



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:06 am BST

PDB ID : 2Y7R  
Title : DntR Inducer Binding Domain  
Authors : Devesse, L.; Smirnova, I.; Lonneborg, R.; Kapp, U.; Brzezinski, P.; Leonard, G.A.; Dian, C.  
Deposited on : 2011-02-01  
Resolution : 2.99 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.

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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) : 1.13  
EDS : 2.11  
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) : 2.11

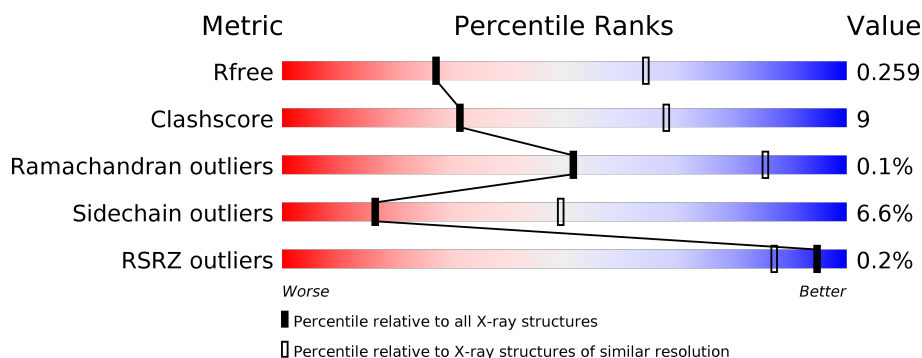
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	218	<div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	B	218	<div> <div>72%</div> <div>25%</div> <div>.</div> </div>
1	C	218	<div> <div>72%</div> <div>22%</div> <div>.</div> <div>.</div> </div>
1	D	218	<div> <div>77%</div> <div>19%</div> <div>.</div> <div>.</div> </div>
1	E	218	<div> <div>72%</div> <div>23%</div> <div>.</div> <div>.</div> </div>
1	F	218	<div> <div>%</div> <div>73%</div> <div>21%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	218	<div><div></div><div>71%</div><div>23%</div><div></div><div></div></div>
1	H	218	<div><div></div><div>71%</div><div>24%</div><div></div><div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12995 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 LYSR-TYPE REGULATORY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1622	1051	281	278	12			
1	B	212	Total	C	N	O	S	0	0	0
			1645	1063	285	285	12			
1	C	210	Total	C	N	O	S	0	0	0
			1623	1048	284	280	11			
1	D	212	Total	C	N	O	S	0	0	0
			1622	1050	284	277	11			
1	E	212	Total	C	N	O	S	0	0	0
			1632	1055	285	280	12			
1	F	211	Total	C	N	O	S	0	0	0
			1613	1047	274	280	12			
1	G	211	Total	C	N	O	S	0	0	0
			1629	1056	286	275	12			
1	H	212	Total	C	N	O	S	0	0	0
			1609	1045	278	274	12			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	MET	PHE	engineered mutation	UNP Q7WT50
A	192	SER	THR	conflict	UNP Q7WT50
A	302	HIS	-	expression tag	UNP Q7WT50
A	303	HIS	-	expression tag	UNP Q7WT50
A	304	HIS	-	expression tag	UNP Q7WT50
A	305	HIS	-	expression tag	UNP Q7WT50
A	306	HIS	-	expression tag	UNP Q7WT50
A	307	HIS	-	expression tag	UNP Q7WT50
B	90	MET	PHE	engineered mutation	UNP Q7WT50
B	192	SER	THR	conflict	UNP Q7WT50
B	302	HIS	-	expression tag	UNP Q7WT50
B	303	HIS	-	expression tag	UNP Q7WT50
B	304	HIS	-	expression tag	UNP Q7WT50

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Chain	Residue	Modelled	Actual	Comment	Reference
B	305	HIS	-	expression tag	UNP Q7WT50
B	306	HIS	-	expression tag	UNP Q7WT50
B	307	HIS	-	expression tag	UNP Q7WT50
C	90	MET	PHE	engineered mutation	UNP Q7WT50
C	192	SER	THR	conflict	UNP Q7WT50
C	302	HIS	-	expression tag	UNP Q7WT50
C	303	HIS	-	expression tag	UNP Q7WT50
C	304	HIS	-	expression tag	UNP Q7WT50
C	305	HIS	-	expression tag	UNP Q7WT50
C	306	HIS	-	expression tag	UNP Q7WT50
C	307	HIS	-	expression tag	UNP Q7WT50
D	90	MET	PHE	engineered mutation	UNP Q7WT50
D	192	SER	THR	conflict	UNP Q7WT50
D	302	HIS	-	expression tag	UNP Q7WT50
D	303	HIS	-	expression tag	UNP Q7WT50
D	304	HIS	-	expression tag	UNP Q7WT50
D	305	HIS	-	expression tag	UNP Q7WT50
D	306	HIS	-	expression tag	UNP Q7WT50
D	307	HIS	-	expression tag	UNP Q7WT50
E	90	MET	PHE	engineered mutation	UNP Q7WT50
E	192	SER	THR	conflict	UNP Q7WT50
E	302	HIS	-	expression tag	UNP Q7WT50
E	303	HIS	-	expression tag	UNP Q7WT50
E	304	HIS	-	expression tag	UNP Q7WT50
E	305	HIS	-	expression tag	UNP Q7WT50
E	306	HIS	-	expression tag	UNP Q7WT50
E	307	HIS	-	expression tag	UNP Q7WT50
F	90	MET	PHE	engineered mutation	UNP Q7WT50
F	192	SER	THR	conflict	UNP Q7WT50
F	302	HIS	-	expression tag	UNP Q7WT50
F	303	HIS	-	expression tag	UNP Q7WT50
F	304	HIS	-	expression tag	UNP Q7WT50
F	305	HIS	-	expression tag	UNP Q7WT50
F	306	HIS	-	expression tag	UNP Q7WT50
F	307	HIS	-	expression tag	UNP Q7WT50
G	90	MET	PHE	engineered mutation	UNP Q7WT50
G	192	SER	THR	conflict	UNP Q7WT50
G	302	HIS	-	expression tag	UNP Q7WT50
G	303	HIS	-	expression tag	UNP Q7WT50
G	304	HIS	-	expression tag	UNP Q7WT50
G	305	HIS	-	expression tag	UNP Q7WT50
G	306	HIS	-	expression tag	UNP Q7WT50

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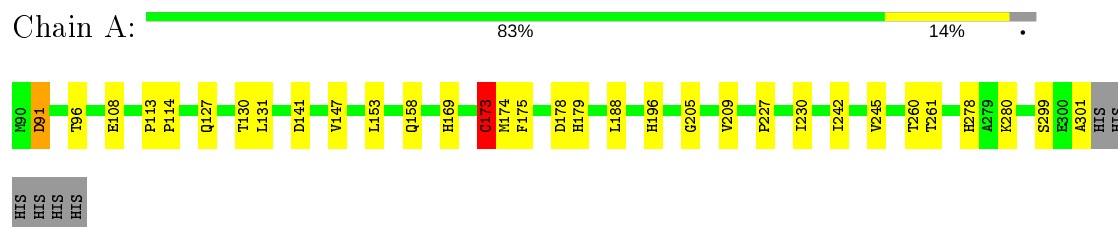
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Chain	Residue	Modelled	Actual	Comment	Reference
G	307	HIS	-	expression tag	UNP Q7WT50
H	90	MET	PHE	engineered mutation	UNP Q7WT50
H	192	SER	THR	conflict	UNP Q7WT50
H	302	HIS	-	expression tag	UNP Q7WT50
H	303	HIS	-	expression tag	UNP Q7WT50
H	304	HIS	-	expression tag	UNP Q7WT50
H	305	HIS	-	expression tag	UNP Q7WT50
H	306	HIS	-	expression tag	UNP Q7WT50
H	307	HIS	-	expression tag	UNP Q7WT50

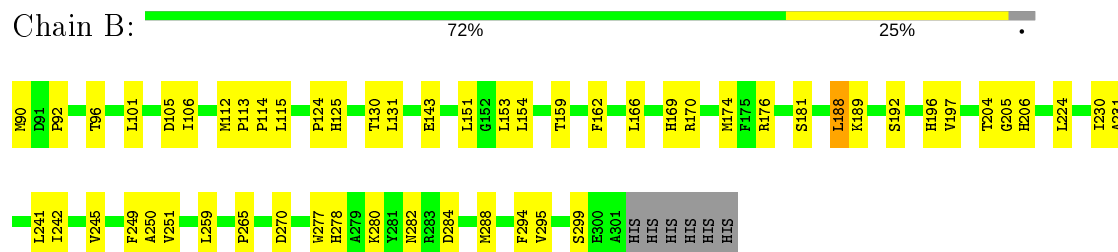
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

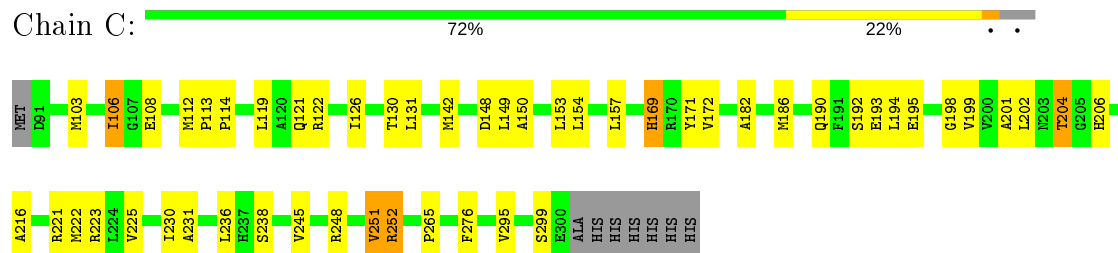
#### • Molecule 1: LYSR-TYPE REGULATORY PROTEIN



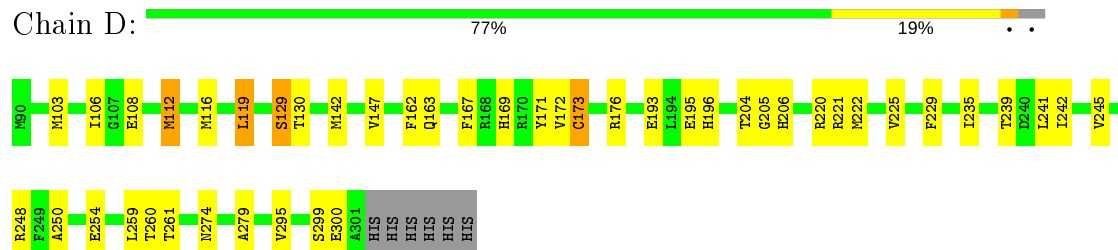
#### • Molecule 1: LYSR-TYPE REGULATORY PROTEIN



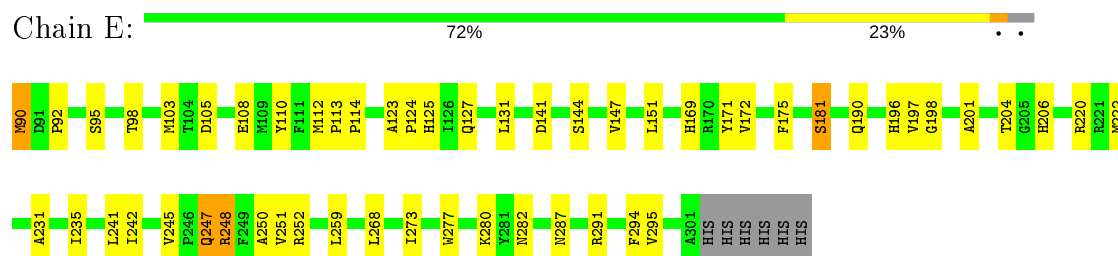
#### • Molecule 1: LYSR-TYPE REGULATORY PROTEIN



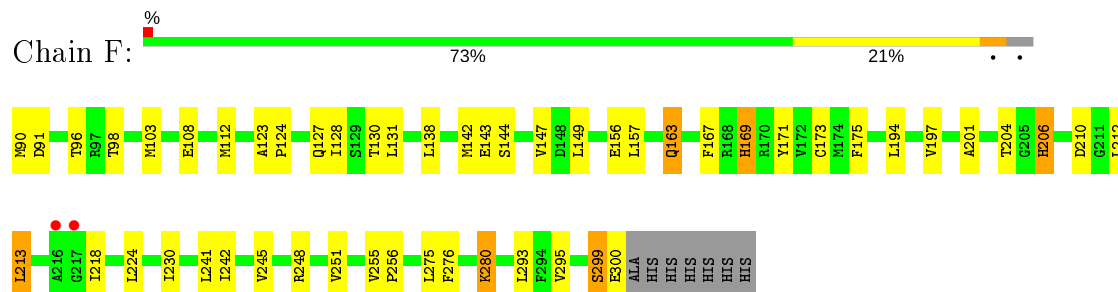
#### • Molecule 1: LYSR-TYPE REGULATORY PROTEIN



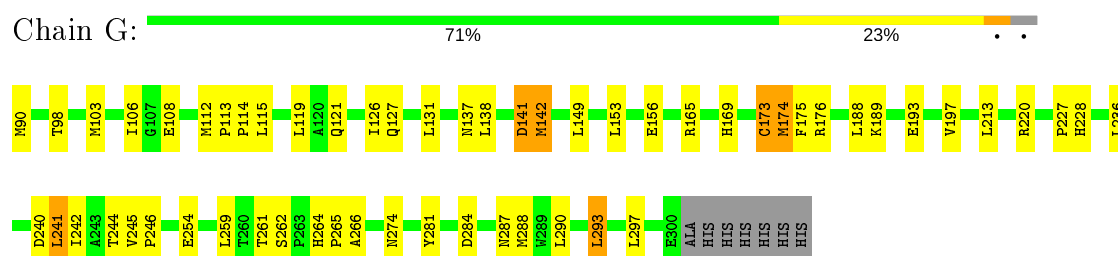
- Molecule 1: LYSR-TYPE REGULATORY PROTEIN



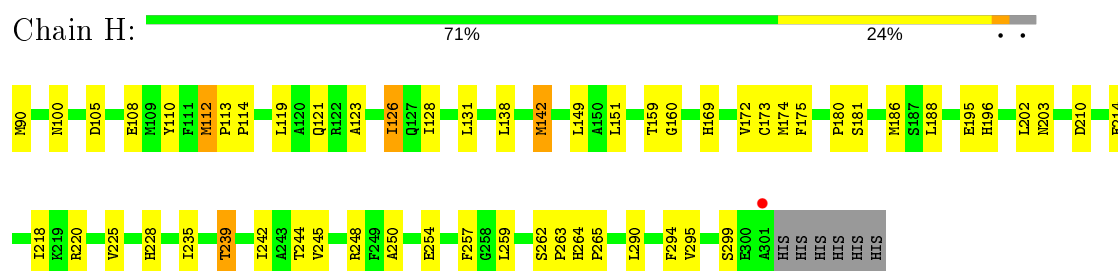
- Molecule 1: LYSR-TYPE REGULATORY PROTEIN



- Molecule 1: LYSR-TYPE REGULATORY PROTEIN



- Molecule 1: LYSR-TYPE REGULATORY PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.47Å 125.00Å 184.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.90 – 2.99 43.88 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.90-2.99) 98.5 (43.88-2.99)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.194 , 0.264 0.191 , 0.259	Depositor DCC
$R_{free}$ test set	1882 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12995	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 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	0.59	1/1667 (0.1%)	0.71	0/2268
1	B	0.59	0/1690	0.71	0/2295
1	C	0.59	0/1668	0.69	0/2268
1	D	0.56	1/1667 (0.1%)	0.71	0/2267
1	E	0.57	0/1677	0.71	0/2280
1	F	0.56	0/1658	0.74	0/2256
1	G	0.59	1/1674 (0.1%)	0.72	0/2273
1	H	0.57	0/1654	0.68	0/2250
All	All	0.58	3/13355 (0.0%)	0.71	0/18157

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	F	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	173	CYS	CB-SG	-7.44	1.69	1.82
1	D	173	CYS	CB-SG	-5.15	1.73	1.81
1	A	173	CYS	CB-SG	-5.04	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	90	MET	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	1622	0	1580	18	0
1	B	1645	0	1615	34	0
1	C	1623	0	1584	30	0
1	D	1622	0	1580	32	0
1	E	1632	0	1598	37	0
1	F	1613	0	1566	27	0
1	G	1629	0	1604	33	0
1	H	1609	0	1558	31	0
All	All	12995	0	12685	232	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (232) 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:F:169:HIS:HD2	1:F:248:ARG:HG3	1.32	0.95
1:C:113:PRO:HB2	1:C:114:PRO:HD3	1.50	0.94
1:C:198:GLY:HA3	1:C:222:MET:HE1	1.51	0.92
1:H:235:ILE:O	1:H:239:THR:HG23	1.72	0.88
1:E:175:PHE:HB3	1:E:242:ILE:HG22	1.54	0.87
1:F:169:HIS:CD2	1:F:248:ARG:HG3	2.12	0.83
1:E:90:MET:O	1:E:92:PRO:HD3	1.79	0.83
1:D:300:GLU:HG3	1:D:300:GLU:O	1.80	0.81
1:H:188:LEU:HD11	1:H:218:ILE:HD11	1.64	0.80
1:D:204:THR:HG22	1:D:205:GLY:H	1.50	0.77
1:H:119:LEU:HD22	1:H:126:ILE:HD11	1.67	0.76
1:B:204:THR:HG22	1:B:206:HIS:H	1.50	0.74
1:H:175:PHE:HB3	1:H:242:ILE:HG22	1.68	0.74
1:A:127:GLN:NE2	1:E:222:MET:O	2.19	0.74
1:F:171:TYR:OH	1:F:206:HIS:HA	1.90	0.72
1:E:201:ALA:O	1:E:204:THR:HG22	1.90	0.71
1:D:112:MET:CE	1:D:112:MET:HA	2.21	0.71
1:F:197:VAL:HG22	1:F:241:LEU:HD13	1.72	0.70
1:G:113:PRO:HB2	1:G:114:PRO:HD3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:THR:OG1	1:F:127:GLN:NE2	2.24	0.69
1:D:204:THR:HG22	1:D:205:GLY:N	2.08	0.67
1:D:176:ARG:HA	1:D:259:LEU:HD23	1.77	0.67
1:A:174:MET:CE	1:A:245:VAL:HG11	2.25	0.67
1:B:277:TRP:HE1	1:B:282:ASN:HD22	1.43	0.66
1:B:124:PRO:HG2	1:B:125:HIS:CE1	2.31	0.66
1:D:112:MET:HA	1:D:112:MET:HE2	1.78	0.66
1:E:248:ARG:O	1:E:251:VAL:HG12	1.96	0.66
1:D:163:GLN:HG2	1:D:274:ASN:HD22	1.60	0.66
1:D:193:GLU:O	1:D:221:ARG:NH1	2.30	0.65
1:F:175:PHE:HB3	1:F:242:ILE:HG22	1.77	0.65
1:C:195:GLU:OE1	1:C:223:ARG:HG3	1.97	0.64
1:H:188:LEU:HD11	1:H:218:ILE:CD1	2.27	0.64
1:G:149:LEU:HD12	1:G:290:LEU:HD23	1.80	0.64
1:C:119:LEU:HD22	1:C:126:ILE:HD11	1.79	0.64
1:H:257:PHE:O	1:H:259:LEU:HD13	1.98	0.64
1:G:119:LEU:HD22	1:G:126:ILE:HD11	1.79	0.64
1:C:153:LEU:O	1:C:154:LEU:HD23	1.98	0.63
1:D:300:GLU:O	1:D:300:GLU:CG	2.46	0.63
1:D:239:THR:HG23	1:D:241:LEU:H	1.65	0.62
1:C:201:ALA:O	1:C:204:THR:HG22	1.99	0.62
1:F:248:ARG:HA	1:F:251:VAL:HG22	1.80	0.61
1:E:113:PRO:HB2	1:E:114:PRO:HD3	1.83	0.61
1:C:113:PRO:HB2	1:C:114:PRO:CD	2.28	0.60
1:E:113:PRO:HB2	1:E:114:PRO:CD	2.31	0.60
1:E:197:VAL:HG22	1:E:241:LEU:HD13	1.83	0.60
1:E:201:ALA:HB1	1:E:204:THR:HG21	1.84	0.60
1:B:113:PRO:HB2	1:B:114:PRO:CD	2.32	0.60
1:G:244:THR:HG23	1:G:264:HIS:CE1	2.37	0.59
1:A:174:MET:HE2	1:A:245:VAL:HG11	1.83	0.59
1:H:196:HIS:CD2	1:H:220:ARG:HB2	2.37	0.59
1:E:181:SER:O	1:E:190:GLN:NE2	2.36	0.59
1:E:151:LEU:HD11	1:E:294:PHE:CE2	2.38	0.58
1:D:103:MET:HE2	1:D:130:THR:HG21	1.84	0.58
1:F:143:GLU:O	1:F:280:LYS:NZ	2.34	0.58
1:D:103:MET:CE	1:D:130:THR:HG21	2.33	0.58
1:G:284:ASP:HB3	1:G:287:ASN:HB2	1.86	0.58
1:H:244:THR:HG23	1:H:264:HIS:CE1	2.39	0.58
1:B:131:LEU:HD12	1:B:131:LEU:C	2.24	0.57
1:D:103:MET:HE2	1:D:130:THR:CG2	2.35	0.57
1:C:119:LEU:CD2	1:C:126:ILE:HD11	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:HIS:HD2	1:F:248:ARG:CG	2.12	0.56
1:E:90:MET:O	1:E:92:PRO:CD	2.50	0.56
1:B:197:VAL:CG2	1:B:241:LEU:HD13	2.35	0.56
1:C:201:ALA:O	1:C:204:THR:CG2	2.54	0.56
1:G:189:LYS:HE2	1:G:193:GLU:OE2	2.06	0.56
1:C:295:VAL:O	1:C:299:SER:HB3	2.06	0.56
1:D:235:ILE:O	1:D:239:THR:HG22	2.06	0.56
1:F:103:MET:HE1	1:F:130:THR:HG21	1.87	0.55
1:G:165:ARG:HA	1:G:274:ASN:OD1	2.05	0.55
1:G:141:ASP:OD1	1:G:141:ASP:N	2.39	0.55
1:D:162:PHE:HE2	1:D:279:ALA:HA	1.73	0.54
1:A:113:PRO:HB2	1:A:114:PRO:HD3	1.88	0.54
1:H:112:MET:HE1	1:H:128:ILE:HG21	1.89	0.54
1:C:171:TYR:OH	1:C:206:HIS:HA	2.08	0.54
1:D:295:VAL:O	1:D:299:SER:HB2	2.07	0.54
1:H:186:MET:O	1:H:265:PRO:HB3	2.07	0.54
1:E:204:THR:HG23	1:E:206:HIS:H	1.73	0.54
1:E:287:ASN:O	1:E:291:ARG:HD3	2.08	0.54
1:D:196:HIS:CE1	1:D:242:ILE:HD11	2.42	0.53
1:B:204:THR:HG22	1:B:205:GLY:N	2.24	0.53
1:B:204:THR:HG22	1:B:206:HIS:N	2.21	0.53
1:H:250:ALA:O	1:H:254:GLU:HG3	2.09	0.53
1:C:182:ALA:HA	1:C:190:GLN:HE22	1.74	0.53
1:E:98:THR:HG23	1:E:127:GLN:HB2	1.90	0.52
1:F:197:VAL:HG13	1:F:224:LEU:HD23	1.91	0.52
1:B:204:THR:CG2	1:B:205:GLY:N	2.73	0.52
1:E:198:GLY:HA3	1:E:222:MET:HE1	1.92	0.52
1:C:130:THR:O	1:G:227:PRO:HD3	2.10	0.52
1:A:230:ILE:HG21	1:E:105:ASP:HB2	1.91	0.51
1:E:171:TYR:CB	1:E:268:LEU:HD12	2.40	0.51
1:B:115:LEU:HD12	1:B:115:LEU:O	2.10	0.51
1:D:162:PHE:CE2	1:D:279:ALA:HA	2.45	0.51
1:G:264:HIS:HD2	1:G:266:ALA:H	1.59	0.51
1:A:141:ASP:HB3	1:A:147:VAL:HG23	1.92	0.51
1:C:169:HIS:CE1	1:C:248:ARG:HB2	2.47	0.50
1:C:103:MET:HE3	1:C:108:GLU:HA	1.92	0.50
1:B:230:ILE:HG23	1:B:231:ALA:N	2.27	0.50
1:C:121:GLN:HG3	1:C:122:ARG:HG3	1.94	0.50
1:E:171:TYR:OH	1:E:206:HIS:HA	2.11	0.50
1:F:123:ALA:N	1:F:124:PRO:CD	2.74	0.50
1:A:196:HIS:CE1	1:A:242:ILE:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:HIS:CE1	1:B:280:LYS:HG3	2.47	0.49
1:F:213:LEU:HD12	1:F:218:ILE:HD12	1.93	0.49
1:A:178:ASP:O	1:A:179:HIS:C	2.50	0.49
1:B:90:MET:O	1:B:92:PRO:HD3	2.12	0.49
1:E:277:TRP:HE1	1:E:282:ASN:HD22	1.60	0.49
1:D:112:MET:O	1:D:116:MET:HG2	2.12	0.49
1:H:112:MET:CE	1:H:128:ILE:HG21	2.41	0.49
1:B:112:MET:HA	1:B:112:MET:CE	2.41	0.49
1:B:90:MET:O	1:B:92:PRO:CD	2.60	0.49
1:D:295:VAL:O	1:D:299:SER:CB	2.60	0.49
1:G:173:CYS:O	1:G:261:THR:HA	2.11	0.49
1:A:91:ASP:OD1	1:A:91:ASP:C	2.51	0.49
1:C:186:MET:O	1:C:265:PRO:HB3	2.11	0.49
1:G:174:MET:HG3	1:G:261:THR:HG22	1.95	0.48
1:G:98:THR:HA	1:G:127:GLN:O	2.12	0.48
1:E:247:GLN:O	1:E:250:ALA:HB3	2.13	0.48
1:F:138:LEU:HG	1:F:142:MET:HE3	1.96	0.48
1:G:138:LEU:O	1:G:142:MET:HB2	2.14	0.48
1:E:169:HIS:CD2	1:E:273:ILE:HD11	2.48	0.48
1:F:142:MET:HE1	1:F:157:LEU:HD13	1.96	0.48
1:H:110:TYR:CE1	1:H:248:ARG:HD3	2.49	0.48
1:C:150:ALA:HB3	1:C:276:PHE:HB2	1.97	0.47
1:B:105:ASP:HB2	1:F:230:ILE:HD13	1.95	0.47
1:C:222:MET:HE2	1:C:225:VAL:HG22	1.96	0.47
1:E:141:ASP:HB3	1:E:147:VAL:HG23	1.95	0.47
1:A:173:CYS:O	1:A:261:THR:HA	2.14	0.47
1:B:197:VAL:HG23	1:B:241:LEU:HB3	1.95	0.47
1:E:103:MET:HE3	1:E:108:GLU:HA	1.96	0.47
1:F:201:ALA:O	1:F:204:THR:OG1	2.32	0.47
1:C:195:GLU:OE1	1:C:223:ARG:CG	2.63	0.47
1:E:110:TYR:HA	1:E:252:ARG:HH11	1.80	0.47
1:B:162:PHE:HZ	1:G:121:GLN:HG2	1.79	0.47
1:B:188:LEU:HD13	1:B:265:PRO:HB2	1.97	0.47
1:F:108:GLU:O	1:F:112:MET:HB2	2.15	0.47
1:G:213:LEU:HD13	1:G:220:ARG:HD2	1.97	0.47
1:H:121:GLN:O	1:H:121:GLN:HG2	2.15	0.46
1:B:162:PHE:CZ	1:G:121:GLN:HG2	2.51	0.46
1:H:105:ASP:OD2	1:H:228:HIS:HB3	2.15	0.46
1:F:255:VAL:HB	1:F:256:PRO:HD3	1.97	0.46
1:D:108:GLU:O	1:D:112:MET:HB2	2.15	0.46
1:B:106:ILE:HD12	1:B:249:PHE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ARG:HG2	1:B:270:ASP:OD1	2.16	0.46
1:E:95:SER:O	1:E:125:HIS:HB2	2.16	0.46
1:D:142:MET:HG2	1:D:147:VAL:HG12	1.97	0.45
1:G:176:ARG:NH2	1:G:240:ASP:OD1	2.46	0.45
1:H:262:SER:O	1:H:263:PRO:C	2.52	0.45
1:E:171:TYR:HB2	1:E:268:LEU:HD12	1.98	0.45
1:A:299:SER:O	1:A:301:ALA:N	2.50	0.45
1:G:106:ILE:HD13	1:G:246:PRO:HG2	1.98	0.45
1:H:149:LEU:CD1	1:H:290:LEU:HD23	2.46	0.45
1:D:222:MET:HG2	1:D:225:VAL:HG22	1.98	0.45
1:F:131:LEU:HD21	1:F:147:VAL:HG22	1.99	0.45
1:G:284:ASP:HB3	1:G:287:ASN:CB	2.47	0.45
1:B:101:LEU:O	1:B:130:THR:HA	2.17	0.45
1:D:112:MET:CA	1:D:112:MET:CE	2.92	0.45
1:B:189:LYS:O	1:B:192:SER:HB2	2.17	0.45
1:B:176:ARG:HA	1:B:259:LEU:HD23	1.99	0.45
1:C:182:ALA:HA	1:C:190:GLN:NE2	2.32	0.44
1:G:137:ASN:O	1:G:141:ASP:OD1	2.35	0.44
1:H:151:LEU:HD11	1:H:294:PHE:CE2	2.53	0.44
1:E:103:MET:HE3	1:E:112:MET:HG2	1.99	0.44
1:E:231:ALA:O	1:E:235:ILE:HG13	2.18	0.44
1:H:210:ASP:O	1:H:214:GLU:HB2	2.17	0.44
1:B:113:PRO:HB2	1:B:114:PRO:HD3	2.00	0.44
1:B:295:VAL:O	1:B:299:SER:HB3	2.18	0.44
1:G:175:PHE:HB3	1:G:242:ILE:HG22	2.00	0.44
1:G:197:VAL:HG22	1:G:241:LEU:HD23	1.99	0.44
1:A:108:GLU:OE2	1:A:130:THR:OG1	2.33	0.44
1:D:171:TYR:OH	1:D:206:HIS:HA	2.18	0.44
1:A:278:HIS:CE1	1:A:280:LYS:HG3	2.53	0.43
1:F:142:MET:HE1	1:F:157:LEU:CD1	2.48	0.43
1:E:291:ARG:O	1:E:295:VAL:HG23	2.18	0.43
1:B:196:HIS:CE1	1:B:242:ILE:HD11	2.53	0.43
1:E:123:ALA:N	1:E:124:PRO:HD3	2.33	0.43
1:F:149:LEU:HD13	1:F:275:LEU:HD11	1.99	0.43
1:B:143:GLU:O	1:B:280:LYS:NZ	2.49	0.43
1:E:196:HIS:CD2	1:E:220:ARG:HG3	2.53	0.43
1:F:295:VAL:O	1:F:299:SER:HB2	2.17	0.43
1:F:163:GLN:HB2	1:F:276:PHE:CD1	2.53	0.43
1:H:138:LEU:O	1:H:142:MET:HB2	2.18	0.43
1:H:257:PHE:O	1:H:259:LEU:CD1	2.64	0.43
1:A:175:PHE:HB3	1:A:242:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:ILE:HD11	1:D:229:PHE:CG	2.53	0.43
1:E:201:ALA:HB1	1:E:204:THR:CG2	2.48	0.43
1:G:254:GLU:HG2	1:G:259:LEU:O	2.19	0.43
1:B:151:LEU:HD21	1:B:294:PHE:CE1	2.53	0.43
1:C:103:MET:HE3	1:C:112:MET:HG2	2.01	0.43
1:G:284:ASP:O	1:G:288:MET:HG3	2.19	0.43
1:A:188:LEU:HD23	1:C:216:ALA:HA	2.01	0.42
1:G:293:LEU:HD22	1:G:297:LEU:CD1	2.49	0.42
1:C:193:GLU:O	1:C:221:ARG:NH1	2.52	0.42
1:D:196:HIS:CD2	1:D:220:ARG:HB3	2.54	0.42
1:C:169:HIS:ND1	1:C:248:ARG:HB2	2.34	0.42
1:G:103:MET:HE3	1:G:108:GLU:HA	2.02	0.42
1:H:113:PRO:HB2	1:H:114:PRO:CD	2.49	0.42
1:H:202:LEU:HD12	1:H:203:ASN:H	1.84	0.42
1:H:295:VAL:O	1:H:299:SER:HB3	2.19	0.42
1:D:167:PHE:CE2	1:D:248:ARG:HD2	2.55	0.42
1:F:210:ASP:C	1:F:212:LEU:H	2.23	0.42
1:G:227:PRO:HB2	1:G:228:HIS:CD2	2.55	0.42
1:A:153:LEU:HD23	1:A:205:GLY:CA	2.50	0.42
1:A:227:PRO:HD2	1:E:108:GLU:OE2	2.20	0.42
1:B:174:MET:HE1	1:B:250:ALA:HA	2.01	0.42
1:C:230:ILE:HG23	1:C:231:ALA:N	2.34	0.41
1:G:103:MET:HE3	1:G:112:MET:HG2	2.02	0.41
1:C:142:MET:CE	1:C:157:LEU:HD11	2.50	0.41
1:C:148:ASP:O	1:C:149:LEU:HD23	2.20	0.41
1:H:174:MET:SD	1:H:259:LEU:HD23	2.60	0.41
1:B:224:LEU:HA	1:F:128:ILE:O	2.20	0.41
1:E:103:MET:CE	1:E:108:GLU:HA	2.49	0.41
1:F:167:PHE:HB3	1:F:300:GLU:HG3	2.02	0.41
1:H:123:ALA:HB1	1:H:126:ILE:HD13	2.01	0.41
1:H:159:THR:HG22	1:H:160:GLY:N	2.35	0.41
1:D:204:THR:CG2	1:D:205:GLY:N	2.78	0.41
1:H:108:GLU:O	1:H:112:MET:HB2	2.20	0.41
1:C:106:ILE:HG21	1:C:106:ILE:HD13	1.74	0.41
1:A:278:HIS:ND1	1:A:280:LYS:HG3	2.35	0.41
1:D:129:SER:HB2	1:H:225:VAL:HB	2.02	0.41
1:D:250:ALA:O	1:D:254:GLU:HG3	2.21	0.41
1:B:153:LEU:O	1:B:154:LEU:C	2.60	0.41
1:G:188:LEU:HD13	1:G:265:PRO:HB2	2.03	0.41
1:G:293:LEU:HD22	1:G:297:LEU:HD12	2.03	0.41
1:H:113:PRO:HB2	1:H:114:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:172:VAL:HG12	1:H:245:VAL:O	2.21	0.41
1:C:251:VAL:HG12	1:C:252:ARG:N	2.35	0.40
1:D:119:LEU:HD12	1:D:119:LEU:HA	1.86	0.40
1:E:280:LYS:HB3	1:E:280:LYS:HE3	1.90	0.40
1:G:281:TYR:N	1:G:281:TYR:CD1	2.89	0.40
1:E:198:GLY:HA3	1:E:222:MET:CE	2.50	0.40
1:G:188:LEU:HA	1:G:188:LEU:HD12	1.85	0.40
1:B:284:ASP:O	1:B:288:MET:HG3	2.21	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	210/218 (96%)	194 (92%)	15 (7%)	1 (0%)	29	68
1	B	210/218 (96%)	200 (95%)	10 (5%)	0	100	100
1	C	208/218 (95%)	198 (95%)	10 (5%)	0	100	100
1	D	210/218 (96%)	197 (94%)	13 (6%)	0	100	100
1	E	210/218 (96%)	199 (95%)	11 (5%)	0	100	100
1	F	209/218 (96%)	194 (93%)	15 (7%)	0	100	100
1	G	209/218 (96%)	200 (96%)	9 (4%)	0	100	100
1	H	210/218 (96%)	194 (92%)	15 (7%)	1 (0%)	29	68
All	All	1676/1744 (96%)	1576 (94%)	98 (6%)	2 (0%)	51	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	180	PRO
1	A	209	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	164/187 (88%)	157 (96%)	7 (4%)	29	66
1	B	169/187 (90%)	161 (95%)	8 (5%)	26	63
1	C	166/187 (89%)	152 (92%)	14 (8%)	11	38
1	D	163/187 (87%)	153 (94%)	10 (6%)	18	53
1	E	167/187 (89%)	158 (95%)	9 (5%)	22	57
1	F	164/187 (88%)	150 (92%)	14 (8%)	10	38
1	G	165/187 (88%)	151 (92%)	14 (8%)	10	38
1	H	159/187 (85%)	148 (93%)	11 (7%)	15	48
All	All	1317/1496 (88%)	1230 (93%)	87 (7%)	16	49

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ASP
1	A	96	THR
1	A	131	LEU
1	A	158	GLN
1	A	169	HIS
1	A	173	CYS
1	A	260	THR
1	B	96	THR
1	B	159	THR
1	B	166	LEU
1	B	169	HIS
1	B	181	SER
1	B	188	LEU
1	B	245	VAL
1	B	251	VAL
1	C	106	ILE
1	C	131	LEU
1	C	169	HIS
1	C	172	VAL

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Mol	Chain	Res	Type
1	C	192	SER
1	C	194	LEU
1	C	199	VAL
1	C	202	LEU
1	C	204	THR
1	C	236	LEU
1	C	238	SER
1	C	245	VAL
1	C	251	VAL
1	C	252	ARG
1	D	112	MET
1	D	119	LEU
1	D	129	SER
1	D	169	HIS
1	D	172	VAL
1	D	173	CYS
1	D	195	GLU
1	D	245	VAL
1	D	260	THR
1	D	261	THR
1	E	90	MET
1	E	131	LEU
1	E	144	SER
1	E	172	VAL
1	E	181	SER
1	E	245	VAL
1	E	247	GLN
1	E	248	ARG
1	E	259	LEU
1	F	91	ASP
1	F	96	THR
1	F	144	SER
1	F	156	GLU
1	F	163	GLN
1	F	169	HIS
1	F	173	CYS
1	F	194	LEU
1	F	206	HIS
1	F	213	LEU
1	F	245	VAL
1	F	280	LYS
1	F	293	LEU

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Mol	Chain	Res	Type
1	F	299	SER
1	G	90	MET
1	G	115	LEU
1	G	131	LEU
1	G	141	ASP
1	G	142	MET
1	G	153	LEU
1	G	156	GLU
1	G	169	HIS
1	G	174	MET
1	G	236	LEU
1	G	241	LEU
1	G	245	VAL
1	G	262	SER
1	G	293	LEU
1	H	90	MET
1	H	100	ASN
1	H	112	MET
1	H	126	ILE
1	H	131	LEU
1	H	142	MET
1	H	169	HIS
1	H	173	CYS
1	H	181	SER
1	H	195	GLU
1	H	239	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	GLN
1	A	274	ASN
1	B	282	ASN
1	C	163	GLN
1	E	121	GLN
1	E	169	HIS
1	E	282	ASN
1	F	127	GLN
1	F	169	HIS
1	G	203	ASN
1	G	228	HIS
1	G	264	HIS

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Mol	Chain	Res	Type
1	G	278	HIS
1	H	196	HIS
1	H	247	GLN
1	H	264	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	212/218 (97%)	-0.49	0	100	100	7, 17, 27, 34	3 (1%)
1	B	212/218 (97%)	-0.44	0	100	100	4, 18, 28, 34	3 (1%)
1	C	210/218 (96%)	-0.48	0	100	100	8, 19, 34, 45	2 (0%)
1	D	212/218 (97%)	-0.46	0	100	100	9, 19, 32, 36	2 (0%)
1	E	212/218 (97%)	-0.39	0	100	100	6, 19, 30, 34	3 (1%)
1	F	211/218 (96%)	-0.28	2 (0%)	84	63	8, 23, 37, 44	2 (0%)
1	G	211/218 (96%)	-0.35	0	100	100	8, 24, 34, 45	0
1	H	212/218 (97%)	-0.35	1 (0%)	91	75	9, 22, 39, 43	2 (0%)
All	All	1692/1744 (97%)	-0.40	3 (0%)	95	87	4, 20, 34, 45	17 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	216	ALA	2.2
1	F	217	GLY	2.1
1	H	301	ALA	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.