



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:20 AM UTC

PDB ID : 6ICY / pdb_00006icy
Title : Crystal structure of H7 hemagglutinin mutant H7-AGTL (V186G, P221T)
from the influenza virus A/Anhui/1/2013 (H7N9)
Authors : Gao, G.F.; Xu, Y.; Qi, J.X.
Deposited on : 2018-09-07
Resolution : 2.40 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

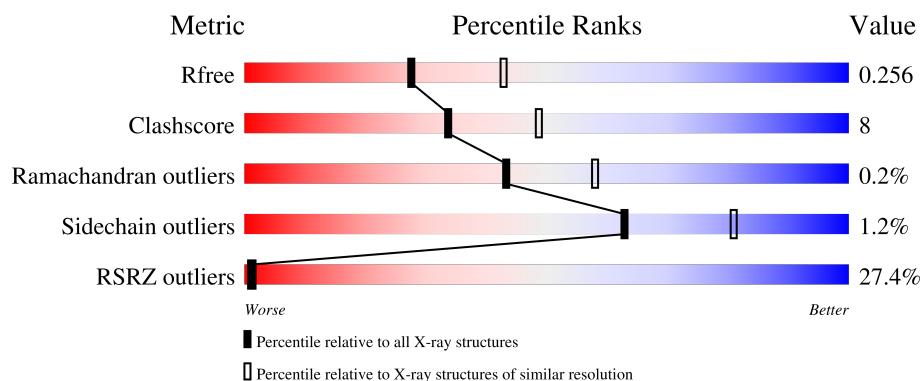
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	321	23% 85% 12% ..
2	B	177	33% 80% 13% .. 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3906 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 HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2392	1484	433	460	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	GLY	VAL	engineered mutation	UNP R4NN21
A	211	THR	PRO	engineered mutation	UNP R4NN21

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	168	1364	843	236	278	7	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

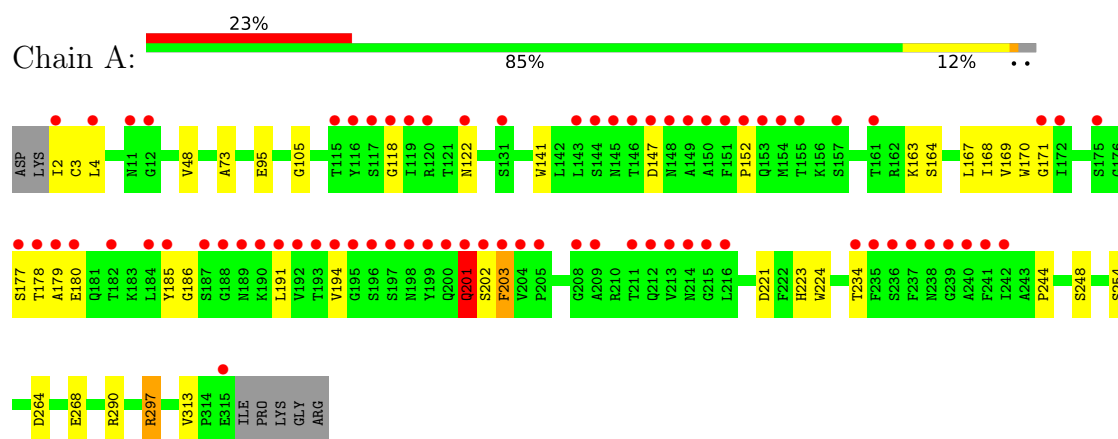
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	80	Total	O	0	0
			80	80		
4	B	28	Total	O	0	0
			28	28		

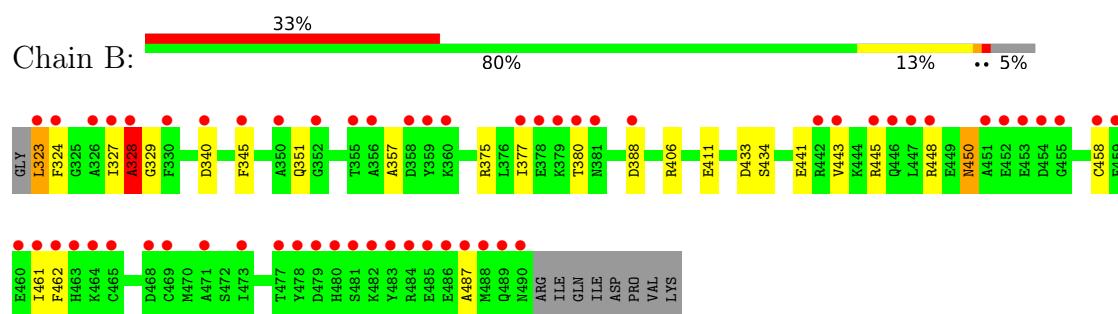
3 Residue-property plots

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: Hemagglutinin HA1 chain



• Molecule 2: Hemagglutinin HA2 chain



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	116.54Å 116.54Å 295.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.35 – 2.40 38.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.0 (38.35-2.40) 90.0 (38.35-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.244 , 0.267 (Not available) , 0.256	Depositor DCC
R_{free} test set	1327 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.019 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.010 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3906	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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	0.11	0/2437	0.39	3/3293 (0.1%)
2	B	0.11	0/1388	0.58	3/1871 (0.2%)
All	All	0.11	0/3825	0.47	6/5164 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	448	ARG	N-CA-C	14.79	127.12	111.14
2	B	328	ALA	CB-CA-C	-12.33	94.86	111.63
2	B	448	ARG	CB-CA-C	-9.17	96.41	110.90
1	A	201	GLN	CA-C-N	6.60	133.58	121.70
1	A	201	GLN	C-N-CA	6.60	133.58	121.70
1	A	203	PHE	CB-CA-C	5.39	121.15	110.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	GLN	Peptide
2	B	328	ALA	Peptide

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	2392	0	2346	38	0
2	B	1364	0	1261	24	1
3	A	28	0	26	1	0
3	B	14	0	13	0	0
4	A	80	0	0	20	0
4	B	28	0	0	9	0
All	All	3906	0	3646	57	1

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 8.

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)
2:B:377:ILE:HG22	4:B:602:HOH:O	1.60	1.00
2:B:411:GLU:OE2	4:B:601:HOH:O	1.83	0.96
1:A:164:SER:OG	4:A:702:HOH:O	1.87	0.93
1:A:179:ALA:N	4:A:707:HOH:O	2.02	0.92
2:B:377:ILE:C	4:B:602:HOH:O	2.12	0.91
2:B:411:GLU:HG2	4:B:601:HOH:O	1.73	0.88
1:A:177:SER:C	4:A:707:HOH:O	2.17	0.87
1:A:118:GLY:O	4:A:705:HOH:O	1.95	0.84
2:B:377:ILE:O	4:B:602:HOH:O	1.96	0.83
1:A:186:GLY:N	4:A:709:HOH:O	2.19	0.75
1:A:95:GLU:OE2	4:A:708:HOH:O	2.05	0.74
1:A:185:TYR:C	4:A:709:HOH:O	2.32	0.72
2:B:328:ALA:N	2:B:329:GLY:HA3	2.05	0.71
1:A:201:GLN:HA	1:A:202:SER:HB3	1.74	0.69
1:A:186:GLY:N	4:A:715:HOH:O	2.26	0.69
2:B:388:ASP:OD2	2:B:406:ARG:NH2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:GLU:CG	4:B:601:HOH:O	2.40	0.65
1:A:122:ASN:HB2	4:A:716:HOH:O	1.96	0.64
1:A:178:THR:N	4:A:707:HOH:O	2.31	0.61
1:A:168:ILE:O	1:A:224:TRP:HA	2.01	0.59
2:B:461:ILE:HD11	4:B:628:HOH:O	2.04	0.57
1:A:4:LEU:HD21	2:B:443:VAL:HG21	1.86	0.56
1:A:178:THR:C	4:A:707:HOH:O	2.43	0.56
1:A:141:TRP:N	4:A:704:HOH:O	1.93	0.55
1:A:313:VAL:N	4:A:703:HOH:O	1.87	0.54
2:B:375:ARG:NH2	4:B:603:HOH:O	2.20	0.53
1:A:201:GLN:CA	1:A:202:SER:HB3	2.39	0.52
2:B:327:ILE:N	2:B:433:ASP:OD1	2.41	0.52
1:A:105:GLY:HA2	1:A:254:SER:HB3	1.91	0.52
1:A:152:PRO:CD	4:A:705:HOH:O	2.57	0.51
1:A:194:VAL:HA	1:A:234:THR:O	2.11	0.51
1:A:264:ASP:OD2	4:A:710:HOH:O	2.19	0.50
2:B:441:GLU:O	2:B:445:ARG:HG2	2.11	0.49
1:A:169:VAL:HG22	1:A:224:TRP:HB3	1.94	0.49
1:A:48:VAL:HG23	1:A:73:ALA:HB2	1.95	0.48
1:A:297:ARG:NH1	2:B:380:THR:OG1	2.45	0.48
1:A:2:ILE:HD11	2:B:345:PHE:HB3	1.95	0.48
2:B:327:ILE:C	2:B:329:GLY:HA3	2.39	0.48
2:B:450:ASN:N	2:B:450:ASN:OD1	2.49	0.46
1:A:163:LYS:NZ	3:A:602:NAG:H3	2.31	0.45
1:A:171:GLY:HA2	1:A:221:ASP:O	2.17	0.44
1:A:3:CYS:HA	2:B:458:CYS:HA	1.98	0.44
1:A:268:GLU:OE2	4:A:712:HOH:O	2.21	0.44
1:A:167:LEU:HB3	1:A:248:SER:HB2	1.99	0.44
1:A:191:LEU:HB2	4:A:740:HOH:O	2.18	0.44
2:B:351:GLN:NE2	4:B:606:HOH:O	2.51	0.43
2:B:462:PHE:HB2	2:B:487:ALA:HB1	1.98	0.43
2:B:324:PHE:CE2	2:B:434:SER:HB2	2.53	0.43
1:A:105:GLY:O	4:A:711:HOH:O	2.21	0.42
1:A:141:TRP:CB	4:A:704:HOH:O	2.67	0.42
1:A:169:VAL:O	1:A:244:PRO:HB3	2.18	0.42
1:A:290:ARG:HE	2:B:388:ASP:HB2	1.85	0.42
2:B:324:PHE:HB2	2:B:433:ASP:OD2	2.20	0.41
1:A:180:GLU:N	4:A:707:HOH:O	2.21	0.41
2:B:340:ASP:HB2	2:B:357:ALA:HB2	2.02	0.41
1:A:170:TRP:CE2	1:A:223:HIS:HB2	2.56	0.40
1:A:297:ARG:H	1:A:297:ARG:HG2	1.61	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:323:LEU:O	2:B:434:SER:OG[3_655]	2.18	0.02

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	312/321 (97%)	293 (94%)	18 (6%)	1 (0%)	36	50
2	B	166/177 (94%)	158 (95%)	8 (5%)	0	100	100
All	All	478/498 (96%)	451 (94%)	26 (5%)	1 (0%)	43	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	PHE

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	262/268 (98%)	259 (99%)	3 (1%)	65	82
2	B	144/152 (95%)	142 (99%)	2 (1%)	59	79
All	All	406/420 (97%)	401 (99%)	5 (1%)	63	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	ASP
1	A	201	GLN
1	A	297	ARG
2	B	323	LEU
2	B	450	ASN

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

Mol	Chain	Res	Type
1	A	16	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	B	501	2	14,14,15	0.33	0	17,19,21	0.50	0
3	NAG	A	602	1	14,14,15	0.27	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	601	1	14,14,15	0.27	0	17,19,21	0.43	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	B	501	2	-	1/6/23/26	0/1/1/1
3	NAG	A	602	1	-	2/6/23/26	0/1/1/1
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAG	O5-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	A	602	NAG	C4-C5-C6-O6
3	A	601	NAG	C4-C5-C6-O6
3	B	501	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NAG	1	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, 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	314/321 (97%)	1.06	74 (23%) 2 1	18, 51, 111, 133	0
2	B	168/177 (94%)	1.52	58 (34%) 1 1	19, 79, 134, 145	0
All	All	482/498 (96%)	1.22	132 (27%) 1 1	18, 59, 125, 145	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	379	LYS	7.5
1	A	202	SER	7.4
1	A	211	THR	6.5
1	A	198	ASN	6.5
1	A	203	PHE	6.5
1	A	189	ASN	5.5
1	A	195	GLY	5.3
2	B	328	ALA	4.9
1	A	179	ALA	4.8
2	B	460	GLU	4.8
1	A	215	GLY	4.8
1	A	118	GLY	4.7
2	B	350	ALA	4.7
1	A	146	THR	4.7
1	A	214	ASN	4.6
2	B	380	THR	4.6
2	B	378	GLU	4.5
1	A	151	PHE	4.5
1	A	143	LEU	4.4
2	B	489	GLN	4.3
2	B	488	MET	4.2
1	A	188	GLY	4.2
1	A	190	LYS	4.2
1	A	144	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	155	THR	4.1
1	A	153	GLN	4.1
2	B	482	LYS	4.1
1	A	193	THR	4.1
1	A	152	PRO	4.0
2	B	462	PHE	4.0
1	A	191	LEU	4.0
1	A	199	TYR	4.0
1	A	178	THR	3.9
2	B	445	ARG	3.9
1	A	147	ASP	3.9
1	A	185	TYR	3.9
1	A	200	GLN	3.9
2	B	452	GLU	3.9
2	B	490	ASN	3.8
1	A	2	ILE	3.8
2	B	451	ALA	3.7
1	A	116	TYR	3.7
2	B	480	HIS	3.7
2	B	487	ALA	3.7
2	B	483	TYR	3.6
1	A	197	SER	3.6
1	A	209	ALA	3.6
2	B	459	PHE	3.6
2	B	469	CYS	3.5
1	A	204	VAL	3.5
1	A	175	SER	3.5
1	A	216	LEU	3.5
1	A	241	PHE	3.5
1	A	117	SER	3.5
2	B	377	ILE	3.4
2	B	447	LEU	3.4
1	A	150	ALA	3.4
2	B	478	TYR	3.4
2	B	461	ILE	3.4
2	B	454	ASP	3.4
1	A	192	VAL	3.4
2	B	464	LYS	3.3
2	B	484	ARG	3.3
2	B	485	GLU	3.3
1	A	149	ALA	3.2
1	A	182	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	120	ARG	3.2
1	A	236	SER	3.2
1	A	187	SER	3.1
1	A	4	LEU	3.1
2	B	465	CYS	3.1
1	A	154	MET	3.1
1	A	196	SER	3.1
1	A	180	GLU	3.1
1	A	184	LEU	3.1
1	A	237	PHE	3.1
1	A	157	SER	3.1
2	B	381	ASN	3.1
1	A	148	ASN	3.0
1	A	238	ASN	3.0
1	A	242	ILE	3.0
1	A	205	PRO	3.0
2	B	388	ASP	3.0
2	B	446	GLN	3.0
1	A	213	VAL	3.0
1	A	115	THR	3.0
1	A	119	ILE	2.8
1	A	194	VAL	2.8
1	A	212	GLN	2.8
1	A	172	ILE	2.8
2	B	455	GLY	2.7
2	B	473	ILE	2.7
2	B	443	VAL	2.7
1	A	208	GLY	2.7
1	A	235	PHE	2.7
1	A	315	GLU	2.7
1	A	240	ALA	2.6
1	A	11	ASN	2.6
2	B	463	HIS	2.6
1	A	234	THR	2.6
2	B	326	ALA	2.6
2	B	458	CYS	2.6
1	A	239	GLY	2.5
1	A	145	ASN	2.5
2	B	448	ARG	2.5
2	B	477	THR	2.5
1	A	201	GLN	2.4
2	B	453	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	358	ASP	2.4
2	B	324	PHE	2.4
2	B	471	ALA	2.4
2	B	356	ALA	2.3
2	B	486	GLU	2.3
2	B	340	ASP	2.3
2	B	468	ASP	2.3
1	A	171	GLY	2.3
2	B	345	PHE	2.3
2	B	442	ARG	2.3
1	A	12	GLY	2.2
1	A	177	SER	2.2
2	B	479	ASP	2.2
2	B	360	LYS	2.2
1	A	122	ASN	2.2
2	B	327	ILE	2.1
2	B	481	SER	2.1
1	A	161	THR	2.1
2	B	323	LEU	2.0
2	B	355	THR	2.0
2	B	359	TYR	2.0
1	A	131	SER	2.0
2	B	330	PHE	2.0
2	B	352	GLY	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	NAG	A	602	14/15	0.50	0.19	78,92,107,113	0
3	NAG	A	601	14/15	0.54	0.24	74,91,119,125	0
3	NAG	B	501	14/15	0.78	0.17	48,60,66,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.