



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:36 AM GMT

PDB ID : 2XNY  
Title : A FRAGMENT OF STREPTOCOCCAL M1 PROTEIN IN COMPLEX WITH HUMAN FIBRINOGEN  
Authors : Macheboeuf, P.; Y Fu, C.; Zinkernagel, A.S.; Johnson, J.E.; Nizet, V.; Ghosh, P.  
Deposited on : 2010-08-06  
Resolution : 7.50 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](mailto: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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

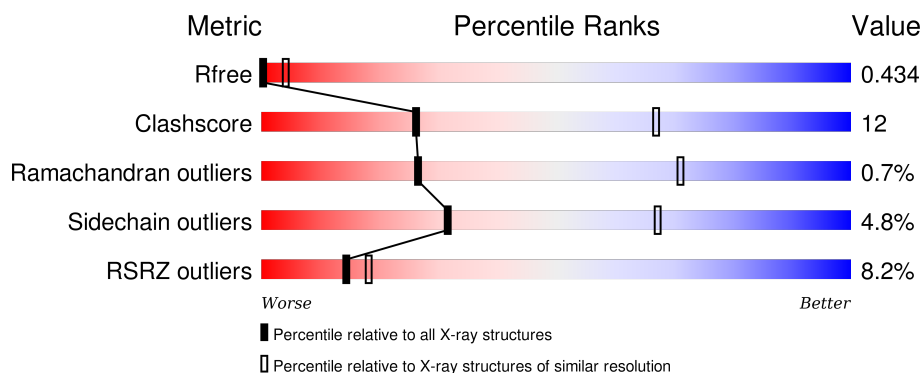
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 7.50 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))
$R_{free}$	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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  $\geq 3$ , 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	87	<div> <div>6%</div> <div>55%</div> <div>9%</div> <div>34%</div> </div>
1	D	87	<div> <div>6%</div> <div>55%</div> <div>9%</div> <div>34%</div> </div>
2	B	328	<div> <div>9%</div> <div>77%</div> <div>11%</div> <div>9%</div> </div>
2	E	328	<div> <div>4%</div> <div>78%</div> <div>11%</div> <div>9%</div> </div>
3	C	319	<div> <div>8%</div> <div>80%</div> <div>9%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	319	<div><div><div></div><div></div><div></div><div></div></div><div>6%80%8%10%</div></div>
4	M	102	<div><div><div></div><div></div><div></div><div></div></div><div>6%8%21%7%64%</div></div>
4	N	102	<div><div><div></div><div></div><div></div><div></div></div><div>8%15%15%6%65%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10956 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 FIBRINOGEN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	57	Total	C	N	O	S	0	0	0
			463	283	88	89	3			
1	D	57	Total	C	N	O	S	0	0	0
			463	283	88	89	3			

- Molecule 2 is a protein called FIBRINOGEN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	0	0
			2392	1494	422	454	22			
2	E	298	Total	C	N	O	S	0	0	0
			2392	1494	422	454	22			

- Molecule 3 is a protein called FIBRINOGEN GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	288	Total	C	N	O	S	0	0	0
			2311	1467	390	443	11			
3	F	288	Total	C	N	O	S	0	0	0
			2311	1467	390	443	11			

- Molecule 4 is a protein called M PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	37	Total	C	N	O	0	0	0
			315	192	58	65			
4	N	36	Total	C	N	O	0	0	0
			309	189	55	65			

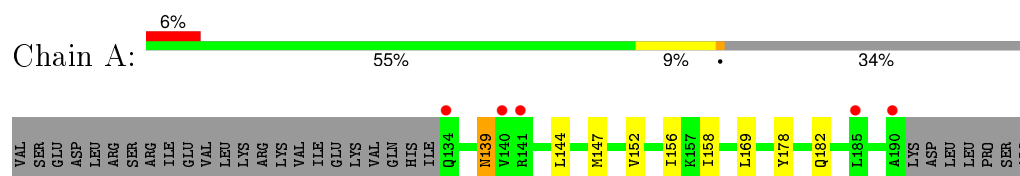
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	40	MET	-	EXPRESSION TAG	UNP Q48WD8
M	41	VAL	-	EXPRESSION TAG	UNP Q48WD8
M	136	HIS	-	EXPRESSION TAG	UNP Q48WD8
M	137	HIS	-	EXPRESSION TAG	UNP Q48WD8
M	138	HIS	-	EXPRESSION TAG	UNP Q48WD8
M	139	HIS	-	EXPRESSION TAG	UNP Q48WD8
M	140	HIS	-	EXPRESSION TAG	UNP Q48WD8
M	141	HIS	-	EXPRESSION TAG	UNP Q48WD8
N	40	MET	-	EXPRESSION TAG	UNP Q48WD8
N	41	VAL	-	EXPRESSION TAG	UNP Q48WD8
N	136	HIS	-	EXPRESSION TAG	UNP Q48WD8
N	137	HIS	-	EXPRESSION TAG	UNP Q48WD8
N	138	HIS	-	EXPRESSION TAG	UNP Q48WD8
N	139	HIS	-	EXPRESSION TAG	UNP Q48WD8
N	140	HIS	-	EXPRESSION TAG	UNP Q48WD8
N	141	HIS	-	EXPRESSION TAG	UNP Q48WD8

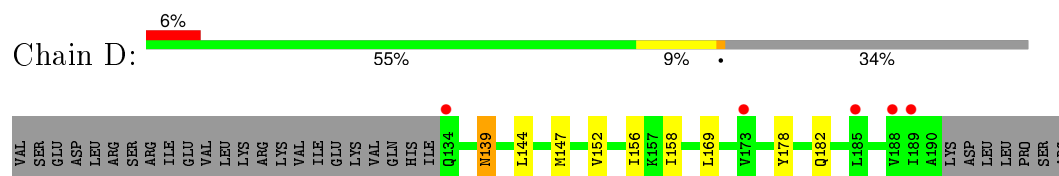
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

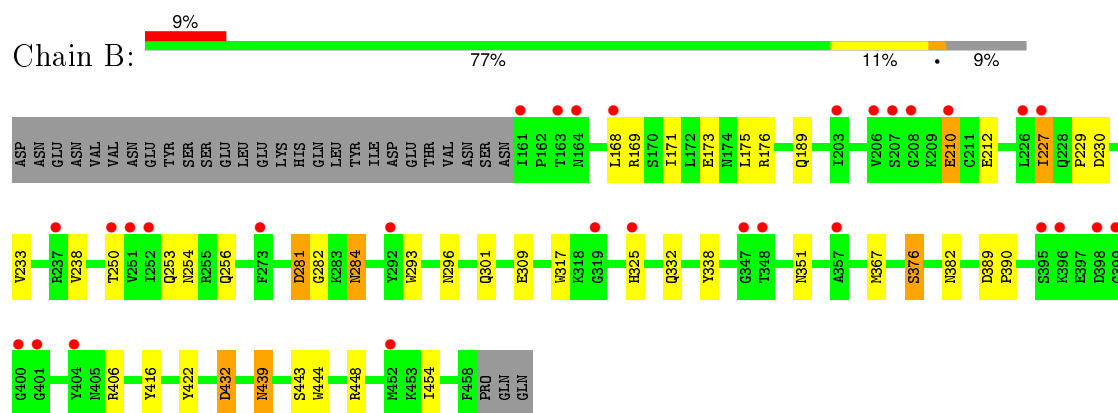
#### • Molecule 1: FIBRINOGEN ALPHA CHAIN



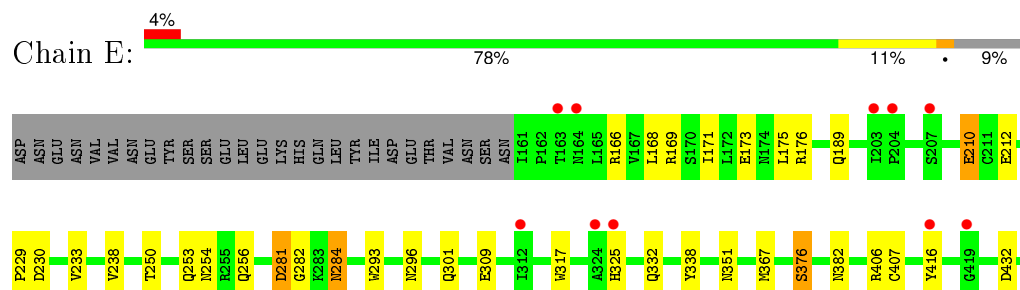
#### • Molecule 1: FIBRINOGEN ALPHA CHAIN



#### • Molecule 2: FIBRINOGEN BETA CHAIN

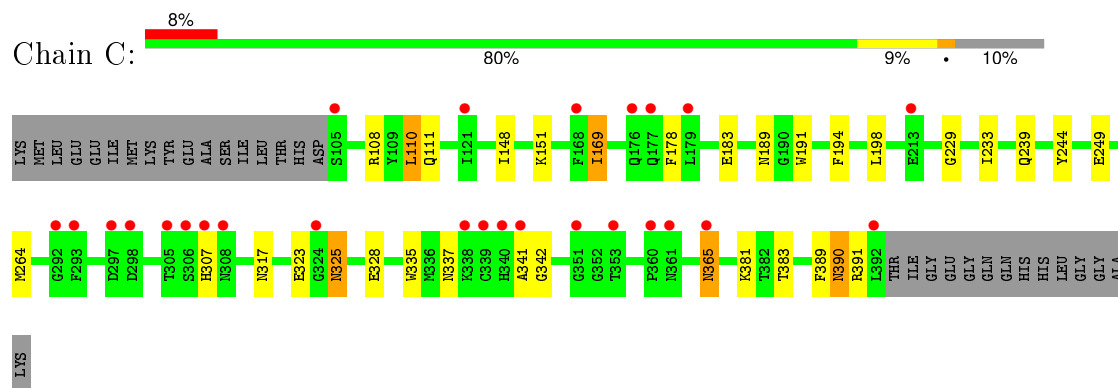


#### • Molecule 2: FIBRINOGEN BETA CHAIN

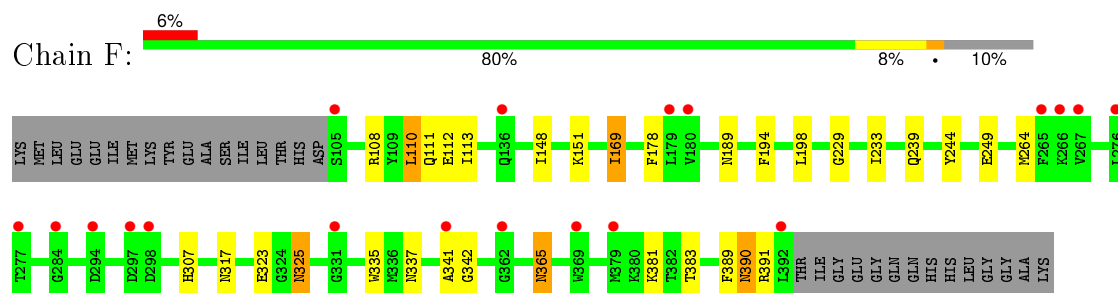




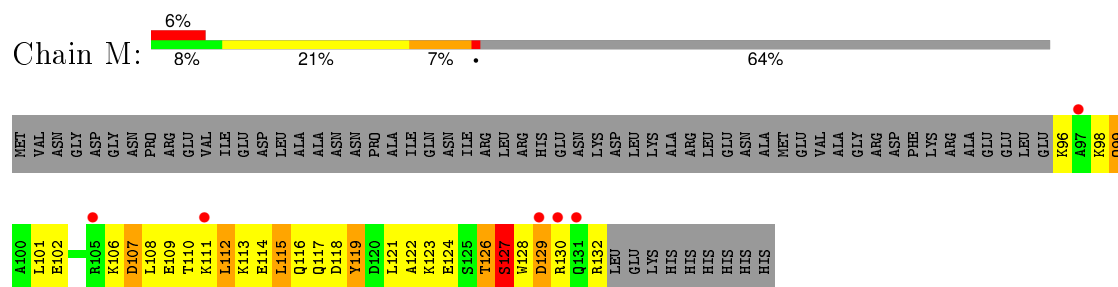
• Molecule 3: FIBRINOGEN GAMMA CHAIN



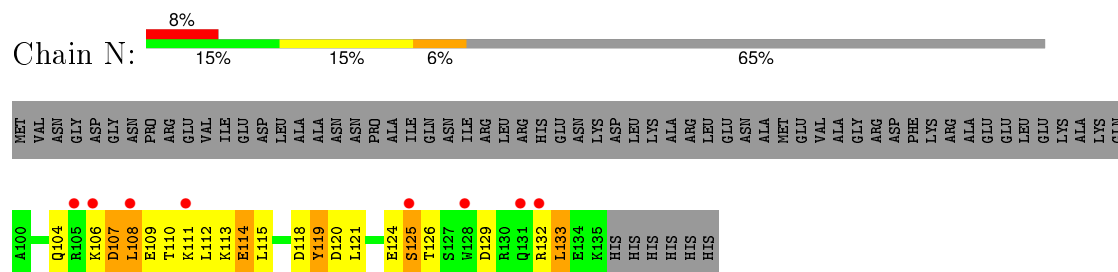
• Molecule 3: FIBRINOGEN GAMMA CHAIN



• Molecule 4: M PROTEIN



• Molecule 4: M PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.69Å 165.69Å 289.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	142.86 – 7.50 47.83 – 6.00	Depositor EDS
% Data completeness (in resolution range)	92.1 (142.86-7.50) 43.9 (47.83-6.00)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 6.15Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.424 , 0.408 0.423 , 0.434	Depositor DCC
$R_{free}$ test set	202 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	98.8	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.4	EDS
Estimated twinning fraction	0.086 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 5265 reflections	Xtriage
$F_o, F_c$ correlation	0.65	EDS
Total number of atoms	10956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.32	0/463	0.52	0/617
1	D	0.32	0/463	0.52	0/617
2	B	0.42	0/2453	0.55	1/3312 (0.0%)
2	E	0.42	0/2453	0.55	1/3312 (0.0%)
3	C	0.50	0/2375	0.58	0/3211
3	F	0.50	0/2375	0.58	0/3211
4	M	1.86	8/317 (2.5%)	1.35	6/421 (1.4%)
4	N	1.63	3/311 (1.0%)	1.31	5/414 (1.2%)
All	All	0.60	11/11210 (0.1%)	0.63	13/15115 (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
4	N	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	124	GLU	CD-OE2	12.07	1.39	1.25
4	M	118	ASP	CG-OD1	11.15	1.51	1.25
4	M	132	ARG	CZ-NH1	9.32	1.45	1.33
4	M	107	ASP	CG-OD2	8.91	1.45	1.25
4	M	127	SER	CB-OG	8.71	1.53	1.42

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	132	ARG	NE-CZ-NH2	-9.71	115.44	120.30
4	N	120	ASP	CB-CG-OD1	8.35	125.82	118.30
4	M	118	ASP	CB-CG-OD2	-7.96	111.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	107	ASP	CB-CG-OD1	-6.89	112.09	118.30
4	M	107	ASP	CB-CG-OD2	-6.86	112.13	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	N	124	GLU	Peptide

## 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	463	0	482	9	0
1	D	463	0	482	9	0
2	B	2392	0	2260	39	3
2	E	2392	0	2257	79	3
3	C	2311	0	2163	46	5
3	F	2311	0	2161	58	0
4	M	315	0	310	112	0
4	N	309	0	301	43	0
All	All	10956	0	10416	263	8

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 263 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)
3:F:110:LEU:CD2	4:M:115:LEU:CD2	1.93	1.45
2:E:166:ARG:HB3	4:M:123:LYS:CE	1.53	1.36
2:E:166:ARG:CB	4:M:123:LYS:HZ1	1.39	1.36
2:E:173:GLU:OE2	4:M:116:GLN:HA	1.19	1.35
2:E:166:ARG:CB	4:M:123:LYS:NZ	1.86	1.35

The worst 5 of 8 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)
3:C:328:GLU:OE2	3:C:328:GLU:OE2[4_556]	1.59	0.61
3:C:328:GLU:OE1	3:C:328:GLU:OE2[4_556]	1.63	0.57
2:B:444:TRP:NE1	2:E:458:PHE:CA[5_445]	1.66	0.54
2:B:444:TRP:CZ2	2:E:458:PHE:O[5_445]	1.68	0.52
3:C:328:GLU:CD	3:C:328:GLU:OE2[4_556]	1.78	0.42

## 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	55/87 (63%)	49 (89%)	6 (11%)	0	100	100
1	D	55/87 (63%)	49 (89%)	6 (11%)	0	100	100
2	B	296/328 (90%)	281 (95%)	14 (5%)	1 (0%)	46	83
2	E	296/328 (90%)	281 (95%)	14 (5%)	1 (0%)	46	83
3	C	286/319 (90%)	272 (95%)	12 (4%)	2 (1%)	26	71
3	F	286/319 (90%)	272 (95%)	12 (4%)	2 (1%)	26	71
4	M	35/102 (34%)	20 (57%)	12 (34%)	3 (9%)	1	17
4	N	34/102 (33%)	24 (71%)	9 (26%)	1 (3%)	6	43
All	All	1343/1672 (80%)	1248 (93%)	85 (6%)	10 (1%)	26	71

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	127	SER
4	M	99	GLN
4	M	107	ASP
3	C	110	LEU
3	C	111	GLN

### 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	52/82 (63%)	50 (96%)	2 (4%)	40	73
1	D	52/82 (63%)	50 (96%)	2 (4%)	40	73
2	B	256/286 (90%)	247 (96%)	9 (4%)	43	74
2	E	256/286 (90%)	247 (96%)	9 (4%)	43	74
3	C	242/267 (91%)	235 (97%)	7 (3%)	50	78
3	F	242/267 (91%)	235 (97%)	7 (3%)	50	78
4	M	34/89 (38%)	24 (71%)	10 (29%)	0	3
4	N	34/89 (38%)	24 (71%)	10 (29%)	0	3
All	All	1168/1448 (81%)	1112 (95%)	56 (5%)	31	67

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	351	ASN
3	F	317	ASN
4	N	121	LEU
2	E	376	SER
2	E	454	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	365	ASN
2	E	253	GLN
3	F	319	ASN
3	C	390	ASN
2	E	164	ASN

### 5.3.3 RNA

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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	57/87 (65%)	0.65	5 (8%)	12 16	34, 65, 96, 97	0
1	D	57/87 (65%)	0.73	5 (8%)	12 16	34, 65, 96, 97	0
2	B	298/328 (90%)	0.43	30 (10%)	9 14	17, 32, 76, 102	0
2	E	298/328 (90%)	0.13	13 (4%)	38 37	17, 32, 76, 102	0
3	C	288/319 (90%)	0.37	26 (9%)	12 16	13, 20, 64, 100	0
3	F	288/319 (90%)	0.44	19 (6%)	22 23	13, 20, 64, 100	0
4	M	37/102 (36%)	0.88	6 (16%)	3 8	24, 37, 82, 116	0
4	N	36/102 (35%)	0.96	8 (22%)	1 6	21, 32, 70, 86	0
All	All	1359/1672 (81%)	0.40	112 (8%)	14 18	13, 28, 84, 116	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	207	SER	7.9
2	B	400	GLY	5.7
2	B	206	VAL	5.1
4	N	106	LYS	4.9
2	E	203	ILE	4.4

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.