



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 09:51 am BST

PDB ID : 4EVN  
Title : Crystal Structure of Fab CR6261 (somatic heavy chain with germline-reverted light chain)  
Authors : Whittle, J.R.R.  
Deposited on : 2012-04-26  
Resolution : 2.85 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

<https://www.wwpdb.org/validation/2017/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  
Xtrriage (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

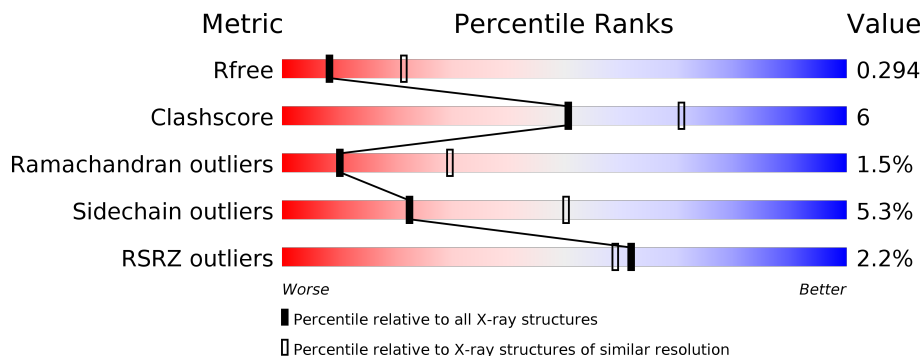
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 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	242	<p>0% 73% 17% • 9%</p>
1	C	242	<p>3% 70% 19% • 9%</p>
1	E	242	<p>2% 71% 18% • 9%</p>
1	G	242	<p>3% 73% 17% • 9%</p>
1	I	242	<p>3% 74% 16% • 9%</p>
1	K	242	<p>2% 70% 19% • 9%</p>

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Mol	Chain	Length	Quality of chain
1	M	242	<p>3% 74% 17% 9%</p>
1	O	242	<p>2% 71% 18% 9%</p>
2	B	217	<p>2% 85% 12% ..</p>
2	D	217	<p>% 83% 15% .</p>
2	F	217	<p>% 84% 13% ..</p>
2	H	217	<p>4% 86% 12% ..</p>
2	J	217	<p>% 83% 14% ..</p>
2	L	217	<p>% 84% 13% .</p>
2	N	217	<p>% 83% 14% ..</p>
2	P	217	<p>3% 86% 12% ..</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 25293 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 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	221	Total 1623	C 1028	N 268	O 318	S 9	0	0	0
1	C	221	Total 1623	C 1028	N 268	O 318	S 9	0	0	0
1	E	221	Total 1625	C 1029	N 269	O 318	S 9	0	0	0
1	G	221	Total 1623	C 1028	N 268	O 318	S 9	0	0	0
1	I	221	Total 1625	C 1029	N 269	O 318	S 9	0	0	0
1	K	221	Total 1623	C 1028	N 268	O 318	S 9	0	0	0
1	M	221	Total 1623	C 1028	N 268	O 318	S 9	0	0	0
1	O	221	Total 1623	C 1028	N 268	O 318	S 9	0	0	0

- Molecule 2 is a protein called Fab Lambda Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	213	Total 1541	C 972	N 251	O 314	S 4	0	0	0
2	D	213	Total 1537	C 969	N 250	O 314	S 4	0	0	0
2	F	213	Total 1537	C 969	N 250	O 314	S 4	0	0	0
2	H	213	Total 1537	C 969	N 250	O 314	S 4	0	0	0
2	J	213	Total 1537	C 969	N 250	O 314	S 4	0	0	0
2	L	213	Total 1540	C 970	N 251	O 315	S 4	0	0	0

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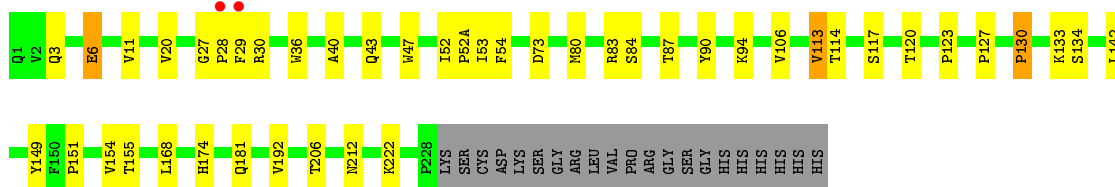
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	N	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	P	213	Total	C	N	O	S	0	0	0
			1539	970	251	314	4			

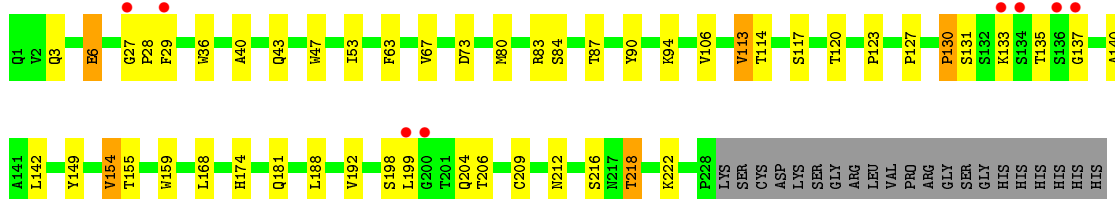
### 3 Residue-property plots [i](#)

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.

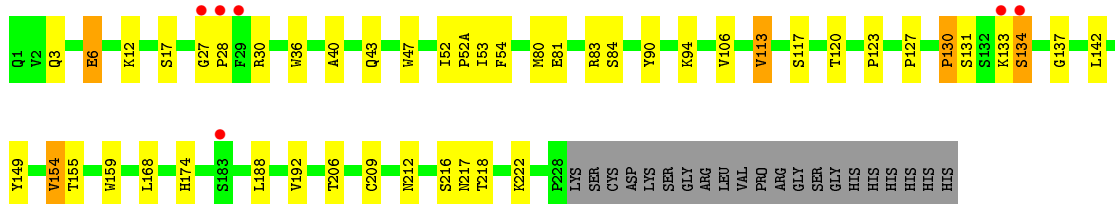
- Molecule 1: Fab Heavy Chain



- Molecule 1: Fab Heavy Chain

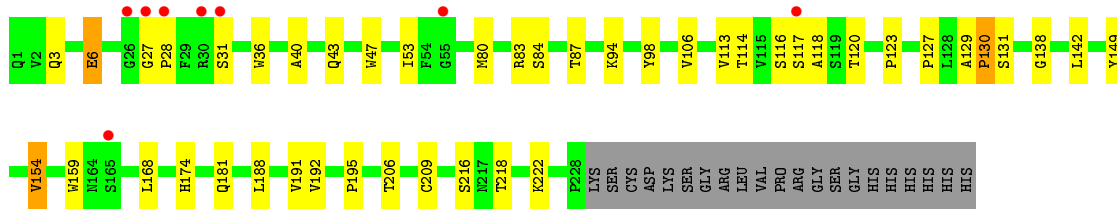


- Molecule 1: Fab Heavy Chain

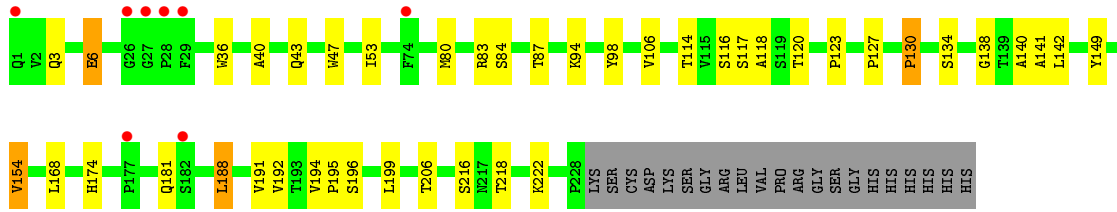


- Molecule 1: Fab Heavy Chain

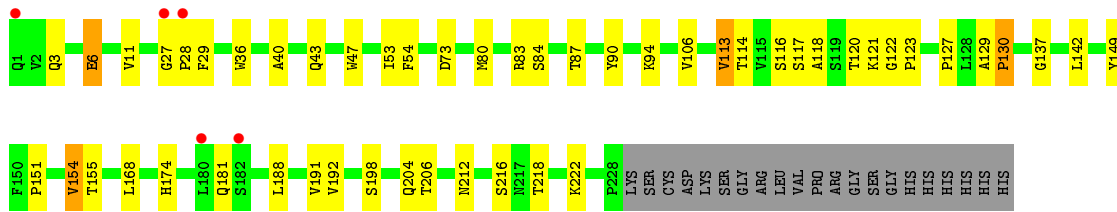




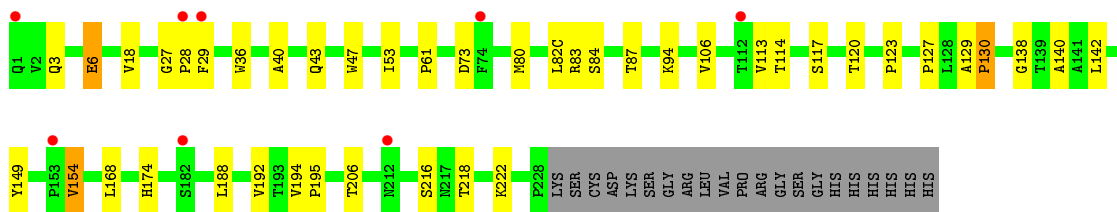
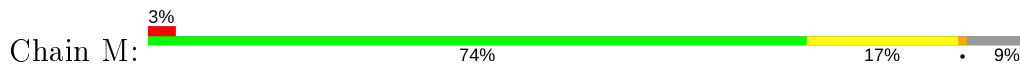
• Molecule 1: Fab Heavy Chain



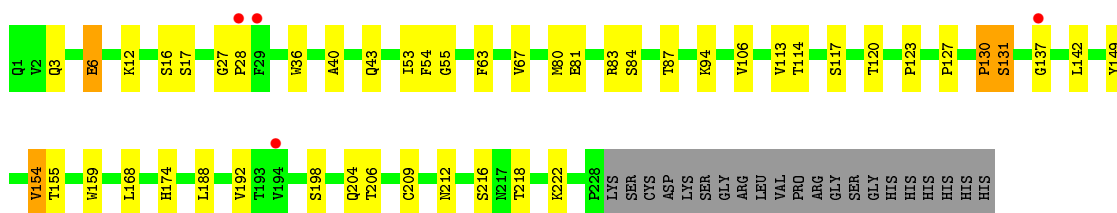
• Molecule 1: Fab Heavy Chain



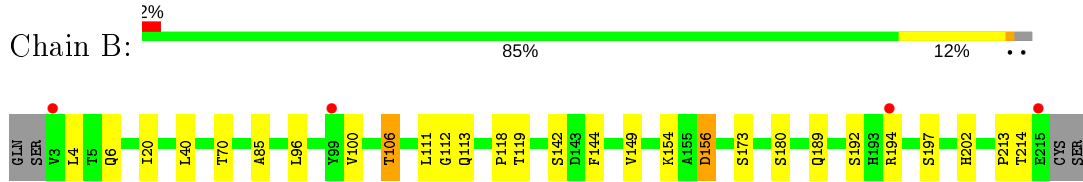
• Molecule 1: Fab Heavy Chain



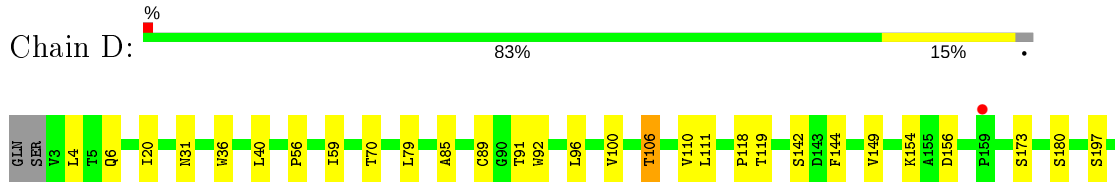
• Molecule 1: Fab Heavy Chain



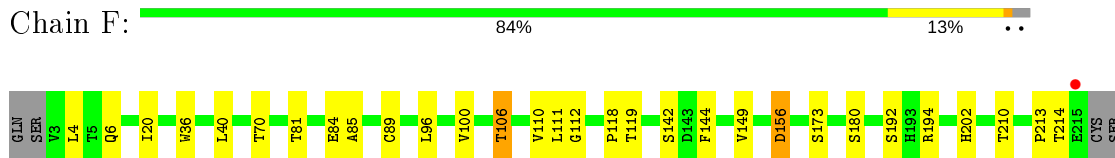
• Molecule 2: Fab Lambda Light Chain



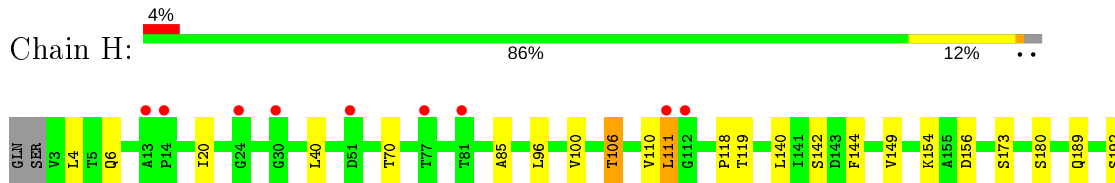
• Molecule 2: Fab Lambda Light Chain



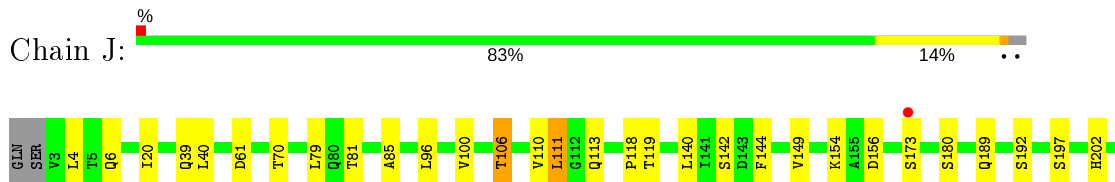
• Molecule 2: Fab Lambda Light Chain



• Molecule 2: Fab Lambda Light Chain



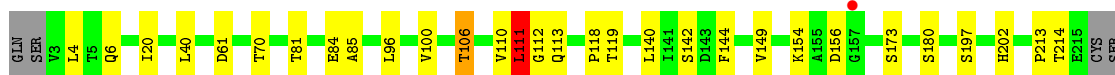
• Molecule 2: Fab Lambda Light Chain



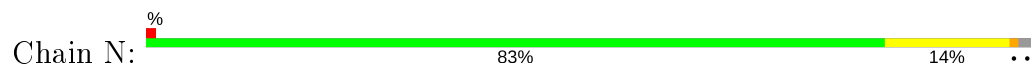
• Molecule 2: Fab Lambda Light Chain



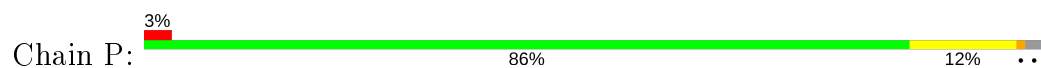




- Molecule 2: Fab Lambda Light Chain



- Molecule 2: Fab Lambda Light Chain



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.11Å 159.27Å 176.44Å 90.00° 89.73° 90.00°	Depositor
Resolution (Å)	55.01 – 2.85 176.44 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.3 (55.01-2.85) 92.7 (176.44-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.230 , 0.293 0.228 , 0.294	Depositor DCC
$R_{free}$ test set	2024 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 2.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.069 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	25293	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.48	0/1664	0.59	0/2270
1	C	0.53	1/1664 (0.1%)	0.62	0/2270
1	E	0.57	0/1666	0.66	0/2272
1	G	0.50	0/1664	0.61	0/2270
1	I	0.52	0/1666	0.63	0/2272
1	K	0.53	0/1664	0.66	0/2270
1	M	0.49	0/1664	0.57	0/2270
1	O	0.51	0/1664	0.62	0/2270
2	B	0.46	0/1580	0.60	1/2168 (0.0%)
2	D	0.48	0/1576	0.61	0/2164
2	F	0.46	0/1576	0.62	0/2164
2	H	0.42	0/1576	0.56	0/2164
2	J	0.44	0/1576	0.59	0/2164
2	L	0.43	0/1579	0.60	0/2168
2	N	0.43	0/1576	0.59	0/2164
2	P	0.45	0/1578	0.60	0/2166
All	All	0.48	1/25933 (0.0%)	0.61	1/35486 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	GLN	CD-NE2	6.42	1.49	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	113	GLN	N-CA-C	-5.67	95.69	111.00

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	1623	0	1580	21	0
1	C	1623	0	1580	23	0
1	E	1625	0	1587	33	0
1	G	1623	0	1580	28	0
1	I	1625	0	1587	23	0
1	K	1623	0	1580	27	0
1	M	1623	0	1580	18	1
1	O	1623	0	1580	25	0
2	B	1541	0	1444	11	0
2	D	1537	0	1433	18	0
2	F	1537	0	1433	15	0
2	H	1537	0	1433	11	0
2	J	1537	0	1433	16	0
2	L	1540	0	1437	15	0
2	N	1537	0	1433	18	0
2	P	1539	0	1440	12	1
All	All	25293	0	24140	282	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 6.

The worst 5 of 282 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:192:SER:HB2	2:P:96:LEU:HD12	1.49	0.94
1:E:81:GLU:OE2	1:O:12:LYS:NZ	2.02	0.93
2:P:81:THR:HA	2:P:110:VAL:HG21	1.52	0.91
1:I:138:GLY:O	1:I:196:SER:N	2.06	0.89
2:D:96:LEU:HD12	2:F:192:SER:HB2	1.51	0.88

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:M:61:PRO:O	2:P:16:GLN:NE2[2_555]	2.08	0.12

## 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	219/242 (90%)	211 (96%)	6 (3%)	2 (1%)	17	43
1	C	219/242 (90%)	210 (96%)	6 (3%)	3 (1%)	11	31
1	E	219/242 (90%)	207 (94%)	9 (4%)	3 (1%)	11	31
1	G	219/242 (90%)	207 (94%)	10 (5%)	2 (1%)	17	43
1	I	219/242 (90%)	209 (95%)	7 (3%)	3 (1%)	11	31
1	K	219/242 (90%)	209 (95%)	7 (3%)	3 (1%)	11	31
1	M	219/242 (90%)	209 (95%)	8 (4%)	2 (1%)	17	43
1	O	219/242 (90%)	208 (95%)	7 (3%)	4 (2%)	8	25
2	B	211/217 (97%)	200 (95%)	7 (3%)	4 (2%)	8	24
2	D	211/217 (97%)	202 (96%)	6 (3%)	3 (1%)	11	31
2	F	211/217 (97%)	201 (95%)	7 (3%)	3 (1%)	11	31
2	H	211/217 (97%)	199 (94%)	8 (4%)	4 (2%)	8	24
2	J	211/217 (97%)	200 (95%)	7 (3%)	4 (2%)	8	24
2	L	211/217 (97%)	199 (94%)	7 (3%)	5 (2%)	6	19
2	N	211/217 (97%)	199 (94%)	8 (4%)	4 (2%)	8	24
2	P	211/217 (97%)	202 (96%)	6 (3%)	3 (1%)	11	31
All	All	3440/3672 (94%)	3272 (95%)	116 (3%)	52 (2%)	10	30

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	130	PRO

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Mol	Chain	Res	Type
2	J	111	LEU
2	L	111	LEU
2	N	111	LEU
2	B	214	THR

### 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	178/202 (88%)	166 (93%)	12 (7%)	16	39
1	C	178/202 (88%)	167 (94%)	11 (6%)	18	43
1	E	179/202 (89%)	168 (94%)	11 (6%)	18	43
1	G	178/202 (88%)	168 (94%)	10 (6%)	21	47
1	I	179/202 (89%)	169 (94%)	10 (6%)	21	47
1	K	178/202 (88%)	168 (94%)	10 (6%)	21	47
1	M	178/202 (88%)	168 (94%)	10 (6%)	21	47
1	O	178/202 (88%)	168 (94%)	10 (6%)	21	47
2	B	164/182 (90%)	156 (95%)	8 (5%)	25	54
2	D	163/182 (90%)	156 (96%)	7 (4%)	29	59
2	F	163/182 (90%)	156 (96%)	7 (4%)	29	59
2	H	163/182 (90%)	154 (94%)	9 (6%)	21	49
2	J	163/182 (90%)	156 (96%)	7 (4%)	29	59
2	L	164/182 (90%)	156 (95%)	8 (5%)	25	54
2	N	163/182 (90%)	155 (95%)	8 (5%)	25	54
2	P	164/182 (90%)	157 (96%)	7 (4%)	29	59
All	All	2733/3072 (89%)	2588 (95%)	145 (5%)	22	50

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	206	THR

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Mol	Chain	Res	Type
1	I	154	VAL
1	O	120	THR
2	H	70	THR
2	H	173	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	217	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 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](#)

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	221/242 (91%)	-0.35	2 (0%) 84 84	35, 65, 111, 200	0
1	C	221/242 (91%)	-0.32	8 (3%) 42 37	32, 60, 132, 231	0
1	E	221/242 (91%)	-0.19	6 (2%) 54 50	24, 57, 123, 199	0
1	G	221/242 (91%)	-0.06	8 (3%) 42 37	52, 75, 130, 200	0
1	I	221/242 (91%)	-0.20	8 (3%) 42 37	38, 72, 122, 200	0
1	K	221/242 (91%)	-0.19	5 (2%) 60 57	31, 64, 111, 198	0
1	M	221/242 (91%)	0.08	8 (3%) 42 37	48, 76, 133, 200	0
1	O	221/242 (91%)	-0.25	4 (1%) 68 66	28, 68, 146, 199	0
2	B	213/217 (98%)	-0.25	4 (1%) 66 64	38, 75, 107, 163	0
2	D	213/217 (98%)	-0.34	3 (1%) 75 74	30, 64, 104, 165	0
2	F	213/217 (98%)	-0.39	1 (0%) 91 90	31, 65, 105, 162	0
2	H	213/217 (98%)	0.24	9 (4%) 36 31	55, 92, 141, 207	0
2	J	213/217 (98%)	-0.33	2 (0%) 84 84	42, 76, 114, 161	0
2	L	213/217 (98%)	-0.28	1 (0%) 91 90	34, 71, 118, 163	0
2	N	213/217 (98%)	-0.32	2 (0%) 84 84	40, 77, 113, 183	0
2	P	213/217 (98%)	-0.25	6 (2%) 53 48	32, 73, 114, 164	0
All	All	3472/3672 (94%)	-0.21	77 (2%) 62 59	24, 72, 123, 231	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	28	PRO	11.5
1	M	29	PHE	8.1
2	J	173	SER	7.2
1	I	26	GLY	6.8
2	D	215	GLU	6.5



## 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.