



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:18 AM BST

PDB ID : 5UKR
Title : Structure of unliganded anti-gp120 CD4bs antibody DH522.2 Fab in complex with a gp120 core
Authors : Nicely, N.I.
Deposited on : 2017-01-23
Resolution : 2.71 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

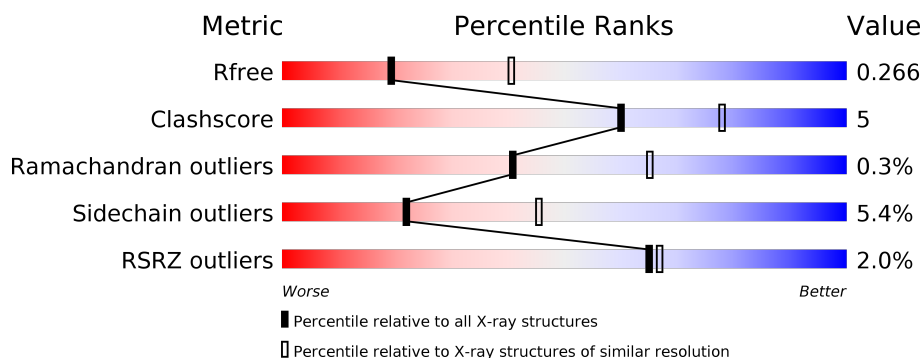
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 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	H	230	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 84% 12% • </div> </div>
2	L	216	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 86% 11% • </div> </div>
3	G	313	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 4% </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 51% 14% • 34% </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	G	406	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4954 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 DH522.2 Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	221	Total	C	N	O	S	0	0	0
			1662	1056	273	328	5			

- Molecule 2 is a protein called DH522.2 Fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	0	0	0
			1566	974	266	322	4			

- Molecule 3 is a protein called Chimeric B.YU2 gp120 core derived from HIV-1 Env.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	207	Total	C	N	O	S	0	0	0
			1625	1013	286	313	13			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

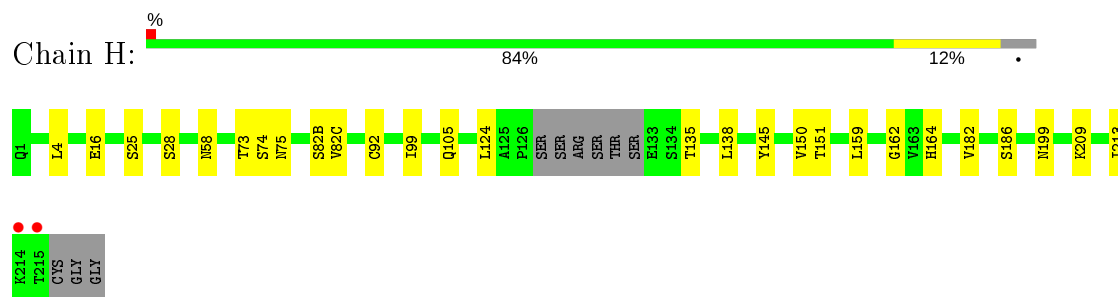
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	9	Total	O	0	0
			9	9		
5	L	7	Total	O	0	0
			7	7		
5	G	1	Total	O	0	0
			1	1		

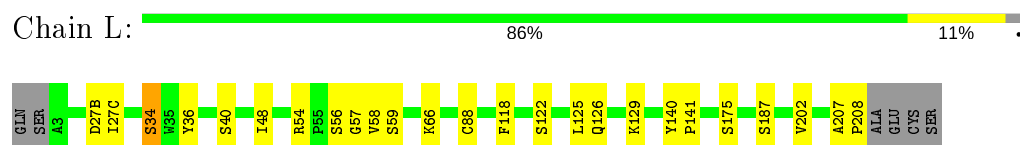
3 Residue-property plots [i](#)

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.

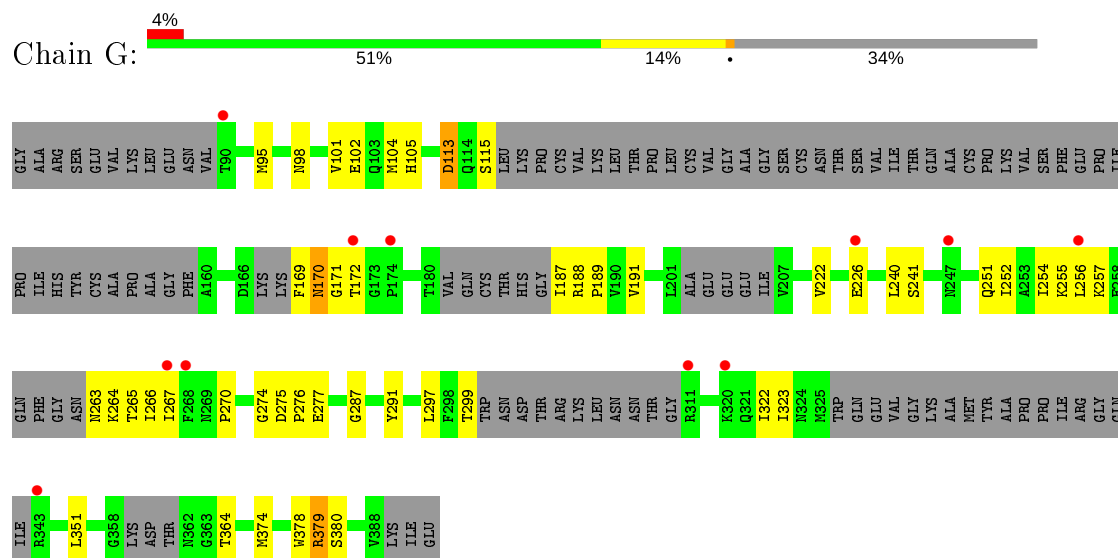
- Molecule 1: DH522.2 Fab fragment heavy chain



- Molecule 2: DH522.2 Fab fragment light chain



- Molecule 3: Chimeric B.YU2 gp120 core derived from HIV-1 Env



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.85Å 71.97Å 252.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.71 49.85 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.85-2.71) 98.2 (49.85-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.201 , 0.265 0.203 , 0.266	Depositor DCC
R_{free} test set	2000 reflections (7.82%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4954	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: 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	H	0.49	0/1703	0.64	0/2326
2	L	0.41	0/1602	0.57	0/2184
3	G	0.36	0/1645	0.56	0/2214
All	All	0.42	0/4950	0.59	0/6724

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	H	1662	0	1623	12	0
2	L	1566	0	1508	8	0
3	G	1625	0	1580	27	0
4	G	84	0	78	0	0
5	G	1	0	0	0	0
5	H	9	0	0	0	0
5	L	7	0	0	0	0
All	All	4954	0	4789	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 5.

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)
3:G:105:HIS:HD1	3:G:378:TRP:HZ3	1.46	0.63
1:H:159:LEU:HD21	1:H:182:VAL:HG21	1.81	0.63
3:G:240:LEU:HD23	3:G:297:LEU:HD21	1.84	0.60
3:G:270:PRO:HD3	3:G:299:THR:HG22	1.84	0.60
3:G:169:PHE:O	3:G:170:ASN:ND2	2.36	0.58
3:G:277:GLU:HG2	3:G:291:TYR:HE2	1.69	0.55
3:G:257:LYS:HG2	3:G:266:ILE:HD13	1.88	0.55
3:G:251:GLN:O	3:G:255:LYS:HG2	2.09	0.52
3:G:105:HIS:HA	3:G:378:TRP:CZ3	2.44	0.52
1:H:138:LEU:HD21	1:H:213:ILE:HD11	1.92	0.51
1:H:58:ASN:OD1	3:G:274:GLY:HA3	2.11	0.50
2:L:34:SER:HB2	2:L:36:TYR:CE1	2.47	0.50
1:H:74:SER:O	1:H:75:ASN:HB2	2.12	0.49
3:G:257:LYS:HB3	3:G:263:ASN:N	2.29	0.48
2:L:122:SER:HA	2:L:125:LEU:HD12	1.97	0.47
3:G:252:ILE:O	3:G:256:LEU:HG	2.16	0.46
3:G:95:MET:HG2	3:G:171:GLY:HA3	1.97	0.46
2:L:48:ILE:HD13	2:L:54:ARG:HG2	1.96	0.46
3:G:267:ILE:HD13	3:G:364:THR:HG23	1.97	0.46
1:H:151:THR:HB	1:H:199:ASN:HB3	1.98	0.45
1:H:4:LEU:N	1:H:4:LEU:HD12	2.32	0.45
1:H:162:GLY:O	1:H:182:VAL:HA	2.17	0.45
3:G:222:VAL:HB	3:G:351:LEU:HB2	1.99	0.44
3:G:264:LYS:HB2	3:G:264:LYS:HE3	1.82	0.44
3:G:275:ASP:HA	3:G:276:PRO:HD3	1.87	0.44
3:G:104:MET:CE	3:G:378:TRP:HB3	2.47	0.44
3:G:277:GLU:HG2	3:G:291:TYR:CE2	2.51	0.43
2:L:56:SER:HA	2:L:57:GLY:HA2	1.47	0.43
3:G:98:ASN:HB3	3:G:101:VAL:HG23	2.00	0.43
3:G:188:ARG:HA	3:G:189:PRO:HD3	1.93	0.43
1:H:145:TYR:CE2	1:H:150:VAL:HG13	2.54	0.42
2:L:27(C):ILE:O	2:L:66:LYS:NZ	2.26	0.42
3:G:287:GLY:O	3:G:322:ILE:HG12	2.18	0.42
3:G:113:ASP:OD1	3:G:113:ASP:N	2.53	0.42
1:H:124:LEU:HB3	2:L:118:PHE:CD1	2.54	0.42
3:G:191:VAL:HA	3:G:374:MET:HE1	2.01	0.42
3:G:297:LEU:HD23	3:G:297:LEU:HA	1.86	0.42
3:G:379:ARG:HE	3:G:379:ARG:HB3	1.55	0.41
1:H:16:GLU:O	1:H:82(C):VAL:HG22	2.21	0.41
2:L:207:ALA:HA	2:L:208:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:140:TYR:CG	2:L:141:PRO:HA	2.55	0.41
3:G:191:VAL:HA	3:G:374:MET:CE	2.51	0.41
1:H:4:LEU:HD23	1:H:92:CYS:SG	2.61	0.41
3:G:105:HIS:HA	3:G:378:TRP:HZ3	1.86	0.41
1:H:135:THR:N	1:H:186:SER:HB2	2.36	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	H	217/230 (94%)	209 (96%)	8 (4%)	0	100	100
2	L	208/216 (96%)	197 (95%)	10 (5%)	1 (0%)	29	53
3	G	189/313 (60%)	172 (91%)	16 (8%)	1 (0%)	29	53
All	All	614/759 (81%)	578 (94%)	34 (6%)	2 (0%)	41	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	59	SER
3	G	170	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	H	190/197 (96%)	182 (96%)	8 (4%)	30	56
2	L	176/181 (97%)	166 (94%)	10 (6%)	20	43
3	G	187/276 (68%)	175 (94%)	12 (6%)	17	37
All	All	553/654 (85%)	523 (95%)	30 (5%)	22	45

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	25	SER
1	H	28	SER
1	H	73	THR
1	H	82(B)	SER
1	H	99	ILE
1	H	105	GLN
1	H	164	HIS
1	H	209	LYS
2	L	27(B)	ASP
2	L	34	SER
2	L	40	SER
2	L	58	VAL
2	L	88	CYS
2	L	126	GLN
2	L	129	LYS
2	L	175	SER
2	L	187	SER
2	L	202	VAL
3	G	102	GLU
3	G	113	ASP
3	G	115	SER
3	G	172	THR
3	G	187	ILE
3	G	226	GLU
3	G	241	SER
3	G	254	ILE
3	G	265	THR
3	G	323	ILE
3	G	379	ARG
3	G	380	SER

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

Mol	Chain	Res	Type
3	G	170	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	G	401	3	14,14,15	0.43	0	17,19,21	0.65	0
4	NAG	G	405	3	14,14,15	0.33	0	17,19,21	0.59	0
4	NAG	G	402	3	14,14,15	0.32	0	17,19,21	0.73	1 (5%)
4	NAG	G	404	3	14,14,15	0.25	0	17,19,21	0.77	0
4	NAG	G	403	3	14,14,15	0.61	0	17,19,21	0.69	0
4	NAG	G	406	3	14,14,15	0.39	0	17,19,21	0.77	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	401	3	-	0/6/23/26	0/1/1/1
4	NAG	G	405	3	-	0/6/23/26	0/1/1/1
4	NAG	G	402	3	-	4/6/23/26	0/1/1/1
4	NAG	G	404	3	-	3/6/23/26	0/1/1/1
4	NAG	G	403	3	-	4/6/23/26	0/1/1/1
4	NAG	G	406	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	406	NAG	C1-O5-C5	2.79	115.97	112.19
4	G	402	NAG	C1-O5-C5	2.46	115.53	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	404	NAG	O5-C5-C6-O6
4	G	403	NAG	O5-C5-C6-O6
4	G	404	NAG	C4-C5-C6-O6
4	G	403	NAG	C4-C5-C6-O6
4	G	402	NAG	C8-C7-N2-C2
4	G	402	NAG	O7-C7-N2-C2
4	G	403	NAG	C8-C7-N2-C2
4	G	403	NAG	O7-C7-N2-C2
4	G	402	NAG	O5-C5-C6-O6
4	G	402	NAG	C4-C5-C6-O6
4	G	404	NAG	C3-C2-N2-C7

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	H	221/230 (96%)	-0.48	2 (0%) 84 85	20, 35, 68, 127	0
2	L	210/216 (97%)	-0.41	0 100 100	29, 48, 71, 92	0
3	G	207/313 (66%)	0.26	11 (5%) 26 25	44, 78, 109, 142	0
All	All	638/759 (84%)	-0.22	13 (2%) 65 67	20, 51, 97, 142	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	215	THR	6.6
3	G	172	THR	3.6
3	G	320	LYS	2.8
3	G	343	ARG	2.8
3	G	247	ASN	2.4
3	G	90	THR	2.1
3	G	174	PRO	2.1
3	G	226	GLU	2.1
1	H	214	LYS	2.1
3	G	311	ARG	2.1
3	G	268	PHE	2.1
3	G	267	ILE	2.0
3	G	256	LEU	2.0

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
4	NAG	G	406	14/15	0.75	0.41	91,112,116,116	0
4	NAG	G	404	14/15	0.80	0.24	92,108,116,118	0
4	NAG	G	403	14/15	0.81	0.20	79,93,105,110	0
4	NAG	G	405	14/15	0.82	0.26	69,93,104,109	0
4	NAG	G	401	14/15	0.88	0.22	67,78,83,84	0
4	NAG	G	402	14/15	0.91	0.22	59,77,87,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.