



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 07:54 PM EDT

PDB ID : 6KI7  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

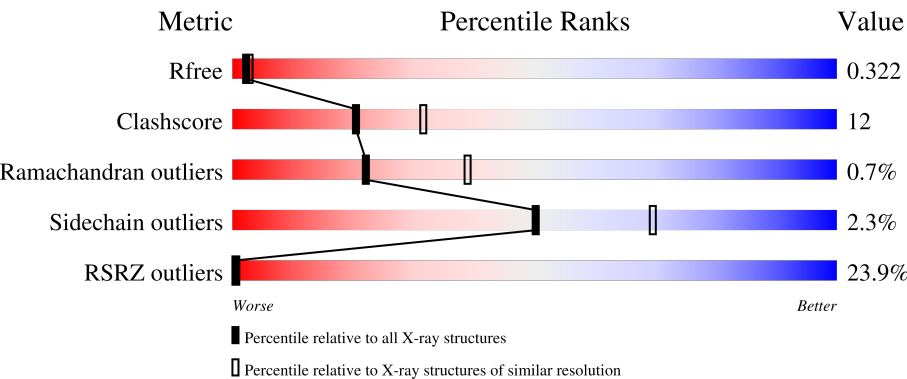
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

# 1 Overall quality at a glance i

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))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	177	<div><div>14%</div><div>82%</div><div>15%</div><div>..</div></div>
1	B	177	<div><div>9%</div><div>74%</div><div>23%</div><div>..</div></div>
1	C	177	<div><div>4%</div><div>84%</div><div>14%</div><div>.</div></div>
1	D	177	<div><div>51%</div><div>54%</div><div>39%</div><div>5%</div><div>.</div></div>
1	E	177	<div><div>18%</div><div>68%</div><div>29%</div><div>.</div></div>

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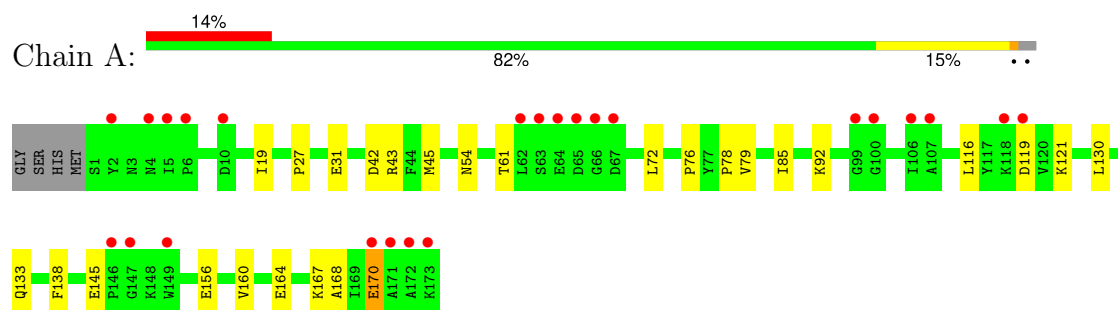
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	O	0	0
			2	2		
2	H	4	Total	O	0	0
			4	4		

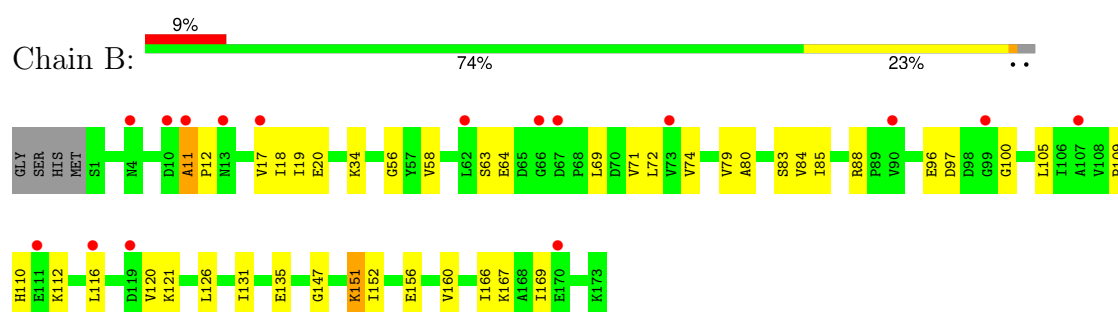
### 3 Residue-property plots [i](#)

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.

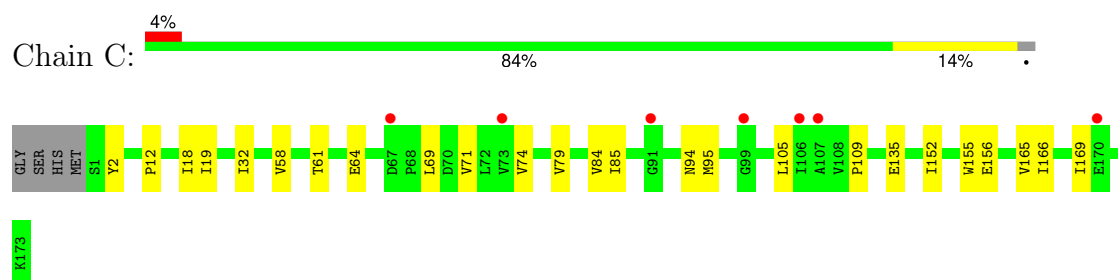
- Molecule 1: Inorganic pyrophosphatase



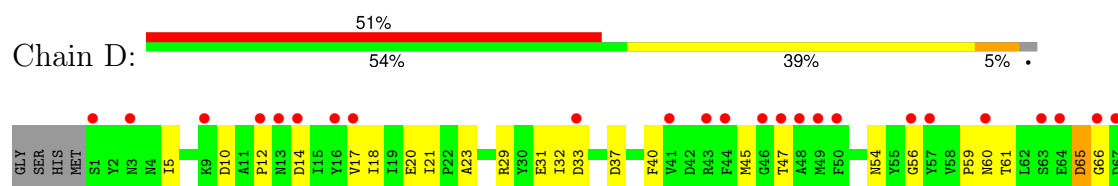
- Molecule 1: Inorganic pyrophosphatase

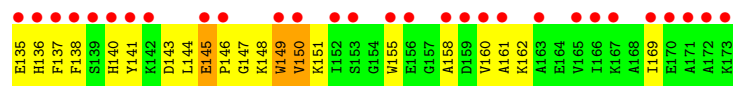
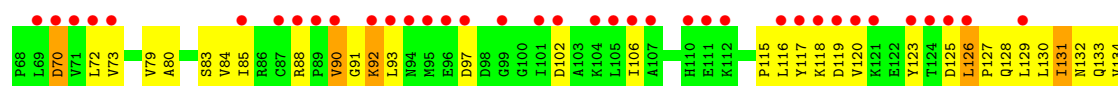


- Molecule 1: Inorganic pyrophosphatase

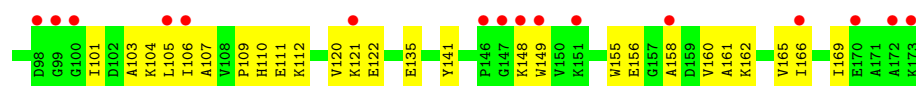
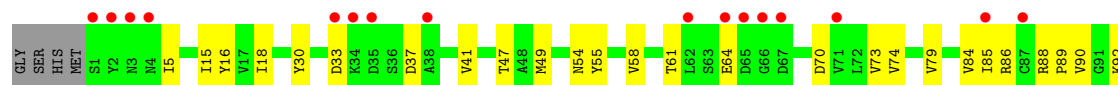


- Molecule 1: Inorganic pyrophosphatase





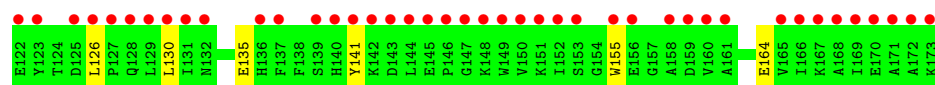
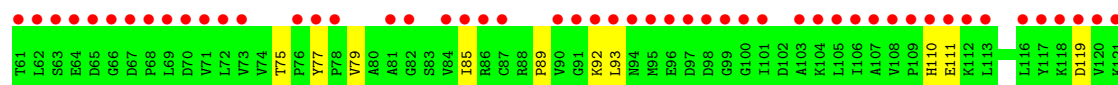
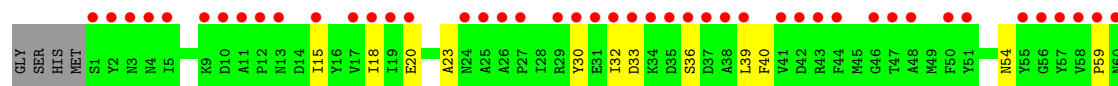
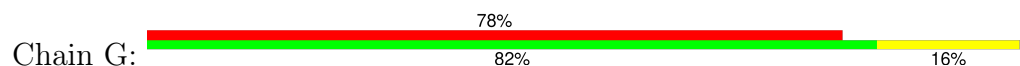
• Molecule 1: Inorganic pyrophosphatase



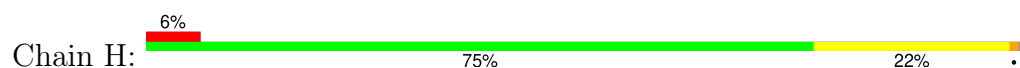
• Molecule 1: Inorganic pyrophosphatase



• 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, $\alpha$ , $\beta$ , $\gamma$	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) 98.4 (19.96-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	1978 reflections (5.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.1	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 69.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [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	0.26	0/1383	0.46	0/1886
1	B	0.28	0/1383	0.46	0/1886
1	C	0.25	0/1383	0.45	0/1886
1	D	0.31	0/1380	0.59	0/1883
1	E	0.27	0/1383	0.47	0/1886
1	F	0.31	0/1383	0.48	0/1886
1	G	0.25	0/1383	0.43	0/1886
1	H	0.26	0/1383	0.48	0/1886
All	All	0.28	0/11061	0.48	0/15085

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 [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	36	0
1	C	1348	0	1330	15	0
1	D	1345	0	1323	84	0
1	E	1348	0	1330	36	0
1	F	1348	0	1330	37	0
1	G	1348	0	1330	14	0
1	H	1348	0	1330	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	265	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 (265) 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: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: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
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:92:LYS:HZ3	1:D:160:VAL:HB	1.49	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:92:LYS:NZ	1:D:160:VAL:HB	2.13	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
1:G:110:HIS:HE1	1:G:111:GLU:OE2	1.83	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:D:45:MET:HE1	1:D:141:TYR:HD2	1.67	0.59
1:H:156:GLU:HB2	1:H:160:VAL:HG11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:170:GLU:HA	1:F:173:LYS:HZ3	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:LYS:HZ1	1:D:161:ALA:N	2.07	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:E:110:HIS:CG	1:E:111:GLU:N	2.79	0.51
1:G:92:LYS:NZ	1:G:164:GLU:OE1	2.30	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: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:D:80:ALA:O	1:D:83:SER:OG	2.25	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:93:LEU:CD2	1:F:95:MET:HE2	2.44	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:F:93:LEU:HD22	1:F:95:MET:CE	2.43	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: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:A:54:ASN:HD21	1:A:78:PRO:HA	1.82	0.45
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:144:LEU:HD13	1:D:144:LEU:C	2.39	0.43
1:A:130:LEU:CD1	1:A:133:GLN:NE2	2.81	0.43
1:F:170:GLU:HA	1:F:173:LYS:NZ	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:65:ASP:OD1	1:F:65:ASP:N	2.53	0.42
1:D:123:TYR:CZ	1:D:155:TRP:HB3	2.54	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:G:30:TYR:HB3	1:G:39:LEU:HG	2.01	0.41
1:A:61:THR:HB	1:A:168:ALA:HB1	2.03	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: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:D:149:TRP:C	1:D:150:VAL:HG22	2.41	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:G:79:VAL:HG21	1:G:85:ILE:HD11	2.03	0.40
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:D:131:ILE:HG12	1:D:131:ILE:H	1.37	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%)	25	42
1	C	171/177 (97%)	165 (96%)	6 (4%)	0	100	100
1	D	171/177 (97%)	138 (81%)	26 (15%)	7 (4%)	3	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%)	25	42
1	H	171/177 (97%)	164 (96%)	6 (4%)	1 (1%)	25	42
All	All	1368/1416 (97%)	1269 (93%)	89 (6%)	10 (1%)	22	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	126	LEU
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%)	142 (99%)	2 (1%)	67	79
1	B	144/147 (98%)	142 (99%)	2 (1%)	67	79
1	C	144/147 (98%)	144 (100%)	0	100	100
1	D	143/147 (97%)	138 (96%)	5 (4%)	36	56
1	E	144/147 (98%)	140 (97%)	4 (3%)	43	63
1	F	144/147 (98%)	137 (95%)	7 (5%)	25	43
1	G	144/147 (98%)	140 (97%)	4 (3%)	43	63
1	H	144/147 (98%)	141 (98%)	3 (2%)	53	71
All	All	1151/1176 (98%)	1124 (98%)	27 (2%)	50	69

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LYS
1	A	170	GLU
1	B	72	LEU
1	B	151	LYS
1	D	70	ASP
1	D	92	LYS
1	D	131	ILE
1	D	149	TRP
1	D	151	LYS
1	E	112	LYS
1	E	141	TYR
1	E	148	LYS
1	E	149	TRP
1	F	13	ASN
1	F	34	LYS
1	F	35	ASP
1	F	43	ARG
1	F	117	TYR
1	F	141	TYR
1	F	151	LYS
1	G	33	ASP
1	G	40	PHE
1	G	119	ASP
1	G	141	TYR

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Mol	Chain	Res	Type
1	H	86	ARG
1	H	141	TYR
1	H	159	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	133	GLN
1	B	110	HIS
1	C	3	ASN
1	C	4	ASN
1	C	140	HIS
1	D	54	ASN
1	D	60	ASN
1	D	136	HIS
1	E	133	GLN
1	F	13	ASN
1	F	94	ASN
1	F	110	HIS
1	F	128	GLN
1	F	140	HIS
1	G	110	HIS
1	H	94	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 monosaccharides 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	173/177 (97%)	0.79	24 (13%) 2 3	40, 63, 92, 101	0
1	B	173/177 (97%)	0.46	16 (9%) 9 10	32, 53, 80, 114	0
1	C	173/177 (97%)	0.15	7 (4%) 38 45	23, 38, 70, 89	0
1	D	173/177 (97%)	2.35	90 (52%) 0 0	40, 97, 129, 163	0
1	E	173/177 (97%)	0.93	32 (18%) 1 1	45, 80, 122, 141	0
1	F	173/177 (97%)	0.51	14 (8%) 12 14	27, 56, 90, 114	0
1	G	173/177 (97%)	4.18	138 (79%) 0 0	99, 139, 181, 228	0
1	H	173/177 (97%)	0.35	10 (5%) 23 28	25, 50, 89, 116	0
All	All	1384/1416 (97%)	1.21	331 (23%) 0 0	23, 64, 145, 228	0

All (331) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	99	GLY	13.9
1	G	38	ALA	12.7
1	G	11	ALA	12.0
1	G	110	HIS	10.9
1	G	107	ALA	10.7
1	G	56	GLY	10.6
1	G	105	LEU	10.4
1	G	39	LEU	10.1
1	G	85	ILE	9.8
1	G	12	PRO	9.5
1	G	171	ALA	9.4
1	D	116	LEU	9.2
1	G	144	LEU	8.9
1	G	112	LYS	8.7
1	G	64	GLU	8.6
1	G	160	VAL	8.4

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Mol	Chain	Res	Type	RSRZ
1	G	91	GLY	8.4
1	G	59	PRO	8.2
1	G	62	LEU	8.1
1	G	65	ASP	8.1
1	D	66	GLY	7.9
1	G	106	ILE	7.9
1	G	9	LYS	7.9
1	G	48	ALA	7.7
1	D	101	ILE	7.6
1	G	60	ASN	7.5
1	E	64	GLU	7.2
1	G	69	LEU	7.1
1	G	67	ASP	7.1
1	G	153	SER	7.1
1	D	124	THR	6.8
1	G	72	LEU	6.8
1	D	155	TRP	6.5
1	G	108	VAL	6.4
1	G	61	THR	6.4
1	D	163	ALA	6.3
1	G	146	PRO	6.2
1	E	3	ASN	6.1
1	D	152	ILE	6.1
1	G	156	GLU	6.0
1	D	48	ALA	6.0
1	G	129	LEU	6.0
1	G	96	GLU	6.0
1	G	101	ILE	5.9
1	G	159	ASP	5.9
1	G	4	ASN	5.9
1	G	92	LYS	5.9
1	G	136	HIS	5.8
1	E	35	ASP	5.8
1	G	155	TRP	5.7
1	G	66	GLY	5.7
1	G	168	ALA	5.7
1	G	120	VAL	5.7
1	A	100	GLY	5.6
1	D	145	GLU	5.5
1	G	2	TYR	5.5
1	G	77	TYR	5.5
1	E	147	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	G	172	ALA	5.4
1	G	98	ASP	5.3
1	G	27	PRO	5.3
1	G	35	ASP	5.3
1	G	170	GLU	5.3
1	D	64	GLU	5.3
1	G	139	SER	5.3
1	G	33	ASP	5.2
1	A	173	LYS	5.2
1	D	47	THR	5.1
1	D	123	TYR	5.1
1	D	117	TYR	5.1
1	G	161	ALA	5.1
1	G	173	LYS	5.0
1	G	26	ALA	5.0
1	G	71	VAL	5.0
1	D	13	ASN	5.0
1	G	121	LYS	5.0
1	D	149	TRP	4.9
1	G	87	CYS	4.9
1	A	2	TYR	4.8
1	G	147	GLY	4.8
1	E	2	TYR	4.8
1	G	152	ILE	4.8
1	G	127	PRO	4.7
1	D	138	PHE	4.7
1	G	97	ASP	4.7
1	G	103	ALA	4.7
1	G	151	LYS	4.7
1	E	62	LEU	4.7
1	G	132	ASN	4.7
1	E	99	GLY	4.6
1	D	120	VAL	4.6
1	E	38	ALA	4.6
1	E	66	GLY	4.5
1	G	57	TYR	4.5
1	D	146	PRO	4.5
1	G	3	ASN	4.4
1	G	32	ILE	4.4
1	G	100	GLY	4.4
1	A	62	LEU	4.4
1	G	93	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	106	ILE	4.4
1	D	140	HIS	4.3
1	G	30	TYR	4.3
1	G	117	TYR	4.3
1	G	141	TYR	4.3
1	G	5	ILE	4.3
1	D	63	SER	4.3
1	E	67	ASP	4.3
1	G	158	ALA	4.3
1	G	13	ASN	4.3
1	G	125	ASP	4.3
1	D	69	LEU	4.3
1	E	151	LYS	4.2
1	D	121	LYS	4.2
1	A	119	ASP	4.2
1	G	123	TYR	4.2
1	G	113	LEU	4.2
1	G	111	GLU	4.2
1	D	160	VAL	4.1
1	A	64	GLU	4.1
1	E	33	ASP	4.1
1	D	105	LEU	4.1
1	G	36	SER	4.0
1	G	118	LYS	4.0
1	G	20	GLU	4.0
1	G	143	ASP	4.0
1	G	169	ILE	4.0
1	D	112	LYS	4.0
1	D	99	GLY	3.9
1	A	99	GLY	3.9
1	F	66	GLY	3.9
1	D	107	ALA	3.8
1	D	49	MET	3.8
1	H	45	MET	3.8
1	H	1	SER	3.8
1	E	146	PRO	3.8
1	D	166	ILE	3.8
1	B	66	GLY	3.8
1	E	173	LYS	3.8
1	G	24	ASN	3.7
1	B	99	GLY	3.7
1	G	104	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	63	SER	3.7
1	D	43	ARG	3.7
1	A	172	ALA	3.7
1	E	1	SER	3.7
1	A	146	PRO	3.7
1	D	111	GLU	3.7
1	G	37	ASP	3.6
1	G	109	PRO	3.6
1	D	50	PHE	3.6
1	D	12	PRO	3.6
1	F	85	ILE	3.5
1	D	172	ALA	3.5
1	G	148	LYS	3.5
1	A	5	ILE	3.5
1	G	50	PHE	3.5
1	G	18	ILE	3.5
1	G	119	ASP	3.5
1	D	46	GLY	3.5
1	D	9	LYS	3.4
1	A	65	ASP	3.4
1	D	137	PHE	3.4
1	D	87	CYS	3.4
1	D	94	ASN	3.4
1	D	72	LEU	3.4
1	D	126	LEU	3.4
1	G	17	VAL	3.4
1	G	145	GLU	3.3
1	H	64	GLU	3.3
1	B	107	ALA	3.3
1	G	95	MET	3.3
1	D	71	VAL	3.3
1	G	31	GLU	3.3
1	D	141	TYR	3.3
1	A	147	GLY	3.3
1	D	17	VAL	3.3
1	E	121	LYS	3.3
1	G	68	PRO	3.3
1	H	35	ASP	3.3
1	G	55	TYR	3.2
1	D	167	LYS	3.2
1	D	159	ASP	3.2
1	G	116	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	106	ILE	3.2
1	F	13	ASN	3.2
1	A	63	SER	3.2
1	D	161	ALA	3.1
1	A	106	ILE	3.1
1	G	70	ASP	3.1
1	D	41	VAL	3.1
1	H	147	GLY	3.1
1	D	85	ILE	3.1
1	G	42	ASP	3.1
1	D	170	GLU	3.1
1	E	148	LYS	3.1
1	D	90	VAL	3.0
1	A	10	ASP	3.0
1	D	119	ASP	3.0
1	D	57	TYR	3.0
1	D	142	LYS	3.0
1	G	46	GLY	3.0
1	B	11	ALA	3.0
1	H	11	ALA	3.0
1	G	73	VAL	3.0
1	G	44	PHE	3.0
1	F	67	ASP	2.9
1	C	170	GLU	2.9
1	G	43	ARG	2.9
1	D	165	VAL	2.9
1	E	87	CYS	2.9
1	G	10	ASP	2.9
1	G	166	ILE	2.9
1	D	156	GLU	2.9
1	G	140	HIS	2.9
1	E	34	LYS	2.9
1	D	67	ASP	2.9
1	D	171	ALA	2.8
1	G	94	ASN	2.8
1	G	149	TRP	2.8
1	E	105	LEU	2.8
1	D	60	ASN	2.8
1	D	110	HIS	2.8
1	D	129	LEU	2.8
1	D	173	LYS	2.8
1	G	142	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	131	ILE	2.7
1	G	128	GLN	2.7
1	D	1	SER	2.7
1	D	73	VAL	2.7
1	F	116	LEU	2.7
1	F	9	LYS	2.7
1	E	100	GLY	2.7
1	D	3	ASN	2.7
1	B	67	ASP	2.7
1	F	172	ALA	2.7
1	C	67	ASP	2.7
1	C	107	ALA	2.7
1	G	76	PRO	2.7
1	D	56	GLY	2.7
1	G	150	VAL	2.7
1	E	106	ILE	2.6
1	F	16	TYR	2.6
1	H	2	TYR	2.6
1	A	6	PRO	2.6
1	D	95	MET	2.6
1	D	135	GLU	2.6
1	B	73	VAL	2.6
1	G	34	LYS	2.6
1	D	92	LYS	2.5
1	A	4	ASN	2.5
1	B	170	GLU	2.5
1	F	121	LYS	2.5
1	A	107	ALA	2.5
1	A	66	GLY	2.5
1	D	102	ASP	2.5
1	G	78	PRO	2.5
1	E	158	ALA	2.5
1	G	25	ALA	2.4
1	G	137	PHE	2.4
1	D	93	LEU	2.4
1	G	90	VAL	2.4
1	G	51	TYR	2.4
1	B	116	LEU	2.4
1	D	139	SER	2.4
1	E	85	ILE	2.4
1	B	13	ASN	2.4
1	G	86	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	87	CYS	2.4
1	G	15	ILE	2.4
1	G	165	VAL	2.4
1	A	171	ALA	2.4
1	G	130	LEU	2.3
1	H	67	ASP	2.3
1	E	4	ASN	2.3
1	H	170	GLU	2.3
1	D	136	HIS	2.3
1	E	149	TRP	2.3
1	D	153	SER	2.3
1	G	47	THR	2.3
1	E	71	VAL	2.3
1	G	41	VAL	2.3
1	D	70	ASP	2.3
1	G	84	VAL	2.3
1	D	169	ILE	2.3
1	D	150	VAL	2.3
1	B	10	ASP	2.3
1	D	118	LYS	2.3
1	E	172	ALA	2.3
1	E	166	ILE	2.2
1	D	96	GLU	2.2
1	F	1	SER	2.2
1	H	173	LYS	2.2
1	G	167	LYS	2.2
1	D	14	ASP	2.2
1	D	125	ASP	2.2
1	E	98	ASP	2.2
1	B	111	GLU	2.2
1	D	33	ASP	2.2
1	D	88	ARG	2.2
1	F	35	ASP	2.2
1	G	81	ALA	2.2
1	B	90	VAL	2.2
1	G	1	SER	2.2
1	B	4	ASN	2.1
1	D	104	LYS	2.1
1	G	82	GLY	2.1
1	B	17	VAL	2.1
1	F	91	GLY	2.1
1	D	16	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	91	GLY	2.1
1	B	62	LEU	2.1
1	G	58	VAL	2.1
1	G	126	LEU	2.1
1	C	99	GLY	2.1
1	E	65	ASP	2.1
1	F	105	LEU	2.1
1	G	19	ILE	2.1
1	B	119	ASP	2.1
1	E	170	GLU	2.1
1	A	149	TRP	2.1
1	D	89	PRO	2.1
1	D	44	PHE	2.1
1	D	97	ASP	2.1
1	C	73	VAL	2.0
1	A	170	GLU	2.0
1	D	158	ALA	2.0
1	G	29	ARG	2.0
1	G	122	GLU	2.0
1	A	67	ASP	2.0
1	A	118	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.