



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2021 – 11:48 am BST

PDB ID : 7BBG
Title : CRYSTAL STRUCTURE OF HLA-A2-WT1-RMF AND FAB 11D06
Authors : Bujotzek, A.; Georges, G.; Hanisch, L.J.; Klein, C.; Benz, J.
Deposited on : 2020-12-17
Resolution : 2.64 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

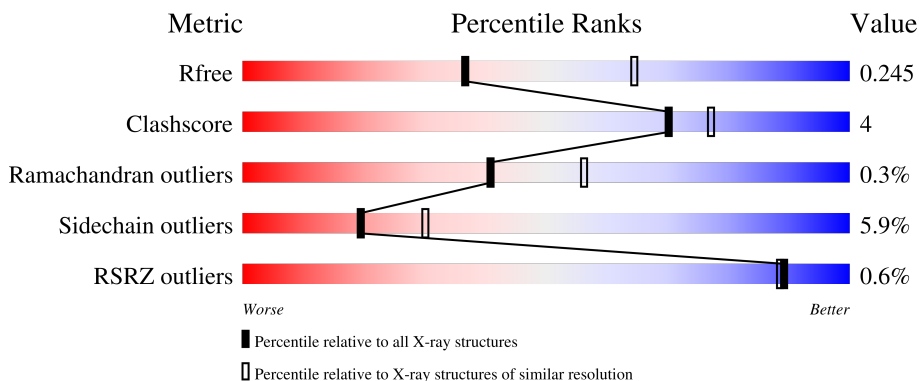
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	309	 73% 15% 11%
2	B	100	 92% 8%
3	C	9	 89% 11%
4	H	223	 81% 15%
5	L	213	 88% 11%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6650 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	2245	1403	411	422	9	0	1	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q861F7
A	276	GLY	-	expression tag	UNP Q861F7
A	277	GLY	-	expression tag	UNP Q861F7
A	278	GLY	-	expression tag	UNP Q861F7
A	279	GLY	-	expression tag	UNP Q861F7
A	280	SER	-	expression tag	UNP Q861F7
A	281	GLY	-	expression tag	UNP Q861F7
A	282	GLY	-	expression tag	UNP Q861F7
A	283	GLY	-	expression tag	UNP Q861F7
A	284	GLY	-	expression tag	UNP Q861F7
A	285	SER	-	expression tag	UNP Q861F7
A	286	GLY	-	expression tag	UNP Q861F7
A	287	SER	-	expression tag	UNP Q861F7
A	288	GLY	-	expression tag	UNP Q861F7
A	289	LEU	-	expression tag	UNP Q861F7
A	290	ASN	-	expression tag	UNP Q861F7
A	291	ASP	-	expression tag	UNP Q861F7
A	292	ILE	-	expression tag	UNP Q861F7
A	293	PHE	-	expression tag	UNP Q861F7
A	294	GLU	-	expression tag	UNP Q861F7
A	295	ALA	-	expression tag	UNP Q861F7
A	296	GLN	-	expression tag	UNP Q861F7
A	297	LYS	-	expression tag	UNP Q861F7
A	298	ILE	-	expression tag	UNP Q861F7
A	299	GLU	-	expression tag	UNP Q861F7
A	300	TRP	-	expression tag	UNP Q861F7
A	301	HIS	-	expression tag	UNP Q861F7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	302	GLU	-	expression tag	UNP Q861F7
A	303	HIS	-	expression tag	UNP Q861F7
A	304	HIS	-	expression tag	UNP Q861F7
A	305	HIS	-	expression tag	UNP Q861F7
A	306	HIS	-	expression tag	UNP Q861F7
A	307	HIS	-	expression tag	UNP Q861F7
A	308	HIS	-	expression tag	UNP Q861F7

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	837	533	141	159	4	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Wilms tumor 1 (WT1) derived peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	9	77	52	13	11	1	0	0	0

- Molecule 4 is a protein called Heavy chain of Fab fragment 11D06.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	215	1603	1019	264	313	7	0	0	0

- Molecule 5 is a protein called Light chain of Fab fragment 11D06.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	L	212	1633	1021	270	337	5	0	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Na 3 3	0	0
6	H	2	Total Na 2 2	0	0

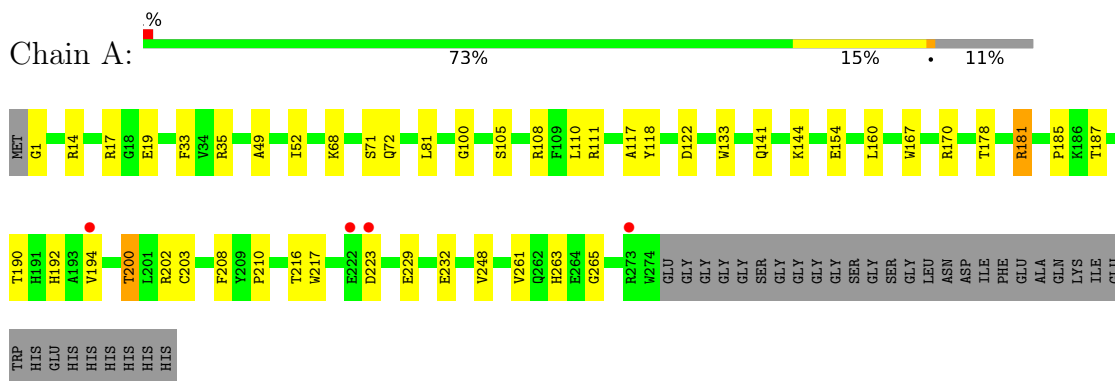
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	77	Total O 77 77	0	0
7	B	32	Total O 32 32	0	0
7	C	2	Total O 2 2	0	0
7	H	67	Total O 67 67	0	0
7	L	72	Total O 72 72	0	0

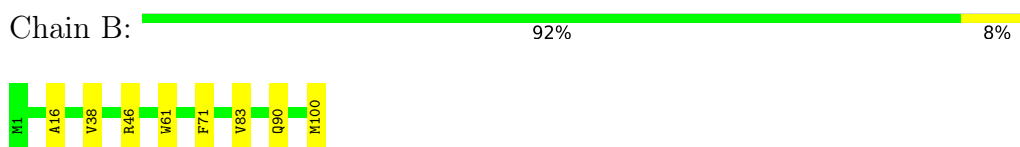
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

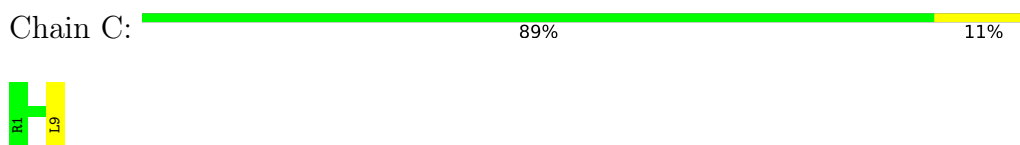
- Molecule 1: MHC class I antigen



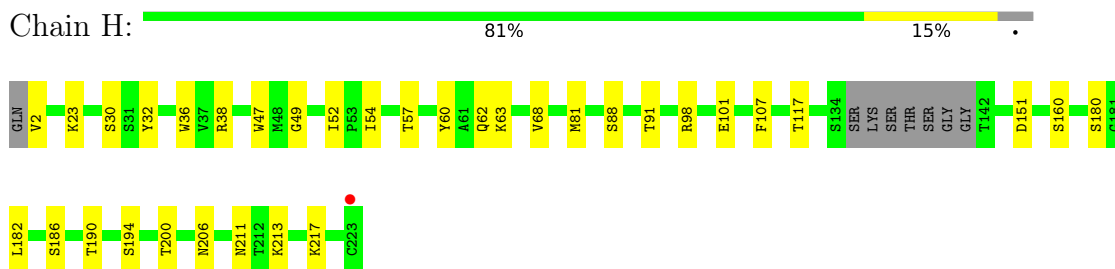
- Molecule 2: Beta-2-microglobulin




- Molecule 3: Wilms tumor 1 (WT1) derived peptide



- Molecule 4: Heavy chain of Fab fragment 11D06



- Molecule 5: Light chain of Fab fragment 11D06

Chain L:  88% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.11Å 67.01Å 139.36Å 90.00° 90.57° 90.00°	Depositor
Resolution (Å)	48.30 – 2.64 48.30 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.30-2.64) 99.9 (48.30-2.64)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.65Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.168 , 0.230 0.179 , 0.245	Depositor DCC
R_{free} test set	1425 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6650	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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

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	0/2313	0.74	0/3139
2	B	0.47	0/860	0.69	0/1162
3	C	0.64	0/80	0.82	0/108
4	H	0.53	0/1643	0.77	0/2239
5	L	0.53	0/1668	0.76	0/2265
All	All	0.52	0/6564	0.75	0/8913

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2245	0	2103	20	0
2	B	837	0	803	2	0
3	C	77	0	78	1	0
4	H	1603	0	1575	12	0
5	L	1633	0	1575	12	0
6	A	3	0	0	0	0
6	H	2	0	0	0	0
7	A	77	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	32	0	0	0	0
7	C	2	0	0	0	0
7	H	67	0	0	1	0
7	L	72	0	0	0	0
All	All	6650	0	6134	45	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 4.

All (45) 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)
4:H:91:THR:HG23	4:H:117:THR:HA	1.78	0.65
4:H:30:SER:HB2	4:H:32:TYR:HD2	1.65	0.61
5:L:89:GLN:HE21	5:L:95:THR:CG2	2.15	0.59
1:A:14:ARG:HB3	1:A:17:ARG:HB2	1.87	0.55
5:L:144:LYS:HB3	5:L:196:THR:HB	1.88	0.55
5:L:116:ILE:HD12	5:L:193:CYS:HB2	1.89	0.54
5:L:11:LEU:CD2	5:L:19:VAL:HG13	2.37	0.54
4:H:36:TRP:CE2	4:H:81:MET:HB2	2.43	0.53
4:H:151:ASP:HB3	4:H:182:LEU:HD13	1.90	0.53
5:L:89:GLN:HE21	5:L:95:THR:HG21	1.74	0.53
1:A:81:LEU:HD11	3:C:9:LEU:HD12	1.91	0.53
4:H:52:ILE:HG22	4:H:54:ILE:HG22	1.92	0.52
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.92	0.51
4:H:101:GLU:HB3	7:H:429:HOH:O	2.09	0.51
1:A:117:ALA:HB2	2:B:61:TRP:CE2	2.47	0.50
1:A:263:HIS:HD2	1:A:265:GLY:H	1.60	0.49
1:A:1:GLY:O	1:A:105:SER:HA	2.12	0.49
1:A:210:PRO:O	1:A:263:HIS:HE1	1.96	0.49
1:A:192:HIS:HB2	1:A:200:THR:HG23	1.94	0.49
4:H:206:ASN:HD22	4:H:213:LYS:HG2	1.78	0.49
1:A:68:LYS:O	1:A:71:SER:HB3	2.13	0.47
4:H:30:SER:HB2	4:H:32:TYR:CD2	2.48	0.47
1:A:49:ALA:O	1:A:52:ILE:HG22	2.15	0.47
1:A:185:PRO:HB3	1:A:208:PHE:CD2	2.51	0.46
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.97	0.46
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.52	0.45
5:L:193:CYS:O	5:L:205:THR:HA	2.16	0.44
1:A:167:TRP:CE3	1:A:170:ARG:HD3	2.52	0.44
1:A:33:PHE:O	1:A:52:ILE:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:162:VAL:HG22	5:L:174:LEU:HD12	1.99	0.43
1:A:178:THR:O	1:A:181:ARG:HD3	2.18	0.43
5:L:145:VAL:HG22	5:L:195:VAL:HG22	2.00	0.43
5:L:11:LEU:HD21	5:L:19:VAL:HG13	2.01	0.43
2:B:38:VAL:HG22	2:B:83:VAL:HG13	2.00	0.42
4:H:47:TRP:CZ2	4:H:49:GLY:HA2	2.54	0.42
4:H:98:ARG:O	4:H:107:PHE:HA	2.20	0.41
5:L:119:PRO:HD3	5:L:131:VAL:HG22	2.02	0.41
1:A:100:GLY:O	1:A:160:LEU:HD22	2.20	0.41
4:H:60:TYR:CD1	4:H:68:VAL:HG13	2.55	0.41
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.56	0.41
5:L:89:GLN:HE21	5:L:95:THR:HG23	1.84	0.41
5:L:181:SER:OG	5:L:184:ASP:HB2	2.19	0.41
4:H:200:THR:HG23	4:H:217:LYS:HE3	2.01	0.41
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.21	0.40
1:A:194:VAL:HG23	1:A:200:THR:HG22	2.02	0.40

There are no symmetry-related clashes.

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	273/309 (88%)	261 (96%)	12 (4%)	0	100	100
2	B	98/100 (98%)	94 (96%)	3 (3%)	1 (1%)	15	22
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	H	211/223 (95%)	205 (97%)	6 (3%)	0	100	100
5	L	210/213 (99%)	199 (95%)	10 (5%)	1 (0%)	29	43
All	All	799/854 (94%)	766 (96%)	31 (4%)	2 (0%)	41	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	16	ALA
5	L	137	ASN

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	231/254 (91%)	214 (93%)	17 (7%)	13	21
2	B	95/95 (100%)	91 (96%)	4 (4%)	30	45
3	C	8/8 (100%)	8 (100%)	0	100	100
4	H	179/185 (97%)	166 (93%)	13 (7%)	14	21
5	L	186/187 (100%)	178 (96%)	8 (4%)	29	45
All	All	699/729 (96%)	657 (94%)	42 (6%)	19	29

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	35	ARG
1	A	72	GLN
1	A	108	ARG
1	A	110	LEU
1	A	111[A]	ARG
1	A	111[B]	ARG
1	A	122	ASP
1	A	141	GLN
1	A	154	GLU
1	A	181	ARG
1	A	200	THR
1	A	216	THR
1	A	223	ASP
1	A	229	GLU
1	A	232	GLU
1	A	248	VAL
2	B	46	ARG

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Mol	Chain	Res	Type
2	B	71	PHE
2	B	90	GLN
2	B	100	MET
4	H	2	VAL
4	H	23	LYS
4	H	38	ARG
4	H	57	THR
4	H	62	GLN
4	H	63	LYS
4	H	88	SER
4	H	160	SER
4	H	180	SER
4	H	186	SER
4	H	190	THR
4	H	194	SER
4	H	211	ASN
5	L	22	THR
5	L	33	LEU
5	L	122	GLU
5	L	153	LEU
5	L	155	SER
5	L	180	LEU
5	L	184	ASP
5	L	186	GLU

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

Mol	Chain	Res	Type
1	A	72	GLN
1	A	180	GLN
1	A	263	HIS
4	H	206	ASN
5	L	146	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	274/309 (88%)	-0.15	4 (1%) 73 71	40, 62, 112, 127	0
2	B	100/100 (100%)	-0.35	0 100 100	49, 75, 103, 106	2 (2%)
3	C	9/9 (100%)	-0.34	0 100 100	45, 50, 54, 55	0
4	H	215/223 (96%)	-0.33	1 (0%) 91 90	40, 63, 96, 139	0
5	L	212/213 (99%)	-0.47	0 100 100	40, 63, 95, 125	0
All	All	810/854 (94%)	-0.31	5 (0%) 89 88	40, 63, 104, 139	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	VAL	2.6
4	H	223	CYS	2.4
1	A	222	GLU	2.4
1	A	223	ASP	2.4
1	A	273	ARG	2.2

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 monosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q < 0.9
6	NA	A	402	1/1	0.83	0.23	62,62,62,62	0
6	NA	H	301	1/1	0.87	0.19	72,72,72,72	0
6	NA	A	401	1/1	0.88	0.37	65,65,65,65	0
6	NA	H	302	1/1	0.88	0.26	70,70,70,70	0
6	NA	A	403	1/1	0.95	0.22	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.