



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2024 – 04:16 PM EDT

PDB ID : 8SM0  
Title : Crystal structure of human complement receptor 2 (CD21) in complex with Epstein-Barr virus major glycoprotein gp350  
Authors : Chen, W.-H.; Bu, W.; Cohen, J.I.; Kanekiyo, M.; Joyce, M.G.  
Deposited on : 2023-04-25  
Resolution : 1.68 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
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) : 2.36.2

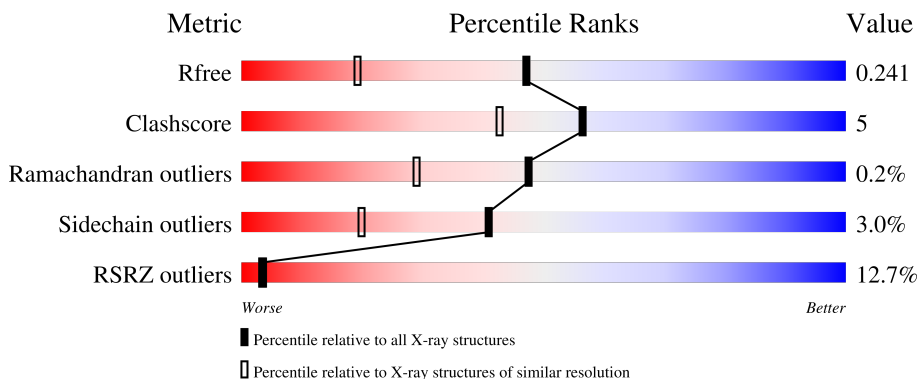
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.68 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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  $\geq 3$ , 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	C	129	 9% 93% 6%
2	G	431	 13% 79% 13% 7%

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
3	NAG	C	601	-	-	-	X
3	NAG	C	602	-	-	-	X
3	NAG	G	504	-	-	-	X
3	NAG	G	506	-	-	-	X
3	NAG	G	507	-	-	-	X
3	NAG	G	510	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8526 atoms, of which 4061 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 Complement receptor type 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	C	129	1945	625	959	169	182	10	0	0	0

- Molecule 2 is a protein called Envelope glycoprotein gp350.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	G	400	6003	1942	2934	496	614	17	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	426	HIS	-	expression tag	UNP P03200
G	427	HIS	-	expression tag	UNP P03200
G	428	HIS	-	expression tag	UNP P03200
G	429	HIS	-	expression tag	UNP P03200
G	430	HIS	-	expression tag	UNP P03200
G	431	HIS	-	expression tag	UNP P03200

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
3	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

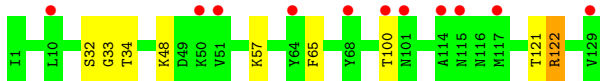
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	77	Total	O	0	0
			77	77		
5	G	160	Total	O	0	0
			160	160		

### 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.

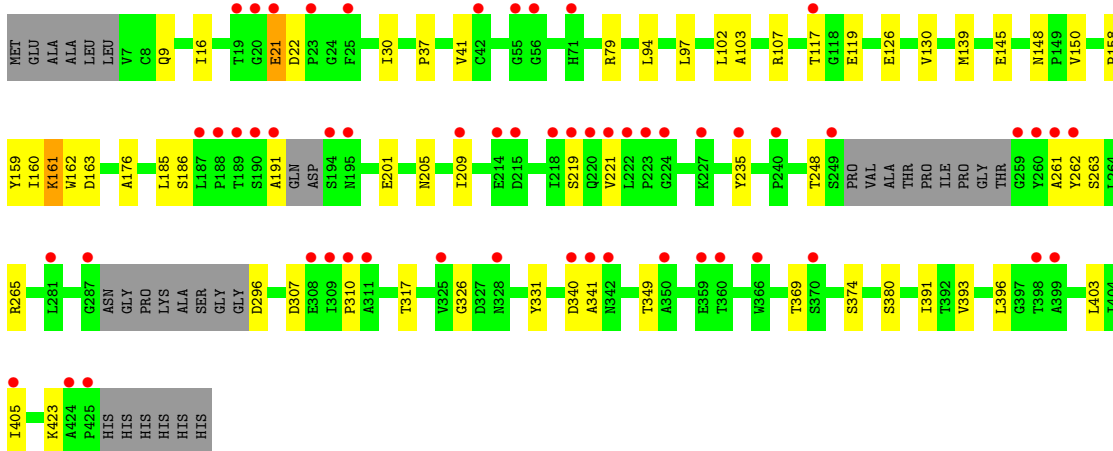
- Molecule 1: Complement receptor type 2

Chain C: 



- Molecule 2: Envelope glycoprotein gp350

Chain G: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.58Å 49.26Å 78.32Å 90.00° 101.64° 90.00°	Depositor
Resolution (Å)	30.68 – 1.68 30.68 – 1.68	Depositor EDS
% Data completeness (in resolution range)	84.2 (30.68-1.68) 84.2 (30.68-1.68)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 1.69Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.212 , 0.241 0.212 , 0.241	Depositor DCC
$R_{free}$ test set	2796 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtrriage
Anisotropy	0.659	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4

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	C	0.26	0/1015	0.46	0/1381
2	G	0.27	0/3140	0.48	0/4291
All	All	0.27	0/4155	0.48	0/5672

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	C	986	959	961	4	0
2	G	3069	2934	2931	36	0
3	C	28	28	26	1	0
3	G	140	140	130	2	0
4	C	5	0	0	0	0
5	C	77	0	0	1	0
5	G	160	0	0	13	0
All	All	4465	4061	4048	41	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 (41) 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:G:176:ALA:HB2	2:G:310:PRO:HG3	1.62	0.81
2:G:326:GLY:O	2:G:423:LYS:NZ	2.14	0.81
3:G:501:NAG:O7	5:G:601:HOH:O	1.99	0.80
2:G:185:LEU:O	5:G:602:HOH:O	2.01	0.78
2:G:126:GLU:OE2	5:G:603:HOH:O	2.03	0.77
2:G:307:ASP:OD2	3:G:505:NAG:O3	2.06	0.72
2:G:162:TRP:NE1	2:G:201:GLU:OE2	2.24	0.70
2:G:119:GLU:OE1	5:G:604:HOH:O	2.10	0.70
2:G:79:ARG:NH2	5:G:610:HOH:O	2.24	0.69
2:G:148:ASN:OD1	5:G:605:HOH:O	2.11	0.67
2:G:159:TYR:OH	5:G:606:HOH:O	2.13	0.67
2:G:117:THR:OG1	5:G:607:HOH:O	2.13	0.66
2:G:9:GLN:OE1	2:G:139:MET:N	2.26	0.66
2:G:340:ASP:O	5:G:608:HOH:O	2.13	0.66
2:G:219:SER:O	5:G:609:HOH:O	2.16	0.63
2:G:161:LYS:NZ	5:G:611:HOH:O	2.28	0.62
1:C:122:ARG:NH1	5:C:703:HOH:O	2.29	0.61
2:G:107:ARG:NH2	2:G:205:ASN:O	2.37	0.56
2:G:94:LEU:HD11	2:G:102:LEU:HD13	1.87	0.55
2:G:191:ALA:HB1	2:G:221:VAL:O	2.11	0.51
2:G:262:TYR:O	5:G:602:HOH:O	2.20	0.50
1:C:34:THR:O	1:C:65:PHE:HB2	2.11	0.50
2:G:37:PRO:HG3	2:G:317:THR:HG21	1.94	0.49
2:G:30:ILE:CD1	2:G:130:VAL:HG21	2.43	0.49
2:G:393:VAL:HG23	2:G:396:LEU:HD11	1.94	0.49
2:G:150:VAL:HG21	2:G:235:TYR:OH	2.13	0.48
2:G:340:ASP:OD1	2:G:341:ALA:N	2.47	0.48
1:C:32:SER:O	1:C:34:THR:N	2.47	0.47
2:G:248:THR:HB	2:G:261:ALA:HB3	1.98	0.46
2:G:30:ILE:HD11	2:G:130:VAL:HG21	1.98	0.45
2:G:158:PRO:O	2:G:160:ILE:HD12	2.17	0.45
2:G:41:VAL:O	2:G:41:VAL:CG1	2.65	0.43
2:G:97:LEU:HD11	2:G:103:ALA:HB2	2.00	0.43
2:G:21:GLU:HG3	2:G:22:ASP:N	2.35	0.42
2:G:201:GLU:HA	2:G:209:ILE:O	2.20	0.42
2:G:403:LEU:HD23	2:G:405:ILE:HD11	2.03	0.41
1:C:121:THR:HG21	3:C:602:NAG:O5	2.21	0.41
2:G:16:ILE:HG22	2:G:235:TYR:CE1	2.56	0.41
2:G:369:THR:O	2:G:369:THR:OG1	2.37	0.40
2:G:349:THR:HG23	5:G:651:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:331:TYR:O	2:G:391:ILE:HG22	2.21	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	C	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19	6
2	G	392/431 (91%)	381 (97%)	11 (3%)	0	100	100
All	All	519/560 (93%)	506 (98%)	12 (2%)	1 (0%)	47	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	33	GLY

### 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	C	112/113 (99%)	108 (96%)	4 (4%)	35	14
2	G	350/373 (94%)	340 (97%)	10 (3%)	42	21
All	All	462/486 (95%)	448 (97%)	14 (3%)	41	20

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	48	LYS
1	C	57	LYS
1	C	100	THR
1	C	122	ARG
2	G	21	GLU
2	G	145	GLU
2	G	161	LYS
2	G	163	ASP
2	G	186	SER
2	G	263	SER
2	G	265	ARG
2	G	296	ASP
2	G	374	SER
2	G	380	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

13 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	$\# Z  > 2$
3	NAG	G	509	2	14,14,15	0.27	0	17,19,21	0.38	0
3	NAG	G	502	2	14,14,15	0.26	0	17,19,21	0.46	0
4	SO4	C	603	-	4,4,4	0.14	0	6,6,6	0.06	0
3	NAG	G	504	2	14,14,15	0.16	0	17,19,21	0.46	0
3	NAG	G	508	2	14,14,15	0.18	0	17,19,21	0.34	0
3	NAG	C	601	1	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	G	506	2	14,14,15	0.34	0	17,19,21	0.38	0
3	NAG	C	602	1	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	G	501	2	14,14,15	0.26	0	17,19,21	0.47	0
3	NAG	G	505	2	14,14,15	0.24	0	17,19,21	0.47	0
3	NAG	G	507	2	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	G	510	2	14,14,15	0.14	0	17,19,21	0.76	1 (5%)
3	NAG	G	503	2	14,14,15	0.21	0	17,19,21	0.41	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
3	NAG	G	509	2	-	2/6/23/26	0/1/1/1
3	NAG	G	502	2	-	4/6/23/26	0/1/1/1
3	NAG	G	504	2	-	1/6/23/26	0/1/1/1
3	NAG	G	508	2	-	1/6/23/26	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
3	NAG	G	506	2	-	3/6/23/26	0/1/1/1
3	NAG	C	602	1	-	0/6/23/26	0/1/1/1
3	NAG	G	501	2	-	4/6/23/26	0/1/1/1
3	NAG	G	505	2	-	2/6/23/26	0/1/1/1
3	NAG	G	507	2	-	1/6/23/26	0/1/1/1
3	NAG	G	510	2	-	3/6/23/26	0/1/1/1
3	NAG	G	503	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	510	NAG	C1-O5-C5	2.52	115.60	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	503	NAG	O5-C5-C6-O6
3	G	502	NAG	O5-C5-C6-O6
3	G	506	NAG	O5-C5-C6-O6
3	G	503	NAG	C4-C5-C6-O6
3	G	502	NAG	C4-C5-C6-O6
3	G	501	NAG	C4-C5-C6-O6
3	G	509	NAG	C4-C5-C6-O6
3	G	501	NAG	C8-C7-N2-C2
3	G	501	NAG	O7-C7-N2-C2
3	G	502	NAG	C8-C7-N2-C2
3	G	502	NAG	O7-C7-N2-C2
3	G	505	NAG	C8-C7-N2-C2
3	G	505	NAG	O7-C7-N2-C2
3	G	501	NAG	O5-C5-C6-O6
3	G	509	NAG	O5-C5-C6-O6
3	G	510	NAG	O5-C5-C6-O6
3	G	506	NAG	C4-C5-C6-O6
3	G	507	NAG	O5-C5-C6-O6
3	G	504	NAG	C3-C2-N2-C7
3	G	508	NAG	O5-C5-C6-O6
3	G	506	NAG	C1-C2-N2-C7
3	G	510	NAG	C4-C5-C6-O6
3	G	510	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	NAG	1	0
3	G	501	NAG	1	0
3	G	505	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 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, 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	C	129/129 (100%)	0.31	11 (8%) 10 11	25, 43, 78, 106	0
2	G	400/431 (92%)	0.96	56 (14%) 2 2	23, 48, 101, 184	0
All	All	529/560 (94%)	0.80	67 (12%) 3 3	23, 47, 95, 184	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	260	TYR	25.2
2	G	249	SER	12.8
2	G	261	ALA	9.7
2	G	309	ILE	8.9
2	G	191	ALA	8.1
2	G	425	PRO	7.7
2	G	310	PRO	6.9
2	G	223	PRO	6.4
2	G	259	GLY	6.1
2	G	117	THR	5.9
2	G	187	LEU	4.8
1	C	114	ALA	4.6
2	G	189	THR	4.2
1	C	64	TYR	4.1
2	G	287	GLY	4.1
2	G	222	LEU	4.0
1	C	51	VAL	3.9
2	G	325	VAL	3.8
2	G	341	ALA	3.8
2	G	308	GLU	3.8
2	G	262	TYR	3.8
2	G	311	ALA	3.6
2	G	209	ILE	3.5
2	G	359	GLU	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	G	20	GLY	3.4
2	G	424	ALA	3.4
2	G	21	GLU	3.4
2	G	194	SER	3.3
2	G	220	GLN	3.3
2	G	56	GLY	3.2
2	G	370	SER	3.0
2	G	195	ASN	3.0
1	C	117	MET	3.0
2	G	19	THR	3.0
2	G	215	ASP	2.9
2	G	218	ILE	2.9
2	G	188	PRO	2.9
2	G	350	ALA	2.9
2	G	240	PRO	2.8
2	G	190	SER	2.7
2	G	227	LYS	2.7
2	G	221	VAL	2.6
1	C	100	THR	2.6
2	G	219	SER	2.5
2	G	398	THR	2.5
2	G	399	ALA	2.5
2	G	42	CYS	2.5
2	G	71	HIS	2.4
2	G	23	PRO	2.4
2	G	340	ASP	2.4
2	G	224	GLY	2.4
1	C	10	LEU	2.3
2	G	366	TRP	2.3
2	G	25	PHE	2.3
2	G	214	GLU	2.3
2	G	55	GLY	2.3
1	C	50	LYS	2.2
2	G	360	THR	2.2
2	G	281	LEU	2.2
1	C	101	ASN	2.2
2	G	405	ILE	2.2
2	G	235	TYR	2.2
1	C	129	VAL	2.2
1	C	115	ASN	2.1
2	G	328	ASN	2.1
1	C	68	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
2	G	342	ASN	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	C	602	14/15	0.22	0.45	76,134,163,168	0
3	NAG	G	510	14/15	0.33	0.62	132,178,226,242	0
3	NAG	G	506	14/15	0.35	0.56	117,166,240,265	0
3	NAG	G	507	14/15	0.62	0.49	121,152,178,185	0
3	NAG	G	504	14/15	0.68	0.62	169,192,226,231	0
3	NAG	G	502	14/15	0.71	0.25	109,139,173,180	0
3	NAG	C	601	14/15	0.73	0.54	155,187,215,216	0
3	NAG	G	503	14/15	0.75	0.26	88,113,135,152	0
3	NAG	G	509	14/15	0.84	0.21	76,107,137,137	0
3	NAG	G	505	14/15	0.87	0.20	58,82,107,107	0
3	NAG	G	501	14/15	0.88	0.19	61,78,98,112	0
3	NAG	G	508	14/15	0.90	0.09	30,44,56,68	0
4	SO4	C	603	5/5	0.90	0.14	86,95,106,128	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.