



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:01 AM GMT

PDB ID : 2JJ1  
Title : THE STRUCTURE OF F1-ATPASE INHIBITED BY PICEATANNOL.  
Authors : Gledhill, J.R.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2007-07-03  
Resolution : 2.70 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

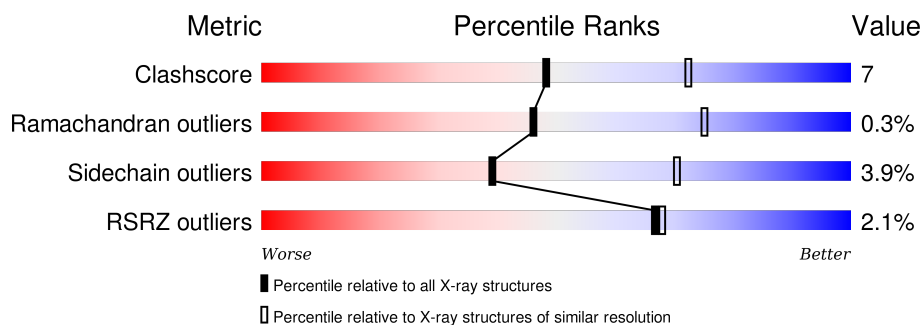
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	510	<div> <div></div> <div>79% 15% • 5%</div> </div>
1	B	510	<div> <div></div> <div>75% 18% • 6%</div> </div>
1	C	510	<div> <div>2%</div> <div>78% 17% • •</div> </div>
1	H	510	<div> <div></div> <div>77% 17% • 5%</div> </div>
1	I	510	<div> <div></div> <div>79% 14% • 6%</div> </div>
1	J	510	<div> <div></div> <div>79% 16% • •</div> </div>
2	D	482	<div> <div></div> <div>81% 15% •</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	482	
2	F	482	
2	K	482	
2	L	482	
2	M	482	
3	G	272	
3	N	272	

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
10	PIT	G	1273	-	-	-	X
10	PIT	N	1273	-	-	-	X
6	GOL	B	1512	-	-	-	X
6	GOL	B	1513	-	-	-	X
6	GOL	H	1514	-	-	-	X
6	GOL	K	1479	-	-	-	X
8	AZI	K	1478	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 47647 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 ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	479	Total	C	N	O	S	0	0	0
			3658	2305	647	694	12			
1	C	495	Total	C	N	O	S	0	0	0
			3768	2374	664	718	12			
1	H	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	I	479	Total	C	N	O	S	0	0	0
			3658	2305	647	694	12			
1	J	495	Total	C	N	O	S	0	0	0
			3768	2374	664	718	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	GLN	SEE REMARK 999	UNP P19483
B	1	GLU	GLN	SEE REMARK 999	UNP P19483
C	1	GLU	GLN	SEE REMARK 999	UNP P19483
H	1	GLU	GLN	SEE REMARK 999	UNP P19483
I	1	GLU	GLN	SEE REMARK 999	UNP P19483
J	1	GLU	GLN	SEE REMARK 999	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	L	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	M	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- | Mol | Chain | Residues | Atoms         |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| 3   | G     | 167      | Total<br>1296 | C<br>810 | N<br>237 | O<br>242 | S<br>7 | 0       | 0       | 0     |
| 3   | N     | 167      | Total<br>1296 | C<br>810 | N<br>237 | O<br>242 | S<br>7 | 0       | 0       | 0     |

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	C	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	F	1	Total 31	C 10	N 6	O 12	P 3	0	0



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	M	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

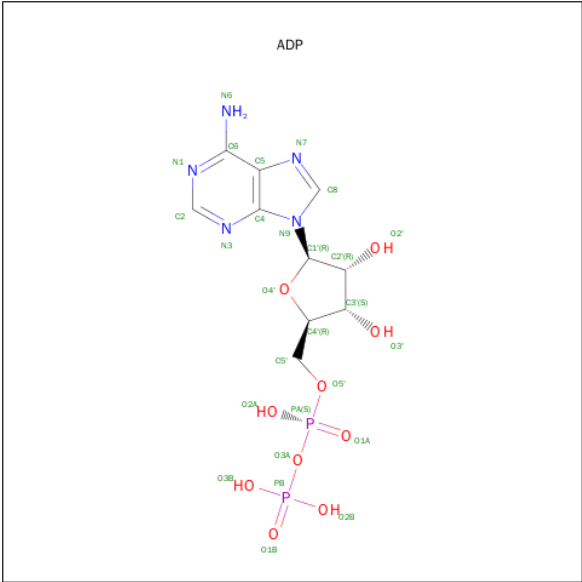
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	M	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



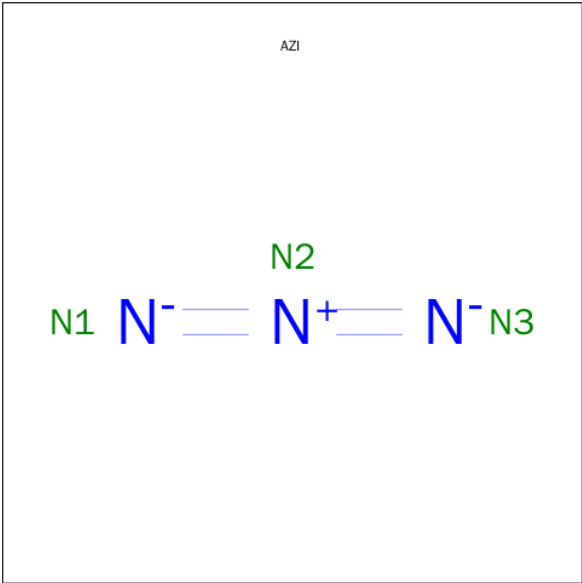
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	J	1	Total	C	O	0	0
			6	3	3		
6	K	1	Total	C	O	0	0
			6	3	3		
6	K	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

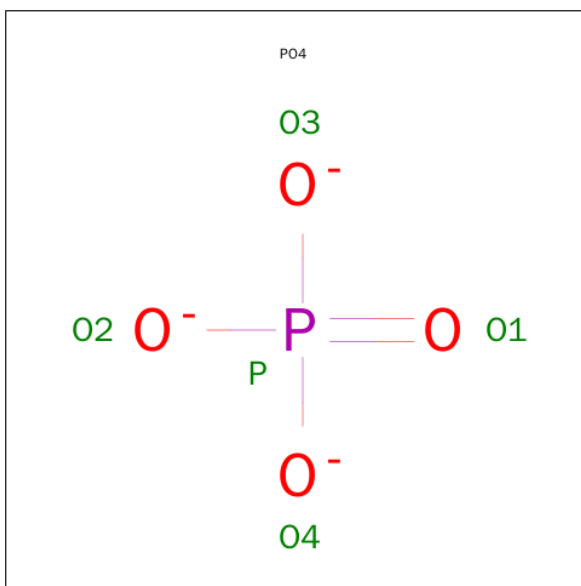
- Molecule 8 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	N	0	0
			3	3		
8	K	1	Total	N	0	0
			3	3		

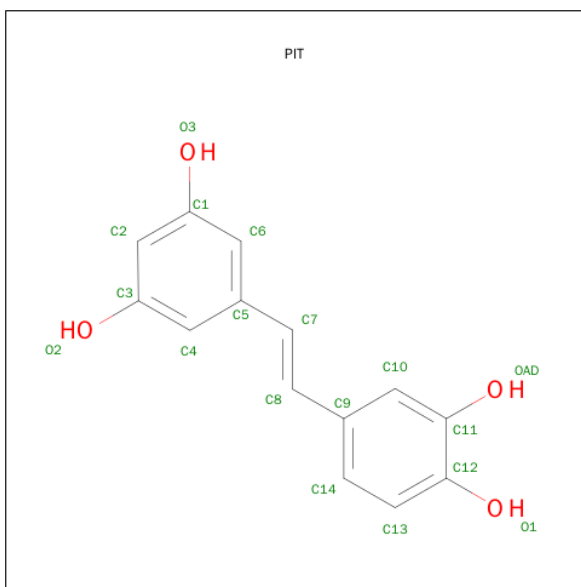


- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	O	P	0	0
			5	4	1		
9	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is PICEATANNOL (three-letter code: PIT) (formula:  $C_{14}H_{12}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	0
			18	14	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	N	1	Total	C	O	0	0
			18	14	4		

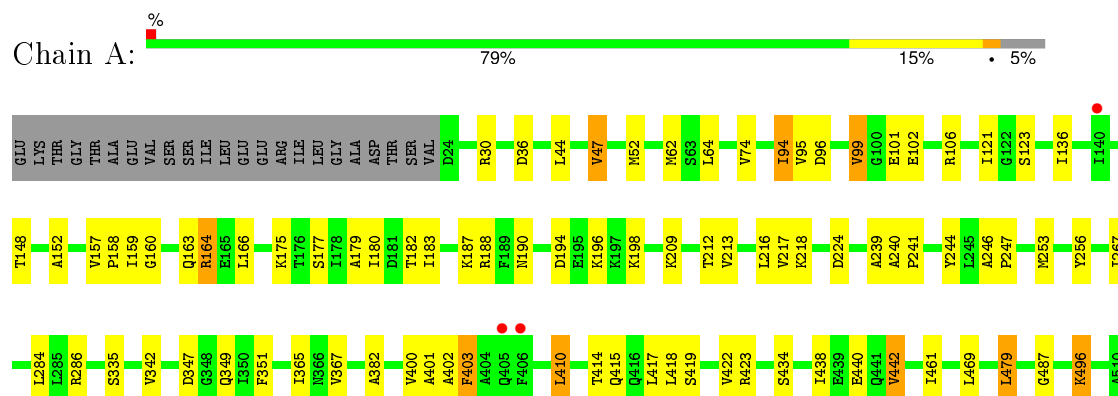
- Molecule 11 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	101	Total	O		0	0
			101	101			
11	B	81	Total	O		0	0
			81	81			
11	C	107	Total	O		0	0
			107	107			
11	D	98	Total	O		0	0
			98	98			
11	E	76	Total	O		0	0
			76	76			
11	F	104	Total	O		0	0
			104	104			
11	G	20	Total	O		0	0
			20	20			
11	H	79	Total	O		0	0
			79	79			
11	I	86	Total	O		0	0
			86	86			
11	J	104	Total	O		0	0
			104	104			
11	K	93	Total	O		0	0
			93	93			
11	L	64	Total	O		0	0
			64	64			
11	M	104	Total	O		0	0
			104	104			
11	N	22	Total	O		0	0
			22	22			

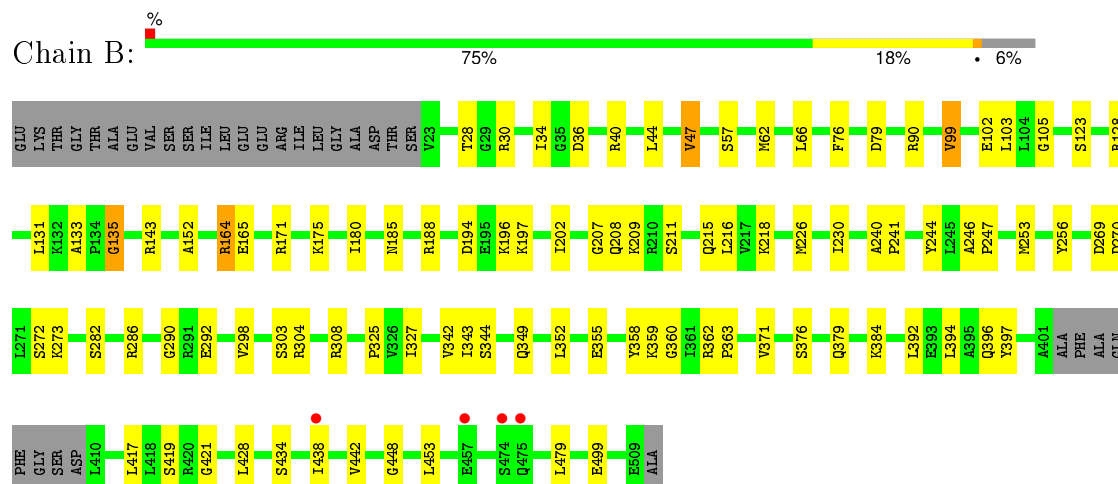
### 3 Residue-property plots [i](#)

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

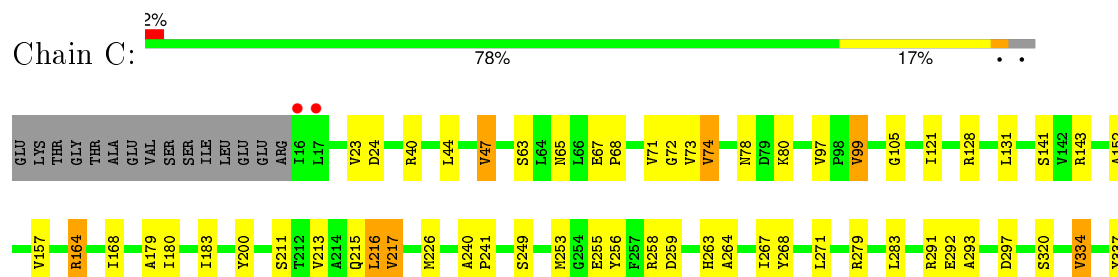
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

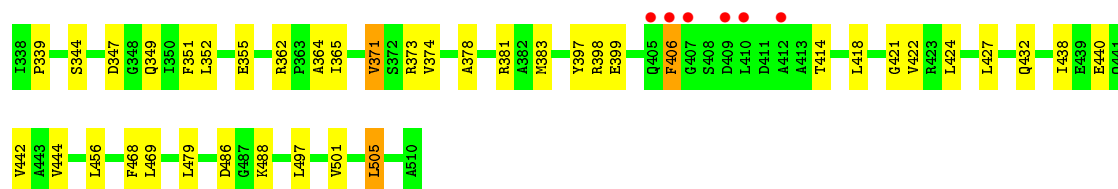


#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

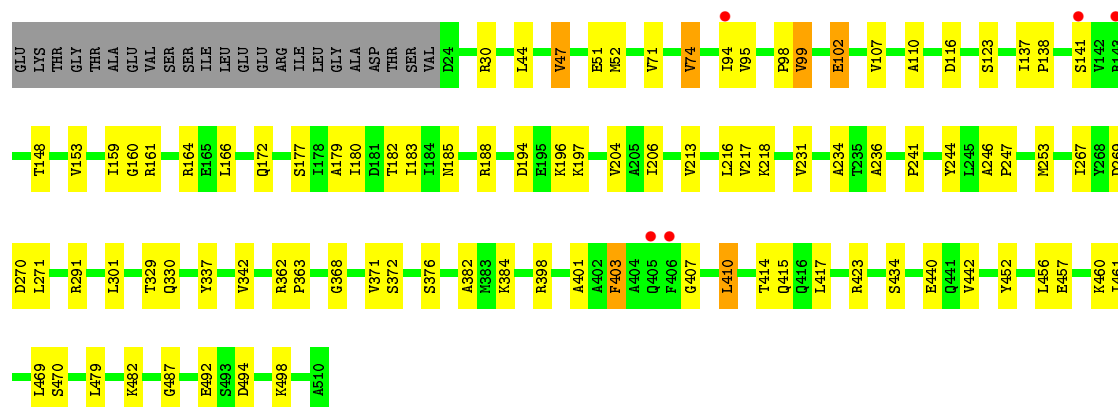


#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

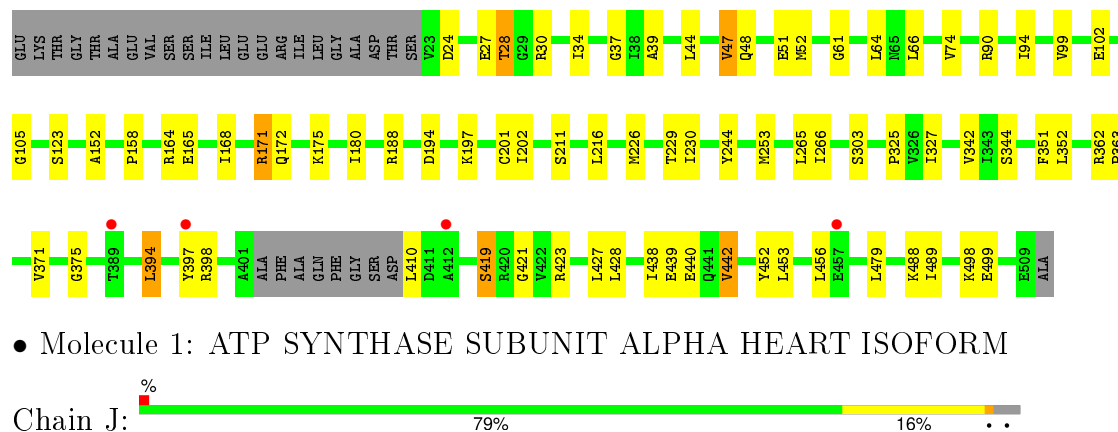
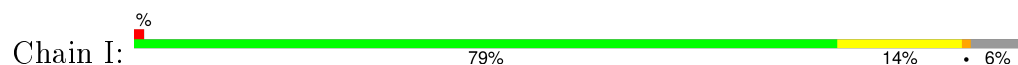




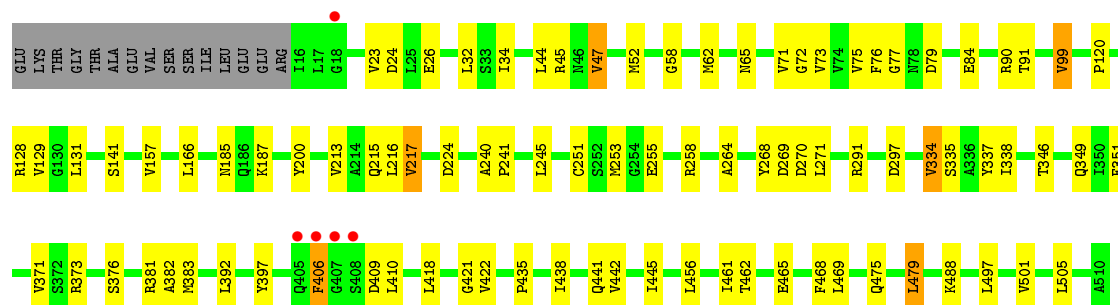
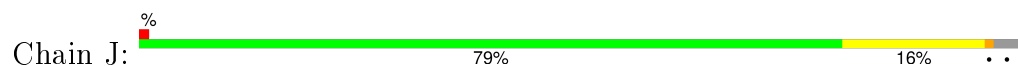
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM



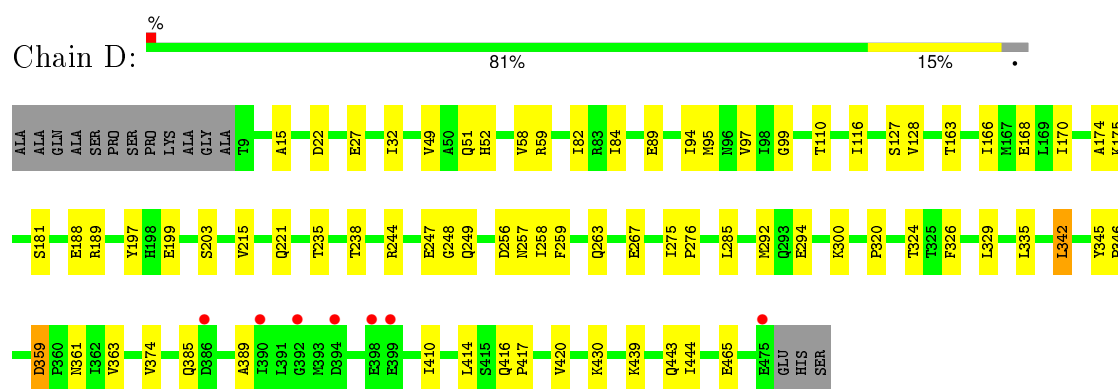
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM



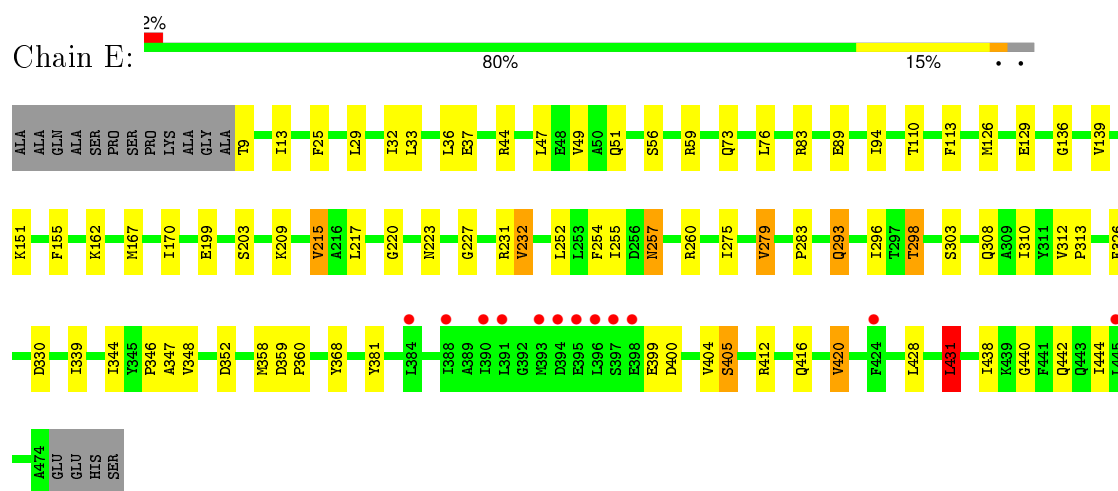
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM



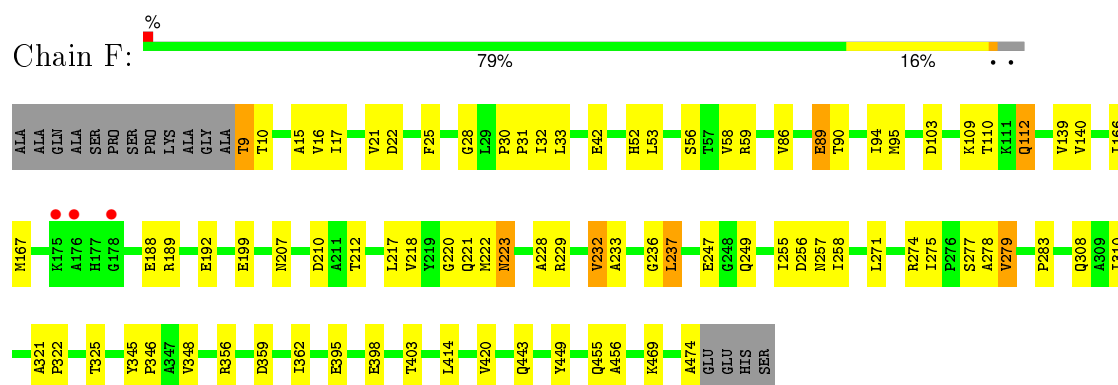
• Molecule 2: ATP SYNTHASE SUBUNIT BETA



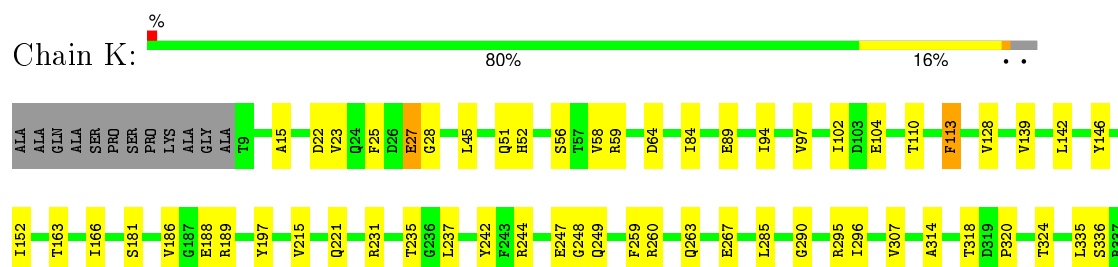
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

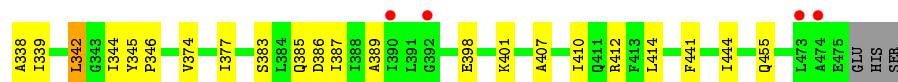


• Molecule 2: ATP SYNTHASE SUBUNIT BETA

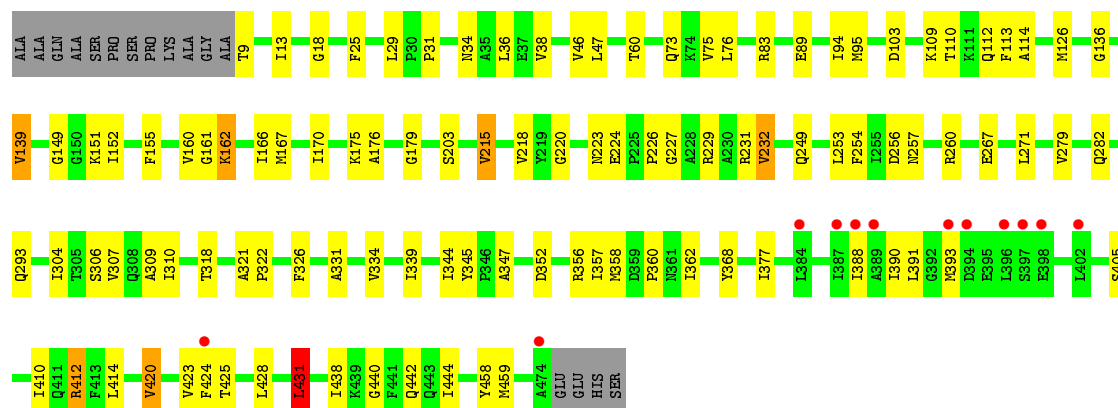
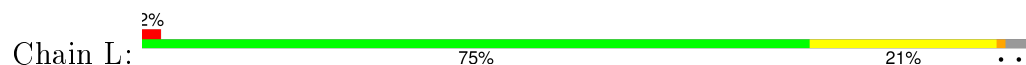


• Molecule 2: ATP SYNTHASE SUBUNIT BETA

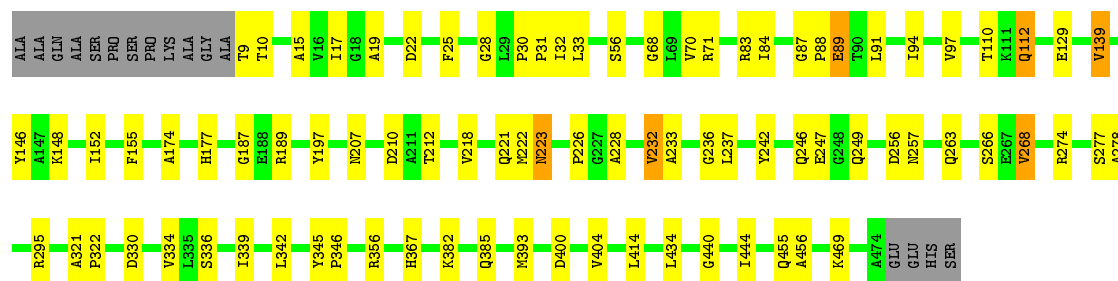
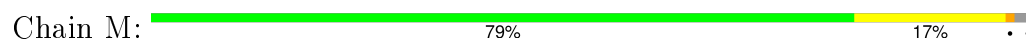




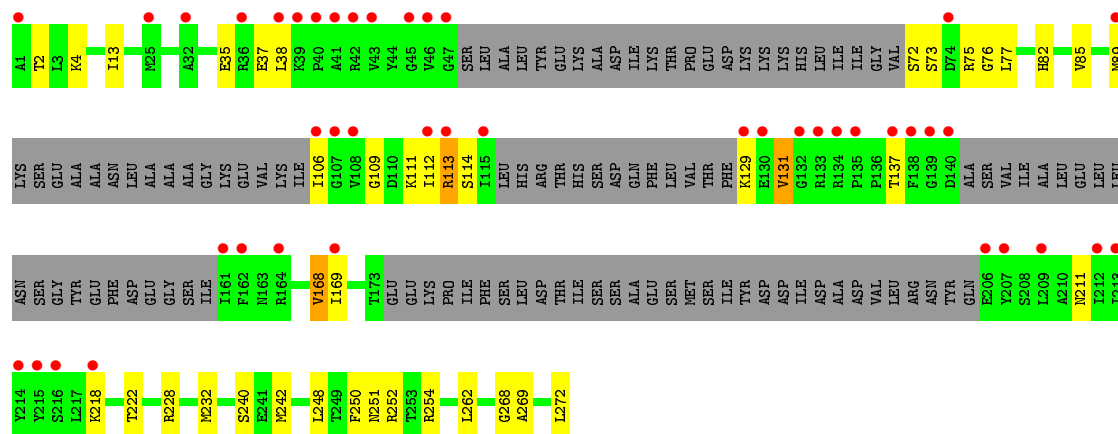
• Molecule 2: ATP SYNTHASE SUBUNIT BETA



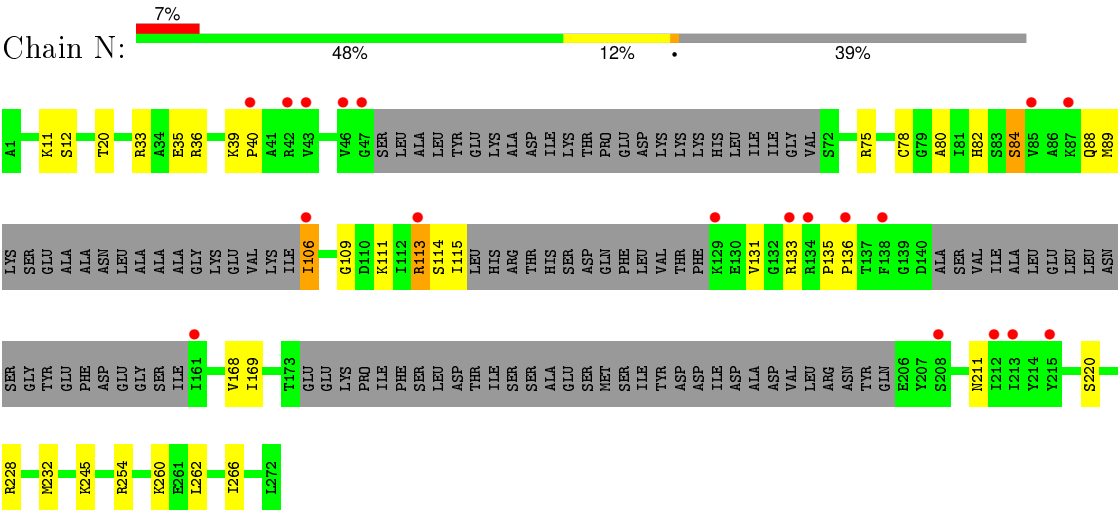
• Molecule 2: ATP SYNTHASE SUBUNIT BETA



• Molecule 3: ATP SYNTHASE GAMMA CHAIN



• Molecule 3: ATP SYNTHASE GAMMA CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.96Å 281.18Å 138.78Å 90.00° 89.58° 90.00°	Depositor
Resolution (Å)	72.74 – 2.70 67.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.0 (72.74-2.70) 88.1 (67.37-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.202 , 0.269 0.207 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 29.8	EDS
Estimated twinning fraction	0.388 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 201330 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	47647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, MG, ADP, GOL, PO4, ANP, PIT

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	0.47	0/3766	0.63	0/5080
1	B	0.47	0/3706	0.62	0/4998
1	C	0.48	0/3819	0.64	0/5153
1	H	0.47	0/3766	0.62	0/5080
1	I	0.46	0/3706	0.62	0/4998
1	J	0.50	0/3819	0.63	0/5153
2	D	0.47	0/3596	0.61	0/4879
2	E	0.44	0/3587	0.61	1/4867 (0.0%)
2	F	0.47	0/3587	0.63	1/4867 (0.0%)
2	K	0.47	0/3596	0.61	0/4879
2	L	0.45	0/3587	0.61	1/4867 (0.0%)
2	M	0.46	0/3587	0.62	0/4867
3	G	0.40	0/1304	0.53	0/1737
3	N	0.40	0/1304	0.53	0/1737
All	All	0.46	0/46730	0.62	3/63162 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	431	LEU	CA-CB-CG	6.01	129.13	115.30
2	F	237	LEU	CA-CB-CG	5.77	128.57	115.30
2	E	431	LEU	CA-CB-CG	5.60	128.18	115.30

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	3715	0	3812	57	0
1	B	3658	0	3767	57	0
1	C	3768	0	3867	64	0
1	H	3715	0	3812	60	0
1	I	3658	0	3767	43	0
1	J	3768	0	3868	58	0
2	D	3539	0	3592	48	0
2	E	3530	0	3587	49	0
2	F	3530	0	3586	58	0
2	K	3539	0	3592	54	0
2	L	3530	0	3587	67	0
2	M	3530	0	3586	57	0
3	G	1296	0	1365	20	0
3	N	1296	0	1365	16	0
4	A	31	0	13	2	0
4	B	31	0	13	1	0
4	C	31	0	13	0	0
4	F	31	0	13	1	0
4	H	31	0	13	1	0
4	I	31	0	13	0	0
4	J	31	0	13	0	0
4	M	31	0	13	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	M	1	0	0	0	0
6	A	12	0	16	0	0
6	B	12	0	16	3	0
6	C	6	0	8	0	0
6	D	6	0	8	0	0
6	H	12	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	6	0	8	0	0
6	J	6	0	8	0	0
6	K	12	0	16	0	0
7	D	27	0	12	1	0
7	K	27	0	12	1	0
8	D	3	0	0	0	0
8	K	3	0	0	0	0
9	E	5	0	0	0	0
9	L	5	0	0	0	0
10	G	18	0	8	2	0
10	N	18	0	8	3	0
11	A	101	0	0	2	0
11	B	81	0	0	8	0
11	C	107	0	0	6	0
11	D	98	0	0	6	0
11	E	76	0	0	7	0
11	F	104	0	0	5	0
11	G	20	0	0	1	0
11	H	79	0	0	7	0
11	I	86	0	0	2	0
11	J	104	0	0	4	0
11	K	93	0	0	2	0
11	L	64	0	0	10	0
11	M	104	0	0	9	0
11	N	22	0	0	3	0
All	All	47647	0	47393	681	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 7.

All (681) 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:A:62:MET:HE3	1:A:64:LEU:HD21	1.32	1.09
1:A:62:MET:CE	1:A:64:LEU:HD21	1.84	1.06
1:A:52:MET:HG3	1:A:95:VAL:HG22	1.47	0.95
1:B:171:ARG:HD3	11:B:2032:HOH:O	1.64	0.95
2:K:104:GLU:HG2	11:K:2022:HOH:O	1.66	0.93
2:F:398:GLU:HG2	11:F:2081:HOH:O	1.72	0.90
2:M:223:ASN:HD22	2:M:223:ASN:H	1.16	0.87
2:F:223:ASN:H	2:F:223:ASN:HD22	1.25	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:58:GLY:HA3	11:J:2011:HOH:O	1.77	0.85
1:C:44:LEU:O	1:C:47:VAL:HG22	1.78	0.83
2:M:15:ALA:HB3	2:M:22:ASP:HB2	1.61	0.82
1:C:183:ILE:HD11	1:C:267:ILE:HD13	1.61	0.82
1:A:44:LEU:O	1:A:47:VAL:HG22	1.78	0.82
1:A:62:MET:HE3	1:A:64:LEU:CD2	2.11	0.81
1:H:52:MET:HG3	1:H:95:VAL:HG22	1.64	0.80
2:E:199:GLU:HG2	11:E:2033:HOH:O	1.82	0.79
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.62	0.79
2:F:112:GLN:HA	11:F:2020:HOH:O	1.83	0.79
1:B:290:GLY:HA3	6:B:1513:GOL:H12	1.65	0.78
2:L:425:THR:HG23	11:L:2062:HOH:O	1.84	0.77
2:F:139:VAL:HG11	2:F:348:VAL:HG21	1.67	0.76
2:L:229:ARG:NH2	2:L:267:GLU:OE1	2.18	0.76
1:H:172:GLN:HG2	11:H:2078:HOH:O	1.84	0.76
1:B:44:LEU:O	1:B:47:VAL:HG22	1.84	0.76
2:L:170:ILE:HG21	2:L:215:VAL:HG22	1.68	0.75
2:F:228:ALA:O	2:F:232:VAL:HG22	1.86	0.75
2:M:129:GLU:HG3	11:M:2031:HOH:O	1.86	0.75
1:I:34:ILE:HD13	1:I:39:ALA:HB2	1.70	0.74
1:H:492:GLU:HB2	11:H:2072:HOH:O	1.88	0.74
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.21	0.73
1:C:362:ARG:HD3	11:C:2078:HOH:O	1.88	0.73
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.19	0.73
2:E:167:MET:HB3	2:E:420:VAL:HG21	1.69	0.73
2:M:330:ASP:OD1	2:M:356:ARG:NH1	2.21	0.73
1:C:179:ALA:HB1	1:C:267:ILE:HG12	1.69	0.73
2:L:9:THR:HB	11:L:2001:HOH:O	1.88	0.72
1:J:441:GLN:O	1:J:445:ILE:HG12	1.90	0.72
1:I:44:LEU:O	1:I:47:VAL:HG22	1.92	0.69
2:D:52:HIS:CD2	2:D:58:VAL:HG12	2.29	0.68
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.73	0.68
1:A:62:MET:HE2	1:A:64:LEU:HD21	1.74	0.67
2:M:223:ASN:HD22	2:M:223:ASN:N	1.90	0.67
1:A:415:GLN:HB3	11:A:2083:HOH:O	1.94	0.67
1:I:172:GLN:NE2	2:L:356:ARG:HE	1.92	0.67
1:C:468:PHE:CE1	1:C:501:VAL:HG12	2.29	0.67
2:E:339:ILE:HG22	2:E:344:ILE:HB	1.74	0.67
2:M:223:ASN:H	2:M:223:ASN:ND2	1.92	0.67
2:L:36:LEU:HB2	2:L:47:LEU:HB2	1.77	0.67
2:K:89:GLU:HB2	2:K:110:THR:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:LEU:O	1:H:47:VAL:HG22	1.96	0.66
1:I:64:LEU:HD22	1:I:74:VAL:CG2	2.26	0.66
2:D:175:LYS:HE3	2:D:203:SER:HB2	1.78	0.66
2:M:218:VAL:HG21	2:M:236:GLY:HA2	1.78	0.65
1:A:183:ILE:HD11	1:A:267:ILE:HD13	1.79	0.65
1:A:62:MET:HE1	1:A:244:TYR:HE2	1.61	0.65
2:E:94:ILE:HG12	2:E:217:LEU:HD12	1.79	0.65
1:B:218:LYS:HE2	11:E:2023:HOH:O	1.96	0.65
2:M:139:VAL:HG13	2:M:414:LEU:HD22	1.79	0.65
1:C:99:VAL:HG22	1:C:253:MET:HA	1.78	0.65
1:J:166:LEU:HB2	1:J:346:THR:HG21	1.79	0.64
2:M:228:ALA:O	2:M:232:VAL:HG22	1.97	0.64
2:E:44:ARG:HD2	11:E:2017:HOH:O	1.97	0.64
2:K:383:SER:O	2:K:387:ILE:HD12	1.98	0.64
2:F:42:GLU:HG3	1:J:120:PRO:HG3	1.80	0.64
2:E:298:THR:HG23	2:E:303:SER:HB3	1.78	0.64
1:I:397:TYR:CD1	1:I:421:GLY:HA3	2.34	0.63
1:J:251:CYS:O	1:J:255:GLU:HG3	1.98	0.63
3:N:115:ILE:HG21	11:N:2004:HOH:O	1.97	0.63
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.78	0.63
2:L:339:ILE:HG22	2:L:344:ILE:HB	1.79	0.63
1:H:102:GLU:HG3	1:H:123:SER:HA	1.80	0.63
2:L:151:LYS:HE2	2:L:293:GLN:HE21	1.64	0.63
1:J:99:VAL:HG22	1:J:253:MET:HA	1.79	0.63
2:M:210:ASP:HB3	2:M:212:THR:H	1.62	0.63
2:E:25:PHE:HB2	2:E:29:LEU:HD23	1.81	0.63
1:J:23:VAL:O	1:J:23:VAL:CG1	2.46	0.62
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.81	0.62
2:M:237:LEU:HD21	2:M:295:ARG:HB3	1.81	0.62
1:A:410:LEU:HD12	1:A:410:LEU:H	1.65	0.62
1:H:244:TYR:HE1	1:H:301:LEU:HD11	1.64	0.62
1:B:175:LYS:HG2	1:B:352:LEU:HD12	1.82	0.62
1:J:468:PHE:CE1	1:J:501:VAL:HG12	2.34	0.62
1:A:177:SER:OG	4:A:1511:ANP:H8	2.00	0.62
2:D:188:GLU:O	2:D:221:GLN:HB3	1.99	0.62
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.35	0.61
1:A:213:VAL:O	1:A:216:LEU:HB3	2.00	0.61
1:A:52:MET:CG	1:A:95:VAL:HG22	2.28	0.61
1:J:373:ARG:HA	7:K:1476:ADP:O3'	2.00	0.61
2:M:233:ALA:O	2:M:237:LEU:HB2	2.01	0.61
2:F:53:LEU:HD21	2:F:59:ARG:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:148:LYS:HE2	11:M:2034:HOH:O	1.99	0.61
2:K:94:ILE:HD11	2:K:197:TYR:CD1	2.36	0.60
2:F:218:VAL:HG21	2:F:236:GLY:HA2	1.84	0.60
2:L:136:GLY:HA3	2:L:431:LEU:HD13	1.82	0.60
2:E:151:LYS:HE3	2:E:296:ILE:HB	1.82	0.60
2:D:94:ILE:HD11	2:D:197:TYR:CD1	2.37	0.60
2:M:277:SER:OG	2:M:278:ALA:N	2.34	0.60
1:H:99:VAL:HG23	1:H:253:MET:HA	1.82	0.60
3:N:39:LYS:HB2	3:N:40:PRO:HD3	1.83	0.60
1:J:456:LEU:HD23	1:J:461:ILE:HD13	1.84	0.60
1:B:355:GLU:HA	11:B:2069:HOH:O	2.01	0.59
1:I:180:ILE:CD1	1:I:216:LEU:HD21	2.33	0.59
1:J:23:VAL:O	1:J:23:VAL:HG12	2.02	0.59
2:F:255:ILE:HD12	2:F:308:GLN:HG2	1.83	0.59
1:H:236:ALA:O	2:K:290:GLY:HA3	2.02	0.59
3:N:75:ARG:HD3	3:N:228:ARG:NH2	2.18	0.59
1:B:196:LYS:HE3	11:B:2034:HOH:O	2.02	0.59
1:A:194:ASP:OD1	1:A:196:LYS:HB2	2.02	0.59
1:J:187:LYS:HE2	1:J:224:ASP:HB3	1.83	0.59
1:C:259:ASP:HB3	11:C:2055:HOH:O	2.02	0.58
2:E:203:SER:HB2	2:E:420:VAL:HG22	1.83	0.58
1:C:23:VAL:CG1	1:C:23:VAL:O	2.52	0.58
1:J:349:GLN:HE22	1:J:371:VAL:HG22	1.68	0.58
1:I:419:SER:O	1:I:423:ARG:NH1	2.33	0.58
1:J:418:LEU:O	1:J:422:VAL:HG23	2.03	0.58
11:J:2075:HOH:O	2:K:344:ILE:HD11	2.03	0.58
1:H:52:MET:CG	1:H:95:VAL:HG22	2.32	0.58
2:E:257:ASN:HD21	2:E:260:ARG:HG3	1.69	0.58
2:K:374:VAL:HG13	2:K:410:ILE:HG21	1.85	0.58
2:E:293:GLN:HA	2:E:293:GLN:HE21	1.68	0.58
1:J:65:ASN:HB2	1:J:72:GLY:HA3	1.86	0.57
3:N:75:ARG:HD2	3:N:133:ARG:HH21	1.69	0.57
1:I:24:ASP:O	1:I:28:THR:HB	2.04	0.57
2:L:167:MET:HB3	2:L:420:VAL:HG21	1.86	0.57
2:L:162:LYS:NZ	2:L:256:ASP:OD2	2.38	0.57
1:C:71:VAL:HG12	1:C:73:VAL:HG23	1.86	0.57
2:M:139:VAL:HG23	11:M:2033:HOH:O	2.04	0.57
2:L:161:GLY:HA3	11:L:2024:HOH:O	2.02	0.57
2:M:87:GLY:HA2	2:M:242:TYR:CE2	2.40	0.57
2:L:377:ILE:HG21	2:L:410:ILE:HD12	1.86	0.57
1:I:99:VAL:HG22	1:I:253:MET:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:424:PHE:HB3	11:L:2062:HOH:O	2.04	0.57
2:F:474:ALA:HB2	11:F:2100:HOH:O	2.05	0.57
2:F:275:ILE:O	2:F:283:PRO:HG3	2.05	0.57
1:J:24:ASP:OD2	1:J:26:GLU:HB2	2.05	0.57
2:D:32:ILE:HA	2:D:49:VAL:HG12	1.86	0.57
1:A:102:GLU:HG3	1:A:123:SER:HA	1.86	0.56
2:D:244:ARG:O	2:D:248:GLY:HA2	2.05	0.56
3:N:113:ARG:HG3	3:N:114:SER:N	2.20	0.56
1:A:106:ARG:NH1	1:A:121:ILE:HD13	2.21	0.56
2:D:89:GLU:HG3	2:D:110:THR:HA	1.88	0.56
2:L:89:GLU:HG3	11:L:2014:HOH:O	2.05	0.56
1:C:23:VAL:HG13	1:C:23:VAL:O	2.05	0.56
2:M:342:LEU:HD23	11:M:2082:HOH:O	2.06	0.56
2:E:257:ASN:ND2	2:E:260:ARG:HG3	2.21	0.55
2:K:244:ARG:O	2:K:248:GLY:HA2	2.06	0.55
1:A:94:ILE:HD13	1:A:96:ASP:HB3	1.86	0.55
1:J:438:ILE:O	1:J:442:VAL:HG23	2.06	0.55
2:D:275:ILE:HG23	3:G:269:ALA:HB2	1.87	0.55
1:C:383:MET:HB2	1:C:438:ILE:HD11	1.87	0.55
2:M:400:ASP:O	2:M:404:VAL:HG23	2.05	0.55
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.89	0.55
1:C:128:ARG:HB2	1:C:131:LEU:HG	1.87	0.55
2:E:227:GLY:O	2:E:231:ARG:HG2	2.06	0.55
2:L:423:VAL:HG23	11:L:2061:HOH:O	2.06	0.55
2:K:414:LEU:HD23	2:K:441:PHE:CZ	2.42	0.55
2:F:210:ASP:HB3	2:F:212:THR:H	1.71	0.55
2:K:186:VAL:HG12	2:K:260:ARG:HB2	1.89	0.55
2:M:9:THR:HA	11:M:2001:HOH:O	2.06	0.55
1:I:327:ILE:HD11	1:I:342:VAL:HG21	1.88	0.55
2:K:52:HIS:CD2	2:K:58:VAL:HG12	2.41	0.54
1:J:406:PHE:CE2	2:K:389:ALA:HA	2.42	0.54
1:J:383:MET:HB2	1:J:438:ILE:HD11	1.88	0.54
2:F:17:ILE:HG13	2:F:271:LEU:HD22	1.90	0.54
2:D:324:THR:O	2:D:324:THR:HG22	2.08	0.54
1:H:107:VAL:HB	1:H:116:ASP:HB3	1.89	0.54
2:K:188:GLU:O	2:K:221:GLN:HB3	2.08	0.54
2:M:89:GLU:HG2	2:M:110:THR:HG22	1.90	0.54
1:B:40:ARG:HG3	11:B:2002:HOH:O	2.08	0.54
1:C:406:PHE:CE2	2:D:389:ALA:HA	2.42	0.54
1:J:44:LEU:HB3	1:J:47:VAL:HG22	1.90	0.54
2:L:89:GLU:HB2	2:L:110:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:9:THR:HB	11:E:2001:HOH:O	2.07	0.54
1:J:268:TYR:HB3	1:J:271:LEU:HD21	1.89	0.54
2:E:275:ILE:O	2:E:283:PRO:HG3	2.08	0.54
2:E:405:SER:HA	11:E:2074:HOH:O	2.08	0.54
2:D:300:LYS:HG2	11:D:2025:HOH:O	2.08	0.53
1:C:157:VAL:HG23	1:C:157:VAL:O	2.08	0.53
2:L:334:VAL:HG21	2:L:352:ASP:HB3	1.89	0.53
2:M:94:ILE:HD11	2:M:197:TYR:CD1	2.43	0.53
1:H:440:GLU:HB3	1:H:469:LEU:HD11	1.91	0.53
1:H:71:VAL:HG23	11:L:2008:HOH:O	2.07	0.53
2:E:36:LEU:HB2	2:E:47:LEU:HB2	1.91	0.53
1:I:165:GLU:O	1:I:325:PRO:HD2	2.08	0.53
1:C:427:LEU:HD22	1:C:444:VAL:HG12	1.89	0.53
1:A:99:VAL:HG22	1:A:253:MET:HA	1.91	0.53
2:L:360:PRO:HD3	2:L:368:TYR:CD1	2.44	0.53
1:H:177:SER:OG	4:H:1511:ANP:H8	2.08	0.53
1:B:165:GLU:O	1:B:325:PRO:HD2	2.08	0.53
1:B:438:ILE:O	1:B:442:VAL:HG13	2.08	0.53
2:L:13:ILE:HD12	2:L:73:GLN:HB3	1.89	0.53
1:I:211:SER:HB3	2:L:126:MET:CE	2.38	0.53
2:F:139:VAL:HG23	2:F:414:LEU:HD22	1.89	0.53
2:E:25:PHE:HB2	2:E:29:LEU:CD2	2.38	0.53
2:M:177:HIS:HB2	11:M:2042:HOH:O	2.08	0.53
1:C:355:GLU:HB2	11:C:2076:HOH:O	2.09	0.53
1:J:479:LEU:HD11	1:J:497:LEU:HG	1.91	0.53
2:M:263:GLN:O	2:M:266:SER:HB3	2.09	0.53
2:L:257:ASN:HD22	2:L:260:ARG:CZ	2.22	0.52
1:J:47:VAL:HG13	1:J:90:ARG:HG2	1.91	0.52
2:L:176:ALA:HB2	2:L:431:LEU:HD21	1.91	0.52
2:L:440:GLY:O	2:L:444:ILE:HG13	2.09	0.52
1:B:99:VAL:HG22	1:B:253:MET:HA	1.91	0.52
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.92	0.52
1:I:66:LEU:O	2:M:15:ALA:HA	2.10	0.52
1:C:65:ASN:HB2	1:C:72:GLY:HA3	1.90	0.52
1:J:157:VAL:HG23	1:J:157:VAL:O	2.09	0.52
2:L:139:VAL:HG23	11:L:2022:HOH:O	2.08	0.52
1:J:215:GLN:HG3	2:M:356:ARG:HH22	1.75	0.52
3:N:109:GLY:HA2	3:N:131:VAL:CG1	2.40	0.52
2:K:51:GLN:HB2	2:K:59:ARG:HB3	1.91	0.52
1:J:410:LEU:HA	11:J:2078:HOH:O	2.08	0.52
2:L:357:ILE:HB	2:L:362:ILE:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:LEU:O	1:C:422:VAL:HG23	2.10	0.52
2:K:444:ILE:HA	11:K:2080:HOH:O	2.10	0.52
1:I:105:GLY:HA2	1:I:226:MET:O	2.10	0.52
2:E:136:GLY:CA	2:E:431:LEU:HD13	2.39	0.52
2:D:52:HIS:HD2	2:D:58:VAL:HG12	1.74	0.52
1:H:457:GLU:HB2	1:H:460:LYS:HD3	1.92	0.52
1:H:213:VAL:O	1:H:216:LEU:HB3	2.09	0.52
2:K:221:GLN:HA	2:K:221:GLN:HE21	1.75	0.52
3:G:76:GLY:O	3:G:228:ARG:NH1	2.43	0.51
2:K:89:GLU:HG3	2:K:110:THR:HA	1.91	0.51
3:G:113:ARG:HG3	3:G:114:SER:N	2.25	0.51
2:L:162:LYS:O	2:L:166:ILE:HG13	2.10	0.51
1:B:202:ILE:HA	1:B:230:ILE:O	2.11	0.51
1:J:34:ILE:HD11	1:J:79:ASP:HB2	1.93	0.51
1:B:171:ARG:CD	11:B:2032:HOH:O	2.41	0.51
1:I:438:ILE:O	1:I:442:VAL:HG13	2.11	0.51
2:F:223:ASN:H	2:F:223:ASN:ND2	2.03	0.51
2:F:139:VAL:HG11	2:F:348:VAL:CG2	2.37	0.51
1:H:99:VAL:CG2	1:H:253:MET:HA	2.40	0.51
2:K:410:ILE:O	2:K:414:LEU:HG	2.11	0.51
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.92	0.51
1:I:168:ILE:HG23	1:I:351:PHE:HD1	1.76	0.51
2:L:257:ASN:HD21	2:L:260:ARG:HG3	1.76	0.51
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.93	0.51
1:H:423:ARG:HG2	1:H:461:ILE:HD11	1.91	0.51
1:J:334:VAL:HG13	1:J:351:PHE:CE1	2.45	0.51
1:I:453:LEU:HA	1:I:456:LEU:HD12	1.93	0.51
1:B:47:VAL:HG13	1:B:90:ARG:HG2	1.93	0.51
1:B:211:SER:HB3	2:E:126:MET:CE	2.41	0.51
1:C:164:ARG:HH22	2:D:189:ARG:HG2	1.76	0.51
1:H:148:THR:HA	1:H:182:THR:HG23	1.93	0.50
1:A:209:LYS:HB2	2:D:294:GLU:OE1	2.11	0.50
2:M:321:ALA:HB3	2:M:322:PRO:CD	2.40	0.50
1:B:66:LEU:O	2:F:15:ALA:HA	2.12	0.50
1:H:368:GLY:HA2	1:H:398:ARG:NH1	2.26	0.50
1:C:399:GLU:HG3	2:D:342:LEU:HD12	1.93	0.50
2:D:363:VAL:HA	11:D:2078:HOH:O	2.11	0.50
2:L:152:ILE:HG13	2:L:331:ALA:HB3	1.93	0.50
1:H:244:TYR:CE1	1:H:301:LEU:HD11	2.45	0.50
2:F:25:PHE:O	2:F:56:SER:HB3	2.10	0.50
2:E:252:LEU:HD13	2:E:254:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:VAL:O	1:A:402:ALA:N	2.45	0.50
1:H:159:ILE:HG22	1:H:160:GLY:N	2.27	0.50
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.47	0.50
2:L:89:GLU:HG2	2:L:109:LYS:O	2.11	0.50
1:H:179:ALA:HB1	1:H:267:ILE:HG12	1.94	0.50
2:E:167:MET:HA	2:E:170:ILE:HD12	1.94	0.50
2:L:321:ALA:HB3	2:L:322:PRO:CD	2.42	0.50
2:D:168:GLU:OE1	2:D:420:VAL:HG23	2.11	0.50
1:B:207:GLY:HA3	1:B:273:LYS:HD3	1.93	0.50
2:F:189:ARG:HB2	2:F:192:GLU:OE1	2.11	0.50
2:K:386:ASP:HB3	3:N:12:SER:HB2	1.93	0.50
1:A:349:GLN:HB2	1:A:351:PHE:CE1	2.47	0.50
2:M:456:ALA:HA	2:M:469:LYS:HD3	1.94	0.50
2:E:346:PRO:HB2	2:E:348:VAL:HG23	1.93	0.50
2:L:139:VAL:HG22	2:L:414:LEU:O	2.12	0.49
1:H:482:LYS:HE2	11:H:2071:HOH:O	2.11	0.49
2:L:149:GLY:HA2	2:L:304:ILE:O	2.12	0.49
3:G:109:GLY:HA2	3:G:131:VAL:HG13	1.94	0.49
2:K:142:LEU:HD21	2:K:374:VAL:HG21	1.94	0.49
2:L:155:PHE:HZ	2:L:326:PHE:CZ	2.31	0.49
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.47	0.49
1:C:263:HIS:HD2	1:C:320:SER:OG	1.94	0.49
1:H:470:SER:HB3	11:H:2069:HOH:O	2.12	0.49
3:G:13:ILE:HD13	3:G:242:MET:SD	2.52	0.49
2:F:94:ILE:HG12	2:F:217:LEU:HD12	1.94	0.49
1:A:164:ARG:HD3	1:A:164:ARG:N	2.27	0.49
1:C:414:THR:O	1:C:418:LEU:HG	2.13	0.49
1:C:373:ARG:HA	7:D:1476:ADP:O3'	2.13	0.49
2:M:89:GLU:HG2	2:M:110:THR:CG2	2.43	0.49
1:B:327:ILE:HD11	1:B:342:VAL:HG21	1.94	0.49
2:M:382:LYS:HA	2:M:385:GLN:HG3	1.95	0.49
1:B:194:ASP:OD2	1:B:197:LYS:HG3	2.13	0.49
1:J:200:TYR:O	1:J:264:ALA:HA	2.13	0.49
1:H:403:PHE:CD2	1:H:403:PHE:N	2.80	0.49
2:K:163:THR:O	2:K:166:ILE:HG22	2.13	0.49
1:I:344:SER:HA	4:M:1475:ANP:O1G	2.13	0.49
3:N:82:HIS:CG	3:N:111:LYS:HG2	2.48	0.48
1:C:397:TYR:CD1	1:C:421:GLY:HA3	2.48	0.48
1:C:279:ARG:O	1:C:283:LEU:HG	2.13	0.48
1:J:44:LEU:O	1:J:47:VAL:HG22	2.13	0.48
3:G:75:ARG:HD3	3:G:228:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLY:HA3	6:B:1513:GOL:C1	2.41	0.48
2:L:257:ASN:ND2	2:L:260:ARG:HG3	2.28	0.48
1:B:344:SER:HA	4:F:1475:ANP:O1G	2.13	0.48
1:B:448:GLY:HA2	1:B:453:LEU:HD12	1.94	0.48
1:H:376:SER:HB3	1:H:384:LYS:HE2	1.95	0.48
2:F:52:HIS:CD2	2:F:58:VAL:HG12	2.47	0.48
1:J:141:SER:HB3	11:J:2031:HOH:O	2.13	0.48
2:L:95:MET:HG2	2:L:218:VAL:HG22	1.95	0.48
2:M:174:ALA:O	2:M:177:HIS:HB3	2.14	0.48
3:G:109:GLY:HA2	3:G:131:VAL:CG1	2.43	0.48
2:K:377:ILE:HG12	2:K:407:ALA:HB2	1.95	0.48
1:I:202:ILE:HG12	1:I:230:ILE:HD12	1.94	0.48
1:A:148:THR:HA	1:A:182:THR:HG23	1.96	0.48
2:D:285:LEU:C	2:D:285:LEU:HD23	2.34	0.48
1:A:410:LEU:HB2	1:A:415:GLN:HG3	1.95	0.48
2:F:189:ARG:O	2:F:221:GLN:NE2	2.46	0.48
2:M:139:VAL:CG2	11:M:2033:HOH:O	2.61	0.48
1:I:202:ILE:HB	1:I:266:ILE:HG13	1.96	0.48
1:I:202:ILE:HA	1:I:230:ILE:O	2.14	0.48
2:D:345:TYR:HA	2:D:346:PRO:C	2.33	0.48
1:I:37:GLY:HA3	11:I:2003:HOH:O	2.14	0.48
1:J:382:ALA:HB2	1:J:488:LYS:HA	1.96	0.48
3:N:245:LYS:HE3	11:N:2015:HOH:O	2.14	0.48
1:A:403:PHE:CD2	1:A:403:PHE:N	2.81	0.48
1:C:74:VAL:HG13	1:C:241:PRO:CG	2.43	0.47
2:F:395:GLU:OE2	3:G:77:LEU:HA	2.14	0.47
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.96	0.47
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.97	0.47
1:C:438:ILE:O	1:C:442:VAL:HG23	2.13	0.47
2:L:25:PHE:HB2	2:L:29:LEU:HD23	1.96	0.47
2:L:388:ILE:HD12	2:L:393:MET:HG3	1.96	0.47
2:K:84:ILE:HG21	2:K:235:THR:HG23	1.96	0.47
3:N:106:ILE:N	11:N:2007:HOH:O	2.46	0.47
1:H:410:LEU:H	1:H:410:LEU:HD12	1.79	0.47
1:C:268:TYR:HB3	1:C:271:LEU:HD21	1.96	0.47
1:I:410:LEU:HB3	11:I:2071:HOH:O	2.14	0.47
2:D:444:ILE:HA	11:D:2091:HOH:O	2.14	0.47
3:N:260:LYS:HG3	10:N:1273:PIT:C9	2.44	0.47
11:M:2076:HOH:O	10:N:1273:PIT:H4	2.13	0.47
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.95	0.47
1:A:209:LYS:NZ	1:A:212:THR:OG1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:80:ALA:O	3:N:84:SER:HB2	2.14	0.47
2:M:84:ILE:HG13	2:M:84:ILE:O	2.15	0.47
1:A:159:ILE:HG22	1:A:160:GLY:N	2.29	0.47
1:H:98:PRO:HG3	11:H:2018:HOH:O	2.14	0.47
2:F:403:THR:HG21	11:F:2082:HOH:O	2.13	0.47
2:F:139:VAL:CG1	2:F:348:VAL:HG21	2.41	0.47
1:C:240:ALA:HB3	1:C:241:PRO:HD3	1.95	0.47
2:K:181:SER:O	2:K:215:VAL:HA	2.15	0.47
2:M:345:TYR:HA	2:M:346:PRO:C	2.34	0.47
2:M:83:ARG:CZ	11:M:2017:HOH:O	2.63	0.47
2:K:237:LEU:HD21	2:K:295:ARG:HB2	1.97	0.47
1:I:48:GLN:HE21	2:M:68:GLY:HA2	1.78	0.47
2:L:224:GLU:O	2:L:229:ARG:HD3	2.15	0.47
1:C:362:ARG:CD	11:C:2078:HOH:O	2.53	0.47
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.45	0.47
2:D:199:GLU:HA	11:D:2041:HOH:O	2.15	0.47
2:E:32:ILE:HG22	2:E:33:LEU:HG	1.96	0.47
2:M:440:GLY:O	2:M:444:ILE:HG13	2.14	0.47
2:E:440:GLY:O	2:E:444:ILE:HG13	2.14	0.47
1:J:213:VAL:O	1:J:217:VAL:HG13	2.15	0.47
2:D:247:GLU:O	2:D:249:GLN:NE2	2.48	0.47
2:L:31:PRO:O	2:L:34:ASN:HB2	2.14	0.47
1:A:438:ILE:O	1:A:442:VAL:HG13	2.15	0.47
2:E:13:ILE:HD12	2:E:73:GLN:HB3	1.97	0.47
2:F:86:VAL:O	2:F:110:THR:HG21	2.14	0.47
1:I:398:ARG:CZ	1:I:398:ARG:HB2	2.45	0.47
1:I:102:GLU:HG3	1:I:123:SER:HA	1.97	0.47
2:L:227:GLY:O	2:L:231:ARG:HG2	2.15	0.46
1:C:141:SER:HB2	1:C:143:ARG:HE	1.80	0.46
2:K:259:PHE:CZ	2:K:263:GLN:HB2	2.50	0.46
1:H:407:GLY:O	1:H:410:LEU:HD11	2.15	0.46
2:M:112:GLN:H	2:M:112:GLN:HE21	1.63	0.46
1:C:292:GLU:O	1:C:293:ALA:HB3	2.15	0.46
2:F:220:GLY:N	2:F:232:VAL:HG11	2.30	0.46
2:K:113:PHE:CD1	2:K:113:PHE:N	2.81	0.46
1:B:99:VAL:HG13	1:B:256:TYR:HB2	1.96	0.46
2:F:89:GLU:HG2	2:F:110:THR:HG23	1.96	0.46
1:I:194:ASP:OD2	1:I:197:LYS:HG3	2.16	0.46
2:M:189:ARG:O	2:M:221:GLN:NE2	2.49	0.46
2:K:27:GLU:HB2	2:K:28:GLY:H	1.49	0.46
1:C:334:VAL:HG13	1:C:351:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:374:VAL:HG13	2:D:410:ILE:HG21	1.95	0.46
3:G:38:LEU:HD22	3:G:222:THR:HG21	1.96	0.46
10:G:1273:PIT:H8	10:G:1273:PIT:H6	1.68	0.46
1:B:164:ARG:HD3	1:B:164:ARG:N	2.30	0.46
2:E:170:ILE:HD13	2:E:215:VAL:CG2	2.46	0.46
2:E:83:ARG:NH2	2:E:113:PHE:HB2	2.30	0.46
1:B:62:MET:HB2	1:B:76:PHE:HE1	1.81	0.46
2:K:285:LEU:HD23	2:K:285:LEU:C	2.36	0.46
2:D:276:PRO:HG3	3:G:268:GLY:HA3	1.97	0.46
2:F:359:ASP:HB3	2:F:362:ILE:HD12	1.96	0.46
1:C:80:LYS:HD3	2:F:33:LEU:HD12	1.96	0.46
1:J:240:ALA:HB3	1:J:241:PRO:HD3	1.98	0.46
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.80	0.46
2:M:256:ASP:HA	2:M:257:ASN:HA	1.69	0.46
1:J:71:VAL:HG12	1:J:73:VAL:HG23	1.96	0.46
1:H:194:ASP:OD1	1:H:196:LYS:HB2	2.16	0.46
2:L:226:PRO:HG2	2:L:271:LEU:HD11	1.96	0.46
1:J:297:ASP:HA	2:K:267:GLU:HG2	1.98	0.46
1:J:349:GLN:NE2	1:J:371:VAL:HG22	2.29	0.46
2:D:51:GLN:HB2	2:D:59:ARG:HB3	1.98	0.46
2:L:390:ILE:HG22	2:L:391:LEU:HG	1.97	0.46
2:K:324:THR:HG22	2:K:324:THR:O	2.16	0.46
1:I:52:MET:HA	1:I:61:GLY:O	2.16	0.45
3:G:248:LEU:HB3	3:G:252:ARG:HH12	1.80	0.45
1:H:337:TYR:CZ	6:H:1514:GOL:H12	2.51	0.45
1:A:157:VAL:N	1:A:158:PRO:CD	2.80	0.45
1:H:74:VAL:CG1	1:H:241:PRO:HB3	2.46	0.45
1:B:102:GLU:HG3	1:B:123:SER:HA	1.98	0.45
1:I:27:GLU:OE1	1:I:90:ARG:HD3	2.16	0.45
2:M:242:TYR:CD1	2:M:246:GLN:HG3	2.52	0.45
1:B:180:ILE:HD12	1:B:216:LEU:HD21	1.95	0.45
1:I:64:LEU:HD22	1:I:74:VAL:HG23	1.97	0.45
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.98	0.45
1:B:343:ILE:HG12	1:B:349:GLN:HG2	1.99	0.45
2:E:381:TYR:HE1	2:E:404:VAL:HG13	1.80	0.45
1:I:201:CYS:O	1:I:229:THR:HA	2.15	0.45
1:H:246:ALA:HB3	1:H:247:PRO:HD3	1.99	0.45
1:A:36:ASP:O	1:A:284:LEU:HD13	2.17	0.45
1:J:52:MET:O	1:J:91:THR:HB	2.17	0.45
2:F:443:GLN:NE2	2:F:449:TYR:OH	2.48	0.45
1:C:213:VAL:O	1:C:217:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:438:ILE:O	2:E:442:GLN:HB2	2.17	0.45
1:J:381:ARG:NH1	1:J:488:LYS:NZ	2.64	0.45
1:B:105:GLY:HA2	1:B:226:MET:O	2.17	0.45
1:B:419:SER:HB3	11:B:2078:HOH:O	2.17	0.45
3:G:251:ASN:HA	3:G:254:ARG:HB3	1.98	0.45
2:E:89:GLU:HB2	2:E:110:THR:HG22	1.98	0.45
2:D:95:MET:HE3	2:D:99:GLY:HA2	1.99	0.45
1:B:303:SER:HB2	2:F:222:MET:SD	2.56	0.45
1:C:297:ASP:HA	2:D:267:GLU:HG2	1.99	0.45
2:K:113:PHE:HD1	2:K:113:PHE:N	2.15	0.45
1:J:381:ARG:HH11	1:J:488:LYS:HZ2	1.64	0.45
11:E:2057:HOH:O	3:G:250:PHE:HE2	2.00	0.45
1:A:166:LEU:HD13	1:A:342:VAL:HG11	1.98	0.45
2:D:359:ASP:OD2	2:D:361:ASN:N	2.50	0.45
1:J:129:VAL:HG21	1:J:245:LEU:HD11	1.98	0.44
2:L:139:VAL:HG13	2:L:414:LEU:HD22	1.99	0.44
2:E:32:ILE:HA	2:E:49:VAL:HG12	1.99	0.44
2:F:277:SER:OG	2:F:278:ALA:N	2.50	0.44
1:B:392:LEU:HG	1:B:396:GLN:HE21	1.82	0.44
2:E:167:MET:CB	2:E:420:VAL:HG21	2.42	0.44
1:H:159:ILE:HG22	1:H:160:GLY:H	1.83	0.44
1:C:397:TYR:CD2	1:C:398:ARG:HG3	2.52	0.44
1:B:343:ILE:HG23	1:B:349:GLN:NE2	2.32	0.44
1:B:396:GLN:HB3	1:B:417:LEU:HD13	1.99	0.44
1:C:67:GLU:HB3	1:C:68:PRO:CD	2.47	0.44
6:B:1513:GOL:H2	2:F:279:VAL:O	2.17	0.44
1:I:394:LEU:HD11	1:I:428:LEU:HD11	2.00	0.44
2:D:84:ILE:HG21	2:D:235:THR:HG23	1.98	0.44
2:E:220:GLY:CA	2:E:232:VAL:HG11	2.47	0.44
1:C:352:LEU:HA	1:C:364:ALA:O	2.17	0.44
2:L:220:GLY:HA3	2:L:232:VAL:HG21	1.99	0.44
3:G:85:VAL:HG23	3:G:112:ILE:HD11	1.99	0.44
3:G:4:LYS:HG3	11:G:2001:HOH:O	2.17	0.44
2:L:253:LEU:O	2:L:306:SER:HA	2.18	0.44
1:H:410:LEU:HB2	1:H:415:GLN:HG3	2.00	0.44
2:F:32:ILE:O	2:F:33:LEU:HB2	2.18	0.44
2:E:381:TYR:CE1	2:E:404:VAL:HG13	2.53	0.44
1:C:488:LYS:HD3	11:C:2097:HOH:O	2.18	0.44
2:D:256:ASP:HA	2:D:257:ASN:HA	1.87	0.44
2:D:15:ALA:HB3	2:D:22:ASP:HB2	1.98	0.44
2:D:127:SER:HB2	11:D:2025:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:255:ILE:HB	2:E:308:GLN:HG2	1.98	0.44
1:I:488:LYS:HG2	1:I:489:ILE:N	2.33	0.44
2:M:226:PRO:HB2	2:M:268:VAL:HG12	1.99	0.44
2:M:187:GLY:O	2:M:222:MET:HB3	2.18	0.44
1:I:175:LYS:HG2	1:I:352:LEU:HD12	1.99	0.44
1:H:371:VAL:HG22	1:H:372:SER:N	2.32	0.44
2:L:83:ARG:NH2	2:L:113:PHE:HB2	2.33	0.44
2:D:163:THR:O	2:D:166:ILE:HG22	2.18	0.44
1:A:187:LYS:HE2	1:A:224:ASP:HB3	2.00	0.44
1:A:94:ILE:CD1	1:A:96:ASP:HB3	2.47	0.44
2:L:322:PRO:O	2:L:326:PHE:HD1	2.01	0.44
2:F:9:THR:HB	2:F:10:THR:H	1.57	0.44
2:D:439:LYS:O	2:D:443:GLN:HG3	2.17	0.44
2:L:345:TYR:H	2:L:459:MET:HE1	1.83	0.44
1:H:110:ALA:HB2	1:H:234:ALA:HB2	1.99	0.44
2:L:36:LEU:O	2:L:46:VAL:HA	2.18	0.43
1:J:26:GLU:HA	1:J:45:ARG:HB2	2.00	0.43
1:A:99:VAL:HG13	1:A:256:TYR:HB2	1.99	0.43
2:F:16:VAL:HG22	2:F:21:VAL:HG22	1.99	0.43
1:C:349:GLN:NE2	1:C:371:VAL:HG22	2.33	0.43
2:M:88:PRO:O	2:M:91:LEU:HD12	2.18	0.43
2:K:247:GLU:O	2:K:249:GLN:NE2	2.50	0.43
1:H:148:THR:HG21	1:H:153:VAL:HG11	2.00	0.43
1:C:486:ASP:HB3	1:C:488:LYS:HG2	2.00	0.43
1:J:128:ARG:HB2	1:J:131:LEU:HG	2.00	0.43
1:C:497:LEU:O	1:C:501:VAL:HG13	2.18	0.43
1:H:456:LEU:HD23	1:H:461:ILE:HD13	2.00	0.43
1:A:240:ALA:N	1:A:241:PRO:HD2	2.33	0.43
2:D:410:ILE:HG13	2:D:444:ILE:HG21	2.00	0.43
2:L:254:PHE:HA	2:L:307:VAL:O	2.19	0.43
1:B:270:ASP:OD1	1:B:272:SER:HB2	2.18	0.43
2:D:430:LYS:HD2	2:D:465:GLU:OE1	2.19	0.43
2:K:345:TYR:HA	2:K:346:PRO:C	2.39	0.43
1:B:362:ARG:HA	1:B:363:PRO:C	2.39	0.43
1:I:439:GLU:HG2	1:I:440:GLU:N	2.32	0.43
2:M:223:ASN:N	2:M:223:ASN:ND2	2.61	0.43
1:C:424:LEU:HA	1:C:427:LEU:HD12	2.00	0.43
2:M:32:ILE:O	2:M:33:LEU:HB2	2.18	0.43
2:D:188:GLU:H	2:D:221:GLN:NE2	2.17	0.43
2:D:416:GLN:HA	2:D:417:PRO:HD2	1.85	0.43
1:H:51:GLU:HG2	1:H:52:MET:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:139:VAL:HG23	2:K:414:LEU:HD22	2.01	0.43
1:J:334:VAL:HG13	1:J:351:PHE:CD1	2.54	0.43
1:H:291:ARG:H	6:H:1514:GOL:H11	1.82	0.43
2:F:256:ASP:HA	2:F:257:ASN:HA	1.76	0.43
1:C:347:ASP:HA	1:C:373:ARG:HD2	2.01	0.43
1:A:166:LEU:HD13	1:A:342:VAL:CG1	2.49	0.43
2:D:84:ILE:HD13	2:D:235:THR:HG23	2.00	0.43
2:F:90:THR:HG22	2:F:95:MET:HE1	2.00	0.43
3:N:20:THR:O	3:N:232:MET:HB3	2.19	0.43
1:C:440:GLU:HB3	1:C:469:LEU:HD11	2.00	0.43
1:H:183:ILE:HD11	1:H:267:ILE:HD13	2.01	0.43
2:K:163:THR:HA	2:K:166:ILE:HG22	2.00	0.43
1:J:337:TYR:CD2	1:J:338:ILE:HD12	2.53	0.43
2:D:258:ILE:HD11	2:D:292:MET:HE2	2.00	0.43
1:B:135:GLY:HA2	11:F:2039:HOH:O	2.19	0.43
2:M:367:HIS:CE1	2:M:434:LEU:HD11	2.54	0.43
1:J:62:MET:HB2	1:J:76:PHE:CZ	2.54	0.43
2:F:30:PRO:HA	2:F:31:PRO:HD2	1.89	0.43
1:I:452:TYR:OH	1:I:498:LYS:HG3	2.18	0.43
3:G:72:SER:OG	3:G:73:SER:N	2.52	0.43
1:J:465:GLU:O	1:J:469:LEU:HB2	2.19	0.43
1:H:410:LEU:HD13	1:H:415:GLN:CG	2.48	0.42
1:J:32:LEU:O	1:J:84:GLU:HG3	2.19	0.42
3:G:37:GLU:HG2	3:G:218:LYS:HE2	2.01	0.42
2:L:94:ILE:HD12	2:L:103:ASP:HB3	2.01	0.42
1:C:249:SER:O	1:C:253:MET:HG3	2.19	0.42
2:K:237:LEU:HD13	2:K:296:ILE:HG12	2.00	0.42
2:F:32:ILE:HG22	2:F:33:LEU:HG	2.01	0.42
1:A:190:ASN:HA	1:A:198:LYS:HG2	2.00	0.42
1:H:382:ALA:HB2	1:H:487:GLY:O	2.19	0.42
1:I:158:PRO:O	1:I:375:GLY:HA3	2.19	0.42
1:B:133:ALA:HB2	1:B:308:ARG:HG3	2.01	0.42
1:C:374:VAL:HG11	1:C:378:ALA:HB2	2.02	0.42
2:K:45:LEU:HD13	2:K:64:ASP:HB3	2.01	0.42
2:K:152:ILE:HB	2:K:307:VAL:HG22	2.00	0.42
2:K:242:TYR:C	2:K:242:TYR:CD2	2.93	0.42
2:K:25:PHE:O	2:K:56:SER:HB3	2.19	0.42
4:B:1510:ANP:O2'	2:E:359:ASP:OD1	2.38	0.42
1:B:240:ALA:HB3	1:B:241:PRO:HD3	2.02	0.42
1:H:218:LYS:HE3	2:K:128:VAL:HG21	2.01	0.42
2:L:412:ARG:HG2	2:L:458:TYR:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:47:LEU:HB3	2:L:60:THR:HB	2.00	0.42
1:B:286:ARG:HA	2:E:275:ILE:CD1	2.50	0.42
1:H:410:LEU:HD13	1:H:415:GLN:HG3	2.02	0.42
2:L:438:ILE:O	2:L:442:GLN:HB2	2.20	0.42
2:F:221:GLN:OE1	2:F:221:GLN:HA	2.20	0.42
2:F:94:ILE:HD12	2:F:103:ASP:HB3	2.00	0.42
1:A:419:SER:O	1:A:422:VAL:HG22	2.19	0.42
11:H:2047:HOH:O	2:L:18:GLY:HA2	2.19	0.42
3:N:78:CYS:HB3	3:N:228:ARG:HB2	2.01	0.42
1:C:121:ILE:HB	11:C:2031:HOH:O	2.19	0.42
2:L:155:PHE:HZ	2:L:326:PHE:HZ	1.67	0.42
2:F:89:GLU:HG2	2:F:110:THR:CG2	2.50	0.42
2:F:345:TYR:HA	2:F:346:PRO:C	2.40	0.42
3:N:135:PRO:HA	3:N:136:PRO:HD2	1.92	0.42
2:L:179:GLY:HA2	2:L:249:GLN:NE2	2.34	0.42
1:H:414:THR:HA	1:H:417:LEU:HD12	2.01	0.42
1:A:218:LYS:HE3	2:D:128:VAL:HG21	2.02	0.42
2:M:30:PRO:HA	2:M:31:PRO:HD2	1.84	0.42
1:J:397:TYR:CD1	1:J:421:GLY:HA3	2.55	0.42
1:I:64:LEU:HD22	1:I:74:VAL:HG21	1.99	0.42
2:L:257:ASN:HB2	2:L:309:ALA:HB3	2.01	0.42
1:A:164:ARG:CD	1:A:164:ARG:N	2.83	0.42
1:B:292:GLU:H	10:G:1273:PIT:C1	2.33	0.42
1:A:418:LEU:O	1:A:422:VAL:HG13	2.20	0.42
2:F:456:ALA:HA	2:F:469:LYS:HD3	2.02	0.42
1:C:200:TYR:O	1:C:264:ALA:HA	2.19	0.42
1:B:379:GLN:OE1	1:B:384:LYS:HG3	2.19	0.42
1:H:137:ILE:N	1:H:138:PRO:CD	2.82	0.42
1:B:128:ARG:HB2	1:B:131:LEU:HG	2.01	0.42
1:B:209:LYS:NZ	2:E:330:ASP:OD2	2.52	0.42
2:F:420:VAL:HG12	2:F:420:VAL:O	2.20	0.42
2:M:321:ALA:HB3	2:M:322:PRO:HD3	2.01	0.41
1:C:78:ASN:ND2	1:C:80:LYS:HE2	2.35	0.41
1:J:62:MET:HB2	1:J:76:PHE:CE1	2.55	0.41
1:A:440:GLU:HB3	1:A:469:LEU:HD11	2.02	0.41
1:A:152:ALA:HB3	1:A:365:ILE:HD12	2.02	0.41
2:D:82:ILE:HB	2:D:116:ILE:HG12	2.01	0.41
1:B:246:ALA:HB3	1:B:247:PRO:HD3	2.02	0.41
1:C:456:LEU:HD22	1:C:505:LEU:HD21	2.01	0.41
1:H:269:ASP:HA	1:H:270:ASP:HA	1.77	0.41
2:K:336:SER:HB3	2:K:339:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:338:ALA:O	2:K:342:LEU:HG	2.19	0.41
2:E:155:PHE:HZ	2:E:326:PHE:CZ	2.38	0.41
1:A:175:LYS:H	4:A:1511:ANP:PB	2.42	0.41
2:E:32:ILE:O	2:E:33:LEU:HB2	2.21	0.41
1:H:185:ASN:O	1:H:188:ARG:HG2	2.20	0.41
2:L:203:SER:HB2	2:L:420:VAL:HG22	2.03	0.41
2:K:188:GLU:HB3	2:K:189:ARG:H	1.68	0.41
1:C:168:ILE:O	1:C:351:PHE:HA	2.20	0.41
2:K:84:ILE:HD13	2:K:235:THR:HG23	2.01	0.41
10:N:1273:PIT:H6	10:N:1273:PIT:H8	1.76	0.41
1:J:240:ALA:N	1:J:241:PRO:CD	2.83	0.41
2:K:23:VAL:HG12	2:K:25:PHE:CE1	2.55	0.41
2:K:398:GLU:HA	2:K:401:LYS:HG2	2.02	0.41
1:H:362:ARG:HA	1:H:363:PRO:C	2.40	0.41
1:A:382:ALA:HB2	1:A:487:GLY:O	2.20	0.41
1:I:362:ARG:HA	1:I:363:PRO:C	2.40	0.41
2:M:70:VAL:HG12	2:M:71:ARG:O	2.20	0.41
2:L:256:ASP:HA	2:L:257:ASN:HA	1.58	0.41
2:L:110:THR:OG1	2:L:112:GLN:O	2.34	0.41
2:M:19:ALA:HB2	2:M:226:PRO:HG2	2.02	0.41
1:I:171:ARG:NH1	1:I:171:ARG:HB2	2.35	0.41
2:E:37:GLU:OE2	2:E:44:ARG:NH2	2.54	0.41
1:A:99:VAL:CG1	1:A:256:TYR:HB2	2.50	0.41
1:A:209:LYS:HD3	11:D:2032:HOH:O	2.19	0.41
1:J:71:VAL:HG12	1:J:73:VAL:CG2	2.51	0.41
1:C:40:ARG:NH1	1:C:67:GLU:OE2	2.54	0.41
2:L:83:ARG:HA	2:L:114:ALA:O	2.20	0.41
1:A:423:ARG:HG2	1:A:461:ILE:HD11	2.01	0.41
2:E:312:VAL:HA	2:E:313:PRO:HD2	1.89	0.41
2:K:412:ARG:HE	2:K:455:GLN:NE2	2.19	0.41
2:D:170:ILE:O	2:D:174:ALA:HB3	2.21	0.41
1:C:99:VAL:CG1	1:C:256:TYR:HB2	2.51	0.41
2:L:110:THR:HB	11:L:2013:HOH:O	2.20	0.41
1:J:291:ARG:HD3	1:J:337:TYR:CE1	2.56	0.41
2:K:146:TYR:CG	2:K:152:ILE:HG12	2.56	0.41
1:B:304:ARG:HB2	11:B:2061:HOH:O	2.19	0.41
1:A:414:THR:HA	1:A:417:LEU:HD12	2.02	0.41
1:A:163:GLN:HG3	1:A:347:ASP:HB2	2.03	0.41
2:L:282:GLN:HB2	11:L:2043:HOH:O	2.19	0.41
3:N:33:ARG:HD2	3:N:36:ARG:HH12	1.86	0.41
2:M:25:PHE:O	2:M:56:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:HG	1:A:496:LYS:HG2	2.03	0.41
2:K:231:ARG:HD3	2:K:231:ARG:HA	1.84	0.41
1:I:152:ALA:HB2	1:I:428:LEU:HB3	2.02	0.41
2:M:336:SER:OG	2:M:339:ILE:HG13	2.19	0.41
2:E:51:GLN:HB2	2:E:59:ARG:HB3	2.03	0.41
1:H:434:SER:HB3	11:H:2066:HOH:O	2.21	0.41
1:H:166:LEU:HD13	1:H:342:VAL:CG1	2.51	0.41
1:C:291:ARG:HD3	1:C:337:TYR:CD1	2.56	0.41
2:K:15:ALA:HB3	2:K:22:ASP:HB2	2.02	0.41
1:H:204:VAL:HG12	1:H:206:ILE:HD11	2.01	0.41
1:C:105:GLY:HA2	1:C:226:MET:O	2.20	0.41
2:F:229:ARG:HA	2:F:232:VAL:CG2	2.50	0.41
2:M:207:ASN:CG	2:M:210:ASP:HB2	2.41	0.41
2:E:29:LEU:HD11	2:E:56:SER:HA	2.02	0.41
2:M:393:MET:SD	2:M:404:VAL:HG11	2.61	0.41
1:B:103:LEU:HD13	1:B:253:MET:HG2	2.03	0.41
2:L:152:ILE:HA	2:L:331:ALA:O	2.21	0.41
1:I:303:SER:HB2	2:M:222:MET:SD	2.61	0.41
1:H:330:GLN:HB3	2:K:318:THR:HB	2.03	0.41
1:J:75:VAL:HG12	1:J:77:GLY:H	1.86	0.41
1:B:358:TYR:C	1:B:360:GLY:H	2.24	0.41
1:J:185:ASN:OD1	1:J:435:PRO:HB2	2.19	0.41
2:F:166:ILE:CG2	2:F:167:MET:N	2.83	0.41
2:M:155:PHE:HB2	2:M:334:VAL:HA	2.03	0.41
1:C:152:ALA:HB3	1:C:365:ILE:HD12	2.03	0.41
2:D:326:PHE:HA	2:D:329:LEU:HD12	2.02	0.41
3:G:82:HIS:CG	3:G:111:LYS:HG2	2.56	0.41
1:C:168:ILE:HD11	1:C:339:PRO:HB3	2.03	0.41
1:A:434:SER:HB3	11:A:2086:HOH:O	2.20	0.41
2:F:233:ALA:O	2:F:237:LEU:HB2	2.20	0.41
1:C:255:GLU:HG2	1:C:258:ARG:NH1	2.36	0.41
1:H:271:LEU:HA	1:H:271:LEU:HD23	1.88	0.41
2:F:139:VAL:HG13	2:F:140:VAL:N	2.36	0.40
2:K:94:ILE:HG22	2:K:102:ILE:HG13	2.03	0.40
1:J:269:ASP:HA	1:J:270:ASP:HA	1.82	0.40
2:F:188:GLU:O	2:F:221:GLN:HB3	2.22	0.40
2:D:84:ILE:HD11	2:D:238:THR:HB	2.02	0.40
1:B:269:ASP:HA	1:B:270:ASP:HA	1.73	0.40
1:B:152:ALA:HA	1:B:428:LEU:HD22	2.02	0.40
1:I:51:GLU:HA	1:I:94:ILE:HA	2.03	0.40
1:H:161:ARG:NH2	1:H:197:LYS:O	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:170:ILE:HD13	2:E:215:VAL:HG22	2.04	0.40
1:J:255:GLU:HG2	1:J:258:ARG:NH1	2.37	0.40
1:A:196:LYS:HB3	1:A:196:LYS:HE3	1.88	0.40
2:L:38:VAL:HG22	2:L:75:VAL:HG22	2.04	0.40
1:A:286:ARG:NH2	3:G:272:LEU:HD13	2.36	0.40
1:B:36:ASP:HA	11:E:2050:HOH:O	2.21	0.40
2:D:259:PHE:CE2	2:D:263:GLN:HB2	2.56	0.40
1:H:107:VAL:HG22	1:H:231:VAL:HB	2.04	0.40
1:H:452:TYR:OH	1:H:498:LYS:HG3	2.22	0.40
1:H:180:ILE:HA	1:H:180:ILE:HD13	1.87	0.40
2:F:207:ASN:CG	2:F:210:ASP:HB2	2.42	0.40
2:D:410:ILE:O	2:D:414:LEU:HG	2.21	0.40
1:A:246:ALA:HB3	1:A:247:PRO:HD3	2.03	0.40
3:G:168:VAL:HG23	3:G:169:ILE:HG13	2.02	0.40
1:J:392:LEU:HD23	1:J:392:LEU:HA	1.93	0.40
1:B:208:GLN:HG2	11:B:2052:HOH:O	2.22	0.40
2:M:146:TYR:HB3	2:M:152:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/510 (95%)	458 (94%)	25 (5%)	2 (0%)	39	69
1	B	475/510 (93%)	457 (96%)	15 (3%)	3 (1%)	30	59
1	C	493/510 (97%)	470 (95%)	23 (5%)	0	100	100
1	H	485/510 (95%)	458 (94%)	26 (5%)	1 (0%)	52	80
1	I	475/510 (93%)	453 (95%)	22 (5%)	0	100	100
1	J	493/510 (97%)	473 (96%)	19 (4%)	1 (0%)	52	80
2	D	465/482 (96%)	436 (94%)	27 (6%)	2 (0%)	39	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	464/482 (96%)	443 (96%)	19 (4%)	2 (0%)	39	69
2	F	464/482 (96%)	436 (94%)	25 (5%)	3 (1%)	30	59
2	K	465/482 (96%)	443 (95%)	19 (4%)	3 (1%)	30	59
2	L	464/482 (96%)	442 (95%)	20 (4%)	2 (0%)	39	69
2	M	464/482 (96%)	440 (95%)	22 (5%)	2 (0%)	39	69
3	G	155/272 (57%)	151 (97%)	4 (3%)	0	100	100
3	N	155/272 (57%)	150 (97%)	5 (3%)	0	100	100
All	All	6002/6496 (92%)	5710 (95%)	271 (4%)	21 (0%)	46	75

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	ALA
1	H	401	ALA
2	K	314	ALA
2	L	347	ALA
2	D	385	GLN
2	E	347	ALA
2	F	455	GLN
1	J	409	ASP
2	K	385	GLN
1	A	239	ALA
2	M	28	GLY
1	B	143	ARG
1	B	135	GLY
1	B	359	LYS
2	K	320	PRO
2	E	279	VAL
2	F	28	GLY
2	L	279	VAL
2	M	17	ILE
2	D	320	PRO
2	F	279	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/413 (95%)	376 (96%)	17 (4%)	35	66
1	B	389/413 (94%)	373 (96%)	16 (4%)	37	69
1	C	399/413 (97%)	381 (96%)	18 (4%)	34	65
1	H	393/413 (95%)	378 (96%)	15 (4%)	40	71
1	I	389/413 (94%)	374 (96%)	15 (4%)	39	70
1	J	399/413 (97%)	387 (97%)	12 (3%)	48	79
2	D	377/386 (98%)	372 (99%)	5 (1%)	76	92
2	E	376/386 (97%)	353 (94%)	23 (6%)	23	49
2	F	376/386 (97%)	365 (97%)	11 (3%)	50	80
2	K	377/386 (98%)	372 (99%)	5 (1%)	76	92
2	L	376/386 (97%)	360 (96%)	16 (4%)	35	66
2	M	376/386 (97%)	364 (97%)	12 (3%)	46	77
3	G	140/230 (61%)	127 (91%)	13 (9%)	11	25
3	N	140/230 (61%)	126 (90%)	14 (10%)	9	22
All	All	4900/5254 (93%)	4708 (96%)	192 (4%)	39	70

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	47	VAL
1	A	74	VAL
1	A	94	ILE
1	A	99	VAL
1	A	101	GLU
1	A	136	ILE
1	A	164	ARG
1	A	188	ARG
1	A	217	VAL
1	A	335	SER
1	A	367	VAL
1	A	403	PHE
1	A	410	LEU
1	A	442	VAL
1	A	479	LEU

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Mol	Chain	Res	Type
1	A	496	LYS
1	B	28	THR
1	B	30	ARG
1	B	47	VAL
1	B	57	SER
1	B	99	VAL
1	B	164	ARG
1	B	215	GLN
1	B	244	TYR
1	B	282	SER
1	B	298	VAL
1	B	371	VAL
1	B	376	SER
1	B	394	LEU
1	B	434	SER
1	B	479	LEU
1	B	499	GLU
1	C	24	ASP
1	C	47	VAL
1	C	63	SER
1	C	74	VAL
1	C	97	VAL
1	C	99	VAL
1	C	164	ARG
1	C	211	SER
1	C	216	LEU
1	C	217	VAL
1	C	334	VAL
1	C	344	SER
1	C	371	VAL
1	C	381	ARG
1	C	406	PHE
1	C	432	GLN
1	C	479	LEU
1	C	505	LEU
2	D	27	GLU
2	D	97	VAL
2	D	335	LEU
2	D	342	LEU
2	D	359	ASP
2	E	76	LEU
2	E	129	GLU

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Mol	Chain	Res	Type
2	E	139	VAL
2	E	162	LYS
2	E	209	LYS
2	E	215	VAL
2	E	223	ASN
2	E	232	VAL
2	E	257	ASN
2	E	279	VAL
2	E	293	GLN
2	E	298	THR
2	E	310	ILE
2	E	352	ASP
2	E	358	MET
2	E	399	GLU
2	E	400	ASP
2	E	405	SER
2	E	412	ARG
2	E	416	GLN
2	E	420	VAL
2	E	428	LEU
2	E	431	LEU
2	F	9	THR
2	F	89	GLU
2	F	109	LYS
2	F	112	GLN
2	F	199	GLU
2	F	223	ASN
2	F	232	VAL
2	F	247	GLU
2	F	249	GLN
2	F	258	ILE
2	F	274	ARG
3	G	2	THR
3	G	35	GLU
3	G	89	MET
3	G	106	ILE
3	G	113	ARG
3	G	129	LYS
3	G	131	VAL
3	G	137	THR
3	G	168	VAL
3	G	211	ASN

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Mol	Chain	Res	Type
3	G	232	MET
3	G	240	SER
3	G	262	LEU
1	H	30	ARG
1	H	47	VAL
1	H	74	VAL
1	H	94	ILE
1	H	99	VAL
1	H	102	GLU
1	H	141	SER
1	H	164	ARG
1	H	217	VAL
1	H	329	THR
1	H	403	PHE
1	H	410	LEU
1	H	442	VAL
1	H	479	LEU
1	H	494	ASP
1	I	28	THR
1	I	30	ARG
1	I	47	VAL
1	I	164	ARG
1	I	171	ARG
1	I	188	ARG
1	I	244	TYR
1	I	265	LEU
1	I	371	VAL
1	I	394	LEU
1	I	419	SER
1	I	427	LEU
1	I	442	VAL
1	I	479	LEU
1	I	499	GLU
1	J	47	VAL
1	J	99	VAL
1	J	216	LEU
1	J	217	VAL
1	J	334	VAL
1	J	335	SER
1	J	376	SER
1	J	406	PHE
1	J	462	THR

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Mol	Chain	Res	Type
1	J	475	GLN
1	J	479	LEU
1	J	505	LEU
2	K	27	GLU
2	K	97	VAL
2	K	113	PHE
2	K	335	LEU
2	K	342	LEU
2	L	76	LEU
2	L	139	VAL
2	L	160	VAL
2	L	162	LYS
2	L	175	LYS
2	L	215	VAL
2	L	223	ASN
2	L	232	VAL
2	L	310	ILE
2	L	318	THR
2	L	358	MET
2	L	405	SER
2	L	412	ARG
2	L	420	VAL
2	L	428	LEU
2	L	431	LEU
2	M	10	THR
2	M	89	GLU
2	M	97	VAL
2	M	112	GLN
2	M	139	VAL
2	M	223	ASN
2	M	232	VAL
2	M	247	GLU
2	M	249	GLN
2	M	268	VAL
2	M	274	ARG
2	M	455	GLN
3	N	11	LYS
3	N	35	GLU
3	N	84	SER
3	N	88	GLN
3	N	89	MET
3	N	106	ILE

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Mol	Chain	Res	Type
3	N	113	ARG
3	N	168	VAL
3	N	169	ILE
3	N	211	ASN
3	N	220	SER
3	N	254	ARG
3	N	262	LEU
3	N	266	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	349	GLN
1	B	415	GLN
1	B	466	ASN
1	B	503	ASN
1	C	263	HIS
1	C	416	GLN
1	C	475	GLN
2	D	112	GLN
2	D	130	GLN
2	D	194	ASN
2	D	221	GLN
2	D	419	GLN
2	E	194	ASN
2	E	223	ASN
2	E	249	GLN
2	E	257	ASN
2	E	263	GLN
2	E	293	GLN
2	E	308	GLN
2	F	112	GLN
2	F	130	GLN
2	F	194	ASN
2	F	198	HIS
2	F	223	ASN
2	F	328	HIS
2	F	419	GLN
2	F	443	GLN
3	G	88	GLN
3	G	211	ASN
1	H	42	HIS

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Mol	Chain	Res	Type
1	H	46	ASN
1	H	396	GLN
1	H	476	HIS
1	I	46	ASN
1	I	48	GLN
1	I	172	GLN
1	I	349	GLN
1	I	415	GLN
1	I	432	GLN
1	I	466	ASN
1	I	471	HIS
1	I	503	ASN
1	J	48	GLN
1	J	263	HIS
1	J	416	GLN
2	K	130	GLN
2	K	194	ASN
2	K	221	GLN
2	L	223	ASN
2	L	249	GLN
2	L	263	GLN
2	L	293	GLN
2	L	308	GLN
2	M	112	GLN
2	M	130	GLN
2	M	194	ASN
2	M	198	HIS
2	M	223	ASN
2	M	385	GLN
2	M	419	GLN
2	M	443	GLN
3	N	88	GLN
3	N	211	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 10 are monoatomic - leaving 28 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	ANP	A	1511	5	27,33,33	2.20	6 (22%)	30,52,52	2.42	6 (20%)
6	GOL	A	1513	-	5,5,5	0.25	0	5,5,5	0.54	0
6	GOL	A	1514	-	5,5,5	0.28	0	5,5,5	0.42	0
4	ANP	B	1510	5	27,33,33	2.08	8 (29%)	30,52,52	2.07	7 (23%)
6	GOL	B	1512	-	5,5,5	0.34	0	5,5,5	0.62	0
6	GOL	B	1513	-	5,5,5	0.37	0	5,5,5	0.46	0
4	ANP	C	1511	5	27,33,33	2.23	9 (33%)	30,52,52	2.22	9 (30%)
6	GOL	C	1513	-	5,5,5	0.34	0	5,5,5	0.36	0
7	ADP	D	1476	5	22,29,29	1.14	2 (9%)	27,45,45	1.92	6 (22%)
8	AZI	D	1478	-	0,2,2	0.00	-	0,1,1	0.00	-
6	GOL	D	1479	-	5,5,5	0.42	0	5,5,5	0.52	0
9	PO4	E	1475	-	4,4,4	0.47	0	6,6,6	0.28	0
4	ANP	F	1475	5	27,33,33	1.96	7 (25%)	30,52,52	2.29	7 (23%)
10	PIT	G	1273	-	19,19,19	0.50	0	26,26,26	0.93	2 (7%)
4	ANP	H	1511	5	27,33,33	2.07	6 (22%)	30,52,52	2.55	6 (20%)
6	GOL	H	1513	-	5,5,5	0.25	0	5,5,5	0.50	0
6	GOL	H	1514	-	5,5,5	0.44	0	5,5,5	0.48	0
4	ANP	I	1510	5	27,33,33	2.14	8 (29%)	30,52,52	2.08	5 (16%)
6	GOL	I	1512	-	5,5,5	0.43	0	5,5,5	0.53	0
4	ANP	J	1511	5	27,33,33	2.18	9 (33%)	30,52,52	2.08	7 (23%)
6	GOL	J	1513	-	5,5,5	0.33	0	5,5,5	0.28	0
7	ADP	K	1476	5	22,29,29	0.99	1 (4%)	27,45,45	1.89	4 (14%)
8	AZI	K	1478	-	0,2,2	0.00	-	0,1,1	0.00	-
6	GOL	K	1479	-	5,5,5	0.47	0	5,5,5	0.42	0
6	GOL	K	1480	-	5,5,5	0.36	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	PO4	L	1475	-	4,4,4	0.43	0	6,6,6	0.28	0
4	ANP	M	1475	5	27,33,33	1.98	8 (29%)	30,52,52	2.22	6 (20%)
10	PIT	N	1273	-	19,19,19	0.32	0	26,26,26	0.83	1 (3%)

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	ANP	A	1511	5	-	1/12/38/38	0/3/3/3
6	GOL	A	1513	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1514	-	-	0/4/4/4	0/0/0/0
4	ANP	B	1510	5	-	0/12/38/38	0/3/3/3
6	GOL	B	1512	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1513	-	-	0/4/4/4	0/0/0/0
4	ANP	C	1511	5	-	0/12/38/38	0/3/3/3
6	GOL	C	1513	-	-	0/4/4/4	0/0/0/0
7	ADP	D	1476	5	-	0/12/32/32	0/3/3/3
8	AZI	D	1478	-	-	0/0/0/0	0/0/0/0
6	GOL	D	1479	-	-	0/4/4/4	0/0/0/0
9	PO4	E	1475	-	-	0/0/0/0	0/0/0/0
4	ANP	F	1475	5	-	0/12/38/38	0/3/3/3
10	PIT	G	1273	-	-	0/5/5/5	0/2/2/2
4	ANP	H	1511	5	-	0/12/38/38	0/3/3/3
6	GOL	H	1513	-	-	0/4/4/4	0/0/0/0
6	GOL	H	1514	-	-	0/4/4/4	0/0/0/0
4	ANP	I	1510	5	-	1/12/38/38	0/3/3/3
6	GOL	I	1512	-	-	0/4/4/4	0/0/0/0
4	ANP	J	1511	5	-	1/12/38/38	0/3/3/3
6	GOL	J	1513	-	-	0/4/4/4	0/0/0/0
7	ADP	K	1476	5	-	0/12/32/32	0/3/3/3
8	AZI	K	1478	-	-	0/0/0/0	0/0/0/0
6	GOL	K	1479	-	-	0/4/4/4	0/0/0/0
6	GOL	K	1480	-	-	0/4/4/4	0/0/0/0
9	PO4	L	1475	-	-	0/0/0/0	0/0/0/0
4	ANP	M	1475	5	-	0/12/38/38	0/3/3/3
10	PIT	N	1273	-	-	0/5/5/5	0/2/2/2

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1511	ANP	PB-O2B	-2.64	1.49	1.56
4	C	1511	ANP	PB-O2B	-2.56	1.49	1.56
4	I	1510	ANP	PB-O2B	-2.41	1.50	1.56
4	A	1511	ANP	PB-O2B	-2.34	1.50	1.56
4	M	1475	ANP	PB-O2B	-2.33	1.50	1.56
4	H	1511	ANP	PB-O2B	-2.30	1.50	1.56
4	C	1511	ANP	PG-O2G	-2.29	1.50	1.56
4	J	1511	ANP	PG-O2G	-2.28	1.50	1.56
4	F	1475	ANP	PB-O2B	-2.22	1.50	1.56
4	I	1510	ANP	PG-O2G	-2.13	1.50	1.56
4	M	1475	ANP	PG-O3G	-2.09	1.50	1.56
4	B	1510	ANP	PG-O3G	-2.01	1.51	1.56
4	B	1510	ANP	C2-N3	2.01	1.35	1.32
4	B	1510	ANP	O4'-C1'	2.03	1.43	1.41
4	C	1511	ANP	O4'-C1'	2.03	1.43	1.41
4	I	1510	ANP	PB-O3A	2.11	1.61	1.59
4	F	1475	ANP	O4'-C1'	2.22	1.44	1.41
4	M	1475	ANP	O4'-C1'	2.22	1.44	1.41
4	J	1511	ANP	O4'-C1'	2.29	1.44	1.41
4	J	1511	ANP	PB-O3A	2.46	1.62	1.59
7	K	1476	ADP	C5-C4	2.56	1.46	1.40
7	D	1476	ADP	O4'-C1'	2.70	1.44	1.41
4	C	1511	ANP	PB-O3A	2.74	1.62	1.59
4	J	1511	ANP	C5-C4	2.81	1.46	1.40
7	D	1476	ADP	C5-C4	3.10	1.47	1.40
4	C	1511	ANP	C5-C4	3.12	1.47	1.40
4	A	1511	ANP	C5-C4	3.20	1.47	1.40
4	M	1475	ANP	C5-C4	3.25	1.47	1.40
4	B	1510	ANP	C5-C4	3.36	1.48	1.40
4	H	1511	ANP	C5-C4	3.41	1.48	1.40
4	I	1510	ANP	C5-C4	3.44	1.48	1.40
4	F	1475	ANP	C5-C4	3.48	1.48	1.40
4	H	1511	ANP	PB-N3B	3.69	1.73	1.63
4	F	1475	ANP	PB-N3B	3.75	1.73	1.63
4	M	1475	ANP	PG-N3B	3.78	1.73	1.63
4	F	1475	ANP	PG-N3B	3.79	1.73	1.63
4	F	1475	ANP	PB-O1B	3.80	1.50	1.46
4	I	1510	ANP	PB-O1B	3.85	1.50	1.46
4	I	1510	ANP	PG-N3B	3.85	1.73	1.63
4	M	1475	ANP	PB-N3B	3.86	1.73	1.63
4	B	1510	ANP	PG-N3B	4.05	1.74	1.63
4	H	1511	ANP	PG-N3B	4.13	1.74	1.63
4	M	1475	ANP	PB-O1B	4.18	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1510	ANP	PB-N3B	4.24	1.74	1.63
4	B	1510	ANP	PB-N3B	4.28	1.74	1.63
4	J	1511	ANP	PG-O1G	4.32	1.51	1.46
4	C	1511	ANP	PG-N3B	4.40	1.75	1.63
4	B	1510	ANP	PB-O1B	4.42	1.51	1.46
4	M	1475	ANP	PG-O1G	4.47	1.51	1.46
4	A	1511	ANP	PB-O1B	4.47	1.51	1.46
4	A	1511	ANP	PB-N3B	4.49	1.75	1.63
4	J	1511	ANP	PG-N3B	4.55	1.75	1.63
4	H	1511	ANP	PB-O1B	4.58	1.51	1.46
4	J	1511	ANP	PB-N3B	4.60	1.75	1.63
4	F	1475	ANP	PG-O1G	4.63	1.51	1.46
4	C	1511	ANP	PB-N3B	4.70	1.75	1.63
4	C	1511	ANP	PG-O1G	4.73	1.51	1.46
4	B	1510	ANP	PG-O1G	4.80	1.51	1.46
4	A	1511	ANP	PG-N3B	4.91	1.76	1.63
4	H	1511	ANP	PG-O1G	4.94	1.51	1.46
4	C	1511	ANP	PB-O1B	5.28	1.52	1.46
4	J	1511	ANP	PB-O1B	5.30	1.52	1.46
4	A	1511	ANP	PG-O1G	5.60	1.52	1.46
4	I	1510	ANP	PG-O1G	5.62	1.52	1.46

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1511	ANP	O1G-PG-N3B	-9.10	97.94	111.90
4	A	1511	ANP	N3-C2-N1	-8.51	122.38	128.89
4	C	1511	ANP	N3-C2-N1	-8.43	122.44	128.89
4	I	1510	ANP	N3-C2-N1	-8.19	122.63	128.89
4	A	1511	ANP	O1G-PG-N3B	-7.30	100.70	111.90
4	H	1511	ANP	N3-C2-N1	-7.20	123.39	128.89
4	B	1510	ANP	N3-C2-N1	-7.00	123.54	128.89
4	J	1511	ANP	N3-C2-N1	-6.83	123.66	128.89
7	D	1476	ADP	N3-C2-N1	-6.68	123.78	128.89
7	K	1476	ADP	N3-C2-N1	-6.43	123.97	128.89
4	M	1475	ANP	N3-C2-N1	-6.40	124.00	128.89
4	F	1475	ANP	N3-C2-N1	-6.37	124.01	128.89
4	M	1475	ANP	O1G-PG-N3B	-6.05	102.62	111.90
4	F	1475	ANP	O1G-PG-N3B	-5.62	103.28	111.90
4	F	1475	ANP	C2'-C1'-N9	-5.26	106.26	114.29
7	K	1476	ADP	C2'-C1'-N9	-4.97	106.69	114.29
4	J	1511	ANP	O1G-PG-N3B	-4.64	104.78	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1511	ANP	O1G-PG-N3B	-4.23	105.41	111.90
4	I	1510	ANP	O1G-PG-N3B	-4.13	105.56	111.90
4	M	1475	ANP	C2'-C1'-N9	-3.96	108.24	114.29
4	M	1475	ANP	C4-C5-N7	-3.82	105.97	109.48
7	D	1476	ADP	C2'-C1'-N9	-3.79	108.50	114.29
4	B	1510	ANP	O1G-PG-N3B	-3.73	106.19	111.90
4	M	1475	ANP	PA-O3A-PB	-3.40	121.26	132.67
4	B	1510	ANP	C4-C5-N7	-3.39	106.36	109.48
4	F	1475	ANP	PA-O3A-PB	-3.26	121.72	132.67
4	H	1511	ANP	PA-O3A-PB	-3.26	121.75	132.67
4	C	1511	ANP	C4-C5-N7	-3.18	106.55	109.48
4	F	1475	ANP	C4-C5-N7	-3.10	106.63	109.48
4	J	1511	ANP	PA-O3A-PB	-2.99	122.63	132.67
4	B	1510	ANP	C2'-C1'-N9	-2.73	110.11	114.29
7	D	1476	ADP	C4-C5-N7	-2.69	107.00	109.48
4	I	1510	ANP	C4-C5-N7	-2.66	107.03	109.48
4	C	1511	ANP	PA-O3A-PB	-2.65	123.78	132.67
4	A	1511	ANP	PA-O3A-PB	-2.64	123.83	132.67
4	B	1510	ANP	PA-O3A-PB	-2.61	123.93	132.67
4	A	1511	ANP	C4-C5-N7	-2.60	107.09	109.48
7	D	1476	ADP	O3A-PA-O5'	-2.48	96.37	102.94
4	J	1511	ANP	C4-C5-N7	-2.45	107.23	109.48
4	J	1511	ANP	C2'-C1'-N9	-2.40	110.63	114.29
7	K	1476	ADP	C4-C5-N7	-2.40	107.28	109.48
10	G	1273	PIT	C5-C7-C8	-2.37	116.83	125.94
10	N	1273	PIT	C5-C7-C8	-2.27	117.19	125.94
7	K	1476	ADP	PA-O3A-PB	-2.24	125.15	132.67
10	G	1273	PIT	C9-C10-C11	-2.20	119.15	120.75
4	H	1511	ANP	C4-C5-N7	-2.16	107.49	109.48
7	D	1476	ADP	PA-O3A-PB	-2.14	125.50	132.67
4	H	1511	ANP	C2'-C1'-N9	-2.10	111.09	114.29
4	C	1511	ANP	C1'-N9-C4	-2.04	123.86	126.94
4	I	1510	ANP	C2'-C3'-C4'	2.02	106.77	102.61
7	D	1476	ADP	O2B-PB-O1B	2.12	117.41	110.58
4	C	1511	ANP	C2-N1-C6	2.20	122.69	118.77
4	C	1511	ANP	C4'-O4'-C1'	2.21	112.15	109.72
4	C	1511	ANP	O3G-PG-O2G	2.24	114.21	107.58
4	A	1511	ANP	C2-N1-C6	2.34	122.95	118.77
4	C	1511	ANP	O2B-PB-O1B	2.36	114.93	110.00
4	J	1511	ANP	O3G-PG-O2G	2.45	114.85	107.58
4	F	1475	ANP	O3G-PG-O2G	2.49	114.97	107.58
4	I	1510	ANP	O2B-PB-O1B	2.78	115.80	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1510	ANP	O3G-PG-O2G	2.97	116.39	107.58
4	J	1511	ANP	O2B-PB-O1B	2.99	116.25	110.00
4	M	1475	ANP	O2B-PB-O1B	3.30	116.88	110.00
4	B	1510	ANP	O2B-PB-O1B	3.40	117.10	110.00
4	A	1511	ANP	O2B-PB-O1B	4.03	118.42	110.00
4	H	1511	ANP	O2B-PB-O1B	4.14	118.63	110.00
4	F	1475	ANP	O2B-PB-O1B	4.21	118.78	110.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1511	ANP	O1B-PB-N3B-PG
4	I	1510	ANP	O1B-PB-N3B-PG
4	A	1511	ANP	O1B-PB-N3B-PG

There are no ring outliers.

11 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1511	ANP	2	0
4	B	1510	ANP	1	0
6	B	1513	GOL	3	0
7	D	1476	ADP	1	0
4	F	1475	ANP	1	0
10	G	1273	PIT	2	0
4	H	1511	ANP	1	0
6	H	1514	GOL	2	0
7	K	1476	ADP	1	0
4	M	1475	ANP	1	0
10	N	1273	PIT	3	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	487/510 (95%)	-0.04	3 (0%) 90 91	14, 34, 57, 88	0
1	B	479/510 (93%)	-0.16	4 (0%) 87 88	14, 31, 67, 88	0
1	C	495/510 (97%)	-0.28	8 (1%) 74 75	15, 28, 47, 82	0
1	H	487/510 (95%)	-0.01	5 (1%) 84 85	16, 34, 57, 88	0
1	I	479/510 (93%)	-0.19	4 (0%) 87 88	12, 31, 66, 87	0
1	J	495/510 (97%)	-0.28	5 (1%) 84 85	12, 28, 48, 83	0
2	D	467/482 (96%)	-0.15	7 (1%) 76 76	12, 29, 58, 79	0
2	E	466/482 (96%)	0.09	12 (2%) 59 59	13, 37, 75, 103	0
2	F	466/482 (96%)	-0.24	3 (0%) 90 91	13, 30, 54, 75	0
2	K	467/482 (96%)	-0.11	4 (0%) 85 86	12, 29, 60, 79	0
2	L	466/482 (96%)	0.12	12 (2%) 59 59	15, 38, 75, 104	0
2	M	466/482 (96%)	-0.26	0 100 100	13, 31, 53, 75	0
3	G	167/272 (61%)	1.08	44 (26%) 1 1	15, 64, 93, 99	0
3	N	167/272 (61%)	0.70	19 (11%) 7 5	11, 62, 96, 100	0
All	All	6054/6496 (93%)	-0.07	130 (2%) 67 68	11, 32, 69, 104	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	42	ARG	7.7
3	G	40	PRO	7.6
3	G	207	TYR	6.8
2	E	424	PHE	6.2
3	G	209	LEU	5.7
2	L	396	LEU	5.7
2	E	390	ILE	5.7
1	A	406	PHE	5.7

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Mol	Chain	Res	Type	RSRZ
2	D	390	ILE	5.5
1	C	407	GLY	5.3
1	C	16	ILE	5.0
2	L	384	LEU	5.0
3	N	87	LYS	4.6
3	G	213	ILE	4.5
3	G	161	ILE	4.5
2	E	395	GLU	4.5
2	E	396	LEU	4.4
3	N	212	ILE	4.4
2	K	390	ILE	4.4
3	G	162	PHE	4.3
3	N	215	TYR	4.2
3	G	43	VAL	4.2
2	L	393	MET	4.2
3	G	214	TYR	4.0
2	L	389	ALA	4.0
3	G	45	GLY	3.9
2	E	393	MET	3.9
3	G	36	ARG	3.9
2	E	394	ASP	3.8
3	N	138	PHE	3.8
3	G	212	ILE	3.8
1	C	409	ASP	3.7
3	G	38	LEU	3.7
3	G	1	ALA	3.7
3	N	46	VAL	3.7
3	G	138	PHE	3.7
3	N	40	PRO	3.6
3	G	130	GLU	3.6
2	L	397	SER	3.6
3	G	115	ILE	3.6
1	J	407	GLY	3.5
3	N	213	ILE	3.5
3	G	39	LYS	3.5
2	L	424	PHE	3.5
3	G	206	GLU	3.4
3	G	216	SER	3.4
2	L	394	ASP	3.3
3	N	43	VAL	3.3
3	N	47	GLY	3.3
2	E	384	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
3	G	139	GLY	3.3
2	D	394	ASP	3.3
3	G	108	VAL	3.2
2	F	175	LYS	3.2
2	D	475	GLU	3.2
3	G	46	VAL	3.1
3	G	134	ARG	3.1
3	G	41	ALA	3.0
1	J	408	SER	3.0
3	N	161	ILE	3.0
3	G	25	MET	3.0
3	N	129	LYS	3.0
2	D	392	GLY	3.0
2	K	474	ALA	3.0
2	L	474	ALA	3.0
1	C	17	LEU	2.9
3	G	218	LYS	2.9
2	L	387	ILE	2.9
3	N	134	ARG	2.9
1	J	406	PHE	2.9
3	G	135	PRO	2.9
1	I	412	ALA	2.9
3	G	133	ARG	2.8
3	N	208	SER	2.8
3	G	89	MET	2.8
3	G	106	ILE	2.8
2	E	397	SER	2.8
3	G	137	THR	2.7
1	B	457	GLU	2.7
2	K	392	GLY	2.7
3	G	140	ASP	2.7
2	L	388	ILE	2.6
1	I	389	THR	2.6
1	H	94	ILE	2.6
1	H	406	PHE	2.6
1	C	405	GLN	2.6
2	K	473	LEU	2.5
1	C	406	PHE	2.5
1	B	474	SER	2.5
1	A	140	ILE	2.4
1	J	18	GLY	2.4
3	G	129	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	G	107	GLY	2.4
1	B	438	ILE	2.4
2	D	398	GLU	2.4
3	G	113	ARG	2.3
3	G	215	TYR	2.3
2	E	391	LEU	2.3
3	G	112	ILE	2.3
1	H	143	ARG	2.3
3	G	132	GLY	2.3
2	D	386	ASP	2.3
3	N	85	VAL	2.2
3	N	133	ARG	2.2
1	H	405	GLN	2.2
1	H	141	SER	2.2
3	G	74	ASP	2.2
1	J	405	GLN	2.2
3	G	164	ARG	2.2
1	C	410	LEU	2.2
3	N	136	PRO	2.2
3	N	113	ARG	2.2
2	E	388	ILE	2.2
2	E	445	LEU	2.2
2	L	398	GLU	2.2
2	F	176	ALA	2.2
3	G	47	GLY	2.1
3	G	32	ALA	2.1
1	I	397	TYR	2.1
1	C	412	ALA	2.1
1	B	475	GLN	2.1
2	D	399	GLU	2.1
1	A	405	GLN	2.0
3	N	106	ILE	2.0
2	L	402	LEU	2.0
3	G	169	ILE	2.0
3	N	42	ARG	2.0
1	I	457	GLU	2.0
2	E	398	GLU	2.0
2	F	178	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	K	1479	6/6	0.94	0.37	7.98	46,48,51,54	0
6	GOL	B	1513	6/6	0.96	0.19	5.47	28,29,32,35	0
10	PIT	G	1273	18/18	0.94	0.20	3.53	46,47,48,48	0
6	GOL	H	1514	6/6	0.92	0.19	2.70	20,31,32,38	0
10	PIT	N	1273	18/18	0.90	0.21	2.60	58,59,60,60	0
8	AZI	K	1478	3/3	0.98	0.18	2.53	9,9,16,19	0
6	GOL	B	1512	6/6	0.96	0.19	2.49	17,21,23,24	0
6	GOL	I	1512	6/6	0.98	0.17	1.99	10,17,19,25	0
6	GOL	K	1480	6/6	0.89	0.24	1.51	60,62,66,67	0
6	GOL	A	1513	6/6	0.94	0.22	1.24	26,27,30,32	0
6	GOL	C	1513	6/6	0.96	0.16	1.09	22,24,28,28	0
8	AZI	D	1478	3/3	0.91	0.15	0.82	20,20,31,33	0
6	GOL	A	1514	6/6	0.93	0.16	0.58	34,38,40,41	0
6	GOL	D	1479	6/6	0.97	0.15	-0.02	36,40,44,45	0
9	PO4	E	1475	5/5	0.94	0.18	-0.17	81,83,85,85	0
6	GOL	H	1513	6/6	0.95	0.17	-0.66	31,32,34,35	0
4	ANP	I	1510	31/31	0.97	0.12	-0.84	19,30,36,39	0
4	ANP	A	1511	31/31	0.96	0.14	-1.07	21,27,31,32	0
4	ANP	F	1475	31/31	0.98	0.10	-1.44	7,21,27,27	0
6	GOL	J	1513	6/6	0.98	0.12	-1.55	18,21,25,29	0
4	ANP	J	1511	31/31	0.98	0.09	-1.58	12,20,26,29	0
9	PO4	L	1475	5/5	0.95	0.14	-1.64	71,71,74,75	0
4	ANP	B	1510	31/31	0.97	0.11	-1.75	14,29,36,39	0
5	MG	K	1477	1/1	0.98	0.11	-1.93	22,22,22,22	0
7	ADP	K	1476	27/27	0.98	0.09	-2.04	16,25,30,32	0
4	ANP	M	1475	31/31	0.98	0.09	-2.04	11,26,31,31	0
7	ADP	D	1476	27/27	0.98	0.10	-2.14	11,32,38,41	0
4	ANP	H	1511	31/31	0.97	0.12	-2.42	11,32,39,40	0
4	ANP	C	1511	31/31	0.98	0.09	-2.70	13,23,27,28	0
5	MG	F	1476	1/1	0.94	0.05	-4.48	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	D	1477	1/1	0.98	0.04	-5.61	18,18,18,18	0
5	MG	M	1476	1/1	0.99	0.03	-11.06	18,18,18,18	0
5	MG	A	1512	1/1	0.98	0.03	-	19,19,19,19	0
5	MG	I	1511	1/1	0.96	0.12	-	24,24,24,24	0
5	MG	C	1512	1/1	0.98	0.05	-	5,5,5,5	0
5	MG	J	1512	1/1	0.95	0.07	-	4,4,4,4	0
5	MG	H	1512	1/1	0.99	0.05	-	28,28,28,28	0
5	MG	B	1511	1/1	0.95	0.05	-	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.