Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 01:06 PM EDT

PDB ID	:	4OM1
Title	:	Crystal structure of antibody VRC07-I30Q, G54W, S58N in complex with clade A/E 93TH057 HIV-1 gp120 core
Authors	:	Kwon, Y.D.; Kwong, P.D.
Deposited on	:	2014-01-25
Resolution	:	2.13 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

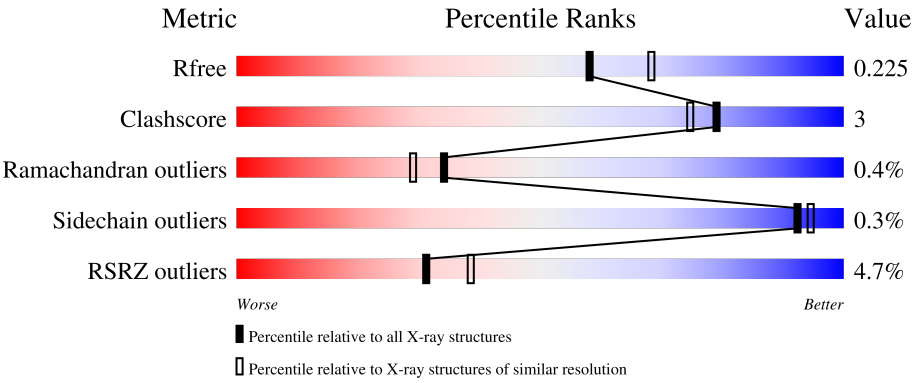
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 <=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	G	353	7% 92% 5%
2	H	228	4% 92% 8%
3	L	210	2% 92% 8%

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	502	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6482 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	344	Total	C	N	O	S	0	0	0
			2687	1686	468	511	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	124	GLY	-	linker	UNP Q0ED31
G	198	GLY	-	linker	UNP Q0ED31
G	318	GLY	-	linker	UNP Q0ED31
G	319	GLY	-	linker	UNP Q0ED31
G	320	SER	-	linker	UNP Q0ED31
G	321	GLY	-	linker	UNP Q0ED31
G	322	SER	-	linker	UNP Q0ED31
G	323	GLY	-	linker	UNP Q0ED31

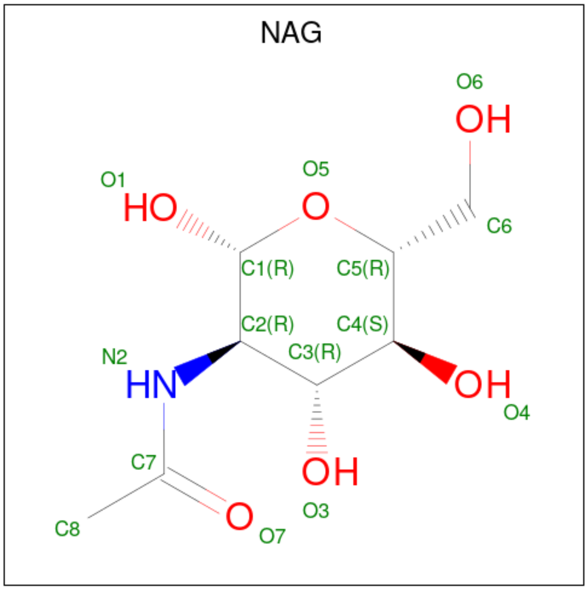
- Molecule 2 is a protein called Antigen binding fragment of heavy chain: Antibody VRC01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	228	Total	C	N	O	S	0	0	0
			1760	1106	307	334	13			

- Molecule 3 is a protein called Antigen binding fragment of light chain: Antibody VRC01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1624	1018	275	326	5			

- 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 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	78	Total O 78 78	0	0
5	H	101	Total O 101 101	0	0

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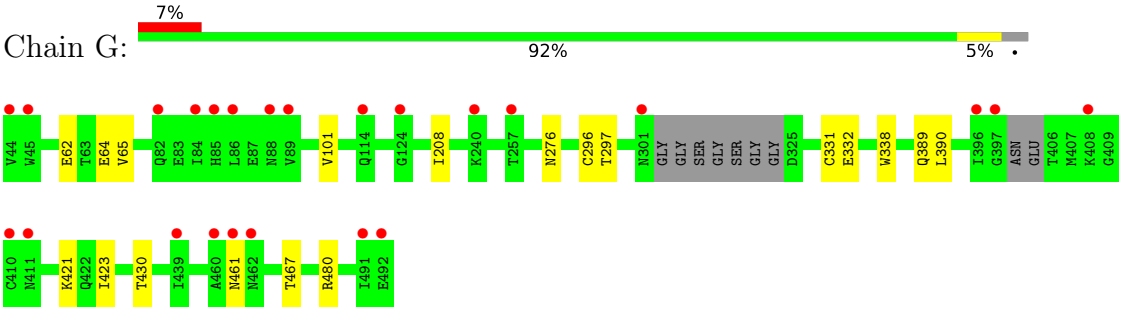
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	92	Total	O	0	0
			92	92		

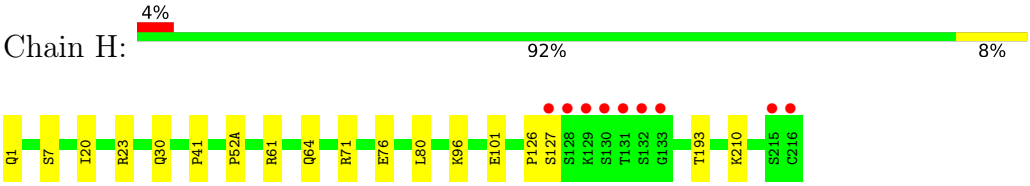
3 Residue-property plots (i)

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.

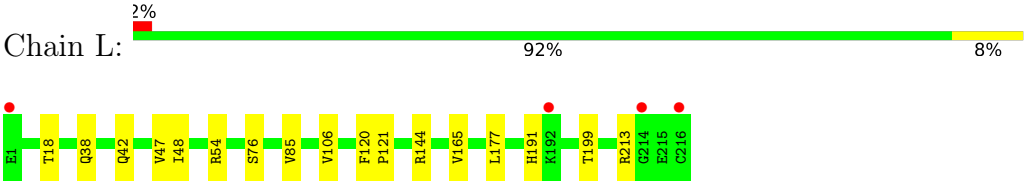
• Molecule 1: Envelope glycoprotein gp160



• Molecule 2: Antigen binding fragment of heavy chain: Antibody VRC01



• Molecule 3: Antigen binding fragment of light chain: Antibody VRC01



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.04Å 76.00Å 199.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.00 – 2.13 47.54 – 2.13	Depositor EDS
% Data completeness (in resolution range)	90.5 (38.00-2.13) 86.6 (47.54-2.13)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.191 , 0.226 0.194 , 0.225	Depositor DCC
R_{free} test set	2000 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6482	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	G	0.22	0/2743	0.40	0/3723
2	H	0.24	0/1808	0.44	0/2456
3	L	0.23	0/1661	0.40	0/2255
All	All	0.23	0/6212	0.41	0/8434

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

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	G	2687	0	2615	12	0
2	H	1760	0	1712	12	0
3	L	1624	0	1562	11	0
4	G	140	0	130	2	0
5	G	78	0	0	4	0
5	H	101	0	0	6	0
5	L	92	0	0	4	0
All	All	6482	0	6019	34	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 3.

All (34) 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:H:23:ARG:NH1	5:H:367:HOH:O	2.15	0.80
1:G:297:THR:OG1	5:G:647:HOH:O	2.06	0.74
2:H:1:GLN:N	5:H:362:HOH:O	2.25	0.69
3:L:191:HIS:O	3:L:213:ARG:NH1	2.26	0.67
1:G:332:GLU:OE2	5:G:671:HOH:O	2.16	0.62
1:G:101:VAL:HG21	1:G:480:ARG:HG2	1.82	0.61
1:G:62:GLU:HG3	1:G:64:GLU:H	1.64	0.60
2:H:64:GLN:OE1	5:H:353:HOH:O	2.16	0.58
3:L:144:ARG:NH1	5:L:312:HOH:O	2.37	0.57
4:G:509:NAG:H83	5:G:666:HOH:O	2.03	0.57
1:G:421:LYS:NZ	1:G:423:ILE:O	2.36	0.56
3:L:199:THR:HG23	5:L:308:HOH:O	2.06	0.55
2:H:7:SER:OG	5:H:303:HOH:O	2.18	0.55
3:L:47:VAL:HG12	3:L:48:ILE:HG12	1.89	0.55
2:H:193:THR:HG23	2:H:210:LYS:HE3	1.90	0.52
2:H:76:GLU:OE2	5:H:339:HOH:O	2.19	0.51
1:G:65:VAL:HG21	1:G:208:ILE:HD12	1.93	0.50
1:G:461:ASN:CG	2:H:61:ARG:HD2	2.32	0.50
2:H:96:LYS:HB2	2:H:101:GLU:HB2	1.95	0.49
3:L:38:GLN:HB3	3:L:85:VAL:HG13	1.94	0.48
1:G:389:GLN:HG2	4:G:509:NAG:H81	1.95	0.48
2:H:30:GLN:HA	2:H:52(A):PRO:HB2	1.97	0.46
3:L:42:GLN:NE2	5:L:361:HOH:O	2.40	0.46
3:L:165:VAL:HG22	3:L:177:LEU:HD12	1.96	0.46
2:H:20:ILE:HD11	2:H:80:LEU:HD23	1.98	0.44
3:L:18:THR:HG22	3:L:76:SER:HA	2.00	0.44
1:G:338:TRP:NE1	1:G:390:LEU:O	2.33	0.42
1:G:208:ILE:HG12	5:G:644:HOH:O	2.20	0.42
1:G:467:THR:N	2:H:61:ARG:HH12	2.18	0.41
2:H:41:PRO:HA	5:H:361:HOH:O	2.20	0.41
1:G:296:CYS:HA	1:G:331:CYS:HA	2.01	0.41
3:L:120:PHE:HA	3:L:121:PRO:HD2	1.94	0.41
3:L:106:VAL:HG12	5:L:314:HOH:O	2.20	0.40
3:L:48:ILE:HD13	3:L:54:ARG:HA	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	G	338/353 (96%)	322 (95%)	15 (4%)	1 (0%)	41 36
2	H	226/228 (99%)	221 (98%)	3 (1%)	2 (1%)	17 10
3	L	208/210 (99%)	204 (98%)	4 (2%)	0	100 100
All	All	772/791 (98%)	747 (97%)	22 (3%)	3 (0%)	34 29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	126	PRO
1	G	430	THR
2	H	127	SER

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	G	305/311 (98%)	304 (100%)	1 (0%)	92 94
2	H	196/196 (100%)	195 (100%)	1 (0%)	88 91
3	L	181/182 (100%)	181 (100%)	0	100 100
All	All	682/689 (99%)	680 (100%)	2 (0%)	92 94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	276	ASN
2	H	71	ARG

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

Mol	Chain	Res	Type
1	G	422	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)

10 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	507	1	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	G	503	1	14,14,15	0.24	0	17,19,21	0.59	0
4	NAG	G	509	1	14,14,15	0.28	0	17,19,21	0.39	0
4	NAG	G	504	1	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	G	506	1	14,14,15	0.30	0	17,19,21	0.44	0
4	NAG	G	502	1	14,14,15	0.41	0	17,19,21	0.62	0
4	NAG	G	505	1	14,14,15	0.27	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	G	510	1	14,14,15	0.29	0	17,19,21	0.48	0
4	NAG	G	508	1	14,14,15	0.36	0	17,19,21	0.54	0
4	NAG	G	501	1	14,14,15	0.26	0	17,19,21	0.32	0

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	507	1	-	0/6/23/26	0/1/1/1
4	NAG	G	503	1	-	2/6/23/26	0/1/1/1
4	NAG	G	509	1	-	4/6/23/26	0/1/1/1
4	NAG	G	504	1	-	2/6/23/26	0/1/1/1
4	NAG	G	506	1	-	2/6/23/26	0/1/1/1
4	NAG	G	502	1	-	0/6/23/26	0/1/1/1
4	NAG	G	505	1	-	2/6/23/26	0/1/1/1
4	NAG	G	510	1	-	4/6/23/26	0/1/1/1
4	NAG	G	508	1	-	2/6/23/26	0/1/1/1
4	NAG	G	501	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	510	NAG	O5-C5-C6-O6
4	G	505	NAG	C8-C7-N2-C2
4	G	505	NAG	O7-C7-N2-C2
4	G	509	NAG	C8-C7-N2-C2
4	G	509	NAG	O7-C7-N2-C2
4	G	510	NAG	C8-C7-N2-C2
4	G	510	NAG	O7-C7-N2-C2
4	G	510	NAG	C4-C5-C6-O6
4	G	506	NAG	O5-C5-C6-O6
4	G	508	NAG	O5-C5-C6-O6
4	G	503	NAG	O5-C5-C6-O6
4	G	506	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	G	504	NAG	O5-C5-C6-O6
4	G	503	NAG	C4-C5-C6-O6
4	G	509	NAG	O5-C5-C6-O6
4	G	509	NAG	C4-C5-C6-O6
4	G	508	NAG	C4-C5-C6-O6
4	G	504	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	509	NAG	2	0

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^{th} 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	G	344/353 (97%)	0.51	24 (6%)	16	21	32, 59, 95, 118	0
2	H	228/228 (100%)	0.20	9 (3%)	39	47	31, 44, 75, 152	0
3	L	210/210 (100%)	-0.09	4 (1%)	66	72	30, 44, 72, 128	0
All	All	782/791 (98%)	0.26	37 (4%)	31	38	30, 50, 91, 152	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	131	THR	13.2
2	H	132	SER	11.2
2	H	216	CYS	10.9
2	H	133	GLY	9.7
1	G	460	ALA	9.0
2	H	130	SER	8.7
2	H	129	LYS	8.5
2	H	128	SER	8.0
3	L	216	CYS	7.3
1	G	44	VAL	6.8
1	G	461	ASN	6.6
2	H	215	SER	6.0
1	G	411	ASN	5.8
1	G	410	CYS	5.2
1	G	462	ASN	4.7
1	G	491	ILE	4.7
1	G	86	LEU	4.5
1	G	492	GLU	4.2
1	G	396	ILE	4.2
3	L	214	GLY	4.1
1	G	45	TRP	3.8
1	G	301	ASN	3.8
1	G	84	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	408	LYS	2.9
3	L	1	GLU	2.8
1	G	124	GLY	2.7
1	G	82	GLN	2.7
1	G	439	ILE	2.5
1	G	88	ASN	2.5
1	G	397	GLY	2.4
3	L	192	LYS	2.3
2	H	127	SER	2.3
1	G	114	GLN	2.2
1	G	85	HIS	2.2
1	G	89	VAL	2.2
1	G	257	THR	2.2
1	G	240	LYS	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, 95^{th} 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	502	14/15	0.67	0.50	99,119,127,128	0
4	NAG	G	510	14/15	0.82	0.23	78,96,100,104	0
4	NAG	G	505	14/15	0.89	0.14	47,63,75,78	0
4	NAG	G	508	14/15	0.89	0.16	55,78,88,91	0
4	NAG	G	509	14/15	0.89	0.30	85,101,111,114	0
4	NAG	G	504	14/15	0.89	0.18	79,95,104,105	0
4	NAG	G	507	14/15	0.90	0.31	78,95,99,100	0
4	NAG	G	501	14/15	0.93	0.10	44,59,71,77	0
4	NAG	G	506	14/15	0.94	0.12	47,63,75,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	G	503	14/15	0.96	0.12	41,49,58,59	0

6.5 Other polymers (i)

There are no such residues in this entry.