



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:21 am BST

PDB ID : 1JI4  
Title : NAP protein from helicobacter pylori  
Authors : Zanotti, G.; Papinutto, E.; Dundon, W.G.; Battistutta, R.; Seveso, M.; Del Giudice, G.; Rappuoli, R.; Montecucco, C.  
Deposited on : 2001-06-29  
Resolution : 2.52 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) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

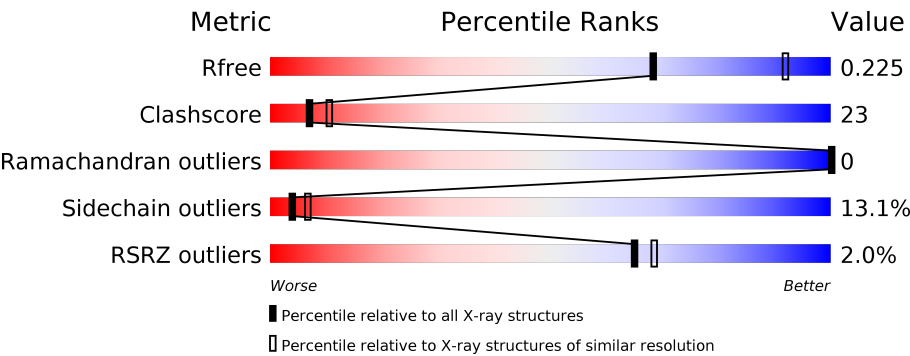
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.52 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	144	<div><div>3%</div><div><div></div><div>60%</div><div>33%</div><div>7%</div></div></div>
1	B	144	<div><div>3%</div><div><div></div><div>60%</div><div>33%</div><div>8%</div></div></div>
1	C	144	<div><div>2%</div><div><div></div><div>59%</div><div>34%</div><div>7%</div></div></div>
1	D	144	<div><div>2%</div><div><div></div><div>60%</div><div>33%</div><div>7%</div></div></div>
1	E	144	<div><div>%</div><div><div></div><div>60%</div><div>34%</div><div>6%</div></div></div>
1	F	144	<div><div>%</div><div><div></div><div>59%</div><div>35%</div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	144	
1	H	144	
1	I	144	
1	J	144	
1	K	144	
1	L	144	

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	UNX	D	808	-	-	-	X
3	UNX	E	810	-	-	-	X
3	UNX	J	820	-	-	-	X
3	UNX	L	824	-	-	-	X
4	MPD	A	700	-	-	-	X
4	MPD	B	701	-	-	-	X
4	MPD	C	702	-	-	-	X
4	MPD	D	703	-	-	-	X
4	MPD	E	704	-	-	-	X
4	MPD	F	705	-	-	-	X
4	MPD	G	706	-	-	-	X
4	MPD	H	707	-	-	-	X
4	MPD	I	708	-	-	-	X
4	MPD	J	709	-	-	-	X
4	MPD	K	710	-	-	-	X
4	MPD	L	711	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15118 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 NEUTROPHIL-ACTIVATING PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1196	773	194	225	4			
1	B	144	Total	C	N	O	S	0	0	0
			1196	773	194	225	4			
1	C	144	Total	C	N	O	S	0	0	0
			1196	773	194	225	4			
1	D	144	Total	C	N	O	S	0	0	0
			1196	773	194	225	4			
1	E	144	Total	C	N	O	S	0	0	0
			1196	773	194	225	4			
1	F	144	Total	C	N	O	S	0	0	0
			1196	773	194	225	4			
1	G	144	Total	C	N	O	S	0	0	0
			1196	773	194	225	4			
1	H	144	Total	C	N	O	S	0	0	0
			1196	773	194	225	4			
1	I	144	Total	C	N	O	S	0	0	0
			1196	773	194	225	4			
1	J	144	Total	C	N	O	S	0	0	0
			1196	773	194	225	4			
1	K	144	Total	C	N	O	S	0	0	0
			1196	773	194	225	4			
1	L	144	Total	C	N	O	S	0	0	0
			1196	773	194	225	4			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Fe	0	0
			1	1		
2	J	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe 1 1	0	0
2	K	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

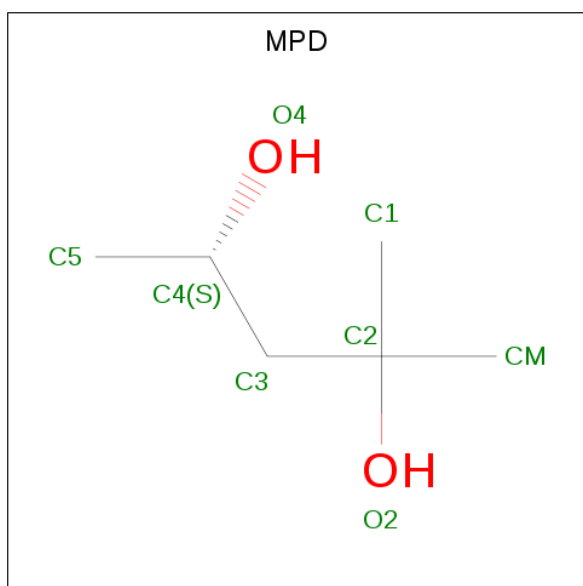
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total X 1 1	0	0
3	J	1	Total X 1 1	0	0
3	D	1	Total X 1 1	0	0
3	K	1	Total X 1 1	0	0
3	E	1	Total X 1 1	0	0
3	H	1	Total X 1 1	0	0
3	B	1	Total X 1 1	0	0
3	I	1	Total X 1 1	0	0
3	C	1	Total X 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	X	0	0
			1	1		
3	L	1	Total	X	0	0
			1	1		
3	F	1	Total	X	0	0
			1	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	D	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	G	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total	C	O	0	0
			8	6	2		
4	J	1	Total	C	O	0	0
			8	6	2		
4	K	1	Total	C	O	0	0
			8	6	2		
4	L	1	Total	C	O	0	0
			8	6	2		

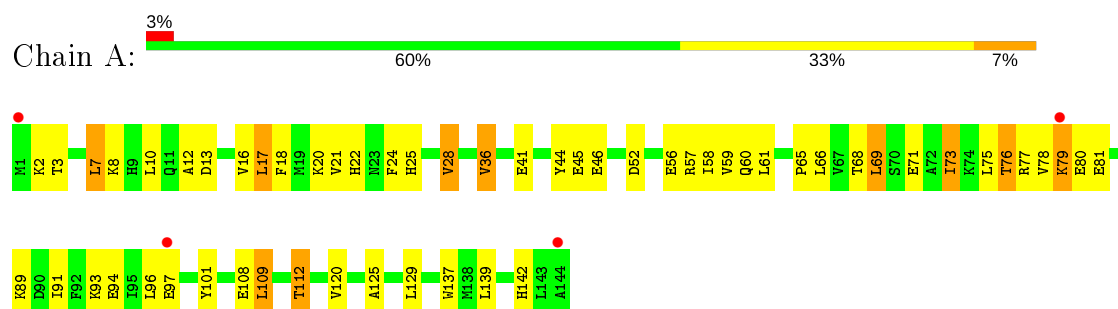
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total	O	0	0
			54	54		
5	B	54	Total	O	0	0
			54	54		
5	C	54	Total	O	0	0
			54	54		
5	D	54	Total	O	0	0
			54	54		
5	E	55	Total	O	0	0
			55	55		
5	F	53	Total	O	0	0
			53	53		
5	G	54	Total	O	0	0
			54	54		
5	H	54	Total	O	0	0
			54	54		
5	I	54	Total	O	0	0
			54	54		
5	J	53	Total	O	0	0
			53	53		
5	K	54	Total	O	0	0
			54	54		
5	L	53	Total	O	0	0
			53	53		

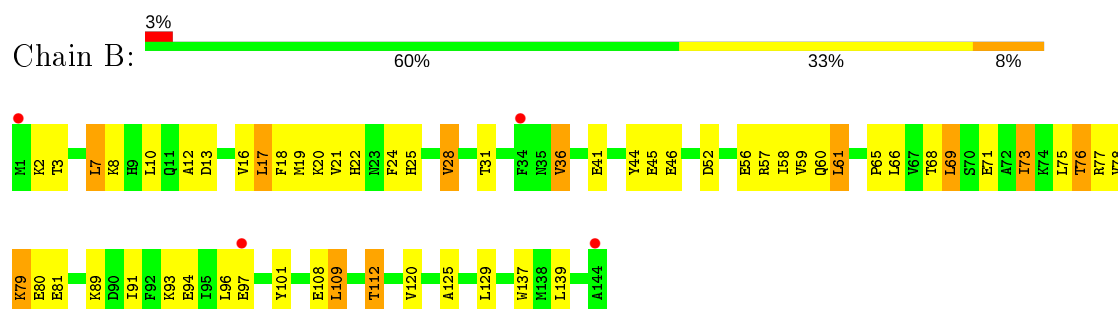
### 3 Residue-property plots [i](#)

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

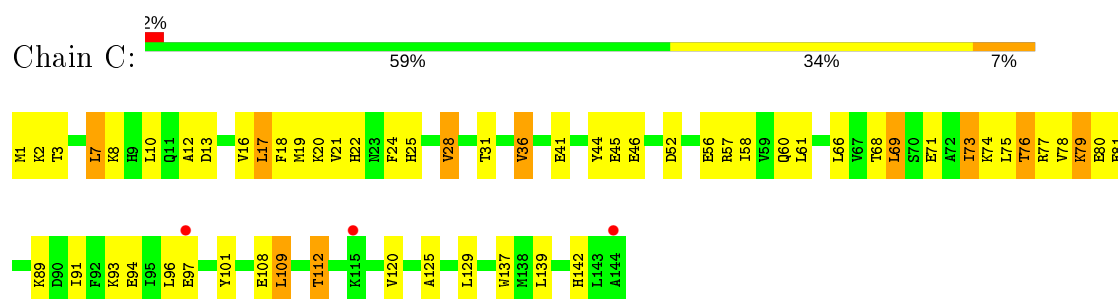
#### • Molecule 1: NEUTROPHIL-ACTIVATING PROTEIN A



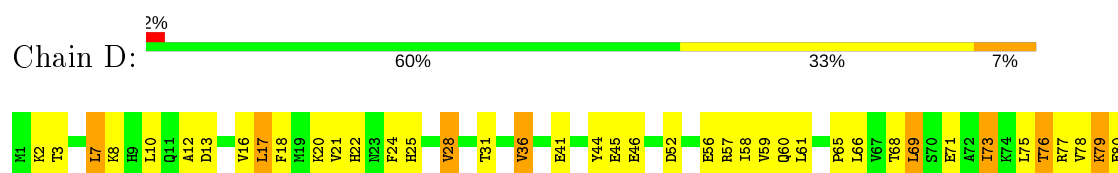
#### • Molecule 1: NEUTROPHIL-ACTIVATING PROTEIN A



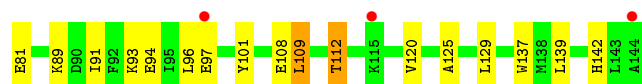
#### • Molecule 1: NEUTROPHIL-ACTIVATING PROTEIN A



#### • Molecule 1: NEUTROPHIL-ACTIVATING PROTEIN A







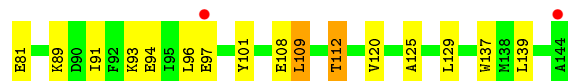
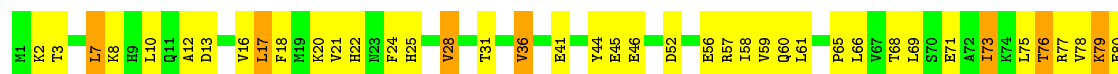
● Molecule 1: NEUTROPHIL-ACTIVATING PROTEIN A



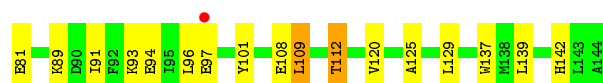
● Molecule 1: NEUTROPHIL-ACTIVATING PROTEIN A



● Molecule 1: NEUTROPHIL-ACTIVATING PROTEIN A

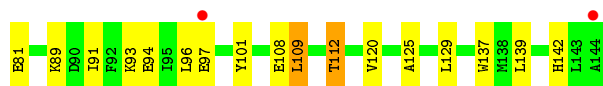


● Molecule 1: NEUTROPHIL-ACTIVATING PROTEIN A



● Molecule 1: NEUTROPHIL-ACTIVATING PROTEIN A





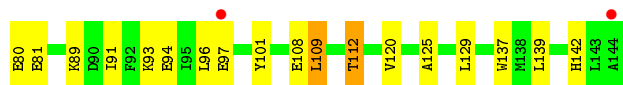
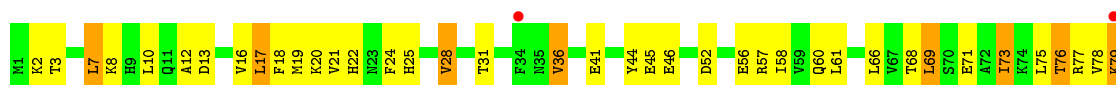
● Molecule 1: NEUTROPHIL-ACTIVATING PROTEIN A



● Molecule 1: NEUTROPHIL-ACTIVATING PROTEIN A



● Molecule 1: NEUTROPHIL-ACTIVATING PROTEIN A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.78 Å 133.22 Å 95.23 Å 90.00° 93.99° 90.00°	Depositor
Resolution (Å)	20.81 – 2.52 20.81 – 2.52	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.81-2.52) 96.8 (20.81-2.52)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.53 (at 2.53 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.215 , 0.224 0.216 , 0.225	Depositor DCC
$R_{free}$ test set	7263 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	15118	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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: UNX, MPD, FE

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	0.42	0/1222	0.64	0/1643
1	B	0.42	0/1222	0.64	0/1643
1	C	0.42	0/1222	0.64	0/1643
1	D	0.42	0/1222	0.64	0/1643
1	E	0.42	0/1222	0.64	0/1643
1	F	0.42	0/1222	0.64	0/1643
1	G	0.42	0/1222	0.64	0/1643
1	H	0.42	0/1222	0.64	0/1643
1	I	0.42	0/1222	0.64	0/1643
1	J	0.42	0/1222	0.64	0/1643
1	K	0.42	0/1222	0.64	0/1643
1	L	0.42	0/1222	0.64	0/1643
All	All	0.42	0/14664	0.64	0/19716

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1196	0	1187	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1196	0	1187	57	0
1	C	1196	0	1187	59	0
1	D	1196	0	1187	61	0
1	E	1196	0	1187	60	0
1	F	1196	0	1187	60	0
1	G	1196	0	1187	57	0
1	H	1196	0	1187	61	0
1	I	1196	0	1187	58	0
1	J	1196	0	1187	56	0
1	K	1196	0	1187	53	0
1	L	1196	0	1187	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	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
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	8	0	14	3	0
4	B	8	0	14	3	0
4	C	8	0	14	4	0
4	D	8	0	14	4	0
4	E	8	0	14	4	0
4	F	8	0	14	4	0
4	G	8	0	14	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	8	0	14	4	0
4	I	8	0	14	4	0
4	J	8	0	14	4	0
4	K	8	0	14	4	0
4	L	8	0	14	3	0
5	A	54	0	0	3	1
5	B	54	0	0	3	1
5	C	54	0	0	4	0
5	D	54	0	0	2	0
5	E	55	0	0	3	1
5	F	53	0	0	3	0
5	G	54	0	0	3	1
5	H	54	0	0	3	0
5	I	54	0	0	3	0
5	J	53	0	0	3	0
5	K	54	0	0	3	0
5	L	53	0	0	3	0
All	All	15118	0	14412	660	2

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 23.

All (660) 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:79:LYS:HA	1:C:79:LYS:HE2	1.52	0.90
1:J:79:LYS:HE2	1:J:79:LYS:HA	1.52	0.90
1:K:79:LYS:HE2	1:K:79:LYS:HA	1.52	0.90
1:E:79:LYS:HE2	1:E:79:LYS:HA	1.52	0.90
1:I:79:LYS:HE2	1:I:79:LYS:HA	1.52	0.90
1:E:73:ILE:HD11	1:H:73:ILE:HD11	1.54	0.90
1:G:79:LYS:HE2	1:G:79:LYS:HA	1.52	0.90
1:H:79:LYS:HE2	1:H:79:LYS:HA	1.52	0.89
1:L:79:LYS:HA	1:L:79:LYS:HE2	1.52	0.89
1:B:79:LYS:HE2	1:B:79:LYS:HA	1.52	0.89
1:F:79:LYS:HA	1:F:79:LYS:HE2	1.52	0.89
1:A:79:LYS:HE2	1:A:79:LYS:HA	1.52	0.89
1:D:79:LYS:HA	1:D:79:LYS:HE2	1.52	0.89
1:E:93:LYS:O	1:E:97:GLU:HG2	1.74	0.88
1:C:93:LYS:O	1:C:97:GLU:HG2	1.74	0.88
1:G:93:LYS:O	1:G:97:GLU:HG2	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LYS:O	1:A:97:GLU:HG2	1.74	0.88
1:B:93:LYS:O	1:B:97:GLU:HG2	1.74	0.88
1:D:93:LYS:O	1:D:97:GLU:HG2	1.74	0.87
1:K:93:LYS:O	1:K:97:GLU:HG2	1.74	0.87
1:H:93:LYS:O	1:H:97:GLU:HG2	1.74	0.87
1:F:93:LYS:O	1:F:97:GLU:HG2	1.74	0.87
1:A:73:ILE:HD11	1:D:73:ILE:HD11	1.57	0.87
1:I:93:LYS:O	1:I:97:GLU:HG2	1.74	0.87
1:L:93:LYS:O	1:L:97:GLU:HG2	1.74	0.86
1:J:93:LYS:O	1:J:97:GLU:HG2	1.74	0.86
1:F:73:ILE:HD11	1:G:73:ILE:HD11	1.58	0.85
1:E:46:GLU:HG2	4:E:704:MPD:H11	1.59	0.84
1:H:46:GLU:HG2	4:H:707:MPD:H11	1.59	0.84
1:I:46:GLU:HG2	4:I:708:MPD:H11	1.59	0.84
1:D:21:VAL:CG2	1:D:44:TYR:HB3	2.08	0.84
1:C:46:GLU:HG2	4:C:702:MPD:H11	1.60	0.84
1:I:21:VAL:CG2	1:I:44:TYR:HB3	2.08	0.84
1:K:21:VAL:CG2	1:K:44:TYR:HB3	2.08	0.84
1:K:46:GLU:HG2	4:K:710:MPD:H11	1.60	0.84
1:E:21:VAL:CG2	1:E:44:TYR:HB3	2.08	0.83
1:L:46:GLU:HG2	4:L:711:MPD:H11	1.59	0.83
1:A:21:VAL:CG2	1:A:44:TYR:HB3	2.08	0.83
1:G:21:VAL:CG2	1:G:44:TYR:HB3	2.08	0.83
1:L:21:VAL:CG2	1:L:44:TYR:HB3	2.08	0.83
1:F:46:GLU:HG2	4:F:705:MPD:H11	1.59	0.83
1:G:46:GLU:HG2	4:G:706:MPD:H11	1.59	0.83
1:B:21:VAL:CG2	1:B:44:TYR:HB3	2.08	0.83
1:J:21:VAL:CG2	1:J:44:TYR:HB3	2.08	0.83
1:H:21:VAL:CG2	1:H:44:TYR:HB3	2.08	0.83
1:A:46:GLU:HG2	4:A:700:MPD:H11	1.59	0.83
1:C:21:VAL:CG2	1:C:44:TYR:HB3	2.08	0.83
1:B:46:GLU:HG2	4:B:701:MPD:H11	1.59	0.82
1:F:21:VAL:CG2	1:F:44:TYR:HB3	2.08	0.82
1:D:46:GLU:HG2	4:D:703:MPD:H11	1.59	0.82
1:B:73:ILE:HD11	1:C:73:ILE:HD11	1.62	0.81
1:J:46:GLU:HG2	4:J:709:MPD:H11	1.59	0.81
1:J:2:LYS:N	1:J:2:LYS:HD2	1.98	0.79
1:K:2:LYS:HD2	1:K:2:LYS:N	1.98	0.79
1:D:2:LYS:N	1:D:2:LYS:HD2	1.98	0.79
1:E:2:LYS:HD2	1:E:2:LYS:N	1.98	0.79
1:H:2:LYS:HD2	1:H:2:LYS:N	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2:LYS:N	1:L:2:LYS:HD2	1.98	0.79
1:B:2:LYS:N	1:B:2:LYS:HD2	1.98	0.79
1:G:2:LYS:N	1:G:2:LYS:HD2	1.98	0.79
1:J:73:ILE:HD11	1:K:73:ILE:HD11	1.65	0.79
1:A:2:LYS:N	1:A:2:LYS:HD2	1.98	0.79
1:I:2:LYS:N	1:I:2:LYS:HD2	1.98	0.78
1:C:2:LYS:HD2	1:C:2:LYS:N	1.98	0.78
1:F:2:LYS:N	1:F:2:LYS:HD2	1.98	0.78
1:D:66:LEU:HD21	1:D:75:LEU:HD22	1.66	0.78
1:C:66:LEU:HD21	1:C:75:LEU:HD22	1.66	0.77
1:A:66:LEU:HD21	1:A:75:LEU:HD22	1.66	0.77
1:I:66:LEU:HD21	1:I:75:LEU:HD22	1.66	0.77
1:B:66:LEU:HD21	1:B:75:LEU:HD22	1.67	0.77
1:F:66:LEU:HD21	1:F:75:LEU:HD22	1.66	0.77
1:F:108:GLU:O	1:F:112:THR:HG23	1.85	0.77
1:K:66:LEU:HD21	1:K:75:LEU:HD22	1.66	0.77
1:B:108:GLU:O	1:B:112:THR:HG23	1.85	0.77
1:D:108:GLU:O	1:D:112:THR:HG23	1.85	0.77
1:K:108:GLU:O	1:K:112:THR:HG23	1.85	0.76
1:A:108:GLU:O	1:A:112:THR:HG23	1.85	0.76
1:E:66:LEU:HD21	1:E:75:LEU:HD22	1.67	0.76
1:C:108:GLU:O	1:C:112:THR:HG23	1.85	0.76
1:H:108:GLU:O	1:H:112:THR:HG23	1.85	0.76
1:L:66:LEU:HD21	1:L:75:LEU:HD22	1.66	0.76
1:A:24:PHE:O	1:A:28:VAL:HG22	1.86	0.76
1:E:108:GLU:O	1:E:112:THR:HG23	1.85	0.76
1:F:24:PHE:O	1:F:28:VAL:HG22	1.86	0.76
1:J:66:LEU:HD21	1:J:75:LEU:HD22	1.66	0.76
1:J:108:GLU:O	1:J:112:THR:HG23	1.85	0.76
1:G:66:LEU:HD21	1:G:75:LEU:HD22	1.66	0.76
1:H:66:LEU:HD21	1:H:75:LEU:HD22	1.66	0.76
1:G:24:PHE:O	1:G:28:VAL:HG22	1.86	0.75
1:H:24:PHE:O	1:H:28:VAL:HG22	1.86	0.75
1:D:24:PHE:O	1:D:28:VAL:HG22	1.86	0.75
1:K:24:PHE:O	1:K:28:VAL:HG22	1.86	0.75
1:J:24:PHE:O	1:J:28:VAL:HG22	1.86	0.75
1:L:108:GLU:O	1:L:112:THR:HG23	1.85	0.75
1:L:24:PHE:O	1:L:28:VAL:HG22	1.86	0.75
1:G:108:GLU:O	1:G:112:THR:HG23	1.85	0.74
1:I:108:GLU:O	1:I:112:THR:HG23	1.85	0.74
1:E:24:PHE:O	1:E:28:VAL:HG22	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:PHE:O	1:C:28:VAL:HG22	1.86	0.74
1:B:24:PHE:O	1:B:28:VAL:HG22	1.86	0.74
1:I:24:PHE:O	1:I:28:VAL:HG22	1.86	0.74
1:H:31:THR:HA	1:L:142:HIS:CE1	2.26	0.70
1:I:73:ILE:HD11	1:L:73:ILE:HD11	1.75	0.69
4:L:711:MPD:O4	4:L:711:MPD:HM3	1.93	0.69
4:D:703:MPD:O4	4:D:703:MPD:HM3	1.93	0.68
4:J:709:MPD:O4	4:J:709:MPD:HM3	1.93	0.68
4:C:702:MPD:HM3	4:C:702:MPD:O4	1.93	0.68
4:A:700:MPD:O4	4:A:700:MPD:HM3	1.93	0.68
4:K:710:MPD:HM3	4:K:710:MPD:O4	1.93	0.67
4:G:706:MPD:O4	4:G:706:MPD:HM3	1.93	0.67
4:F:705:MPD:HM3	4:F:705:MPD:O4	1.93	0.67
4:I:708:MPD:HM3	4:I:708:MPD:O4	1.93	0.67
4:H:707:MPD:HM3	4:H:707:MPD:O4	1.93	0.66
1:A:77:ARG:HG3	1:A:77:ARG:HH11	1.61	0.66
4:B:701:MPD:HM3	4:B:701:MPD:O4	1.93	0.66
1:K:77:ARG:HG3	1:K:77:ARG:HH11	1.61	0.66
4:E:704:MPD:O4	4:E:704:MPD:HM3	1.93	0.66
1:I:77:ARG:HG3	1:I:77:ARG:HH11	1.61	0.66
1:J:77:ARG:HG3	1:J:77:ARG:HH11	1.61	0.66
1:F:77:ARG:HG3	1:F:77:ARG:HH11	1.61	0.66
1:L:77:ARG:HG3	1:L:77:ARG:HH11	1.61	0.65
1:E:77:ARG:HG3	1:E:77:ARG:HH11	1.61	0.65
1:G:77:ARG:HH11	1:G:77:ARG:HG3	1.61	0.65
1:G:97:GLU:HB2	5:G:832:HOH:O	1.97	0.65
1:B:77:ARG:HH11	1:B:77:ARG:HG3	1.61	0.65
1:C:77:ARG:HG3	1:C:77:ARG:HH11	1.61	0.65
1:H:77:ARG:HG3	1:H:77:ARG:HH11	1.61	0.65
1:I:97:GLU:HB2	5:I:459:HOH:O	1.97	0.65
1:D:77:ARG:HG3	1:D:77:ARG:HH11	1.61	0.65
1:E:97:GLU:HB2	5:E:825:HOH:O	1.97	0.65
1:A:20:LYS:HE2	1:A:94:GLU:OE1	1.97	0.65
1:G:20:LYS:HE2	1:G:94:GLU:OE1	1.97	0.65
1:F:20:LYS:HE2	1:F:94:GLU:OE1	1.97	0.65
1:L:20:LYS:HE2	1:L:94:GLU:OE1	1.97	0.65
1:J:20:LYS:HE2	1:J:94:GLU:OE1	1.97	0.64
1:F:97:GLU:HB2	5:F:824:HOH:O	1.97	0.64
1:H:97:GLU:HB2	5:H:834:HOH:O	1.97	0.64
1:C:97:GLU:HB2	5:C:819:HOH:O	1.97	0.64
1:B:20:LYS:HE2	1:B:94:GLU:OE1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:GLU:HB2	5:D:822:HOH:O	1.97	0.64
1:C:20:LYS:HE2	1:C:94:GLU:OE1	1.97	0.64
1:I:20:LYS:HE2	1:I:94:GLU:OE1	1.97	0.64
1:K:97:GLU:HB2	5:K:842:HOH:O	1.97	0.64
1:D:20:LYS:HE2	1:D:94:GLU:OE1	1.97	0.64
1:A:97:GLU:HB2	5:A:814:HOH:O	1.97	0.64
1:D:57:ARG:HH11	1:D:60:GLN:HE21	1.46	0.64
1:B:97:GLU:HB2	5:B:812:HOH:O	1.97	0.64
1:L:97:GLU:HB2	5:L:843:HOH:O	1.97	0.64
1:K:20:LYS:HE2	1:K:94:GLU:OE1	1.97	0.64
1:E:20:LYS:HE2	1:E:94:GLU:OE1	1.97	0.63
1:J:97:GLU:HB2	5:J:834:HOH:O	1.97	0.63
1:L:109:LEU:HD13	1:L:125:ALA:HB2	1.81	0.63
1:E:57:ARG:HH11	1:E:60:GLN:HE21	1.46	0.63
1:E:80:GLU:HG2	1:H:68:THR:HG22	1.80	0.63
1:I:2:LYS:H	1:I:2:LYS:HD2	1.63	0.63
1:F:57:ARG:HH11	1:F:60:GLN:HE21	1.46	0.63
1:E:16:VAL:HG21	1:E:76:THR:HG21	1.81	0.63
1:H:20:LYS:HE2	1:H:94:GLU:OE1	1.97	0.63
1:L:57:ARG:HH11	1:L:60:GLN:HE21	1.46	0.63
1:I:57:ARG:HH11	1:I:60:GLN:HE21	1.46	0.63
1:A:109:LEU:HD13	1:A:125:ALA:HB2	1.81	0.63
1:B:16:VAL:HG21	1:B:76:THR:HG21	1.81	0.63
1:D:2:LYS:H	1:D:2:LYS:HD2	1.63	0.63
1:I:16:VAL:HG21	1:I:76:THR:HG21	1.81	0.63
1:D:109:LEU:HD13	1:D:125:ALA:HB2	1.81	0.62
1:F:16:VAL:HG21	1:F:76:THR:HG21	1.81	0.62
1:H:57:ARG:HH11	1:H:60:GLN:HE21	1.46	0.62
1:J:16:VAL:HG21	1:J:76:THR:HG21	1.81	0.62
1:L:16:VAL:HG21	1:L:76:THR:HG21	1.81	0.62
1:A:16:VAL:HG21	1:A:76:THR:HG21	1.81	0.62
1:C:57:ARG:HH11	1:C:60:GLN:HE21	1.46	0.62
1:G:2:LYS:H	1:G:2:LYS:HD2	1.64	0.62
1:B:109:LEU:HD13	1:B:125:ALA:HB2	1.81	0.62
1:C:109:LEU:HD13	1:C:125:ALA:HB2	1.80	0.62
1:D:16:VAL:HG21	1:D:76:THR:HG21	1.81	0.62
1:H:109:LEU:HD13	1:H:125:ALA:HB2	1.81	0.62
1:K:16:VAL:HG21	1:K:76:THR:HG21	1.81	0.62
1:G:109:LEU:HD13	1:G:125:ALA:HB2	1.81	0.62
1:I:109:LEU:HD13	1:I:125:ALA:HB2	1.81	0.62
1:G:57:ARG:HH11	1:G:60:GLN:HE21	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LYS:H	1:A:2:LYS:HD2	1.63	0.62
1:F:80:GLU:HG2	1:G:68:THR:HG22	1.82	0.62
1:K:57:ARG:HH11	1:K:60:GLN:HE21	1.46	0.62
1:F:109:LEU:HD13	1:F:125:ALA:HB2	1.81	0.62
1:J:57:ARG:HH11	1:J:60:GLN:HE21	1.46	0.62
1:A:57:ARG:HH11	1:A:60:GLN:HE21	1.46	0.62
1:B:57:ARG:HH11	1:B:60:GLN:HE21	1.46	0.62
1:H:16:VAL:HG21	1:H:76:THR:HG21	1.81	0.62
1:C:16:VAL:HG21	1:C:76:THR:HG21	1.81	0.62
1:E:2:LYS:HD2	1:E:2:LYS:H	1.64	0.61
1:G:16:VAL:HG21	1:G:76:THR:HG21	1.81	0.61
1:H:2:LYS:HD2	1:H:2:LYS:H	1.64	0.61
1:K:109:LEU:HD13	1:K:125:ALA:HB2	1.81	0.61
1:A:57:ARG:HH11	1:A:60:GLN:NE2	1.98	0.61
1:B:57:ARG:HH11	1:B:60:GLN:NE2	1.98	0.61
1:C:2:LYS:H	1:C:2:LYS:HD2	1.63	0.61
1:F:57:ARG:HH11	1:F:60:GLN:NE2	1.98	0.61
1:J:109:LEU:HD13	1:J:125:ALA:HB2	1.81	0.61
1:J:2:LYS:H	1:J:2:LYS:HD2	1.64	0.61
1:J:57:ARG:HH11	1:J:60:GLN:NE2	1.98	0.61
1:B:2:LYS:H	1:B:2:LYS:HD2	1.63	0.61
1:E:109:LEU:HD13	1:E:125:ALA:HB2	1.81	0.61
1:H:57:ARG:HH11	1:H:60:GLN:NE2	1.98	0.61
1:E:68:THR:HG22	1:H:80:GLU:HG2	1.81	0.61
1:K:57:ARG:HH11	1:K:60:GLN:NE2	1.98	0.61
1:E:80:GLU:HG2	1:H:68:THR:CG2	2.31	0.61
1:G:57:ARG:HH11	1:G:60:GLN:NE2	1.98	0.61
1:D:57:ARG:HH11	1:D:60:GLN:NE2	1.98	0.61
1:C:57:ARG:HH11	1:C:60:GLN:NE2	1.98	0.61
1:L:57:ARG:HH11	1:L:60:GLN:NE2	1.98	0.60
1:A:46:GLU:CG	4:A:700:MPD:H11	2.32	0.60
1:L:2:LYS:H	1:L:2:LYS:HD2	1.63	0.60
1:E:68:THR:CG2	1:H:80:GLU:HG2	2.31	0.60
1:E:57:ARG:HH11	1:E:60:GLN:NE2	1.98	0.60
1:D:46:GLU:CG	4:D:703:MPD:H11	2.32	0.60
1:K:2:LYS:HD2	1:K:2:LYS:H	1.63	0.60
1:B:46:GLU:CG	4:B:701:MPD:H11	2.32	0.59
1:I:57:ARG:HH11	1:I:60:GLN:NE2	1.98	0.59
1:A:68:THR:HG22	1:D:80:GLU:HG2	1.84	0.59
1:K:46:GLU:CG	4:K:710:MPD:H11	2.32	0.59
1:L:46:GLU:CG	4:L:711:MPD:H11	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ALA:HB2	1:B:66:LEU:HD11	1.85	0.59
1:E:46:GLU:CG	4:E:704:MPD:H11	2.32	0.59
1:F:46:GLU:CG	4:F:705:MPD:H11	2.31	0.59
1:F:2:LYS:H	1:F:2:LYS:HD2	1.64	0.59
1:H:41:GLU:O	1:H:45:GLU:HG2	2.03	0.59
1:I:41:GLU:O	1:I:45:GLU:HG2	2.03	0.59
1:G:41:GLU:O	1:G:45:GLU:HG2	2.03	0.58
1:E:12:ALA:HB2	1:E:66:LEU:HD11	1.85	0.58
1:E:41:GLU:O	1:E:45:GLU:HG2	2.03	0.58
1:D:41:GLU:O	1:D:45:GLU:HG2	2.03	0.58
1:L:41:GLU:O	1:L:45:GLU:HG2	2.03	0.58
1:A:13:ASP:OD1	1:A:76:THR:HG22	2.04	0.58
1:D:13:ASP:OD1	1:D:76:THR:HG22	2.04	0.58
1:G:12:ALA:HB2	1:G:66:LEU:HD11	1.85	0.58
1:K:12:ALA:HB2	1:K:66:LEU:HD11	1.85	0.58
1:L:12:ALA:HB2	1:L:66:LEU:HD11	1.85	0.58
1:F:12:ALA:HB2	1:F:66:LEU:HD11	1.85	0.58
1:H:12:ALA:HB2	1:H:66:LEU:HD11	1.85	0.58
1:J:41:GLU:O	1:J:45:GLU:HG2	2.03	0.58
1:B:41:GLU:O	1:B:45:GLU:HG2	2.03	0.58
1:C:41:GLU:O	1:C:45:GLU:HG2	2.03	0.58
1:I:13:ASP:OD1	1:I:76:THR:HG22	2.04	0.58
1:K:13:ASP:OD1	1:K:76:THR:HG22	2.04	0.58
1:A:12:ALA:HB2	1:A:66:LEU:HD11	1.85	0.58
1:F:13:ASP:OD1	1:F:76:THR:HG22	2.04	0.58
1:B:13:ASP:OD1	1:B:76:THR:HG22	2.04	0.58
1:D:12:ALA:HB2	1:D:66:LEU:HD11	1.85	0.57
1:F:80:GLU:HG2	1:G:68:THR:CG2	2.34	0.57
1:J:12:ALA:HB2	1:J:66:LEU:HD11	1.85	0.57
1:L:13:ASP:OD1	1:L:76:THR:HG22	2.04	0.57
1:A:41:GLU:O	1:A:45:GLU:HG2	2.03	0.57
1:C:12:ALA:HB2	1:C:66:LEU:HD11	1.85	0.57
1:C:46:GLU:CG	4:C:702:MPD:H11	2.32	0.57
1:H:46:GLU:CG	4:H:707:MPD:H11	2.32	0.57
1:I:46:GLU:CG	4:I:708:MPD:H11	2.32	0.57
1:I:12:ALA:HB2	1:I:66:LEU:HD11	1.85	0.57
1:H:13:ASP:OD1	1:H:76:THR:HG22	2.04	0.57
1:F:41:GLU:O	1:F:45:GLU:HG2	2.03	0.57
1:J:13:ASP:OD1	1:J:76:THR:HG22	2.04	0.57
1:K:41:GLU:O	1:K:45:GLU:HG2	2.03	0.57
1:G:13:ASP:OD1	1:G:76:THR:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:46:GLU:CG	4:J:709:MPD:H11	2.32	0.57
1:G:46:GLU:CG	4:G:706:MPD:H11	2.32	0.57
1:E:13:ASP:OD1	1:E:76:THR:HG22	2.04	0.56
1:C:13:ASP:OD1	1:C:76:THR:HG22	2.04	0.56
1:D:18:PHE:O	1:D:22:HIS:HD2	1.89	0.56
1:G:18:PHE:O	1:G:22:HIS:HD2	1.89	0.56
1:A:68:THR:CG2	1:D:80:GLU:HG2	2.35	0.56
1:B:68:THR:OG1	1:B:71:GLU:HG3	2.07	0.56
1:J:18:PHE:O	1:J:22:HIS:HD2	1.89	0.56
1:B:18:PHE:O	1:B:22:HIS:HD2	1.89	0.55
1:I:18:PHE:O	1:I:22:HIS:HD2	1.89	0.55
1:K:68:THR:OG1	1:K:71:GLU:HG3	2.07	0.55
1:A:18:PHE:O	1:A:22:HIS:HD2	1.89	0.55
1:G:68:THR:OG1	1:G:71:GLU:HG3	2.07	0.55
1:H:18:PHE:O	1:H:22:HIS:HD2	1.89	0.55
1:J:68:THR:OG1	1:J:71:GLU:HG3	2.06	0.55
1:L:18:PHE:O	1:L:22:HIS:HD2	1.89	0.55
1:A:68:THR:OG1	1:A:71:GLU:HG3	2.07	0.55
1:C:68:THR:OG1	1:C:71:GLU:HG3	2.07	0.55
1:D:68:THR:OG1	1:D:71:GLU:HG3	2.07	0.55
1:D:77:ARG:HG3	1:D:77:ARG:NH1	2.22	0.55
1:F:68:THR:HG22	1:G:80:GLU:HG2	1.88	0.55
1:L:77:ARG:NH1	1:L:77:ARG:HG3	2.22	0.55
1:E:68:THR:OG1	1:E:71:GLU:HG3	2.07	0.55
1:F:68:THR:CG2	1:G:80:GLU:HG2	2.37	0.55
1:A:80:GLU:HG2	1:D:68:THR:HG22	1.89	0.55
1:E:18:PHE:O	1:E:22:HIS:HD2	1.89	0.55
1:F:18:PHE:O	1:F:22:HIS:HD2	1.89	0.55
1:L:68:THR:OG1	1:L:71:GLU:HG3	2.07	0.55
1:H:77:ARG:HG3	1:H:77:ARG:NH1	2.22	0.54
1:B:77:ARG:NH1	1:B:77:ARG:HG3	2.22	0.54
1:C:18:PHE:O	1:C:22:HIS:HD2	1.89	0.54
1:I:77:ARG:HG3	1:I:77:ARG:NH1	2.22	0.54
1:F:68:THR:OG1	1:F:71:GLU:HG3	2.06	0.54
1:H:68:THR:OG1	1:H:71:GLU:HG3	2.07	0.54
1:K:18:PHE:O	1:K:22:HIS:HD2	1.89	0.54
1:I:68:THR:OG1	1:I:71:GLU:HG3	2.06	0.54
1:K:77:ARG:NH1	1:K:77:ARG:HG3	2.22	0.54
1:C:77:ARG:NH1	1:C:77:ARG:HG3	2.22	0.53
1:E:77:ARG:HG3	1:E:77:ARG:NH1	2.22	0.53
1:B:28:VAL:HG21	1:B:36:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HG2	1:D:68:THR:CG2	2.39	0.53
1:J:28:VAL:HG21	1:J:36:VAL:HG22	1.91	0.53
1:J:69:LEU:HD13	1:K:19:MET:HG2	1.90	0.53
1:A:77:ARG:NH1	1:A:77:ARG:HG3	2.22	0.53
1:L:28:VAL:HG21	1:L:36:VAL:HG22	1.91	0.53
1:J:77:ARG:NH1	1:J:77:ARG:HG3	2.22	0.53
1:C:28:VAL:HG21	1:C:36:VAL:HG22	1.91	0.53
1:D:28:VAL:HG13	1:D:91:ILE:HD12	1.91	0.53
1:K:28:VAL:HG21	1:K:36:VAL:HG22	1.91	0.53
1:F:77:ARG:HG3	1:F:77:ARG:NH1	2.22	0.53
1:G:77:ARG:HG3	1:G:77:ARG:NH1	2.22	0.53
1:D:28:VAL:HG21	1:D:36:VAL:HG22	1.91	0.53
1:A:28:VAL:HG21	1:A:36:VAL:HG22	1.91	0.52
1:F:28:VAL:HG21	1:F:36:VAL:HG22	1.91	0.52
1:I:28:VAL:HG13	1:I:91:ILE:HD12	1.91	0.52
1:H:28:VAL:HG13	1:H:91:ILE:HD12	1.91	0.52
1:I:28:VAL:HG21	1:I:36:VAL:HG22	1.91	0.52
1:J:19:MET:HG2	1:K:69:LEU:HD13	1.91	0.52
1:B:28:VAL:HG13	1:B:91:ILE:HD12	1.91	0.52
1:K:28:VAL:HG13	1:K:91:ILE:HD12	1.91	0.52
1:C:28:VAL:HG13	1:C:91:ILE:HD12	1.91	0.52
1:L:79:LYS:NZ	1:L:80:GLU:H	2.08	0.52
1:A:28:VAL:HG13	1:A:91:ILE:HD12	1.91	0.52
1:E:79:LYS:NZ	1:E:80:GLU:H	2.08	0.52
1:E:80:GLU:HG2	1:H:68:THR:HB	1.91	0.52
1:F:28:VAL:HG13	1:F:91:ILE:HD12	1.91	0.52
1:I:79:LYS:NZ	1:I:80:GLU:H	2.08	0.52
1:K:79:LYS:NZ	1:K:80:GLU:H	2.08	0.52
1:E:28:VAL:HG21	1:E:36:VAL:HG22	1.91	0.51
1:E:68:THR:HB	1:H:80:GLU:HG2	1.91	0.51
1:L:28:VAL:HG13	1:L:91:ILE:HD12	1.91	0.51
1:G:28:VAL:HG21	1:G:36:VAL:HG22	1.91	0.51
1:J:79:LYS:NZ	1:J:80:GLU:H	2.08	0.51
1:J:28:VAL:HG13	1:J:91:ILE:HD12	1.91	0.51
1:A:79:LYS:HA	1:A:79:LYS:CE	2.34	0.51
1:B:79:LYS:NZ	1:B:80:GLU:H	2.08	0.51
1:H:79:LYS:NZ	1:H:80:GLU:H	2.08	0.51
1:D:79:LYS:HD3	1:D:80:GLU:N	2.26	0.51
1:G:79:LYS:NZ	1:G:80:GLU:H	2.08	0.51
1:G:28:VAL:HG13	1:G:91:ILE:HD12	1.91	0.51
1:H:28:VAL:HG21	1:H:36:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LYS:HD3	1:B:80:GLU:N	2.26	0.51
1:G:52:ASP:O	1:G:56:GLU:HG3	2.11	0.51
1:J:52:ASP:O	1:J:56:GLU:HG3	2.11	0.51
1:C:79:LYS:NZ	1:C:80:GLU:H	2.08	0.51
1:D:31:THR:HA	1:H:142:HIS:CE1	2.46	0.51
1:D:79:LYS:NZ	1:D:80:GLU:H	2.08	0.51
1:C:79:LYS:HD3	1:C:80:GLU:N	2.26	0.51
1:H:79:LYS:HD3	1:H:80:GLU:N	2.26	0.51
1:L:52:ASP:O	1:L:56:GLU:HG3	2.11	0.51
1:L:79:LYS:HD3	1:L:80:GLU:N	2.26	0.51
1:A:52:ASP:O	1:A:56:GLU:HG3	2.11	0.51
1:D:52:ASP:O	1:D:56:GLU:HG3	2.11	0.51
1:E:28:VAL:HG13	1:E:91:ILE:HD12	1.91	0.51
1:K:52:ASP:O	1:K:56:GLU:HG3	2.11	0.51
1:K:79:LYS:HD3	1:K:80:GLU:N	2.26	0.50
1:F:52:ASP:O	1:F:56:GLU:HG3	2.11	0.50
1:F:79:LYS:NZ	1:F:80:GLU:H	2.08	0.50
1:I:52:ASP:O	1:I:56:GLU:HG3	2.11	0.50
1:A:79:LYS:NZ	1:A:80:GLU:H	2.08	0.50
1:G:79:LYS:HD3	1:G:80:GLU:N	2.26	0.50
1:H:52:ASP:O	1:H:56:GLU:HG3	2.11	0.50
1:A:79:LYS:HD3	1:A:80:GLU:N	2.26	0.50
1:E:77:ARG:HB2	1:E:101:TYR:CZ	2.47	0.50
1:D:77:ARG:HB2	1:D:101:TYR:CZ	2.47	0.50
1:F:77:ARG:HB2	1:F:101:TYR:CZ	2.47	0.50
1:F:79:LYS:HD3	1:F:80:GLU:N	2.26	0.50
1:E:79:LYS:HD3	1:E:80:GLU:N	2.26	0.50
1:I:77:ARG:HB2	1:I:101:TYR:CZ	2.47	0.50
1:I:68:THR:HG22	1:L:80:GLU:HG2	1.94	0.50
1:L:28:VAL:HG13	1:L:91:ILE:CD1	2.42	0.50
1:B:28:VAL:HG13	1:B:91:ILE:CD1	2.42	0.50
1:C:28:VAL:HG13	1:C:91:ILE:CD1	2.42	0.50
1:H:89:LYS:HE2	1:H:93:LYS:HE3	1.94	0.50
1:L:77:ARG:HB2	1:L:101:TYR:CZ	2.47	0.50
1:B:52:ASP:O	1:B:56:GLU:HG3	2.11	0.50
1:E:80:GLU:HG2	1:H:68:THR:CB	2.41	0.50
1:L:89:LYS:HE2	1:L:93:LYS:HE3	1.94	0.50
1:A:28:VAL:HG13	1:A:91:ILE:CD1	2.42	0.50
1:J:79:LYS:HD3	1:J:80:GLU:N	2.26	0.50
1:J:28:VAL:HG13	1:J:91:ILE:CD1	2.42	0.50
1:K:77:ARG:HB2	1:K:101:TYR:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ARG:HB2	1:C:101:TYR:CZ	2.47	0.49
1:F:28:VAL:HG13	1:F:91:ILE:CD1	2.42	0.49
1:F:68:THR:HB	1:G:80:GLU:HG2	1.94	0.49
1:I:79:LYS:HD3	1:I:80:GLU:N	2.26	0.49
1:A:68:THR:HB	1:D:80:GLU:HG2	1.93	0.49
1:B:89:LYS:HE2	1:B:93:LYS:HE3	1.94	0.49
1:E:52:ASP:O	1:E:56:GLU:HG3	2.11	0.49
1:B:69:LEU:HD13	1:C:19:MET:HG2	1.94	0.49
1:H:77:ARG:HB2	1:H:101:TYR:CZ	2.47	0.49
1:I:89:LYS:HE2	1:I:93:LYS:HE3	1.94	0.49
1:G:77:ARG:HB2	1:G:101:TYR:CZ	2.47	0.49
1:I:28:VAL:HG13	1:I:91:ILE:CD1	2.42	0.49
1:E:68:THR:CB	1:H:80:GLU:HG2	2.42	0.49
1:J:77:ARG:HB2	1:J:101:TYR:CZ	2.47	0.49
1:A:77:ARG:HB2	1:A:101:TYR:CZ	2.47	0.49
1:B:79:LYS:CE	1:B:80:GLU:H	2.26	0.49
1:C:52:ASP:O	1:C:56:GLU:HG3	2.11	0.49
1:C:79:LYS:CE	1:C:80:GLU:H	2.26	0.49
1:D:89:LYS:HE2	1:D:93:LYS:HE3	1.94	0.49
1:E:89:LYS:HE2	1:E:93:LYS:HE3	1.94	0.49
1:E:28:VAL:HG13	1:E:91:ILE:CD1	2.42	0.49
1:H:28:VAL:HG13	1:H:91:ILE:CD1	2.42	0.49
1:D:28:VAL:HG13	1:D:91:ILE:CD1	2.42	0.49
1:D:79:LYS:CE	1:D:80:GLU:H	2.26	0.49
1:B:77:ARG:HB2	1:B:101:TYR:CZ	2.47	0.49
1:G:28:VAL:HG13	1:G:91:ILE:CD1	2.42	0.49
1:K:17:LEU:HD13	1:K:78:VAL:HG11	1.95	0.49
1:F:89:LYS:HE2	1:F:93:LYS:HE3	1.94	0.49
1:H:79:LYS:CE	1:H:80:GLU:H	2.26	0.49
1:J:89:LYS:HE2	1:J:93:LYS:HE3	1.94	0.49
1:C:17:LEU:HD13	1:C:78:VAL:HG11	1.95	0.49
1:I:17:LEU:HD13	1:I:78:VAL:HG11	1.95	0.49
1:L:79:LYS:CE	1:L:80:GLU:H	2.26	0.49
1:A:41:GLU:HA	1:A:44:TYR:CE2	2.48	0.48
1:G:89:LYS:HE2	1:G:93:LYS:HE3	1.94	0.48
1:J:22:HIS:HE1	5:K:843:HOH:O	1.96	0.48
1:K:41:GLU:HA	1:K:44:TYR:CE2	2.48	0.48
1:K:89:LYS:HE2	1:K:93:LYS:HE3	1.94	0.48
1:L:41:GLU:HA	1:L:44:TYR:CE2	2.48	0.48
1:I:80:GLU:HG2	1:L:68:THR:HG22	1.94	0.48
1:F:80:GLU:HG2	1:G:68:THR:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:28:VAL:HG13	1:K:91:ILE:CD1	2.42	0.48
1:K:79:LYS:CE	1:K:80:GLU:H	2.26	0.48
1:C:89:LYS:HE2	1:C:93:LYS:HE3	1.94	0.48
1:A:17:LEU:HD13	1:A:78:VAL:HG11	1.95	0.48
1:E:79:LYS:CE	1:E:80:GLU:H	2.26	0.48
1:G:79:LYS:CE	1:G:80:GLU:H	2.26	0.48
1:J:79:LYS:CE	1:J:80:GLU:H	2.26	0.48
1:C:74:LYS:NZ	5:C:857:HOH:O	2.47	0.48
1:E:17:LEU:HD13	1:E:78:VAL:HG11	1.95	0.48
1:F:74:LYS:NZ	5:F:816:HOH:O	2.46	0.48
1:A:79:LYS:CE	1:A:80:GLU:H	2.26	0.48
1:B:80:GLU:HG2	1:C:68:THR:HG22	1.95	0.48
1:D:41:GLU:HA	1:D:44:TYR:CE2	2.49	0.48
1:C:31:THR:HA	1:F:142:HIS:CE1	2.48	0.48
1:H:41:GLU:HA	1:H:44:TYR:CE2	2.48	0.48
1:B:41:GLU:HA	1:B:44:TYR:CE2	2.49	0.48
1:G:41:GLU:HA	1:G:44:TYR:CE2	2.48	0.48
1:A:89:LYS:HE2	1:A:93:LYS:HE3	1.94	0.48
1:B:19:MET:HG2	1:C:69:LEU:HD13	1.94	0.48
1:E:41:GLU:HA	1:E:44:TYR:CE2	2.48	0.48
1:J:17:LEU:HD13	1:J:78:VAL:HG11	1.95	0.48
1:B:17:LEU:HD13	1:B:78:VAL:HG11	1.95	0.48
1:F:79:LYS:CE	1:F:80:GLU:H	2.26	0.48
1:H:80:GLU:HG3	5:H:829:HOH:O	2.14	0.48
1:L:17:LEU:HD13	1:L:78:VAL:HG11	1.95	0.48
1:F:41:GLU:HA	1:F:44:TYR:CE2	2.49	0.48
1:I:41:GLU:HA	1:I:44:TYR:CE2	2.48	0.48
1:A:21:VAL:HG23	1:A:44:TYR:HB3	1.95	0.47
1:B:80:GLU:HG2	1:C:68:THR:CG2	2.44	0.47
1:C:41:GLU:HA	1:C:44:TYR:CE2	2.48	0.47
1:G:17:LEU:HD13	1:G:78:VAL:HG11	1.95	0.47
1:I:80:GLU:HG3	5:I:452:HOH:O	2.14	0.47
1:D:17:LEU:HD13	1:D:78:VAL:HG11	1.95	0.47
1:E:80:GLU:HG3	5:E:820:HOH:O	2.14	0.47
1:F:17:LEU:HD13	1:F:78:VAL:HG11	1.95	0.47
1:A:68:THR:CB	1:D:80:GLU:HG2	2.45	0.47
1:E:31:THR:HA	1:K:142:HIS:CE1	2.49	0.47
1:L:80:GLU:HG3	5:L:838:HOH:O	2.14	0.47
1:A:80:GLU:HG3	5:A:809:HOH:O	2.14	0.47
1:B:80:GLU:HG2	1:C:68:THR:HB	1.95	0.47
1:B:80:GLU:HG3	5:B:807:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:GLU:HG3	5:D:817:HOH:O	2.14	0.47
1:B:31:THR:HA	1:E:142:HIS:CE1	2.50	0.47
1:H:17:LEU:HD13	1:H:78:VAL:HG11	1.95	0.47
1:I:79:LYS:CE	1:I:80:GLU:H	2.26	0.47
1:J:41:GLU:HA	1:J:44:TYR:CE2	2.48	0.47
1:D:77:ARG:HG3	1:D:101:TYR:OH	2.15	0.47
1:F:22:HIS:HE1	5:G:833:HOH:O	1.98	0.47
1:F:21:VAL:HG23	1:F:44:TYR:HB3	1.95	0.47
1:L:77:ARG:HG3	1:L:101:TYR:OH	2.15	0.47
1:A:80:GLU:HG2	1:D:68:THR:HB	1.96	0.47
5:I:460:HOH:O	1:L:22:HIS:HE1	1.98	0.47
1:E:22:HIS:HE1	5:H:835:HOH:O	1.97	0.47
1:H:77:ARG:HG3	1:H:101:TYR:OH	2.15	0.47
1:L:21:VAL:HG23	1:L:44:TYR:HB3	1.95	0.47
1:B:77:ARG:HG3	1:B:101:TYR:OH	2.15	0.46
1:C:80:GLU:HG3	5:C:814:HOH:O	2.14	0.46
1:F:77:ARG:HG3	1:F:101:TYR:OH	2.15	0.46
1:F:31:THR:HA	1:I:142:HIS:CE1	2.50	0.46
5:B:813:HOH:O	1:C:22:HIS:HE1	1.97	0.46
1:F:80:GLU:HG3	5:F:819:HOH:O	2.14	0.46
1:E:57:ARG:CZ	1:E:120:VAL:HG22	2.46	0.46
1:G:77:ARG:HG3	1:G:101:TYR:OH	2.15	0.46
1:F:80:GLU:HG2	1:G:68:THR:CB	2.45	0.46
1:E:77:ARG:HG3	1:E:101:TYR:OH	2.15	0.46
1:G:57:ARG:CZ	1:G:120:VAL:HG22	2.46	0.46
1:G:80:GLU:HG3	5:G:827:HOH:O	2.14	0.46
5:E:826:HOH:O	1:H:22:HIS:HE1	1.97	0.46
1:J:57:ARG:CZ	1:J:120:VAL:HG22	2.46	0.46
1:A:57:ARG:CZ	1:A:120:VAL:HG22	2.46	0.46
1:F:57:ARG:CZ	1:F:120:VAL:HG22	2.46	0.46
1:I:22:HIS:HE1	5:L:844:HOH:O	1.97	0.46
1:E:21:VAL:HG23	1:E:44:TYR:HB3	1.95	0.46
1:C:77:ARG:HG3	1:C:101:TYR:OH	2.15	0.46
1:H:57:ARG:CZ	1:H:120:VAL:HG22	2.46	0.46
1:J:77:ARG:HG3	1:J:101:TYR:OH	2.15	0.46
1:J:80:GLU:HG3	5:J:829:HOH:O	2.14	0.46
1:K:77:ARG:HG3	1:K:101:TYR:OH	2.15	0.46
1:A:77:ARG:HG3	1:A:101:TYR:OH	2.15	0.46
1:B:22:HIS:HE1	5:C:820:HOH:O	1.99	0.46
1:C:57:ARG:CZ	1:C:120:VAL:HG22	2.46	0.46
1:D:142:HIS:CE1	1:L:31:THR:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:57:ARG:CZ	1:I:120:VAL:HG22	2.46	0.46
1:K:80:GLU:HG3	5:K:837:HOH:O	2.14	0.46
1:H:57:ARG:NH2	1:H:120:VAL:HG22	2.32	0.45
1:B:57:ARG:NH2	1:B:120:VAL:HG22	2.32	0.45
1:B:57:ARG:CZ	1:B:120:VAL:HG22	2.46	0.45
1:E:57:ARG:NH2	1:E:120:VAL:HG22	2.32	0.45
1:L:57:ARG:CZ	1:L:120:VAL:HG22	2.46	0.45
1:G:57:ARG:NH2	1:G:120:VAL:HG22	2.32	0.45
4:J:709:MPD:H4	4:J:709:MPD:H13	1.61	0.45
1:K:57:ARG:CZ	1:K:120:VAL:HG22	2.46	0.45
1:A:57:ARG:NH2	1:A:120:VAL:HG22	2.32	0.45
1:K:57:ARG:NH2	1:K:120:VAL:HG22	2.32	0.45
1:L:57:ARG:NH2	1:L:120:VAL:HG22	2.31	0.45
1:I:57:ARG:NH2	1:I:120:VAL:HG22	2.32	0.45
1:D:57:ARG:NH2	1:D:120:VAL:HG22	2.32	0.45
1:I:77:ARG:HG3	1:I:101:TYR:OH	2.15	0.45
4:C:702:MPD:H13	4:C:702:MPD:H4	1.61	0.45
1:D:57:ARG:CZ	1:D:120:VAL:HG22	2.46	0.45
1:J:57:ARG:NH2	1:J:120:VAL:HG22	2.32	0.45
1:J:79:LYS:HA	1:J:79:LYS:CE	2.34	0.45
1:F:57:ARG:NH2	1:F:120:VAL:HG22	2.32	0.44
1:K:21:VAL:HG23	1:K:44:TYR:HB3	1.95	0.44
4:E:704:MPD:H13	4:E:704:MPD:H4	1.61	0.44
1:C:57:ARG:NH2	1:C:120:VAL:HG22	2.32	0.44
1:D:21:VAL:HG23	1:D:44:TYR:HB3	1.95	0.44
4:I:708:MPD:H13	4:I:708:MPD:H4	1.61	0.44
1:J:21:VAL:HG23	1:J:44:TYR:HB3	1.95	0.44
1:C:57:ARG:NH1	1:C:60:GLN:HE21	2.15	0.44
1:A:8:LYS:HG2	1:A:58:ILE:HD13	2.00	0.44
1:H:79:LYS:CE	1:H:79:LYS:HA	2.34	0.44
5:J:835:HOH:O	1:K:22:HIS:HE1	1.99	0.44
1:C:1:MET:HE2	1:C:77:ARG:HH22	1.82	0.44
4:H:707:MPD:H4	4:H:707:MPD:H13	1.61	0.44
1:H:8:LYS:HG2	1:H:58:ILE:HD13	2.00	0.44
1:I:8:LYS:HG2	1:I:58:ILE:HD13	2.00	0.44
1:I:69:LEU:HG	1:L:69:LEU:HG	2.00	0.44
1:F:68:THR:CB	1:G:80:GLU:HG2	2.47	0.44
1:L:79:LYS:CE	1:L:79:LYS:HA	2.34	0.43
1:F:16:VAL:CG2	1:F:76:THR:HG21	2.48	0.43
1:A:22:HIS:O	1:A:25:HIS:HB3	2.19	0.43
1:B:22:HIS:O	1:B:25:HIS:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:22:HIS:O	1:H:25:HIS:HB3	2.19	0.43
1:I:22:HIS:O	1:I:25:HIS:HB3	2.19	0.43
1:C:142:HIS:CE1	1:I:31:THR:HA	2.52	0.43
1:L:8:LYS:HG2	1:L:58:ILE:HD13	2.00	0.43
1:D:22:HIS:O	1:D:25:HIS:HB3	2.19	0.43
1:E:22:HIS:O	1:E:25:HIS:HB3	2.19	0.43
1:E:8:LYS:HG2	1:E:58:ILE:HD13	2.00	0.43
1:F:22:HIS:O	1:F:25:HIS:HB3	2.19	0.43
1:C:8:LYS:HG2	1:C:58:ILE:HD13	2.00	0.43
4:K:710:MPD:H13	4:K:710:MPD:H4	1.61	0.43
1:I:57:ARG:NH1	1:I:60:GLN:HE21	2.15	0.43
1:D:8:LYS:HG2	1:D:58:ILE:HD13	2.00	0.43
1:F:8:LYS:HG2	1:F:58:ILE:HD13	2.00	0.43
1:I:16:VAL:CG2	1:I:76:THR:HG21	2.48	0.43
1:J:22:HIS:O	1:J:25:HIS:HB3	2.19	0.43
1:K:1:MET:HE2	1:K:77:ARG:HH22	1.84	0.43
1:L:22:HIS:O	1:L:25:HIS:HB3	2.19	0.43
1:C:16:VAL:CG2	1:C:76:THR:HG21	2.48	0.43
1:C:3:THR:HG22	1:C:7:LEU:HD22	2.01	0.43
5:A:815:HOH:O	1:D:22:HIS:HE1	2.01	0.43
1:A:80:GLU:HG2	1:D:68:THR:CB	2.49	0.43
1:E:3:THR:HG22	1:E:7:LEU:HD22	2.01	0.43
4:F:705:MPD:H4	4:F:705:MPD:H13	1.61	0.43
1:G:21:VAL:HG23	1:G:44:TYR:HB3	1.95	0.43
1:I:3:THR:HG22	1:I:7:LEU:HD22	2.01	0.43
1:B:8:LYS:HG2	1:B:58:ILE:HD13	2.00	0.43
1:H:57:ARG:NH1	1:H:60:GLN:HE21	2.15	0.43
1:A:56:GLU:O	1:A:60:GLN:HG3	2.19	0.43
1:A:3:THR:HG22	1:A:7:LEU:HD22	2.01	0.43
1:D:56:GLU:O	1:D:60:GLN:HG3	2.19	0.43
1:G:56:GLU:O	1:G:60:GLN:HG3	2.19	0.43
1:G:16:VAL:CG2	1:G:76:THR:HG21	2.48	0.43
1:K:22:HIS:O	1:K:25:HIS:HB3	2.19	0.43
1:K:8:LYS:HG2	1:K:58:ILE:HD13	2.00	0.43
1:B:3:THR:HG22	1:B:7:LEU:HD22	2.01	0.42
1:C:22:HIS:O	1:C:25:HIS:HB3	2.19	0.42
1:C:21:VAL:HG22	1:C:44:TYR:HB3	1.98	0.42
1:D:16:VAL:CG2	1:D:76:THR:HG21	2.48	0.42
1:F:56:GLU:O	1:F:60:GLN:HG3	2.19	0.42
1:I:68:THR:CG2	1:L:80:GLU:HG2	2.49	0.42
1:K:3:THR:HG22	1:K:7:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ARG:NH1	1:A:60:GLN:HE21	2.15	0.42
1:G:22:HIS:O	1:G:25:HIS:HB3	2.19	0.42
1:L:56:GLU:O	1:L:60:GLN:HG3	2.19	0.42
1:B:56:GLU:O	1:B:60:GLN:HG3	2.19	0.42
1:D:57:ARG:NH1	1:D:60:GLN:HE21	2.15	0.42
1:D:3:THR:HG22	1:D:7:LEU:HD22	2.01	0.42
1:H:16:VAL:CG2	1:H:76:THR:HG21	2.48	0.42
1:K:56:GLU:O	1:K:60:GLN:HG3	2.19	0.42
1:I:56:GLU:O	1:I:60:GLN:HG3	2.19	0.42
1:G:21:VAL:HG22	1:G:44:TYR:HB3	1.98	0.42
1:J:8:LYS:HG2	1:J:58:ILE:HD13	2.00	0.42
1:L:3:THR:HG22	1:L:7:LEU:HD22	2.01	0.42
1:G:8:LYS:HG2	1:G:58:ILE:HD13	2.00	0.42
1:I:80:GLU:HG2	1:L:68:THR:CG2	2.49	0.42
1:J:56:GLU:O	1:J:60:GLN:HG3	2.19	0.42
1:L:57:ARG:NH1	1:L:60:GLN:HE21	2.15	0.42
1:G:3:THR:HG22	1:G:7:LEU:HD22	2.01	0.42
1:C:56:GLU:O	1:C:60:GLN:HG3	2.19	0.42
1:H:56:GLU:O	1:H:60:GLN:HG3	2.19	0.42
1:J:21:VAL:HG22	1:J:44:TYR:HB3	1.98	0.42
1:B:61:LEU:HD12	1:B:61:LEU:HA	1.94	0.42
1:D:21:VAL:HG22	1:D:44:TYR:HB3	1.98	0.42
1:F:21:VAL:HG22	1:F:44:TYR:HB3	1.98	0.42
1:H:21:VAL:HG23	1:H:44:TYR:HB3	1.95	0.42
1:E:56:GLU:O	1:E:60:GLN:HG3	2.19	0.41
1:G:59:VAL:HG12	1:G:65:PRO:HD3	2.02	0.41
1:K:59:VAL:HG12	1:K:65:PRO:HD3	2.02	0.41
1:L:16:VAL:CG2	1:L:76:THR:HG21	2.48	0.41
1:J:57:ARG:NH1	1:J:60:GLN:HE21	2.15	0.41
1:B:16:VAL:CG2	1:B:76:THR:HG21	2.48	0.41
1:D:59:VAL:HG12	1:D:65:PRO:HD3	2.02	0.41
4:D:703:MPD:H4	4:D:703:MPD:H13	1.61	0.41
1:E:57:ARG:NH1	1:E:60:GLN:HE21	2.15	0.41
1:H:3:THR:HG22	1:H:7:LEU:HD22	2.01	0.41
1:J:3:THR:HG22	1:J:7:LEU:HD22	2.01	0.41
1:I:21:VAL:HG23	1:I:44:TYR:HB3	1.95	0.41
1:J:68:THR:HB	1:K:80:GLU:HG2	2.02	0.41
1:I:69:LEU:HD13	1:L:19:MET:HG2	2.02	0.41
1:A:16:VAL:HG21	1:A:76:THR:CG2	2.50	0.41
1:E:59:VAL:HG12	1:E:65:PRO:HD3	2.02	0.41
1:I:59:VAL:HG12	1:I:65:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:16:VAL:HG21	1:L:76:THR:CG2	2.50	0.41
1:A:59:VAL:HG12	1:A:65:PRO:HD3	2.02	0.41
1:B:57:ARG:NH1	1:B:60:GLN:HE21	2.15	0.41
1:F:3:THR:HG22	1:F:7:LEU:HD22	2.01	0.41
1:B:80:GLU:HG2	1:C:68:THR:CB	2.51	0.41
1:E:16:VAL:CG2	1:E:76:THR:HG21	2.48	0.41
1:G:31:THR:HA	1:J:142:HIS:CE1	2.56	0.41
1:H:1:MET:HE2	1:H:77:ARG:HH22	1.85	0.41
1:J:59:VAL:HG12	1:J:65:PRO:HD3	2.02	0.41
1:B:21:VAL:HG23	1:B:44:TYR:HB3	1.95	0.41
1:B:59:VAL:HG12	1:B:65:PRO:HD3	2.02	0.41
1:G:57:ARG:NH1	1:G:60:GLN:HE21	2.15	0.41
1:I:19:MET:HG2	1:L:69:LEU:HD13	2.02	0.41
1:C:21:VAL:HG23	1:C:44:TYR:HB3	1.95	0.41
1:A:69:LEU:HG	1:D:69:LEU:HG	2.03	0.41
1:K:16:VAL:CG2	1:K:76:THR:HG21	2.48	0.41
1:H:59:VAL:HG12	1:H:65:PRO:HD3	2.02	0.41
1:A:142:HIS:CE1	1:J:31:THR:HA	2.56	0.41
1:J:16:VAL:CG2	1:J:76:THR:HG21	2.48	0.41
1:D:57:ARG:HA	1:D:57:ARG:HD2	1.89	0.40
1:J:16:VAL:HG21	1:J:76:THR:CG2	2.50	0.40
1:F:59:VAL:HG12	1:F:65:PRO:HD3	2.02	0.40
1:B:16:VAL:HG21	1:B:76:THR:CG2	2.50	0.40
1:C:79:LYS:HA	1:C:79:LYS:CE	2.34	0.40
1:E:21:VAL:HG22	1:E:44:TYR:HB3	1.98	0.40
1:I:16:VAL:HG21	1:I:76:THR:CG2	2.50	0.40
1:K:16:VAL:HG21	1:K:76:THR:CG2	2.50	0.40
1:E:80:GLU:CD	1:H:68:THR:HB	2.42	0.40
1:F:17:LEU:HD12	1:F:17:LEU:HA	1.94	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:808:HOH:O	5:E:819:HOH:O[2_655]	1.70	0.50
5:B:806:HOH:O	5:G:826:HOH:O[2_546]	1.72	0.48

## 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	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	B	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	C	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	D	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	E	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	F	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	G	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	H	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	I	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	J	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	K	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	L	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
All	All	1704/1728 (99%)	1668 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	130/130 (100%)	113 (87%)	17 (13%)	4	7
1	B	130/130 (100%)	113 (87%)	17 (13%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	130/130 (100%)	113 (87%)	17 (13%)	4	7
1	D	130/130 (100%)	113 (87%)	17 (13%)	4	7
1	E	130/130 (100%)	113 (87%)	17 (13%)	4	7
1	F	130/130 (100%)	113 (87%)	17 (13%)	4	7
1	G	130/130 (100%)	113 (87%)	17 (13%)	4	7
1	H	130/130 (100%)	113 (87%)	17 (13%)	4	7
1	I	130/130 (100%)	113 (87%)	17 (13%)	4	7
1	J	130/130 (100%)	113 (87%)	17 (13%)	4	7
1	K	130/130 (100%)	113 (87%)	17 (13%)	4	7
1	L	130/130 (100%)	113 (87%)	17 (13%)	4	7
All	All	1560/1560 (100%)	1356 (87%)	204 (13%)	4	7

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	10	LEU
1	A	17	LEU
1	A	28	VAL
1	A	36	VAL
1	A	61	LEU
1	A	69	LEU
1	A	73	ILE
1	A	76	THR
1	A	79	LYS
1	A	81	GLU
1	A	96	LEU
1	A	109	LEU
1	A	112	THR
1	A	129	LEU
1	A	137	TRP
1	A	139	LEU
1	B	7	LEU
1	B	10	LEU
1	B	17	LEU
1	B	28	VAL
1	B	36	VAL
1	B	61	LEU

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Mol	Chain	Res	Type
1	B	69	LEU
1	B	73	ILE
1	B	76	THR
1	B	79	LYS
1	B	81	GLU
1	B	96	LEU
1	B	109	LEU
1	B	112	THR
1	B	129	LEU
1	B	137	TRP
1	B	139	LEU
1	C	7	LEU
1	C	10	LEU
1	C	17	LEU
1	C	28	VAL
1	C	36	VAL
1	C	61	LEU
1	C	69	LEU
1	C	73	ILE
1	C	76	THR
1	C	79	LYS
1	C	81	GLU
1	C	96	LEU
1	C	109	LEU
1	C	112	THR
1	C	129	LEU
1	C	137	TRP
1	C	139	LEU
1	D	7	LEU
1	D	10	LEU
1	D	17	LEU
1	D	28	VAL
1	D	36	VAL
1	D	61	LEU
1	D	69	LEU
1	D	73	ILE
1	D	76	THR
1	D	79	LYS
1	D	81	GLU
1	D	96	LEU
1	D	109	LEU
1	D	112	THR

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Mol	Chain	Res	Type
1	D	129	LEU
1	D	137	TRP
1	D	139	LEU
1	E	7	LEU
1	E	10	LEU
1	E	17	LEU
1	E	28	VAL
1	E	36	VAL
1	E	61	LEU
1	E	69	LEU
1	E	73	ILE
1	E	76	THR
1	E	79	LYS
1	E	81	GLU
1	E	96	LEU
1	E	109	LEU
1	E	112	THR
1	E	129	LEU
1	E	137	TRP
1	E	139	LEU
1	F	7	LEU
1	F	10	LEU
1	F	17	LEU
1	F	28	VAL
1	F	36	VAL
1	F	61	LEU
1	F	69	LEU
1	F	73	ILE
1	F	76	THR
1	F	79	LYS
1	F	81	GLU
1	F	96	LEU
1	F	109	LEU
1	F	112	THR
1	F	129	LEU
1	F	137	TRP
1	F	139	LEU
1	G	7	LEU
1	G	10	LEU
1	G	17	LEU
1	G	28	VAL
1	G	36	VAL

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Mol	Chain	Res	Type
1	G	61	LEU
1	G	69	LEU
1	G	73	ILE
1	G	76	THR
1	G	79	LYS
1	G	81	GLU
1	G	96	LEU
1	G	109	LEU
1	G	112	THR
1	G	129	LEU
1	G	137	TRP
1	G	139	LEU
1	H	7	LEU
1	H	10	LEU
1	H	17	LEU
1	H	28	VAL
1	H	36	VAL
1	H	61	LEU
1	H	69	LEU
1	H	73	ILE
1	H	76	THR
1	H	79	LYS
1	H	81	GLU
1	H	96	LEU
1	H	109	LEU
1	H	112	THR
1	H	129	LEU
1	H	137	TRP
1	H	139	LEU
1	I	7	LEU
1	I	10	LEU
1	I	17	LEU
1	I	28	VAL
1	I	36	VAL
1	I	61	LEU
1	I	69	LEU
1	I	73	ILE
1	I	76	THR
1	I	79	LYS
1	I	81	GLU
1	I	96	LEU
1	I	109	LEU

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Mol	Chain	Res	Type
1	I	112	THR
1	I	129	LEU
1	I	137	TRP
1	I	139	LEU
1	J	7	LEU
1	J	10	LEU
1	J	17	LEU
1	J	28	VAL
1	J	36	VAL
1	J	61	LEU
1	J	69	LEU
1	J	73	ILE
1	J	76	THR
1	J	79	LYS
1	J	81	GLU
1	J	96	LEU
1	J	109	LEU
1	J	112	THR
1	J	129	LEU
1	J	137	TRP
1	J	139	LEU
1	K	7	LEU
1	K	10	LEU
1	K	17	LEU
1	K	28	VAL
1	K	36	VAL
1	K	61	LEU
1	K	69	LEU
1	K	73	ILE
1	K	76	THR
1	K	79	LYS
1	K	81	GLU
1	K	96	LEU
1	K	109	LEU
1	K	112	THR
1	K	129	LEU
1	K	137	TRP
1	K	139	LEU
1	L	7	LEU
1	L	10	LEU
1	L	17	LEU
1	L	28	VAL

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Mol	Chain	Res	Type
1	L	36	VAL
1	L	61	LEU
1	L	69	LEU
1	L	73	ILE
1	L	76	THR
1	L	79	LYS
1	L	81	GLU
1	L	96	LEU
1	L	109	LEU
1	L	112	THR
1	L	129	LEU
1	L	137	TRP
1	L	139	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	22	HIS
1	A	27	ASN
1	A	60	GLN
1	A	111	ASN
1	A	140	GLN
1	B	9	HIS
1	B	22	HIS
1	B	27	ASN
1	B	60	GLN
1	B	111	ASN
1	B	140	GLN
1	C	9	HIS
1	C	22	HIS
1	C	27	ASN
1	C	60	GLN
1	C	111	ASN
1	C	140	GLN
1	D	9	HIS
1	D	22	HIS
1	D	27	ASN
1	D	60	GLN
1	D	111	ASN
1	D	140	GLN
1	E	9	HIS

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Mol	Chain	Res	Type
1	E	22	HIS
1	E	27	ASN
1	E	60	GLN
1	E	111	ASN
1	E	140	GLN
1	F	9	HIS
1	F	22	HIS
1	F	27	ASN
1	F	60	GLN
1	F	111	ASN
1	F	140	GLN
1	G	9	HIS
1	G	22	HIS
1	G	27	ASN
1	G	60	GLN
1	G	111	ASN
1	G	140	GLN
1	H	9	HIS
1	H	22	HIS
1	H	27	ASN
1	H	60	GLN
1	H	111	ASN
1	H	140	GLN
1	I	9	HIS
1	I	22	HIS
1	I	27	ASN
1	I	60	GLN
1	I	111	ASN
1	I	140	GLN
1	J	9	HIS
1	J	22	HIS
1	J	27	ASN
1	J	60	GLN
1	J	111	ASN
1	J	140	GLN
1	K	9	HIS
1	K	22	HIS
1	K	27	ASN
1	K	60	GLN
1	K	111	ASN
1	K	140	GLN
1	L	9	HIS

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Mol	Chain	Res	Type
1	L	22	HIS
1	L	27	ASN
1	L	60	GLN
1	L	111	ASN
1	L	140	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 12 are unknown and 12 are monoatomic - leaving 12 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	D	703	-	7,7,7	1.09	1 (14%)	9,10,10	4.16	6 (66%)
4	MPD	L	711	-	7,7,7	1.09	1 (14%)	9,10,10	4.15	6 (66%)
4	MPD	K	710	-	7,7,7	1.08	1 (14%)	9,10,10	4.16	6 (66%)
4	MPD	A	700	-	7,7,7	1.09	1 (14%)	9,10,10	4.16	6 (66%)
4	MPD	C	702	-	7,7,7	1.09	1 (14%)	9,10,10	4.16	6 (66%)
4	MPD	B	701	-	7,7,7	1.09	1 (14%)	9,10,10	4.16	6 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MPD	I	708	-	7,7,7	1.09	1 (14%)	9,10,10	4.16	6 (66%)
4	MPD	G	706	-	7,7,7	1.10	1 (14%)	9,10,10	4.16	6 (66%)
4	MPD	H	707	-	7,7,7	1.09	1 (14%)	9,10,10	4.16	6 (66%)
4	MPD	E	704	-	7,7,7	1.09	1 (14%)	9,10,10	4.16	6 (66%)
4	MPD	J	709	-	7,7,7	1.09	1 (14%)	9,10,10	4.16	6 (66%)
4	MPD	F	705	-	7,7,7	1.10	1 (14%)	9,10,10	4.16	6 (66%)

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	D	703	-	-	0/5/5/5	-
4	MPD	L	711	-	-	0/5/5/5	-
4	MPD	K	710	-	-	0/5/5/5	-
4	MPD	A	700	-	-	0/5/5/5	-
4	MPD	C	702	-	-	0/5/5/5	-
4	MPD	B	701	-	-	0/5/5/5	-
4	MPD	I	708	-	-	0/5/5/5	-
4	MPD	G	706	-	-	0/5/5/5	-
4	MPD	H	707	-	-	0/5/5/5	-
4	MPD	E	704	-	-	0/5/5/5	-
4	MPD	J	709	-	-	0/5/5/5	-
4	MPD	F	705	-	-	0/5/5/5	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	705	MPD	C3-C2	2.62	1.60	1.53
4	G	706	MPD	C3-C2	2.61	1.60	1.53
4	C	702	MPD	C3-C2	2.61	1.60	1.53
4	B	701	MPD	C3-C2	2.60	1.60	1.53
4	I	708	MPD	C3-C2	2.60	1.60	1.53
4	H	707	MPD	C3-C2	2.60	1.60	1.53
4	A	700	MPD	C3-C2	2.60	1.60	1.53
4	E	704	MPD	C3-C2	2.60	1.60	1.53
4	L	711	MPD	C3-C2	2.59	1.60	1.53
4	D	703	MPD	C3-C2	2.58	1.60	1.53
4	J	709	MPD	C3-C2	2.58	1.60	1.53
4	K	710	MPD	C3-C2	2.56	1.60	1.53



All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	705	MPD	O2-C2-C3	-8.21	78.96	109.80
4	E	704	MPD	O2-C2-C3	-8.20	78.98	109.80
4	K	710	MPD	O2-C2-C3	-8.20	78.98	109.80
4	B	701	MPD	O2-C2-C3	-8.20	78.98	109.80
4	H	707	MPD	O2-C2-C3	-8.20	78.98	109.80
4	A	700	MPD	O2-C2-C3	-8.20	78.98	109.80
4	I	708	MPD	O2-C2-C3	-8.20	78.99	109.80
4	D	703	MPD	O2-C2-C3	-8.20	78.99	109.80
4	C	702	MPD	O2-C2-C3	-8.20	78.99	109.80
4	G	706	MPD	O2-C2-C3	-8.20	79.00	109.80
4	J	709	MPD	O2-C2-C3	-8.20	79.01	109.80
4	L	711	MPD	O2-C2-C3	-8.19	79.02	109.80
4	B	701	MPD	CM-C2-C3	-5.16	85.94	109.96
4	I	708	MPD	CM-C2-C3	-5.16	85.94	109.96
4	C	702	MPD	CM-C2-C3	-5.16	85.95	109.96
4	G	706	MPD	CM-C2-C3	-5.16	85.96	109.96
4	J	709	MPD	CM-C2-C3	-5.15	85.96	109.96
4	A	700	MPD	CM-C2-C3	-5.15	85.96	109.96
4	D	703	MPD	CM-C2-C3	-5.15	85.97	109.96
4	K	710	MPD	CM-C2-C3	-5.15	85.98	109.96
4	L	711	MPD	CM-C2-C3	-5.15	85.98	109.96
4	H	707	MPD	CM-C2-C3	-5.15	85.98	109.96
4	F	705	MPD	CM-C2-C3	-5.15	85.98	109.96
4	E	704	MPD	CM-C2-C3	-5.15	85.99	109.96
4	I	708	MPD	CM-C2-C1	4.69	120.36	110.57
4	K	710	MPD	CM-C2-C1	4.69	120.35	110.57
4	J	709	MPD	CM-C2-C1	4.68	120.33	110.57
4	E	704	MPD	CM-C2-C1	4.68	120.33	110.57
4	H	707	MPD	CM-C2-C1	4.68	120.33	110.57
4	L	711	MPD	CM-C2-C1	4.68	120.32	110.57
4	B	701	MPD	CM-C2-C1	4.68	120.32	110.57
4	C	702	MPD	CM-C2-C1	4.67	120.31	110.57
4	A	700	MPD	CM-C2-C1	4.67	120.31	110.57
4	G	706	MPD	CM-C2-C1	4.67	120.31	110.57
4	F	705	MPD	CM-C2-C1	4.67	120.31	110.57
4	D	703	MPD	CM-C2-C1	4.67	120.30	110.57
4	B	701	MPD	C1-C2-C3	-4.05	91.12	109.96
4	G	706	MPD	C1-C2-C3	-4.04	91.13	109.96
4	D	703	MPD	C1-C2-C3	-4.04	91.14	109.96
4	I	708	MPD	C1-C2-C3	-4.04	91.14	109.96
4	F	705	MPD	C1-C2-C3	-4.04	91.14	109.96
4	C	702	MPD	C1-C2-C3	-4.04	91.15	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	MPD	C1-C2-C3	-4.04	91.15	109.96
4	J	709	MPD	C1-C2-C3	-4.04	91.16	109.96
4	H	707	MPD	C1-C2-C3	-4.04	91.16	109.96
4	L	711	MPD	C1-C2-C3	-4.04	91.17	109.96
4	E	704	MPD	C1-C2-C3	-4.03	91.18	109.96
4	K	710	MPD	C1-C2-C3	-4.03	91.18	109.96
4	D	703	MPD	O2-C2-CM	3.75	120.12	108.08
4	L	711	MPD	O2-C2-CM	3.74	120.08	108.08
4	G	706	MPD	O2-C2-CM	3.74	120.08	108.08
4	C	702	MPD	O2-C2-CM	3.74	120.08	108.08
4	A	700	MPD	O2-C2-CM	3.74	120.08	108.08
4	F	705	MPD	O2-C2-CM	3.74	120.07	108.08
4	B	701	MPD	O2-C2-CM	3.74	120.07	108.08
4	H	707	MPD	O2-C2-CM	3.74	120.06	108.08
4	J	709	MPD	O2-C2-CM	3.74	120.06	108.08
4	K	710	MPD	O2-C2-CM	3.73	120.06	108.08
4	E	704	MPD	O2-C2-CM	3.73	120.04	108.08
4	I	708	MPD	O2-C2-CM	3.72	120.02	108.08
4	E	704	MPD	O2-C2-C1	3.00	117.70	108.08
4	H	707	MPD	O2-C2-C1	2.99	117.67	108.08
4	F	705	MPD	O2-C2-C1	2.99	117.67	108.08
4	I	708	MPD	O2-C2-C1	2.99	117.67	108.08
4	A	700	MPD	O2-C2-C1	2.99	117.67	108.08
4	L	711	MPD	O2-C2-C1	2.99	117.67	108.08
4	J	709	MPD	O2-C2-C1	2.99	117.66	108.08
4	C	702	MPD	O2-C2-C1	2.99	117.66	108.08
4	K	710	MPD	O2-C2-C1	2.99	117.66	108.08
4	G	706	MPD	O2-C2-C1	2.98	117.66	108.08
4	B	701	MPD	O2-C2-C1	2.98	117.65	108.08
4	D	703	MPD	O2-C2-C1	2.98	117.64	108.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	703	MPD	4	0
4	L	711	MPD	3	0
4	K	710	MPD	4	0
4	A	700	MPD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	702	MPD	4	0
4	B	701	MPD	3	0
4	I	708	MPD	4	0
4	G	706	MPD	3	0
4	H	707	MPD	4	0
4	E	704	MPD	4	0
4	J	709	MPD	4	0
4	F	705	MPD	4	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 ⓘ

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	144/144 (100%)	0.09	4 (2%)	53	57	17, 27, 42, 48	0
1	B	144/144 (100%)	0.10	4 (2%)	53	57	17, 27, 42, 48	0
1	C	144/144 (100%)	0.04	3 (2%)	63	67	17, 27, 42, 48	0
1	D	144/144 (100%)	0.07	3 (2%)	63	67	17, 27, 42, 48	0
1	E	144/144 (100%)	0.13	2 (1%)	75	78	17, 27, 42, 48	0
1	F	144/144 (100%)	0.07	2 (1%)	75	78	17, 27, 42, 48	0
1	G	144/144 (100%)	0.06	2 (1%)	75	78	17, 27, 42, 48	0
1	H	144/144 (100%)	0.00	2 (1%)	75	78	17, 27, 42, 48	0
1	I	144/144 (100%)	0.14	2 (1%)	75	78	17, 27, 42, 48	0
1	J	144/144 (100%)	0.07	3 (2%)	63	67	17, 27, 42, 48	0
1	K	144/144 (100%)	0.01	3 (2%)	63	67	17, 27, 42, 48	0
1	L	144/144 (100%)	0.28	4 (2%)	53	57	17, 27, 42, 48	0
All	All	1728/1728 (100%)	0.09	34 (1%)	65	68	17, 27, 42, 48	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	97	GLU	4.1
1	C	144	ALA	4.1
1	D	144	ALA	3.8
1	G	144	ALA	3.6
1	B	144	ALA	3.5
1	I	97	GLU	3.4
1	K	97	GLU	3.4
1	B	97	GLU	3.2
1	F	97	GLU	3.2
1	L	97	GLU	3.1
1	H	97	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	115	LYS	3.0
1	J	1	MET	2.9
1	E	97	GLU	2.9
1	A	144	ALA	2.9
1	D	115	LYS	2.8
1	C	97	GLU	2.7
1	F	2	LYS	2.7
1	A	1	MET	2.7
1	B	34	PHE	2.6
1	G	97	GLU	2.5
1	L	34	PHE	2.5
1	J	97	GLU	2.5
1	A	79	LYS	2.5
1	H	2	LYS	2.5
1	E	144	ALA	2.4
1	K	144	ALA	2.3
1	L	79	LYS	2.3
1	D	97	GLU	2.2
1	B	1	MET	2.2
1	L	144	ALA	2.1
1	K	115	LYS	2.1
1	I	144	ALA	2.1
1	J	2	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MPD	F	705	8/8	0.43	0.76	36,39,41,42	8
3	UNX	D	808	1/1	0.51	0.98	18,18,18,18	1
4	MPD	L	711	8/8	0.55	0.63	36,39,41,42	8
4	MPD	J	709	8/8	0.57	0.62	36,39,41,42	8
4	MPD	E	704	8/8	0.57	0.66	36,39,41,42	8
4	MPD	A	700	8/8	0.59	0.60	36,39,41,42	8
4	MPD	H	707	8/8	0.61	0.64	36,39,41,42	8
4	MPD	K	710	8/8	0.61	0.58	36,39,41,42	8
4	MPD	I	708	8/8	0.62	0.61	36,39,41,42	8
4	MPD	B	701	8/8	0.63	0.60	36,39,41,42	8
4	MPD	C	702	8/8	0.64	0.57	36,39,41,42	8
4	MPD	D	703	8/8	0.64	0.58	36,39,41,42	8
3	UNX	L	824	1/1	0.64	0.88	18,18,18,18	1
4	MPD	G	706	8/8	0.66	0.61	36,39,41,42	8
3	UNX	E	810	1/1	0.68	0.92	18,18,18,18	1
3	UNX	J	820	1/1	0.77	0.95	18,18,18,18	1
3	UNX	C	806	1/1	0.80	0.96	18,18,18,18	1
3	UNX	G	814	1/1	0.82	0.94	18,18,18,18	1
3	UNX	K	822	1/1	0.85	0.92	18,18,18,18	1
3	UNX	H	816	1/1	0.90	0.93	18,18,18,18	1
3	UNX	F	812	1/1	0.91	0.94	18,18,18,18	1
3	UNX	A	802	1/1	0.92	0.98	18,18,18,18	1
3	UNX	B	804	1/1	0.93	0.94	18,18,18,18	1
3	UNX	I	818	1/1	0.93	0.93	18,18,18,18	1
2	FE	A	807	1/1	0.95	0.09	26,26,26,26	0
2	FE	G	811	1/1	0.96	0.09	26,26,26,26	0
2	FE	B	805	1/1	0.96	0.07	26,26,26,26	0
2	FE	I	823	1/1	0.97	0.08	26,26,26,26	0
2	FE	K	819	1/1	0.97	0.04	26,26,26,26	0
2	FE	J	821	1/1	0.98	0.06	26,26,26,26	0
2	FE	E	815	1/1	0.98	0.07	26,26,26,26	0
2	FE	D	801	1/1	0.98	0.04	26,26,26,26	0
2	FE	C	803	1/1	0.98	0.05	26,26,26,26	0
2	FE	H	809	1/1	0.98	0.09	26,26,26,26	0
2	FE	L	817	1/1	0.99	0.04	26,26,26,26	0
2	FE	F	813	1/1	0.99	0.07	26,26,26,26	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.