



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:53 PM UTC

PDB ID : 6KI7 / pdb_00006ki7
Title : Pyrophosphatase mutant K30R from *Acinetobacter baumannii*
Authors : Su, J.
Deposited on : 2019-07-17
Resolution : 2.75 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

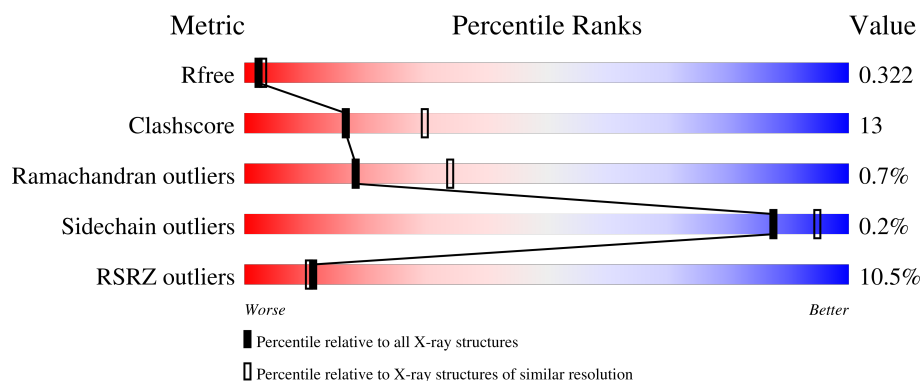
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	177	5% 83% 15% .
1	B	177	2% 74% 23% ..
1	C	177	% 84% 14% .
1	D	177	49% 54% 39% ...
1	E	177	2% 69% 29% .

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Mol	Chain	Length	Quality of chain
1	F	177	
1	G	177	
1	H	177	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10804 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 Inorganic pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			
1	B	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			
1	C	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			
1	D	173	Total	C	N	O	S	0	0	0
			1345	868	216	258	3			
1	E	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			
1	F	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			
1	G	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			
1	H	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP N9S5K0
A	-2	SER	-	expression tag	UNP N9S5K0
A	-1	HIS	-	expression tag	UNP N9S5K0
A	29	ARG	LYS	engineered mutation	UNP N9S5K0
A	139	SER	ALA	engineered mutation	UNP N9S5K0
B	-3	GLY	-	expression tag	UNP N9S5K0
B	-2	SER	-	expression tag	UNP N9S5K0
B	-1	HIS	-	expression tag	UNP N9S5K0
B	29	ARG	LYS	engineered mutation	UNP N9S5K0
B	139	SER	ALA	engineered mutation	UNP N9S5K0
C	-3	GLY	-	expression tag	UNP N9S5K0
C	-2	SER	-	expression tag	UNP N9S5K0
C	-1	HIS	-	expression tag	UNP N9S5K0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	29	ARG	LYS	engineered mutation	UNP N9S5K0
C	139	SER	ALA	engineered mutation	UNP N9S5K0
D	-3	GLY	-	expression tag	UNP N9S5K0
D	-2	SER	-	expression tag	UNP N9S5K0
D	-1	HIS	-	expression tag	UNP N9S5K0
D	29	ARG	LYS	engineered mutation	UNP N9S5K0
D	139	SER	ALA	engineered mutation	UNP N9S5K0
E	-3	GLY	-	expression tag	UNP N9S5K0
E	-2	SER	-	expression tag	UNP N9S5K0
E	-1	HIS	-	expression tag	UNP N9S5K0
E	29	ARG	LYS	engineered mutation	UNP N9S5K0
E	139	SER	ALA	engineered mutation	UNP N9S5K0
F	-3	GLY	-	expression tag	UNP N9S5K0
F	-2	SER	-	expression tag	UNP N9S5K0
F	-1	HIS	-	expression tag	UNP N9S5K0
F	29	ARG	LYS	engineered mutation	UNP N9S5K0
F	139	SER	ALA	engineered mutation	UNP N9S5K0
G	-3	GLY	-	expression tag	UNP N9S5K0
G	-2	SER	-	expression tag	UNP N9S5K0
G	-1	HIS	-	expression tag	UNP N9S5K0
G	29	ARG	LYS	engineered mutation	UNP N9S5K0
G	139	SER	ALA	engineered mutation	UNP N9S5K0
H	-3	GLY	-	expression tag	UNP N9S5K0
H	-2	SER	-	expression tag	UNP N9S5K0
H	-1	HIS	-	expression tag	UNP N9S5K0
H	29	ARG	LYS	engineered mutation	UNP N9S5K0
H	139	SER	ALA	engineered mutation	UNP N9S5K0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	2	Total O 2 2	0	0
2	C	2	Total O 2 2	0	0
2	D	3	Total O 3 3	0	0
2	E	2	Total O 2 2	0	0
2	F	4	Total O 4 4	0	0

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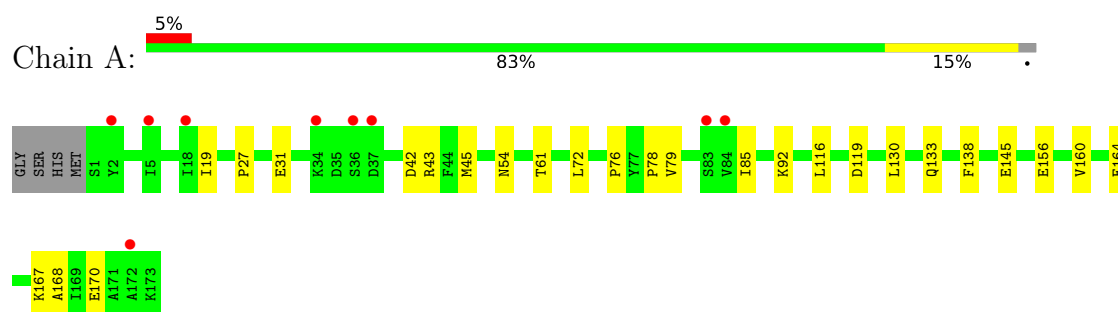
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	O	0	0
			2	2		
2	H	4	Total	O	0	0
			4	4		

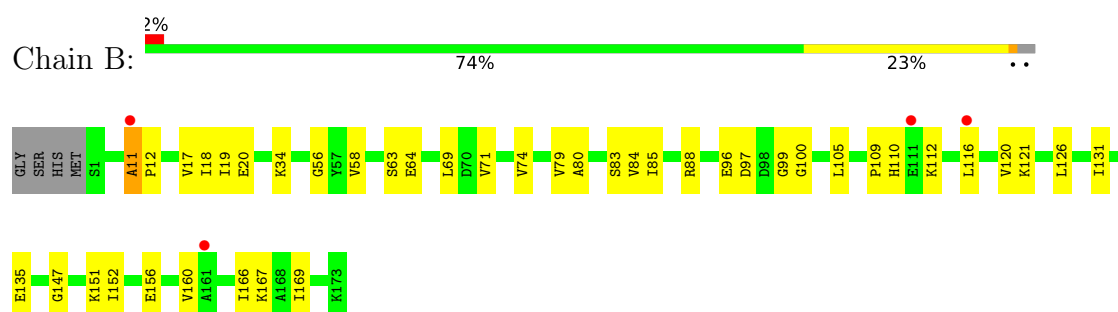
3 Residue-property plots [i](#)

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.

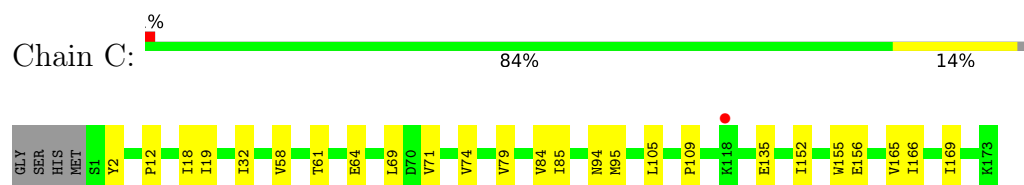
- Molecule 1: Inorganic pyrophosphatase



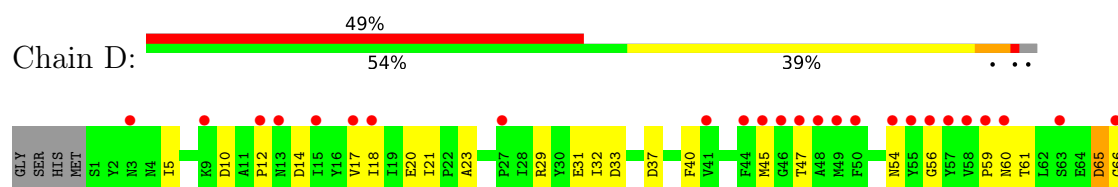
- Molecule 1: Inorganic pyrophosphatase

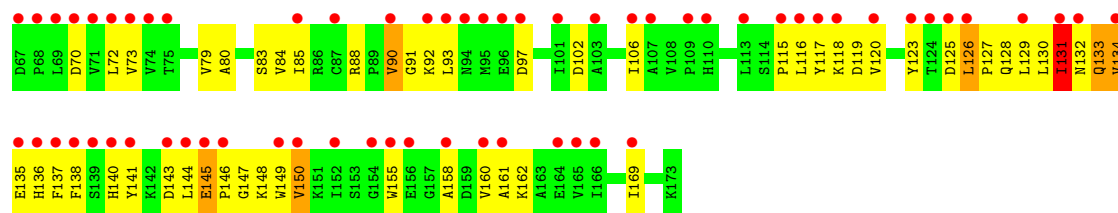


- Molecule 1: Inorganic pyrophosphatase



- Molecule 1: Inorganic pyrophosphatase





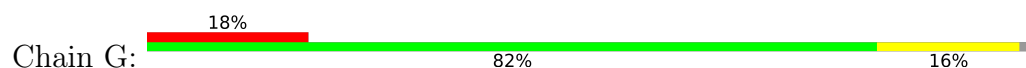
• Molecule 1: Inorganic pyrophosphatase



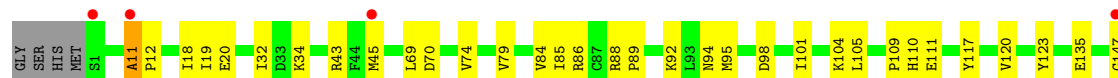
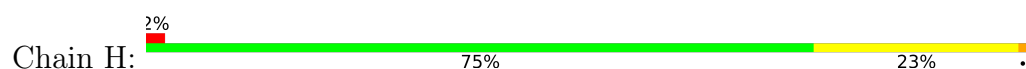
• Molecule 1: Inorganic pyrophosphatase



• Molecule 1: Inorganic pyrophosphatase



• Molecule 1: Inorganic pyrophosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	113.05Å 113.05Å 551.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.75 19.96 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.96-2.75) 98.1 (19.96-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.75Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.292 , 0.324 0.293 , 0.322	Depositor DCC
R_{free} test set	2000 reflections (5.55%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10804	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 78.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4797e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.13	0/1383	0.33	0/1886
1	B	0.15	0/1383	0.39	0/1886
1	C	0.12	0/1383	0.32	0/1886
1	D	0.26	0/1380	0.67	3/1883 (0.2%)
1	E	0.19	0/1383	0.39	0/1886
1	F	0.19	0/1383	0.41	0/1886
1	G	0.12	0/1383	0.33	0/1886
1	H	0.14	0/1383	0.39	0/1886
All	All	0.17	0/11061	0.42	3/15085 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	GLN	N-CA-C	-7.09	103.48	111.07
1	D	131	ILE	N-CA-C	-5.27	104.46	111.05
1	D	134	VAL	N-CA-C	-5.12	104.99	110.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1348	0	1330	21	0
1	B	1348	0	1330	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1348	0	1330	15	0
1	D	1345	0	1323	83	0
1	E	1348	0	1330	38	0
1	F	1348	0	1330	39	0
1	G	1348	0	1330	16	0
1	H	1348	0	1330	31	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	2	0
2	E	2	0	0	0	0
2	F	4	0	0	0	0
2	G	2	0	0	0	0
2	H	4	0	0	0	0
All	All	10804	0	10633	274	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 13.

All (274) 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:D:126:LEU:CG	1:D:127:PRO:HD3	1.76	1.15
1:D:126:LEU:CG	1:D:127:PRO:CD	2.30	1.09
1:D:126:LEU:HG	1:D:127:PRO:CD	1.85	1.05
1:D:92:LYS:HZ1	1:D:160:VAL:HB	1.26	1.00
1:D:126:LEU:HG	1:D:127:PRO:HD3	1.02	1.00
1:D:126:LEU:HD23	1:D:127:PRO:HD2	1.42	0.98
1:F:93:LEU:HD22	1:F:95:MET:HE3	1.47	0.96
1:D:126:LEU:CB	1:D:127:PRO:CD	2.48	0.92
1:D:126:LEU:CD2	1:D:127:PRO:HD2	2.02	0.90
1:F:110:HIS:HD2	1:F:112:LYS:H	1.16	0.89
1:D:126:LEU:HB3	1:D:127:PRO:HD2	1.54	0.88
1:E:165:VAL:O	1:E:169:ILE:HG13	1.73	0.88
1:B:110:HIS:HD2	1:B:112:LYS:H	1.12	0.87
1:G:110:HIS:CE1	1:G:111:GLU:OE2	2.27	0.87
1:B:110:HIS:CD2	1:B:112:LYS:H	1.93	0.87
1:D:120:VAL:HA	1:D:125:ASP:OD1	1.74	0.86
1:D:126:LEU:CG	1:D:127:PRO:HD2	2.06	0.85
1:D:126:LEU:HD23	1:D:127:PRO:CD	2.06	0.85
1:D:126:LEU:CB	1:D:127:PRO:HD2	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:HIS:CD2	1:F:112:LYS:H	1.98	0.81
1:D:126:LEU:CD2	1:D:127:PRO:CD	2.57	0.80
1:D:79:VAL:HG11	1:D:85:ILE:HD11	1.63	0.78
1:D:116:LEU:HG	1:D:117:TYR:CE1	2.21	0.75
1:F:93:LEU:HD12	1:F:155:TRP:CZ2	2.23	0.74
1:F:122:GLU:OE1	1:F:157:GLY:CA	2.36	0.73
1:D:5:ILE:HD11	1:D:18:ILE:HD11	1.71	0.73
1:D:149:TRP:O	1:D:150:VAL:HG22	1.88	0.73
1:D:128:GLN:O	1:D:131:ILE:HG12	1.89	0.72
1:D:97:ASP:HA	1:D:150:VAL:CG1	2.18	0.72
1:H:79:VAL:HG21	1:H:85:ILE:HD11	1.71	0.72
1:H:89:PRO:HG2	1:H:162:LYS:HG2	1.71	0.72
1:F:122:GLU:OE1	1:F:157:GLY:HA3	1.88	0.71
1:F:79:VAL:HG21	1:F:85:ILE:HD11	1.70	0.71
1:B:79:VAL:HG21	1:B:85:ILE:HD11	1.75	0.69
1:D:126:LEU:HB3	1:D:127:PRO:CD	2.19	0.69
1:E:73:VAL:HG21	1:E:85:ILE:HD12	1.75	0.69
1:F:93:LEU:CD2	1:F:95:MET:HE3	2.21	0.68
1:D:97:ASP:HA	1:D:150:VAL:HG12	1.74	0.68
1:F:90:VAL:HA	1:F:158:ALA:HB2	1.76	0.68
1:B:156:GLU:OE1	1:B:160:VAL:HG11	1.93	0.68
1:E:79:VAL:HG21	1:E:85:ILE:HD11	1.75	0.68
1:A:170:GLU:HG3	1:B:160:VAL:HG23	1.77	0.67
1:E:89:PRO:HG2	1:E:162:LYS:HG2	1.75	0.67
1:D:145:GLU:O	1:D:147:GLY:N	2.28	0.66
1:F:16:TYR:HE1	1:F:86:ARG:HB2	1.61	0.66
1:D:93:LEU:HD12	1:D:155:TRP:NE1	2.10	0.66
1:B:17:VAL:HG22	1:B:58:VAL:HG12	1.77	0.66
1:H:92:LYS:HE2	1:H:94:ASN:HD21	1.61	0.65
1:D:20:GLU:OE2	1:D:32:ILE:N	2.27	0.65
1:E:121:LYS:NZ	1:E:122:GLU:OE1	2.29	0.64
1:D:129:LEU:H	1:D:129:LEU:HD23	1.63	0.63
1:F:156:GLU:HB3	1:F:160:VAL:HG11	1.81	0.63
1:D:144:LEU:HD22	1:D:145:GLU:H	1.64	0.62
1:H:12:PRO:HB2	1:H:162:LYS:HB3	1.80	0.62
1:D:92:LYS:HD2	1:D:161:ALA:HB2	1.81	0.62
1:B:58:VAL:HG22	1:B:69:LEU:HB3	1.80	0.61
1:F:122:GLU:OE1	1:F:157:GLY:HA2	2.01	0.61
1:B:11:ALA:HB1	1:B:12:PRO:HD2	1.83	0.61
1:C:165:VAL:O	1:C:169:ILE:HG12	2.00	0.61
1:F:158:ALA:HA	1:F:161:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:HIS:HE1	1:G:111:GLU:OE2	1.83	0.60
1:G:92:LYS:NZ	1:G:164:GLU:OE1	2.30	0.60
1:H:11:ALA:HB1	1:H:12:PRO:HD2	1.84	0.60
1:A:27:PRO:HB2	1:A:45:MET:HB2	1.84	0.60
1:B:96:GLU:HG3	1:B:151:LYS:HB2	1.84	0.60
1:D:127:PRO:O	1:D:131:ILE:HD11	2.03	0.59
1:H:156:GLU:HB2	1:H:160:VAL:HG11	1.83	0.59
1:E:55:TYR:HE1	1:E:70:ASP:HB3	1.68	0.59
1:D:133:GLN:O	1:D:137:PHE:N	2.32	0.58
1:F:170:GLU:HA	1:F:173:LYS:HZ3	1.67	0.58
1:D:129:LEU:HA	1:D:132:ASN:HB3	1.86	0.58
1:F:32:ILE:HG13	1:F:39:LEU:HD12	1.86	0.58
1:D:21:ILE:HD11	1:D:29:ARG:HA	1.83	0.58
1:F:16:TYR:CE1	1:F:86:ARG:HB2	2.39	0.58
1:C:95:MET:HG2	1:C:152:ILE:HD13	1.86	0.57
1:D:65:ASP:OD1	1:D:66:GLY:N	2.34	0.57
1:E:70:ASP:OD2	1:E:104:LYS:NZ	2.35	0.57
1:D:128:GLN:O	1:D:131:ILE:CG1	2.51	0.57
1:D:10:ASP:H	1:D:14:ASP:HB3	1.69	0.57
1:F:9:LYS:HE2	1:F:16:TYR:HE2	1.70	0.57
1:D:23:ALA:H	1:D:54:ASN:HD22	1.53	0.57
1:E:156:GLU:HB3	1:E:160:VAL:HG11	1.86	0.57
1:F:9:LYS:HE2	1:F:16:TYR:CE2	2.40	0.56
1:F:80:ALA:O	1:F:83:SER:OG	2.21	0.56
1:F:145:GLU:HG2	1:F:148:LYS:HE3	1.88	0.56
1:B:110:HIS:CD2	1:B:112:LYS:HG3	2.41	0.56
1:D:115:PRO:O	1:D:118:LYS:N	2.34	0.56
1:D:134:VAL:O	1:D:138:PHE:HB2	2.06	0.56
1:C:79:VAL:HG21	1:C:85:ILE:HD11	1.88	0.55
1:E:110:HIS:NE2	1:E:111:GLU:HG2	2.21	0.55
1:A:130:LEU:HD13	1:A:133:GLN:NE2	2.21	0.55
1:D:118:LYS:HG3	1:D:119:ASP:H	1.70	0.55
1:D:18:ILE:HG12	1:D:84:VAL:HG12	1.88	0.55
1:D:80:ALA:O	1:D:83:SER:OG	2.25	0.55
1:B:64:GLU:N	1:B:64:GLU:OE2	2.38	0.55
1:D:73:VAL:HG11	1:D:85:ILE:HG21	1.89	0.55
1:E:92:LYS:HG3	1:E:105:LEU:HD23	1.89	0.55
1:H:111:GLU:N	1:H:111:GLU:OE1	2.39	0.54
1:D:120:VAL:CA	1:D:125:ASP:OD1	2.51	0.54
1:H:11:ALA:HB1	1:H:12:PRO:CD	2.37	0.54
1:F:130:LEU:O	1:F:134:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:LEU:HD12	1:D:155:TRP:HE1	1.72	0.53
1:A:130:LEU:HD13	1:A:133:GLN:HE21	1.74	0.53
1:E:33:ASP:OD1	1:E:37:ASP:N	2.42	0.53
1:F:61:THR:HG23	1:F:168:ALA:HB1	1.90	0.53
1:F:111:GLU:H	1:F:111:GLU:CD	2.16	0.53
1:D:144:LEU:HD13	1:D:145:GLU:N	2.24	0.53
1:E:86:ARG:NH1	1:E:110:HIS:CG	2.77	0.52
1:B:116:LEU:HD23	1:B:116:LEU:O	2.10	0.52
1:A:170:GLU:HG3	1:B:160:VAL:CG2	2.40	0.52
1:D:127:PRO:HB2	1:D:130:LEU:HB3	1.92	0.51
1:A:130:LEU:CD1	1:A:133:GLN:HE21	2.23	0.51
1:D:123:TYR:O	1:D:131:ILE:HD12	2.09	0.51
1:D:91:GLY:H	1:D:158:ALA:HA	1.76	0.51
1:H:162:LYS:HA	1:H:165:VAL:HG12	1.92	0.51
1:E:18:ILE:HG12	1:E:84:VAL:HG22	1.92	0.51
1:E:73:VAL:HG12	1:E:107:ALA:HB3	1.92	0.51
1:H:135:GLU:OE2	1:H:155:TRP:NE1	2.42	0.51
1:A:167:LYS:HG3	1:B:160:VAL:HG22	1.92	0.51
1:D:127:PRO:O	1:D:131:ILE:CD1	2.58	0.51
1:E:110:HIS:CG	1:E:111:GLU:N	2.79	0.51
1:E:54:ASN:HB2	1:E:73:VAL:HG22	1.93	0.51
1:D:5:ILE:O	1:D:60:ASN:ND2	2.43	0.50
1:G:49:MET:HE1	1:G:137:PHE:HA	1.93	0.50
1:H:109:PRO:HD2	1:H:117:TYR:CD2	2.45	0.50
1:D:23:ALA:H	1:D:54:ASN:ND2	2.09	0.50
1:D:88:ARG:HG2	1:D:90:VAL:HG23	1.93	0.50
1:E:110:HIS:CE1	1:E:111:GLU:HG2	2.47	0.50
1:H:20:GLU:HG2	1:H:32:ILE:HG13	1.93	0.50
1:A:79:VAL:HG21	1:A:85:ILE:HD11	1.93	0.50
1:E:92:LYS:HB3	1:E:156:GLU:HB2	1.92	0.50
1:A:72:LEU:HD21	1:A:138:PHE:HZ	1.78	0.49
1:H:43:ARG:HH21	1:H:45:MET:CE	2.25	0.49
1:A:160:VAL:HG13	1:B:167:LYS:HG2	1.94	0.49
1:A:31:GLU:HG2	1:A:42:ASP:HB2	1.95	0.49
1:H:18:ILE:HG12	1:H:84:VAL:HG22	1.95	0.49
1:D:18:ILE:O	1:D:56:GLY:HA3	2.12	0.49
1:B:126:LEU:HB2	1:B:131:ILE:HD11	1.94	0.49
1:E:90:VAL:HG23	1:E:106:ILE:HG23	1.94	0.49
1:B:58:VAL:CG2	1:B:69:LEU:HB3	2.43	0.49
1:E:92:LYS:HE2	1:E:103:ALA:HB1	1.94	0.49
1:B:12:PRO:HD3	1:B:166:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLU:OE2	1:C:155:TRP:NE1	2.45	0.48
1:F:74:VAL:O	1:F:109:PRO:HD3	2.13	0.48
1:F:139:SER:HB2	1:F:140:HIS:CD2	2.48	0.48
1:B:166:ILE:HA	1:B:169:ILE:HD12	1.94	0.48
1:E:86:ARG:HH12	1:E:110:HIS:CD2	2.31	0.48
1:E:162:LYS:O	1:E:166:ILE:HG13	2.14	0.48
1:B:97:ASP:OD1	1:B:100:GLY:N	2.46	0.48
1:E:158:ALA:HA	1:E:161:ALA:HB3	1.95	0.48
1:F:135:GLU:OE1	1:F:155:TRP:NE1	2.43	0.48
1:A:76:PRO:HG3	1:A:116:LEU:HD12	1.96	0.48
1:A:156:GLU:OE1	1:A:160:VAL:HG11	2.14	0.48
1:C:61:THR:HG22	1:C:169:ILE:HD13	1.96	0.48
1:F:71:VAL:HG22	1:F:105:LEU:HB2	1.96	0.47
1:C:58:VAL:HG12	1:C:69:LEU:HB3	1.95	0.47
1:D:129:LEU:HD23	1:D:129:LEU:N	2.29	0.47
1:F:13:ASN:O	1:F:13:ASN:ND2	2.48	0.47
1:G:135:GLU:CG	1:G:155:TRP:HE1	2.26	0.47
1:E:16:TYR:HE1	1:E:86:ARG:HB2	1.80	0.47
1:G:18:ILE:HG13	1:G:59:PRO:HD3	1.97	0.47
1:H:74:VAL:O	1:H:109:PRO:HD3	2.14	0.47
1:G:75:THR:HG22	1:G:77:TYR:H	1.80	0.47
1:D:144:LEU:HD13	1:D:144:LEU:C	2.39	0.47
1:F:18:ILE:HG12	1:F:84:VAL:HG22	1.95	0.47
1:D:12:PRO:HG2	1:D:162:LYS:HB3	1.97	0.47
1:D:31:GLU:O	1:D:40:PHE:N	2.48	0.46
1:D:61:THR:HG23	1:D:169:ILE:HA	1.98	0.46
1:F:13:ASN:HD21	1:F:88:ARG:CD	2.28	0.46
1:H:162:LYS:O	1:H:166:ILE:HG13	2.16	0.46
1:B:69:LEU:HD21	1:B:105:LEU:HD11	1.97	0.46
1:B:74:VAL:O	1:B:109:PRO:HD3	2.15	0.46
1:D:97:ASP:OD2	1:D:102:ASP:N	2.49	0.46
1:E:5:ILE:HD13	1:E:84:VAL:HG21	1.97	0.46
1:G:23:ALA:N	1:G:54:ASN:OD1	2.49	0.46
1:D:129:LEU:O	1:D:133:GLN:N	2.49	0.46
1:E:88:ARG:NH1	1:E:120:VAL:O	2.48	0.46
1:A:119:ASP:N	1:A:119:ASP:OD1	2.44	0.46
1:B:80:ALA:O	1:B:83:SER:OG	2.30	0.46
1:D:136:HIS:CE1	1:D:140:HIS:NE2	2.84	0.46
1:B:34:LYS:HD3	1:B:34:LYS:N	2.30	0.45
1:D:149:TRP:C	1:D:150:VAL:HG22	2.41	0.45
1:A:54:ASN:HD21	1:A:78:PRO:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ARG:NH1	1:B:120:VAL:O	2.31	0.45
1:D:129:LEU:HA	1:D:132:ASN:CB	2.47	0.45
1:D:45:MET:HE1	1:D:141:TYR:HD2	1.81	0.45
1:E:90:VAL:HA	1:E:158:ALA:HB2	1.99	0.45
1:H:69:LEU:HD21	1:H:105:LEU:HD11	1.99	0.45
1:H:165:VAL:O	1:H:169:ILE:HG22	2.16	0.45
1:G:20:GLU:HG2	1:G:32:ILE:HG13	1.99	0.45
1:C:18:ILE:HG12	1:C:84:VAL:HG22	1.99	0.45
1:G:93:LEU:HD13	1:G:155:TRP:CE2	2.52	0.45
1:H:92:LYS:HE2	1:H:94:ASN:ND2	2.30	0.45
1:B:17:VAL:HG22	1:B:58:VAL:CG1	2.47	0.44
1:G:15:ILE:HG12	1:G:89:PRO:HD3	1.98	0.44
1:B:71:VAL:HG22	1:B:105:LEU:HB2	1.98	0.44
1:H:98:ASP:CG	1:H:148:LYS:HD2	2.43	0.44
1:D:126:LEU:CD2	1:D:127:PRO:HD3	2.34	0.44
1:F:54:ASN:O	1:F:72:LEU:HA	2.17	0.44
1:E:92:LYS:HD3	1:E:156:GLU:OE2	2.17	0.44
1:E:30:TYR:CE1	1:E:41:VAL:HG12	2.53	0.44
1:H:34:LYS:H	1:H:34:LYS:HD2	1.83	0.44
1:H:19:ILE:HG13	1:H:79:VAL:HG21	1.99	0.44
1:E:58:VAL:HG13	1:E:61:THR:OG1	2.18	0.43
1:E:47:THR:HB	1:E:49:MET:HG3	2.00	0.43
1:H:147:GLY:C	1:H:148:LYS:HD3	2.42	0.43
1:C:94:ASN:ND2	1:C:156:GLU:HG3	2.32	0.43
1:E:135:GLU:OE1	1:E:155:TRP:NE1	2.48	0.43
1:F:54:ASN:ND2	1:F:79:VAL:HG22	2.33	0.43
1:F:128:GLN:NE2	1:H:123:TYR:OH	2.51	0.43
1:B:20:GLU:HG3	1:B:56:GLY:HA2	2.00	0.43
1:C:71:VAL:HG22	1:C:105:LEU:HB2	2.00	0.43
1:A:92:LYS:HE3	1:A:164:GLU:HG3	1.99	0.43
1:B:112:LYS:HE3	1:B:112:LYS:HB2	1.53	0.43
1:D:132:ASN:O	1:D:136:HIS:N	2.32	0.43
1:B:135:GLU:HG2	1:B:152:ILE:HG21	2.00	0.43
1:B:18:ILE:HG12	1:B:84:VAL:HG22	2.01	0.43
1:D:5:ILE:HG13	1:D:59:PRO:HG3	2.00	0.43
1:D:33:ASP:O	1:D:37:ASP:N	2.49	0.43
1:A:130:LEU:CD1	1:A:133:GLN:NE2	2.81	0.43
1:E:74:VAL:O	1:E:109:PRO:HD3	2.18	0.43
1:A:72:LEU:HD21	1:A:138:PHE:CZ	2.54	0.42
1:A:19:ILE:HD13	1:A:19:ILE:HA	1.84	0.42
1:B:19:ILE:HD13	1:B:19:ILE:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:SER:OG	1:B:64:GLU:N	2.51	0.42
1:F:93:LEU:HD12	1:F:155:TRP:CE2	2.53	0.42
1:H:86:ARG:HD3	1:H:110:HIS:CB	2.49	0.42
1:D:118:LYS:HG3	1:D:119:ASP:N	2.34	0.42
1:D:119:ASP:O	1:D:125:ASP:OD1	2.37	0.42
1:B:166:ILE:HA	1:B:166:ILE:HD13	1.95	0.42
1:A:43:ARG:CZ	1:A:145:GLU:HG3	2.48	0.42
1:D:90:VAL:N	2:D:202:HOH:O	2.52	0.42
1:D:90:VAL:O	1:D:90:VAL:HG12	2.20	0.42
1:D:17:VAL:O	1:D:84:VAL:HA	2.19	0.42
1:E:15:ILE:HG12	1:E:89:PRO:HD3	2.02	0.42
1:E:49:MET:HE1	1:E:137:PHE:HA	2.00	0.42
1:D:123:TYR:CZ	1:D:155:TRP:HB3	2.54	0.42
1:F:170:GLU:HA	1:F:173:LYS:NZ	2.33	0.42
1:G:126:LEU:HD22	1:G:130:LEU:HD23	2.01	0.42
1:B:121:LYS:HE3	1:B:121:LYS:HA	2.01	0.41
1:C:74:VAL:O	1:C:109:PRO:HD3	2.19	0.41
1:D:72:LEU:O	1:D:106:ILE:HA	2.20	0.41
1:F:65:ASP:OD1	1:F:65:ASP:N	2.53	0.41
1:G:30:TYR:HB3	1:G:39:LEU:HG	2.01	0.41
1:D:45:MET:HE2	1:D:45:MET:HB3	1.86	0.41
1:A:61:THR:HB	1:A:168:ALA:HB1	2.03	0.41
1:E:149:TRP:CD1	1:E:149:TRP:C	2.98	0.41
1:H:98:ASP:OD2	1:H:148:LYS:HD2	2.21	0.41
1:F:94:ASN:HD21	1:F:156:GLU:HG3	1.85	0.41
1:G:26:ALA:C	1:G:28:ILE:H	2.28	0.41
1:C:64:GLU:OE2	1:C:64:GLU:N	2.54	0.41
1:D:47:THR:HG21	1:D:140:HIS:O	2.20	0.41
1:E:122:GLU:HG2	1:E:158:ALA:H	1.85	0.41
1:C:58:VAL:CG1	1:C:69:LEU:HB3	2.50	0.41
1:B:147:GLY:HA2	1:H:101:ILE:HD13	2.03	0.41
1:C:12:PRO:HD3	1:C:166:ILE:HD11	2.03	0.41
1:H:88:ARG:NH1	1:H:120:VAL:O	2.48	0.41
1:C:19:ILE:HD13	1:C:19:ILE:HA	1.83	0.41
1:D:135:GLU:HG2	1:D:155:TRP:HE1	1.86	0.41
1:E:64:GLU:OE1	1:E:101:ILE:HD11	2.20	0.41
1:F:117:TYR:O	1:F:120:VAL:HG22	2.21	0.41
1:H:12:PRO:HG3	1:H:166:ILE:HD11	2.02	0.41
1:D:70:ASP:N	1:D:70:ASP:OD1	2.53	0.40
1:F:93:LEU:C	1:F:93:LEU:HD23	2.46	0.40
1:G:79:VAL:HG21	1:G:85:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:GLU:H	1:G:111:GLU:HG3	1.74	0.40
1:D:91:GLY:N	2:D:202:HOH:O	2.53	0.40
1:H:95:MET:HE3	1:H:95:MET:HB2	1.94	0.40
1:D:131:ILE:HG12	1:D:131:ILE:H	1.37	0.40
1:B:97:ASP:CG	1:B:99:GLY:H	2.29	0.40
1:C:2:TYR:CE2	1:C:32:ILE:HD13	2.56	0.40
1:D:47:THR:CG2	1:D:143:ASP:HB2	2.51	0.40
1:D:115:PRO:O	1:D:118:LYS:HG2	2.21	0.40
1:H:70:ASP:OD2	1:H:104:LYS:NZ	2.54	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	171/177 (97%)	165 (96%)	6 (4%)	0	100	100
1	B	171/177 (97%)	164 (96%)	6 (4%)	1 (1%)	21	38
1	C	171/177 (97%)	165 (96%)	6 (4%)	0	100	100
1	D	171/177 (97%)	138 (81%)	26 (15%)	7 (4%)	2	3
1	E	171/177 (97%)	159 (93%)	12 (7%)	0	100	100
1	F	171/177 (97%)	161 (94%)	10 (6%)	0	100	100
1	G	171/177 (97%)	153 (90%)	17 (10%)	1 (1%)	21	38
1	H	171/177 (97%)	164 (96%)	6 (4%)	1 (1%)	21	38
All	All	1368/1416 (97%)	1269 (93%)	89 (6%)	10 (1%)	18	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	126	LEU

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Mol	Chain	Res	Type
1	D	145	GLU
1	B	11	ALA
1	D	150	VAL
1	H	11	ALA
1	D	146	PRO
1	D	65	ASP
1	D	148	LYS
1	G	36	SER
1	D	90	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	144/147 (98%)	144 (100%)	0	100	100
1	B	144/147 (98%)	144 (100%)	0	100	100
1	C	144/147 (98%)	144 (100%)	0	100	100
1	D	143/147 (97%)	142 (99%)	1 (1%)	76	86
1	E	144/147 (98%)	143 (99%)	1 (1%)	76	86
1	F	144/147 (98%)	144 (100%)	0	100	100
1	G	144/147 (98%)	144 (100%)	0	100	100
1	H	144/147 (98%)	144 (100%)	0	100	100
All	All	1151/1176 (98%)	1149 (100%)	2 (0%)	87	95

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

Mol	Chain	Res	Type
1	D	131	ILE
1	E	148	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	133	GLN
1	A	136	HIS
1	A	140	HIS
1	B	110	HIS
1	C	3	ASN
1	C	60	ASN
1	C	128	GLN
1	C	140	HIS
1	D	54	ASN
1	D	60	ASN
1	D	136	HIS
1	E	3	ASN
1	E	4	ASN
1	E	60	ASN
1	E	128	GLN
1	E	133	GLN
1	F	13	ASN
1	F	24	ASN
1	F	54	ASN
1	F	60	ASN
1	F	94	ASN
1	F	110	HIS
1	F	128	GLN
1	F	140	HIS
1	G	110	HIS
1	H	13	ASN
1	H	60	ASN
1	H	94	ASN
1	H	128	GLN

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	173/177 (97%)	0.46	9 (5%)	33	32	40, 63, 92, 101	0
1	B	173/177 (97%)	0.38	4 (2%)	61	59	32, 53, 80, 114	0
1	C	173/177 (97%)	-0.12	1 (0%)	85	86	23, 38, 70, 89	0
1	D	173/177 (97%)	2.04	87 (50%)	0	0	40, 97, 129, 163	0
1	E	173/177 (97%)	0.35	3 (1%)	69	67	45, 80, 122, 141	0
1	F	173/177 (97%)	0.42	5 (2%)	53	52	27, 56, 90, 114	0
1	G	173/177 (97%)	1.33	32 (18%)	3	2	99, 139, 181, 228	0
1	H	173/177 (97%)	0.15	4 (2%)	61	59	25, 50, 89, 116	0
All	All	1384/1416 (97%)	0.63	145 (10%)	11	11	23, 64, 145, 228	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	152	ILE	5.6
1	D	47	THR	5.2
1	D	63	SER	4.8
1	D	116	LEU	4.8
1	D	48	ALA	4.8
1	D	155	TRP	4.6
1	D	120	VAL	4.5
1	A	2	TYR	4.5
1	H	45	MET	4.5
1	D	137	PHE	4.5
1	D	117	TYR	4.4
1	D	138	PHE	4.2
1	D	141	TYR	4.2
1	D	145	GLU	4.2
1	D	154	GLY	4.2
1	G	101	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	11	ALA	4.0
1	D	123	TYR	4.0
1	D	107	ALA	3.9
1	D	134	VAL	3.9
1	D	49	MET	3.8
1	D	56	GLY	3.8
1	D	149	TRP	3.8
1	D	90	VAL	3.7
1	D	92	LYS	3.7
1	H	11	ALA	3.7
1	D	101	ILE	3.7
1	D	140	HIS	3.5
1	D	69	LEU	3.5
1	D	118	LYS	3.4
1	D	73	VAL	3.4
1	D	136	HIS	3.4
1	D	124	THR	3.3
1	G	168	ALA	3.3
1	D	129	LEU	3.3
1	D	150	VAL	3.3
1	D	109	PRO	3.3
1	D	139	SER	3.2
1	D	161	ALA	3.2
1	D	93	LEU	3.2
1	B	11	ALA	3.2
1	G	146	PRO	3.1
1	G	103	ALA	3.1
1	G	85	ILE	3.1
1	D	17	VAL	3.1
1	D	160	VAL	3.1
1	G	62	LEU	3.1
1	E	33	ASP	3.1
1	G	152	ILE	3.1
1	D	144	LEU	3.0
1	D	41	VAL	3.0
1	D	165	VAL	3.0
1	A	36	SER	3.0
1	D	50	PHE	3.0
1	G	139	SER	2.9
1	D	158	ALA	2.9
1	D	94	ASN	2.9
1	G	72	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	135	GLU	2.8
1	D	95	MET	2.8
1	G	108	VAL	2.7
1	D	146	PRO	2.7
1	G	99	GLY	2.7
1	B	161	ALA	2.7
1	D	131	ILE	2.6
1	D	169	ILE	2.6
1	B	116	LEU	2.6
1	D	72	LEU	2.6
1	D	9	LYS	2.6
1	D	71	VAL	2.6
1	G	120	VAL	2.6
1	D	67	ASP	2.6
1	D	85	ILE	2.6
1	G	66	GLY	2.6
1	D	60	ASN	2.6
1	G	127	PRO	2.6
1	D	96	GLU	2.6
1	A	172	ALA	2.6
1	A	18	ILE	2.5
1	C	118	LYS	2.5
1	D	46	GLY	2.5
1	D	156	GLU	2.5
1	D	166	ILE	2.5
1	D	15	ILE	2.5
1	G	110	HIS	2.5
1	D	68	PRO	2.4
1	G	109	PRO	2.4
1	G	160	VAL	2.4
1	D	75	THR	2.4
1	D	54	ASN	2.4
1	D	45	MET	2.4
1	A	84	VAL	2.4
1	D	55	TYR	2.4
1	D	3	ASN	2.4
1	D	59	PRO	2.4
1	D	66	GLY	2.4
1	D	74	VAL	2.4
1	D	143	ASP	2.4
1	D	27	PRO	2.4
1	D	44	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	39	LEU	2.3
1	A	37	ASP	2.3
1	D	12	PRO	2.3
1	F	165	VAL	2.3
1	G	166	ILE	2.3
1	H	147	GLY	2.3
1	D	87	CYS	2.3
1	G	144	LEU	2.3
1	D	103	ALA	2.3
1	D	57	TYR	2.3
1	D	70	ASP	2.3
1	D	97	ASP	2.3
1	G	56	GLY	2.3
1	G	161	ALA	2.2
1	A	5	ILE	2.2
1	D	110	HIS	2.2
1	D	125	ASP	2.2
1	G	113	LEU	2.2
1	G	17	VAL	2.2
1	G	30	TYR	2.2
1	G	158	ALA	2.2
1	F	159	ASP	2.2
1	E	158	ALA	2.1
1	D	132	ASN	2.1
1	G	18	ILE	2.1
1	D	164	GLU	2.1
1	G	105	LEU	2.1
1	D	115	PRO	2.1
1	D	126	LEU	2.1
1	F	16	TYR	2.1
1	D	18	ILE	2.1
1	G	169	ILE	2.1
1	D	13	ASN	2.1
1	D	106	ILE	2.1
1	D	58	VAL	2.1
1	G	71	VAL	2.1
1	B	111	GLU	2.0
1	A	83	SER	2.0
1	F	151	LYS	2.0
1	D	113	LEU	2.0
1	G	69	LEU	2.0
1	G	141	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	34	LYS	2.0
1	H	1	SER	2.0
1	F	8	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.