WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 11:29 pm BST

PDB ID	:	5HYJ
Title	:	1E6 TCR in Complex with HLA-A02 carrying AQWGPDPAAA
Authors	:	Rizkallah, P.J.; Bulek, A.M.; Cole, D.K.; Sewell, A.K.
Deposited on	:	2016-02-01
Resolution	:	3.06 Å(reported)

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

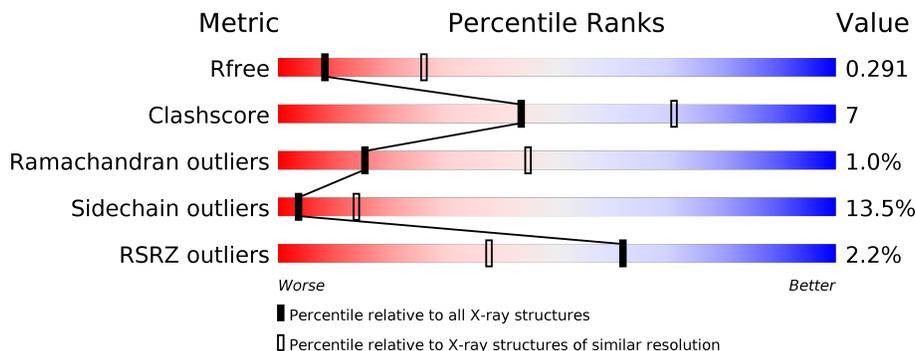|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	Percentile Ranks	Value
Rfree		0.291
Clashscore		7
Ramachandran outliers		1.0%
Sidechain outliers		13.5%
RSRZ outliers		2.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 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	276	75% 21% •
1	F	276	77% 18% •
2	B	100	76% 21% •
2	G	100	76% 17% 7%
3	C	10	60% 30% 10%
3	H	10	70% 30%

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Mol	Chain	Length	Quality of chain
4	D	193	5% · · · 60% · 31% · 8% ·
4	I	193	8% · · · 62% · 31% · 7%
5	E	246	% · · · 76% · 21% ·
5	J	246	2% · · · 76% · 23% ·

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 13392 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total 2254	C 1408	N 410	O 427	S 9	0	0	0
1	F	276	Total 2254	C 1408	N 410	O 427	S 9	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	G	100	Total 837	C 533	N 141	O 159	S 4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called ALA-GLN-TRP-GLY-PRO-ASP-PRO-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total 70	C 44	N 12	O 14	0	0	0
3	H	10	Total 70	C 44	N 12	O 14	0	0	0

- Molecule 4 is a protein called Human T-cell Receptor, Class I, Light alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	193	Total 1520	C 950	N 253	O 307	S 10	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	193	Total 1520	C 950	N 253	O 307	S 10	0	0	0

- Molecule 5 is a protein called Human T-cell Receptor, Class I, Heavy beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total 1974	C 1249	N 341	O 374	S 10	0	0	0
5	J	246	Total 1974	C 1249	N 341	O 374	S 10	0	0	0

- Molecule 6 is water.

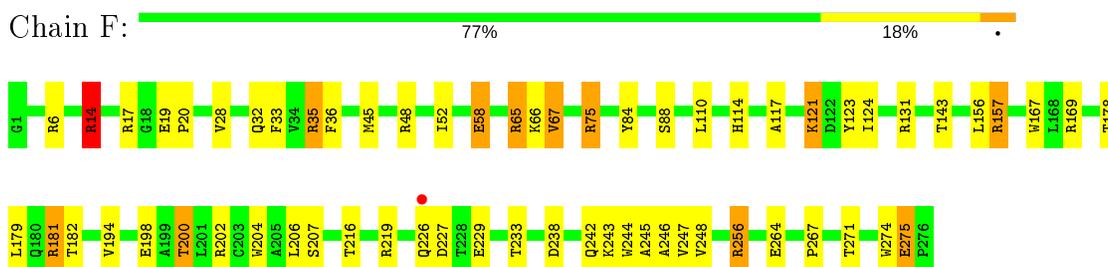| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total 12	O 12	0	0
6	B	2	Total 2	O 2	0	0
6	D	14	Total 14	O 14	0	0
6	E	13	Total 13	O 13	0	0
6	F	20	Total 20	O 20	0	0
6	G	2	Total 2	O 2	0	0
6	I	11	Total 11	O 11	0	0
6	J	8	Total 8	O 8	0	0

3 Residue-property plots ⓘ

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.
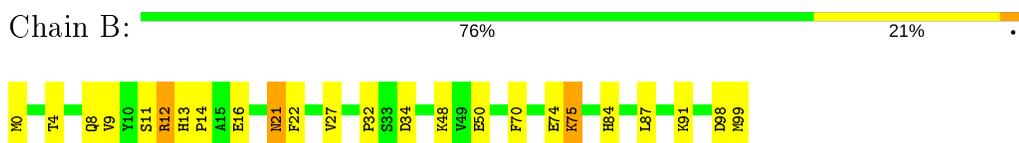
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain
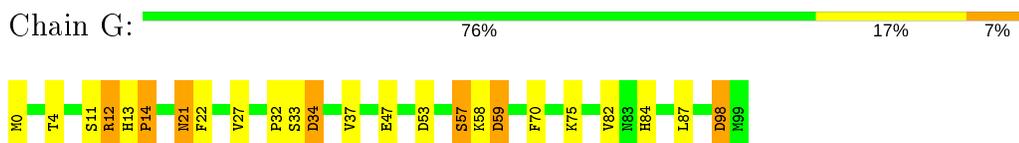
Chain A:

- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain F:

- Molecule 2: Beta-2-microglobulin

Chain B:

- Molecule 2: Beta-2-microglobulin

Chain G:
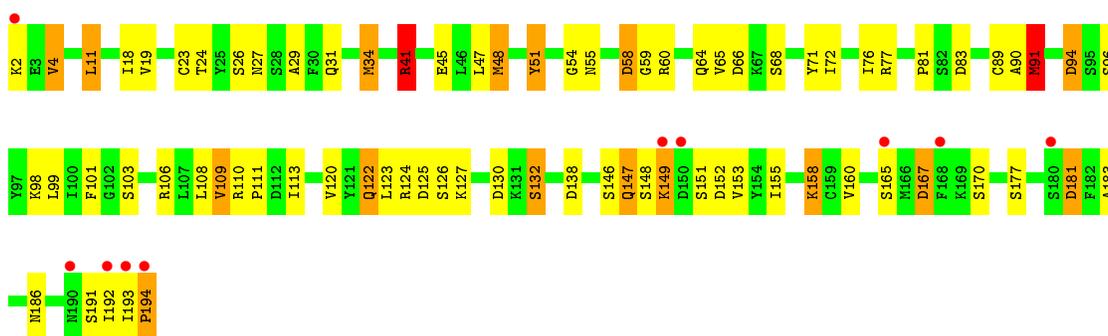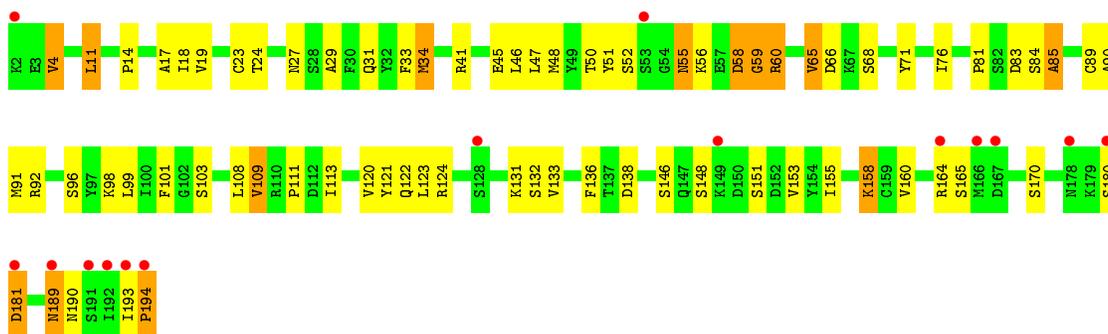
- Molecule 3: ALA-GLN-TRP-GLY-PRO-ASP-PRO-ALA-ALA-ALA

Chain C:

A1 Q2 W3 G4 P5 A9 A10

• Molecule 3: ALA-GLN-TRP-GLY-PRO-ASP-PRO-ALA-ALA-ALA

Chain H:

70%   30%

A1 A8 A9 A10

• Molecule 4: Human T-cell Receptor, Class I, Light alpha Chain

Chain D:

5%

60%   31%   8%

K2 E3 V4 L11 I18 V19 C23 T24 Y25 S26 N27 S28 A29 F30 Q31 M34 R41 E45 L46 L47 M48 Y51 G54 N55 D58 G59 R60 Q64 V65 D66 K67 S68 Y71 I72 I76 R77 P81 S82 D83 C89 A90 M91 D94 S95 S96

Y97 K98 L99 I100 F101 G102 S103 R106 L107 L108 V109 R110 P111 D112 I113 V120 Y121 Q122 L123 R124 D125 S126 K127 D130 K131 S132 D138 S146 Q147 S148 K149 D150 S151 D152 V153 Y154 I155 K158 C159 V160 S165 M166 D167 F168 K169 S170 S177 S180 D181 F182 A183

M186 N190 S191 I192 I193 P194

• Molecule 4: Human T-cell Receptor, Class I, Light alpha Chain

Chain I:

8%

62%   31%   7%

K2 E3 V4 L11 P14 A17 I18 V19 C23 T24 N27 S28 A29 F30 Q31 Y32 F33 M34 R41 E45 L46 L47 M48 Y49 T50 Y51 S52 S53 G54 N55 K56 E57 D58 G59 R60 V65 D66 K67 S68 Y71 I76 P81 S82 D83 S84 A85 C89 A90

M91 R92 S96 Y97 K98 L99 I100 F101 G102 S103 L108 V109 R110 P111 D112 I113 V120 Y121 Q122 L123 R124 S128 K131 S132 V133 F136 T137 D138 S146 Q147 S148 K149 D150 S151 D152 V153 Y154 I155 K158 C159 V160 R164 S165 M166 D167 S170 N178 K179 S180

D181 N189 N190 S191 I192 I193 P194

• Molecule 5: Human T-cell Receptor, Class I, Heavy beta Chain

Chain E:

%

76%   21%

D1 S7 P8 R9 H10 M15 V19 T20 L21 R22 H29 D30 R36 M39 M40 R41 G42 L43 E44 L45 L46 E62 D63 R64 S73 T76 L77 K78 I79 Q80 P84 R85 D86 S87 A88 V89 Y90 W97 E98 K99 N103 T111 E117 K120

V129 F130 E131 P132 S138 K142 A143 V157 E158 L159 S160 V168 L179 L185 N186 R195 L196 R197 R207 Y217 E221 N222 W225 T226 Q227 D228 R229 I246

• Molecule 5: Human T-cell Receptor, Class I, Heavy beta Chain

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.44Å 97.31Å 121.37Å 97.29° 97.66° 92.73°	Depositor
Resolution (Å)	38.63 – 3.06 38.63 – 3.06	Depositor EDS
% Data completeness (in resolution range)	97.2 (38.63-3.06) 97.2 (38.63-3.06)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.36 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.212 , 0.293 0.213 , 0.291	Depositor DCC
R_{free} test set	1726 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.6	EDS
L-test for twinning[2]	$<\vert L\vert>\; =\; 0.49,\; <L^2>\; =\; 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13392	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<\vert L\vert>$, $<L^2>$ 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	A	0.89	0/2320	1.05	10/3149 (0.3%)
1	F	0.95	2/2320 (0.1%)	1.09	15/3149 (0.5%)
2	B	0.90	0/860	1.02	2/1162 (0.2%)
2	G	0.97	1/860 (0.1%)	1.12	5/1162 (0.4%)
3	C	1.14	0/73	0.96	0/100
3	H	1.15	0/73	1.13	0/100
4	D	0.91	1/1553 (0.1%)	1.08	10/2100 (0.5%)
4	I	0.85	1/1553 (0.1%)	1.01	4/2100 (0.2%)
5	E	0.84	1/2029 (0.0%)	1.00	4/2759 (0.1%)
5	J	0.75	1/2029 (0.0%)	0.97	6/2759 (0.2%)
All	All	0.88	7/13670 (0.1%)	1.04	56/18540 (0.3%)

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	2
2	G	0	1
3	C	0	1
3	H	0	1
4	D	0	2
4	I	0	2
5	E	0	2
All	All	0	11

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	194	PRO	C-O	10.49	1.44	1.23
4	I	194	PRO	C-O	10.06	1.43	1.23
1	F	58	GLU	CB-CG	7.30	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	58	GLU	CG-CD	7.08	1.62	1.51
5	J	44	GLU	CD-OE1	5.14	1.31	1.25

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	14	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	A	44	ARG	NE-CZ-NH1	8.98	124.79	120.30
2	G	12	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	F	14	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	A	48	ARG	NE-CZ-NH2	8.00	124.30	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ASP	Peptide
1	A	226	GLN	Peptide
3	C	9	ALA	Peptide
4	D	149	LYS	Peptide
4	D	158	LYS	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	2254	0	2103	26	0
1	F	2254	0	2103	21	0
2	B	837	0	803	12	0
2	G	837	0	803	10	0
3	C	70	0	61	4	0
3	H	70	0	61	2	0
4	D	1520	0	1447	36	0
4	I	1520	0	1447	30	0
5	E	1974	0	1887	28	0
5	J	1974	0	1887	25	0
6	A	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	2	0	0	0	0
6	D	14	0	0	1	0
6	E	13	0	0	1	0
6	F	20	0	0	1	0
6	G	2	0	0	1	0
6	I	11	0	0	0	0
6	J	8	0	0	0	0
All	All	13392	0	12602	174	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 7.

The worst 5 of 174 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:41:ARG:NH2	5:E:157:VAL:O	2.06	0.87
4:I:34:MET:HE2	5:J:103:ASN:HB2	1.58	0.85
2:B:21:ASN:HD22	2:B:22:PHE:H	1.27	0.82
4:D:183:ALA:HB3	4:D:186:ASN:HD21	1.46	0.80
5:E:15:MET:CE	5:E:117:GLU:HA	2.15	0.77

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	274/276 (99%)	245 (89%)	25 (9%)	4 (2%)	10	35
1	F	274/276 (99%)	253 (92%)	19 (7%)	2 (1%)	22	52
2	B	98/100 (98%)	91 (93%)	6 (6%)	1 (1%)	15	45
2	G	98/100 (98%)	96 (98%)	1 (1%)	1 (1%)	15	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	H	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
4	D	191/193 (99%)	166 (87%)	22 (12%)	3 (2%)	9	33
4	I	191/193 (99%)	167 (87%)	19 (10%)	5 (3%)	5	22
5	E	244/246 (99%)	226 (93%)	17 (7%)	1 (0%)	34	64
5	J	244/246 (99%)	225 (92%)	19 (8%)	0	100	100
All	All	1630/1650 (99%)	1484 (91%)	129 (8%)	17 (1%)	15	45

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	GLY
1	A	137	ASP
4	D	181	ASP
4	I	158	LYS
4	D	158	LYS

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	232/232 (100%)	206 (89%)	26 (11%)	6	21
1	F	232/232 (100%)	207 (89%)	25 (11%)	6	22
2	B	95/95 (100%)	84 (88%)	11 (12%)	5	19
2	G	95/95 (100%)	84 (88%)	11 (12%)	5	19
3	C	5/5 (100%)	5 (100%)	0	100	100
3	H	5/5 (100%)	5 (100%)	0	100	100
4	D	174/174 (100%)	137 (79%)	37 (21%)	1	4
4	I	174/174 (100%)	139 (80%)	35 (20%)	1	4
5	E	216/216 (100%)	191 (88%)	25 (12%)	5	19
5	J	216/216 (100%)	191 (88%)	25 (12%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1444/1444 (100%)	1249 (86%)	195 (14%)	4 14

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	131	GLU
1	F	121	LYS
5	J	68	LYS
5	E	168	VAL
1	F	14	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	29	HIS
1	F	174	ASN
4	I	189	ASN
5	E	141	GLN
1	F	54	GLN

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 (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	A	276/276 (100%)	-0.18	3 (1%) 80	60	45, 65, 108, 138	0
1	F	276/276 (100%)	-0.18	1 (0%) 92	82	30, 57, 123, 169	0
2	B	100/100 (100%)	-0.33	0 100	100	47, 60, 88, 109	0
2	G	100/100 (100%)	-0.45	0 100	100	38, 55, 76, 91	0
3	C	10/10 (100%)	-0.40	0 100	100	47, 54, 56, 61	0
3	H	10/10 (100%)	-0.23	0 100	100	42, 50, 59, 60	0
4	D	193/193 (100%)	0.17	10 (5%) 27	11	46, 77, 130, 155	0
4	I	193/193 (100%)	0.30	15 (7%) 13	4	51, 86, 144, 173	0
5	E	246/246 (100%)	-0.18	3 (1%) 79	58	34, 63, 120, 143	0
5	J	246/246 (100%)	0.03	5 (2%) 65	41	49, 80, 117, 151	0
All	All	1650/1650 (100%)	-0.08	37 (2%) 62	38	30, 67, 126, 173	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	150	ASP	7.4
4	D	194	PRO	6.7
4	I	180	SER	5.0
4	I	194	PRO	4.9
5	J	1	ASP	4.7

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 carbohydrates 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.