wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2021 – 07:24 AM EDT

PDB ID	:	3C60
Title	:	Crystal structure of mouse MHC class II I-Ab/3K peptide complexed with mouse TCR YAe62
Authors	:	Dai, S.
Deposited on	:	2008-02-01
Resolution	:	3.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

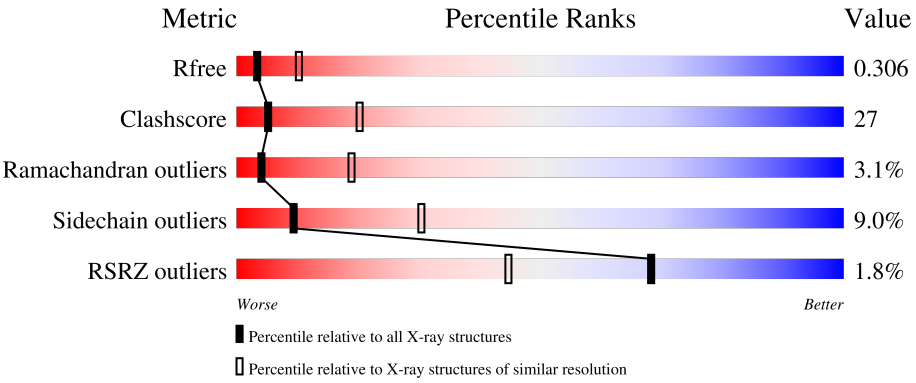
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	A	199	49% 45% 6%
1	E	199	6% 51% 42% 7%
2	B	236	2% 51% 41% 7%
2	F	236	3% 49% 43% 8%
3	C	182	% 62% 32% 5%

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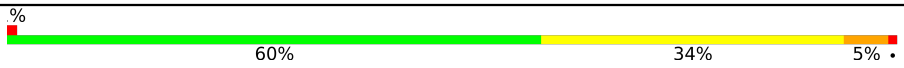
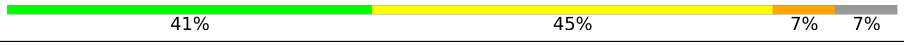
Mol	Chain	Length	Quality of chain
3	G	182	
4	D	217	
4	H	217	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13102 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 TCR YAe62 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1554	971	252	323	8			
1	E	199	Total	C	N	O	S	0	0	0
			1554	971	252	323	8			

- Molecule 2 is a protein called TCR YAe62 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	0
			1869	1177	325	361	6			
2	F	236	Total	C	N	O	S	0	0	0
			1869	1177	325	361	6			

- Molecule 3 is a protein called H-2 class II histocompatibility antigen, A-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	182	Total	C	N	O	S	0	0	0
			1459	944	230	282	3			
3	G	182	Total	C	N	O	S	0	0	0
			1459	944	230	282	3			

- Molecule 4 is a protein called 3K peptide, Linker, and H-2 class II histocompatibility antigen (A beta chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	201	Total	C	N	O	S	0	0	0
			1669	1045	303	314	7			
4	H	201	Total	C	N	O	S	0	0	0
			1669	1045	303	314	7			

There are 32 discrepancies between the modelled and reference sequences:

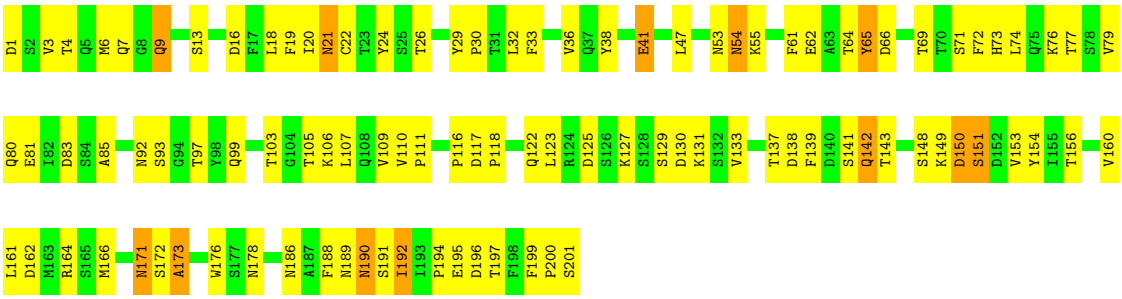
Chain	Residue	Modelled	Actual	Comment	Reference
D	14	GLY	-	linker	UNP P14483
D	15	GLY	-	linker	UNP P14483
D	16	GLY	-	linker	UNP P14483
D	17	GLY	-	linker	UNP P14483
D	18	SER	-	linker	UNP P14483
D	19	LEU	-	linker	UNP P14483
D	20	VAL	-	linker	UNP P14483
D	21	PRO	-	linker	UNP P14483
D	22	ARG	-	linker	UNP P14483
D	23	GLY	-	linker	UNP P14483
D	24	SER	-	linker	UNP P14483
D	25	GLY	-	linker	UNP P14483
D	26	GLY	-	linker	UNP P14483
D	27	GLY	-	linker	UNP P14483
D	28	GLY	-	linker	UNP P14483
D	216	LYS	ARG	engineered mutation	UNP P14483
H	14	GLY	-	linker	UNP P14483
H	15	GLY	-	linker	UNP P14483
H	16	GLY	-	linker	UNP P14483
H	17	GLY	-	linker	UNP P14483
H	18	SER	-	linker	UNP P14483
H	19	LEU	-	linker	UNP P14483
H	20	VAL	-	linker	UNP P14483
H	21	PRO	-	linker	UNP P14483
H	22	ARG	-	linker	UNP P14483
H	23	GLY	-	linker	UNP P14483
H	24	SER	-	linker	UNP P14483
H	25	GLY	-	linker	UNP P14483
H	26	GLY	-	linker	UNP P14483
H	27	GLY	-	linker	UNP P14483
H	28	GLY	-	linker	UNP P14483
H	216	LYS	ARG	engineered mutation	UNP P14483

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.

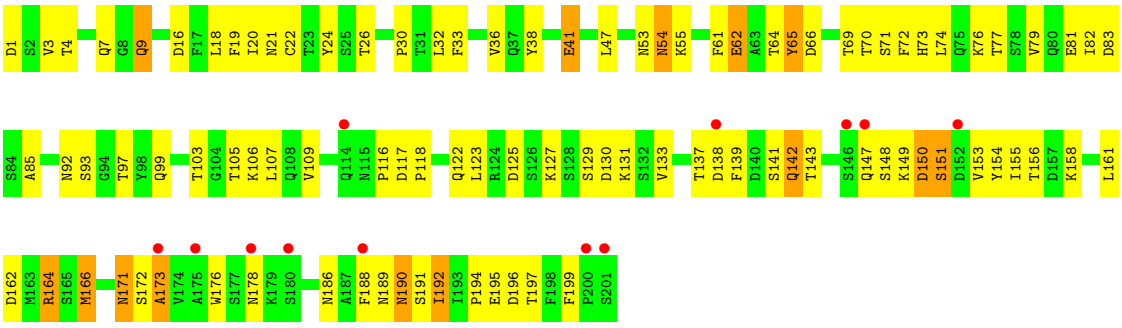
• Molecule 1: TCR YAe62 alpha chain

Chain A:



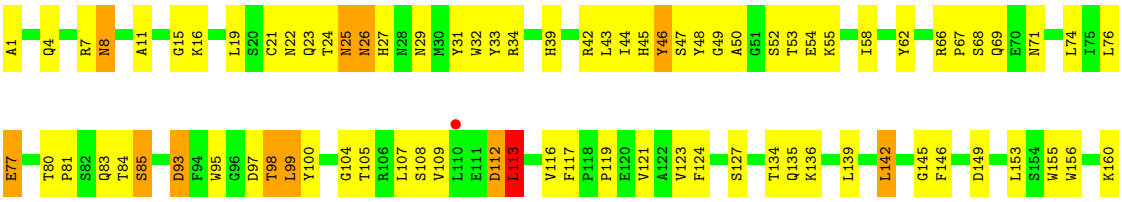
• Molecule 1: TCR YAe62 alpha chain

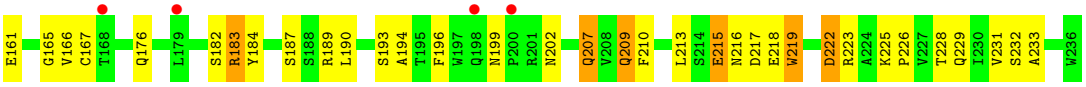
Chain E:



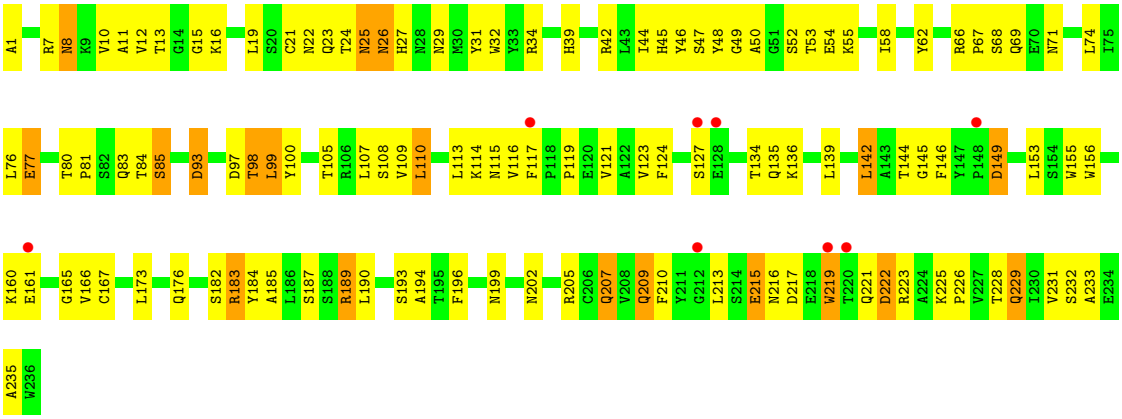
• Molecule 2: TCR YAe62 beta chain

Chain B:

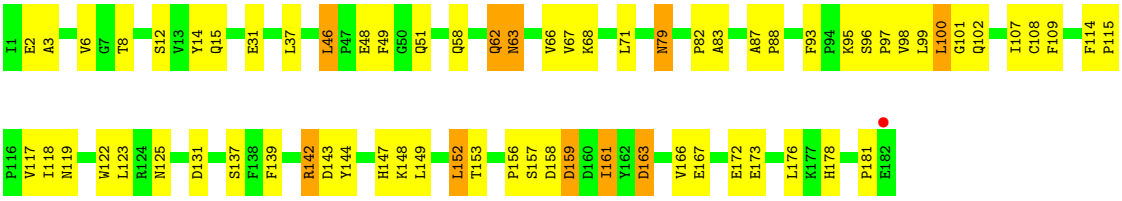




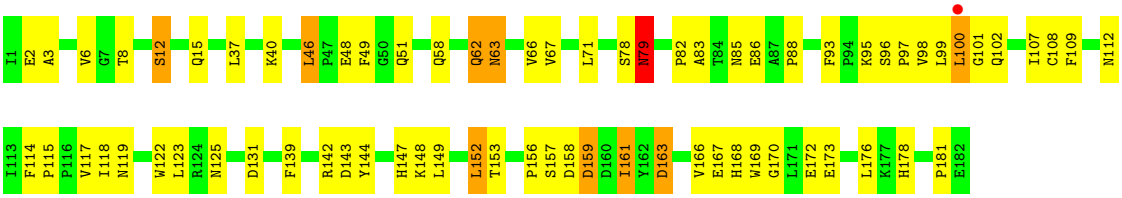
• Molecule 2: TCR YAe62 beta chain



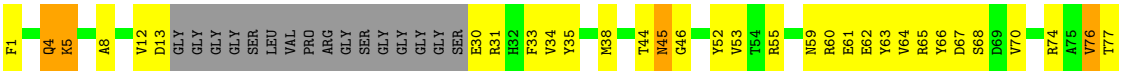
• Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain

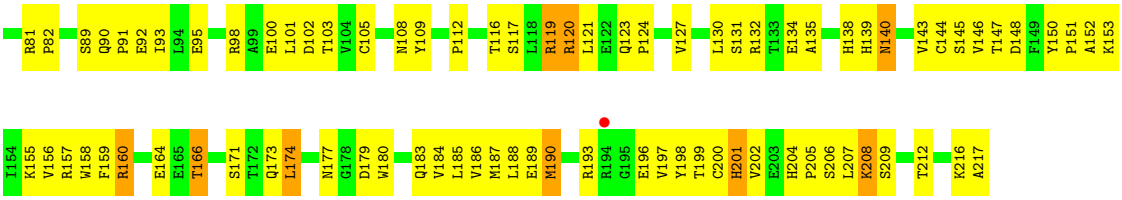


• Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain



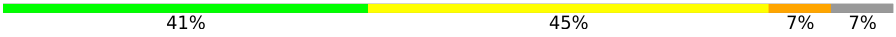
• Molecule 4: 3K peptide, Linker, and H-2 class II histocompatibility antigen (A beta chain)

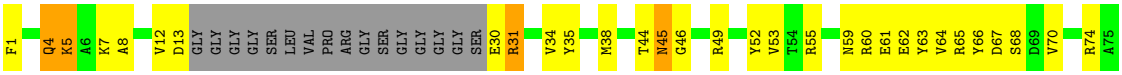


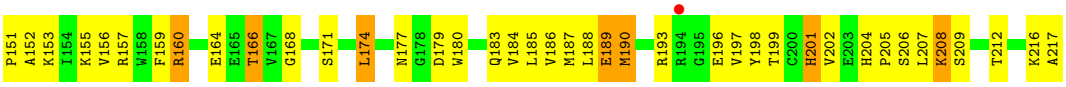


• Molecule 4: 3K peptide, Linker, and H-2 class II histocompatibility antigen (A beta chain)

Chain H:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.06Å 126.17Å 277.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.92 – 3.05 40.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.6 (40.92-3.05) 90.7 (40.91-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.267 , 0.309 0.266 , 0.306	Depositor DCC
R_{free} test set	2372 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	73.1	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13102	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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	0.45	0/1588	0.61	0/2157
1	E	0.47	0/1588	0.61	0/2157
2	B	0.42	0/1922	0.57	0/2620
2	F	0.43	0/1922	0.57	0/2620
3	C	0.56	0/1504	0.67	0/2054
3	G	0.55	0/1504	0.67	0/2054
4	D	0.50	0/1709	0.62	0/2316
4	H	0.49	0/1709	0.64	0/2316
All	All	0.48	0/13446	0.62	0/18294

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	C	0	1
3	G	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	144	TYR	Sidechain
3	G	144	TYR	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	A	1554	0	1454	79	0
1	E	1554	0	1454	75	0
2	B	1869	0	1763	99	0
2	F	1869	0	1763	117	0
3	C	1459	0	1386	63	0
3	G	1459	0	1386	64	0
4	D	1669	0	1600	119	0
4	H	1669	0	1600	119	0
All	All	13102	0	12406	682	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 27.

The worst 5 of 682 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)
4:D:208:LYS:HE3	4:D:208:LYS:H	1.14	1.12
4:H:208:LYS:H	4:H:208:LYS:HE3	1.18	1.09
4:D:174:LEU:HD13	4:D:174:LEU:H	1.34	0.93
2:F:48:TYR:CE1	3:G:62:GLN:HG2	2.05	0.91
2:F:16:LYS:HD2	2:F:77:GLU:HA	1.51	0.90

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	A	197/199 (99%)	159 (81%)	27 (14%)	11 (6%)	2 9
1	E	197/199 (99%)	160 (81%)	25 (13%)	12 (6%)	1 7
2	B	234/236 (99%)	192 (82%)	33 (14%)	9 (4%)	3 15
2	F	234/236 (99%)	193 (82%)	33 (14%)	8 (3%)	3 17
3	C	180/182 (99%)	162 (90%)	17 (9%)	1 (1%)	25 55
3	G	180/182 (99%)	161 (89%)	18 (10%)	1 (1%)	25 55
4	D	197/217 (91%)	166 (84%)	27 (14%)	4 (2%)	7 27
4	H	197/217 (91%)	166 (84%)	27 (14%)	4 (2%)	7 27
All	All	1616/1668 (97%)	1359 (84%)	207 (13%)	50 (3%)	4 19

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	E	142	GLN
2	F	215	GLU
1	A	150	ASP
1	A	151	SER

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	178/178 (100%)	167 (94%)	11 (6%)	18 46
1	E	178/178 (100%)	167 (94%)	11 (6%)	18 46
2	B	203/203 (100%)	185 (91%)	18 (9%)	9 31
2	F	203/203 (100%)	186 (92%)	17 (8%)	11 34
3	C	163/163 (100%)	147 (90%)	16 (10%)	8 26
3	G	163/163 (100%)	147 (90%)	16 (10%)	8 26
4	D	182/189 (96%)	162 (89%)	20 (11%)	6 22
4	H	182/189 (96%)	161 (88%)	21 (12%)	5 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1452/1466 (99%)	1322 (91%)	130 (9%)	9 30

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	76	VAL
4	H	102	ASP
4	D	38	MET
4	D	30	GLU
4	H	120	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	168	HIS
4	H	32	HIS
4	H	177	ASN
4	D	36	GLN
4	D	4	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 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

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	199/199 (100%)	-0.05	0 100 100	29, 84, 130, 140	0
1	E	199/199 (100%)	0.21	12 (6%) 21 9	29, 85, 131, 140	0
2	B	236/236 (100%)	0.07	5 (2%) 63 39	26, 89, 139, 159	0
2	F	236/236 (100%)	0.17	8 (3%) 45 22	29, 90, 139, 158	0
3	C	182/182 (100%)	-0.25	1 (0%) 91 79	23, 55, 107, 128	0
3	G	182/182 (100%)	-0.24	1 (0%) 91 79	26, 56, 106, 130	0
4	D	201/217 (92%)	-0.03	1 (0%) 91 79	26, 72, 113, 128	0
4	H	201/217 (92%)	-0.11	1 (0%) 91 79	30, 72, 112, 127	0
All	All	1636/1668 (98%)	-0.02	29 (1%) 68 45	23, 74, 129, 159	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	128	GLU	3.6
1	E	152	ASP	3.5
2	F	161	GLU	3.3
1	E	147	GLN	3.2
2	F	148	PRO	3.0

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 monosaccharides 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.