



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2024 – 10:33 PM EDT

PDB ID : 1SF8  
Title : Crystal structure of the carboxy-terminal domain of htpG, the E. coli Hsp90  
Authors : Harris, S.F.; Shiau, A.K.; Agard, D.A.  
Deposited on : 2004-02-19  
Resolution : 2.60 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  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

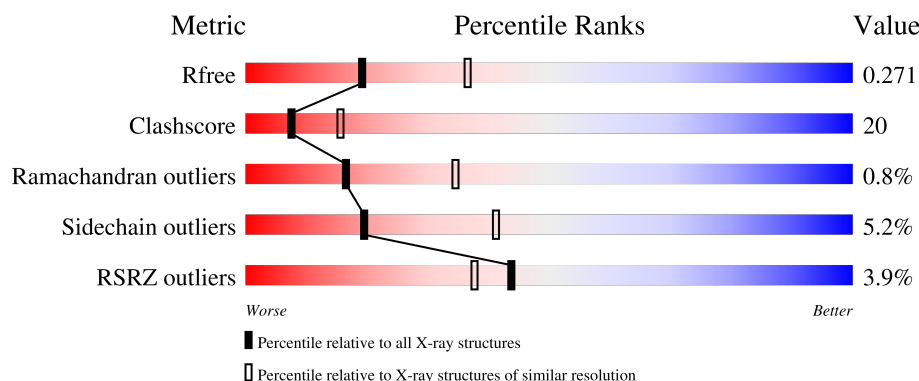
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	126	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>25%</div> <div>• • 9%</div> </div> </div>
1	B	126	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>30%</div> <div>• 9%</div> </div> </div>
1	C	126	<div> <div>12%</div> <div> <div></div> <div>56%</div> <div>33%</div> <div>6% • 5%</div> </div> </div>
1	D	126	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>34%</div> <div>• 9%</div> </div> </div>
1	E	126	<div> <div>0%</div> <div> <div></div> <div>63%</div> <div>26%</div> <div>• 9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	126	
1	G	126	
1	H	126	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	H	705	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7915 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 Chaperone protein htpG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	Se	0	0	0
			916	579	158	176	3			
1	B	115	Total	C	N	O	Se	0	0	0
			916	579	158	176	3			
1	C	120	Total	C	N	O	Se	0	0	0
			960	605	171	181	3			
1	D	115	Total	C	N	O	Se	0	0	0
			916	579	158	176	3			
1	E	115	Total	C	N	O	Se	0	0	0
			916	579	158	176	3			
1	F	115	Total	C	N	O	Se	0	0	0
			916	579	158	176	3			
1	G	121	Total	C	N	O	Se	0	0	0
			965	608	172	182	3			
1	H	116	Total	C	N	O	Se	0	0	0
			920	581	159	177	3			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	499	MET	-	cloning artifact	UNP P0A6Z3
A	500	ARG	-	cloning artifact	UNP P0A6Z3
A	501	GLY	-	cloning artifact	UNP P0A6Z3
A	502	SER	-	cloning artifact	UNP P0A6Z3
A	503	HIS	-	cloning artifact	UNP P0A6Z3
A	504	HIS	-	cloning artifact	UNP P0A6Z3
A	505	HIS	-	cloning artifact	UNP P0A6Z3
A	506	HIS	-	cloning artifact	UNP P0A6Z3
A	507	HIS	-	cloning artifact	UNP P0A6Z3
A	508	HIS	-	cloning artifact	UNP P0A6Z3
A	509	GLY	-	cloning artifact	UNP P0A6Z3
A	510	SER	-	cloning artifact	UNP P0A6Z3
A	546	MSE	MET	modified residue	UNP P0A6Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	550	MSE	MET	modified residue	UNP P0A6Z3
A	618	MSE	MET	modified residue	UNP P0A6Z3
B	499	MET	-	cloning artifact	UNP P0A6Z3
B	500	ARG	-	cloning artifact	UNP P0A6Z3
B	501	GLY	-	cloning artifact	UNP P0A6Z3
B	502	SER	-	cloning artifact	UNP P0A6Z3
B	503	HIS	-	cloning artifact	UNP P0A6Z3
B	504	HIS	-	cloning artifact	UNP P0A6Z3
B	505	HIS	-	cloning artifact	UNP P0A6Z3
B	506	HIS	-	cloning artifact	UNP P0A6Z3
B	507	HIS	-	cloning artifact	UNP P0A6Z3
B	508	HIS	-	cloning artifact	UNP P0A6Z3
B	509	GLY	-	cloning artifact	UNP P0A6Z3
B	510	SER	-	cloning artifact	UNP P0A6Z3
B	546	MSE	MET	modified residue	UNP P0A6Z3
B	550	MSE	MET	modified residue	UNP P0A6Z3
B	618	MSE	MET	modified residue	UNP P0A6Z3
C	499	MET	-	cloning artifact	UNP P0A6Z3
C	500	ARG	-	cloning artifact	UNP P0A6Z3
C	501	GLY	-	cloning artifact	UNP P0A6Z3
C	502	SER	-	cloning artifact	UNP P0A6Z3
C	503	HIS	-	cloning artifact	UNP P0A6Z3
C	504	HIS	-	cloning artifact	UNP P0A6Z3
C	505	HIS	-	cloning artifact	UNP P0A6Z3
C	506	HIS	-	cloning artifact	UNP P0A6Z3
C	507	HIS	-	cloning artifact	UNP P0A6Z3
C	508	HIS	-	cloning artifact	UNP P0A6Z3
C	509	GLY	-	cloning artifact	UNP P0A6Z3
C	510	SER	-	cloning artifact	UNP P0A6Z3
C	546	MSE	MET	modified residue	UNP P0A6Z3
C	550	MSE	MET	modified residue	UNP P0A6Z3
C	618	MSE	MET	modified residue	UNP P0A6Z3
D	499	MET	-	cloning artifact	UNP P0A6Z3
D	500	ARG	-	cloning artifact	UNP P0A6Z3
D	501	GLY	-	cloning artifact	UNP P0A6Z3
D	502	SER	-	cloning artifact	UNP P0A6Z3
D	503	HIS	-	cloning artifact	UNP P0A6Z3
D	504	HIS	-	cloning artifact	UNP P0A6Z3
D	505	HIS	-	cloning artifact	UNP P0A6Z3
D	506	HIS	-	cloning artifact	UNP P0A6Z3
D	507	HIS	-	cloning artifact	UNP P0A6Z3
D	508	HIS	-	cloning artifact	UNP P0A6Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	509	GLY	-	cloning artifact	UNP P0A6Z3
D	510	SER	-	cloning artifact	UNP P0A6Z3
D	546	MSE	MET	modified residue	UNP P0A6Z3
D	550	MSE	MET	modified residue	UNP P0A6Z3
D	618	MSE	MET	modified residue	UNP P0A6Z3
E	499	MET	-	cloning artifact	UNP P0A6Z3
E	500	ARG	-	cloning artifact	UNP P0A6Z3
E	501	GLY	-	cloning artifact	UNP P0A6Z3
E	502	SER	-	cloning artifact	UNP P0A6Z3
E	503	HIS	-	cloning artifact	UNP P0A6Z3
E	504	HIS	-	cloning artifact	UNP P0A6Z3
E	505	HIS	-	cloning artifact	UNP P0A6Z3
E	506	HIS	-	cloning artifact	UNP P0A6Z3
E	507	HIS	-	cloning artifact	UNP P0A6Z3
E	508	HIS	-	cloning artifact	UNP P0A6Z3
E	509	GLY	-	cloning artifact	UNP P0A6Z3
E	510	SER	-	cloning artifact	UNP P0A6Z3
E	546	MSE	MET	modified residue	UNP P0A6Z3
E	550	MSE	MET	modified residue	UNP P0A6Z3
E	618	MSE	MET	modified residue	UNP P0A6Z3
F	499	MET	-	cloning artifact	UNP P0A6Z3
F	500	ARG	-	cloning artifact	UNP P0A6Z3
F	501	GLY	-	cloning artifact	UNP P0A6Z3
F	502	SER	-	cloning artifact	UNP P0A6Z3
F	503	HIS	-	cloning artifact	UNP P0A6Z3
F	504	HIS	-	cloning artifact	UNP P0A6Z3
F	505	HIS	-	cloning artifact	UNP P0A6Z3
F	506	HIS	-	cloning artifact	UNP P0A6Z3
F	507	HIS	-	cloning artifact	UNP P0A6Z3
F	508	HIS	-	cloning artifact	UNP P0A6Z3
F	509	GLY	-	cloning artifact	UNP P0A6Z3
F	510	SER	-	cloning artifact	UNP P0A6Z3
F	546	MSE	MET	modified residue	UNP P0A6Z3
F	550	MSE	MET	modified residue	UNP P0A6Z3
F	618	MSE	MET	modified residue	UNP P0A6Z3
G	499	MET	-	cloning artifact	UNP P0A6Z3
G	500	ARG	-	cloning artifact	UNP P0A6Z3
G	501	GLY	-	cloning artifact	UNP P0A6Z3
G	502	SER	-	cloning artifact	UNP P0A6Z3
G	503	HIS	-	cloning artifact	UNP P0A6Z3
G	504	HIS	-	cloning artifact	UNP P0A6Z3
G	505	HIS	-	cloning artifact	UNP P0A6Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	506	HIS	-	cloning artifact	UNP P0A6Z3
G	507	HIS	-	cloning artifact	UNP P0A6Z3
G	508	HIS	-	cloning artifact	UNP P0A6Z3
G	509	GLY	-	cloning artifact	UNP P0A6Z3
G	510	SER	-	cloning artifact	UNP P0A6Z3
G	546	MSE	MET	modified residue	UNP P0A6Z3
G	550	MSE	MET	modified residue	UNP P0A6Z3
G	618	MSE	MET	modified residue	UNP P0A6Z3
H	499	MET	-	cloning artifact	UNP P0A6Z3
H	500	ARG	-	cloning artifact	UNP P0A6Z3
H	501	GLY	-	cloning artifact	UNP P0A6Z3
H	502	SER	-	cloning artifact	UNP P0A6Z3
H	503	HIS	-	cloning artifact	UNP P0A6Z3
H	504	HIS	-	cloning artifact	UNP P0A6Z3
H	505	HIS	-	cloning artifact	UNP P0A6Z3
H	506	HIS	-	cloning artifact	UNP P0A6Z3
H	507	HIS	-	cloning artifact	UNP P0A6Z3
H	508	HIS	-	cloning artifact	UNP P0A6Z3
H	509	GLY	-	cloning artifact	UNP P0A6Z3
H	510	SER	-	cloning artifact	UNP P0A6Z3
H	546	MSE	MET	modified residue	UNP P0A6Z3
H	550	MSE	MET	modified residue	UNP P0A6Z3
H	618	MSE	MET	modified residue	UNP P0A6Z3

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Ni 1 1	0	0
2	D	1	Total Ni 1 1	0	0
2	G	1	Total Ni 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

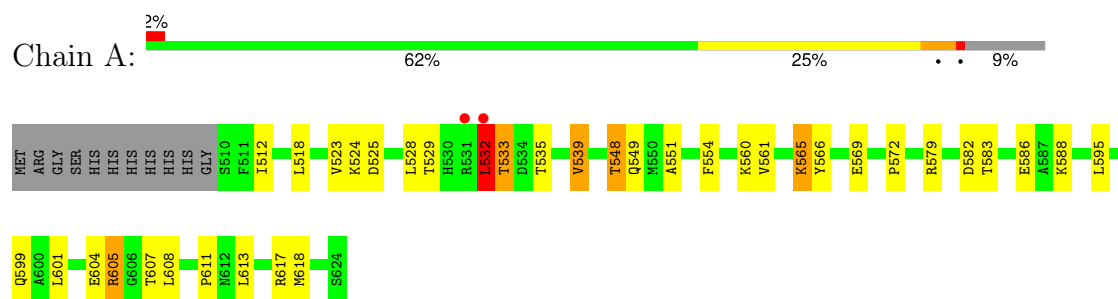
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	55	Total	O	0	0
			55	55		
4	C	42	Total	O	0	0
			42	42		
4	D	45	Total	O	0	0
			45	45		
4	E	45	Total	O	0	0
			45	45		
4	F	57	Total	O	0	0
			57	57		
4	G	70	Total	O	0	0
			70	70		
4	H	112	Total	O	0	0
			112	112		



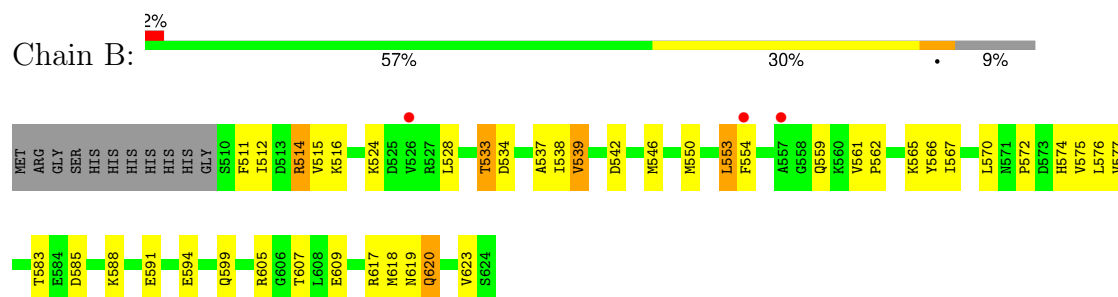
### 3 Residue-property plots [i](#)

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.

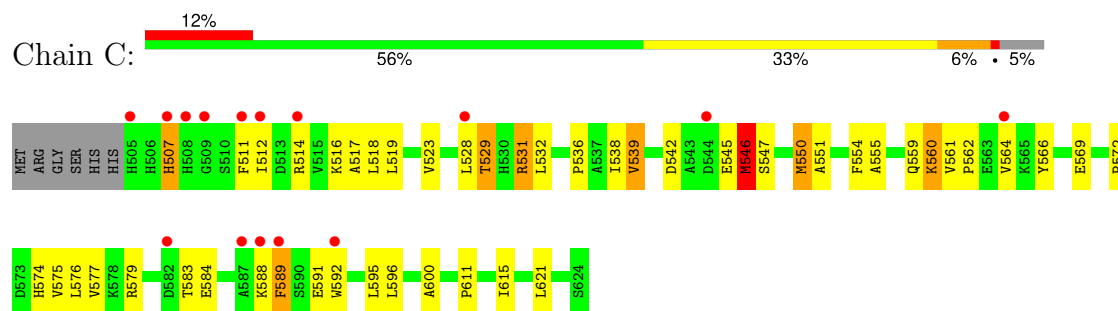
#### • Molecule 1: Chaperone protein htpG



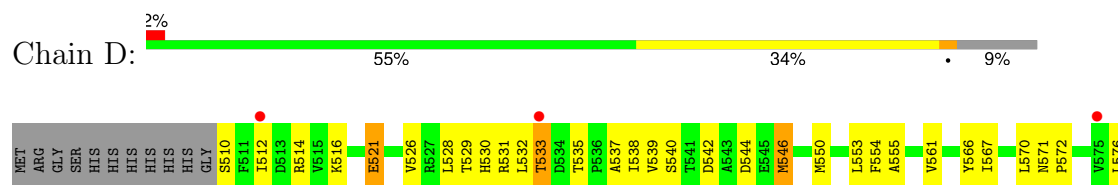
#### • Molecule 1: Chaperone protein htpG

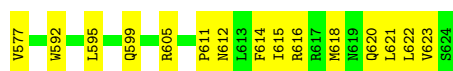


#### • Molecule 1: Chaperone protein htpG

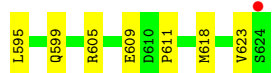
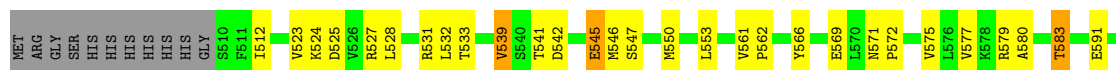


#### • Molecule 1: Chaperone protein htpG

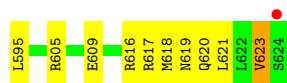




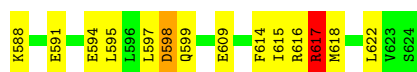
• Molecule 1: Chaperone protein htpG



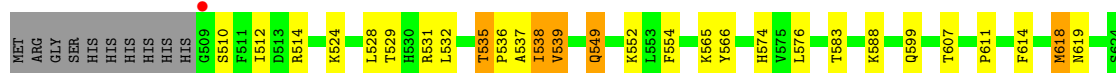
• Molecule 1: Chaperone protein htpG



• Molecule 1: Chaperone protein htpG



• Molecule 1: Chaperone protein htpG



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.52Å 103.52Å 249.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.60 29.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.3 (29.90-2.60) 90.2 (29.90-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.62Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.223 , 0.261 0.235 , 0.271	Depositor DCC
$R_{free}$ test set	1997 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7915	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, CL

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	0.44	0/926	0.67	0/1246
1	B	0.41	0/926	0.60	0/1246
1	C	0.36	0/974	0.55	0/1311
1	D	0.37	0/926	0.55	0/1246
1	E	0.43	0/926	0.59	0/1246
1	F	0.35	0/926	0.53	0/1246
1	G	0.48	0/979	0.68	2/1318 (0.2%)
1	H	0.47	0/930	0.63	0/1251
All	All	0.42	0/7513	0.60	2/10110 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	617	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	G	617	ARG	NE-CZ-NH1	-5.46	117.57	120.30

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	916	0	930	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	916	0	930	41	0
1	C	960	0	961	52	0
1	D	916	0	930	46	0
1	E	916	0	930	36	0
1	F	916	0	930	32	0
1	G	965	0	963	44	0
1	H	920	0	933	39	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	G	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	7	0
4	A	58	0	0	9	0
4	B	55	0	0	8	0
4	C	42	0	0	14	0
4	D	45	0	0	9	0
4	E	45	0	0	12	0
4	F	57	0	0	10	0
4	G	70	0	0	11	0
4	H	112	0	0	9	0
All	All	7915	0	7507	297	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 20.

All (297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:LEU:HD22	1:C:572:PRO:HG3	1.50	0.94
1:C:519:LEU:HD13	1:C:523:VAL:HG21	1.54	0.89
1:C:550:MSE:HG2	1:D:550:MSE:SE	2.25	0.87
1:E:562:PRO:HB2	4:E:1240:HOH:O	1.76	0.86
1:E:512:ILE:HD11	1:E:528:LEU:HG	1.57	0.83
1:A:528:LEU:HD22	1:A:572:PRO:HG3	1.60	0.83
1:C:595:LEU:HD11	1:E:618:MSE:HE1	1.60	0.81
1:D:529:THR:HG22	1:D:531:ARG:H	1.42	0.81
1:E:546:MSE:SE	4:E:1240:HOH:O	2.51	0.79
1:A:595:LEU:HD11	1:G:618:MSE:HE1	1.64	0.79
1:F:512:ILE:HD11	1:F:528:LEU:HG	1.65	0.78
1:B:605:ARG:HD3	4:B:995:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:523:VAL:HG12	1:G:525:ASP:H	1.49	0.78
1:F:539:VAL:HG22	1:F:566:TYR:HB3	1.67	0.77
1:H:510:SER:HA	4:H:1113:HOH:O	1.85	0.76
1:C:512:ILE:HD11	1:C:528:LEU:HD12	1.67	0.76
1:B:512:ILE:HD11	1:B:528:LEU:HG	1.68	0.76
1:A:548:THR:HG21	1:A:604:GLU:OE2	1.87	0.74
1:B:539:VAL:HG22	1:B:566:TYR:HB3	1.70	0.73
1:G:539:VAL:HG22	1:G:566:TYR:HB3	1.70	0.73
1:C:579:ARG:HD2	4:C:1262:HOH:O	1.89	0.73
1:B:575:VAL:HG23	4:B:1056:HOH:O	1.89	0.72
1:C:514:ARG:HD3	4:C:1222:HOH:O	1.88	0.72
1:C:579:ARG:HH22	1:E:623:VAL:HA	1.52	0.72
1:G:542:ASP:O	1:G:545:GLU:HB2	1.90	0.72
1:A:586:GLU:HG2	4:A:1218:HOH:O	1.90	0.71
1:G:561:VAL:HG22	4:G:1090:HOH:O	1.89	0.71
1:C:546:MSE:HE2	1:C:551:ALA:HA	1.70	0.71
1:A:549:GLN:HB3	4:A:1205:HOH:O	1.91	0.70
1:B:574:HIS:HD2	1:B:576:LEU:H	1.39	0.70
1:H:583:THR:HG21	1:H:588:LYS:HB3	1.75	0.69
1:H:536:PRO:HD2	3:H:705:CL:CL	2.30	0.69
1:B:599:GLN:NE2	1:H:619:ASN:HD21	1.90	0.68
1:F:518:LEU:HD21	1:F:590:SER:HA	1.74	0.68
1:G:510:SER:HA	4:G:848:HOH:O	1.91	0.68
1:B:599:GLN:OE1	1:H:618:MSE:HE3	1.92	0.68
1:A:539:VAL:HG22	1:A:566:TYR:HB3	1.74	0.68
1:A:595:LEU:HD21	1:G:618:MSE:CE	2.24	0.68
1:F:519:LEU:HD13	1:F:523:VAL:HG21	1.75	0.67
1:C:546:MSE:HE3	4:C:1215:HOH:O	1.93	0.67
1:H:538:ILE:HD13	4:H:874:HOH:O	1.95	0.67
1:C:579:ARG:NH2	1:E:623:VAL:HA	2.10	0.67
1:D:528:LEU:HD22	1:D:572:PRO:HG3	1.77	0.67
1:G:570:LEU:O	1:G:572:PRO:HD3	1.96	0.66
1:F:532:LEU:HD22	1:F:535:THR:HB	1.78	0.66
1:C:574:HIS:HB3	1:C:577:VAL:HG23	1.78	0.66
1:C:542:ASP:O	1:C:545:GLU:HB3	1.94	0.65
1:B:534:ASP:HB2	4:B:979:HOH:O	1.95	0.65
1:H:536:PRO:CD	3:H:705:CL:CL	2.82	0.65
1:B:619:ASN:O	1:B:623:VAL:HG23	1.97	0.65
1:F:524:LYS:HE3	1:F:542:ASP:OD2	1.97	0.64
1:C:591:GLU:HA	4:C:1275:HOH:O	1.97	0.64
1:H:538:ILE:HD13	1:H:539:VAL:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:ARG:HB2	4:A:1209:HOH:O	1.99	0.63
1:C:550:MSE:HB3	4:C:1215:HOH:O	1.96	0.63
1:A:617:ARG:HB2	4:A:1125:HOH:O	1.98	0.63
1:H:574:HIS:HD2	1:H:576:LEU:H	1.45	0.63
1:F:616:ARG:O	1:F:620:GLN:HG3	1.99	0.62
1:D:532:LEU:HB2	1:D:571:ASN:HD22	1.65	0.62
1:H:532:LEU:HD13	1:H:535:THR:HG22	1.82	0.61
1:E:542:ASP:HB2	1:E:545:GLU:HG3	1.82	0.61
1:E:611:PRO:HG3	4:E:927:HOH:O	2.01	0.61
1:F:562:PRO:HD2	4:F:1279:HOH:O	1.99	0.61
1:G:594:GLU:CB	1:G:617:ARG:NH1	2.63	0.61
4:F:1239:HOH:O	1:H:554:PHE:CE2	2.51	0.61
1:E:533:THR:HA	4:E:1101:HOH:O	2.01	0.61
1:F:528:LEU:HD22	1:F:572:PRO:HB3	1.83	0.61
1:F:605:ARG:HD3	4:F:972:HOH:O	2.00	0.60
1:D:615:ILE:HA	1:D:618:MSE:HE3	1.83	0.60
1:G:617:ARG:NH1	4:G:1096:HOH:O	2.33	0.60
1:D:595:LEU:O	1:D:599:GLN:HG2	2.01	0.60
1:H:535:THR:HG23	3:H:705:CL:CL	2.38	0.60
1:D:529:THR:HG22	1:D:530:HIS:N	2.16	0.60
1:B:607:THR:HG22	1:H:607:THR:HG22	1.83	0.60
1:D:555:ALA:HB2	1:D:561:VAL:HG22	1.82	0.60
1:E:591:GLU:HG3	4:E:1278:HOH:O	2.02	0.60
1:H:536:PRO:HD3	1:H:574:HIS:CE1	2.37	0.60
1:B:554:PHE:HB3	4:B:1235:HOH:O	2.01	0.59
1:D:595:LEU:HD22	1:D:621:LEU:HD12	1.83	0.59
1:E:539:VAL:HG22	1:E:566:TYR:HB3	1.83	0.59
1:H:536:PRO:HG2	3:H:705:CL:CL	2.40	0.59
1:B:599:GLN:HE22	1:H:619:ASN:HD21	1.50	0.59
1:H:524:LYS:HB2	1:H:565:LYS:HB3	1.85	0.59
1:D:550:MSE:HE2	1:D:554:PHE:CE1	2.38	0.59
1:C:584:GLU:HB2	4:C:1268:HOH:O	2.02	0.58
1:C:560:LYS:CD	1:C:560:LYS:H	2.15	0.58
1:C:512:ILE:O	1:C:516:LYS:HG3	2.04	0.57
1:A:548:THR:HB	1:A:566:TYR:OH	2.05	0.57
1:F:594:GLU:HB3	1:F:617:ARG:NH1	2.20	0.57
1:B:583:THR:HG21	1:B:588:LYS:HB3	1.86	0.57
1:H:618:MSE:SE	4:H:1214:HOH:O	2.72	0.57
1:B:546:MSE:HE3	1:B:561:VAL:HB	1.87	0.56
1:A:607:THR:HG22	1:A:608:LEU:N	2.19	0.56
1:C:511:PHE:HA	1:C:514:ARG:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:LYS:H	1:C:560:LYS:HD2	1.71	0.56
1:E:562:PRO:CB	4:E:1240:HOH:O	2.43	0.56
1:G:591:GLU:OE1	1:G:617:ARG:HD3	2.06	0.56
1:C:560:LYS:HD2	1:C:560:LYS:N	2.21	0.55
1:F:575:VAL:HG23	4:F:881:HOH:O	2.05	0.55
1:H:512:ILE:HD11	1:H:528:LEU:HG	1.88	0.55
1:A:595:LEU:HD21	1:G:618:MSE:HE1	1.87	0.55
1:D:539:VAL:CG2	1:D:566:TYR:HB3	2.36	0.55
1:F:512:ILE:O	1:F:516:LYS:HG3	2.07	0.55
1:C:536:PRO:HB2	1:C:596:LEU:HD22	1.88	0.55
1:A:524:LYS:HB2	1:A:565:LYS:HB3	1.89	0.54
1:C:539:VAL:HG22	1:C:566:TYR:HB3	1.88	0.54
1:G:536:PRO:HG2	4:G:992:HOH:O	2.08	0.54
1:C:559:GLN:HE22	1:C:560:LYS:HZ1	1.55	0.54
1:D:512:ILE:HD11	1:D:528:LEU:HG	1.88	0.54
1:D:567:ILE:HD12	4:D:1171:HOH:O	2.06	0.54
1:G:509:GLY:HA3	4:G:1135:HOH:O	2.06	0.54
1:E:524:LYS:NZ	1:E:542:ASP:OD2	2.39	0.54
1:F:510:SER:N	4:F:1246:HOH:O	2.40	0.54
1:D:535:THR:HB	4:D:1025:HOH:O	2.07	0.54
1:E:605:ARG:HD2	4:E:841:HOH:O	2.08	0.54
1:A:613:LEU:O	1:A:617:ARG:HG2	2.07	0.53
1:C:574:HIS:HB3	1:C:577:VAL:CG2	2.38	0.53
1:F:609:GLU:HB3	4:F:1251:HOH:O	2.07	0.53
1:G:594:GLU:HG3	1:G:617:ARG:HH12	1.73	0.53
1:D:529:THR:HG21	1:D:531:ARG:HG2	1.90	0.53
1:F:542:ASP:HB2	1:F:545:GLU:OE2	2.08	0.53
1:G:574:HIS:HD2	1:G:576:LEU:H	1.57	0.53
1:H:611:PRO:HG3	4:H:858:HOH:O	2.09	0.53
1:C:517:ALA:HB3	4:C:1234:HOH:O	2.09	0.53
1:E:562:PRO:HD2	4:E:1240:HOH:O	2.07	0.53
4:F:1239:HOH:O	1:H:554:PHE:CZ	2.62	0.52
1:H:532:LEU:HB2	4:H:830:HOH:O	2.08	0.52
1:C:532:LEU:HD12	1:D:538:ILE:HG22	1.91	0.52
1:C:575:VAL:HG23	4:C:997:HOH:O	2.09	0.52
1:H:599:GLN:NE2	3:H:705:CL:CL	2.80	0.52
1:D:576:LEU:HD22	1:D:592:TRP:CZ3	2.44	0.52
1:B:591:GLU:HG2	4:B:1237:HOH:O	2.09	0.52
1:C:547:SER:OG	1:C:550:MSE:HB2	2.10	0.52
1:F:594:GLU:OE1	1:F:594:GLU:HA	2.10	0.51
1:G:585:ASP:OD2	1:G:587:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:562:PRO:CG	4:E:1240:HOH:O	2.58	0.51
1:F:511:PHE:O	1:F:514:ARG:HB3	2.10	0.51
1:C:591:GLU:HB3	1:C:621:LEU:HD21	1.92	0.51
1:G:591:GLU:HG2	4:G:895:HOH:O	2.10	0.51
1:H:529:THR:OG1	1:H:531:ARG:HG2	2.11	0.51
1:A:617:ARG:NH1	4:A:937:HOH:O	2.40	0.51
1:A:611:PRO:HG3	4:A:851:HOH:O	2.11	0.51
1:B:512:ILE:HG22	1:B:516:LYS:HE3	1.93	0.51
1:D:616:ARG:O	1:D:620:GLN:HG2	2.10	0.51
1:G:616:ARG:HG2	4:G:1108:HOH:O	2.09	0.51
1:H:549:GLN:CD	1:H:549:GLN:H	2.15	0.51
1:C:559:GLN:HE22	1:C:560:LYS:NZ	2.09	0.51
1:B:583:THR:HG22	1:B:585:ASP:H	1.77	0.50
1:C:555:ALA:HB2	1:C:561:VAL:HG21	1.93	0.50
1:C:579:ARG:O	1:C:583:THR:HG23	2.12	0.50
1:E:531:ARG:HH21	1:E:569:GLU:CD	2.15	0.50
1:C:550:MSE:HE3	4:C:1215:HOH:O	2.11	0.50
1:B:524:LYS:HB2	1:B:565:LYS:HB3	1.93	0.50
1:H:510:SER:O	1:H:514:ARG:HG3	2.11	0.50
1:A:523:VAL:HG12	1:A:525:ASP:H	1.76	0.50
1:E:575:VAL:HG23	4:E:963:HOH:O	2.11	0.50
1:G:524:LYS:O	1:G:525:ASP:HB2	2.11	0.50
1:E:579:ARG:O	1:E:583:THR:HG22	2.12	0.49
1:D:510:SER:O	1:D:514:ARG:HB2	2.12	0.49
1:F:537:ALA:HB1	1:F:568:PHE:CE1	2.48	0.49
1:G:506:HIS:ND1	1:G:506:HIS:N	2.59	0.49
1:G:554:PHE:HD2	1:G:559:GLN:HB2	1.77	0.49
1:F:555:ALA:HB2	1:F:561:VAL:HG21	1.95	0.49
1:A:551:ALA:HB1	1:A:561:VAL:HG13	1.94	0.49
1:H:539:VAL:HG22	1:H:566:TYR:HB3	1.93	0.49
1:C:574:HIS:CD2	1:C:576:LEU:H	2.29	0.49
1:A:599:GLN:CG	1:G:615:ILE:HG23	2.43	0.49
1:B:561:VAL:HG12	1:C:559:GLN:HE21	1.77	0.49
1:C:539:VAL:HB	1:C:600:ALA:HB1	1.93	0.49
1:E:528:LEU:HD22	1:E:572:PRO:HG3	1.95	0.49
1:E:541:THR:HG21	1:E:547:SER:HA	1.95	0.49
1:E:539:VAL:HG13	1:E:566:TYR:CD2	2.48	0.48
1:B:562:PRO:CD	1:C:559:GLN:HE22	2.26	0.48
1:D:521:GLU:H	1:D:521:GLU:CD	2.15	0.48
1:D:531:ARG:HG2	1:D:531:ARG:HH11	1.77	0.48
1:D:532:LEU:HB2	4:D:991:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:GLN:HE21	1:B:620:GLN:HA	1.77	0.48
1:D:571:ASN:O	1:D:577:VAL:HG21	2.13	0.48
4:F:1239:HOH:O	1:H:554:PHE:HE2	1.93	0.48
1:A:529:THR:HG22	1:A:569:GLU:HB3	1.95	0.48
1:A:518:LEU:HD11	4:A:1071:HOH:O	2.13	0.48
1:E:523:VAL:HG13	1:E:566:TYR:O	2.13	0.48
1:A:533:THR:HG23	1:A:535:THR:H	1.79	0.48
1:H:574:HIS:HD2	1:H:576:LEU:N	2.11	0.48
1:A:601:LEU:O	1:A:605:ARG:HG2	2.13	0.48
1:G:539:VAL:HG13	1:G:566:TYR:CD2	2.48	0.48
1:F:554:PHE:CD1	1:F:554:PHE:N	2.81	0.47
1:B:609:GLU:HG2	4:B:983:HOH:O	2.13	0.47
1:A:554:PHE:CE2	1:D:546:MSE:HE2	2.49	0.47
1:F:546:MSE:HE1	1:F:554:PHE:HE2	1.79	0.47
1:G:521:GLU:HG2	4:G:1091:HOH:O	2.13	0.47
1:A:579:ARG:HD3	4:A:1084:HOH:O	2.14	0.47
1:B:574:HIS:HB3	1:B:577:VAL:HG23	1.97	0.47
1:G:508:HIS:HA	4:G:1001:HOH:O	2.15	0.47
1:G:574:HIS:CD2	1:G:576:LEU:H	2.33	0.46
1:G:568:PHE:CE1	1:G:597:LEU:HA	2.50	0.46
1:H:574:HIS:CD2	1:H:576:LEU:H	2.30	0.46
1:A:523:VAL:HG13	1:A:566:TYR:O	2.16	0.46
1:B:528:LEU:HD22	1:B:572:PRO:HG3	1.96	0.46
1:A:583:THR:HG21	1:A:588:LYS:HB3	1.97	0.46
1:H:536:PRO:CG	3:H:705:CL:CL	3.00	0.46
1:D:611:PRO:HG3	4:F:959:HOH:O	2.14	0.46
1:E:523:VAL:HG12	1:E:525:ASP:H	1.79	0.46
1:G:537:ALA:HB2	1:G:570:LEU:HD23	1.98	0.46
1:G:539:VAL:HG22	1:G:566:TYR:CB	2.42	0.46
1:B:537:ALA:HB2	1:B:570:LEU:HD23	1.98	0.46
1:G:594:GLU:HB2	1:G:617:ARG:NH1	2.31	0.46
1:D:539:VAL:HG12	4:D:813:HOH:O	2.16	0.46
1:G:588:LYS:HE2	4:G:984:HOH:O	2.15	0.46
1:G:595:LEU:O	1:G:599:GLN:HG3	2.15	0.46
1:A:548:THR:CG2	1:A:604:GLU:OE2	2.60	0.45
1:F:537:ALA:HB1	1:F:568:PHE:HE1	1.81	0.45
1:G:598:ASP:HB3	1:G:614:PHE:CD1	2.51	0.45
1:H:538:ILE:HD13	1:H:539:VAL:N	2.29	0.45
1:B:546:MSE:HA	1:B:550:MSE:HE2	1.98	0.45
1:D:612:ASN:ND2	4:D:935:HOH:O	2.48	0.45
1:G:618:MSE:HE3	1:G:622:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:MSE:SE	1:H:618:MSE:SE	3.34	0.45
1:D:614:PHE:CZ	1:F:618:MSE:HE1	2.51	0.45
1:E:562:PRO:CD	4:E:1240:HOH:O	2.63	0.45
1:H:552:LYS:HG3	4:H:945:HOH:O	2.16	0.45
1:H:539:VAL:CG2	1:H:566:TYR:HB3	2.46	0.45
1:E:595:LEU:O	1:E:599:GLN:HG3	2.16	0.45
1:D:529:THR:CG2	1:D:531:ARG:HG2	2.47	0.45
1:C:554:PHE:CE2	1:C:562:PRO:HD3	2.52	0.45
1:B:511:PHE:O	1:B:515:VAL:HG23	2.18	0.44
1:B:539:VAL:HG13	1:B:566:TYR:CD2	2.53	0.44
1:F:512:ILE:C	1:F:514:ARG:H	2.21	0.44
1:A:605:ARG:HG2	1:A:605:ARG:H	1.64	0.44
1:E:571:ASN:O	1:E:577:VAL:HG21	2.18	0.44
1:F:554:PHE:CE1	4:F:1207:HOH:O	2.56	0.44
1:D:516:LYS:HG2	1:D:526:VAL:HG23	2.00	0.44
1:E:580:ALA:O	1:E:583:THR:CG2	2.66	0.44
1:G:512:ILE:HG22	1:G:516:LYS:HE3	2.00	0.44
1:B:619:ASN:HD21	1:H:599:GLN:HE22	1.64	0.44
1:D:529:THR:CG2	1:D:530:HIS:N	2.81	0.44
1:F:619:ASN:O	1:F:623:VAL:HG23	2.18	0.44
1:B:605:ARG:NH1	4:B:1023:HOH:O	2.47	0.44
1:C:560:LYS:HG2	4:C:1284:HOH:O	2.17	0.44
1:E:553:LEU:HD13	1:G:553:LEU:CD1	2.48	0.44
1:F:595:LEU:HD22	1:F:621:LEU:CD1	2.48	0.44
1:E:542:ASP:CB	1:E:545:GLU:HG3	2.47	0.43
1:A:607:THR:CG2	1:A:608:LEU:N	2.79	0.43
1:B:511:PHE:O	1:B:514:ARG:HG2	2.18	0.43
1:A:554:PHE:HE2	1:D:546:MSE:HE2	1.83	0.43
1:C:564:VAL:HG22	4:C:1055:HOH:O	2.18	0.43
1:C:589:PHE:N	4:C:1230:HOH:O	2.51	0.43
1:C:531:ARG:HD2	1:C:538:ILE:HG23	1.99	0.43
1:D:529:THR:HG21	1:D:531:ARG:NH1	2.33	0.43
1:D:540:SER:HB2	4:D:1005:HOH:O	2.19	0.43
1:E:532:LEU:HB2	4:E:883:HOH:O	2.18	0.43
1:G:561:VAL:HB	1:G:562:PRO:HD2	1.99	0.43
1:C:611:PRO:O	1:C:615:ILE:HG13	2.19	0.43
1:C:529:THR:HG23	1:C:569:GLU:HB3	2.01	0.43
1:D:533:THR:HB	4:D:1252:HOH:O	2.17	0.43
1:C:518:LEU:HB2	4:C:1111:HOH:O	2.19	0.43
1:D:614:PHE:CE2	1:F:618:MSE:HE1	2.54	0.43
1:E:553:LEU:HD13	1:G:553:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:GLU:HG3	4:C:1140:HOH:O	2.18	0.42
1:G:594:GLU:HB3	1:G:617:ARG:NH1	2.33	0.42
1:D:605:ARG:HD3	4:D:876:HOH:O	2.19	0.42
1:B:553:LEU:HD11	1:D:554:PHE:CZ	2.54	0.42
1:G:588:LYS:HB3	4:G:910:HOH:O	2.19	0.42
1:C:554:PHE:O	1:C:559:GLN:HB2	2.20	0.42
1:D:539:VAL:HG21	1:D:566:TYR:HB3	2.02	0.42
1:D:537:ALA:HB2	1:D:570:LEU:HD23	2.01	0.42
1:G:617:ARG:HE	1:G:617:ARG:HB2	1.61	0.42
1:G:523:VAL:HG12	1:G:525:ASP:N	2.26	0.42
1:B:618:MSE:SE	4:H:1274:HOH:O	2.88	0.42
1:C:507:HIS:CD2	1:C:507:HIS:N	2.88	0.42
1:C:532:LEU:CD1	1:D:538:ILE:HG22	2.50	0.42
1:E:527:ARG:O	1:E:569:GLU:HA	2.20	0.42
1:E:546:MSE:SE	1:E:550:MSE:HG2	2.70	0.42
1:D:533:THR:CB	4:D:1252:HOH:O	2.67	0.42
1:D:622:LEU:HD11	1:F:595:LEU:HD21	2.00	0.42
1:G:531:ARG:HE	1:G:538:ILE:HG12	1.85	0.42
1:A:532:LEU:O	1:A:533:THR:HB	2.20	0.41
1:C:595:LEU:HD21	1:E:618:MSE:HE2	2.01	0.41
1:F:609:GLU:O	1:F:609:GLU:HG2	2.20	0.41
1:A:618:MSE:HE3	1:A:618:MSE:HB2	1.90	0.41
1:B:594:GLU:HB2	1:B:617:ARG:HD3	2.02	0.41
1:D:542:ASP:HB3	1:D:544:ASP:OD1	2.21	0.41
1:D:553:LEU:HD23	1:D:553:LEU:HA	1.90	0.41
1:F:571:ASN:HA	1:F:572:PRO:HD2	1.96	0.41
1:H:537:ALA:N	3:H:705:CL:CL	2.70	0.41
1:H:614:PHE:CZ	4:H:1214:HOH:O	2.74	0.41
1:A:512:ILE:HD13	4:A:875:HOH:O	2.20	0.41
1:B:512:ILE:O	1:B:516:LYS:HG3	2.21	0.41
1:B:538:ILE:HG12	1:B:539:VAL:H	1.85	0.41
1:B:605:ARG:HD3	4:B:1094:HOH:O	2.20	0.41
1:A:560:LYS:HE3	1:D:544:ASP:OD2	2.21	0.41
1:C:576:LEU:HD13	1:C:592:TRP:HZ3	1.85	0.41
1:B:542:ASP:OD2	1:B:567:ILE:HD11	2.21	0.40
1:H:588:LYS:HD2	4:H:1193:HOH:O	2.21	0.40
1:B:546:MSE:HA	1:B:550:MSE:CE	2.51	0.40
1:B:565:LYS:HA	1:B:565:LYS:HD3	1.83	0.40
1:E:561:VAL:HA	1:E:562:PRO:HD3	1.96	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	113/126 (90%)	105 (93%)	6 (5%)	2 (2%)	7	14
1	B	113/126 (90%)	107 (95%)	5 (4%)	1 (1%)	14	31
1	C	118/126 (94%)	106 (90%)	10 (8%)	2 (2%)	7	16
1	D	113/126 (90%)	105 (93%)	7 (6%)	1 (1%)	14	31
1	E	113/126 (90%)	112 (99%)	1 (1%)	0	100	100
1	F	113/126 (90%)	107 (95%)	5 (4%)	1 (1%)	14	31
1	G	119/126 (94%)	113 (95%)	6 (5%)	0	100	100
1	H	114/126 (90%)	111 (97%)	3 (3%)	0	100	100
All	All	916/1008 (91%)	866 (94%)	43 (5%)	7 (1%)	16	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	533	THR
1	F	623	VAL
1	A	532	LEU
1	A	533	THR
1	C	546	MSE
1	C	589	PHE
1	D	623	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	100/106 (94%)	94 (94%)	6 (6%)	16	35
1	B	100/106 (94%)	94 (94%)	6 (6%)	16	35
1	C	104/106 (98%)	96 (92%)	8 (8%)	10	22
1	D	100/106 (94%)	97 (97%)	3 (3%)	36	63
1	E	100/106 (94%)	96 (96%)	4 (4%)	27	52
1	F	100/106 (94%)	99 (99%)	1 (1%)	73	88
1	G	104/106 (98%)	95 (91%)	9 (9%)	8	17
1	H	100/106 (94%)	95 (95%)	5 (5%)	20	43
All	All	808/848 (95%)	766 (95%)	42 (5%)	19	41

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	532	LEU
1	A	539	VAL
1	A	548	THR
1	A	565	LYS
1	A	582	ASP
1	A	605	ARG
1	B	514	ARG
1	B	533	THR
1	B	539	VAL
1	B	553	LEU
1	B	559	GLN
1	B	620	GLN
1	C	507	HIS
1	C	529	THR
1	C	531	ARG
1	C	539	VAL
1	C	546	MSE
1	C	550	MSE
1	C	560	LYS
1	C	588	LYS
1	D	521	GLU
1	D	533	THR
1	D	546	MSE
1	E	539	VAL
1	E	545	GLU
1	E	583	THR
1	E	609	GLU

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Mol	Chain	Res	Type
1	F	539	VAL
1	G	506	HIS
1	G	531	ARG
1	G	534	ASP
1	G	539	VAL
1	G	553	LEU
1	G	554	PHE
1	G	598	ASP
1	G	609	GLU
1	G	617	ARG
1	H	535	THR
1	H	538	ILE
1	H	539	VAL
1	H	549	GLN
1	H	618	MSE

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

Mol	Chain	Res	Type
1	A	559	GLN
1	B	559	GLN
1	B	574	HIS
1	B	599	GLN
1	B	620	GLN
1	C	559	GLN
1	C	574	HIS
1	C	612	ASN
1	D	549	GLN
1	E	559	GLN
1	E	599	GLN
1	G	574	HIS
1	G	599	GLN
1	H	549	GLN
1	H	574	HIS
1	H	599	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	112/126 (88%)	-0.11	2 (1%) 67 62	29, 50, 77, 85	0
1	B	112/126 (88%)	0.44	3 (2%) 56 50	30, 68, 96, 108	0
1	C	117/126 (92%)	0.97	15 (12%) 9 7	47, 75, 114, 142	0
1	D	112/126 (88%)	0.47	3 (2%) 56 50	45, 69, 100, 112	0
1	E	112/126 (88%)	-0.08	1 (0%) 81 77	36, 51, 69, 84	0
1	F	112/126 (88%)	0.52	6 (5%) 32 27	43, 73, 99, 107	0
1	G	118/126 (93%)	-0.07	4 (3%) 48 42	29, 44, 78, 88	0
1	H	113/126 (89%)	-0.39	1 (0%) 81 77	30, 43, 64, 79	0
All	All	908/1008 (90%)	0.22	35 (3%) 44 38	29, 57, 99, 142	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	532	LEU	4.3
1	C	592	TRP	4.1
1	E	624	SER	4.1
1	D	533	THR	3.6
1	C	544	ASP	3.5
1	B	554	PHE	3.2
1	C	589	PHE	3.1
1	C	514	ARG	3.1
1	C	511	PHE	3.0
1	H	509	GLY	3.0
1	G	504	HIS	2.8
1	G	506	HIS	2.7
1	C	512	ILE	2.6
1	C	588	LYS	2.6
1	C	507	HIS	2.5
1	C	587	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	557	ALA	2.4
1	C	582	ASP	2.4
1	C	509	GLY	2.4
1	G	509	GLY	2.3
1	F	513	ASP	2.3
1	C	508	HIS	2.3
1	F	554	PHE	2.3
1	F	510	SER	2.3
1	D	575	VAL	2.2
1	C	528	LEU	2.2
1	G	563	GLU	2.2
1	B	526	VAL	2.2
1	C	564	VAL	2.1
1	C	505	HIS	2.1
1	D	512	ILE	2.1
1	F	561	VAL	2.1
1	F	564	VAL	2.1
1	A	531	ARG	2.1
1	F	624	SER	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	F	704	1/1	0.78	0.20	91,91,91,91	0
3	CL	E	703	1/1	0.90	0.14	64,64,64,64	0
3	CL	H	705	1/1	0.91	0.22	85,85,85,85	0
2	NI	D	701	1/1	0.94	0.06	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NI	C	700	1/1	0.96	0.07	86,86,86,86	0
2	NI	G	702	1/1	1.00	0.01	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.