



wwPDB X-ray Structure Validation Summary Report i

Apr 10, 2014 – 05:23 PM EDT

PDB ID : 4J4P
Title : The complex of human IgE-Fc with two bound Fab fragments
Authors : Drinkwater, N.; Sutton, B.J.
Deposited on : 2013-02-07
Resolution : 2.91 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

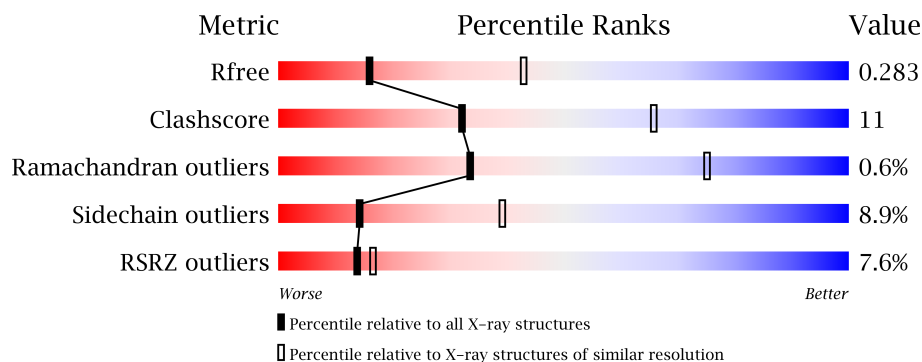
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	dev-1439
EDS	:	stable22978
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.91 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}	66092	1172 (2.94-2.90)
Clashscore	79885	1461 (2.94-2.90)
Ramachandran outliers	78287	1419 (2.94-2.90)
Sidechain outliers	78261	1421 (2.94-2.90)
RSRZ outliers	66119	1173 (2.94-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	323	
1	B	323	
2	C	249	
2	H	249	
3	D	235	
3	L	235	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11702 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ig epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	6	0	0
			2461	1535	438	477	11			
1	B	317	Total	C	N	O	S	6	0	0
			2480	1548	441	480	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLN	ASN	ENGINEERED MUTATION	UNP P01854
A	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854
B	265	GLN	ASN	ENGINEERED MUTATION	UNP P01854
B	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854

- Molecule 2 is a protein called Immunoglobulin G Fab Fragment Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1715	1081	288	339	7			
2	C	222	Total	C	N	O	S	6	0	0
			1701	1074	286	335	6			

- Molecule 3 is a protein called Immunoglobulin G Fab Fragment Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1591	993	262	332	4			
3	D	215	Total	C	N	O	S	0	0	0
			1591	993	262	332	4			

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		
4	B	5	Total	C	N	O	0	0
			61	34	2	25		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLN	ASN	ENGINEERED MUTATION	UNP P01854
A	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854
B	265	GLN	ASN	ENGINEERED MUTATION	UNP P01854
B	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854

- Molecule 5 is water.

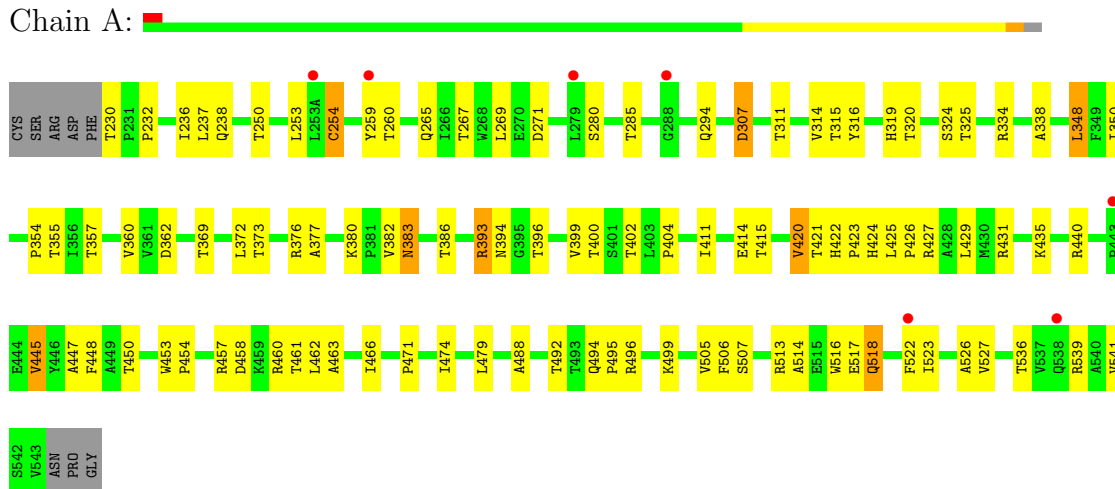
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	8	Total	O	0	0
			8	8		
5	H	9	Total	O	0	0
			9	9		
5	L	2	Total	O	0	0
			2	2		
5	C	5	Total	O	0	0
			5	5		
5	D	6	Total	O	0	0
			6	6		

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.

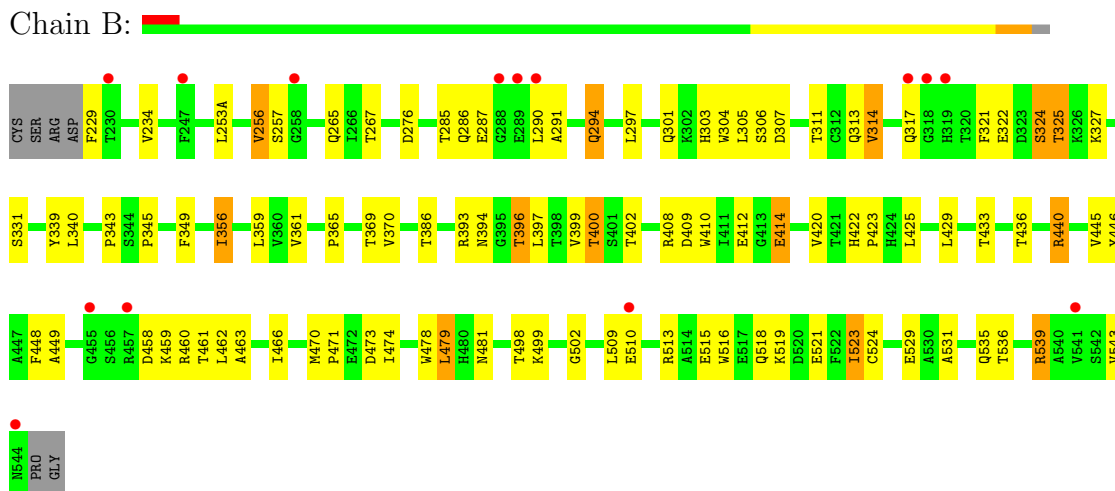
- Molecule 1: Ig epsilon chain C region

Chain A:



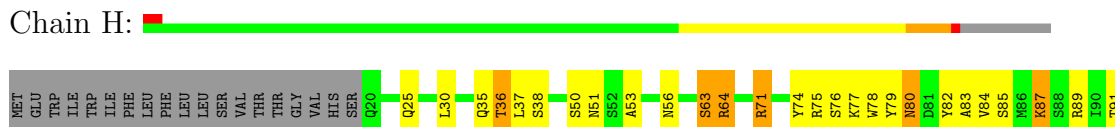
- Molecule 1: Ig epsilon chain C region

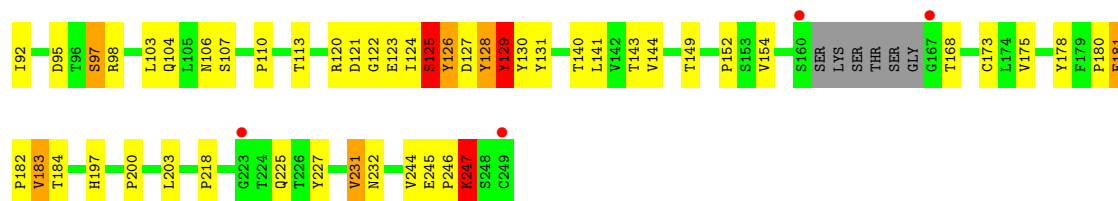
Chain B:



- Molecule 2: Immunoglobulin G Fab Fragment Heavy Chain

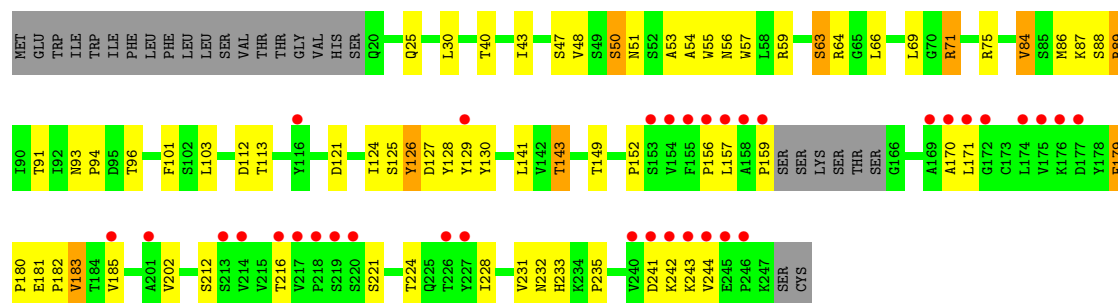
Chain H:





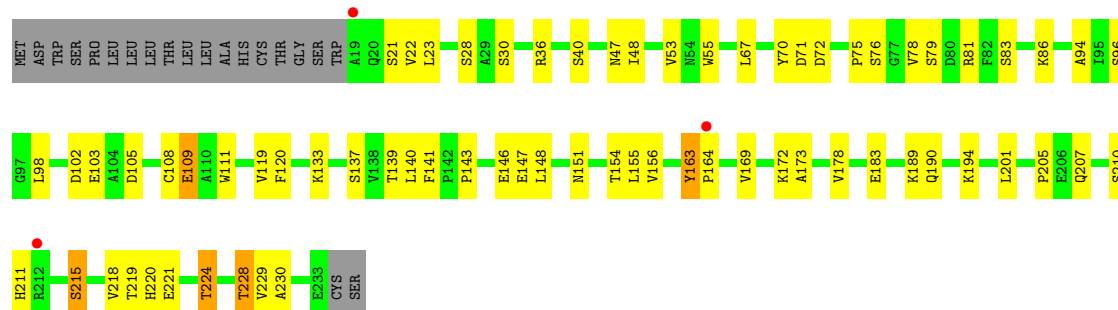
• Molecule 2: Immunoglobulin G Fab Fragment Heavy Chain

Chain C:



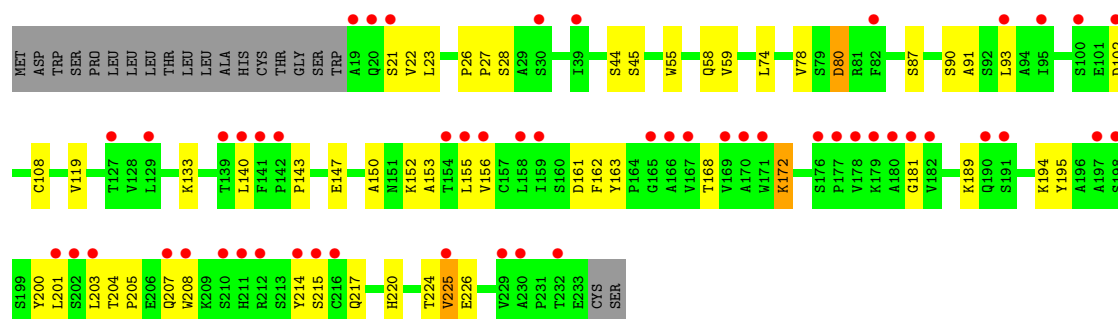
• Molecule 3: Immunoglobulin G Fab Fragment Light Chain

Chain L:



• Molecule 3: Immunoglobulin G Fab Fragment Light Chain

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.59Å 100.81Å 219.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.02 – 2.91 67.02 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.7 (67.02-2.91) 99.7 (67.02-2.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.236 , 0.284 0.235 , 0.283	Depositor DCC
R_{free} test set	2116 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	87.9	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 57.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 41915 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11702	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.51	0/2521	0.72	2/3436 (0.1%)
1	B	0.47	0/2541	0.68	1/3463 (0.0%)
2	C	0.46	0/1745	0.71	0/2383
2	H	0.60	0/1759	0.85	1/2402 (0.0%)
3	D	0.49	1/1629 (0.1%)	0.62	0/2226
3	L	0.56	0/1629	0.77	0/2226
All	All	0.51	1/11824 (0.0%)	0.72	4/16136 (0.0%)

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
2	C	0	2
2	H	0	4
3	D	0	1
3	L	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	215	SER	CB-OG	11.26	1.56	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	84	VAL	N-CA-C	-6.22	94.22	111.00
1	A	334	ARG	N-CA-C	-5.29	96.70	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	GLN	N-CA-C	-5.16	97.08	111.00
1	B	414	GLU	N-CA-C	5.12	124.82	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	124	ILE	Peptide
2	H	181	GLU	Peptide
2	H	247	LYS	Peptide
2	H	83	ALA	Peptide
3	L	163	TYR	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2461	0	2408	60	0
1	B	2480	0	2423	59	0
2	C	1701	0	1648	38	0
2	H	1715	0	1660	44	0
3	D	1591	0	1530	31	0
3	L	1591	0	1530	41	0
4	A	61	0	52	2	0
4	B	61	0	52	2	0
5	A	11	0	0	0	0
5	B	8	0	0	0	0
5	C	5	0	0	0	0
5	D	6	0	0	0	0
5	H	9	0	0	0	0
5	L	2	0	0	1	0
All	All	11702	0	11303	261	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 261 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:232:PRO:HB3	1:A:259:TYR:HB3	1.58	0.86
2:H:125:SER:OG	2:H:126:TYR:N	2.09	0.81
1:B:460:ARG:HH22	1:B:543:VAL:HG21	1.45	0.81
3:L:133:LYS:HD2	3:L:221:GLU:HG3	1.63	0.79
3:L:172:LYS:HB2	3:L:215:SER:HB2	1.66	0.78

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	313/323 (97%)	299 (96%)	13 (4%)	1 (0%)	50	85
1	B	315/323 (98%)	298 (95%)	17 (5%)	0	100	100
2	C	218/249 (88%)	198 (91%)	18 (8%)	2 (1%)	25	65
2	H	220/249 (88%)	197 (90%)	17 (8%)	6 (3%)	8	30
3	D	213/235 (91%)	194 (91%)	19 (9%)	0	100	100
3	L	213/235 (91%)	199 (93%)	14 (7%)	0	100	100
All	All	1492/1614 (92%)	1385 (93%)	98 (7%)	9 (1%)	33	75

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	125	SER
2	H	182	PRO
2	H	183	VAL
2	C	182	PRO
2	C	183	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	279/286 (98%)	253 (91%)	26 (9%)	13	37
1	B	281/286 (98%)	260 (92%)	21 (8%)	19	49
2	C	193/219 (88%)	173 (90%)	20 (10%)	10	29
2	H	196/219 (90%)	169 (86%)	27 (14%)	5	14
3	D	180/198 (91%)	172 (96%)	8 (4%)	39	76
3	L	180/198 (91%)	166 (92%)	14 (8%)	18	46
All	All	1309/1406 (93%)	1193 (91%)	116 (9%)	14	39

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	80	ASN
2	H	128	TYR
2	C	202	VAL
2	H	89	ARG
2	H	103	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	286	GLN
1	B	422	HIS
1	B	484	GLN
2	H	225	GLN
2	C	233	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.8 Polymer linkage issues

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	315/323 (97%)	0.05	7 (2%) 59 67	58, 92, 132, 142	4 (1%)
1	B	317/323 (98%)	0.08	14 (4%) 33 40	65, 94, 164, 193	6 (1%)
2	C	222/249 (89%)	0.66	35 (15%) 3 3	63, 102, 214, 225	5 (2%)
2	H	224/249 (89%)	-0.02	4 (1%) 65 75	50, 80, 159, 189	2 (0%)
3	D	215/235 (91%)	1.14	53 (24%) 1 2	64, 139, 199, 211	0
3	L	215/235 (91%)	-0.03	3 (1%) 72 80	53, 85, 123, 159	0
All	All	1508/1614 (93%)	0.28	116 (7%) 14 16	50, 93, 186, 225	17 (1%)

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	169	ALA	8.7
3	L	19	ALA	7.9
3	D	178	VAL	7.2
3	D	230	ALA	7.0
3	D	208	TRP	7.0

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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BMA	A	603	11/12	0.25	0.89	97,101,112,115	0
4	BMA	B	604	11/12	0.18	0.44	117,127,129,129	0
4	BMA	A	605	11/12	0.21	0.27	120,131,135,138	0
4	NAG	A	602	14/15	0.22	-0.08	79,85,89,90	0
4	NAG	B	601	14/15	0.23	-0.23	80,92,96,102	0
4	NAG	A	601	14/15	0.21	-0.25	70,76,82,86	0
4	NAG	B	602	14/15	0.23	-0.43	94,101,105,107	0
4	BMA	B	603	11/12	0.18	-1.36	110,114,120,123	0
4	BMA	B	605	11/12	0.22	-	129,132,140,142	0
4	BMA	A	604	11/12	0.20	-	117,126,139,140	0

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.