



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2017 – 11:48 PM EST

PDB ID : 1FVE
Title : X-RAY STRUCTURES OF THE ANTIGEN-BINDING DOMAINS FROM
THREE VARIANTS OF HUMANIZED ANTI-P185-HER2 ANTIBODY 4D5
AND COMPARISON WITH MOLECULAR MODELING
Authors : Eigenbrot, C.; Randal, M.; Presta, L.; Kossiakoff, A.A.
Deposited on : unknown
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

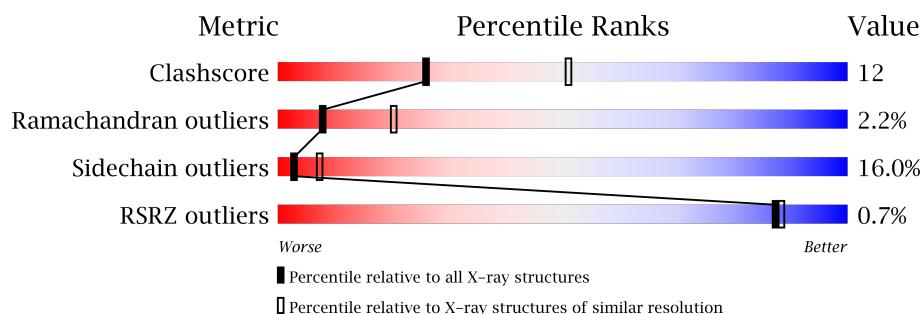
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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. 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	214	<div> <div>54%</div> <div>36%</div> <div>8%</div> <div>.</div> </div>
1	C	214	<div> <div>55%</div> <div>36%</div> <div>7%</div> <div>.</div> </div>
2	B	223	<div> <div>59%</div> <div>32%</div> <div>8%</div> <div>.</div> </div>
2	D	223	<div> <div>60%</div> <div>30%</div> <div>9%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6687 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 IGG1-KAPPA 4D5 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	19	0	0
			1647	1028	277	336	6			
1	C	214	Total	C	N	O	S	20	0	0
			1647	1028	277	336	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SER	PHE	CONFLICT	EMBL X95750
A	28	ASP	SER	CONFLICT	EMBL X95750
A	29	VAL	ILE	CONFLICT	EMBL X95750
A	30	ASN	SER	CONFLICT	EMBL X95750
A	31	THR	SER	CONFLICT	EMBL X95750
A	32	ALA	TYR	CONFLICT	EMBL X95750
A	33	VAL	LEU	CONFLICT	EMBL X95750
A	34	ALA	ASN	CONFLICT	EMBL X95750
A	50	SER	ALA	CONFLICT	EMBL X95750
A	53	PHE	SER	CONFLICT	EMBL X95750
A	55	GLU	GLN	CONFLICT	EMBL X95750
A	66	ARG	GLY	CONFLICT	EMBL X95750
A	91	HIS	SER	CONFLICT	EMBL X95750
A	92	TYR	HIS	CONFLICT	EMBL X95750
A	93	THR	SER	CONFLICT	EMBL X95750
A	96	PRO	TYR	CONFLICT	EMBL X95750
A	103	LYS	ASN	CONFLICT	EMBL X95750
A	104	VAL	LEU	CONFLICT	EMBL X95750
C	14	SER	PHE	CONFLICT	EMBL X95750
C	28	ASP	SER	CONFLICT	EMBL X95750
C	29	VAL	ILE	CONFLICT	EMBL X95750
C	30	ASN	SER	CONFLICT	EMBL X95750
C	31	THR	SER	CONFLICT	EMBL X95750
C	32	ALA	TYR	CONFLICT	EMBL X95750
C	33	VAL	LEU	CONFLICT	EMBL X95750

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Chain	Residue	Modelled	Actual	Comment	Reference
C	34	ALA	ASN	CONFLICT	EMBL X95750
C	50	SER	ALA	CONFLICT	EMBL X95750
C	53	PHE	SER	CONFLICT	EMBL X95750
C	55	GLU	GLN	CONFLICT	EMBL X95750
C	66	ARG	GLY	CONFLICT	EMBL X95750
C	91	HIS	SER	CONFLICT	EMBL X95750
C	92	TYR	HIS	CONFLICT	EMBL X95750
C	93	THR	SER	CONFLICT	EMBL X95750
C	96	PRO	TYR	CONFLICT	EMBL X95750
C	103	LYS	ASN	CONFLICT	EMBL X95750
C	104	VAL	LEU	CONFLICT	EMBL X95750

- Molecule 2 is a protein called IGG1-KAPPA 4D5 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	223	Total	C	N	O	S	44	0	0
			1671	1054	282	328	7			
2	D	223	Total	C	N	O	S	44	0	0
			1671	1054	282	328	7			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASN	ALA	CONFLICT	EMBL Y14735
B	29	ILE	TYR	CONFLICT	EMBL Y14735
B	30	LYS	SER	CONFLICT	EMBL Y14735
B	31	ASP	SER	CONFLICT	EMBL Y14735
B	32	THR	PHE	CONFLICT	EMBL Y14735
B	33	TYR	TRP	CONFLICT	EMBL Y14735
B	34	ILE	MET	CONFLICT	EMBL Y14735
B	43	LYS	ARG	CONFLICT	EMBL Y14735
B	46	GLU	VAL	CONFLICT	EMBL Y14735
B	49	ALA	SER	CONFLICT	EMBL Y14735
B	52	TYR	ASN	CONFLICT	EMBL Y14735
B	54	THR	ASP	CONFLICT	EMBL Y14735
B	55	ASN	GLY	CONFLICT	EMBL Y14735
B	56	GLY	ARG	CONFLICT	EMBL Y14735
B	57	TYR	ILE	CONFLICT	EMBL Y14735
B	59	ARG	VAL	CONFLICT	EMBL Y14735
B	63	SER	ALA	CONFLICT	EMBL Y14735
B	72	ALA	ARG	CONFLICT	EMBL Y14735
B	74	THR	ASN	CONFLICT	EMBL Y14735

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Chain	Residue	Modelled	Actual	Comment	Reference
B	75	SER	ALA	CONFLICT	EMBL Y14735
B	79	ALA	LEU	CONFLICT	EMBL Y14735
B	85	SER	ASN	CONFLICT	EMBL Y14735
B	97	SER	ALA	CONFLICT	EMBL Y14735
B	99	TRP	-	INSERTION	EMBL Y14735
B	100	GLY	-	INSERTION	EMBL Y14735
B	102	ASP	THR	CONFLICT	EMBL Y14735
B	103	GLY	ARG	CONFLICT	EMBL Y14735
B	?	-	LEU	DELETION	EMBL Y14735
B	?	-	GLU	DELETION	EMBL Y14735
B	?	-	LEU	DELETION	EMBL Y14735
B	?	-	THR	DELETION	EMBL Y14735
B	?	-	SER	DELETION	EMBL Y14735
B	?	-	ARG	DELETION	EMBL Y14735
B	105	TYR	GLY	CONFLICT	EMBL Y14735
B	106	ALA	GLN	CONFLICT	EMBL Y14735
B	109	TYR	GLN	CONFLICT	EMBL Y14735
D	28	ASN	ALA	CONFLICT	EMBL Y14735
D	29	ILE	TYR	CONFLICT	EMBL Y14735
D	30	LYS	SER	CONFLICT	EMBL Y14735
D	31	ASP	SER	CONFLICT	EMBL Y14735
D	32	THR	PHE	CONFLICT	EMBL Y14735
D	33	TYR	TRP	CONFLICT	EMBL Y14735
D	34	ILE	MET	CONFLICT	EMBL Y14735
D	43	LYS	ARG	CONFLICT	EMBL Y14735
D	46	GLU	VAL	CONFLICT	EMBL Y14735
D	49	ALA	SER	CONFLICT	EMBL Y14735
D	52	TYR	ASN	CONFLICT	EMBL Y14735
D	54	THR	ASP	CONFLICT	EMBL Y14735
D	55	ASN	GLY	CONFLICT	EMBL Y14735
D	56	GLY	ARG	CONFLICT	EMBL Y14735
D	57	TYR	ILE	CONFLICT	EMBL Y14735
D	59	ARG	VAL	CONFLICT	EMBL Y14735
D	63	SER	ALA	CONFLICT	EMBL Y14735
D	72	ALA	ARG	CONFLICT	EMBL Y14735
D	74	THR	ASN	CONFLICT	EMBL Y14735
D	75	SER	ALA	CONFLICT	EMBL Y14735
D	79	ALA	LEU	CONFLICT	EMBL Y14735
D	85	SER	ASN	CONFLICT	EMBL Y14735
D	97	SER	ALA	CONFLICT	EMBL Y14735
D	99	TRP	-	INSERTION	EMBL Y14735
D	100	GLY	-	INSERTION	EMBL Y14735

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Chain	Residue	Modelled	Actual	Comment	Reference
D	102	ASP	THR	CONFLICT	EMBL Y14735
D	103	GLY	ARG	CONFLICT	EMBL Y14735
D	?	-	LEU	DELETION	EMBL Y14735
D	?	-	GLU	DELETION	EMBL Y14735
D	?	-	LEU	DELETION	EMBL Y14735
D	?	-	THR	DELETION	EMBL Y14735
D	?	-	SER	DELETION	EMBL Y14735
D	?	-	ARG	DELETION	EMBL Y14735
D	105	TYR	GLY	CONFLICT	EMBL Y14735
D	106	ALA	GLN	CONFLICT	EMBL Y14735
D	109	TYR	GLN	CONFLICT	EMBL Y14735

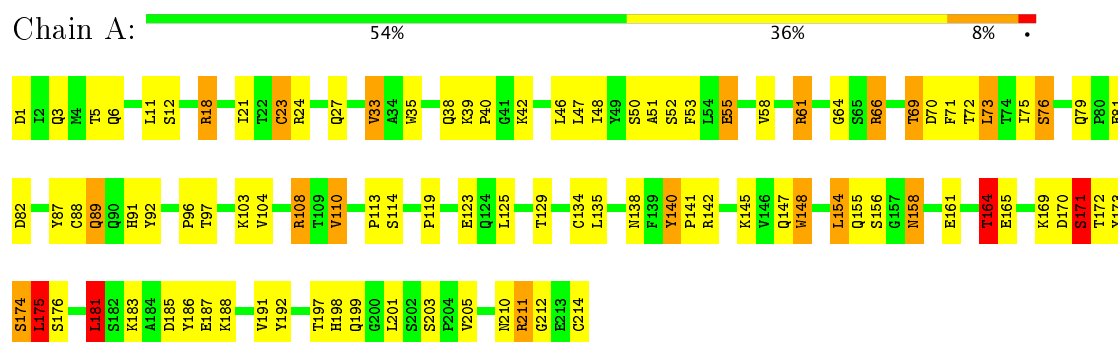
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	12	Total O 12 12	0	0
3	C	10	Total O 10 10	0	0
3	D	18	Total O 18 18	0	0

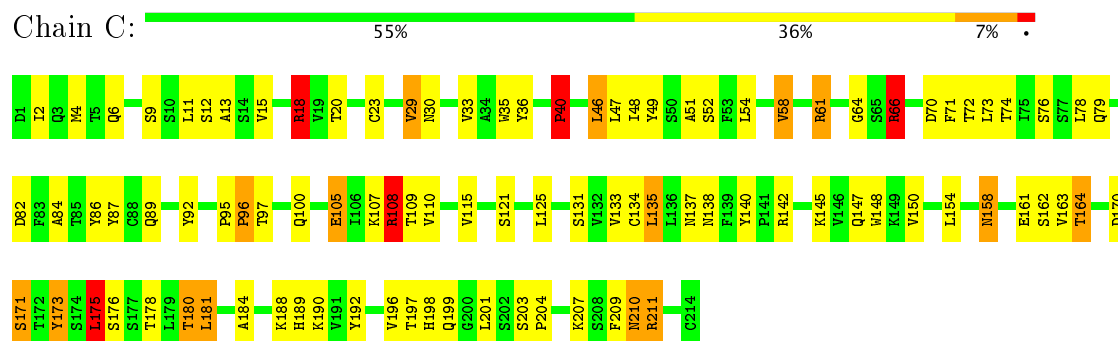
3 Residue-property plots [i](#)

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.

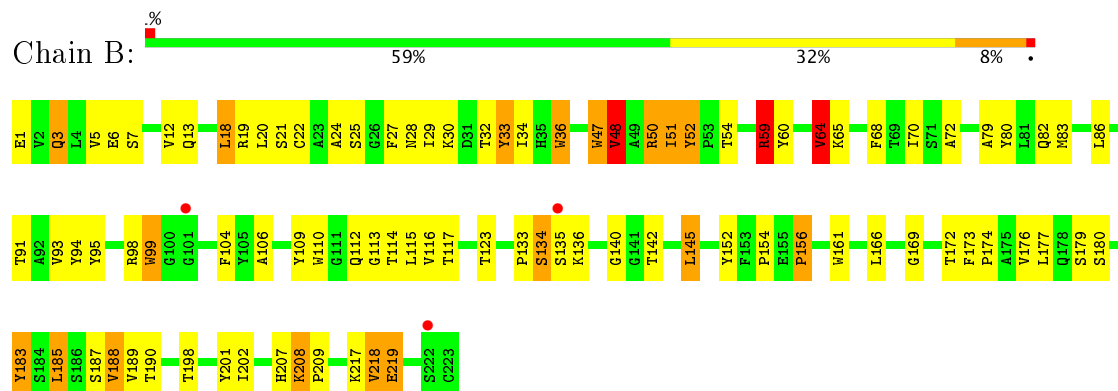
• Molecule 1: IGG1-KAPPA 4D5 FAB (LIGHT CHAIN)



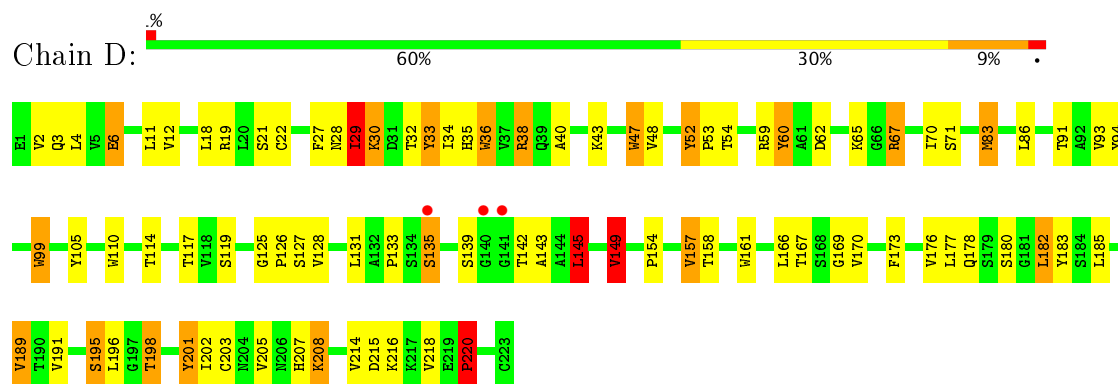
• Molecule 1: IGG1-KAPPA 4D5 FAB (LIGHT CHAIN)



• Molecule 2: IGG1-KAPPA 4D5 FAB (HEAVY CHAIN)



● Molecule 2: IGG1-KAPPA 4D5 FAB (HEAVY CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	39.20 Å 80.20 Å 86.10 Å 113.10° 92.70° 102.60°	Depositor
Resolution (Å)	10.00 – 2.70 10.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 67.1 (10.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.171 , (Not available) 0.163 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 63.5	EDS
L-test for twinning ¹	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6687	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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

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	0.92	0/1683	1.73	28/2286 (1.2%)
1	C	0.94	0/1683	1.85	43/2286 (1.9%)
2	B	1.02	0/1713	1.88	49/2333 (2.1%)
2	D	1.03	2/1713 (0.1%)	1.88	43/2333 (1.8%)
All	All	0.98	2/6792 (0.0%)	1.84	163/9238 (1.8%)

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
1	C	0	1
2	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	99	TRP	CG-CD2	-6.72	1.32	1.43
2	D	99	TRP	CA-CB	-5.50	1.41	1.53

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	ARG	NE-CZ-NH1	14.19	127.39	120.30
1	C	66	ARG	NE-CZ-NH2	-13.04	113.78	120.30
1	C	108	ARG	NE-CZ-NH1	12.05	126.32	120.30
2	D	38	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	A	33	VAL	CG1-CB-CG2	-11.33	92.77	110.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	TYR	Sidechain
1	C	95	PRO	Peptide
2	D	33	TYR	Sidechain

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	1647	0	1596	41	0
1	C	1647	0	1596	34	0
2	B	1671	0	1628	41	0
2	D	1671	0	1628	41	0
3	A	11	0	0	0	0
3	B	12	0	0	1	0
3	C	10	0	0	0	0
3	D	18	0	0	0	0
All	All	6687	0	6448	152	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 152 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:B:91:THR:HG23	2:B:117:THR:HA	1.51	0.92
2:D:133:PRO:HG3	2:D:145:LEU:HD12	1.60	0.82
2:D:133:PRO:HD3	2:D:145:LEU:HB3	1.72	0.71
2:B:104:PHE:HD2	2:B:106:ALA:HB3	1.56	0.70
2:D:128:VAL:HG21	2:D:205:VAL:HG21	1.74	0.70

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	212/214 (99%)	188 (89%)	19 (9%)	5 (2%)	7	17
1	C	212/214 (99%)	190 (90%)	16 (8%)	6 (3%)	6	14
2	B	221/223 (99%)	203 (92%)	14 (6%)	4 (2%)	10	25
2	D	221/223 (99%)	200 (90%)	17 (8%)	4 (2%)	10	25
All	All	866/874 (99%)	781 (90%)	66 (8%)	19 (2%)	8	20

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	133	PRO
2	B	134	SER
1	C	158	ASN
1	C	171	SER
1	A	110	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	189/189 (100%)	155 (82%)	34 (18%)	2	5
1	C	189/189 (100%)	156 (82%)	33 (18%)	2	5
2	B	184/184 (100%)	159 (86%)	25 (14%)	4	10
2	D	184/184 (100%)	157 (85%)	27 (15%)	3	9
All	All	746/746 (100%)	627 (84%)	119 (16%)	3	7

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	190	THR
1	C	40	PRO
2	D	157	VAL
2	B	208	LYS
1	C	15	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	28	ASN
2	B	112	GLN
1	C	100	GLN
1	A	210	ASN
2	B	207	HIS

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 carbohydrates 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 ⓘ

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	212/214 (99%)	-0.90	0	100 100	3, 18, 37, 49	1 (0%)
1	C	211/214 (98%)	-0.92	0	100 100	2, 17, 38, 46	0
2	B	216/223 (96%)	-0.98	3 (1%)	75 76	2, 10, 40, 59	0
2	D	217/223 (97%)	-0.97	3 (1%)	75 76	2, 11, 39, 61	0
All	All	856/874 (97%)	-0.94	6 (0%)	87 88	2, 14, 38, 61	1 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	135	SER	3.4
2	D	140	GLY	3.0
2	D	141	GLY	2.6
2	B	135	SER	2.3
2	B	101	GLY	2.1

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.