



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:41 AM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

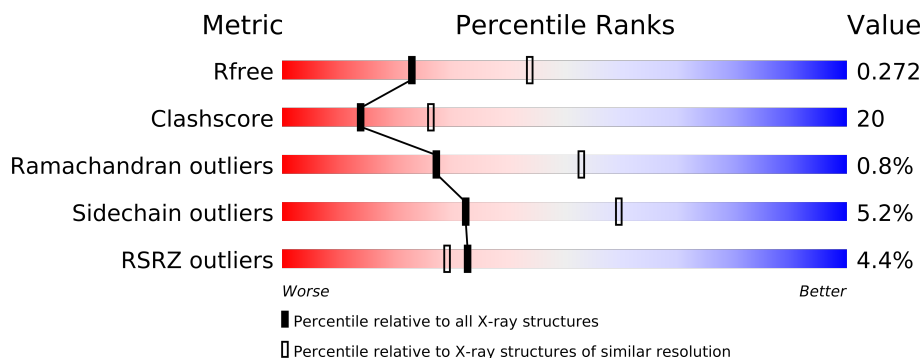
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	126	
1	B	126	
1	C	126	
1	D	126	
1	E	126	
1	F	126	
1	G	126	
1	H	126	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7915 atoms, of which 0 are hydrogen and 0 are deuterium.

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	G	1	Total Ni 1 1	0	0
2	D	1	Total Ni 1 1	0	0
2	C	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	H	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	E	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

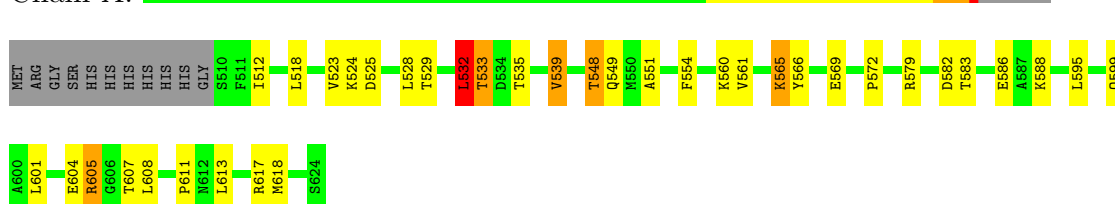
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	55	Total	O	0	0
			55	55		
4	C	42	Total	O	0	0
			42	42		
4	D	45	Total	O	0	0
			45	45		
4	E	45	Total	O	0	0
			45	45		
4	F	57	Total	O	0	0
			57	57		
4	G	70	Total	O	0	0
			70	70		
4	H	112	Total	O	0	0
			112	112		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

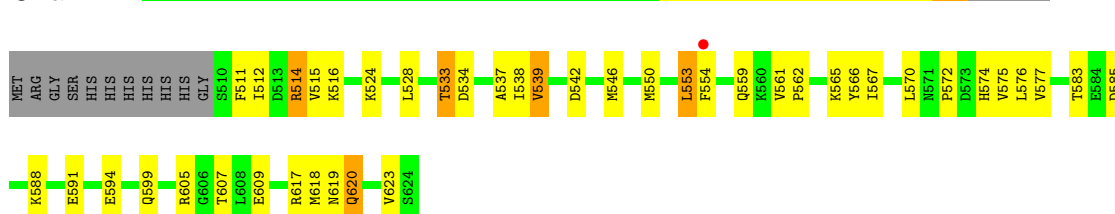
• Molecule 1: Chaperone protein htpG

Chain A:



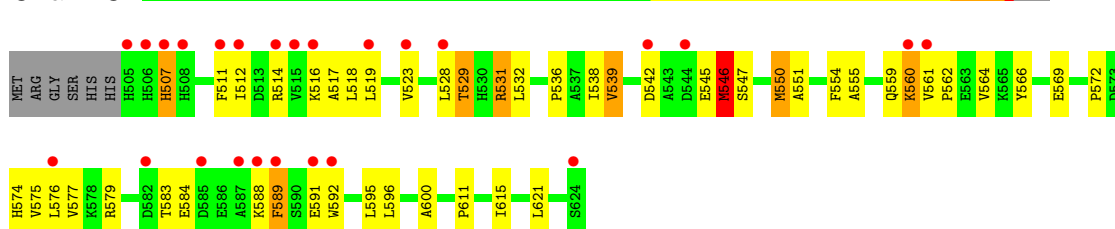
• Molecule 1: Chaperone protein htpG

Chain B:



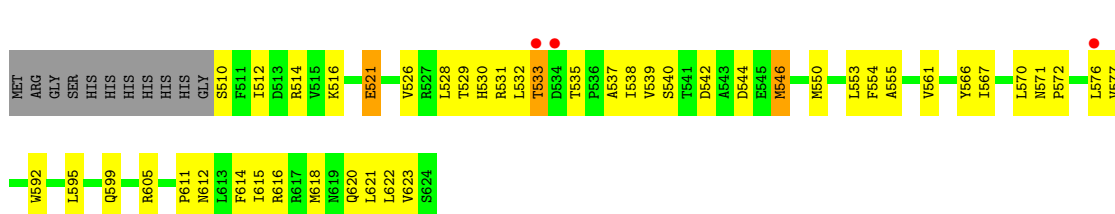
• Molecule 1: Chaperone protein htpG

Chain C:

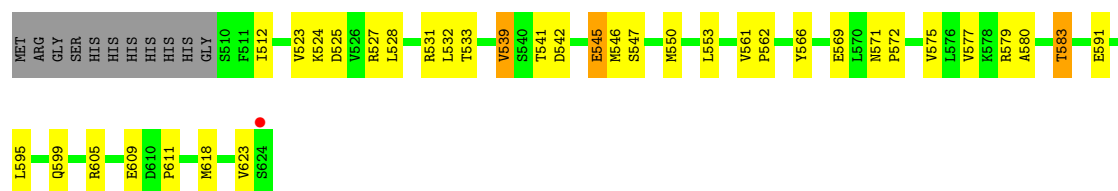


• Molecule 1: Chaperone protein htpG

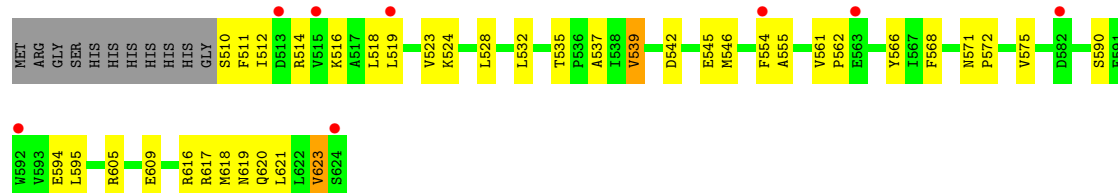
Chain D:



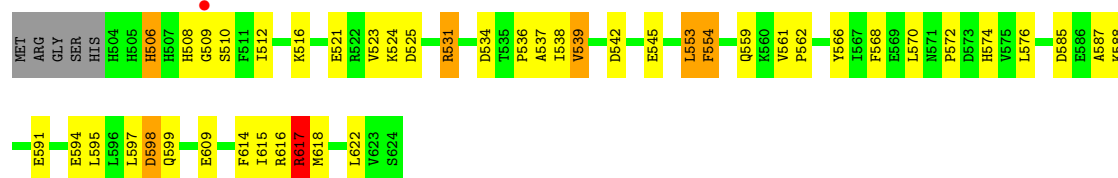
• Molecule 1: Chaperone protein htpG

Chain E: 

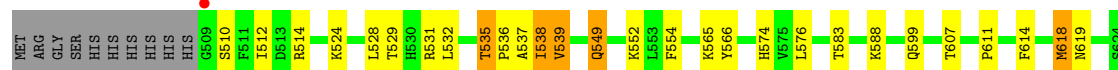
- Molecule 1: Chaperone protein htpG

Chain F: 

- Molecule 1: Chaperone protein htpG

Chain G: 

- Molecule 1: Chaperone protein htpG

Chain H: 

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.52Å 103.52Å 249.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.60 95.63 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.3 (29.90-2.60) 93.8 (95.63-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.62Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.261 0.235 , 0.272	Depositor DCC
R_{free} test set	1998 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 79708 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7915	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	916	0	930	35	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (297) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:574:HIS:HD2	1:B:576:LEU:H	1.39	0.70
1:A:549:GLN:HB3	4:A:1205:HOH:O	1.91	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
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:H:574:HIS:HD2	1:H:576:LEU:H	1.45	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:617:ARG:HB2	4:A:1125:HOH:O	1.98	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:G:594:GLU:CB	1:G:617:ARG:NH1	2.63	0.61
1:F:562:PRO:HD2	4:F:1279:HOH:O	1.99	0.61
4:F:1239:HOH:O	1:H:554:PHE:CE2	2.51	0.61
1:F:528:LEU:HD22	1:F:572:PRO:HB3	1.83	0.61
1:E:533:THR:HA	4:E:1101:HOH:O	2.01	0.61
1:F:605:ARG:HD3	4:F:972:HOH:O	2.00	0.60
1:G:617:ARG:NH1	4:G:1096:HOH:O	2.33	0.60
1:D:615:ILE:HA	1:D:618:MSE:HE3	1.83	0.60
1:H:535:THR:HG23	3:H:705:CL:CL	2.38	0.60
1:D:595:LEU:O	1:D:599:GLN:HG2	2.01	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:H	1:C:560:LYS:CD	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:H:618:MSE:SE	4:H:1214:HOH:O	2.72	0.57
1:B:583:THR:HG21	1:B:588:LYS:HB3	1.86	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:539:VAL:HG22	1:C:566:TYR:HB3	1.88	0.54
1:A:524:LYS:HB2	1:A:565:LYS:HB3	1.89	0.54
1:G:536:PRO:HG2	4:G:992:HOH:O	2.08	0.54
1:D:512:ILE:HD11	1:D:528:LEU:HG	1.88	0.54
1:C:559:GLN:HE22	1:C:560:LYS:HZ1	1.55	0.54
1:G:509:GLY:HA3	4:G:1135:HOH:O	2.06	0.54
1:D:567:ILE:HD12	4:D:1171: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:C:574:HIS:HB3	1:C:577:VAL:CG2	2.38	0.53
1:A:613:LEU:O	1:A:617:ARG:HG2	2.07	0.53
1:G:594:GLU:HG3	1:G:617:ARG:HH12	1.73	0.53
1:F:609:GLU:HB3	4:F:1251:HOH:O	2.07	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
1:H:532:LEU:HB2	4:H:830:HOH:O	2.08	0.52
4:F:1239:HOH:O	1:H:554:PHE:CZ	2.62	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:C:547:SER:OG	1:C:550:MSE:HB2	2.10	0.52
1:B:591:GLU:HG2	4:B:1237:HOH:O	2.09	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:617:ARG:NH1	4:A:937:HOH:O	2.40	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:H:549:GLN:CD	1:H:549:GLN:H	2.15	0.51
1:G:616:ARG:HG2	4:G:1108:HOH:O	2.09	0.51
1:A:611:PRO:HG3	4:A:851:HOH:O	2.11	0.51
1:C:559:GLN:HE22	1:C:560:LYS:NZ	2.09	0.51
1:C:579:ARG:O	1:C:583:THR:HG23	2.12	0.50
1:B:583:THR:HG22	1:B:585:ASP:H	1.77	0.50
1:E:531:ARG:HH21	1:E:569:GLU:CD	2.15	0.50
1:C:555:ALA:HB2	1:C:561:VAL:HG21	1.93	0.50
1:C:550:MSE:HE3	4:C:1215:HOH:O	2.11	0.50
1:H:510:SER:O	1:H:514:ARG:HG3	2.11	0.50
1:B:524:LYS:HB2	1:B:565:LYS:HB3	1.93	0.50
1:G:524:LYS:O	1:G:525:ASP:HB2	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:E:579:ARG:O	1:E:583:THR:HG22	2.12	0.49
1:G:554:PHE:HD2	1:G:559:GLN:HB2	1.77	0.49
1:D:510:SER:O	1:D:514:ARG:HB2	2.12	0.49
1:G:506:HIS:ND1	1:G:506:HIS:N	2.59	0.49
1:F:537:ALA:HB1	1:F:568:PHE:CE1	2.48	0.49
1:F:555:ALA:HB2	1:F:561:VAL:HG21	1.95	0.49
1:H:539:VAL:HG22	1:H:566:TYR:HB3	1.93	0.49
1:A:551:ALA:HB1	1:A:561:VAL:HG13	1.94	0.49
1:C:574:HIS:CD2	1:C:576:LEU:H	2.29	0.49
1:B:561:VAL:HG12	1:C:559:GLN:HE21	1.77	0.49
1:A:599:GLN:CG	1:G:615:ILE:HG23	2.43	0.49
1:E:528:LEU:HD22	1:E:572:PRO:HG3	1.95	0.49
1:C:539:VAL:HB	1:C:600:ALA:HB1	1.93	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:D:531:ARG:HH11	1:D:531:ARG:HG2	1.77	0.48
1:D:532:LEU:HB2	4:D:991:HOH:O	2.13	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: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:B:620:GLN:HA	1:B:620:GLN:HE21	1.77	0.48
1:A:529:THR:HG22	1:A:569:GLU:HB3	1.95	0.48
1:E:523:VAL:HG13	1:E:566:TYR:O	2.13	0.48
1:A:518:LEU:HD11	4:A:1071:HOH:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:574:HIS:HD2	1:H:576:LEU:N	2.11	0.48
1:A:533:THR:HG23	1:A:535:THR:H	1.79	0.48
1:G:539:VAL:HG13	1:G:566:TYR:CD2	2.48	0.48
1:A:601:LEU:O	1:A:605:ARG:HG2	2.13	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:F:546:MSE:HE1	1:F:554:PHE:HE2	1.79	0.47
1:A:554:PHE:CE2	1:D:546:MSE:HE2	2.49	0.47
1:G:521:GLU:HG2	4:G:1091:HOH:O	2.13	0.47
1:B:574:HIS:HB3	1:B:577:VAL:HG23	1.97	0.47
1:A:579:ARG:HD3	4:A:1084:HOH:O	2.14	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:H:574:HIS:CD2	1:H:576:LEU:H	2.30	0.46
1:G:568:PHE:CE1	1:G:597:LEU:HA	2.50	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:H:536:PRO:CG	3:H:705:CL:CL	3.00	0.46
1:A:583:THR:HG21	1:A:588:LYS:HB3	1.97	0.46
1:D:611:PRO:HG3	4:F:959:HOH:O	2.14	0.46
1:G:539:VAL:HG22	1:G:566:TYR:CB	2.42	0.46
1:G:537:ALA:HB2	1:G:570:LEU:HD23	1.98	0.46
1:E:523:VAL:HG12	1:E:525:ASP:H	1.79	0.46
1:G:594:GLU:HB2	1:G:617:ARG:NH1	2.31	0.46
1:B:537:ALA:HB2	1:B:570:LEU:HD23	1.98	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:H:538:ILE:HD13	1:H:539:VAL:N	2.29	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:G:618:MSE:HE3	1:G:622:LEU:HD11	1.99	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:F:512:ILE:C	1:F:514:ARG:H	2.21	0.44
1:B:539:VAL:HG13	1:B:566:TYR:CD2	2.53	0.44
1:A:605:ARG:HG2	1:A:605:ARG:H	1.64	0.44
1:F:554:PHE:CE1	4:F:1207:HOH:O	2.56	0.44
1:E:571:ASN:O	1:E:577:VAL:HG21	2.18	0.44
1:E:580:ALA:O	1:E:583:THR:CG2	2.66	0.44
1:D:516:LYS:HG2	1:D:526:VAL:HG23	2.00	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:G:561:VAL:HB	1:G:562:PRO:HD2	1.99	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: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: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
1:C:518:LEU:HB2	4:C:1111:HOH:O	2.19	0.43
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:G:617:ARG:HE	1:G:617:ARG:HB2	1.61	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:537:ALA:HB2	1:D:570:LEU:HD23	2.01	0.42
1:G:523:VAL:HG12	1:G:525:ASP:N	2.26	0.42
1:E:546:MSE:SE	1:E:550:MSE:HG2	2.70	0.42
1:B:618:MSE:SE	4:H:1274:HOH:O	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:C:507:HIS:CD2	1:C:507:HIS:N	2.88	0.42
1:D:622:LEU:HD11	1:F:595:LEU:HD21	2.00	0.42
1:D:533:THR:CB	4:D:1252:HOH:O	2.67	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:HG2	1:F:609:GLU:O	2.20	0.41
1:A:618:MSE:HB2	1:A:618:MSE:HE3	1.90	0.41
1:D:542:ASP:HB3	1:D:544:ASP:OD1	2.21	0.41
1:B:594:GLU:HB2	1:B:617:ARG:HD3	2.02	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:B:605:ARG:HD3	4:B:1094: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:A:512:ILE:HD13	4:A:875:HOH:O	2.20	0.41
1:C:576:LEU:HD13	1:C:592:TRP:HZ3	1.85	0.41
1:A:560:LYS:HE3	1:D:544:ASP:OD2	2.21	0.41
1:H:588:LYS:HD2	4:H:1193:HOH:O	2.21	0.40
1:B:542:ASP:OD2	1:B:567:ILE:HD11	2.21	0.40
1:B:546:MSE:HA	1:B:550:MSE:CE	2.51	0.40
1:B:565:LYS:HD3	1:B:565:LYS:HA	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%)	13	25
1	B	113/126 (90%)	107 (95%)	5 (4%)	1 (1%)	25	49
1	C	118/126 (94%)	106 (90%)	10 (8%)	2 (2%)	14	26
1	D	113/126 (90%)	105 (93%)	7 (6%)	1 (1%)	25	49
1	E	113/126 (90%)	112 (99%)	1 (1%)	0	100	100
1	F	113/126 (90%)	107 (95%)	5 (4%)	1 (1%)	25	49
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%)	27	53

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%)	27	51
1	B	100/106 (94%)	94 (94%)	6 (6%)	27	51
1	C	104/106 (98%)	96 (92%)	8 (8%)	18	35
1	D	100/106 (94%)	97 (97%)	3 (3%)	53	82
1	E	100/106 (94%)	96 (96%)	4 (4%)	42	73
1	F	100/106 (94%)	99 (99%)	1 (1%)	85	96
1	G	104/106 (98%)	95 (91%)	9 (9%)	15	28
1	H	100/106 (94%)	95 (95%)	5 (5%)	34	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	808/848 (95%)	766 (95%)	42 (5%)	32 59

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
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

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Mol	Chain	Res	Type
1	H	535	THR
1	H	538	ILE
1	H	539	VAL
1	H	549	GLN
1	H	618	MSE

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	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 chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	115/126 (91%)	0.24	0 100 100	29, 50, 77, 85	0
1	B	115/126 (91%)	0.42	1 (0%) 81 82	30, 68, 96, 108	0
1	C	120/126 (95%)	1.06	25 (20%) 1 1	46, 75, 114, 142	0
1	D	115/126 (91%)	0.45	3 (2%) 53 50	45, 68, 100, 112	0
1	E	115/126 (91%)	0.15	1 (0%) 81 82	36, 51, 69, 84	0
1	F	115/126 (91%)	0.68	8 (6%) 16 13	43, 72, 99, 107	0
1	G	121/126 (96%)	0.23	1 (0%) 83 85	29, 44, 77, 88	0
1	H	116/126 (92%)	0.06	1 (0%) 81 82	30, 43, 64, 79	0
All	All	932/1008 (92%)	0.41	40 (4%) 33 30	29, 57, 99, 142	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	508	HIS	5.5
1	C	592	TRP	4.4
1	E	624	SER	4.2
1	C	507	HIS	4.0
1	C	587	ALA	3.8
1	H	509	GLY	3.8
1	G	509	GLY	3.6
1	C	506	HIS	3.6
1	C	519	LEU	3.5
1	C	544	ASP	3.5
1	D	533	THR	3.4
1	C	528	LEU	3.2
1	C	515	VAL	3.2
1	C	505	HIS	2.8
1	C	588	LYS	2.7
1	C	514	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	589	PHE	2.6
1	C	591	GLU	2.6
1	F	519	LEU	2.5
1	F	563	GLU	2.5
1	C	523	VAL	2.5
1	C	512	ILE	2.5
1	C	561	VAL	2.4
1	F	554	PHE	2.4
1	C	516	LYS	2.3
1	C	585	ASP	2.3
1	C	542	ASP	2.2
1	C	624	SER	2.2
1	D	576	LEU	2.2
1	C	576	LEU	2.2
1	D	534	ASP	2.2
1	F	582	ASP	2.2
1	F	515	VAL	2.1
1	C	511	PHE	2.1
1	F	592	TRP	2.1
1	F	624	SER	2.1
1	C	582	ASP	2.1
1	C	560	LYS	2.1
1	F	513	ASP	2.0
1	B	554	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CL	H	705	1/1	0.60	16.39	85,85,85,85	0
2	NI	G	702	1/1	0.16	-1.35	40,40,40,40	0
3	CL	E	703	1/1	0.12	-1.99	64,64,64,64	0
2	NI	D	701	1/1	0.12	-2.00	78,78,78,78	0
2	NI	C	700	1/1	0.06	-2.09	86,86,86,86	0
3	CL	F	704	1/1	0.11	-2.99	91,91,91,91	0

6.5 Other polymers ⓘ

There are no such residues in this entry.