



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:23 PM GMT

PDB ID : 1AHW
Title : A COMPLEX OF EXTRACELLULAR DOMAIN OF TISSUE FACTOR
WITH AN INHIBITORY FAB (5G9)
Authors : Huang, M.; Syed, R.; Stura, E.A.; Stone, M.J.; Stefanko, R.S.; Ruf, W.;
Edgington, T.S.; Wilson, I.A.
Deposited on : 1997-04-10
Resolution : 3.00 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

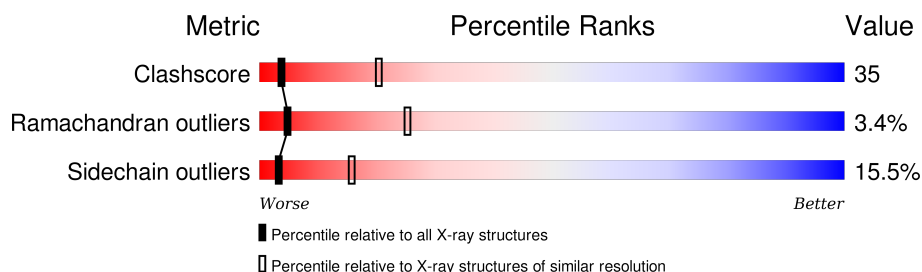
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	
1	D	214	
2	B	214	
2	E	214	
3	C	219	
3	F	219	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9830 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 IMMUNOGLOBULIN FAB 5G9 (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1672	1040	278	346	8			
1	D	214	Total	C	N	O	S	0	0	0
			1672	1040	278	346	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ARG	TYR	CONFLICT	UNP P01837
A	31	LYS	SER	CONFLICT	UNP P01837
A	34	ASN	SER	CONFLICT	UNP P01837
A	36	TYR	PHE	CONFLICT	UNP P01837
A	41	TRP	GLY	CONFLICT	UNP P01837
A	50	TYR	ARG	CONFLICT	UNP P01837
A	52	THR	ASN	CONFLICT	UNP P01837
A	53	SER	ARG	CONFLICT	UNP P01837
A	55	ALA	VAL	CONFLICT	UNP P01837
A	80	SER	TYR	CONFLICT	UNP P01837
A	81	ASP	GLU	CONFLICT	UNP P01837
A	83	THR	LEU	CONFLICT	UNP P01837
A	84	ALA	GLY	CONFLICT	UNP P01837
A	85	THR	ILE	CONFLICT	UNP P01837
A	91	HIS	PHE	CONFLICT	UNP P01837
A	92	GLY	ASP	CONFLICT	UNP P01837
A	94	SER	PHE	CONFLICT	UNP P01837
A	107	ASN	LYS	CONFLICT	UNP P01837
D	30	ARG	TYR	CONFLICT	UNP P01837
D	31	LYS	SER	CONFLICT	UNP P01837
D	34	ASN	SER	CONFLICT	UNP P01837
D	36	TYR	PHE	CONFLICT	UNP P01837
D	41	TRP	GLY	CONFLICT	UNP P01837
D	50	TYR	ARG	CONFLICT	UNP P01837
D	52	THR	ASN	CONFLICT	UNP P01837

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Chain	Residue	Modelled	Actual	Comment	Reference
D	53	SER	ARG	CONFLICT	UNP P01837
D	55	ALA	VAL	CONFLICT	UNP P01837
D	80	SER	TYR	CONFLICT	UNP P01837
D	81	ASP	GLU	CONFLICT	UNP P01837
D	83	THR	LEU	CONFLICT	UNP P01837
D	84	ALA	GLY	CONFLICT	UNP P01837
D	85	THR	ILE	CONFLICT	UNP P01837
D	91	HIS	PHE	CONFLICT	UNP P01837
D	92	GLY	ASP	CONFLICT	UNP P01837
D	94	SER	PHE	CONFLICT	UNP P01837
D	107	ASN	LYS	CONFLICT	UNP P01837

- Molecule 2 is a protein called IMMUNOGLOBULIN FAB 5G9 (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1632	1034	263	329	6			
2	E	214	Total	C	N	O	S	0	0	0
			1632	1034	263	329	6			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLU	-	INSERTION	PIR S49220
B	2	ILE	-	INSERTION	PIR S49220
B	?	-	VAL	DELETION	PIR S49220
B	?	-	LYS	DELETION	PIR S49220
B	5	GLN	LEU	CONFLICT	PIR S49220
B	6	GLN	GLU	CONFLICT	PIR S49220
B	13	ARG	LYS	CONFLICT	PIR S49220
B	14	PRO	SER	CONFLICT	PIR S49220
B	17	LEU	SER	CONFLICT	PIR S49220
B	23	LYS	THR	CONFLICT	PIR S49220
B	32	TYR	THR	CONFLICT	PIR S49220
B	50	LEU	ARG	CONFLICT	PIR S49220
B	54	GLU	ALA	CONFLICT	PIR S49220
B	57	ASN	GLU	CONFLICT	PIR S49220
B	58	THR	ILE	CONFLICT	PIR S49220
B	59	ILE	LYS	CONFLICT	PIR S49220
B	67	LYS	THR	CONFLICT	PIR S49220
B	69	SER	THR	CONFLICT	PIR S49220
B	76	SER	THR	CONFLICT	PIR S49220

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Chain	Residue	Modelled	Actual	Comment	Reference
B	97	ALA	VAL	CONFLICT	PIR S49220
B	?	-	ARG	DELETION	PIR S49220
B	?	-	GLY	DELETION	PIR S49220
B	99	ASP	TYR	CONFLICT	PIR S49220
B	100	ASN	GLY	CONFLICT	PIR S49220
B	102	TYR	SER	CONFLICT	PIR S49220
B	103	TYR	GLN	CONFLICT	PIR S49220
B	104	PHE	GLU	CONFLICT	PIR S49220
B	105	ASP	PRO	CONFLICT	PIR S49220
E	1	GLU	-	INSERTION	PIR S49220
E	2	ILE	-	INSERTION	PIR S49220
E	?	-	VAL	DELETION	PIR S49220
E	?	-	LYS	DELETION	PIR S49220
E	5	GLN	LEU	CONFLICT	PIR S49220
E	6	GLN	GLU	CONFLICT	PIR S49220
E	13	ARG	LYS	CONFLICT	PIR S49220
E	14	PRO	SER	CONFLICT	PIR S49220
E	17	LEU	SER	CONFLICT	PIR S49220
E	23	LYS	THR	CONFLICT	PIR S49220
E	32	TYR	THR	CONFLICT	PIR S49220
E	50	LEU	ARG	CONFLICT	PIR S49220
E	54	GLU	ALA	CONFLICT	PIR S49220
E	57	ASN	GLU	CONFLICT	PIR S49220
E	58	THR	ILE	CONFLICT	PIR S49220
E	59	ILE	LYS	CONFLICT	PIR S49220
E	67	LYS	THR	CONFLICT	PIR S49220
E	69	SER	THR	CONFLICT	PIR S49220
E	76	SER	THR	CONFLICT	PIR S49220
E	97	ALA	VAL	CONFLICT	PIR S49220
E	?	-	ARG	DELETION	PIR S49220
E	?	-	GLY	DELETION	PIR S49220
E	99	ASP	TYR	CONFLICT	PIR S49220
E	100	ASN	GLY	CONFLICT	PIR S49220
E	102	TYR	SER	CONFLICT	PIR S49220
E	103	TYR	GLN	CONFLICT	PIR S49220
E	104	PHE	GLU	CONFLICT	PIR S49220
E	105	ASP	PRO	CONFLICT	PIR S49220

- Molecule 3 is a protein called TISSUE FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	200	Total	C	N	O	S	0	0	0
			1611	1021	262	323	5			

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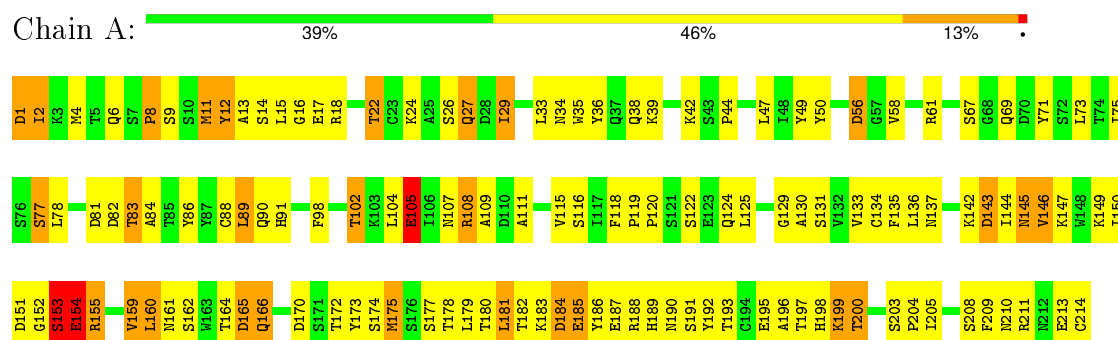
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	200	Total	C	N	O	S	0	0	0
			1611	1021	262	323	5			

3 Residue-property plots

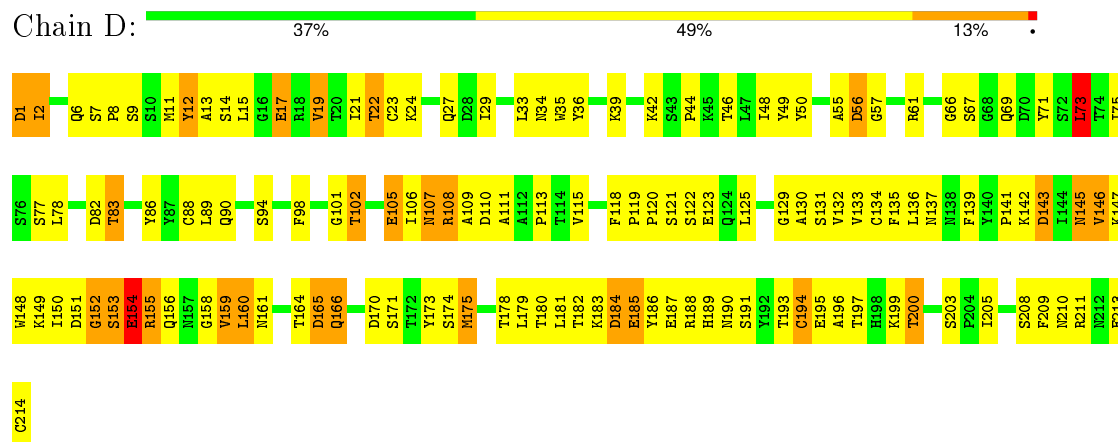
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

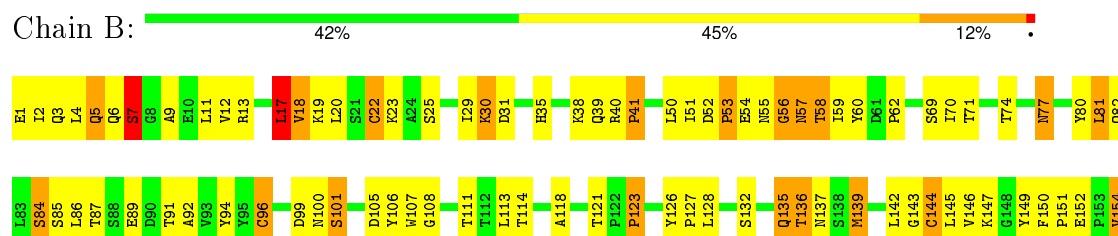
• Molecule 1: IMMUNOGLOBULIN FAB 5G9 (LIGHT CHAIN)

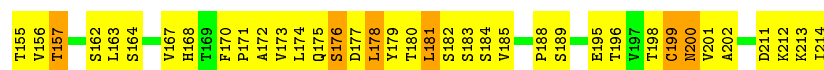


• Molecule 1: IMMUNOGLOBULIN FAB 5G9 (LIGHT CHAIN)



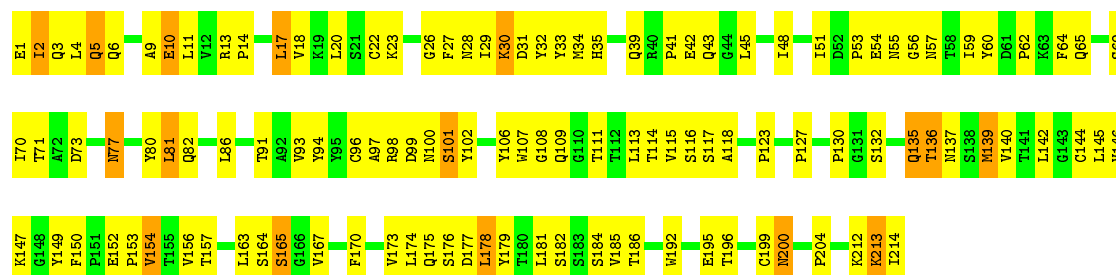
• Molecule 2: IMMUNOGLOBULIN FAB 5G9 (HEAVY CHAIN)





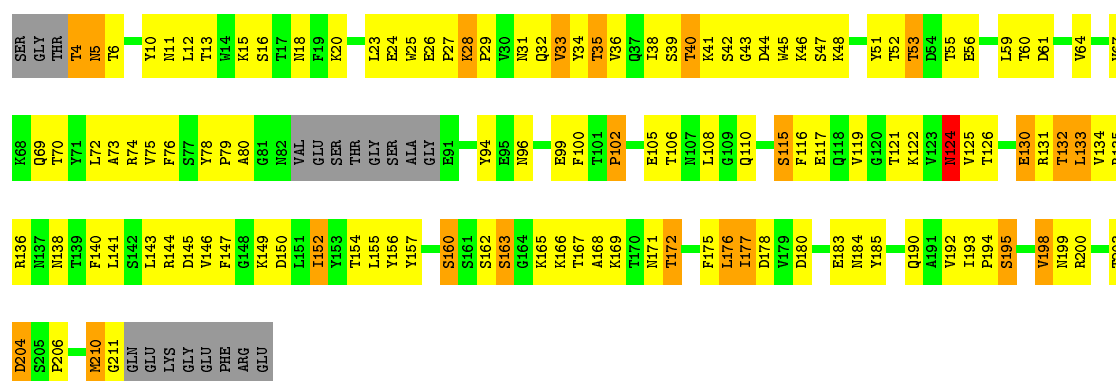
• Molecule 2: IMMUNOGLOBULIN FAB 5G9 (HEAVY CHAIN)

Chain E: 44% 49% 7%



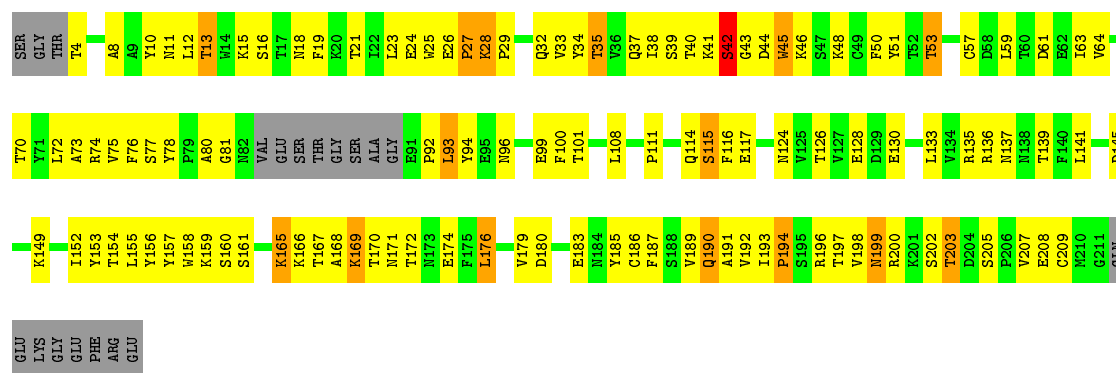
• Molecule 3: TISSUE FACTOR

Chain C: 34% 47% 10% 9%



• Molecule 3: TISSUE FACTOR

Chain F: 37% 47% 7% 9%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.30Å 73.31Å 115.83Å 90.00° 90.89° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00	Depositor
% Data completeness (in resolution range)	78.1 (7.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.217 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9830	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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	0.86	1/1711 (0.1%)	1.04	1/2321 (0.0%)
1	D	0.84	0/1711	0.98	2/2321 (0.1%)
2	B	0.86	0/1675	1.03	4/2292 (0.2%)
2	E	0.77	0/1675	1.00	2/2292 (0.1%)
3	C	0.78	0/1646	0.96	1/2239 (0.0%)
3	F	0.74	1/1646 (0.1%)	0.92	0/2239
All	All	0.81	2/10064 (0.0%)	0.99	10/13704 (0.1%)

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	E	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	45	TRP	CB-CG	-5.79	1.39	1.50
1	A	105	GLU	CG-CD	5.20	1.59	1.51

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	81	LEU	CA-CB-CG	7.35	132.20	115.30
2	E	213	LYS	N-CA-C	-6.22	94.20	111.00
2	B	56	GLY	N-CA-C	5.98	128.04	113.10
1	A	89	LEU	CA-CB-CG	5.90	128.87	115.30
3	C	133	LEU	CA-CB-CG	-5.84	101.88	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	TYR	Sidechain
2	E	94	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	1672	0	1590	125	0
1	D	1672	0	1590	131	0
2	B	1632	0	1580	106	0
2	E	1632	0	1580	110	0
3	C	1611	0	1564	111	0
3	F	1611	0	1564	130	0
All	All	9830	0	9468	679	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 35.

The worst 5 of 679 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:E:91:THR:HG23	2:E:114:THR:HA	1.35	1.06
3:F:136:ARG:HB3	3:F:141:LEU:HD11	1.35	1.05
1:D:6:GLN:HE21	1:D:102:THR:HG23	1.29	0.94
1:D:196:ALA:HB3	1:D:205:ILE:HB	1.51	0.92
2:E:4:LEU:HD23	2:E:22:CYS:SG	2.11	0.90

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%)	176 (83%)	29 (14%)	7 (3%)	5	26
1	D	212/214 (99%)	177 (84%)	29 (14%)	6 (3%)	6	30
2	B	212/214 (99%)	177 (84%)	26 (12%)	9 (4%)	3	20
2	E	212/214 (99%)	175 (82%)	30 (14%)	7 (3%)	5	26
3	C	196/219 (90%)	158 (81%)	31 (16%)	7 (4%)	4	24
3	F	196/219 (90%)	161 (82%)	29 (15%)	6 (3%)	5	28
All	All	1240/1294 (96%)	1024 (83%)	174 (14%)	42 (3%)	5	25

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
1	A	153	SER
2	B	41	PRO
2	B	56	GLY
3	C	5	ASN

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	191/191 (100%)	154 (81%)	37 (19%)	2	9
1	D	191/191 (100%)	154 (81%)	37 (19%)	2	9
2	B	185/185 (100%)	155 (84%)	30 (16%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	185/185 (100%)	167 (90%)	18 (10%)	10	37
3	C	186/200 (93%)	158 (85%)	28 (15%)	3	17
3	F	186/200 (93%)	162 (87%)	24 (13%)	5	23
All	All	1124/1152 (98%)	950 (84%)	174 (16%)	3	16

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	102	PRO
1	D	7	SER
3	F	101	THR
3	C	117	GLU
3	C	172	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	184	ASN
1	D	145	ASN
3	F	137	ASN
1	D	34	ASN
1	D	124	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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.