wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 05:37 am BST

PDB ID	:	6RCV
Title	:	PfRH5 bound to monoclonal antibodies R5.011 and R5.016
Authors	:	Alanine, D.W.G.; Draper, S.J.; Higgins, M.K.
Deposited on	:	2019-04-11
Resolution	:	3.58 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:

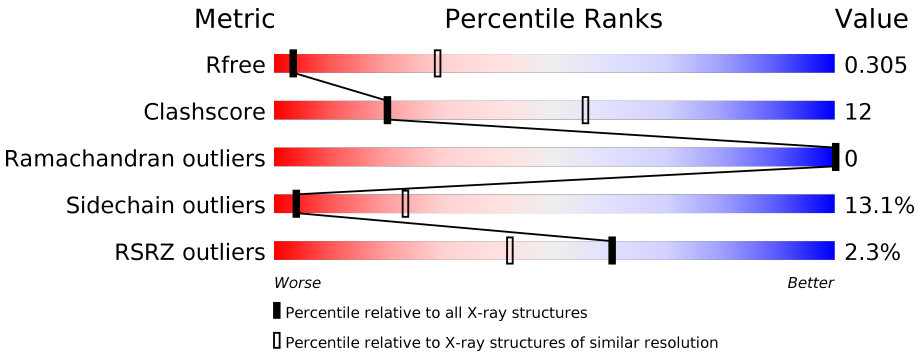
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.58 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	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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	501	% 43% 15% 40%
1	F	501	% 42% 15% 40%
2	B	217	67% 25% 5%
2	G	217	63% 31%
3	C	240	67% 25% 7%
3	H	240	63% 28% 7%

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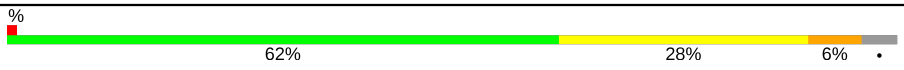
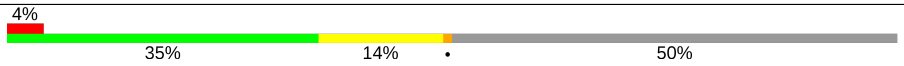
Mol	Chain	Length	Quality of chain
4	D	219	
4	I	219	
5	E	464	
5	J	464	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18311 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 Reticulocyte binding protein homologue 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2540	1640	426	459	15			
1	F	299	Total	C	N	O	S	0	0	0
			2540	1640	426	459	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLN	ASN	conflict	UNP Q8IFM5
A	216	ALA	THR	conflict	UNP Q8IFM5
F	38	GLN	ASN	conflict	UNP Q8IFM5
F	216	ALA	THR	conflict	UNP Q8IFM5

- Molecule 2 is a protein called R5.011 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1579	985	267	323	4			
2	G	210	Total	C	N	O	S	0	0	0
			1574	982	266	322	4			

- Molecule 3 is a protein called R5.011 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	224	Total	C	N	O	S	0	0	0
			1695	1081	272	336	6			
3	H	223	Total	C	N	O	S	0	0	0
			1691	1079	271	335	6			

- Molecule 4 is a protein called R5.016 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	210	Total	C	N	O	S	0	0	0
			1624	1017	275	327	5			
4	I	210	Total	C	N	O	S	0	0	0
			1624	1017	275	327	5			

- Molecule 5 is a protein called R5.016 heavy chain.

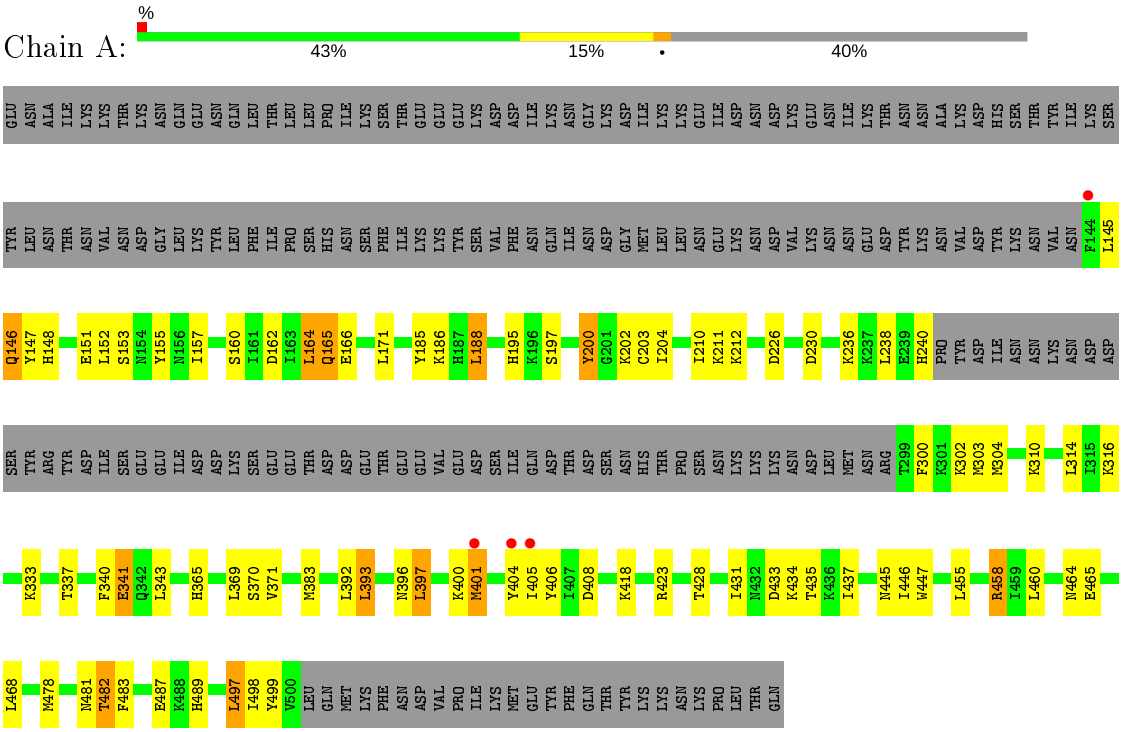
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	232	Total	C	N	O	S	0	0	0
			1746	1098	290	349	9			
5	J	224	Total	C	N	O	S	0	0	0
			1698	1072	281	336	9			

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.

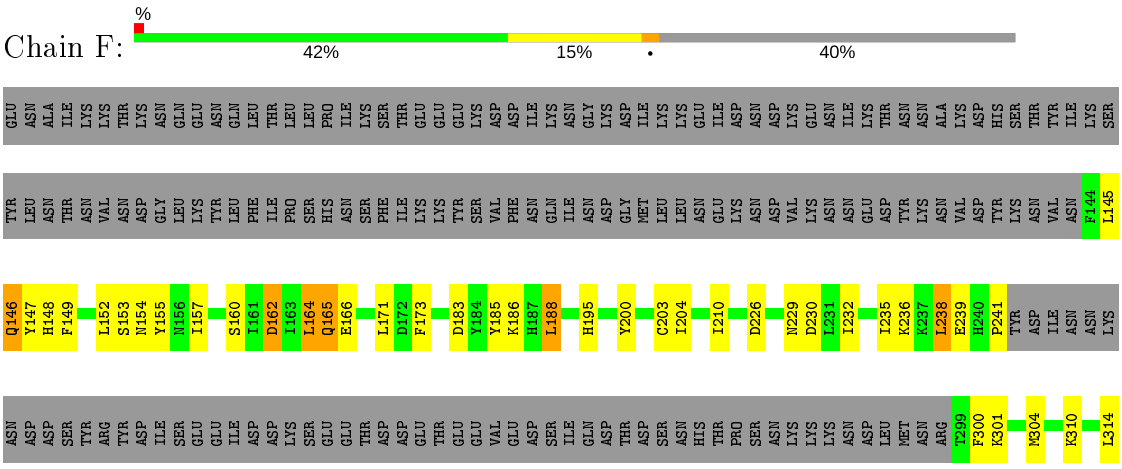
- Molecule 1: Reticulocyte binding protein homologue 5

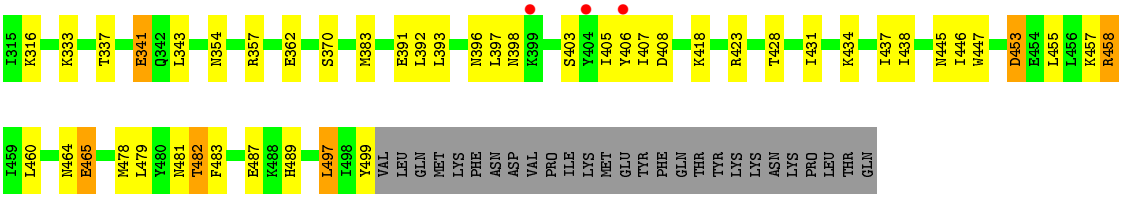
Chain A:



- Molecule 1: Reticulocyte binding protein homologue 5

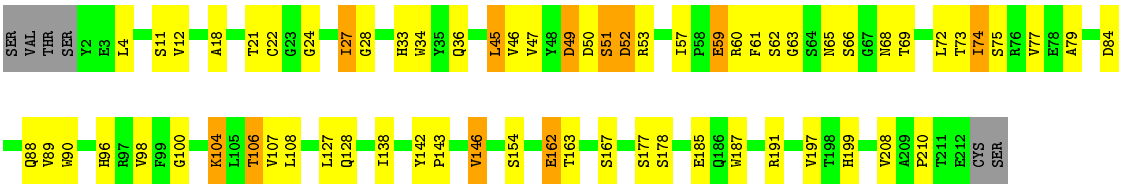
Chain F:





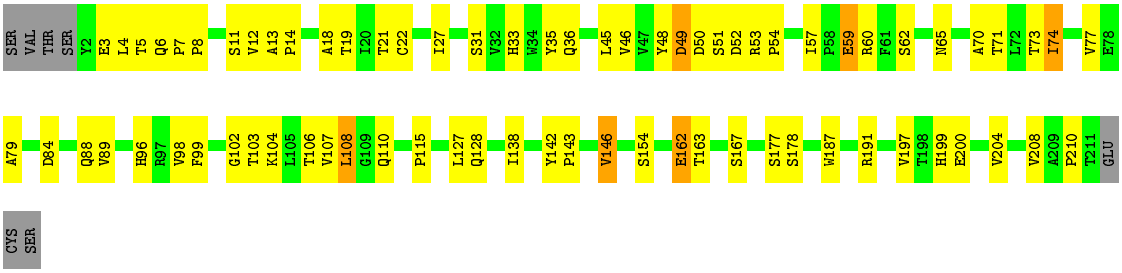
- Molecule 2: R5.011 light chain

Chain B:



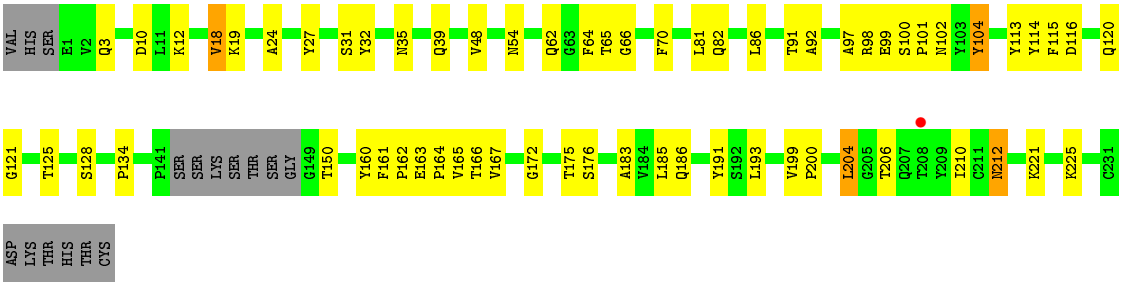
- Molecule 2: R5.011 light chain

Chain G:



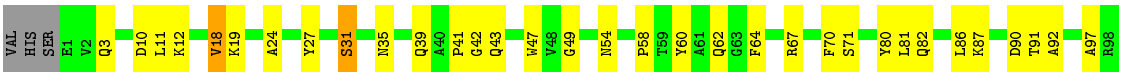
- Molecule 3: R5.011 heavy chain

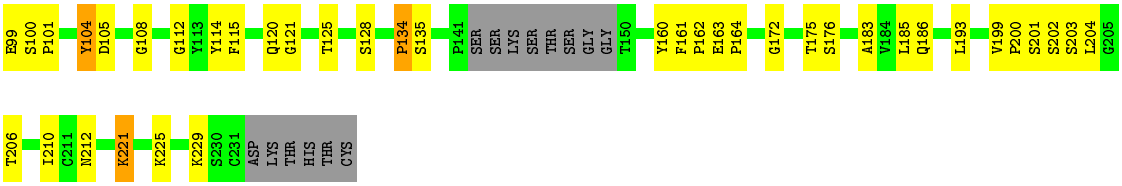
Chain C:



- Molecule 3: R5.011 heavy chain

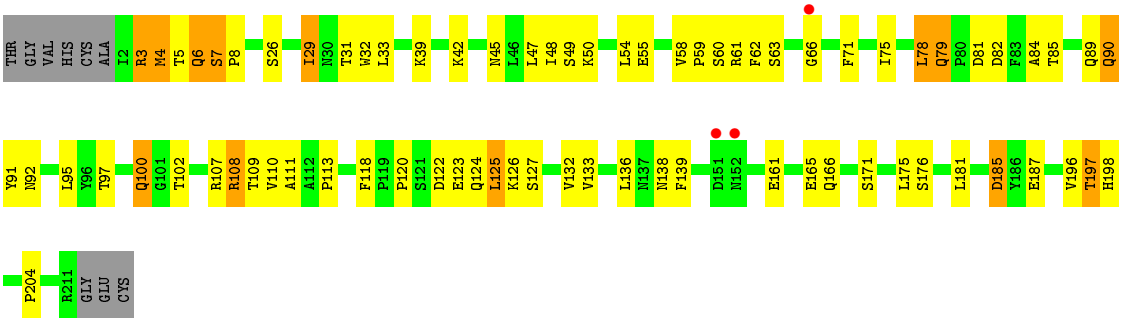
Chain H:





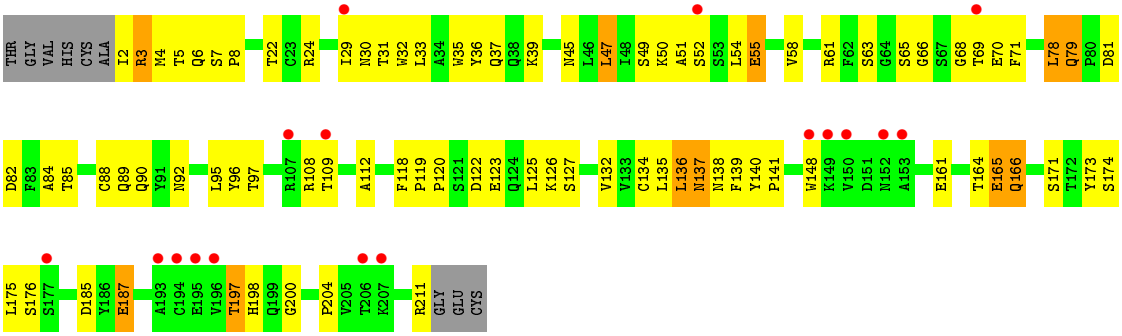
• Molecule 4: R5.016 light chain

Chain D:



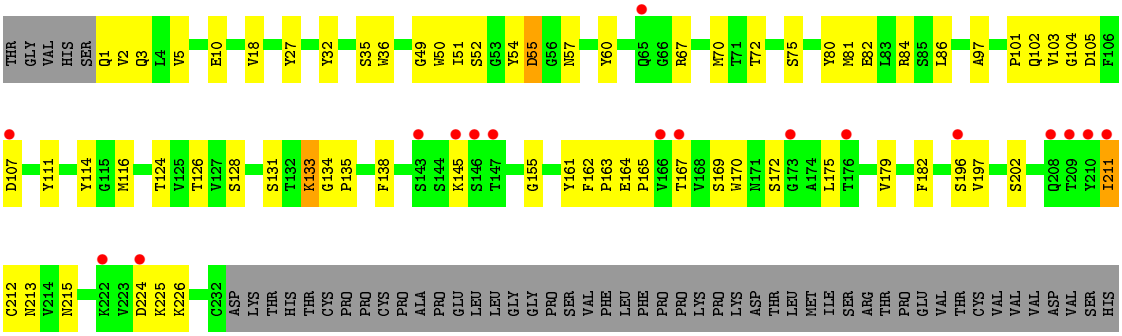
• Molecule 4: R5.016 light chain

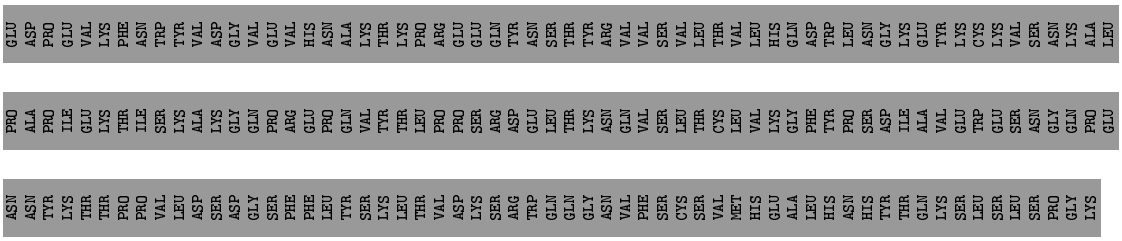
Chain I:



• Molecule 5: R5.016 heavy chain

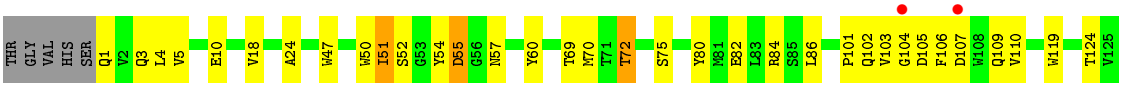
Chain E:

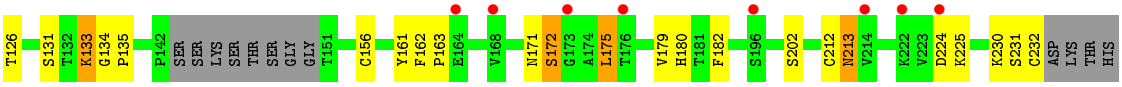




- Molecule 5: R5.016 heavy chain

Chain J:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	140.99Å 150.99Å 163.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.16 – 3.58 49.16 – 3.58	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.16-3.58) 99.2 (49.16-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.280 , 0.305 0.280 , 0.305	Depositor DCC
R_{free} test set	2037 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	73.2	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	18311	wwPDB-VP
Average B, all atoms (Å^2)	75.0	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 57.09 % 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 2.4904e-05. 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, 0.333 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	0.30	0/2594	0.55	0/3479
1	F	0.33	0/2595	0.59	0/3481
2	B	0.33	0/1619	0.68	0/2214
2	G	0.39	0/1614	0.67	0/2207
3	C	0.31	0/1742	0.63	0/2380
3	H	0.41	0/1738	0.70	0/2375
4	D	0.33	0/1659	0.67	0/2253
4	I	0.41	0/1659	0.72	0/2253
5	E	0.44	0/1790	0.68	0/2442
5	J	0.38	0/1741	0.69	0/2376
All	All	0.36	0/18751	0.65	0/25460

There are no bond length outliers.

There are no bond angle outliers.

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	2540	0	2554	52	0
1	F	2540	0	2552	54	0
2	B	1579	0	1515	36	0
2	G	1574	0	1513	56	0
3	C	1695	0	1627	44	0
3	H	1691	0	1624	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1624	0	1581	46	0
4	I	1624	0	1581	70	0
5	E	1746	0	1685	47	0
5	J	1698	0	1640	43	0
All	All	18311	0	17872	451	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 12.

The worst 5 of 451 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:446:ILE:HG23	1:A:447:TRP:CD1	1.93	1.04
3:H:163:GLU:HG2	3:H:164:PRO:HA	1.42	0.98
3:H:134:PRO:HB3	3:H:160:TYR:HB3	1.54	0.90
1:F:434:LYS:HA	1:F:437:ILE:HG22	1.54	0.89
2:G:6:GLN:NE2	2:G:102:GLY:C	2.30	0.85

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	295/501 (59%)	280 (95%)	15 (5%)	0	100	100
1	F	295/501 (59%)	281 (95%)	14 (5%)	0	100	100
2	B	209/217 (96%)	197 (94%)	12 (6%)	0	100	100
2	G	208/217 (96%)	196 (94%)	12 (6%)	0	100	100
3	C	220/240 (92%)	204 (93%)	16 (7%)	0	100	100
3	H	219/240 (91%)	206 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	208/219 (95%)	192 (92%)	16 (8%)	0	100	100
4	I	208/219 (95%)	187 (90%)	21 (10%)	0	100	100
5	E	230/464 (50%)	215 (94%)	15 (6%)	0	100	100
5	J	220/464 (47%)	207 (94%)	13 (6%)	0	100	100
All	All	2312/3282 (70%)	2165 (94%)	147 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	289/486 (60%)	252 (87%)	37 (13%)	4	24
1	F	289/486 (60%)	254 (88%)	35 (12%)	5	26
2	B	177/184 (96%)	148 (84%)	29 (16%)	2	15
2	G	177/184 (96%)	149 (84%)	28 (16%)	2	17
3	C	189/204 (93%)	169 (89%)	20 (11%)	6	33
3	H	189/204 (93%)	168 (89%)	21 (11%)	6	31
4	D	186/192 (97%)	153 (82%)	33 (18%)	2	11
4	I	186/192 (97%)	159 (86%)	27 (14%)	3	20
5	E	195/409 (48%)	176 (90%)	19 (10%)	8	36
5	J	189/409 (46%)	168 (89%)	21 (11%)	6	31
All	All	2066/2950 (70%)	1796 (87%)	270 (13%)	4	23

5 of 270 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	10	GLU
1	F	301	LYS
5	J	1	GLN
5	E	55	ASP

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Mol	Chain	Res	Type
5	E	211	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	6	GLN
4	I	90	GLN
4	I	137	ASN
1	F	154	ASN
4	I	92	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	299/501 (59%)	-0.07	4 (1%) 77 61	37, 58, 108, 147	0
1	F	299/501 (59%)	0.04	3 (1%) 82 69	43, 62, 113, 143	0
2	B	211/217 (97%)	-0.03	0 100 100	45, 58, 112, 130	0
2	G	210/217 (96%)	-0.07	0 100 100	38, 58, 88, 102	0
3	C	224/240 (93%)	0.11	1 (0%) 92 86	45, 70, 126, 152	0
3	H	223/240 (92%)	0.02	0 100 100	46, 65, 109, 140	0
4	D	210/219 (95%)	0.32	3 (1%) 75 59	49, 99, 135, 161	0
4	I	210/219 (95%)	0.52	17 (8%) 12 6	53, 96, 135, 148	0
5	E	232/464 (50%)	0.30	17 (7%) 15 8	48, 80, 137, 144	0
5	J	224/464 (48%)	0.29	10 (4%) 33 19	47, 73, 135, 148	0
All	All	2342/3282 (71%)	0.13	55 (2%) 60 42	37, 67, 129, 161	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	146	SER	4.3
4	I	149	LYS	3.9
4	I	150	VAL	3.8
5	E	176	THR	3.7
5	E	145	LYS	3.6

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 (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.