



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 08:46 am BST

PDB ID : 5WLG
Title : Crystal Structure of H-2Db with the GAP501 peptide (SQL)
Authors : Gras, S.; Farenc, C.; Josephs, T.; Rossjohn, J.
Deposited on : 2017-07-26
Resolution : 2.10 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

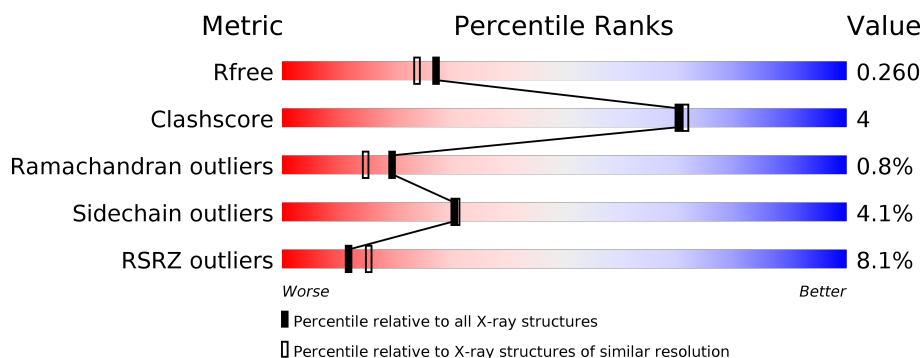
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 $\leq 5\%$. 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	278	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>
1	F	278	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>13%</div> </div> </div>
2	B	99	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
2	G	99	<div> <div>11%</div> <div> <div></div> <div>87%</div> <div>9%</div> </div> </div>
3	C	9	<div> <div></div> <div>100%</div> </div>
3	H	9	<div> <div></div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	182	<div><div></div><div>4%</div><div>87%</div><div>12%</div><div>..</div></div>
4	I	182	<div><div></div><div>16%</div><div>83%</div><div>13%</div><div>..</div></div>
5	E	243	<div><div></div><div>7%</div><div>90%</div><div>9%</div><div></div></div>
5	J	243	<div><div></div><div>14%</div><div>90%</div><div>8%</div><div>..</div></div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13901 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 I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	1	0
			2290	1446	406	429	9			
1	F	277	Total	C	N	O	S	0	0	0
			2271	1435	401	426	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			810	517	137	149	7			
2	G	98	Total	C	N	O	S	0	0	0
			810	517	137	149	7			

- Molecule 3 is a protein called GAP50 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			74	48	12	14			
3	H	9	Total	C	N	O	0	0	0
			74	48	12	14			

- Molecule 4 is a protein called T cell receptor alpha variable 8D-2,Human nkt tcr alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	182	Total	C	N	O	S	0	2	0
			1431	879	249	293	10			
4	I	177	Total	C	N	O	S	0	2	0
			1386	851	242	283	10			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	91	VAL	-	linker	UNP A0A075B616
D	92	TYR	-	linker	UNP A0A075B616
D	93	ALA	-	linker	UNP A0A075B616
D	94	GLN	-	linker	UNP A0A075B616
D	95	GLY	-	linker	UNP A0A075B616
D	96	LEU	-	linker	UNP A0A075B616
D	97	THR	-	linker	UNP A0A075B616
D	98	PHE	-	linker	UNP A0A075B616
D	99	GLY	-	linker	UNP A0A075B616
D	100	LEU	-	linker	UNP A0A075B616
D	101	GLY	-	linker	UNP A0A075B616
D	102	THR	-	linker	UNP A0A075B616
D	103	ARG	-	linker	UNP A0A075B616
D	104	VAL	-	linker	UNP A0A075B616
D	105	SER	-	linker	UNP A0A075B616
D	106	VAL	-	linker	UNP A0A075B616
D	107	PHE	-	linker	UNP A0A075B616
D	108	PRO	-	linker	UNP A0A075B616
D	109	ASN	-	linker	UNP A0A075B616
I	92	VAL	-	linker	UNP A0A075B616
I	93	TYR	-	linker	UNP A0A075B616
I	94	ALA	-	linker	UNP A0A075B616
I	95	GLN	-	linker	UNP A0A075B616
I	96	GLY	-	linker	UNP A0A075B616
I	97	LEU	-	linker	UNP A0A075B616
I	98	THR	-	linker	UNP A0A075B616
I	99	PHE	-	linker	UNP A0A075B616
I	100	GLY	-	linker	UNP A0A075B616
I	101	LEU	-	linker	UNP A0A075B616
I	102	GLY	-	linker	UNP A0A075B616
I	103	THR	-	linker	UNP A0A075B616
I	104	ARG	-	linker	UNP A0A075B616
I	105	VAL	-	linker	UNP A0A075B616
I	106	SER	-	linker	UNP A0A075B616
I	107	VAL	-	linker	UNP A0A075B616
I	108	PHE	-	linker	UNP A0A075B616
I	109	PRO	-	linker	UNP A0A075B616
I	110	ASN	-	linker	UNP A0A075B616

- Molecule 5 is a protein called T-cell receptor beta chain V region C5,Human nkt tcr beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total 1933	C 1215	N 333	O 378	S 7	0	1	0
5	J	241	Total 1928	C 1212	N 333	O 376	S 7	0	2	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	95	ASP	GLY	conflict	UNP P04213
E	96	TRP	THR	conflict	UNP P04213
E	?	-	GLY	deletion	UNP P04213
E	?	-	ALA	deletion	UNP P04213
E	?	-	LEU	deletion	UNP P04213
E	100	GLY	-	insertion	UNP P04213
E	102	LEU	-	insertion	UNP P04213
E	106	GLU	PRO	conflict	UNP P04213
E	108	SER	THR	conflict	UNP P04213
E	109	LYS	ARG	conflict	UNP P04213
E	111	THR	LEU	conflict	UNP P04213
J	95	ASP	GLY	conflict	UNP P04213
J	96	TRP	THR	conflict	UNP P04213
J	?	-	GLY	deletion	UNP P04213
J	?	-	ALA	deletion	UNP P04213
J	?	-	LEU	deletion	UNP P04213
J	100	GLY	-	insertion	UNP P04213
J	102	LEU	-	insertion	UNP P04213
J	106	GLU	PRO	conflict	UNP P04213
J	108	SER	THR	conflict	UNP P04213
J	109	LYS	ARG	conflict	UNP P04213
J	111	THR	LEU	conflict	UNP P04213

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total 1	Na 1	0	0
6	I	1	Total 1	Na 1	0	0
6	A	1	Total 1	Na 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

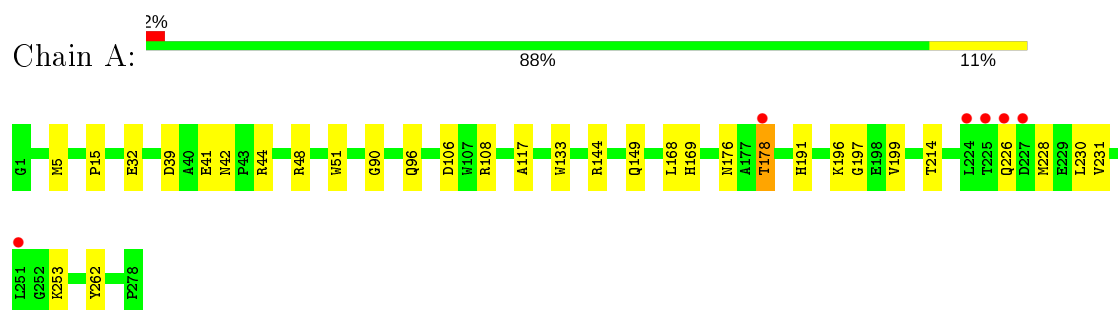
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	215	Total O 215 215	0	0
8	B	97	Total O 97 97	0	0
8	C	1	Total O 1 1	0	0
8	D	97	Total O 97 97	0	0
8	E	120	Total O 120 120	0	0
8	F	139	Total O 139 139	0	0
8	G	47	Total O 47 47	0	0
8	H	1	Total O 1 1	0	0
8	I	66	Total O 66 66	0	0
8	J	107	Total O 107 107	0	0

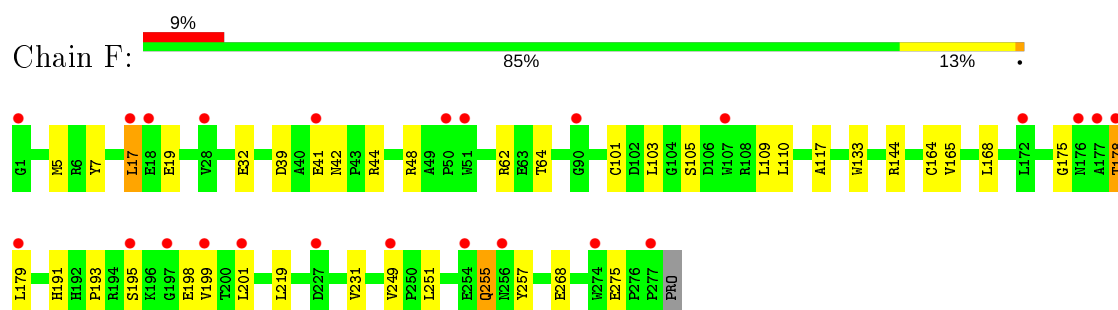
3 Residue-property plots [i](#)

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.

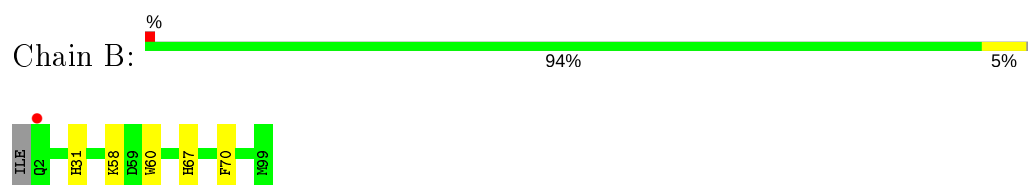
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



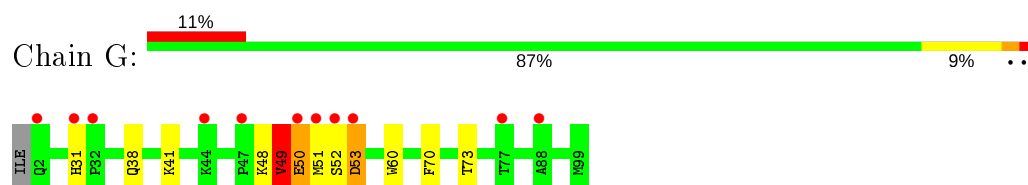
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin




- Molecule 3: GAP50 peptide

Chain C:  100%


There are no outlier residues recorded for this chain.

- Molecule 3: GAP50 peptide

Chain H:  89% 11%




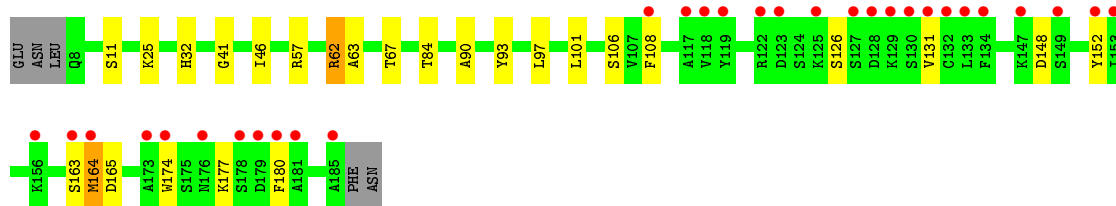
- Molecule 4: T cell receptor alpha variable 8D-2,Human nkt tcr alpha chain

Chain D:  4% 87% 12% ..




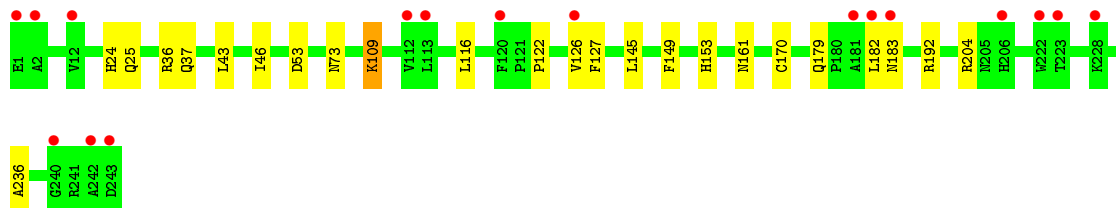
- Molecule 4: T cell receptor alpha variable 8D-2,Human nkt tcr alpha chain

Chain I:  16% 83% 13% ..




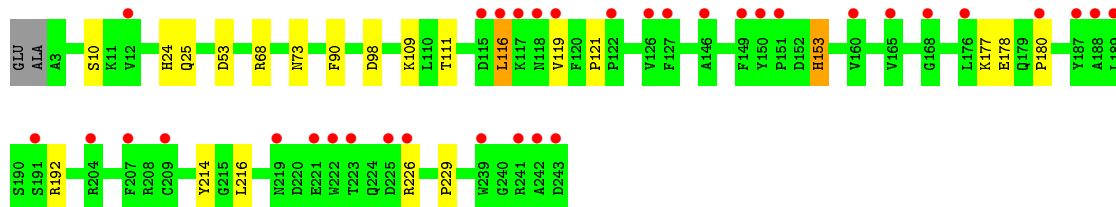
- Molecule 5: T-cell receptor beta chain V region C5,Human nkt tcr beta chain

Chain E:  7% 90% 9%



- Molecule 5: T-cell receptor beta chain V region C5,Human nkt tcr beta chain

Chain J:  14% 90% 8% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.73 Å 70.21 Å 116.49 Å 90.00° 108.28° 90.00°	Depositor
Resolution (Å)	47.05 – 2.10 47.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.05-2.10) 99.9 (47.05-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.10 Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.218 , 0.249 0.227 , 0.260	Depositor DCC
R_{free} test set	5105 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13901	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL

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	0.41	0/2359	0.69	0/3204
1	F	0.40	0/2339	0.71	0/3178
2	B	0.42	0/836	0.65	0/1133
2	G	0.42	0/836	0.69	0/1133
3	C	0.47	0/74	0.77	0/97
3	H	0.51	0/74	0.93	0/97
4	D	0.41	0/1454	0.71	0/1967
4	I	0.38	0/1408	0.69	0/1906
5	E	0.38	0/1986	0.67	0/2705
5	J	0.38	0/1981	0.65	0/2698
All	All	0.40	0/13347	0.69	0/18118

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	2290	0	2162	17	0
1	F	2271	0	2145	20	0
2	B	810	0	783	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	810	0	783	8	0
3	C	74	0	81	0	0
3	H	74	0	81	2	0
4	D	1431	0	1368	11	0
4	I	1386	0	1330	14	0
5	E	1933	0	1817	12	0
5	J	1928	0	1812	13	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
7	A	1	0	0	0	0
8	A	215	0	0	1	0
8	B	97	0	0	2	0
8	C	1	0	0	0	0
8	D	97	0	0	0	0
8	E	120	0	0	0	0
8	F	139	0	0	1	0
8	G	47	0	0	1	0
8	H	1	0	0	0	0
8	I	66	0	0	0	0
8	J	107	0	0	0	0
All	All	13901	0	12362	89	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 4.

The worst 5 of 89 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)
2:G:48:LYS:HA	2:G:49:VAL:HG12	1.18	1.10
2:G:48:LYS:HA	2:G:49:VAL:CG1	2.00	0.91
1:A:196:LYS:HB3	1:A:197:GLY:HA3	1.54	0.90
1:F:103:LEU:HD11	1:F:165:VAL:HG22	1.52	0.90
1:A:196:LYS:CB	1:A:197:GLY:HA3	2.07	0.83

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	277/278 (100%)	262 (95%)	13 (5%)	2 (1%)	22	18
1	F	275/278 (99%)	261 (95%)	11 (4%)	3 (1%)	14	9
2	B	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
2	G	96/99 (97%)	91 (95%)	3 (3%)	2 (2%)	7	3
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	182/182 (100%)	174 (96%)	5 (3%)	3 (2%)	9	5
4	I	177/182 (97%)	169 (96%)	6 (3%)	2 (1%)	14	9
5	E	242/243 (100%)	236 (98%)	5 (2%)	1 (0%)	34	32
5	J	241/243 (99%)	233 (97%)	8 (3%)	0	100	100
All	All	1600/1622 (99%)	1532 (96%)	55 (3%)	13 (1%)	19	15

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	163	MET
1	F	178	THR
2	G	53	ASP
1	A	176	ASN
2	G	49	VAL

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	237/236 (100%)	228 (96%)	9 (4%)	33	34
1	F	235/236 (100%)	222 (94%)	13 (6%)	21	19
2	B	92/93 (99%)	90 (98%)	2 (2%)	52	57
2	G	92/93 (99%)	85 (92%)	7 (8%)	13	10
3	C	8/8 (100%)	8 (100%)	0	100	100
3	H	8/8 (100%)	8 (100%)	0	100	100
4	D	163/161 (101%)	156 (96%)	7 (4%)	29	29
4	I	158/161 (98%)	152 (96%)	6 (4%)	33	34
5	E	210/209 (100%)	202 (96%)	8 (4%)	33	34
5	J	210/209 (100%)	203 (97%)	7 (3%)	38	40
All	All	1413/1414 (100%)	1354 (96%)	59 (4%)	30	30

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	17	LEU
1	F	178	THR
5	J	109	LYS
1	F	19	GLU
1	F	41	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	73	ASN
5	E	183	ASN
5	J	24	HIS
5	E	24	HIS
5	E	37	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	278/278 (100%)	0.11	6 (2%) 62 66	18, 32, 70, 102	4 (1%)
1	F	277/278 (99%)	0.67	24 (8%) 10 13	28, 49, 92, 132	5 (1%)
2	B	98/99 (98%)	-0.15	1 (1%) 82 85	21, 36, 63, 87	1 (1%)
2	G	98/99 (98%)	0.79	11 (11%) 5 6	36, 57, 89, 102	1 (1%)
3	C	9/9 (100%)	-0.18	0 100 100	19, 21, 29, 30	0
3	H	9/9 (100%)	0.02	0 100 100	27, 30, 40, 41	0
4	D	182/182 (100%)	0.34	7 (3%) 40 46	27, 47, 99, 119	0
4	I	177/182 (97%)	0.90	30 (16%) 1 2	30, 58, 127, 158	6 (3%)
5	E	243/243 (100%)	0.57	17 (6%) 16 20	21, 52, 81, 120	0
5	J	241/243 (99%)	0.84	35 (14%) 2 3	28, 58, 114, 138	2 (0%)
All	All	1612/1622 (99%)	0.52	131 (8%) 12 15	18, 48, 97, 158	19 (1%)

The worst 5 of 131 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	17	LEU	20.2
4	I	174	TRP	6.9
4	I	125	LYS	6.4
1	F	197	GLY	6.3
5	E	243	ASP	6.3

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NA	I	201	1/1	0.84	0.17	61,61,61,61	0
7	CL	A	302	1/1	0.85	0.13	67,67,67,67	0
6	NA	G	101	1/1	0.90	0.14	66,66,66,66	0
6	NA	A	301	1/1	0.96	0.11	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.