



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 04:35 AM EDT

PDB ID : 2Z6M  
Title : Crystal structure of Human Ferritin H8 as biotemplate for noble metal nanoparticle synthesis  
Authors : Di Costanzo, L.; Christianson, D.W.  
Deposited on : 2007-08-04  
Resolution : 2.72 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

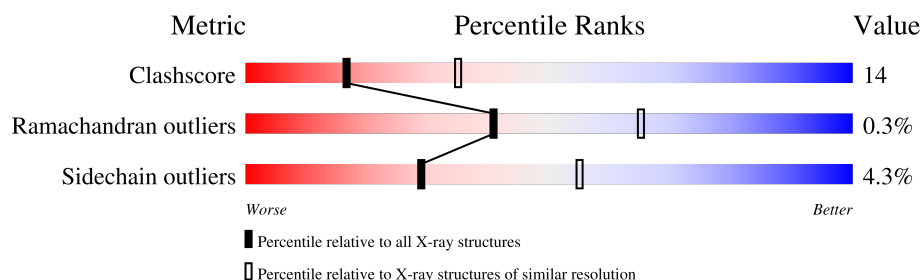
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 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))
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)





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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	176	
1	B	176	
1	C	176	
1	D	176	
1	E	176	
1	F	176	
1	G	176	
1	H	176	

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Mol	Chain	Length	Quality of chain
1	I	176	 69%27%..
1	J	176	 76%21%..
1	K	176	 76%20%..
1	L	176	 70%25%..

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
4	MPD	B	630	X	-	-	-
4	MPD	C	535	X	-	-	-
4	MPD	E	631	X	-	-	-
4	MPD	F	533	X	-	-	-
4	MPD	H	538	X	-	-	-
4	MPD	I	539	X	-	-	-
4	MPD	L	537	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17273 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 Ferritin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1403	877	247	270	9			
1	B	172	Total	C	N	O	S	0	0	0
			1403	877	247	270	9			
1	C	172	Total	C	N	O	S	0	0	0
			1403	877	247	270	9			
1	D	172	Total	C	N	O	S	0	1	0
			1404	877	247	270	10			
1	E	172	Total	C	N	O	S	0	1	0
			1404	877	247	270	10			
1	F	172	Total	C	N	O	S	0	1	0
			1404	877	247	270	10			
1	G	172	Total	C	N	O	S	0	0	0
			1403	877	247	270	9			
1	H	172	Total	C	N	O	S	0	0	0
			1403	877	247	270	9			
1	I	172	Total	C	N	O	S	0	0	0
			1403	877	247	270	9			
1	J	172	Total	C	N	O	S	0	0	0
			1403	877	247	270	9			
1	K	172	Total	C	N	O	S	0	1	0
			1404	877	247	270	10			
1	L	172	Total	C	N	O	S	0	0	0
			1403	877	247	270	9			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASP	HIS	engineered mutation	UNP P02794
A	64	CYS	GLU	engineered mutation	UNP P02794
A	90	ARG	CYS	engineered mutation	UNP P02794
A	102	ALA	CYS	engineered mutation	UNP P02794
A	105	GLN	HIS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
A	140	CYS	GLU	engineered mutation	UNP P02794
A	143	CYS	LYS	engineered mutation	UNP P02794
A	147	CYS	GLU	engineered mutation	UNP P02794
B	13	ASP	HIS	engineered mutation	UNP P02794
B	64	CYS	GLU	engineered mutation	UNP P02794
B	90	ARG	CYS	engineered mutation	UNP P02794
B	102	ALA	CYS	engineered mutation	UNP P02794
B	105	GLN	HIS	engineered mutation	UNP P02794
B	140	CYS	GLU	engineered mutation	UNP P02794
B	143	CYS	LYS	engineered mutation	UNP P02794
B	147	CYS	GLU	engineered mutation	UNP P02794
C	13	ASP	HIS	engineered mutation	UNP P02794
C	64	CYS	GLU	engineered mutation	UNP P02794
C	90	ARG	CYS	engineered mutation	UNP P02794
C	102	ALA	CYS	engineered mutation	UNP P02794
C	105	GLN	HIS	engineered mutation	UNP P02794
C	140	CYS	GLU	engineered mutation	UNP P02794
C	143	CYS	LYS	engineered mutation	UNP P02794
C	147	CYS	GLU	engineered mutation	UNP P02794
D	13	ASP	HIS	engineered mutation	UNP P02794
D	64	CYS	GLU	engineered mutation	UNP P02794
D	90	ARG	CYS	engineered mutation	UNP P02794
D	102	ALA	CYS	engineered mutation	UNP P02794
D	105	GLN	HIS	engineered mutation	UNP P02794
D	140	CYS	GLU	engineered mutation	UNP P02794
D	143	CYS	LYS	engineered mutation	UNP P02794
D	147	CYS	GLU	engineered mutation	UNP P02794
E	13	ASP	HIS	engineered mutation	UNP P02794
E	64	CYS	GLU	engineered mutation	UNP P02794
E	90	ARG	CYS	engineered mutation	UNP P02794
E	102	ALA	CYS	engineered mutation	UNP P02794
E	105	GLN	HIS	engineered mutation	UNP P02794
E	140	CYS	GLU	engineered mutation	UNP P02794
E	143	CYS	LYS	engineered mutation	UNP P02794
E	147	CYS	GLU	engineered mutation	UNP P02794
F	13	ASP	HIS	engineered mutation	UNP P02794
F	64	CYS	GLU	engineered mutation	UNP P02794
F	90	ARG	CYS	engineered mutation	UNP P02794
F	102	ALA	CYS	engineered mutation	UNP P02794
F	105	GLN	HIS	engineered mutation	UNP P02794
F	140	CYS	GLU	engineered mutation	UNP P02794
F	143	CYS	LYS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
F	147	CYS	GLU	engineered mutation	UNP P02794
G	13	ASP	HIS	engineered mutation	UNP P02794
G	64	CYS	GLU	engineered mutation	UNP P02794
G	90	ARG	CYS	engineered mutation	UNP P02794
G	102	ALA	CYS	engineered mutation	UNP P02794
G	105	GLN	HIS	engineered mutation	UNP P02794
G	140	CYS	GLU	engineered mutation	UNP P02794
G	143	CYS	LYS	engineered mutation	UNP P02794
G	147	CYS	GLU	engineered mutation	UNP P02794
H	13	ASP	HIS	engineered mutation	UNP P02794
H	64	CYS	GLU	engineered mutation	UNP P02794
H	90	ARG	CYS	engineered mutation	UNP P02794
H	102	ALA	CYS	engineered mutation	UNP P02794
H	105	GLN	HIS	engineered mutation	UNP P02794
H	140	CYS	GLU	engineered mutation	UNP P02794
H	143	CYS	LYS	engineered mutation	UNP P02794
H	147	CYS	GLU	engineered mutation	UNP P02794
I	13	ASP	HIS	engineered mutation	UNP P02794
I	64	CYS	GLU	engineered mutation	UNP P02794
I	90	ARG	CYS	engineered mutation	UNP P02794
I	102	ALA	CYS	engineered mutation	UNP P02794
I	105	GLN	HIS	engineered mutation	UNP P02794
I	140	CYS	GLU	engineered mutation	UNP P02794
I	143	CYS	LYS	engineered mutation	UNP P02794
I	147	CYS	GLU	engineered mutation	UNP P02794
J	13	ASP	HIS	engineered mutation	UNP P02794
J	64	CYS	GLU	engineered mutation	UNP P02794
J	90	ARG	CYS	engineered mutation	UNP P02794
J	102	ALA	CYS	engineered mutation	UNP P02794
J	105	GLN	HIS	engineered mutation	UNP P02794
J	140	CYS	GLU	engineered mutation	UNP P02794
J	143	CYS	LYS	engineered mutation	UNP P02794
J	147	CYS	GLU	engineered mutation	UNP P02794
K	13	ASP	HIS	engineered mutation	UNP P02794
K	64	CYS	GLU	engineered mutation	UNP P02794
K	90	ARG	CYS	engineered mutation	UNP P02794
K	102	ALA	CYS	engineered mutation	UNP P02794
K	105	GLN	HIS	engineered mutation	UNP P02794
K	140	CYS	GLU	engineered mutation	UNP P02794
K	143	CYS	LYS	engineered mutation	UNP P02794
K	147	CYS	GLU	engineered mutation	UNP P02794
L	13	ASP	HIS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
L	64	CYS	GLU	engineered mutation	UNP P02794
L	90	ARG	CYS	engineered mutation	UNP P02794
L	102	ALA	CYS	engineered mutation	UNP P02794
L	105	GLN	HIS	engineered mutation	UNP P02794
L	140	CYS	GLU	engineered mutation	UNP P02794
L	143	CYS	LYS	engineered mutation	UNP P02794
L	147	CYS	GLU	engineered mutation	UNP P02794

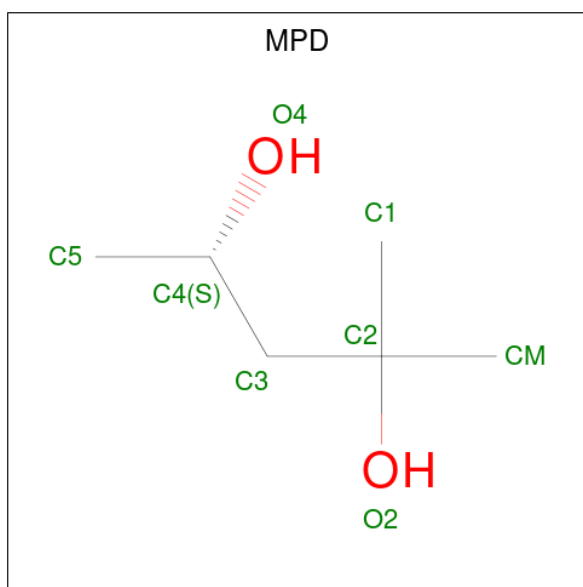
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	L	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total	O	0	0
			37	37		
5	B	34	Total	O	0	0
			34	34		
5	C	43	Total	O	0	0
			43	43		
5	D	35	Total	O	0	0
			35	35		
5	E	33	Total	O	0	0
			33	33		

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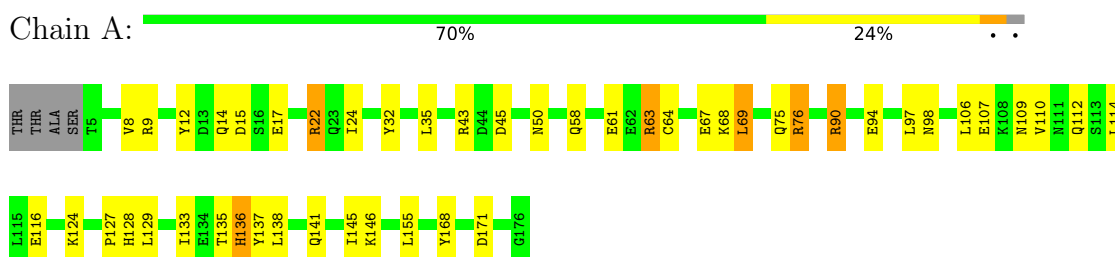
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	30	Total 30	O 30	0	0
5	G	22	Total 22	O 22	0	0
5	H	22	Total 22	O 22	0	0
5	I	42	Total 42	O 42	0	0
5	J	23	Total 23	O 23	0	0
5	K	21	Total 21	O 21	0	0
5	L	26	Total 26	O 26	0	0

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

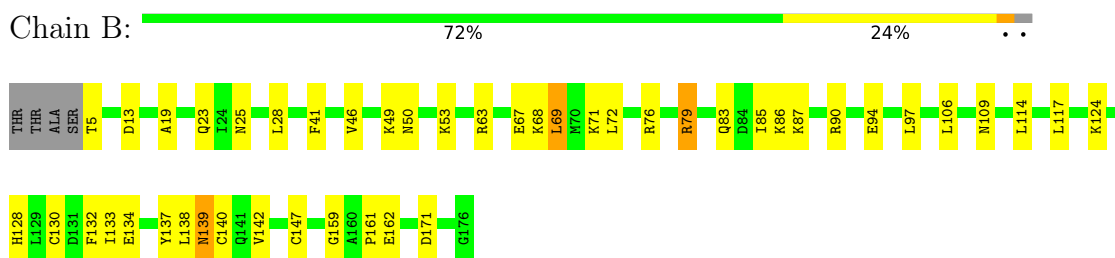
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

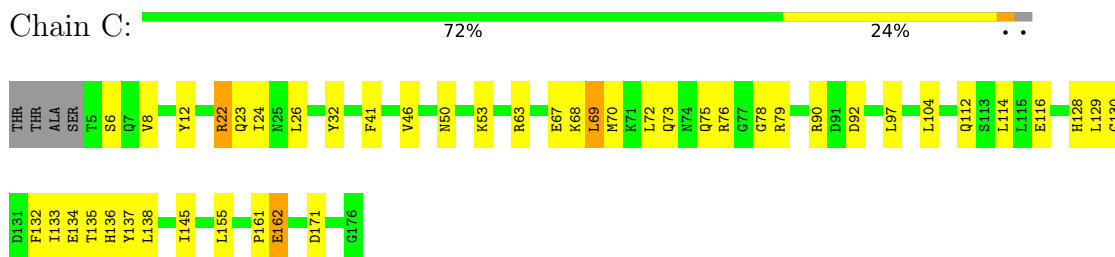
- Molecule 1: Ferritin heavy chain



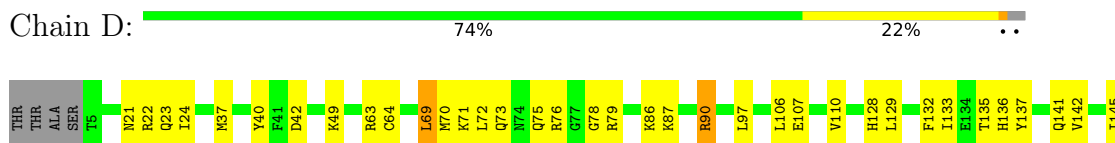
- Molecule 1: Ferritin heavy chain

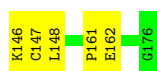


- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain





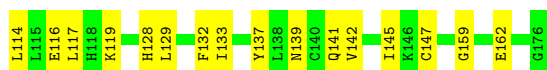
• Molecule 1: Ferritin heavy chain

Chain E: 75% 22% ..



• Molecule 1: Ferritin heavy chain

Chain F: 70% 26% ..



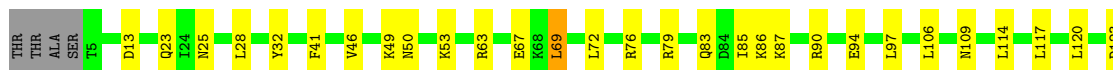
• Molecule 1: Ferritin heavy chain

Chain G: 70% 23% ..



• Molecule 1: Ferritin heavy chain

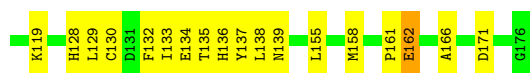
Chain H: 72% 25% ..



• Molecule 1: Ferritin heavy chain

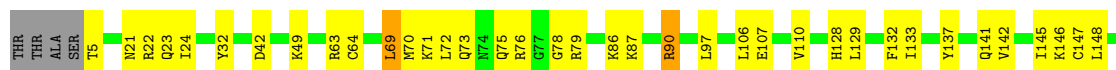
Chain I: 69% 27% ..





- Molecule 1: Ferritin heavy chain

Chain J: 76% 21% ..



- Molecule 1: Ferritin heavy chain

Chain K: 76% 20% ..



- Molecule 1: Ferritin heavy chain

Chain L: 70% 25% ..



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.29Å 171.29Å 190.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.72	Depositor
% Data completeness (in resolution range)	96.0 (50.00-2.72)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.215 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17273	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, MPD

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	0.38	0/1430	0.57	0/1925
1	B	0.36	0/1430	0.56	0/1925
1	C	0.38	0/1430	0.55	0/1925
1	D	0.38	0/1436	0.57	0/1933
1	E	0.40	0/1436	0.55	0/1933
1	F	0.37	0/1436	0.57	0/1933
1	G	0.39	0/1430	0.58	0/1925
1	H	0.38	0/1430	0.57	0/1925
1	I	0.37	0/1430	0.55	0/1925
1	J	0.39	0/1430	0.57	0/1925
1	K	0.39	0/1436	0.55	0/1933
1	L	0.37	0/1430	0.57	0/1925
All	All	0.38	0/17184	0.56	0/23132

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	1403	0	1352	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1403	0	1352	45	0
1	C	1403	0	1352	32	0
1	D	1404	0	1353	38	0
1	E	1404	0	1353	36	0
1	F	1404	0	1353	59	0
1	G	1403	0	1352	50	0
1	H	1403	0	1352	46	0
1	I	1403	0	1352	38	0
1	J	1403	0	1352	32	0
1	K	1404	0	1353	30	0
1	L	1403	0	1352	59	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	B	8	0	13	0	0
4	C	8	0	13	0	0
4	E	8	0	13	0	0
4	F	8	0	13	0	0
4	H	8	0	13	1	0
4	I	8	0	13	0	0
4	L	8	0	13	1	0
5	A	37	0	0	1	0
5	B	34	0	0	4	0
5	C	43	0	0	3	0
5	D	35	0	0	3	0
5	E	33	0	0	4	0
5	F	30	0	0	2	0
5	G	22	0	0	2	0
5	H	22	0	0	1	0
5	I	42	0	0	6	0
5	J	23	0	0	2	0
5	K	21	0	0	1	0
5	L	26	0	0	6	0
All	All	17273	0	16319	471	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 14.

All (471) 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:90:ARG:HH22	1:H:86:LYS:HE3	1.01	1.10
1:A:76:ARG:HG2	1:A:76:ARG:HH11	1.12	1.09
1:G:76:ARG:HG2	1:G:76:ARG:HH11	1.13	1.06
1:F:94:GLU:OE2	1:H:86:LYS:HE2	1.59	1.01
1:F:90:ARG:NH2	1:H:86:LYS:HE3	1.85	0.91
1:F:76:ARG:HH11	1:F:76:ARG:HB3	1.36	0.89
1:A:35:LEU:HD21	1:F:70:MET:HE1	1.55	0.86
1:L:76:ARG:HH11	1:L:76:ARG:HB3	1.36	0.86
1:J:24:ILE:HD13	1:J:70:MET:HG2	1.56	0.86
1:G:35:LEU:HD21	1:L:70:MET:HE1	1.55	0.84
1:K:76:ARG:HH11	1:K:76:ARG:HG2	1.43	0.83
1:F:21:ASN:ND2	1:F:73:GLN:HE21	1.76	0.82
1:B:97:LEU:HD23	1:B:161:PRO:HD3	1.61	0.82
1:D:24:ILE:HD13	1:D:70:MET:HG2	1.59	0.82
1:H:97:LEU:HD23	1:H:161:PRO:HD3	1.61	0.82
1:E:76:ARG:HG2	1:E:76:ARG:HH11	1.45	0.80
1:L:21:ASN:ND2	1:L:73:GLN:HE21	1.78	0.80
1:C:63:ARG:HD3	5:C:544:HOH:O	1.82	0.79
1:G:63:ARG:NH2	1:L:63:ARG:HH21	1.80	0.79
1:F:94:GLU:CD	1:H:86:LYS:HE2	2.04	0.79
1:A:63:ARG:NH2	1:F:63:ARG:HH21	1.80	0.78
1:G:141:GLN:O	1:G:145:ILE:HG12	1.84	0.78
1:A:68:LYS:HD3	1:A:136:HIS:HD2	1.51	0.76
1:A:76:ARG:HG2	1:A:76:ARG:NH1	1.90	0.76
1:I:76:ARG:HD2	1:I:128:HIS:HD2	1.51	0.76
1:A:141:GLN:O	1:A:145:ILE:HG12	1.84	0.76
1:I:158:MET:HB3	5:I:748:HOH:O	1.85	0.75
1:K:134:GLU:HA	1:K:138:LEU:HD12	1.69	0.75
1:G:68:LYS:HD3	1:G:136:HIS:HD2	1.51	0.75
1:E:134:GLU:HA	1:E:138:LEU:HD12	1.68	0.75
1:C:76:ARG:HD2	1:C:128:HIS:HD2	1.52	0.74
1:B:90:ARG:HG3	1:B:90:ARG:HH11	1.52	0.74
1:I:76:ARG:HD2	1:I:128:HIS:CD2	2.23	0.74
1:G:76:ARG:HG2	1:G:76:ARG:NH1	1.91	0.74
1:L:76:ARG:HH11	1:L:76:ARG:CB	2.02	0.73
1:H:76:ARG:HD3	1:H:128:HIS:CD2	2.23	0.73
1:C:76:ARG:HD2	1:C:128:HIS:CD2	2.23	0.72
1:B:76:ARG:HD3	1:B:128:HIS:CD2	2.25	0.72
1:D:86:LYS:HD3	1:D:87:LYS:N	2.04	0.72
1:J:86:LYS:HD3	1:J:87:LYS:N	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:ARG:HH11	1:F:76:ARG:CB	2.02	0.72
1:E:90:ARG:HG2	1:E:90:ARG:HH11	1.56	0.71
1:J:5:THR:N	5:J:184:HOH:O	2.24	0.71
1:H:90:ARG:HG3	1:H:90:ARG:HH11	1.56	0.70
1:G:63:ARG:HH21	1:L:63:ARG:HH21	1.37	0.70
1:A:9:ARG:NH1	1:A:12:TYR:O	2.24	0.70
1:F:49:LYS:HD3	5:F:549:HOH:O	1.92	0.70
1:I:24:ILE:HD13	1:I:70:MET:HG2	1.73	0.70
1:G:9:ARG:NH1	1:G:12:TYR:O	2.25	0.69
1:A:63:ARG:HH21	1:F:63:ARG:HH21	1.38	0.69
1:C:114:LEU:HD13	1:C:137:TYR:HB3	1.76	0.68
1:K:90:ARG:HG2	1:K:90:ARG:HH11	1.58	0.68
1:D:71:LYS:O	1:D:75:GLN:HG3	1.94	0.68
1:A:22:ARG:HH11	1:A:22:ARG:HG2	1.57	0.68
1:B:139:ASN:HD22	1:B:140:CYS:H	1.42	0.68
1:I:129:LEU:O	1:I:133:ILE:HG12	1.94	0.68
1:E:24:ILE:HG12	1:E:69:LEU:HB3	1.76	0.68
1:G:22:ARG:HG2	1:G:22:ARG:HH11	1.57	0.68
1:C:24:ILE:HD13	1:C:70:MET:HG2	1.76	0.67
1:J:69:LEU:HD13	1:J:137:TYR:OH	1.95	0.67
1:C:129:LEU:O	1:C:133:ILE:HG12	1.95	0.67
1:I:158:MET:HE2	5:I:748:HOH:O	1.94	0.67
1:J:71:LYS:O	1:J:75:GLN:HG3	1.94	0.67
1:I:114:LEU:HD13	1:I:137:TYR:HB3	1.76	0.66
1:K:24:ILE:HG12	1:K:69:LEU:HB3	1.78	0.66
1:B:63:ARG:HD2	1:B:67:GLU:OE2	1.97	0.65
1:H:139:ASN:HD22	1:H:140:CYS:H	1.44	0.65
1:B:114:LEU:HD13	1:B:137:TYR:HB3	1.78	0.65
1:D:69:LEU:HD13	1:D:137:TYR:OH	1.97	0.65
1:K:76:ARG:HG2	1:K:76:ARG:NH1	2.09	0.65
1:K:76:ARG:HD2	1:K:128:HIS:HD2	1.62	0.65
1:G:63:ARG:HH11	1:G:63:ARG:HB3	1.61	0.64
1:H:139:ASN:N	1:H:139:ASN:ND2	2.45	0.64
1:H:76:ARG:HH11	1:H:128:HIS:HD2	1.44	0.64
1:B:49:LYS:O	1:B:53:LYS:HG3	1.97	0.64
1:B:139:ASN:N	1:B:139:ASN:ND2	2.46	0.64
1:H:114:LEU:HD13	1:H:137:TYR:HB3	1.78	0.63
1:H:128:HIS:CE1	1:L:142:VAL:HG21	2.34	0.63
1:F:68:LYS:HZ2	1:F:68:LYS:CB	2.11	0.63
1:D:23:GLN:HG3	1:D:69:LEU:HD21	1.79	0.63
1:E:76:ARG:HG2	1:E:76:ARG:NH1	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:CYS:O	1:C:134:GLU:HG3	1.99	0.62
1:E:76:ARG:HD2	1:E:128:HIS:HD2	1.63	0.62
1:B:130:CYS:O	1:B:134:GLU:HG3	1.99	0.62
1:H:130:CYS:O	1:H:134:GLU:HG3	1.99	0.62
1:E:49:LYS:HD3	5:E:654:HOH:O	1.98	0.62
1:J:23:GLN:HG3	1:J:69:LEU:HD21	1.80	0.62
1:A:63:ARG:HH11	1:A:63:ARG:HB3	1.64	0.61
1:B:76:ARG:HH11	1:B:128:HIS:HD2	1.46	0.61
1:H:49:LYS:O	1:H:53:LYS:HG3	2.00	0.61
1:H:139:ASN:HD22	1:H:139:ASN:N	1.97	0.61
1:L:21:ASN:ND2	1:L:73:GLN:NE2	2.49	0.61
1:F:21:ASN:ND2	1:F:73:GLN:NE2	2.47	0.61
1:A:76:ARG:HD2	1:A:128:HIS:CD2	2.36	0.61
5:H:812:HOH:O	1:L:142:VAL:HG13	2.00	0.61
1:L:68:LYS:NZ	1:L:68:LYS:HB3	2.16	0.61
1:G:63:ARG:HB3	1:G:63:ARG:NH1	2.15	0.61
1:I:130:CYS:O	1:I:134:GLU:HG3	2.01	0.60
1:B:79:ARG:NH2	5:B:818:HOH:O	2.34	0.60
1:J:22:ARG:HD3	5:J:197:HOH:O	2.00	0.60
1:K:24:ILE:HD13	1:K:70:MET:HG2	1.83	0.60
1:J:90:ARG:HG2	1:J:90:ARG:HH11	1.67	0.60
1:I:139:ASN:HB2	5:I:747:HOH:O	2.00	0.60
1:L:5:THR:N	5:L:559:HOH:O	2.35	0.60
1:H:90:ARG:HG3	1:H:90:ARG:NH1	2.16	0.60
1:A:129:LEU:O	1:A:133:ILE:HG12	2.02	0.60
1:F:68:LYS:NZ	1:F:68:LYS:HB3	2.16	0.59
1:H:72:LEU:HD22	1:H:132:PHE:CD2	2.37	0.59
1:B:72:LEU:HD22	1:B:132:PHE:CD2	2.38	0.59
1:D:90:ARG:HG2	1:D:90:ARG:HH11	1.67	0.59
1:G:76:ARG:HD2	1:G:128:HIS:CD2	2.37	0.59
1:G:129:LEU:O	1:G:133:ILE:HG12	2.02	0.59
1:A:63:ARG:NH2	1:F:63:ARG:NH2	2.51	0.59
1:A:109:ASN:O	1:A:112:GLN:HB3	2.01	0.59
1:A:63:ARG:HB3	1:A:63:ARG:NH1	2.17	0.58
1:F:90:ARG:HG2	1:F:90:ARG:HH11	1.68	0.58
1:F:109:ASN:O	1:F:112:GLN:HB3	2.03	0.58
1:B:139:ASN:HD22	1:B:140:CYS:N	2.01	0.58
1:H:86:LYS:HD3	1:H:87:LYS:N	2.17	0.58
1:L:109:ASN:O	1:L:112:GLN:HB3	2.02	0.58
1:G:109:ASN:O	1:G:112:GLN:HB3	2.03	0.58
1:B:128:HIS:CE1	1:F:142:VAL:HG21	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5:THR:N	5:L:541:HOH:O	2.36	0.58
1:L:21:ASN:HD22	1:L:73:GLN:HE21	1.51	0.58
1:B:139:ASN:HD22	1:B:139:ASN:N	1.99	0.58
1:G:114:LEU:HD13	1:G:137:TYR:HB3	1.85	0.58
1:I:72:LEU:HD22	1:I:132:PHE:CD2	2.39	0.58
1:A:68:LYS:HD3	1:A:136:HIS:CD2	2.37	0.58
1:B:86:LYS:HD3	1:B:87:LYS:N	2.18	0.58
1:D:90:ARG:HG2	1:D:90:ARG:NH1	2.19	0.58
1:L:90:ARG:HG2	1:L:90:ARG:HH11	1.69	0.58
1:C:72:LEU:HD22	1:C:132:PHE:CD2	2.39	0.58
1:B:90:ARG:HG3	1:B:90:ARG:NH1	2.13	0.58
1:E:97:LEU:HD23	1:E:161:PRO:HD3	1.86	0.58
1:E:24:ILE:HD13	1:E:70:MET:HG2	1.86	0.57
1:E:162:GLU:H	1:E:162:GLU:CD	2.08	0.57
1:K:20:ILE:HD12	1:K:117:LEU:HD21	1.86	0.57
1:K:76:ARG:HD2	1:K:128:HIS:CD2	2.38	0.57
1:A:114:LEU:HD13	1:A:137:TYR:HB3	1.86	0.57
1:I:24:ILE:HG12	1:I:69:LEU:HB3	1.87	0.57
1:J:90:ARG:HG2	1:J:90:ARG:NH1	2.18	0.57
1:B:86:LYS:HD3	1:B:87:LYS:H	1.70	0.57
1:H:86:LYS:HD3	1:H:87:LYS:H	1.70	0.57
1:K:97:LEU:HD23	1:K:161:PRO:HD3	1.86	0.57
1:C:24:ILE:HG12	1:C:69:LEU:HB3	1.85	0.57
1:E:63:ARG:HD2	1:E:67:GLU:OE2	2.05	0.57
1:E:20:ILE:HD12	1:E:117:LEU:HD21	1.84	0.56
1:E:76:ARG:HD2	1:E:128:HIS:CD2	2.40	0.56
1:I:97:LEU:HD23	1:I:161:PRO:HD3	1.87	0.56
1:B:142:VAL:HG21	1:D:128:HIS:CE1	2.40	0.56
1:F:114:LEU:HD13	1:F:137:TYR:HB3	1.88	0.56
1:H:139:ASN:HD22	1:H:140:CYS:N	2.03	0.56
1:B:23:GLN:HG3	1:B:69:LEU:HD21	1.88	0.56
1:D:71:LYS:HG2	1:D:75:GLN:HE21	1.70	0.56
1:J:71:LYS:HG2	1:J:75:GLN:HE21	1.70	0.56
1:H:142:VAL:HG21	1:J:128:HIS:CE1	2.41	0.56
1:J:71:LYS:HG2	1:J:75:GLN:NE2	2.19	0.56
1:F:24:ILE:HG12	1:F:69:LEU:HB3	1.88	0.56
1:I:112:GLN:O	1:I:116:GLU:HG3	2.05	0.56
1:D:71:LYS:HG2	1:D:75:GLN:NE2	2.21	0.56
1:K:162:GLU:CD	1:K:162:GLU:H	2.08	0.56
1:G:63:ARG:NH2	1:L:63:ARG:NH2	2.51	0.55
1:C:112:GLN:O	1:C:116:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:ASN:HD22	1:F:73:GLN:HE21	1.49	0.55
1:L:114:LEU:HD13	1:L:137:TYR:HB3	1.88	0.55
1:L:159:GLY:O	1:L:162:GLU:HG2	2.06	0.55
1:I:135:THR:HG22	1:I:136:HIS:CD2	2.42	0.55
1:L:68:LYS:HZ2	1:L:68:LYS:CB	2.20	0.55
1:F:68:LYS:HZ2	1:F:68:LYS:HB3	1.72	0.55
1:K:63:ARG:HD2	1:K:67:GLU:OE2	2.07	0.55
1:H:69:LEU:HD13	1:H:137:TYR:OH	2.07	0.55
1:L:63:ARG:HD3	5:L:542:HOH:O	2.08	0.55
1:A:90:ARG:NH1	1:A:98:ASN:HD21	2.05	0.54
1:E:19:ALA:HB1	1:E:117:LEU:CD1	2.37	0.54
1:G:68:LYS:HD3	1:G:136:HIS:CD2	2.37	0.54
1:H:50:ASN:HB2	1:H:171:ASP:OD1	2.07	0.54
1:J:141:GLN:O	1:J:145:ILE:HG12	2.07	0.54
1:A:107:GLU:HA	1:A:107:GLU:OE1	2.08	0.54
1:C:97:LEU:HD23	1:C:161:PRO:HD3	1.88	0.54
1:B:69:LEU:HD13	1:B:137:TYR:OH	2.07	0.54
1:C:161:PRO:HD2	1:C:162:GLU:OE2	2.07	0.54
1:H:139:ASN:ND2	1:H:139:ASN:H	2.04	0.54
1:L:76:ARG:HH11	1:L:76:ARG:CG	2.21	0.54
1:A:76:ARG:NH1	1:A:76:ARG:CG	2.64	0.54
1:F:72:LEU:HD22	1:F:132:PHE:CD2	2.43	0.54
1:K:19:ALA:HB1	1:K:117:LEU:CD1	2.37	0.54
1:E:106:LEU:O	1:E:110:VAL:HG23	2.08	0.54
1:F:159:GLY:O	1:F:162:GLU:HG2	2.07	0.54
1:D:141:GLN:O	1:D:145:ILE:HG12	2.08	0.54
1:L:72:LEU:HD22	1:L:132:PHE:CD2	2.43	0.54
1:H:23:GLN:HG3	1:H:69:LEU:HD21	1.90	0.54
1:F:76:ARG:HH11	1:F:76:ARG:CG	2.20	0.53
1:C:135:THR:HG22	1:C:136:HIS:CD2	2.44	0.53
1:G:50:ASN:HB2	1:G:171:ASP:OD1	2.08	0.53
1:D:129:LEU:O	1:D:133:ILE:HG12	2.08	0.53
1:F:97:LEU:O	1:F:101:GLU:HG3	2.08	0.53
1:G:63:ARG:HD3	5:L:563:HOH:O	2.08	0.53
1:C:12:TYR:OH	1:C:73:GLN:NE2	2.42	0.53
1:G:135:THR:HG22	1:G:135:THR:O	2.08	0.53
1:J:129:LEU:O	1:J:133:ILE:HG12	2.08	0.53
1:B:50:ASN:HB2	1:B:171:ASP:OD1	2.09	0.53
1:E:49:LYS:O	1:E:52:ALA:HB3	2.09	0.53
1:G:76:ARG:HH11	1:G:76:ARG:CG	1.99	0.53
1:J:78:GLY:O	1:J:79:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:CYS:HB2	5:G:833:HOH:O	2.08	0.52
1:I:68:LYS:NZ	1:I:136:HIS:HB3	2.24	0.52
1:L:24:ILE:HG12	1:L:69:LEU:HB3	1.90	0.52
1:G:90:ARG:NH1	1:G:98:ASN:HD21	2.06	0.52
1:G:107:GLU:OE1	1:G:107:GLU:HA	2.08	0.52
1:B:139:ASN:ND2	1:B:139:ASN:H	2.05	0.52
1:J:69:LEU:HD13	1:J:137:TYR:CZ	2.44	0.52
1:C:68:LYS:NZ	1:C:136:HIS:HB3	2.25	0.52
1:G:112:GLN:O	1:G:116:GLU:HG2	2.10	0.52
1:H:159:GLY:O	1:H:162:GLU:HG2	2.10	0.52
1:D:22:ARG:NE	5:D:181:HOH:O	2.41	0.52
1:L:19:ALA:HB1	1:L:117:LEU:HD13	1.91	0.52
1:E:141:GLN:HE21	1:E:141:GLN:HA	1.74	0.52
1:L:172:LYS:HE2	5:L:556:HOH:O	2.09	0.52
1:K:5:THR:N	5:K:184:HOH:O	2.43	0.52
1:E:114:LEU:HD13	1:E:137:TYR:HB3	1.92	0.52
1:I:161:PRO:HD2	1:I:162:GLU:OE2	2.09	0.52
1:L:72:LEU:HD22	1:L:132:PHE:CE2	2.45	0.52
1:D:69:LEU:HD13	1:D:137:TYR:CZ	2.45	0.51
1:F:24:ILE:HD13	1:F:70:MET:HG2	1.92	0.51
1:L:20:ILE:HD11	1:L:129:LEU:HD11	1.92	0.51
1:A:35:LEU:CD2	1:F:70:MET:HE1	2.34	0.51
1:F:68:LYS:CB	1:F:68:LYS:NZ	2.73	0.51
1:D:90:ARG:HD3	1:D:90:ARG:N	2.26	0.51
1:F:72:LEU:HD22	1:F:132:PHE:CE2	2.45	0.51
1:K:141:GLN:HE21	1:K:141:GLN:HA	1.74	0.51
1:A:50:ASN:HB2	1:A:171:ASP:OD1	2.10	0.51
1:A:112:GLN:O	1:A:116:GLU:HG2	2.11	0.51
1:K:106:LEU:O	1:K:110:VAL:HG23	2.11	0.51
1:F:19:ALA:HB1	1:F:117:LEU:HD13	1.93	0.51
1:K:49:LYS:O	1:K:52:ALA:HB3	2.10	0.51
1:J:72:LEU:HD22	1:J:132:PHE:CD2	2.46	0.51
1:A:135:THR:O	1:A:135:THR:HG22	2.10	0.51
1:I:97:LEU:HA	1:I:155:LEU:HD13	1.94	0.50
1:L:68:LYS:NZ	1:L:68:LYS:CB	2.74	0.50
1:F:20:ILE:HD11	1:F:129:LEU:HD11	1.91	0.50
1:G:35:LEU:HD11	1:L:70:MET:HE3	1.93	0.50
1:L:97:LEU:O	1:L:101:GLU:HG3	2.11	0.50
1:H:76:ARG:NH1	1:H:128:HIS:HD2	2.09	0.50
1:B:159:GLY:O	1:B:162:GLU:HG2	2.11	0.50
1:D:145:ILE:HG22	1:F:8:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:GLN:OE1	1:F:58:GLN:HA	2.12	0.50
1:G:35:LEU:CD2	1:L:70:MET:HE1	2.37	0.50
1:I:22:ARG:HG2	1:I:22:ARG:HH11	1.76	0.50
1:F:21:ASN:HD22	1:F:73:GLN:NE2	2.07	0.50
1:C:133:ILE:HG22	1:C:138:LEU:HG	1.94	0.50
1:D:78:GLY:O	1:D:79:ARG:NH1	2.44	0.50
1:G:15:ASP:OD2	1:G:124:LYS:NZ	2.45	0.50
1:H:63:ARG:HD2	1:H:67:GLU:OE2	2.12	0.50
1:A:15:ASP:OD2	1:A:124:LYS:NZ	2.45	0.49
1:F:116:GLU:HG2	1:H:123:ASP:OD2	2.12	0.49
1:H:25:ASN:ND2	1:H:83:GLN:HB2	2.27	0.49
1:H:13:ASP:OD2	1:H:124:LYS:HD2	2.12	0.49
1:H:134:GLU:HA	1:H:138:LEU:HD12	1.94	0.49
1:C:97:LEU:HA	1:C:155:LEU:HD13	1.93	0.49
1:L:24:ILE:HD13	1:L:70:MET:HG2	1.94	0.49
1:A:127:PRO:HB3	1:E:118:HIS:CE1	2.47	0.49
1:J:24:ILE:HG12	1:J:69:LEU:HB3	1.95	0.49
1:J:90:ARG:HD3	1:J:90:ARG:N	2.27	0.49
1:A:90:ARG:HH12	1:A:98:ASN:HD21	1.60	0.49
1:B:139:ASN:HA	1:D:128:HIS:CE1	2.48	0.49
1:G:76:ARG:HD2	1:G:128:HIS:HD2	1.78	0.49
1:H:63:ARG:HG3	4:H:538:MPD:CM	2.43	0.49
1:A:64:CYS:SG	5:A:813:HOH:O	2.48	0.49
1:B:90:ARG:HH11	1:B:90:ARG:CG	2.25	0.49
1:J:145:ILE:HG22	1:L:8:VAL:HB	1.94	0.49
1:I:12:TYR:OH	1:I:73:GLN:NE2	2.45	0.49
1:B:63:ARG:HD3	5:B:821:HOH:O	2.13	0.49
1:H:86:LYS:NZ	1:H:87:LYS:HG2	2.27	0.49
1:H:106:LEU:O	1:H:109:ASN:HB2	2.12	0.49
1:L:72:LEU:HD13	1:L:132:PHE:CD1	2.48	0.49
1:I:133:ILE:HG22	1:I:138:LEU:HG	1.94	0.48
1:A:63:ARG:HH21	1:F:63:ARG:NH2	2.09	0.48
1:L:90:ARG:HG2	1:L:90:ARG:NH1	2.28	0.48
1:B:13:ASP:OD2	1:B:124:LYS:HD2	2.12	0.48
1:D:72:LEU:HD22	1:D:132:PHE:CD2	2.48	0.48
1:D:90:ARG:CG	5:D:186:HOH:O	2.61	0.48
1:G:67:GLU:OE2	1:L:56:LEU:HD11	2.13	0.48
1:J:162:GLU:H	1:J:162:GLU:CD	2.16	0.48
1:B:25:ASN:ND2	1:B:83:GLN:HB2	2.28	0.48
1:F:12:TYR:HB2	1:F:76:ARG:NH1	2.29	0.48
1:F:72:LEU:HD13	1:F:132:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:ALA:HA	5:I:748:HOH:O	2.12	0.48
1:L:12:TYR:HB2	1:L:76:ARG:NH1	2.28	0.48
1:C:78:GLY:O	1:C:79:ARG:HD3	2.14	0.48
1:E:141:GLN:HA	1:E:141:GLN:NE2	2.29	0.48
1:L:22:ARG:HG2	1:L:22:ARG:HH11	1.79	0.48
1:A:76:ARG:HD2	1:A:128:HIS:HD2	1.77	0.48
1:B:86:LYS:NZ	1:B:87:LYS:HG2	2.29	0.48
1:D:161:PRO:HD2	1:D:162:GLU:OE2	2.14	0.48
1:I:72:LEU:HD22	1:I:132:PHE:CE2	2.49	0.48
1:L:21:ASN:HD22	1:L:73:GLN:NE2	2.09	0.48
1:L:58:GLN:HA	1:L:58:GLN:OE1	2.13	0.48
1:H:139:ASN:HA	1:J:128:HIS:CE1	2.49	0.48
1:K:141:GLN:HA	1:K:141:GLN:NE2	2.29	0.48
1:D:24:ILE:HG12	1:D:69:LEU:HB3	1.96	0.48
1:F:90:ARG:HG2	1:F:90:ARG:NH1	2.27	0.48
1:F:21:ASN:HD21	1:F:73:GLN:HE21	1.59	0.47
1:F:71:LYS:O	1:F:75:GLN:HG3	2.15	0.47
1:B:76:ARG:NH1	1:B:128:HIS:HD2	2.11	0.47
1:G:90:ARG:HH12	1:G:98:ASN:HD21	1.62	0.47
1:K:114:LEU:HD13	1:K:137:TYR:HB3	1.94	0.47
1:D:162:GLU:CD	1:D:162:GLU:H	2.17	0.47
1:I:162:GLU:CD	1:I:162:GLU:H	2.18	0.47
1:A:67:GLU:OE2	1:F:56:LEU:HD11	2.13	0.47
1:B:106:LEU:O	1:B:109:ASN:HB2	2.13	0.47
1:B:134:GLU:HA	1:B:138:LEU:HD12	1.96	0.47
1:A:133:ILE:HG22	1:A:138:LEU:HG	1.97	0.47
1:G:127:PRO:HB3	1:K:118:HIS:CE1	2.50	0.47
1:I:78:GLY:O	1:I:79:ARG:HD3	2.15	0.47
1:J:161:PRO:HD2	1:J:162:GLU:OE2	2.14	0.47
1:A:106:LEU:O	1:A:110:VAL:HG23	2.15	0.47
1:G:63:ARG:HH21	1:L:63:ARG:NH2	2.08	0.47
1:C:72:LEU:HD22	1:C:132:PHE:CE2	2.49	0.46
1:H:41:PHE:HA	1:H:46:VAL:HG11	1.96	0.46
1:C:162:GLU:H	1:C:162:GLU:CD	2.18	0.46
1:L:71:LYS:O	1:L:75:GLN:HG3	2.16	0.46
1:F:22:ARG:HH11	1:F:22:ARG:HG2	1.80	0.46
1:G:58:GLN:O	1:G:61:GLU:HB2	2.15	0.46
1:C:22:ARG:HG2	1:C:22:ARG:HH11	1.81	0.46
1:G:133:ILE:HG22	1:G:138:LEU:HG	1.97	0.46
1:L:21:ASN:HD21	1:L:73:GLN:HE21	1.59	0.46
1:E:20:ILE:CD1	1:E:117:LEU:HD21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:PHE:HA	1:B:46:VAL:HG11	1.98	0.46
1:G:106:LEU:O	1:G:110:VAL:HG23	2.16	0.46
1:B:71:LYS:HE2	5:B:833:HOH:O	2.15	0.46
1:C:23:GLN:HE22	1:C:26:LEU:HD23	1.81	0.46
1:D:90:ARG:HG2	5:D:186:HOH:O	2.14	0.46
1:C:73:GLN:NE2	1:C:78:GLY:HA3	2.30	0.46
1:A:35:LEU:HD11	1:F:70:MET:HE3	1.98	0.45
1:A:22:ARG:HH11	1:A:22:ARG:CG	2.29	0.45
1:B:23:GLN:CG	1:B:69:LEU:HD21	2.45	0.45
1:E:5:THR:N	5:E:653:HOH:O	2.49	0.45
1:E:139:ASN:HB2	5:E:649:HOH:O	2.15	0.45
1:I:69:LEU:HD12	1:I:69:LEU:HA	1.79	0.45
1:A:97:LEU:HA	1:A:155:LEU:HD13	1.98	0.45
1:C:50:ASN:HB2	1:C:171:ASP:OD1	2.17	0.45
1:L:63:ARG:HG3	4:L:537:MPD:HM1	1.98	0.45
1:L:114:LEU:HD12	1:L:141:GLN:HG3	1.99	0.45
1:A:9:ARG:NH2	1:A:17:GLU:OE2	2.49	0.45
1:C:41:PHE:HA	1:C:46:VAL:HG11	1.98	0.45
1:F:114:LEU:HD12	1:F:141:GLN:HG3	1.98	0.45
1:I:68:LYS:HZ3	1:I:136:HIS:HB3	1.81	0.45
1:L:26:LEU:HD21	1:L:110:VAL:HA	1.99	0.45
1:B:28:LEU:HD13	1:B:85:ILE:HD11	1.99	0.45
1:H:49:LYS:HA	1:H:49:LYS:HD3	1.84	0.45
1:J:142:VAL:HG21	1:L:128:HIS:CD2	2.52	0.45
1:C:138:LEU:HD22	5:C:565:HOH:O	2.15	0.45
1:E:139:ASN:CB	5:E:649:HOH:O	2.64	0.45
1:E:141:GLN:HE21	1:E:141:GLN:CA	2.29	0.45
1:I:73:GLN:NE2	1:I:78:GLY:HA3	2.32	0.45
1:B:5:THR:N	5:B:829:HOH:O	2.49	0.45
1:I:6:SER:OG	1:I:8:VAL:HG22	2.17	0.45
1:A:168:TYR:O	1:A:171:ASP:HB3	2.17	0.45
1:H:23:GLN:CG	1:H:69:LEU:HD21	2.47	0.45
1:I:50:ASN:HB2	1:I:171:ASP:OD1	2.17	0.45
1:E:101:GLU:OE2	1:E:156:ARG:NH1	2.50	0.45
1:G:24:ILE:HG12	1:G:69:LEU:HB3	1.99	0.44
1:D:142:VAL:HG21	1:F:128:HIS:CD2	2.53	0.44
1:H:117:LEU:HG	1:H:133:ILE:CD1	2.48	0.44
1:I:134:GLU:HA	1:I:138:LEU:HD12	1.99	0.44
1:A:146:LYS:HD3	1:C:75:GLN:HA	2.00	0.44
1:C:134:GLU:HA	1:C:138:LEU:HD12	1.98	0.44
1:F:63:ARG:NH1	1:F:64[B]:CYS:SG	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:63:ARG:HG2	1:J:63:ARG:HH11	1.82	0.44
1:K:101:GLU:OE2	1:K:156:ARG:NH1	2.50	0.44
1:B:68:LYS:HB2	1:B:68:LYS:HE3	1.81	0.44
1:D:63:ARG:HG2	1:D:63:ARG:HH11	1.83	0.44
1:K:107:GLU:OE2	1:K:107:GLU:HA	2.18	0.44
1:A:58:GLN:O	1:A:61:GLU:HB2	2.18	0.44
1:G:168:TYR:O	1:G:171:ASP:HB3	2.17	0.44
1:B:69:LEU:HD12	1:B:69:LEU:HA	1.87	0.44
1:E:159:GLY:O	1:E:162:GLU:HG2	2.17	0.44
1:G:76:ARG:NH1	1:G:76:ARG:CG	2.65	0.44
1:E:107:GLU:HA	1:E:107:GLU:OE2	2.18	0.43
1:G:97:LEU:HA	1:G:155:LEU:HD13	2.00	0.43
1:G:146:LYS:HD3	1:I:75:GLN:HA	2.00	0.43
1:H:69:LEU:HD12	1:H:69:LEU:HA	1.86	0.43
1:L:76:ARG:CG	1:L:76:ARG:NH1	2.80	0.43
1:F:72:LEU:HD13	1:F:132:PHE:CE1	2.53	0.43
1:I:119:LYS:HA	5:I:732:HOH:O	2.18	0.43
1:D:42:ASP:OD1	1:D:49:LYS:HE3	2.18	0.43
1:B:49:LYS:HA	1:B:49:LYS:HD3	1.84	0.43
1:B:117:LEU:HG	1:B:133:ILE:CD1	2.48	0.43
1:D:97:LEU:HD23	1:D:161:PRO:HD3	2.00	0.43
1:I:23:GLN:HE22	1:I:26:LEU:HD23	1.83	0.43
1:L:72:LEU:HD13	1:L:132:PHE:CE1	2.54	0.43
1:D:23:GLN:CG	1:D:69:LEU:HD21	2.46	0.43
1:K:20:ILE:CD1	1:K:117:LEU:HD21	2.47	0.43
1:D:76:ARG:HD2	1:D:76:ARG:HA	1.81	0.43
1:E:90:ARG:HH11	1:E:90:ARG:CG	2.26	0.43
1:J:76:ARG:HD2	1:J:76:ARG:HA	1.79	0.43
1:I:82:LEU:HA	5:I:743:HOH:O	2.18	0.43
1:J:42:ASP:OD1	1:J:49:LYS:HE3	2.18	0.43
1:J:76:ARG:HH11	1:J:128:HIS:HD2	1.66	0.43
1:K:33:VAL:O	1:K:36:SER:HB3	2.19	0.43
1:I:79:ARG:HD3	1:I:79:ARG:HA	1.80	0.43
1:J:106:LEU:O	1:J:110:VAL:HG23	2.18	0.43
1:A:63:ARG:HD3	5:F:542:HOH:O	2.17	0.43
1:I:63:ARG:HD2	1:I:67:GLU:OE2	2.19	0.43
1:K:159:GLY:O	1:K:162:GLU:HG2	2.17	0.43
1:E:134:GLU:HA	1:E:138:LEU:CD1	2.44	0.42
1:A:24:ILE:HG12	1:A:69:LEU:HB3	1.99	0.42
1:C:6:SER:OG	1:C:8:VAL:HG22	2.19	0.42
1:C:63:ARG:NH1	5:C:563:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:ARG:HA	1:G:79:ARG:HD3	1.81	0.42
1:D:135:THR:HG22	1:D:136:HIS:CD2	2.55	0.42
1:J:97:LEU:HD23	1:J:161:PRO:HD3	2.00	0.42
1:K:90:ARG:HH11	1:K:90:ARG:CG	2.27	0.42
1:L:9:ARG:NH2	1:L:12:TYR:O	2.47	0.42
1:A:22:ARG:HG2	1:A:22:ARG:NH1	2.30	0.42
1:B:28:LEU:HB3	1:B:85:ILE:HD12	2.00	0.42
1:C:63:ARG:HD2	1:C:67:GLU:OE2	2.20	0.42
1:H:90:ARG:HH11	1:H:90:ARG:CG	2.28	0.42
1:K:141:GLN:HE21	1:K:141:GLN:CA	2.29	0.42
1:L:19:ALA:CB	1:L:117:LEU:HD13	2.49	0.42
1:D:76:ARG:HH11	1:D:128:HIS:HD2	1.68	0.42
1:K:104:LEU:HD12	1:K:104:LEU:O	2.20	0.42
1:L:139:ASN:ND2	5:L:561:HOH:O	2.33	0.42
1:A:35:LEU:HD11	1:F:70:MET:CE	2.50	0.42
1:I:41:PHE:HA	1:I:46:VAL:HG11	2.01	0.42
1:A:43:ARG:HB3	1:A:45:ASP:OD1	2.20	0.42
1:F:9:ARG:NH2	1:F:12:TYR:O	2.48	0.42
1:F:26:LEU:HD21	1:F:110:VAL:HA	2.00	0.42
1:F:117:LEU:HG	1:F:133:ILE:HD11	2.01	0.42
1:B:19:ALA:HB1	1:B:117:LEU:HD13	2.02	0.41
1:G:9:ARG:NH2	1:G:17:GLU:OE2	2.51	0.41
1:H:28:LEU:HD13	1:H:85:ILE:HD11	2.02	0.41
1:A:75:GLN:HA	1:E:146:LYS:HD3	2.02	0.41
1:D:107:GLU:HG3	1:D:148:LEU:HD12	2.02	0.41
1:E:83:GLN:O	1:E:84:ASP:C	2.59	0.41
1:J:21:ASN:ND2	1:J:73:GLN:NE2	2.68	0.41
1:D:90:ARG:HH11	1:D:90:ARG:CG	2.32	0.41
1:D:106:LEU:O	1:D:110:VAL:HG23	2.21	0.41
1:C:104:LEU:HD11	1:C:145:ILE:HG23	2.03	0.41
1:E:104:LEU:O	1:E:104:LEU:HD12	2.20	0.41
1:G:22:ARG:HG2	1:G:22:ARG:NH1	2.30	0.41
1:L:89:ASP:C	1:L:90:ARG:HG3	2.41	0.41
1:B:124:LYS:HD3	1:B:124:LYS:HA	1.92	0.41
1:F:112:GLN:O	1:F:116:GLU:HG3	2.21	0.41
1:G:75:GLN:HA	1:K:146:LYS:HD3	2.03	0.41
1:J:107:GLU:HG3	1:J:148:LEU:HD12	2.01	0.41
1:L:117:LEU:HG	1:L:133:ILE:HD11	2.02	0.41
1:A:8:VAL:HB	1:E:145:ILE:HG22	2.03	0.41
1:D:21:ASN:ND2	1:D:73:GLN:NE2	2.69	0.41
1:F:20:ILE:O	1:F:24:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:ARG:HB3	1:G:45:ASP:OD1	2.20	0.41
1:L:119:LYS:HD3	1:L:119:LYS:O	2.21	0.41
1:F:112:GLN:OE1	1:H:120:LEU:HD22	2.21	0.41
1:G:17:GLU:HB2	5:G:835:HOH:O	2.21	0.41
1:I:106:LEU:O	1:I:110:VAL:HG23	2.21	0.41
1:A:63:ARG:HH21	1:F:63:ARG:HE	1.69	0.41
1:D:37:MET:O	1:D:40:TYR:HB3	2.21	0.41
1:G:67:GLU:HB3	1:L:39:TYR:OH	2.21	0.41
1:H:28:LEU:HB3	1:H:85:ILE:HD12	2.03	0.40
1:K:24:ILE:CG1	1:K:69:LEU:HB3	2.48	0.40
1:L:50:ASN:HB2	1:L:171:ASP:OD1	2.21	0.40
1:E:90:ARG:CG	1:E:90:ARG:NH1	2.84	0.40
1:F:104:LEU:CD1	1:F:145:ILE:HG23	2.51	0.40
1:G:14:GLN:H	1:G:14:GLN:HG2	1.49	0.40
1:H:127:PRO:HB3	1:L:118:HIS:CE1	2.55	0.40
1:D:49:LYS:HD3	1:D:49:LYS:HA	1.97	0.40
1:F:21:ASN:OD1	1:F:81:PHE:N	2.52	0.40
1:G:135:THR:O	1:G:135:THR:CG2	2.69	0.40
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.90	0.40
1:E:90:ARG:HG2	1:E:90:ARG:NH1	2.30	0.40
1:L:68:LYS:HB3	1:L:68:LYS:HZ2	1.80	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	170/176 (97%)	161 (95%)	8 (5%)	1 (1%)	25	48
1	B	170/176 (97%)	162 (95%)	7 (4%)	1 (1%)	25	48
1	C	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	D	171/176 (97%)	164 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	171/176 (97%)	165 (96%)	5 (3%)	1 (1%)	25	48
1	F	171/176 (97%)	167 (98%)	4 (2%)	0	100	100
1	G	170/176 (97%)	160 (94%)	9 (5%)	1 (1%)	25	48
1	H	170/176 (97%)	162 (95%)	7 (4%)	1 (1%)	25	48
1	I	170/176 (97%)	163 (96%)	7 (4%)	0	100	100
1	J	170/176 (97%)	163 (96%)	7 (4%)	0	100	100
1	K	171/176 (97%)	164 (96%)	6 (4%)	1 (1%)	25	48
1	L	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
All	All	2044/2112 (97%)	1960 (96%)	78 (4%)	6 (0%)	41	65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	GLU
1	B	94	GLU
1	G	94	GLU
1	H	94	GLU
1	E	94	GLU
1	K	94	GLU

### 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	152/155 (98%)	144 (95%)	8 (5%)	22	46
1	B	152/155 (98%)	148 (97%)	4 (3%)	46	73
1	C	152/155 (98%)	145 (95%)	7 (5%)	27	52
1	D	153/155 (99%)	147 (96%)	6 (4%)	32	59
1	E	153/155 (99%)	147 (96%)	6 (4%)	32	59
1	F	153/155 (99%)	145 (95%)	8 (5%)	23	47
1	G	152/155 (98%)	144 (95%)	8 (5%)	22	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	152/155 (98%)	147 (97%)	5 (3%)	38	66
1	I	152/155 (98%)	145 (95%)	7 (5%)	27	52
1	J	152/155 (98%)	146 (96%)	6 (4%)	32	59
1	K	153/155 (99%)	147 (96%)	6 (4%)	32	59
1	L	152/155 (98%)	144 (95%)	8 (5%)	22	46
All	All	1828/1860 (98%)	1749 (96%)	79 (4%)	29	55

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	22	ARG
1	A	32	TYR
1	A	63	ARG
1	A	69	LEU
1	A	76	ARG
1	A	90	ARG
1	A	136	HIS
1	B	69	LEU
1	B	79	ARG
1	B	139	ASN
1	B	147	CYS
1	C	22	ARG
1	C	32	TYR
1	C	53	LYS
1	C	69	LEU
1	C	90	ARG
1	C	92	ASP
1	C	162	GLU
1	D	64[A]	CYS
1	D	64[B]	CYS
1	D	69	LEU
1	D	90	ARG
1	D	146	LYS
1	D	147	CYS
1	E	20	ILE
1	E	22	ARG
1	E	32	TYR
1	E	69	LEU
1	E	75	GLN

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Mol	Chain	Res	Type
1	E	147	CYS
1	F	32	TYR
1	F	68	LYS
1	F	69	LEU
1	F	76	ARG
1	F	86	LYS
1	F	119	LYS
1	F	139	ASN
1	F	147	CYS
1	G	14	GLN
1	G	22	ARG
1	G	32	TYR
1	G	63	ARG
1	G	69	LEU
1	G	76	ARG
1	G	90	ARG
1	G	136	HIS
1	H	32	TYR
1	H	69	LEU
1	H	79	ARG
1	H	139	ASN
1	H	147	CYS
1	I	22	ARG
1	I	32	TYR
1	I	53	LYS
1	I	69	LEU
1	I	90	ARG
1	I	92	ASP
1	I	162	GLU
1	J	32	TYR
1	J	64	CYS
1	J	69	LEU
1	J	90	ARG
1	J	146	LYS
1	J	147	CYS
1	K	20	ILE
1	K	22	ARG
1	K	32	TYR
1	K	69	LEU
1	K	75	GLN
1	K	147	CYS
1	L	32	TYR

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Mol	Chain	Res	Type
1	L	68	LYS
1	L	69	LEU
1	L	76	ARG
1	L	86	LYS
1	L	119	LYS
1	L	139	ASN
1	L	147	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	128	HIS
1	A	139	ASN
1	B	14	GLN
1	B	25	ASN
1	B	125	ASN
1	B	128	HIS
1	B	139	ASN
1	C	23	GLN
1	C	73	GLN
1	C	75	GLN
1	C	109	ASN
1	C	128	HIS
1	C	154	ASN
1	D	75	GLN
1	D	128	HIS
1	D	154	ASN
1	E	58	GLN
1	E	65	HIS
1	E	73	GLN
1	E	75	GLN
1	E	105	GLN
1	E	109	ASN
1	E	128	HIS
1	E	141	GLN
1	E	154	ASN
1	F	14	GLN
1	F	21	ASN
1	F	109	ASN
1	F	136	HIS
1	F	139	ASN

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Mol	Chain	Res	Type
1	F	154	ASN
1	G	25	ASN
1	G	98	ASN
1	G	128	HIS
1	G	139	ASN
1	H	7	GLN
1	H	14	GLN
1	H	125	ASN
1	H	128	HIS
1	H	139	ASN
1	I	23	GLN
1	I	73	GLN
1	I	75	GLN
1	I	109	ASN
1	I	128	HIS
1	I	154	ASN
1	J	75	GLN
1	J	128	HIS
1	J	154	ASN
1	K	73	GLN
1	K	75	GLN
1	K	105	GLN
1	K	109	ASN
1	K	128	HIS
1	K	141	GLN
1	K	154	ASN
1	L	14	GLN
1	L	21	ASN
1	L	109	ASN
1	L	136	HIS
1	L	154	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	MPD	I	539	-	7,7,7	1.47	1 (14%)	9,10,10	1.39	2 (22%)
4	MPD	F	533	-	7,7,7	1.13	1 (14%)	9,10,10	1.50	1 (11%)
4	MPD	H	538	-	7,7,7	1.37	1 (14%)	9,10,10	1.49	2 (22%)
4	MPD	L	537	-	7,7,7	1.22	1 (14%)	9,10,10	1.50	1 (11%)
4	MPD	B	630	-	7,7,7	1.11	1 (14%)	9,10,10	1.52	2 (22%)
4	MPD	E	631	-	7,7,7	1.12	1 (14%)	9,10,10	1.52	2 (22%)
4	MPD	C	535	-	7,7,7	1.32	1 (14%)	9,10,10	1.43	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	I	539	-	1/1/2/2	2/5/5/5	-
4	MPD	F	533	-	1/1/2/2	0/5/5/5	-
4	MPD	H	538	-	1/1/2/2	3/5/5/5	-
4	MPD	L	537	-	1/1/2/2	1/5/5/5	-
4	MPD	B	630	-	1/1/2/2	2/5/5/5	-
4	MPD	E	631	-	1/1/2/2	2/5/5/5	-
4	MPD	C	535	-	1/1/2/2	1/5/5/5	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	539	MPD	O2-C2	-2.93	1.37	1.44
4	C	535	MPD	O2-C2	-2.71	1.37	1.44
4	L	537	MPD	O2-C2	-2.68	1.37	1.44
4	H	538	MPD	O2-C2	-2.58	1.38	1.44
4	F	533	MPD	O2-C2	-2.27	1.38	1.44
4	E	631	MPD	O2-C2	-2.15	1.39	1.44
4	B	630	MPD	O2-C2	-2.14	1.39	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	533	MPD	O4-C4-C3	3.63	126.01	111.36
4	E	631	MPD	O4-C4-C3	3.59	125.86	111.36
4	B	630	MPD	O4-C4-C3	3.59	125.85	111.36
4	L	537	MPD	O4-C4-C3	3.54	125.66	111.36
4	H	538	MPD	O4-C4-C3	3.46	125.32	111.36
4	C	535	MPD	O4-C4-C3	3.44	125.26	111.36
4	I	539	MPD	O4-C4-C3	3.21	124.31	111.36
4	B	630	MPD	CM-C2-C1	-2.30	105.79	110.57
4	E	631	MPD	CM-C2-C1	-2.27	105.84	110.57
4	H	538	MPD	CM-C2-C1	-2.18	106.04	110.57
4	I	539	MPD	O4-C4-C5	-2.10	100.28	109.38

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	630	MPD	C4
4	C	535	MPD	C4
4	E	631	MPD	C4
4	F	533	MPD	C4
4	H	538	MPD	C4
4	I	539	MPD	C4
4	L	537	MPD	C4

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	538	MPD	O2-C2-C3-C4
4	H	538	MPD	CM-C2-C3-C4
4	B	630	MPD	O2-C2-C3-C4
4	E	631	MPD	O2-C2-C3-C4
4	I	539	MPD	O2-C2-C3-C4
4	B	630	MPD	CM-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	E	631	MPD	CM-C2-C3-C4
4	H	538	MPD	C1-C2-C3-C4
4	I	539	MPD	C1-C2-C3-C4
4	C	535	MPD	O2-C2-C3-C4
4	L	537	MPD	O2-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	538	MPD	1	0
4	L	537	MPD	1	0

## 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.