wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2024 – 04:18 PM JST

PDB ID	:	8JEL
Title	:	Crystal structure of TIGIT in complexed with Ociperlimab, crystal form I
Authors	:	Sun, J.; Zhang, X.X.; Song, J.
Deposited on	:	2023-05-16
Resolution	:	2.45 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 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:

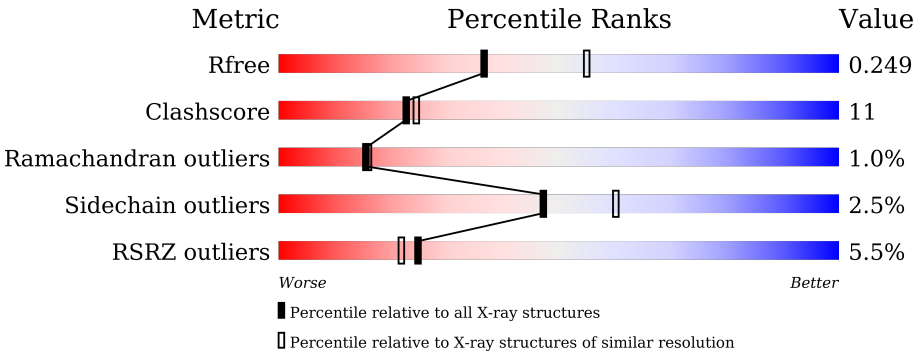
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	222	9% 73% 21%
1	C	222	2% 79% 18%
1	F	222	7% 67% 28%
1	I	222	69% 27%
2	B	214	8% 78% 19%
2	D	214	3% 78% 21%

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Mol	Chain	Length	Quality of chain
2	G	214	
2	K	214	
3	E	115	
3	H	115	
3	J	115	
3	L	115	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17094 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 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	216	Total	C	N	O	S	0	0	0
			1634	1037	269	320	8			
1	A	216	Total	C	N	O	S	0	0	0
			1634	1037	269	320	8			
1	F	213	Total	C	N	O	S	0	0	0
			1613	1025	265	316	7			
1	I	214	Total	C	N	O	S	0	0	0
			1622	1031	267	317	7			

- Molecule 2 is a protein called antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	214	Total	C	N	O	S	0	0	0
			1638	1027	275	330	6			
2	B	214	Total	C	N	O	S	0	0	0
			1638	1027	275	330	6			
2	G	208	Total	C	N	O	S	0	0	0
			1589	998	265	321	5			
2	K	212	Total	C	N	O	S	0	0	0
			1623	1019	273	326	5			

- Molecule 3 is a protein called T-cell immunoreceptor with Ig and ITIM domains.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	108	Total	C	N	O	S	0	0	0
			827	522	135	165	5			
3	E	108	Total	C	N	O	S	0	0	0
			828	522	135	167	4			
3	H	107	Total	C	N	O	S	0	0	0
			819	517	134	164	4			
3	L	106	Total	C	N	O	S	0	0	0
			811	511	133	163	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	129	LEU	-	expression tag	UNP Q495A1
J	130	GLU	-	expression tag	UNP Q495A1
J	131	HIS	-	expression tag	UNP Q495A1
J	132	HIS	-	expression tag	UNP Q495A1
J	133	HIS	-	expression tag	UNP Q495A1
J	134	HIS	-	expression tag	UNP Q495A1
J	135	HIS	-	expression tag	UNP Q495A1
J	136	HIS	-	expression tag	UNP Q495A1
E	129	LEU	-	expression tag	UNP Q495A1
E	130	GLU	-	expression tag	UNP Q495A1
E	131	HIS	-	expression tag	UNP Q495A1
E	132	HIS	-	expression tag	UNP Q495A1
E	133	HIS	-	expression tag	UNP Q495A1
E	134	HIS	-	expression tag	UNP Q495A1
E	135	HIS	-	expression tag	UNP Q495A1
E	136	HIS	-	expression tag	UNP Q495A1
H	129	LEU	-	expression tag	UNP Q495A1
H	130	GLU	-	expression tag	UNP Q495A1
H	131	HIS	-	expression tag	UNP Q495A1
H	132	HIS	-	expression tag	UNP Q495A1
H	133	HIS	-	expression tag	UNP Q495A1
H	134	HIS	-	expression tag	UNP Q495A1
H	135	HIS	-	expression tag	UNP Q495A1
H	136	HIS	-	expression tag	UNP Q495A1
L	129	LEU	-	expression tag	UNP Q495A1
L	130	GLU	-	expression tag	UNP Q495A1
L	131	HIS	-	expression tag	UNP Q495A1
L	132	HIS	-	expression tag	UNP Q495A1
L	133	HIS	-	expression tag	UNP Q495A1
L	134	HIS	-	expression tag	UNP Q495A1
L	135	HIS	-	expression tag	UNP Q495A1
L	136	HIS	-	expression tag	UNP Q495A1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	78	Total O 78 78	0	0
4	D	97	Total O 97 97	0	0
4	J	50	Total O 50 50	0	0

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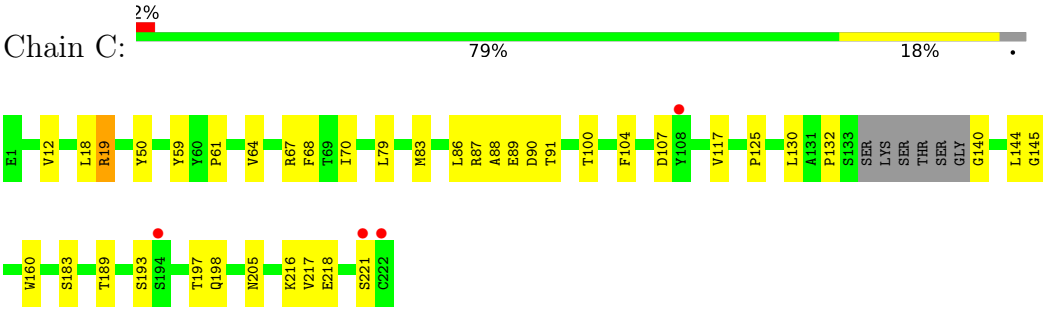
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	90	Total O 90 90	0	0
4	B	76	Total O 76 76	0	0
4	E	49	Total O 49 49	0	0
4	F	41	Total O 41 41	0	0
4	G	67	Total O 67 67	0	0
4	H	54	Total O 54 54	0	0
4	I	78	Total O 78 78	0	0
4	K	88	Total O 88 88	0	0
4	L	50	Total O 50 50	0	0

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.

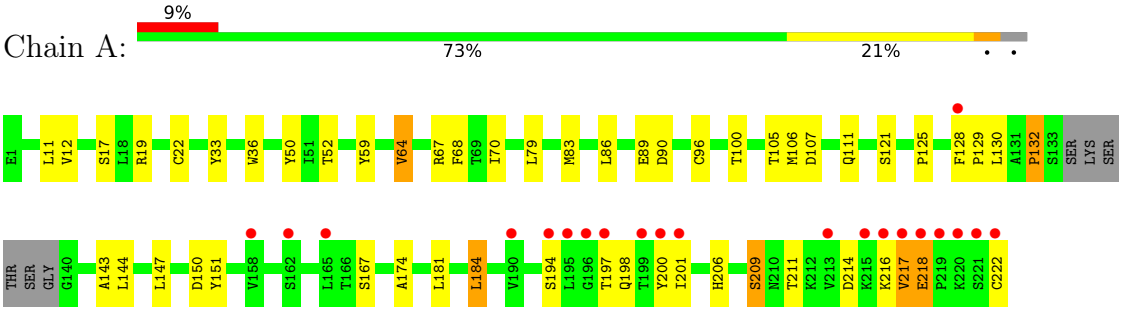
• Molecule 1: antibody heavy chain

Chain C:



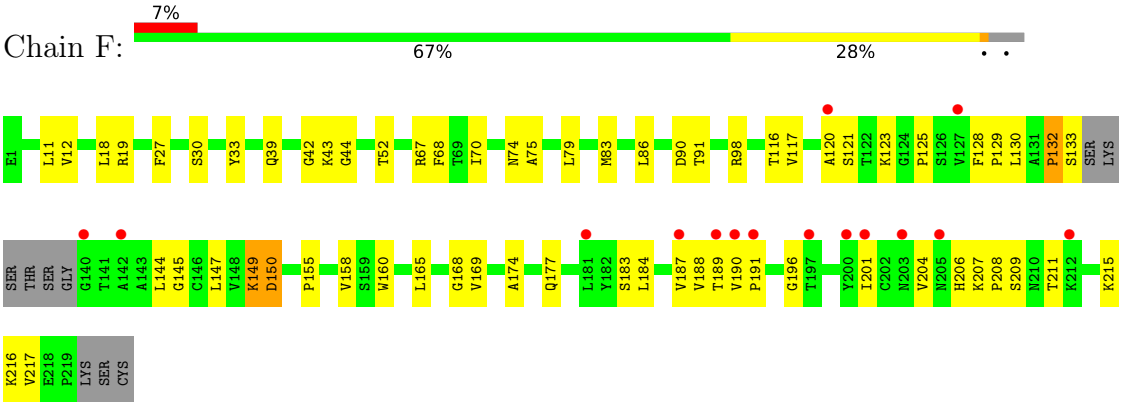
• Molecule 1: antibody heavy chain

Chain A:



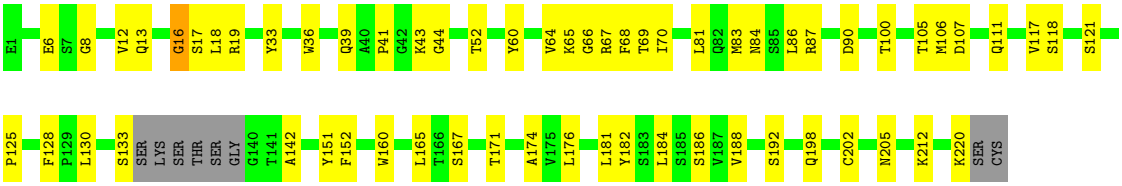
• Molecule 1: antibody heavy chain

Chain F:

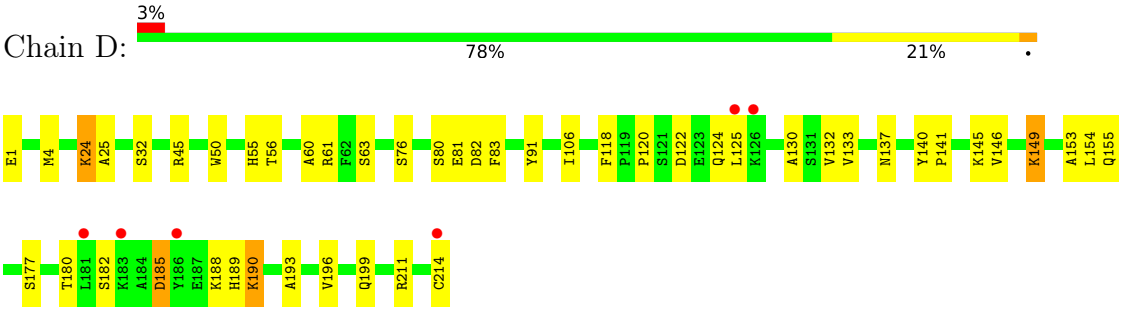


• Molecule 1: antibody heavy chain

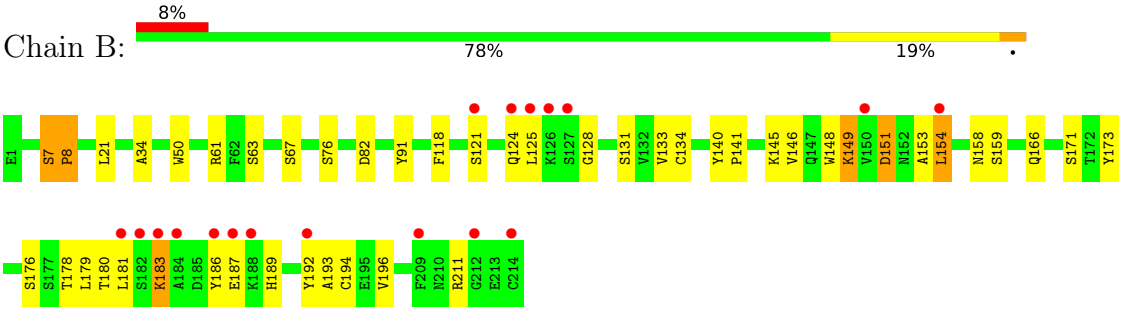
Chain I:



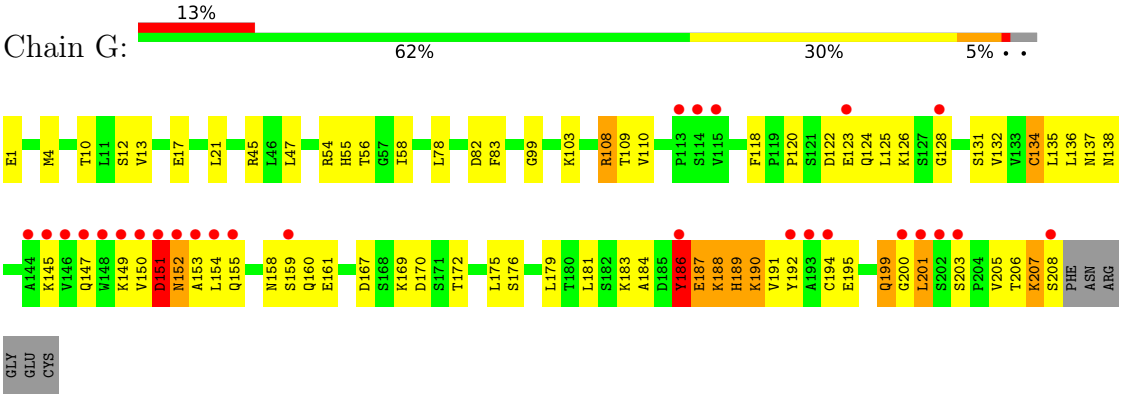
• Molecule 2: antibody light chain



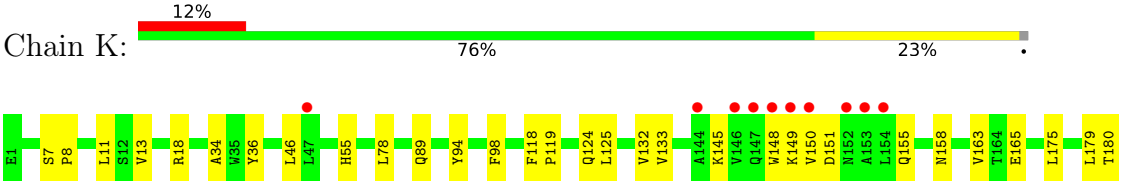
• Molecule 2: antibody light chain

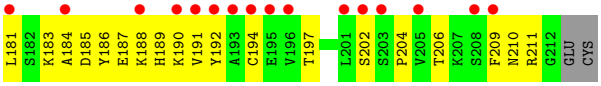


• Molecule 2: antibody light chain



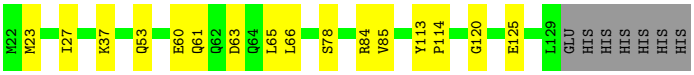
• Molecule 2: antibody light chain





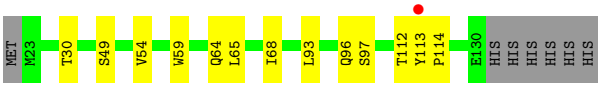
• Molecule 3: T-cell immunoreceptor with Ig and ITIM domains

Chain J:



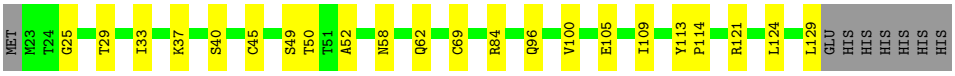
• Molecule 3: T-cell immunoreceptor with Ig and ITIM domains

Chain E:



• Molecule 3: T-cell immunoreceptor with Ig and ITIM domains

Chain H:



• Molecule 3: T-cell immunoreceptor with Ig and ITIM domains

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.53Å 138.31Å 196.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.40 – 2.45 48.40 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.40-2.45) 100.0 (48.40-2.45)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.192 , 0.249 0.192 , 0.249	Depositor DCC
R_{free} test set	6942 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17094	wwPDB-VP
Average B, all atoms (Å^2)	79.0	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 25.59 % 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 3.0831e-03. 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	0.50	1/1675 (0.1%)	0.64	1/2282 (0.0%)
1	C	0.41	0/1675	0.60	0/2282
1	F	0.42	0/1654	0.65	0/2255
1	I	0.41	0/1663	0.61	0/2266
2	B	0.41	0/1675	0.61	0/2276
2	D	0.45	0/1675	0.59	0/2276
2	G	0.40	0/1625	0.65	0/2210
2	K	0.45	0/1660	0.65	0/2256
3	E	0.45	0/845	0.66	0/1153
3	H	0.56	0/836	0.76	1/1141 (0.1%)
3	J	0.48	0/844	0.67	0/1151
3	L	0.48	0/828	0.67	0/1130
All	All	0.45	1/16655 (0.0%)	0.64	2/22678 (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
1	A	0	1
2	B	0	1
2	G	0	4
2	K	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	CYS	CB-SG	-6.81	1.70	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	113	TYR	CA-CB-CG	-7.97	98.26	113.40
1	A	184	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	VAL	Peptide
2	B	7	SER	Peptide
2	G	151	ASP	Peptide
2	G	186	TYR	Peptide
2	G	187	GLU	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	1634	0	1586	36	1
1	C	1634	0	1586	34	0
1	F	1613	0	1564	54	0
1	I	1622	0	1577	47	0
2	B	1638	0	1588	40	0
2	D	1638	0	1588	36	0
2	G	1589	0	1547	74	1
2	K	1623	0	1578	40	0
3	E	828	0	796	8	0
3	H	819	0	790	13	0
3	J	827	0	799	10	0
3	L	811	0	779	5	0
4	A	90	0	0	6	0
4	B	76	0	0	5	0
4	C	78	0	0	5	0
4	D	97	0	0	4	0
4	E	49	0	0	3	0
4	F	41	0	0	1	0
4	G	67	0	0	5	0
4	H	54	0	0	1	0
4	I	78	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	50	0	0	2	0
4	K	88	0	0	3	0
4	L	50	0	0	2	0
All	All	17094	0	15778	367	1

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.

The worst 5 of 367 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:F:27:PHE:CG	1:F:98:ARG:NH2	2.22	1.07
2:G:110:VAL:HG21	2:G:199:GLN:OE1	1.60	0.99
2:G:149:LYS:HG2	2:G:154:LEU:H	1.29	0.98
3:H:69:CYS:SG	4:H:247:HOH:O	2.29	0.90
2:G:188:LYS:O	2:G:190:LYS:N	2.12	0.82

All (1) 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)
1:A:89:GLU:OE1	2:G:152:ASN:ND2[4_455]	2.19	0.01

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	212/222 (96%)	197 (93%)	12 (6%)	3 (1%)	11 9
1	C	212/222 (96%)	198 (93%)	14 (7%)	0	100 100
1	F	209/222 (94%)	187 (90%)	17 (8%)	5 (2%)	6 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	210/222 (95%)	198 (94%)	11 (5%)	1 (0%)	29 34
2	B	212/214 (99%)	201 (95%)	10 (5%)	1 (0%)	29 34
2	D	212/214 (99%)	204 (96%)	8 (4%)	0	100 100
2	G	206/214 (96%)	177 (86%)	23 (11%)	6 (3%)	4 2
2	K	210/214 (98%)	194 (92%)	12 (6%)	4 (2%)	8 6
3	E	106/115 (92%)	103 (97%)	2 (2%)	1 (1%)	17 19
3	H	105/115 (91%)	101 (96%)	3 (3%)	1 (1%)	15 16
3	J	106/115 (92%)	101 (95%)	5 (5%)	0	100 100
3	L	104/115 (90%)	99 (95%)	5 (5%)	0	100 100
All	All	2104/2204 (96%)	1960 (93%)	122 (6%)	22 (1%)	15 16

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	PRO
2	G	151	ASP
2	G	152	ASN
2	G	188	LYS
2	G	201	LEU

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	181/186 (97%)	176 (97%)	5 (3%)	43 56
1	C	181/186 (97%)	177 (98%)	4 (2%)	52 64
1	F	178/186 (96%)	175 (98%)	3 (2%)	60 73
1	I	179/186 (96%)	176 (98%)	3 (2%)	60 73
2	B	184/184 (100%)	176 (96%)	8 (4%)	29 38
2	D	184/184 (100%)	174 (95%)	10 (5%)	22 28
2	G	179/184 (97%)	172 (96%)	7 (4%)	32 42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	K	182/184 (99%)	181 (100%)	1 (0%)	88 93
3	E	92/99 (93%)	91 (99%)	1 (1%)	73 82
3	H	91/99 (92%)	90 (99%)	1 (1%)	73 82
3	J	92/99 (93%)	91 (99%)	1 (1%)	73 82
3	L	90/99 (91%)	88 (98%)	2 (2%)	52 64
All	All	1813/1876 (97%)	1767 (98%)	46 (2%)	47 60

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	49	SER
2	G	176	SER
1	F	30	SER
2	G	12	SER
2	G	186	TYR

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

Mol	Chain	Res	Type
1	I	13	GLN
1	I	84	ASN
2	K	158	ASN
2	B	79	GLN
1	F	210	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

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	216/222 (97%)	0.67	21 (9%) 7 5	46, 78, 141, 180	0
1	C	216/222 (97%)	0.35	4 (1%) 66 64	54, 83, 109, 167	0
1	F	213/222 (95%)	0.61	15 (7%) 16 13	53, 93, 134, 202	0
1	I	214/222 (96%)	0.15	0 100 100	51, 77, 99, 113	0
2	B	214/214 (100%)	0.57	18 (8%) 11 8	43, 72, 127, 169	0
2	D	214/214 (100%)	0.28	6 (2%) 53 49	50, 70, 107, 158	0
2	G	208/214 (97%)	0.80	27 (12%) 3 2	49, 84, 146, 184	0
2	K	212/214 (99%)	0.80	26 (12%) 4 2	50, 75, 131, 164	0
3	E	108/115 (93%)	0.27	1 (0%) 84 85	43, 60, 92, 126	0
3	H	107/115 (93%)	0.41	0 100 100	50, 62, 101, 118	0
3	J	108/115 (93%)	0.24	0 100 100	50, 60, 89, 120	0
3	L	106/115 (92%)	0.05	0 100 100	51, 64, 97, 145	0
All	All	2136/2204 (96%)	0.47	118 (5%) 25 22	43, 75, 128, 202	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	CYS	7.8
2	G	152	ASN	7.2
1	C	222	CYS	6.7
1	A	222	CYS	6.7
1	F	197	THR	6.7

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 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.