



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:27 PM UTC

PDB ID : 6L6P / pdb_00006l6p
Title : hASIC2a co-crystallized with Mamb-1
Authors : Lei, F.; Jian, S.
Deposited on : 2019-10-29
Resolution : 3.08 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
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

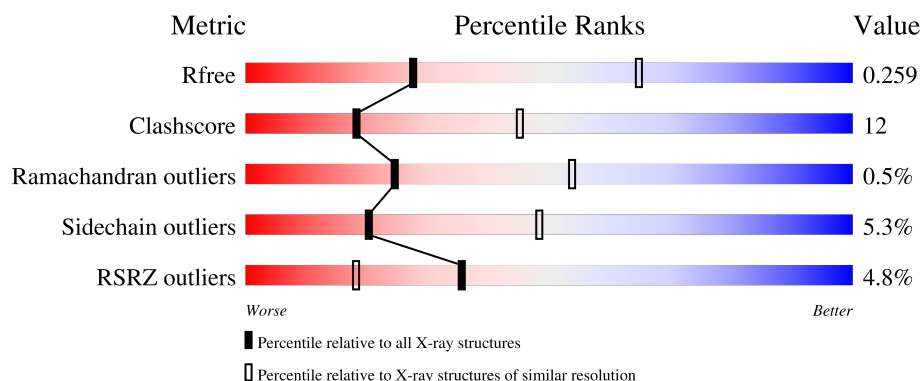
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

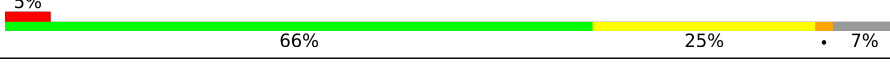
The reported resolution of this entry is 3.08 Å.

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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	463	
1	B	463	
1	C	463	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10369 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 Acid-sensing ion channel 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3468	2239	565	641	23			
1	B	433	Total	C	N	O	S	0	0	0
			3459	2235	563	638	23			
1	C	430	Total	C	N	O	S	0	0	0
			3436	2221	560	633	22			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q16515
A	0	SER	-	expression tag	UNP Q16515
A	1	GLY	-	expression tag	UNP Q16515
A	2	GLY	-	expression tag	UNP Q16515
A	3	SER	-	expression tag	UNP Q16515
A	4	GLY	-	expression tag	UNP Q16515
A	5	LEU	-	expression tag	UNP Q16515
A	6	GLU	-	expression tag	UNP Q16515
A	7	VAL	-	expression tag	UNP Q16515
A	8	LEU	-	expression tag	UNP Q16515
A	9	PHE	-	expression tag	UNP Q16515
A	10	GLN	-	expression tag	UNP Q16515
A	11	GLY	-	expression tag	UNP Q16515
A	12	PRO	-	expression tag	UNP Q16515
B	-1	GLY	-	expression tag	UNP Q16515
B	0	SER	-	expression tag	UNP Q16515
B	1	GLY	-	expression tag	UNP Q16515
B	2	GLY	-	expression tag	UNP Q16515
B	3	SER	-	expression tag	UNP Q16515
B	4	GLY	-	expression tag	UNP Q16515
B	5	LEU	-	expression tag	UNP Q16515
B	6	GLU	-	expression tag	UNP Q16515
B	7	VAL	-	expression tag	UNP Q16515

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	LEU	-	expression tag	UNP Q16515
B	9	PHE	-	expression tag	UNP Q16515
B	10	GLN	-	expression tag	UNP Q16515
B	11	GLY	-	expression tag	UNP Q16515
B	12	PRO	-	expression tag	UNP Q16515
C	-1	GLY	-	expression tag	UNP Q16515
C	0	SER	-	expression tag	UNP Q16515
C	1	GLY	-	expression tag	UNP Q16515
C	2	GLY	-	expression tag	UNP Q16515
C	3	SER	-	expression tag	UNP Q16515
C	4	GLY	-	expression tag	UNP Q16515
C	5	LEU	-	expression tag	UNP Q16515
C	6	GLU	-	expression tag	UNP Q16515
C	7	VAL	-	expression tag	UNP Q16515
C	8	LEU	-	expression tag	UNP Q16515
C	9	PHE	-	expression tag	UNP Q16515
C	10	GLN	-	expression tag	UNP Q16515
C	11	GLY	-	expression tag	UNP Q16515
C	12	PRO	-	expression tag	UNP Q16515

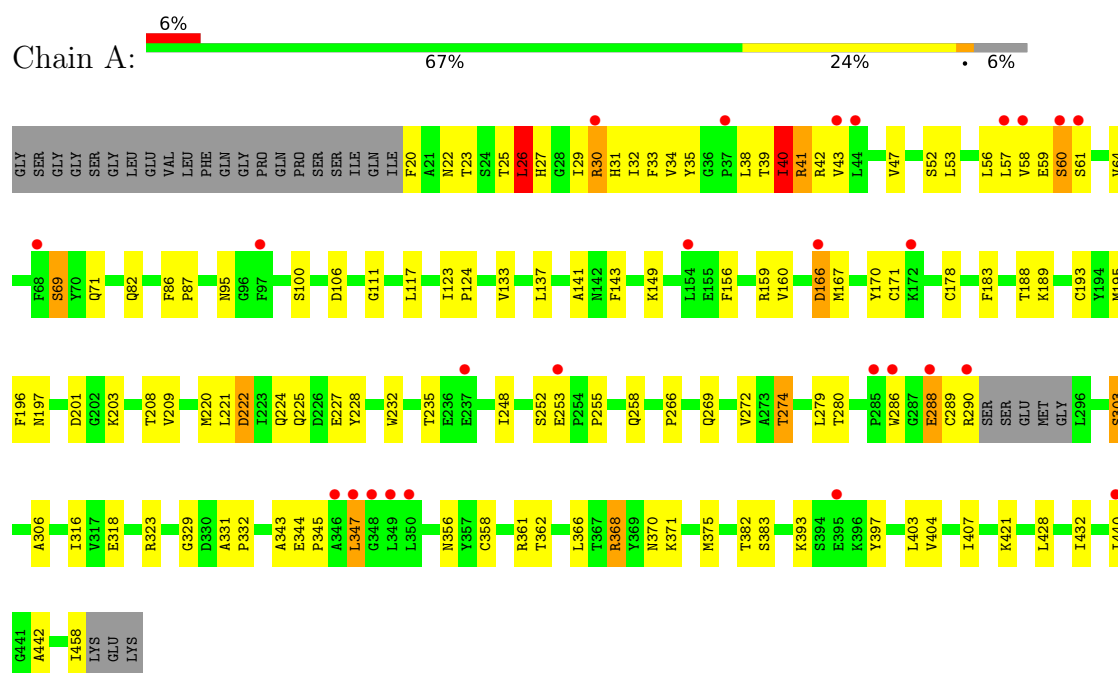
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0
2	B	2	Total O 2 2	0	0
2	C	2	Total O 2 2	0	0

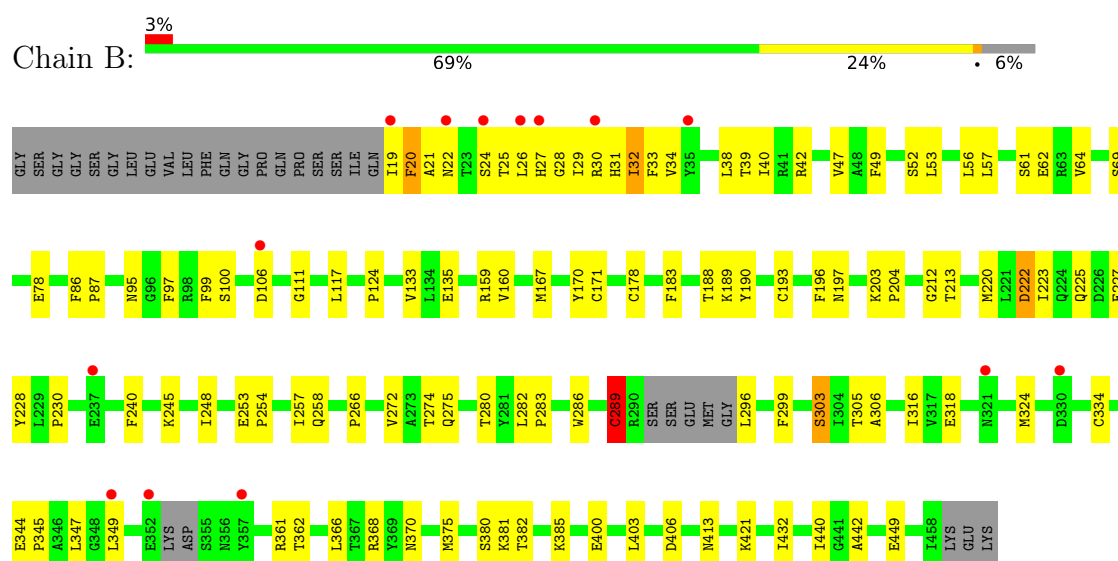
3 Residue-property plots [i](#)

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.

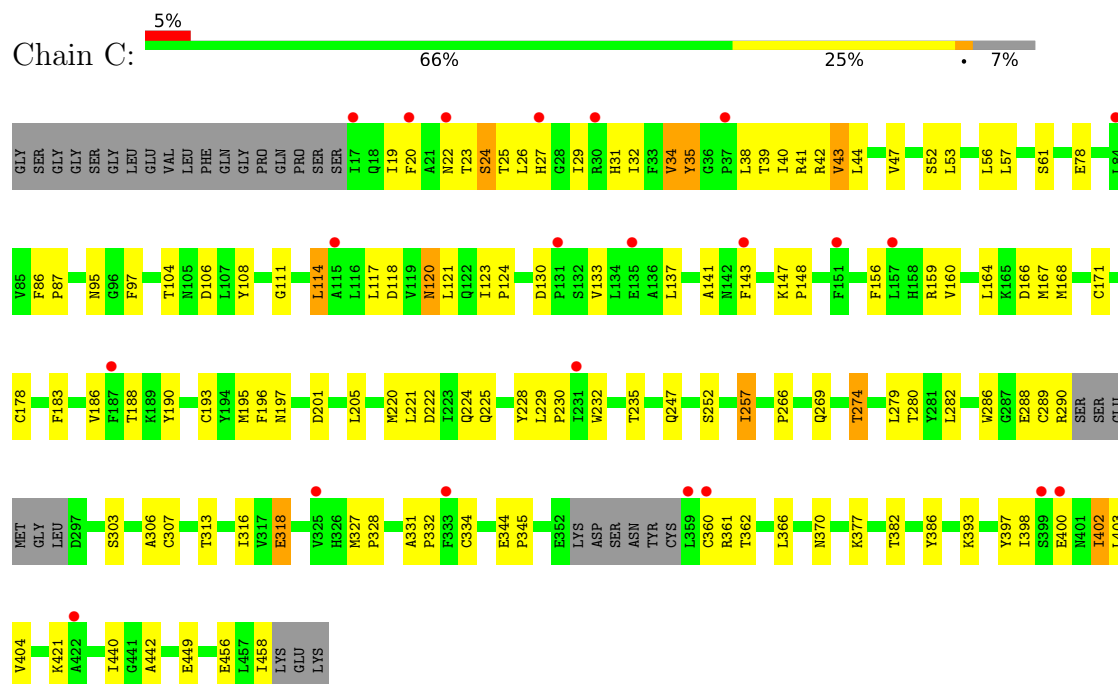
• Molecule 1: Acid-sensing ion channel 2



• Molecule 1: Acid-sensing ion channel 2



● Molecule 1: Acid-sensing ion channel 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.86Å 155.66Å 156.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.23 – 3.08 49.23 – 3.08	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.23-3.08) 98.8 (49.23-3.08)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.231 , 0.282 (Not available) , 0.259	Depositor DCC
R_{free} test set	2474 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	95.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10369	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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

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	1.01	0/3553	1.46	14/4814 (0.3%)
1	B	1.00	0/3543	1.46	10/4800 (0.2%)
1	C	0.99	0/3519	1.47	7/4767 (0.1%)
All	All	1.00	0/10615	1.46	31/14381 (0.2%)

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	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	GLU	CB-CA-C	7.78	119.42	108.76
1	C	147	LYS	CB-CA-C	7.50	118.39	109.85
1	A	27	HIS	CA-C-N	7.32	128.41	120.44
1	A	27	HIS	C-N-CA	7.32	128.41	120.44
1	C	104	THR	CB-CA-C	6.34	120.92	110.90
1	C	27	HIS	CA-C-N	6.23	126.02	120.10
1	C	27	HIS	C-N-CA	6.23	126.02	120.10
1	A	33	PHE	CB-CA-C	-5.96	102.86	111.14
1	B	289	CYS	CA-C-N	5.89	132.29	121.70
1	B	289	CYS	C-N-CA	5.89	132.29	121.70
1	A	253	GLU	CB-CA-C	5.85	116.77	108.76
1	C	43	VAL	N-CA-C	-5.82	106.06	113.22
1	B	27	HIS	CA-C-N	5.71	125.53	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	HIS	C-N-CA	5.71	125.53	120.10
1	B	245	LYS	CB-CA-C	5.68	119.11	109.50
1	B	212	GLY	CA-C-N	5.61	128.06	120.38
1	B	212	GLY	C-N-CA	5.61	128.06	120.38
1	A	166	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	26	LEU	CA-C-N	5.52	131.05	122.49
1	A	26	LEU	C-N-CA	5.52	131.05	122.49
1	C	34	VAL	N-CA-C	-5.44	107.18	112.29
1	B	222	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	43	VAL	N-CA-C	-5.36	106.63	113.22
1	A	356	ASN	CA-C-N	5.35	127.45	120.28
1	A	356	ASN	C-N-CA	5.35	127.45	120.28
1	C	120	ASN	N-CA-C	-5.22	102.79	110.52
1	A	30	ARG	CA-C-O	-5.10	116.26	121.87
1	A	222	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	40	ILE	CA-C-N	5.00	131.10	121.54
1	A	40	ILE	C-N-CA	5.00	131.10	121.54
1	B	28	GLY	CA-C-O	-5.00	116.01	121.71

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	LEU	Peptide
1	A	40	ILE	Peptide
1	C	35	TYR	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	3468	0	3413	82	0
1	B	3459	0	3406	75	0
1	C	3436	0	3391	106	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10369	0	10210	248	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 12.

All (248) 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:C:290:ARG:NH2	1:C:361:ARG:CZ	1.90	1.32
1:C:29:ILE:HD13	1:C:449:GLU:OE1	1.25	1.30
1:C:29:ILE:CD1	1:C:449:GLU:OE1	1.90	1.19
1:B:275:GLN:HE21	1:B:413:ASN:HD21	1.11	0.97
1:A:225:GLN:HE21	1:B:381:LYS:H	1.06	0.96
1:A:26:LEU:HD23	1:A:32:ILE:O	1.63	0.96
1:C:313:THR:HG22	1:C:327:MET:HB3	1.51	0.92
1:A:20:PHE:O	1:A:23:THR:OG1	1.87	0.91
1:A:225:GLN:HE21	1:B:381:LYS:N	1.67	0.90
1:C:290:ARG:NH2	1:C:361:ARG:NE	2.21	0.87
1:C:313:THR:HG21	1:C:328:PRO:HD2	1.54	0.87
1:C:290:ARG:CZ	1:C:361:ARG:CZ	2.56	0.83
1:C:290:ARG:NH2	1:C:361:ARG:NH1	2.27	0.81
1:C:290:ARG:CZ	1:C:361:ARG:NE	2.44	0.81
1:A:38:LEU:HD12	1:A:39:THR:N	1.96	0.79
1:C:290:ARG:HH21	1:C:361:ARG:CZ	1.95	0.78
1:C:225:GLN:NE2	1:C:400:GLU:O	2.17	0.78
1:C:29:ILE:CD1	1:C:449:GLU:CD	2.58	0.77
1:B:225:GLN:NE2	1:B:400:GLU:O	2.17	0.77
1:B:275:GLN:HE21	1:B:413:ASN:ND2	1.82	0.76
1:C:186:VAL:HG21	1:C:195:MET:HE3	1.68	0.75
1:A:375:MET:HE1	1:B:375:MET:HE1	1.71	0.72
1:C:290:ARG:NH2	1:C:361:ARG:NH2	2.38	0.71
1:A:323:ARG:NH1	1:A:329:GLY:O	2.25	0.70
1:B:53:LEU:HD13	1:B:440:ILE:HD11	1.74	0.70
1:C:290:ARG:HH22	1:C:361:ARG:CZ	2.01	0.70
1:C:53:LEU:HD13	1:C:440:ILE:HD11	1.74	0.69
1:C:40:ILE:HG13	1:C:42:ARG:H	1.57	0.69
1:B:275:GLN:NE2	1:B:413:ASN:HD21	1.88	0.67
1:A:22:ASN:O	1:A:25:THR:HG22	1.95	0.67
1:C:130:ASP:O	1:C:133:VAL:HG12	1.95	0.66
1:B:345:PRO:O	1:B:349:LEU:HD13	1.96	0.66
1:C:26:LEU:C	1:C:26:LEU:HD12	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ILE:HD12	1:C:41:ARG:H	1.62	0.65
1:A:166:ASP:HB3	1:A:224:GLN:NE2	2.12	0.64
1:A:225:GLN:NE2	1:B:380:SER:HA	2.13	0.64
1:A:53:LEU:HD13	1:A:440:ILE:HD11	1.80	0.63
1:C:123:ILE:HD11	1:C:137:LEU:HB3	1.80	0.63
1:A:26:LEU:CD2	1:A:32:ILE:O	2.41	0.63
1:B:254:PRO:O	1:B:305:THR:HG21	1.99	0.62
1:B:171:CYS:SG	1:B:178:CYS:CB	2.87	0.62
1:B:303:SER:HB2	1:B:306:ALA:H	1.63	0.62
1:A:171:CYS:SG	1:A:178:CYS:CB	2.88	0.62
1:B:240:PHE:CD2	1:C:220:MET:HE1	2.35	0.61
1:A:32:ILE:HG22	1:A:34:VAL:H	1.65	0.61
1:B:213:THR:HG23	1:B:406:ASP:OD2	2.00	0.61
1:A:32:ILE:HG21	1:A:35:TYR:CE2	2.35	0.60
1:A:195:MET:HE2	1:A:255:PRO:HG3	1.83	0.60
1:A:38:LEU:HD12	1:A:39:THR:H	1.63	0.60
1:A:166:ASP:HB3	1:A:224:GLN:HE22	1.67	0.60
1:A:303:SER:HB2	1:A:306:ALA:H	1.66	0.60
1:B:32:ILE:HG22	1:B:34:VAL:H	1.66	0.60
1:C:106:ASP:OD2	1:C:159:ARG:NH2	2.35	0.60
1:C:32:ILE:HG21	1:C:35:TYR:CE2	2.36	0.60
1:C:166:ASP:HB3	1:C:224:GLN:NE2	2.17	0.60
1:C:313:THR:HG22	1:C:327:MET:CB	2.26	0.59
1:A:29:ILE:HG21	1:C:31:HIS:CE1	2.37	0.59
1:A:106:ASP:OD2	1:A:159:ARG:NH2	2.35	0.59
1:B:106:ASP:OD2	1:B:159:ARG:NH2	2.35	0.59
1:C:188:THR:CG2	1:C:193:CYS:SG	2.90	0.59
1:C:171:CYS:SG	1:C:178:CYS:CB	2.90	0.59
1:C:29:ILE:HD11	1:C:449:GLU:OE1	1.98	0.59
1:C:303:SER:HB2	1:C:306:ALA:H	1.67	0.59
1:B:22:ASN:O	1:B:25:THR:HG22	2.03	0.58
1:C:20:PHE:HB3	1:C:24:SER:HB2	1.85	0.58
1:A:171:CYS:SG	1:A:178:CYS:HB2	2.44	0.58
1:B:97:PHE:HA	1:B:160:VAL:HG12	1.86	0.58
1:A:189:LYS:HB2	1:A:258:GLN:HG3	1.86	0.57
1:B:171:CYS:SG	1:B:178:CYS:HB2	2.45	0.57
1:C:38:LEU:C	1:C:38:LEU:HD23	2.30	0.57
1:C:313:THR:CG2	1:C:327:MET:HB3	2.29	0.57
1:C:32:ILE:HG22	1:C:34:VAL:H	1.69	0.57
1:A:31:HIS:CE1	1:B:29:ILE:HG21	2.41	0.56
1:A:30:ARG:HE	1:A:32:ILE:HD11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HG12	1:B:42:ARG:H	1.71	0.56
1:B:248:ILE:HD11	1:B:272:VAL:HG11	1.87	0.56
1:C:290:ARG:CZ	1:C:361:ARG:NH2	2.67	0.56
1:B:296:LEU:HD23	1:B:299:PHE:HB2	1.87	0.55
1:C:22:ASN:HD22	1:C:22:ASN:H	1.55	0.55
1:C:171:CYS:SG	1:C:178:CYS:HB2	2.47	0.55
1:C:232:TRP:O	1:C:235:THR:HG23	2.07	0.55
1:A:188:THR:CG2	1:A:193:CYS:SG	2.94	0.55
1:A:22:ASN:ND2	1:A:35:TYR:CE1	2.76	0.54
1:B:57:LEU:O	1:B:61:SER:OG	2.25	0.54
1:B:171:CYS:SG	1:B:178:CYS:HB3	2.47	0.54
1:A:232:TRP:O	1:A:235:THR:HG23	2.08	0.54
1:C:25:THR:HG21	2:C:502:HOH:O	2.08	0.54
1:A:40:ILE:HG12	1:A:41:ARG:N	2.24	0.53
1:C:40:ILE:O	1:C:43:VAL:HG13	2.07	0.53
1:B:188:THR:CG2	1:B:193:CYS:SG	2.97	0.53
1:B:274:THR:HA	1:B:370:ASN:O	2.09	0.53
1:B:282:LEU:O	1:B:289:CYS:HB2	2.09	0.53
1:C:290:ARG:NH1	1:C:361:ARG:NE	2.56	0.53
1:B:25:THR:HG23	1:B:25:THR:O	2.08	0.53
1:A:56:LEU:O	1:A:60:SER:HB2	2.09	0.53
1:C:26:LEU:HD12	1:C:26:LEU:O	2.09	0.53
1:A:171:CYS:SG	1:A:178:CYS:HB3	2.48	0.52
1:A:25:THR:HG23	1:A:26:LEU:HD12	1.91	0.52
1:B:189:LYS:HE2	1:B:258:GLN:HE21	1.75	0.52
1:C:166:ASP:HB3	1:C:224:GLN:HE22	1.73	0.52
1:C:118:ASP:OD1	1:C:120:ASN:O	2.28	0.52
1:C:288:GLU:CG	1:C:361:ARG:NH1	2.73	0.52
1:A:166:ASP:CB	1:A:224:GLN:HE22	2.22	0.52
1:A:34:VAL:O	1:A:34:VAL:HG12	2.10	0.52
1:C:398:ILE:HD13	1:C:402:ILE:HD12	1.92	0.51
1:A:274:THR:HA	1:A:370:ASN:O	2.10	0.51
1:A:366:LEU:HD12	1:A:366:LEU:C	2.36	0.51
1:B:135:GLU:HA	1:B:135:GLU:OE1	2.11	0.51
1:B:282:LEU:C	1:B:289:CYS:HB2	2.36	0.51
1:B:283:PRO:HA	1:B:289:CYS:HB2	1.93	0.51
1:C:118:ASP:O	1:C:120:ASN:O	2.29	0.51
1:A:201:ASP:HB2	1:A:203:LYS:HE3	1.92	0.51
1:A:225:GLN:NE2	1:B:381:LYS:N	2.48	0.51
1:A:288:GLU:OE1	1:A:288:GLU:N	2.35	0.50
1:B:33:PHE:CZ	1:C:449:GLU:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ILE:HD11	1:A:137:LEU:HB3	1.92	0.50
1:A:440:ILE:CG2	1:A:442:ALA:HB2	2.41	0.50
1:C:171:CYS:SG	1:C:178:CYS:HB3	2.52	0.50
1:A:57:LEU:O	1:A:61:SER:OG	2.27	0.50
1:C:57:LEU:O	1:C:61:SER:OG	2.28	0.50
1:C:274:THR:HA	1:C:370:ASN:O	2.12	0.50
1:B:19:ILE:C	1:B:20:PHE:CD1	2.90	0.49
1:C:366:LEU:HD12	1:C:366:LEU:C	2.37	0.49
1:A:167:MET:HG3	1:A:222:ASP:O	2.12	0.49
1:A:343:ALA:O	1:A:347:LEU:HD22	2.13	0.49
1:C:398:ILE:CD1	1:C:402:ILE:HD12	2.42	0.49
1:A:26:LEU:HD12	1:A:26:LEU:N	2.28	0.49
1:B:223:ILE:HD13	1:B:266:PRO:HG3	1.95	0.49
1:C:86:PHE:CG	1:C:87:PRO:HD2	2.48	0.49
1:A:86:PHE:CG	1:A:87:PRO:HD2	2.48	0.48
1:A:393:LYS:HE2	1:A:397:TYR:CE2	2.48	0.48
1:B:366:LEU:C	1:B:366:LEU:HD12	2.38	0.48
1:A:323:ARG:NH1	1:A:329:GLY:C	2.72	0.48
1:A:368:ARG:NH2	1:B:78:GLU:OE2	2.47	0.48
1:C:133:VAL:CG2	1:C:230:PRO:HG2	2.44	0.48
1:A:64:VAL:CG2	1:A:432:ILE:HD11	2.43	0.48
1:C:440:ILE:CG2	1:C:442:ALA:HB2	2.44	0.48
1:A:111:GLY:HA3	1:A:117:LEU:HD12	1.95	0.47
1:B:167:MET:HG3	1:B:222:ASP:O	2.14	0.47
1:C:29:ILE:HD12	1:C:29:ILE:N	2.29	0.47
1:A:220:MET:C	1:A:221:LEU:HD12	2.39	0.47
1:B:30:ARG:HD2	1:B:49:PHE:CZ	2.50	0.47
1:C:386:TYR:CD1	1:C:386:TYR:C	2.93	0.47
1:C:289:CYS:C	1:C:290:ARG:HG3	2.40	0.47
1:B:30:ARG:HE	1:B:32:ILE:HD11	1.80	0.46
1:B:440:ILE:CG2	1:B:442:ALA:HB2	2.45	0.46
1:B:86:PHE:O	1:B:197:ASN:ND2	2.48	0.46
1:C:167:MET:HG3	1:C:222:ASP:O	2.16	0.46
1:C:279:LEU:N	1:C:279:LEU:HD12	2.31	0.46
1:A:225:GLN:NE2	1:B:381:LYS:H	1.91	0.46
1:A:440:ILE:HG22	1:A:442:ALA:HB2	1.96	0.46
1:B:86:PHE:CG	1:B:87:PRO:HD2	2.50	0.46
1:C:266:PRO:HA	1:C:403:LEU:HB3	1.96	0.46
1:A:141:ALA:HA	1:A:143:PHE:CZ	2.51	0.46
1:A:40:ILE:HG12	1:A:41:ARG:HB2	1.97	0.46
1:B:29:ILE:HG12	1:B:449:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:LEU:N	1:C:114:LEU:HD23	2.30	0.46
1:B:248:ILE:CD1	1:B:272:VAL:HG11	2.45	0.46
1:B:344:GLU:N	1:B:345:PRO:HD2	2.31	0.46
1:A:248:ILE:HD11	1:A:407:ILE:HG12	1.98	0.45
1:B:64:VAL:CG2	1:B:432:ILE:HD11	2.46	0.45
1:B:266:PRO:HA	1:B:403:LEU:HB3	1.99	0.45
1:C:166:ASP:CB	1:C:224:GLN:HE22	2.30	0.45
1:A:286:TRP:CZ2	1:A:421:LYS:HD3	2.52	0.45
1:B:111:GLY:HA3	1:B:117:LEU:HD12	1.99	0.45
1:C:38:LEU:HD23	1:C:39:THR:O	2.16	0.45
1:B:21:ALA:HB3	1:B:24:SER:HB3	1.98	0.45
1:C:111:GLY:HA3	1:C:117:LEU:HD12	1.98	0.45
1:C:247:GLN:HB2	1:C:257:ILE:HG12	1.97	0.45
1:C:86:PHE:CD1	1:C:87:PRO:HD2	2.51	0.45
1:C:86:PHE:O	1:C:197:ASN:ND2	2.50	0.45
1:C:97:PHE:HB2	1:C:229:LEU:HD21	1.99	0.45
1:C:34:VAL:HG12	1:C:34:VAL:O	2.16	0.45
1:C:286:TRP:CZ2	1:C:421:LYS:HD3	2.51	0.45
1:A:344:GLU:N	1:A:345:PRO:HD2	2.32	0.45
1:A:58:VAL:HG12	1:A:59:GLU:OE2	2.18	0.44
1:A:279:LEU:N	1:A:279:LEU:HD12	2.32	0.44
1:A:289:CYS:O	1:A:290:ARG:HB2	2.18	0.44
1:A:343:ALA:O	1:A:347:LEU:CD2	2.65	0.44
1:C:19:ILE:HD13	1:C:456:GLU:HB3	2.00	0.44
1:C:288:GLU:HG2	1:C:361:ARG:NH1	2.33	0.44
1:C:108:TYR:CE1	1:C:121:LEU:HD22	2.52	0.44
1:B:34:VAL:HG12	1:B:34:VAL:O	2.17	0.44
1:C:205:LEU:HD22	1:C:205:LEU:H	1.82	0.44
1:C:40:ILE:HD12	1:C:41:ARG:N	2.30	0.44
1:A:183:PHE:CE2	1:A:196:PHE:HB2	2.53	0.44
1:B:64:VAL:HG23	1:B:432:ILE:HD11	2.00	0.44
1:B:183:PHE:CE2	1:B:196:PHE:HB2	2.53	0.44
1:C:108:TYR:CD1	1:C:121:LEU:CD2	3.00	0.44
1:A:64:VAL:HG23	1:A:432:ILE:HD11	1.99	0.44
1:A:86:PHE:O	1:A:197:ASN:ND2	2.50	0.44
1:A:375:MET:HE1	1:B:375:MET:CE	2.42	0.44
1:C:44:LEU:O	1:C:47:VAL:HB	2.18	0.44
1:C:121:LEU:HB3	1:C:143:PHE:CD2	2.53	0.44
1:C:331:ALA:HB1	1:C:332:PRO:HD2	2.00	0.44
1:B:286:TRP:CZ2	1:B:421:LYS:HD3	2.53	0.43
1:C:23:THR:HA	1:C:35:TYR:HB3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PRO:HD2	1:C:377:LYS:HB2	1.99	0.43
1:A:266:PRO:HA	1:A:403:LEU:HB3	1.99	0.43
1:C:313:THR:HG22	1:C:327:MET:CG	2.49	0.43
1:C:141:ALA:HA	1:C:143:PHE:CZ	2.54	0.43
1:B:31:HIS:CE1	1:C:29:ILE:HG21	2.54	0.43
1:B:100:SER:HB3	1:B:227:GLU:OE1	2.18	0.43
1:B:21:ALA:HB3	1:B:24:SER:CB	2.49	0.43
1:B:56:LEU:HD22	1:B:440:ILE:HD12	2.01	0.43
1:C:95:ASN:CG	1:C:228:TYR:HA	2.44	0.42
1:B:368:ARG:NH1	1:C:78:GLU:OE1	2.52	0.42
1:A:170:TYR:CE1	1:A:220:MET:HB2	2.54	0.42
1:B:275:GLN:NE2	1:B:413:ASN:ND2	2.56	0.42
1:C:183:PHE:CE2	1:C:196:PHE:HB2	2.54	0.42
1:A:248:ILE:CD1	1:A:272:VAL:HG11	2.49	0.42
1:C:108:TYR:CE2	1:C:148:PRO:HG3	2.54	0.42
1:A:189:LYS:HE3	1:A:258:GLN:HE21	1.85	0.42
1:C:220:MET:C	1:C:221:LEU:HD12	2.44	0.42
1:B:95:ASN:CG	1:B:228:TYR:HA	2.44	0.42
1:C:290:ARG:HH22	1:C:361:ARG:NE	2.08	0.42
1:C:344:GLU:HB2	1:C:345:PRO:HD3	2.02	0.42
1:A:40:ILE:HG12	1:A:42:ARG:H	1.85	0.42
1:C:393:LYS:HE2	1:C:397:TYR:CE2	2.54	0.42
1:C:168:MET:HE1	1:C:183:PHE:CZ	2.54	0.41
1:A:100:SER:HB3	1:A:227:GLU:OE1	2.20	0.41
1:A:279:LEU:N	1:A:279:LEU:CD1	2.83	0.41
1:B:99:PHE:CD2	1:B:230:PRO:HD3	2.56	0.41
1:C:56:LEU:HD22	1:C:440:ILE:HD12	2.01	0.41
1:A:26:LEU:HD21	1:A:32:ILE:HB	2.02	0.41
1:C:19:ILE:HD13	1:C:456:GLU:O	2.20	0.41
1:C:269:GLN:HA	1:C:404:VAL:O	2.20	0.41
1:B:283:PRO:HA	1:B:289:CYS:CB	2.51	0.41
1:B:324:MET:HE1	1:B:347:LEU:CD1	2.51	0.41
1:C:440:ILE:HG22	1:C:442:ALA:HB2	2.03	0.41
1:A:30:ARG:NE	1:A:32:ILE:HD11	2.34	0.41
1:A:331:ALA:HB1	1:A:332:PRO:HD2	2.01	0.41
1:C:156:PHE:O	1:C:160:VAL:HG22	2.20	0.41
1:A:40:ILE:CG1	1:A:41:ARG:N	2.83	0.41
1:A:69:SER:OG	1:A:71:GLN:HG2	2.21	0.41
1:A:95:ASN:CG	1:A:228:TYR:HA	2.45	0.41
1:A:269:GLN:HA	1:A:404:VAL:O	2.20	0.41
1:B:19:ILE:C	1:B:20:PHE:HD1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:HD23	1:C:44:LEU:N	2.36	0.41
1:B:170:TYR:CE1	1:B:220:MET:HB2	2.55	0.40
1:C:164:LEU:HD21	1:C:168:MET:SD	2.61	0.40
1:C:221:LEU:O	1:C:402:ILE:HA	2.21	0.40
1:A:156:PHE:O	1:A:160:VAL:HG22	2.21	0.40
1:B:38:LEU:HD12	1:B:39:THR:N	2.36	0.40
1:B:190:TYR:HD2	1:B:257:ILE:HG23	1.86	0.40
1:B:203:LYS:HB3	1:B:204:PRO:HD2	2.02	0.40
1:C:290:ARG:HH22	1:C:361:ARG:NH1	2.11	0.40
1:C:188:THR:C	1:C:190:TYR:H	2.30	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	430/463 (93%)	401 (93%)	26 (6%)	3 (1%)	18	46
1	B	427/463 (92%)	402 (94%)	23 (5%)	2 (0%)	24	54
1	C	424/463 (92%)	385 (91%)	37 (9%)	2 (0%)	24	54
All	All	1281/1389 (92%)	1188 (93%)	86 (7%)	7 (0%)	24	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	318	GLU
1	B	318	GLU
1	A	124	PRO
1	C	124	PRO
1	C	318	GLU
1	B	124	PRO

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	381/404 (94%)	356 (93%)	25 (7%)	15	41
1	B	380/404 (94%)	363 (96%)	17 (4%)	24	53
1	C	377/404 (93%)	359 (95%)	18 (5%)	23	51
All	All	1138/1212 (94%)	1078 (95%)	60 (5%)	20	48

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	52	SER
1	A	60	SER
1	A	69	SER
1	A	82	GLN
1	A	133	VAL
1	A	149	LYS
1	A	208	THR
1	A	209	VAL
1	A	252	SER
1	A	274	THR
1	A	280	THR
1	A	288	GLU
1	A	303	SER
1	A	316	ILE
1	A	347	LEU
1	A	358	CYS
1	A	361	ARG
1	A	362	THR
1	A	368	ARG
1	A	371	LYS
1	A	382	THR
1	A	383	SER
1	A	428	LEU
1	A	458	ILE
1	B	20	PHE

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Mol	Chain	Res	Type
1	B	26	LEU
1	B	32	ILE
1	B	47	VAL
1	B	52	SER
1	B	62	GLU
1	B	69	SER
1	B	133	VAL
1	B	280	THR
1	B	289	CYS
1	B	303	SER
1	B	316	ILE
1	B	334	CYS
1	B	361	ARG
1	B	362	THR
1	B	382	THR
1	B	385	LYS
1	C	24	SER
1	C	52	SER
1	C	114	LEU
1	C	201	ASP
1	C	252	SER
1	C	257	ILE
1	C	274	THR
1	C	280	THR
1	C	282	LEU
1	C	307	CYS
1	C	316	ILE
1	C	318	GLU
1	C	334	CYS
1	C	360	CYS
1	C	362	THR
1	C	382	THR
1	C	402	ILE
1	C	458	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	31	HIS
1	A	120	ASN
1	A	180	HIS

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Mol	Chain	Res	Type
1	A	181	GLN
1	A	225	GLN
1	A	275	GLN
1	A	365	ASN
1	A	413	ASN
1	B	22	ASN
1	B	95	ASN
1	B	356	ASN
1	B	413	ASN
1	C	22	ASN
1	C	120	ASN
1	C	142	ASN
1	C	145	HIS
1	C	158	HIS
1	C	215	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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, 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	434/463 (93%)	0.25	26 (5%)	27 14	65, 98, 143, 191	0
1	B	433/463 (93%)	0.12	14 (3%)	50 28	64, 95, 146, 196	0
1	C	430/463 (92%)	0.36	22 (5%)	33 17	72, 116, 179, 215	0
All	All	1297/1389 (93%)	0.24	62 (4%)	35 18	64, 102, 162, 215	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	HIS	6.3
1	A	30	ARG	6.1
1	B	35	TYR	4.9
1	B	30	ARG	4.6
1	C	27	HIS	4.5
1	B	26	LEU	4.2
1	C	360	CYS	4.2
1	B	24	SER	4.0
1	B	357	TYR	3.7
1	A	57	LEU	3.7
1	A	237	GLU	3.7
1	A	350	LEU	3.6
1	C	131	PRO	3.5
1	A	285	PRO	3.2
1	B	19	ILE	3.1
1	C	325	VAL	3.0
1	A	58	VAL	3.0
1	A	60	SER	3.0
1	C	359	LEU	2.9
1	A	288	GLU	2.9
1	C	333	PHE	2.9
1	A	395	GLU	2.8
1	C	22	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	68	PHE	2.6
1	A	166	ASP	2.6
1	A	290	ARG	2.6
1	A	61	SER	2.6
1	B	237	GLU	2.6
1	A	286	TRP	2.6
1	C	17	ILE	2.6
1	B	22	ASN	2.6
1	A	349	LEU	2.6
1	C	30	ARG	2.6
1	C	37	PRO	2.5
1	A	154	LEU	2.5
1	C	400	GLU	2.5
1	B	330	ASP	2.5
1	C	187	PHE	2.5
1	C	20	PHE	2.4
1	A	172	LYS	2.4
1	A	347	LEU	2.4
1	C	399	SER	2.4
1	C	157	LEU	2.4
1	A	37	PRO	2.4
1	A	43	VAL	2.4
1	B	349	LEU	2.3
1	C	231	ILE	2.3
1	C	422	ALA	2.2
1	C	143	PHE	2.2
1	B	321	ASN	2.2
1	A	97	PHE	2.2
1	A	348	GLY	2.2
1	C	151	PHE	2.2
1	A	44	LEU	2.1
1	B	352	GLU	2.1
1	C	115	ALA	2.1
1	B	106	ASP	2.1
1	C	135	GLU	2.1
1	A	346	ALA	2.1
1	A	440	ILE	2.1
1	A	253	GLU	2.1
1	C	84	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.