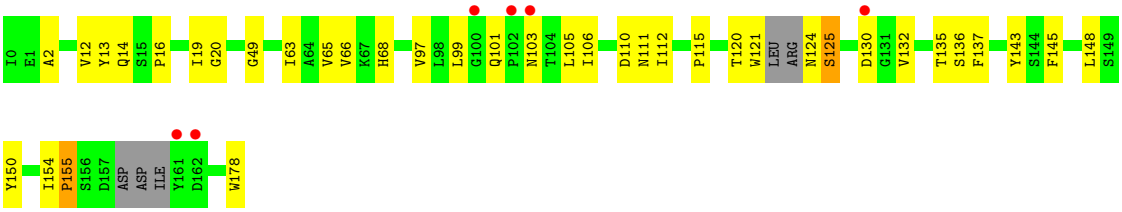
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	239	1806	1144	319	337	6	0	0	0

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.

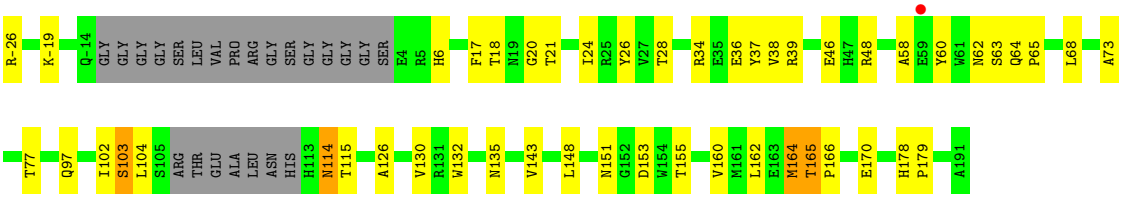
- Molecule 1: H-2 class II histocompatibility antigen, A-B alpha chain

Chain C:



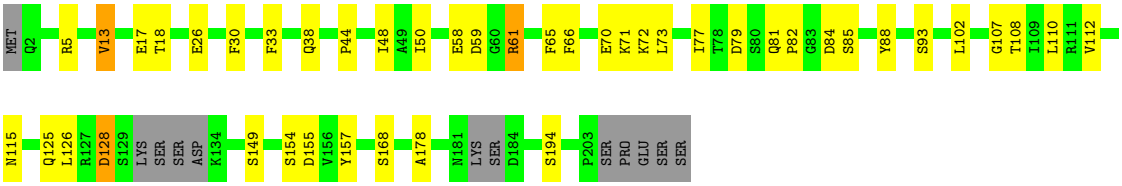
- Molecule 2: Padi4 (92-105) peptide and MHC Class II I-Ab beta chain

Chain D:



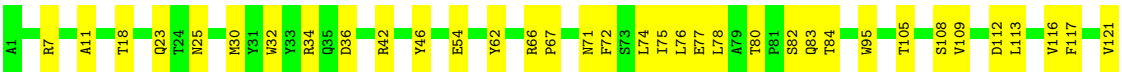
- Molecule 3: 6236 TCR alpha chain

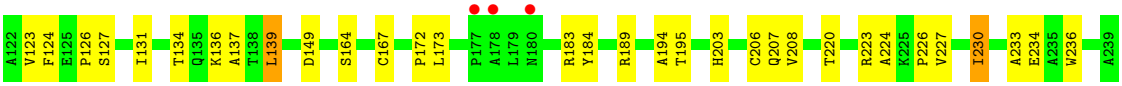
Chain A:



- Molecule 4: 6236 TCR beta chain

Chain B:




A122
V123
F124
E125
P126
S127
I131
T134
Q135
K136
A137
T138
L139
D149
S164
C167
P172
L173
P177
A178
L179
N180
R183
Y184
R189
A194
T195
H203
C206
Q207
V208
T220
R223
A224
K225
P226
V227
I230
A233
E234
A235
W236
A239

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	250.41Å 68.87Å 64.47Å 90.00° 91.97° 90.00°	Depositor
Resolution (Å)	29.62 – 2.83 29.62 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.62-2.83) 99.5 (29.62-2.83)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.219 , 0.262 0.219 , 0.262	Depositor DCC
R_{free} test set	1985 reflections (7.55%)	wwPDB-VP
Wilson B-factor (Å^2)	62.5	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 37.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6102	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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 (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	C	0.59	0/1345	0.64	1/1846 (0.1%)
2	D	0.68	1/1578 (0.1%)	0.61	0/2154
3	A	0.65	0/1491	0.63	0/2038
4	B	0.57	1/1859 (0.1%)	0.60	1/2546 (0.0%)
All	All	0.62	2/6273 (0.0%)	0.62	2/8584 (0.0%)

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
3	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	166	PRO	N-CD	9.08	1.60	1.47
4	B	206	CYS	CB-SG	-5.35	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	139	LEU	CA-CB-CG	5.22	127.31	115.30
1	C	130	ASP	CB-CG-OD2	5.16	122.94	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	61	ARG	Sidechain

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	C	1304	0	1152	31	0
2	D	1538	0	1412	37	0
3	A	1454	0	1286	25	0
4	B	1806	0	1652	45	0
All	All	6102	0	5502	129	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 11.

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)
3:A:154:SER:O	3:A:155:ASP:CB	2.37	0.72
3:A:93:SER:HB3	3:A:102:LEU:HD12	1.73	0.70
2:D:60:TYR:OH	2:D:64:GLN:OE1	2.08	0.69
1:C:14:GLN:HE21	1:C:19:ILE:HD12	1.59	0.68
3:A:61:ARG:NH2	3:A:84:ASP:OD2	2.29	0.65
3:A:82:PRO:HA	3:A:112:VAL:HB	1.76	0.65
4:B:80:THR:HG22	4:B:82:SER:H	1.62	0.63
1:C:124:ASN:O	1:C:125:SER:HB2	1.97	0.63
2:D:37:TYR:CD2	2:D:38:VAL:HG23	2.34	0.63
2:D:58:ALA:O	2:D:62:ASN:ND2	2.32	0.62
1:C:2:ALA:HA	2:D:18:THR:HG22	1.82	0.62
1:C:135:THR:CG2	1:C:148:LEU:H	2.12	0.62
2:D:135:ASN:HD21	2:D:170:GLU:HG2	1.63	0.62
3:A:128:ASP:OD2	3:A:128:ASP:N	2.30	0.61
3:A:149:SER:H	3:A:194:SER:HB3	1.63	0.61
1:C:13:TYR:HB2	1:C:66:VAL:HG12	1.83	0.61
4:B:76:LEU:HD23	4:B:83:GLN:OE1	2.01	0.60
4:B:80:THR:HB	4:B:83:GLN:HG3	1.81	0.60
4:B:134:THR:HG22	4:B:134:THR:O	2.00	0.60
2:D:143:VAL:CG2	2:D:162:LEU:HD13	2.32	0.60
4:B:84:THR:HG23	4:B:108:SER:HA	1.84	0.60
4:B:126:PRO:HD3	4:B:139:LEU:HD13	1.83	0.60
1:C:120:THR:HG23	1:C:121:TRP:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:THR:HG22	1:C:148:LEU:H	1.65	0.59
4:B:32:TRP:CG	4:B:74:LEU:HD22	2.38	0.59
2:D:102:ILE:HG22	2:D:103:SER:N	2.18	0.59
4:B:208:VAL:HG13	4:B:208:VAL:O	2.03	0.58
1:C:106:ILE:HG12	1:C:150:TYR:CD1	2.39	0.57
1:C:49:GLY:O	2:D:-26:ARG:NH1	2.31	0.57
1:C:14:GLN:HE21	1:C:19:ILE:CD1	2.17	0.56
4:B:112:ASP:OD1	4:B:113:LEU:N	2.38	0.56
4:B:203:HIS:HB3	4:B:236:TRP:CE3	2.40	0.56
3:A:13:VAL:HG13	3:A:17:GLU:HB2	1.86	0.56
2:D:37:TYR:CE2	2:D:38:VAL:HG23	2.41	0.56
4:B:149:ASP:HB2	4:B:172:PRO:HG2	1.88	0.56
3:A:79:ASP:O	3:A:81:GLN:NE2	2.39	0.56
4:B:32:TRP:CD2	4:B:74:LEU:HD22	2.41	0.56
1:C:97:VAL:HA	1:C:103:ASN:ND2	2.20	0.55
3:A:168:SER:HA	4:B:164:SER:HA	1.88	0.55
1:C:101:GLN:O	1:C:155:PRO:CD	2.55	0.55
1:C:132:VAL:HA	1:C:150:TYR:O	2.07	0.55
4:B:123:VAL:HG23	4:B:233:ALA:HB3	1.89	0.54
2:D:143:VAL:HG22	2:D:162:LEU:HD13	1.89	0.54
4:B:46:TYR:CE2	4:B:54:GLU:HB2	2.43	0.54
1:C:115:PRO:HG3	1:C:145:PHE:CD2	2.43	0.53
3:A:66:PHE:HD1	3:A:73:LEU:HD13	1.73	0.53
1:C:110:ASP:OD2	1:C:111:ASN:N	2.33	0.52
2:D:104:LEU:HD12	2:D:164:MET:HE1	1.90	0.52
2:D:104:LEU:CD1	2:D:164:MET:HE1	2.40	0.52
4:B:67:PRO:HG2	4:B:71:ASN:HD22	1.75	0.52
3:A:61:ARG:NH2	3:A:81:GLN:H	2.07	0.51
1:C:16:PRO:HD2	2:D:6:HIS:ND1	2.26	0.51
1:C:132:VAL:HG13	1:C:150:TYR:O	2.11	0.50
1:C:97:VAL:HA	1:C:103:ASN:HD22	1.75	0.50
2:D:102:ILE:CG2	2:D:103:SER:N	2.74	0.50
2:D:62:ASN:HA	2:D:68:LEU:HD13	1.94	0.50
4:B:116:VAL:O	4:B:226:PRO:HG3	2.11	0.50
2:D:26:TYR:CZ	2:D:28:THR:CG2	2.94	0.50
4:B:203:HIS:HB3	4:B:236:TRP:CZ3	2.46	0.50
3:A:26:GLU:O	3:A:71:LYS:NZ	2.44	0.49
3:A:125:GLN:O	4:B:127:SER:HB3	2.12	0.49
2:D:132:TRP:CD1	2:D:162:LEU:HB2	2.47	0.49
4:B:34:ARG:NH2	4:B:82:SER:O	2.46	0.48
4:B:77:GLU:O	4:B:78:LEU:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:VAL:O	1:C:20:GLY:HA2	2.13	0.48
1:C:115:PRO:HG3	1:C:145:PHE:CE2	2.49	0.48
2:D:60:TYR:CZ	2:D:64:GLN:OE1	2.67	0.47
4:B:34:ARG:NH1	4:B:36:ASP:OD1	2.46	0.47
2:D:165:THR:O	2:D:165:THR:HG22	2.13	0.47
4:B:131:ILE:HG23	4:B:194:ALA:HB1	1.96	0.47
2:D:73:ALA:O	2:D:77:THR:HG23	2.14	0.47
2:D:178:HIS:CG	2:D:179:PRO:HD2	2.49	0.47
1:C:14:GLN:CG	1:C:19:ILE:HB	2.45	0.46
3:A:48:ILE:HD12	3:A:59:ASP:HB3	1.97	0.46
3:A:157:TYR:O	3:A:178:ALA:HA	2.15	0.46
4:B:134:THR:HG22	4:B:136:LYS:HG3	1.97	0.46
4:B:30:MET:SD	4:B:72:PHE:HB2	2.56	0.46
4:B:173:LEU:O	4:B:184:TYR:HA	2.16	0.46
1:C:135:THR:HG23	1:C:136:SER:O	2.15	0.46
3:A:70:GLU:O	3:A:72:LYS:HG3	2.16	0.46
4:B:134:THR:O	4:B:134:THR:CG2	2.63	0.46
2:D:46:GLU:HG3	2:D:62:ASN:OD1	2.15	0.46
4:B:18:THR:HG23	4:B:75:ILE:HG13	1.97	0.46
1:C:154:ILE:O	1:C:155:PRO:C	2.55	0.46
1:C:143:TYR:HB2	2:D:34:ARG:HG3	1.99	0.45
2:D:151:ASN:HB2	2:D:155:THR:O	2.16	0.45
1:C:99:LEU:HA	1:C:155:PRO:HB2	1.97	0.45
2:D:21:THR:HG22	2:D:24:ILE:HD11	1.99	0.45
3:A:128:ASP:HA	4:B:124:PHE:CD2	2.51	0.45
2:D:36:GLU:CD	2:D:39:ARG:HH21	2.20	0.45
1:C:65:VAL:O	1:C:68:HIS:HB3	2.17	0.44
3:A:5:ARG:HH21	3:A:26:GLU:HG3	1.82	0.44
4:B:126:PRO:HG2	4:B:137:ALA:HB1	2.00	0.44
4:B:113:LEU:O	4:B:116:VAL:HG22	2.17	0.44
2:D:153:ASP:OD2	2:D:155:THR:OG1	2.36	0.44
4:B:116:VAL:HG23	4:B:226:PRO:HG3	1.99	0.44
4:B:207:GLN:CD	4:B:230:ILE:HD13	2.38	0.44
1:C:105:LEU:HA	1:C:105:LEU:HD12	1.72	0.44
3:A:30:PHE:HB3	3:A:33:PHE:CZ	2.53	0.44
2:D:-19:LYS:HB3	4:B:95:TRP:CE2	2.54	0.43
1:C:63:ILE:HD12	1:C:63:ILE:HG23	1.84	0.43
2:D:63:SER:O	2:D:65:PRO:HD3	2.18	0.43
4:B:7:ARG:C	4:B:105:THR:HG23	2.39	0.43
4:B:32:TRP:CD1	4:B:74:LEU:HB2	2.54	0.42
3:A:50:ILE:HD13	3:A:66:PHE:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:GLN:O	1:C:155:PRO:HD2	2.19	0.42
3:A:88:TYR:O	3:A:107:GLY:HA2	2.18	0.42
2:D:104:LEU:HD21	2:D:114:ASN:CG	2.40	0.42
4:B:220:THR:O	4:B:220:THR:OG1	2.34	0.42
2:D:130:VAL:HG11	2:D:160:VAL:HG21	2.01	0.41
2:D:46:GLU:CD	2:D:48:ARG:HH21	2.22	0.41
4:B:223:ARG:HG2	4:B:224:ALA:N	2.35	0.41
2:D:17:PHE:HB3	2:D:20:GLY:O	2.19	0.41
4:B:121:VAL:HG21	4:B:208:VAL:HG11	2.02	0.41
2:D:-19:LYS:HD2	4:B:95:TRP:CD2	2.55	0.41
4:B:11:ALA:O	4:B:109:VAL:HA	2.20	0.41
2:D:38:VAL:HG12	2:D:39:ARG:N	2.36	0.41
1:C:112:ILE:HG21	1:C:137:PHE:HE1	1.85	0.41
4:B:134:THR:CG2	4:B:136:LYS:HB2	2.51	0.41
4:B:223:ARG:HD2	4:B:224:ALA:O	2.21	0.41
2:D:126:ALA:HB1	2:D:148:LEU:HD21	2.02	0.41
2:D:143:VAL:HG22	2:D:162:LEU:CD1	2.50	0.41
3:A:38:GLN:HG3	3:A:44:PRO:N	2.36	0.41
3:A:65:PHE:O	3:A:73:LEU:HD12	2.21	0.41
4:B:117:PHE:CD1	4:B:183:ARG:HD3	2.56	0.41
1:C:120:THR:C	1:C:121:TRP:CD1	2.94	0.40
3:A:18:THR:HA	3:A:77:ILE:O	2.21	0.40
3:A:85:SER:HA	3:A:110:LEU:O	2.21	0.40
4:B:195:THR:H	4:B:195:THR:HG23	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	168/179 (94%)	156 (93%)	11 (6%)	1 (1%)	25 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	188/217 (87%)	178 (95%)	10 (5%)	0	100	100
3	A	190/208 (91%)	175 (92%)	15 (8%)	0	100	100
4	B	237/239 (99%)	224 (94%)	12 (5%)	1 (0%)	34	56
All	All	783/843 (93%)	733 (94%)	48 (6%)	2 (0%)	41	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	155	PRO
4	B	227	VAL

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	C	129/160 (81%)	127 (98%)	2 (2%)	62	81
2	D	161/192 (84%)	155 (96%)	6 (4%)	34	59
3	A	145/185 (78%)	139 (96%)	6 (4%)	30	56
4	B	181/204 (89%)	172 (95%)	9 (5%)	24	46
All	All	616/741 (83%)	593 (96%)	23 (4%)	34	59

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	125	SER
1	C	178	TRP
2	D	97	GLN
2	D	103	SER
2	D	114	ASN
2	D	115	THR
2	D	164	MET
2	D	165	THR
3	A	13	VAL

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Mol	Chain	Res	Type
3	A	58	GLU
3	A	108	THR
3	A	115	ASN
3	A	126	LEU
3	A	128	ASP
4	B	23	GLN
4	B	25	ASN
4	B	42	ARG
4	B	62	TYR
4	B	66	ARG
4	B	167	CYS
4	B	189	ARG
4	B	230	ILE
4	B	234	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	14	GLN
4	B	71	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	C	174/179 (97%)	-0.03	6 (3%) 45 37	26, 51, 72, 89	0
2	D	194/217 (89%)	-0.18	1 (0%) 91 89	29, 45, 65, 84	0
3	A	196/208 (94%)	-0.29	0 100 100	27, 46, 65, 73	0
4	B	239/239 (100%)	-0.26	3 (1%) 77 74	29, 45, 76, 86	0
All	All	803/843 (95%)	-0.20	10 (1%) 79 76	26, 45, 69, 89	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	GLY	4.9
1	C	102	PRO	4.3
4	B	178	ALA	3.5
1	C	103	ASN	3.3
1	C	161	TYR	2.9
2	D	59	GLU	2.3
4	B	180	ASN	2.3
1	C	162	ASP	2.2
1	C	130	ASP	2.2
4	B	177	PRO	2.1

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 monosaccharides 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.