



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:43 am GMT

PDB ID : 2ZB6
Title : Crystal structure of the measles virus hemagglutinin (oligo-sugar type)
Authors : Hashiguchi, T.; Kajikawa, M.; Maita, N.; Takeda, M.; Kuroki, K.; Sasaki, K.; Kohda, D.; Yanagi, Y.; Maenaka, K.
Deposited on : 2007-10-16
Resolution : 2.60 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

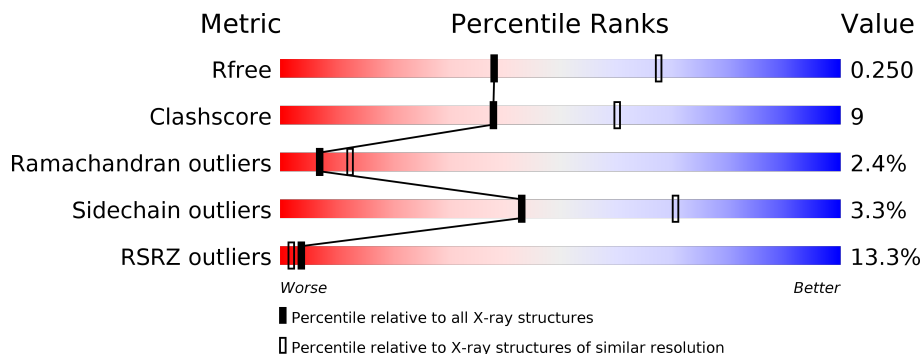
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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	481	<div> <div>12%</div> <div>69%</div> <div>18%</div> <div>•</div> <div>11%</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
3	NAG	A	12	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3391 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 Hemagglutinin protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	3276	2095	544	613	24	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	GLU	-	EXPRESSION TAG	UNP Q83625
A	147	THR	-	EXPRESSION TAG	UNP Q83625
A	148	GLY	-	EXPRESSION TAG	UNP Q83625
A	484	THR	ASN	ENGINEERED	UNP Q83625
A	492	GLY	GLU	ENGINEERED	UNP Q83625
A	618	GLY	-	EXPRESSION TAG	UNP Q83625
A	619	THR	-	EXPRESSION TAG	UNP Q83625
A	620	LYS	-	EXPRESSION TAG	UNP Q83625
A	621	HIS	-	EXPRESSION TAG	UNP Q83625
A	622	HIS	-	EXPRESSION TAG	UNP Q83625
A	623	HIS	-	EXPRESSION TAG	UNP Q83625
A	624	HIS	-	EXPRESSION TAG	UNP Q83625
A	625	HIS	-	EXPRESSION TAG	UNP Q83625
A	626	HIS	-	EXPRESSION TAG	UNP Q83625

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

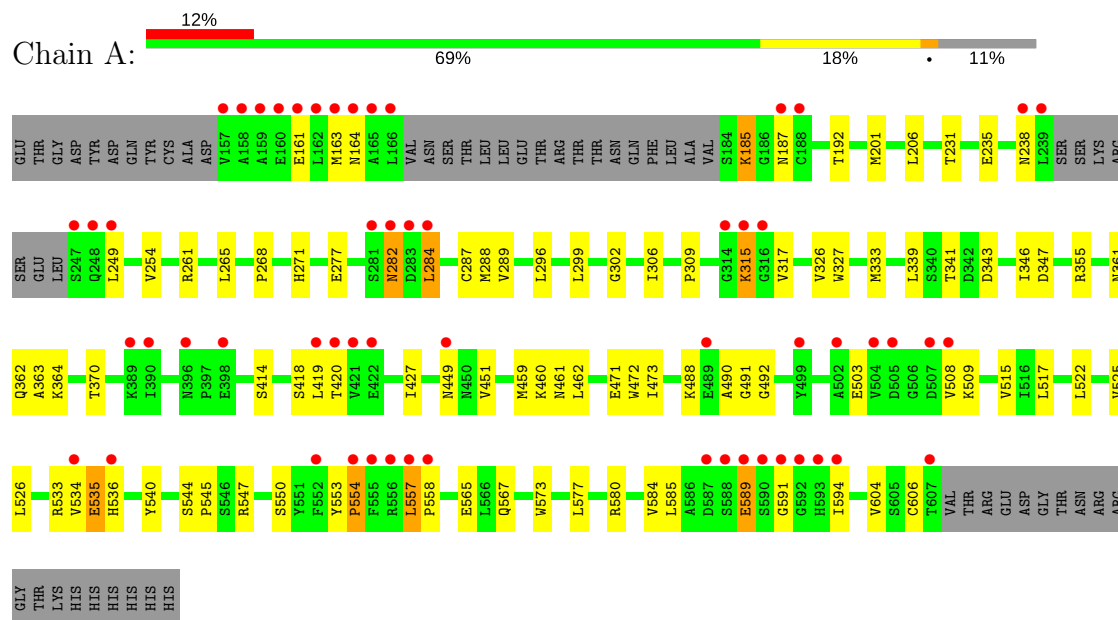
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Hemagglutinin protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.09Å 134.09Å 100.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.60) 99.3 (29.98-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.22 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.248 0.226 , 0.250	Depositor DCC
R_{free} test set	1968 reflections (6.88%)	DCC
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3391	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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

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	A	0.36	0/3358	0.64	0/4573

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	A	3276	0	3195	56	0
2	A	14	0	13	0	0
3	A	28	0	25	2	0
4	A	73	0	0	0	0
All	All	3391	0	3233	57	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 9.

All (57) 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)
1:A:254:VAL:HG22	1:A:277:GLU:HG3	1.52	0.90
1:A:459:MET:HB3	1:A:462:LEU:HD22	1.74	0.70
1:A:557:LEU:H	1:A:558:PRO:CD	2.07	0.68
1:A:261:ARG:HH11	1:A:261:ARG:HG3	1.59	0.67
1:A:192:THR:HG22	1:A:606:CYS:HB3	1.82	0.62
1:A:185:LYS:HE3	1:A:544:SER:HB2	1.81	0.61
1:A:235:GLU:HG2	1:A:249:LEU:HD22	1.86	0.57
1:A:161:GLU:HA	1:A:164:ASN:HD22	1.70	0.57
1:A:306:ILE:HG21	1:A:317:VAL:HG11	1.88	0.56
1:A:361:ASN:ND2	1:A:418:SER:HB3	2.20	0.56
1:A:451:VAL:HG22	1:A:471:GLU:HG2	1.86	0.56
1:A:339:LEU:HD11	1:A:427:ILE:HD11	1.86	0.56
1:A:284:LEU:HD22	1:A:302:GLY:O	2.06	0.55
1:A:309:PRO:HG2	1:A:341:THR:HG22	1.88	0.55
1:A:315:LYS:HD2	1:A:315:LYS:O	2.07	0.55
1:A:557:LEU:H	1:A:558:PRO:HD2	1.71	0.54
1:A:347:ASP:HB3	1:A:370:THR:OG1	2.09	0.53
1:A:261:ARG:NH1	1:A:271:HIS:ND1	2.54	0.53
1:A:461:ASN:HA	1:A:509:LYS:HB3	1.89	0.53
1:A:565:GLU:HB3	1:A:584:VAL:HB	1.91	0.52
1:A:355:ARG:NH2	1:A:567:GLN:HG3	2.24	0.52
1:A:231:THR:HG21	1:A:287:CYS:HB2	1.90	0.52
1:A:261:ARG:HG3	1:A:261:ARG:NH1	2.26	0.51
1:A:460:LYS:HE3	1:A:508:VAL:HG13	1.93	0.50
1:A:161:GLU:HA	1:A:164:ASN:ND2	2.28	0.49
1:A:557:LEU:N	1:A:558:PRO:CD	2.74	0.49
1:A:418:SER:C	1:A:420:THR:H	2.16	0.48
1:A:533:ARG:HB3	1:A:535:GLU:OE1	2.13	0.48
1:A:517:LEU:HD11	1:A:525:VAL:CG2	2.42	0.48
1:A:472:TRP:CD1	1:A:473:ILE:HG13	2.49	0.48
1:A:589:GLU:O	1:A:589:GLU:HG2	2.14	0.48
1:A:585:LEU:HB2	1:A:594:ILE:HG23	1.96	0.48
1:A:522:LEU:O	1:A:545:PRO:HD3	2.15	0.47
1:A:343:ASP:HB3	1:A:346:ILE:HG12	1.96	0.47
1:A:201:MET:SD	1:A:265:LEU:HD13	2.55	0.46
1:A:343:ASP:HB3	1:A:346:ILE:CD1	2.46	0.46
1:A:362:GLN:NE2	1:A:364:LYS:HE2	2.30	0.45
1:A:187:ASN:HD22	1:A:604:VAL:HB	1.82	0.45
1:A:343:ASP:HB3	1:A:346:ILE:HD11	1.97	0.45
1:A:288:MET:CE	1:A:299:LEU:HD23	2.47	0.44
1:A:282:ASN:HD22	1:A:282:ASN:N	2.16	0.44
1:A:363:ALA:O	1:A:414:SER:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:TYR:CD2	1:A:554:PRO:HD2	2.53	0.44
1:A:544:SER:HB3	1:A:547:ARG:O	2.17	0.44
1:A:282:ASN:N	1:A:282:ASN:ND2	2.67	0.43
1:A:361:ASN:HD21	1:A:418:SER:HB3	1.83	0.43
1:A:540:TYR:O	1:A:550:SER:HA	2.19	0.43
1:A:580:ARG:HG3	1:A:580:ARG:HH11	1.84	0.43
1:A:268:PRO:HD3	1:A:573:TRP:CE3	2.54	0.42
1:A:289:VAL:HG13	1:A:296:LEU:HD11	2.02	0.42
1:A:591:GLY:HA2	3:A:12:NAG:H61	2.02	0.42
1:A:490:ALA:O	1:A:492:GLY:N	2.53	0.41
3:A:11:NAG:H61	3:A:12:NAG:H83	2.03	0.41
1:A:261:ARG:HH21	1:A:327:TRP:HH2	1.68	0.41
1:A:533:ARG:O	1:A:535:GLU:HG2	2.20	0.41
1:A:488:LYS:N	1:A:488:LYS:HD2	2.37	0.40
1:A:343:ASP:HB3	1:A:346:ILE:CG1	2.52	0.40

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	421/481 (88%)	372 (88%)	39 (9%)	10 (2%)	7 12

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	PRO
1	A	557	LEU
1	A	185	LYS
1	A	535	GLU
1	A	536	HIS
1	A	503	GLU

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Mol	Chain	Res	Type
1	A	589	GLU
1	A	238	ASN
1	A	491	GLY
1	A	534	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	361/420 (86%)	349 (97%)	12 (3%)	43 70

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	MET
1	A	206	LEU
1	A	282	ASN
1	A	284	LEU
1	A	315	LYS
1	A	326	VAL
1	A	333	MET
1	A	419	LEU
1	A	449	ASN
1	A	515	VAL
1	A	526	LEU
1	A	577	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	A	187	ASN
1	A	225	GLN
1	A	278	GLN
1	A	282	ASN

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Mol	Chain	Res	Type
1	A	320	GLN
1	A	361	ASN
1	A	362	GLN
1	A	384	GLN
1	A	396	ASN
1	A	437	HIS
1	A	449	ASN
1	A	575	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](#)

2 carbohydrates 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	A	11	1,3	14,14,15	0.67	0	15,19,21	0.97	1 (6%)
3	NAG	A	12	3	14,14,15	0.58	0	15,19,21	0.66	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	A	11	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	12	3	-	0/6/23/26	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	A	11	NAG	C2-N2-C7	-2.12	119.86	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	11	NAG	1	0
3	A	12	NAG	2	0

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
2	NAG	A	1	1	14,14,15	0.53	0	15,19,21	0.74	1 (6%)

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
2	NAG	A	1	1	-	0/6/23/26	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($^{\circ}$)	Ideal($^{\circ}$)
2	A	1	NAG	C2-N2-C7	-2.03	119.98	122.94

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 ⓘ

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	427/481 (88%)	0.45	57 (13%) 4 2	22, 44, 102, 117	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	590	SER	8.9
1	A	555	PHE	7.3
1	A	158	ALA	5.2
1	A	420	THR	5.2
1	A	591	GLY	5.1
1	A	314	GLY	4.9
1	A	536	HIS	4.9
1	A	163	MET	4.7
1	A	588	SER	4.7
1	A	238	ASN	4.7
1	A	504	VAL	4.7
1	A	164	ASN	4.6
1	A	165	ALA	4.5
1	A	315	LYS	4.4
1	A	587	ASP	4.3
1	A	534	VAL	4.2
1	A	247	SER	4.2
1	A	162	LEU	4.1
1	A	421	VAL	4.1
1	A	239	LEU	4.1
1	A	160	GLU	4.0
1	A	390	ILE	3.9
1	A	502	ALA	3.8
1	A	248	GLN	3.7
1	A	187	ASN	3.7
1	A	283	ASP	3.7
1	A	594	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	249	LEU	3.5
1	A	281	SER	3.4
1	A	161	GLU	3.3
1	A	554	PRO	3.2
1	A	589	GLU	3.1
1	A	592	GLY	3.1
1	A	157	VAL	3.1
1	A	188	CYS	3.0
1	A	508	VAL	2.9
1	A	284	LEU	2.9
1	A	282	ASN	2.9
1	A	558	PRO	2.9
1	A	607	THR	2.8
1	A	316	GLY	2.7
1	A	159	ALA	2.7
1	A	507	ASP	2.7
1	A	593	HIS	2.7
1	A	422	GLU	2.6
1	A	556	ARG	2.6
1	A	166	LEU	2.6
1	A	398	GLU	2.6
1	A	419	LEU	2.4
1	A	505	ASP	2.3
1	A	396	ASN	2.3
1	A	557	LEU	2.3
1	A	449	ASN	2.3
1	A	489	GLU	2.3
1	A	552	PHE	2.3
1	A	499	TYR	2.2
1	A	389	LYS	2.1

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](#)

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	11	14/15	0.79	0.39	0.49	90,96,98,101	0
3	NAG	A	12	14/15	0.73	0.46	0.26	104,105,106,106	0

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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	1	14/15	0.75	0.39	-	76,81,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.