



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:30 pm GMT

PDB ID : 2JJ2  
Title : THE STRUCTURE OF F1-ATPASE INHIBITED BY QUERCETIN.  
Authors : Gledhill, J.R.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2007-07-03  
Resolution : 2.40 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : trunk28620

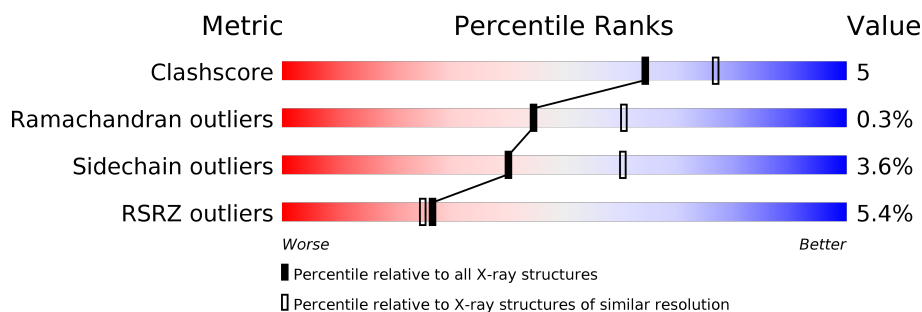
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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>2%</div> <div>85% 10% • 5%</div> </div>
1	B	510	<div> <div>5%</div> <div>83% 10% • 6%</div> </div>
1	C	510	<div> <div>%</div> <div>82% 13% • •</div> </div>
1	H	510	<div> <div>2%</div> <div>83% 12% • 5%</div> </div>
1	I	510	<div> <div>7%</div> <div>81% 12% • 6%</div> </div>
1	J	510	<div> <div>2%</div> <div>81% 14% • •</div> </div>
2	D	482	<div> <div>3%</div> <div>88% 9% • •</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	QUE	G	1273[A]	-	-	-	X
10	QUE	N	1273[A]	-	-	-	X
10	QUE	N	1273[B]	-	-	-	X
6	GOL	A	1513	-	-	X	X
6	GOL	A	1514	-	-	-	X
6	GOL	B	1512	-	-	-	X
6	GOL	B	1513	-	-	-	X
6	GOL	C	1513	-	-	-	X
6	GOL	H	1514	-	-	-	X
6	GOL	J	1513	-	-	-	X
6	GOL	K	1480	-	-	-	X
8	AZI	D	1478	-	-	-	X
8	AZI	K	1478	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48794 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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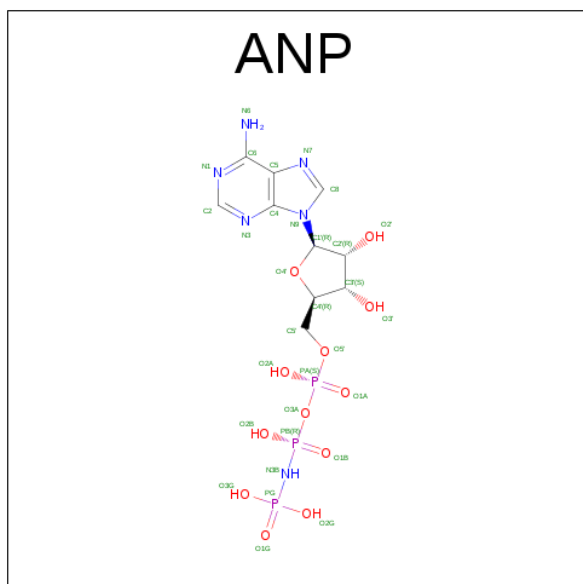
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	L	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	M	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE GAMMA CHAIN.

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



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

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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).

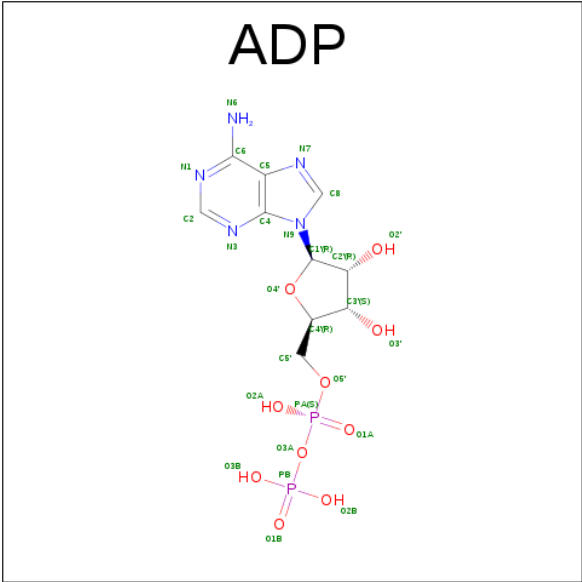
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	M	1	Total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



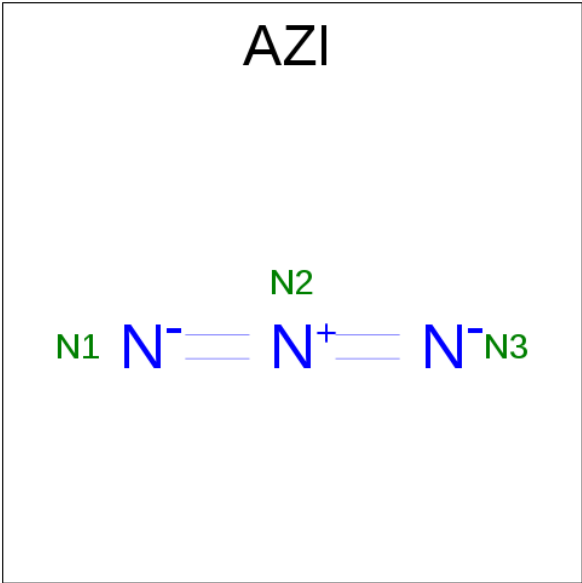
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	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 27	C 10	N 5	O 10	P 2	0	0
7	K	1	Total 27	C 10	N 5	O 10	P 2	0	0

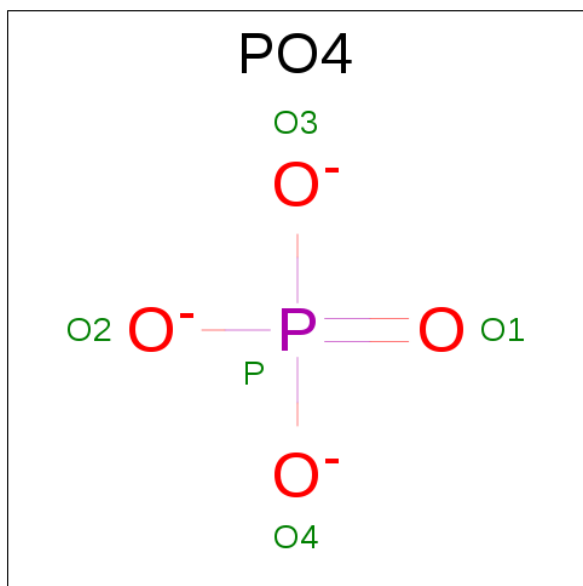
- Molecule 8 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



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

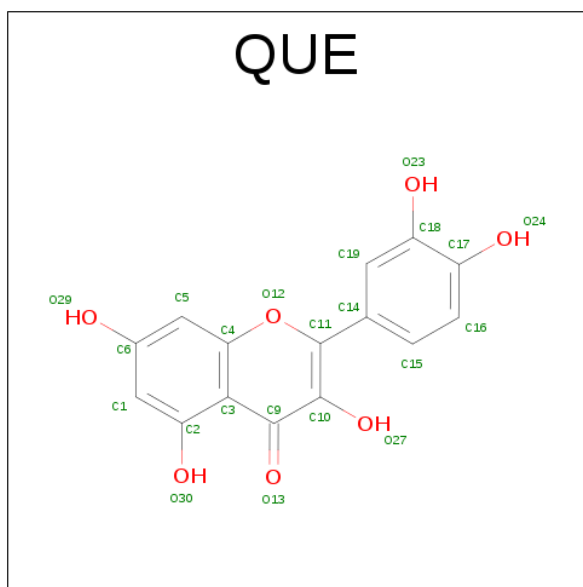


- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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 3,5,7,3',4'-PENTAHYDROXYFLAVONE (three-letter code: QUE) (formula:  $C_{15}H_{10}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	1
			44	30	14		
10	N	1	Total	C	O	0	1
			44	30	14		

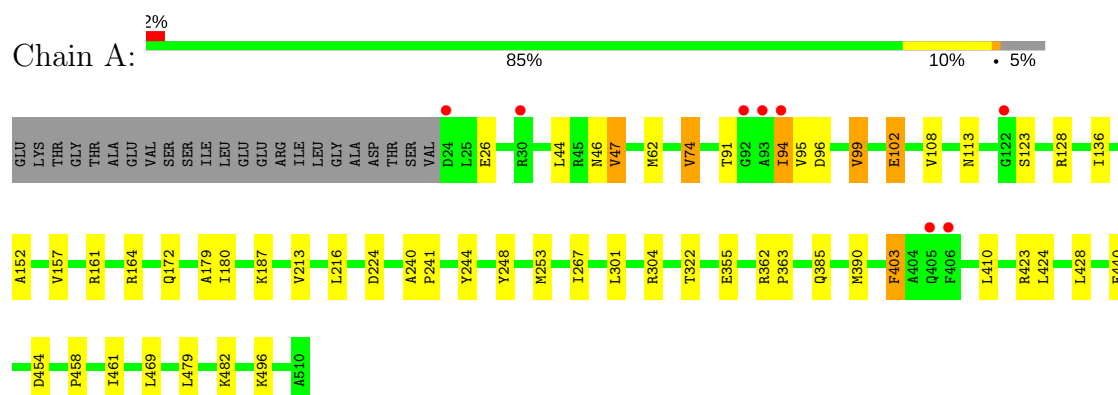
- Molecule 11 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	180	Total	O		0	0
			180	180			
11	B	153	Total	O		0	0
			153	153			
11	C	229	Total	O		0	0
			229	229			
11	D	179	Total	O		0	0
			179	179			
11	E	114	Total	O		0	0
			114	114			
11	F	205	Total	O		0	0
			205	205			
11	G	40	Total	O		0	0
			40	40			
11	H	207	Total	O		0	0
			207	207			
11	I	153	Total	O		0	0
			153	153			
11	J	236	Total	O		0	0
			236	236			
11	K	175	Total	O		0	0
			175	175			
11	L	122	Total	O		0	0
			122	122			
11	M	202	Total	O		0	0
			202	202			
11	N	39	Total	O		0	0
			39	39			

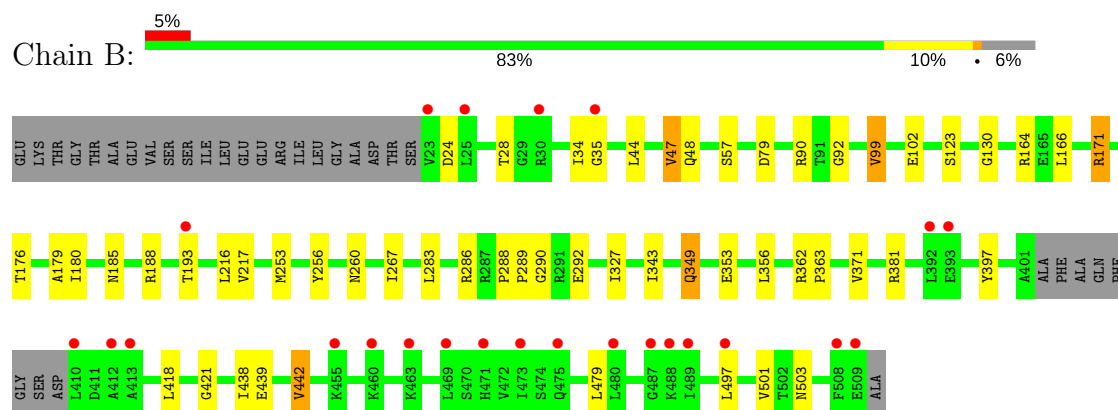
### 3 Residue-property plots [i](#)

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.

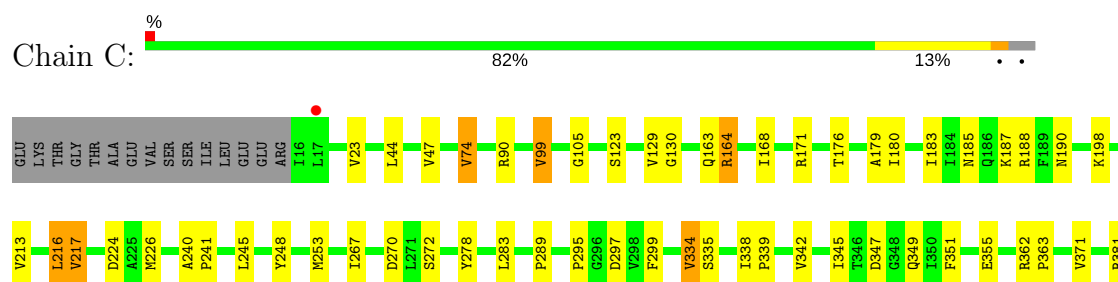
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM



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

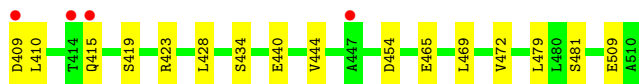
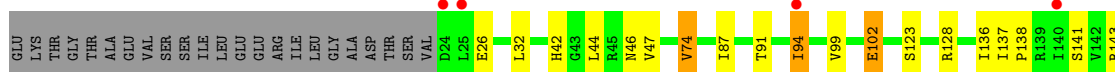
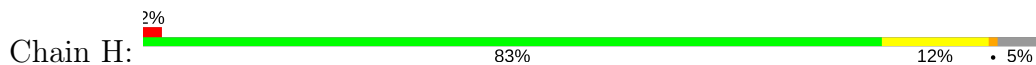


#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

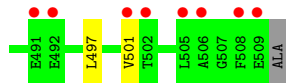
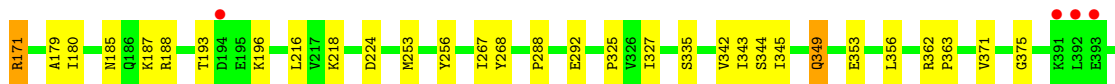
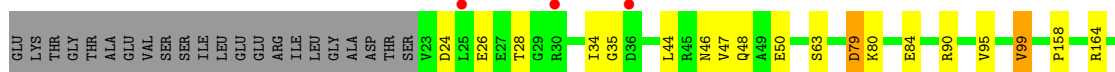
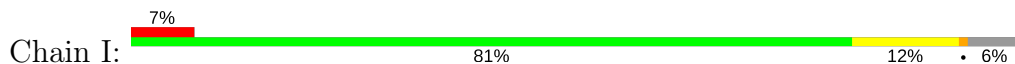




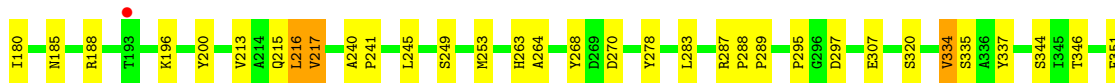
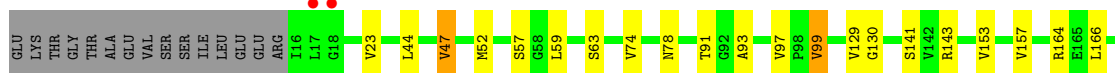
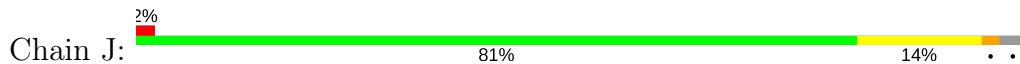
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM



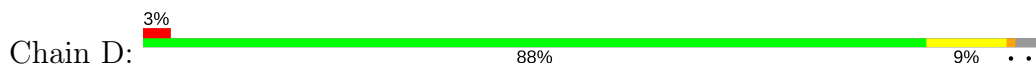
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

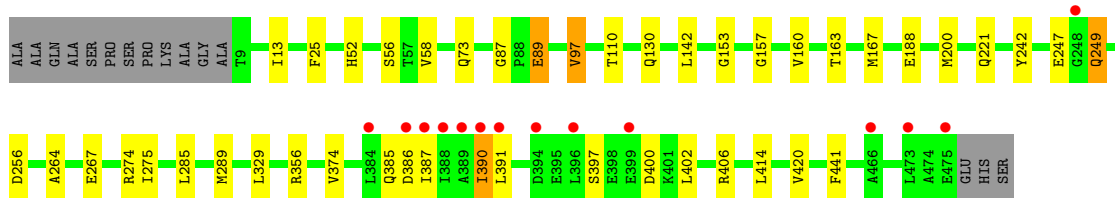


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

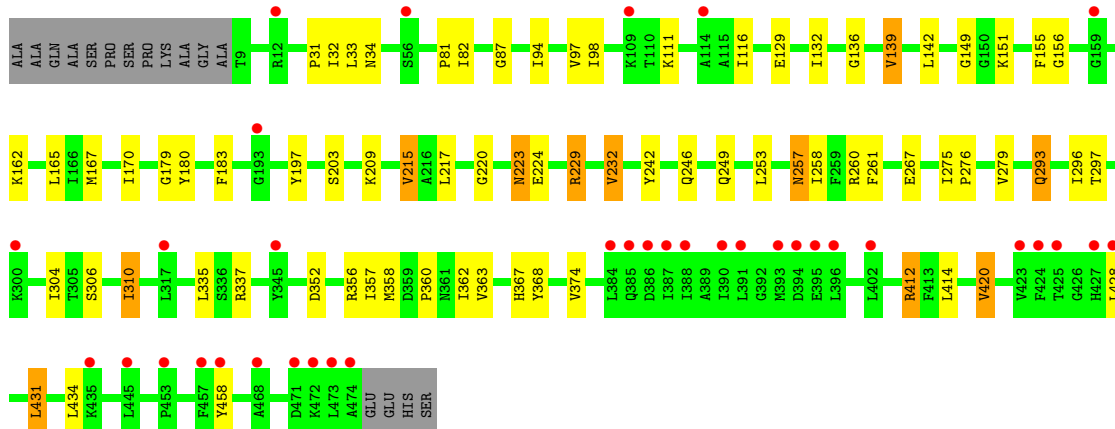
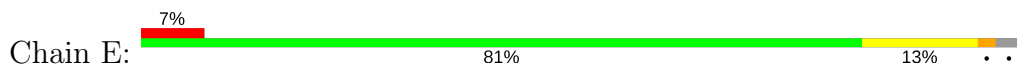


• Molecule 2: ATP SYNTHASE SUBUNIT BETA

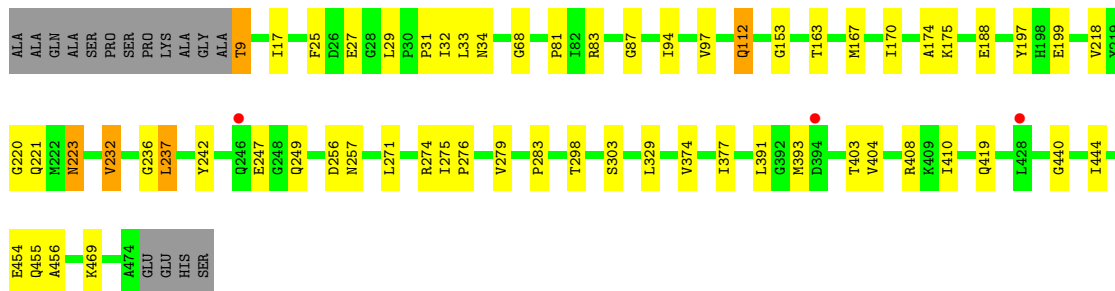
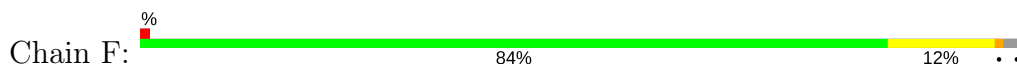




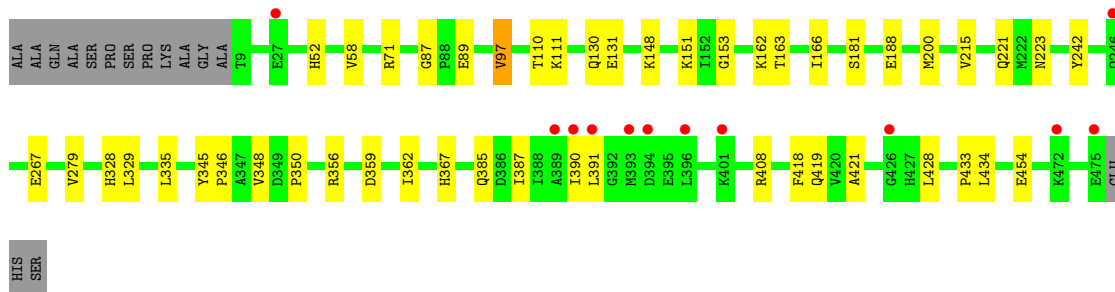
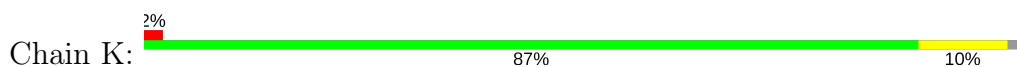
• Molecule 2: ATP SYNTHASE SUBUNIT BETA



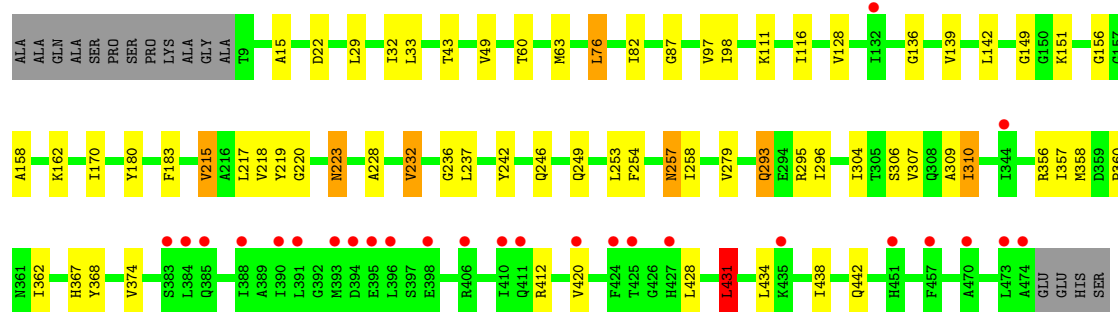
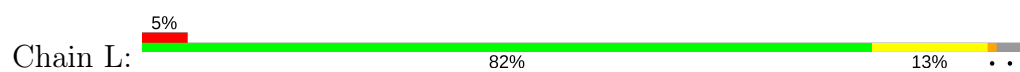
• Molecule 2: ATP SYNTHASE SUBUNIT BETA



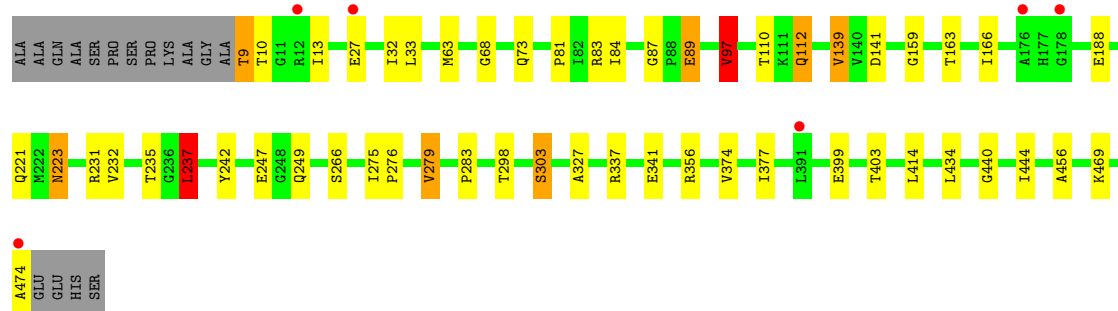
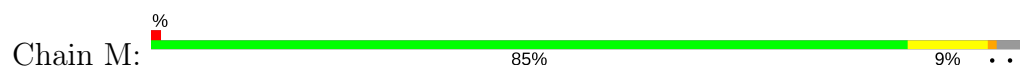
• Molecule 2: ATP SYNTHASE SUBUNIT BETA



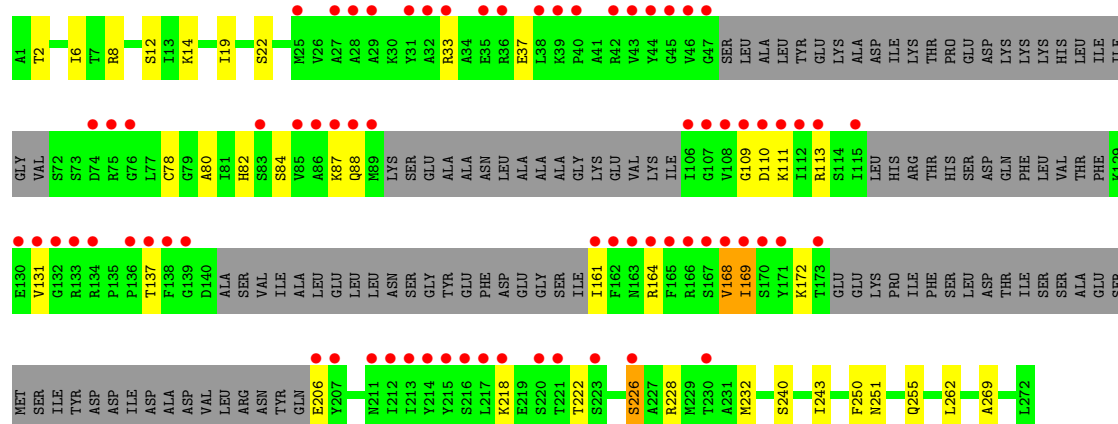
• Molecule 2: ATP SYNTHASE SUBUNIT BETA



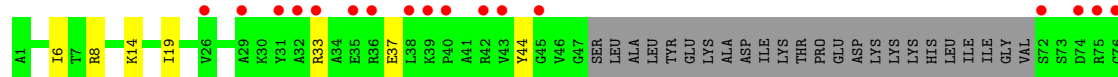
• Molecule 2: ATP SYNTHASE SUBUNIT BETA



• 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, $\alpha$ , $\beta$ , $\gamma$	106.40Å 282.02Å 138.09Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	80.58 – 2.40 80.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.1 (80.58-2.40) 92.1 (80.48-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.188 , 0.238 0.188 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.328 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	48794	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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

### 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, QUE, ANP

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	0.41	0/3766	0.56	0/5080
1	B	0.40	0/3706	0.57	0/4998
1	C	0.43	0/3819	0.59	0/5153
1	H	0.40	0/3766	0.56	0/5080
1	I	0.41	0/3706	0.56	0/4998
1	J	0.43	0/3819	0.60	1/5153 (0.0%)
2	D	0.42	0/3596	0.57	1/4879 (0.0%)
2	E	0.39	0/3587	0.56	1/4867 (0.0%)
2	F	0.41	0/3587	0.58	1/4867 (0.0%)
2	K	0.42	0/3596	0.57	1/4879 (0.0%)
2	L	0.38	0/3587	0.57	2/4867 (0.0%)
2	M	0.42	0/3587	0.59	2/4867 (0.0%)
3	G	0.36	0/1304	0.48	0/1737
3	N	0.36	0/1304	0.49	0/1737
All	All	0.41	0/46730	0.57	9/63162 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	237	LEU	CA-CB-CG	7.28	132.04	115.30
2	M	237	LEU	CA-CB-CG	6.81	130.96	115.30
2	L	431	LEU	CA-CB-CG	6.09	129.30	115.30
2	D	97	VAL	CB-CA-C	-5.67	100.62	111.40
1	J	216	LEU	CA-CB-CG	5.67	128.35	115.30
2	L	76	LEU	CA-CB-CG	5.33	127.55	115.30
2	K	97	VAL	CB-CA-C	-5.33	101.28	111.40
2	M	97	VAL	CB-CA-C	-5.09	101.72	111.40
2	E	229	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	33	0
1	B	3658	0	3767	36	0
1	C	3768	0	3867	45	0
1	H	3715	0	3812	43	0
1	I	3658	0	3767	40	0
1	J	3768	0	3867	42	0
2	D	3539	0	3592	31	0
2	E	3530	0	3587	47	0
2	F	3530	0	3586	33	0
2	K	3539	0	3592	26	0
2	L	3530	0	3587	37	0
2	M	3530	0	3586	31	0
3	G	1296	0	1365	19	0
3	N	1296	0	1365	13	0
4	A	31	0	13	1	0
4	B	31	0	13	0	0
4	C	31	0	13	0	0
4	F	31	0	13	0	0
4	H	31	0	13	0	0
4	I	31	0	13	0	0
4	J	31	0	13	0	0
4	M	31	0	13	2	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	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	12	0	16	2	0
6	C	6	0	8	2	0
6	D	6	0	8	0	0
6	H	12	0	16	0	0
6	I	6	0	8	0	0
6	J	6	0	8	2	0
6	K	12	0	16	0	0
7	D	27	0	12	0	0
7	K	27	0	12	0	0
8	D	3	0	0	0	0
8	K	3	0	0	1	0
9	E	5	0	0	0	0
9	L	5	0	0	0	0
10	G	44	0	12	4	0
10	N	44	0	15	2	0
11	A	180	0	0	3	0
11	B	153	0	0	3	0
11	C	229	0	0	2	0
11	D	179	0	0	3	0
11	E	114	0	0	1	0
11	F	205	0	0	4	0
11	G	40	0	0	3	0
11	H	207	0	0	5	0
11	I	153	0	0	4	0
11	J	236	0	0	2	0
11	K	175	0	0	2	0
11	L	122	0	0	0	0
11	M	202	0	0	5	0
11	N	39	0	0	1	0
All	All	48794	0	47403	453	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 5.

All (453) 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)
2:E:223:ASN:H	2:E:223:ASN:HD22	1.25	0.83
1:B:290:GLY:HA3	6:B:1513:GOL:H12	1.62	0.81
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.15	0.81
2:L:183:PHE:HB3	2:L:217:LEU:HD23	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:180:ILE:HD11	1:J:216:LEU:HD21	1.66	0.78
1:A:304:ARG:HE	6:A:1513:GOL:H31	1.51	0.76
2:D:386:ASP:HB3	3:G:12:SER:HB2	1.69	0.75
1:A:94:ILE:HD11	1:A:128:ARG:HG2	1.69	0.75
1:A:44:LEU:O	1:A:47:VAL:HG22	1.88	0.74
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.70	0.73
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.18	0.73
1:C:418:LEU:O	1:C:422:VAL:HG23	1.90	0.72
2:D:387:ILE:HG23	3:G:19:ILE:HD13	1.71	0.72
2:E:203:SER:HB2	2:E:420:VAL:HG22	1.70	0.72
1:J:52:MET:O	1:J:91:THR:HB	1.90	0.71
1:J:23:VAL:O	1:J:23:VAL:HG12	1.91	0.70
1:H:180:ILE:HD11	1:H:216:LEU:HD21	1.73	0.70
1:I:180:ILE:HD11	1:I:216:LEU:HD21	1.74	0.69
1:J:418:LEU:O	1:J:422:VAL:HG23	1.93	0.69
2:L:136:GLY:HA3	2:L:431:LEU:HD13	1.76	0.68
2:K:391:LEU:HD13	3:N:19:ILE:HG21	1.76	0.68
1:B:180:ILE:HD12	1:B:216:LEU:HD21	1.77	0.67
1:I:437:ALA:HB3	1:I:440:GLU:HG3	1.75	0.67
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.77	0.67
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.60	0.66
2:L:170:ILE:HG21	2:L:215:VAL:HG22	1.76	0.66
2:K:387:ILE:HG23	3:N:19:ILE:HD13	1.78	0.66
1:C:407:GLY:HA2	11:C:2180:HOH:O	1.96	0.66
1:C:355:GLU:HB2	11:C:2158:HOH:O	1.95	0.66
1:J:130:GLY:HA2	6:J:1513:GOL:H11	1.78	0.66
2:E:167:MET:HB3	2:E:420:VAL:HG21	1.78	0.65
1:I:196:LYS:HD3	11:I:2060:HOH:O	1.94	0.65
2:K:130:GLN:HE22	2:K:356:ARG:HD2	1.60	0.65
1:H:44:LEU:O	1:H:47:VAL:HG22	1.97	0.65
1:J:441:GLN:O	1:J:445:ILE:HG12	1.97	0.65
1:J:440:GLU:O	1:J:444:VAL:HG13	1.96	0.64
1:J:44:LEU:O	1:J:47:VAL:HG22	1.97	0.64
1:A:244:TYR:CE1	1:A:301:LEU:HD11	2.33	0.64
2:E:179:GLY:HA2	2:E:249:GLN:HE21	1.63	0.62
1:H:244:TYR:HE1	1:H:301:LEU:HD11	1.64	0.62
1:A:304:ARG:NE	6:A:1513:GOL:H31	2.14	0.62
1:B:44:LEU:O	1:B:47:VAL:HG22	2.00	0.62
1:I:99:VAL:HG22	1:I:253:MET:HA	1.80	0.62
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.35	0.61
1:J:196:LYS:HG3	11:J:2094:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:180:ILE:CD1	1:I:216:LEU:HD21	2.31	0.61
2:K:408:ARG:NE	2:K:454:GLU:OE1	2.26	0.61
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.83	0.61
2:E:132:ILE:HD11	2:E:363:VAL:HG12	1.82	0.61
2:F:223:ASN:H	2:F:223:ASN:HD22	1.49	0.61
2:F:275:ILE:O	2:F:283:PRO:HG3	2.01	0.61
1:H:187:LYS:HE2	1:H:224:ASP:HB3	1.83	0.61
1:J:468:PHE:CE1	1:J:501:VAL:HG12	2.36	0.61
1:I:185:ASN:OD1	1:I:188:ARG:NH1	2.34	0.60
2:M:63:MET:HE1	2:M:231:ARG:HB2	1.83	0.60
1:H:403:PHE:HD2	1:H:403:PHE:N	1.99	0.60
3:G:78:CYS:HB3	3:G:228:ARG:HB2	1.83	0.60
2:M:223:ASN:HD22	2:M:223:ASN:H	1.47	0.60
1:C:179:ALA:HB1	1:C:267:ILE:HG12	1.84	0.59
1:B:349:GLN:NE2	11:B:2122:HOH:O	2.36	0.59
1:H:403:PHE:CD2	1:H:403:PHE:N	2.70	0.59
1:C:185:ASN:OD1	1:C:188:ARG:NH1	2.36	0.59
1:B:292:GLU:HA	10:G:1273[A]:QUE:O29	2.02	0.59
2:E:82:ILE:HB	2:E:116:ILE:HG12	1.85	0.59
2:M:298:THR:HG23	2:M:303:SER:HA	1.83	0.59
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.85	0.58
1:J:129:VAL:HG21	1:J:245:LEU:HD11	1.85	0.58
1:A:248:TYR:CE2	6:A:1513:GOL:H32	2.38	0.58
1:H:102:GLU:HG3	1:H:123:SER:HA	1.84	0.58
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.39	0.58
1:J:59:LEU:HD11	1:J:78:ASN:O	2.03	0.58
2:K:87:GLY:HA2	2:K:242:TYR:CE2	2.38	0.58
2:D:247:GLU:O	2:D:249:GLN:NE2	2.37	0.58
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.85	0.58
2:M:275:ILE:O	2:M:283:PRO:HG3	2.04	0.58
1:J:185:ASN:OD1	1:J:188:ARG:NH1	2.34	0.57
1:C:129:VAL:HG21	1:C:245:LEU:HD11	1.87	0.57
2:E:293:GLN:HA	2:E:293:GLN:HE21	1.70	0.57
2:E:223:ASN:N	2:E:223:ASN:HD22	1.94	0.56
1:B:102:GLU:HG3	1:B:123:SER:HA	1.87	0.56
1:C:349:GLN:NE2	1:C:371:VAL:HG22	2.21	0.56
2:F:81:PRO:O	2:F:83:ARG:HG3	2.06	0.56
1:I:438:ILE:O	1:I:442:VAL:HG12	2.06	0.56
1:J:99:VAL:HG22	1:J:253:MET:HA	1.87	0.56
2:M:163:THR:O	2:M:166:ILE:HG22	2.06	0.56
2:M:159:GLY:HA2	4:M:1475:ANP:HNB1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:229:ARG:NH2	2:E:267:GLU:OE1	2.34	0.56
1:H:244:TYR:CE1	1:H:301:LEU:HD11	2.41	0.56
2:F:220:GLY:HA3	2:F:232:VAL:HG11	1.86	0.56
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.38	0.55
1:I:327:ILE:HD11	1:I:342:VAL:HG21	1.87	0.55
2:K:89:GLU:HG3	2:K:110:THR:HA	1.88	0.55
2:M:89:GLU:HG2	2:M:110:THR:HG22	1.88	0.55
1:C:402:ALA:O	1:C:405:GLN:HB2	2.07	0.55
2:E:180:TYR:H	2:E:249:GLN:NE2	2.03	0.55
2:D:13:ILE:HD12	2:D:73:GLN:HB3	1.88	0.55
1:H:74:VAL:HG13	1:H:241:PRO:HG3	1.88	0.55
3:N:164:ARG:NH2	3:N:172:LYS:HD3	2.22	0.54
1:B:24:ASP:O	1:B:28:THR:HB	2.07	0.54
1:B:497:LEU:O	1:B:501:VAL:HG23	2.07	0.54
2:E:209:LYS:HD2	11:E:2052:HOH:O	2.08	0.54
1:I:44:LEU:O	1:I:47:VAL:HG22	2.07	0.54
1:C:468:PHE:CE1	1:C:501:VAL:HG12	2.43	0.54
1:C:44:LEU:O	1:C:47:VAL:HG22	2.06	0.54
1:I:187:LYS:HE2	1:I:224:ASP:HB3	1.89	0.54
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.43	0.54
2:L:293:GLN:HA	2:L:293:GLN:HE21	1.73	0.54
3:G:80:ALA:O	3:G:84:SER:HB2	2.08	0.53
1:J:278:TYR:CE2	1:J:295:PRO:HG2	2.43	0.53
1:C:342:VAL:HA	1:C:345:ILE:HD12	1.90	0.53
1:I:441:GLN:O	1:I:445:ILE:HG12	2.09	0.53
1:H:373:ARG:HD2	2:L:158:ALA:HB2	1.89	0.53
2:L:257:ASN:HB2	2:L:309:ALA:O	2.07	0.53
2:L:136:GLY:HA3	2:L:431:LEU:CD1	2.38	0.53
1:H:94:ILE:HD11	1:H:128:ARG:HG2	1.90	0.53
2:D:130:GLN:HE22	2:D:356:ARG:HD2	1.73	0.53
2:D:414:LEU:HD23	2:D:441:PHE:CZ	2.44	0.52
1:I:343:ILE:HG12	1:I:349:GLN:HG2	1.90	0.52
1:B:99:VAL:HG22	1:B:253:MET:HA	1.91	0.52
2:F:25:PHE:HB2	2:F:29:LEU:HD12	1.89	0.52
2:E:97:VAL:HG13	2:E:98:ILE:HG23	1.91	0.52
1:H:87:ILE:HD12	1:H:87:ILE:H	1.75	0.52
1:C:23:VAL:HG12	1:C:23:VAL:O	2.09	0.52
1:J:283:LEU:HD21	1:J:289:PRO:HB3	1.91	0.52
2:D:391:LEU:HD13	3:G:19:ILE:HG21	1.91	0.52
1:H:172:GLN:HG2	11:K:2136:HOH:O	2.10	0.52
2:L:151:LYS:HE3	2:L:296:ILE:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:ALA:HB3	1:C:241:PRO:HD3	1.92	0.52
2:K:52:HIS:CD2	2:K:58:VAL:HG12	2.45	0.52
3:N:14:LYS:HA	3:N:243:ILE:HD11	1.90	0.52
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.45	0.52
1:C:338:ILE:HB	1:C:339:PRO:HD3	1.91	0.52
2:D:89:GLU:HG3	2:D:110:THR:HA	1.91	0.52
1:I:497:LEU:O	1:I:501:VAL:HG23	2.10	0.52
1:C:130:GLY:HA2	6:C:1513:GOL:H11	1.92	0.52
2:E:94:ILE:HD11	2:E:197:TYR:CD1	2.45	0.51
1:J:240:ALA:HB3	1:J:241:PRO:HD3	1.92	0.51
3:N:82:HIS:CG	3:N:111:LYS:HG2	2.45	0.51
1:B:362:ARG:HA	1:B:363:PRO:C	2.31	0.51
2:E:179:GLY:HA2	2:E:249:GLN:NE2	2.26	0.51
1:I:171:ARG:HD3	11:I:2050:HOH:O	2.09	0.51
3:G:222:THR:O	3:G:226:SER:OG	2.28	0.51
2:L:87:GLY:HA2	2:L:242:TYR:CE2	2.45	0.51
1:B:479:LEU:HD11	1:B:497:LEU:HD13	1.92	0.51
1:H:362:ARG:HA	1:H:363:PRO:C	2.31	0.51
1:A:440:GLU:HB3	1:A:469:LEU:HD11	1.92	0.51
1:H:440:GLU:HB3	1:H:469:LEU:HD11	1.93	0.51
1:J:153:VAL:HA	1:J:157:VAL:HG23	1.93	0.51
2:L:360:PRO:HD3	2:L:368:TYR:CD1	2.46	0.51
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.93	0.51
1:A:213:VAL:O	1:A:216:LEU:HB3	2.12	0.50
1:H:180:ILE:HD11	1:H:216:LEU:CD2	2.41	0.50
1:H:423:ARG:HD3	1:H:454:ASP:HA	1.93	0.50
3:G:82:HIS:CG	3:G:111:LYS:HG2	2.46	0.50
1:J:97:VAL:HG11	1:J:249:SER:HB3	1.93	0.50
1:C:47:VAL:HG12	1:C:90:ARG:HG2	1.93	0.50
1:C:99:VAL:HG22	1:C:253:MET:HA	1.92	0.50
1:H:327:ILE:HD11	1:H:342:VAL:HG21	1.93	0.50
1:J:334:VAL:HG13	1:J:351:PHE:CE1	2.47	0.50
2:M:63:MET:CE	2:M:231:ARG:HB2	2.41	0.50
1:B:288:PRO:HB3	2:F:276:PRO:HG3	1.93	0.50
2:D:221:GLN:HA	2:D:221:GLN:HE21	1.77	0.50
1:I:218:LYS:HG3	2:L:128:VAL:HB	1.94	0.50
2:L:63:MET:HE1	2:L:228:ALA:HA	1.93	0.50
1:A:403:PHE:N	1:A:403:PHE:HD2	2.10	0.49
1:B:256:TYR:O	1:B:260:ASN:ND2	2.44	0.49
1:J:91:THR:HG22	1:J:93:ALA:HB3	1.93	0.49
1:B:185:ASN:O	1:B:188:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:164:ARG:NH2	3:G:172:LYS:HD3	2.27	0.49
1:C:465:GLU:O	1:C:469:LEU:HB2	2.12	0.49
2:F:374:VAL:HG13	2:F:410:ILE:HG21	1.94	0.49
3:N:251:ASN:O	3:N:255:GLN:HG3	2.13	0.49
3:N:44:TYR:HH	3:N:138:PHE:HE1	1.57	0.49
1:A:95:VAL:HG23	11:A:2029:HOH:O	2.11	0.49
1:J:384:LYS:HE2	11:J:2189:HOH:O	2.12	0.49
2:L:82:ILE:HB	2:L:116:ILE:HG12	1.95	0.49
10:N:1273[A]:QUE:H19	10:N:1273[A]:QUE:O27	2.12	0.49
1:A:423:ARG:HD3	1:A:454:ASP:HA	1.95	0.49
2:E:151:LYS:HE3	2:E:296:ILE:HB	1.95	0.49
1:C:74:VAL:HG13	1:C:241:PRO:HG3	1.95	0.49
2:K:151:LYS:HD3	2:K:328:HIS:O	2.13	0.49
1:A:403:PHE:N	1:A:403:PHE:CD2	2.79	0.48
2:M:139:VAL:HG13	2:M:414:LEU:HD22	1.95	0.48
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.42	0.48
2:E:180:TYR:H	2:E:249:GLN:HE22	1.61	0.48
1:C:406:PHE:CE2	11:D:2159:HOH:O	2.55	0.48
1:C:74:VAL:HG13	1:C:241:PRO:CG	2.43	0.48
1:C:47:VAL:CG1	1:C:90:ARG:HG2	2.44	0.48
2:E:257:ASN:ND2	2:E:260:ARG:HG3	2.28	0.48
1:I:24:ASP:O	1:I:28:THR:HB	2.12	0.48
1:J:200:TYR:O	1:J:264:ALA:HA	2.13	0.48
1:A:482:LYS:HG2	11:A:2169:HOH:O	2.13	0.48
10:G:1273[A]:QUE:O27	10:G:1273[A]:QUE:H19	2.13	0.48
2:L:357:ILE:HB	2:L:362:ILE:HG21	1.96	0.48
2:E:223:ASN:ND2	2:E:223:ASN:H	2.01	0.48
3:G:161:ILE:N	11:G:2016:HOH:O	2.46	0.48
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.95	0.48
1:I:344:SER:HA	4:M:1475:ANP:O1G	2.13	0.48
3:G:251:ASN:O	3:G:255:GLN:HG3	2.14	0.48
1:H:481:SER:CA	11:H:2188:HOH:O	2.62	0.48
2:M:87:GLY:HA2	2:M:242:TYR:CE2	2.48	0.48
1:I:292:GLU:HA	10:N:1273[A]:QUE:O29	2.13	0.48
1:I:448:GLY:HA2	1:I:453:LEU:HD12	1.95	0.48
1:J:130:GLY:HA2	6:J:1513:GOL:C1	2.42	0.48
1:J:402:ALA:O	1:J:405:GLN:HB2	2.14	0.48
2:E:357:ILE:HB	2:E:362:ILE:HG21	1.96	0.47
2:F:188:GLU:O	2:F:221:GLN:HB3	2.14	0.47
1:H:179:ALA:HB1	1:H:267:ILE:HG12	1.95	0.47
2:K:345:TYR:HA	2:K:346:PRO:C	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:180:TYR:H	2:L:249:GLN:NE2	2.12	0.47
1:J:465:GLU:O	1:J:469:LEU:HB2	2.14	0.47
2:K:188:GLU:H	2:K:221:GLN:NE2	2.12	0.47
3:N:168:VAL:HG23	3:N:169:ILE:HG13	1.95	0.47
2:K:163:THR:HA	2:K:166:ILE:HG22	1.96	0.47
2:F:94:ILE:HD11	2:F:197:TYR:CD1	2.50	0.47
1:H:136:ILE:CD1	2:L:219:TYR:HD1	2.27	0.47
1:A:244:TYR:HE1	1:A:301:LEU:CD1	2.25	0.47
1:B:343:ILE:HG12	1:B:349:GLN:HG2	1.96	0.47
1:B:99:VAL:HG13	1:B:256:TYR:HB2	1.95	0.47
1:C:381:ARG:O	1:C:385:GLN:HG3	2.15	0.47
1:H:143:ARG:HG3	11:H:2059:HOH:O	2.15	0.47
1:J:505:LEU:HD22	1:J:509:GLU:HG3	1.97	0.47
2:M:112:GLN:HB3	11:M:2053:HOH:O	2.14	0.47
1:A:390:MET:HG3	1:A:424:LEU:HD22	1.96	0.47
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.97	0.47
1:C:299:PHE:HB3	11:D:2101:HOH:O	2.13	0.47
2:E:136:GLY:HA3	2:E:431:LEU:HD12	1.93	0.47
3:G:33:ARG:O	3:G:37:GLU:HB2	2.13	0.47
1:I:34:ILE:HD11	1:I:79:ASP:HB2	1.97	0.47
1:B:292:GLU:H	10:G:1273[A]:QUE:C6	2.27	0.47
2:K:359:ASP:HB3	2:K:362:ILE:HD12	1.97	0.47
2:L:367:HIS:CE1	2:L:434:LEU:HD11	2.50	0.47
2:M:9:THR:HB	2:M:10:THR:H	1.53	0.47
1:C:362:ARG:HA	1:C:363:PRO:C	2.36	0.47
2:D:221:GLN:HA	2:D:221:GLN:NE2	2.29	0.47
2:E:258:ILE:HG21	2:E:310:ILE:HD13	1.97	0.47
1:J:297:ASP:HA	2:K:267:GLU:HG2	1.97	0.47
2:L:149:GLY:HA2	2:L:304:ILE:O	2.15	0.47
2:D:167:MET:HB2	2:D:420:VAL:HG11	1.97	0.46
1:I:48:GLN:HB3	2:M:68:GLY:HA2	1.97	0.46
1:B:90:ARG:HH21	1:B:92:GLY:HA2	1.81	0.46
2:D:249:GLN:OE1	2:D:249:GLN:HA	2.15	0.46
2:L:49:VAL:HA	2:L:60:THR:HG22	1.97	0.46
1:A:248:TYR:CD2	6:A:1513:GOL:H32	2.50	0.46
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.51	0.46
3:G:22:SER:HB3	11:G:2006:HOH:O	2.14	0.46
1:H:152:ALA:HA	1:H:428:LEU:HD22	1.96	0.46
1:H:74:VAL:HG13	1:H:241:PRO:CG	2.46	0.46
2:D:188:GLU:O	2:D:221:GLN:HB3	2.15	0.46
2:D:153:GLY:HA3	2:D:329:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:342:VAL:HA	1:I:345:ILE:HD12	1.98	0.46
1:C:176:THR:O	1:C:180:ILE:HG12	2.16	0.46
2:F:298:THR:HG23	2:F:303:SER:HA	1.96	0.46
1:I:471:HIS:HB2	11:I:2149:HOH:O	2.16	0.46
1:J:213:VAL:O	1:J:217:VAL:HG13	2.15	0.46
2:K:131:GLU:HG3	2:K:148:LYS:HD2	1.97	0.46
2:L:242:TYR:CD1	2:L:246:GLN:HG3	2.51	0.46
2:F:218:VAL:HG21	2:F:236:GLY:HA2	1.97	0.46
1:I:453:LEU:HA	1:I:456:LEU:HD12	1.97	0.46
2:L:15:ALA:HB3	2:L:22:ASP:HB2	1.97	0.46
1:I:362:ARG:HA	1:I:363:PRO:C	2.37	0.46
2:F:170:ILE:O	2:F:174:ALA:HB3	2.16	0.46
1:I:179:ALA:HB1	1:I:267:ILE:HD13	1.98	0.46
1:J:381:ARG:O	1:J:385:GLN:HG3	2.16	0.46
2:L:237:LEU:HD21	2:L:295:ARG:HB2	1.97	0.46
2:D:397:SER:HB3	2:D:400:ASP:OD1	2.16	0.45
2:F:163:THR:O	2:F:167:MET:HG2	2.16	0.45
2:F:440:GLY:O	2:F:444:ILE:HG13	2.15	0.45
2:F:456:ALA:HA	2:F:469:LYS:HD3	1.97	0.45
3:G:14:LYS:HA	3:G:243:ILE:HD11	1.98	0.45
1:H:99:VAL:CG1	1:H:256:TYR:HB2	2.46	0.45
2:D:188:GLU:H	2:D:221:GLN:NE2	2.15	0.45
2:E:367:HIS:CE1	2:E:434:LEU:HD11	2.52	0.45
1:H:362:ARG:HD3	11:H:2152:HOH:O	2.16	0.45
1:H:87:ILE:HD12	1:H:87:ILE:N	2.31	0.45
2:K:367:HIS:CE1	2:K:434:LEU:HD11	2.51	0.45
2:M:474:ALA:HB3	11:M:2198:HOH:O	2.17	0.45
2:E:32:ILE:O	2:E:33:LEU:HB2	2.17	0.45
3:N:78:CYS:HB3	3:N:228:ARG:HB2	1.98	0.45
2:D:25:PHE:O	2:D:56:SER:HB3	2.17	0.45
1:J:215:GLN:HG3	2:M:356:ARG:HH22	1.82	0.45
2:F:32:ILE:O	2:F:33:LEU:HB2	2.15	0.45
1:I:185:ASN:O	1:I:188:ARG:HG2	2.17	0.45
2:L:438:ILE:O	2:L:442:GLN:HB2	2.17	0.45
2:F:97:VAL:HB	2:F:232:VAL:HG13	1.99	0.45
1:I:26:GLU:HB3	1:I:46:ASN:ND2	2.32	0.45
2:M:81:PRO:O	2:M:83:ARG:HG3	2.15	0.45
1:C:349:GLN:HE22	1:C:371:VAL:HG22	1.81	0.45
2:F:419:GLN:HG2	11:F:2182:HOH:O	2.15	0.45
2:M:237:LEU:HD23	2:M:237:LEU:C	2.37	0.45
2:M:32:ILE:O	2:M:33:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:402:LEU:O	2:D:406:ARG:HG3	2.17	0.45
1:B:171:ARG:HH12	2:E:356:ARG:HH21	1.64	0.45
2:K:418:PHE:HB2	2:K:421:ALA:HB3	1.99	0.44
1:B:123:SER:HB3	11:B:2024:HOH:O	2.16	0.44
1:B:176:THR:O	1:B:180:ILE:HG12	2.17	0.44
2:F:455:GLN:HG2	11:F:2199:HOH:O	2.17	0.44
1:I:84:GLU:HB3	2:L:29:LEU:HD12	1.98	0.44
1:J:141:SER:O	1:J:143:ARG:HG3	2.17	0.44
2:E:242:TYR:CD1	2:E:246:GLN:HG3	2.53	0.44
1:H:244:TYR:HE1	1:H:301:LEU:CD1	2.28	0.44
2:K:162:LYS:HB2	2:K:162:LYS:HE2	1.80	0.44
2:E:165:LEU:HD22	2:E:335:LEU:HD21	1.99	0.44
1:B:439:GLU:HA	1:B:442:VAL:HG13	2.00	0.44
1:C:396:GLN:O	1:C:400:VAL:HG23	2.18	0.44
2:F:31:PRO:HG2	2:F:34:ASN:OD1	2.18	0.44
2:K:188:GLU:O	2:K:221:GLN:HB3	2.18	0.44
1:C:183:ILE:HD11	1:C:267:ILE:HD13	2.00	0.44
1:I:99:VAL:HG13	1:I:256:TYR:HB2	2.00	0.44
2:M:188:GLU:O	2:M:221:GLN:HB3	2.17	0.44
1:C:440:GLU:HB3	1:C:469:LEU:HD11	1.99	0.44
1:I:50:GLU:O	1:I:95:VAL:HG23	2.18	0.44
2:L:223:ASN:HD22	2:L:223:ASN:N	2.15	0.44
2:L:258:ILE:HG21	2:L:310:ILE:HD13	1.99	0.44
2:E:220:GLY:CA	2:E:232:VAL:HG11	2.48	0.44
1:I:349:GLN:NE2	11:I:2124:HOH:O	2.48	0.44
2:M:223:ASN:N	2:M:223:ASN:HD22	2.15	0.44
2:F:393:MET:CE	2:F:404:VAL:HG11	2.48	0.43
3:G:168:VAL:HG23	3:G:169:ILE:HG13	1.99	0.43
1:J:501:VAL:O	1:J:505:LEU:HB2	2.18	0.43
2:M:456:ALA:HA	2:M:469:LYS:HD3	1.99	0.43
2:E:149:GLY:HA2	2:E:304:ILE:O	2.17	0.43
2:E:223:ASN:ND2	2:E:223:ASN:N	2.65	0.43
3:G:109:GLY:HA2	3:G:131:VAL:CG1	2.49	0.43
1:H:469:LEU:HA	1:H:472:VAL:HG22	2.00	0.43
2:D:289:MET:HG3	11:D:2116:HOH:O	2.17	0.43
2:D:390:ILE:O	2:F:391:LEU:HD11	2.19	0.43
2:E:183:PHE:HB3	2:E:217:LEU:CD2	2.48	0.43
2:E:275:ILE:HA	2:E:276:PRO:HD3	1.89	0.43
1:I:397:TYR:CD1	1:I:421:GLY:HA3	2.54	0.43
2:M:337:ARG:O	2:M:341:GLU:HG3	2.17	0.43
2:K:153:GLY:HA3	2:K:329:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:220:GLY:CA	2:L:232:VAL:HG11	2.48	0.43
1:A:240:ALA:N	1:A:241:PRO:HD2	2.33	0.43
2:D:157:GLY:O	2:D:160:VAL:HG22	2.19	0.43
1:H:240:ALA:HB3	1:H:241:PRO:HD3	2.00	0.43
1:A:187:LYS:HE2	1:A:224:ASP:HB3	2.00	0.43
2:F:175:LYS:HG3	11:F:2075:HOH:O	2.18	0.43
1:H:444:VAL:HG13	1:H:465:GLU:HG3	1.99	0.43
1:J:307:GLU:OE2	2:K:223:ASN:HB3	2.18	0.43
2:E:258:ILE:O	2:E:261:PHE:HB3	2.19	0.43
2:F:17:ILE:HG13	2:F:271:LEU:HD22	2.01	0.43
1:J:268:TYR:O	1:J:270:ASP:HA	2.19	0.43
2:K:348:VAL:O	2:K:350:PRO:HD3	2.19	0.43
1:A:102:GLU:HG3	1:A:123:SER:HA	2.01	0.43
2:E:97:VAL:HB	2:E:232:VAL:HG13	2.01	0.43
2:F:374:VAL:O	2:F:377:ILE:HG22	2.18	0.43
10:G:1273[B]:QUE:H15	10:G:1273[B]:QUE:O27	2.19	0.43
1:J:166:LEU:HB2	1:J:346:THR:HG21	2.01	0.43
2:E:142:LEU:HD21	2:E:374:VAL:HG21	2.01	0.42
1:I:171:ARG:HH12	2:L:356:ARG:HH21	1.66	0.42
1:C:213:VAL:O	1:C:217:VAL:HG13	2.19	0.42
1:C:248:TYR:CD2	6:C:1513:GOL:H12	2.54	0.42
3:G:6:ILE:HG21	3:G:250:PHE:HB2	2.00	0.42
1:A:161:ARG:HA	1:A:322:THR:OG1	2.18	0.42
1:A:362:ARG:HA	1:A:363:PRO:C	2.39	0.42
1:A:62:MET:HB3	1:A:74:VAL:HG12	2.00	0.42
1:B:166:LEU:HD11	1:B:327:ILE:HB	1.99	0.42
1:C:270:ASP:OD1	1:C:272:SER:HB2	2.19	0.42
2:D:275:ILE:HG23	3:G:269:ALA:HB2	2.02	0.42
1:A:94:ILE:HD13	1:A:96:ASP:HB3	2.01	0.42
1:B:47:VAL:HG13	1:B:90:ARG:HG2	2.02	0.42
2:E:412:ARG:HG2	2:E:458:TYR:HB2	2.00	0.42
2:M:97:VAL:HG22	11:M:2045:HOH:O	2.19	0.42
1:C:105:GLY:HA2	1:C:226:MET:O	2.20	0.42
2:E:224:GLU:O	2:E:229:ARG:HD3	2.19	0.42
2:F:256:ASP:HA	2:F:257:ASN:HA	1.77	0.42
3:N:109:GLY:HA2	3:N:131:VAL:CG1	2.50	0.42
1:H:509:GLU:HG2	11:H:2179:HOH:O	2.20	0.42
2:L:253:LEU:O	2:L:306:SER:HA	2.19	0.42
1:C:456:LEU:HD23	1:C:461:ILE:HD13	2.00	0.42
2:D:163:THR:OG1	2:D:256:ASP:OD2	2.38	0.42
3:N:33:ARG:O	3:N:37:GLU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:PRO:O	1:A:461:ILE:HG12	2.20	0.42
2:F:223:ASN:N	2:F:223:ASN:HD22	2.15	0.42
2:F:9:THR:HG22	11:F:2002:HOH:O	2.19	0.42
1:B:283:LEU:HD21	1:B:289:PRO:HB3	2.02	0.42
1:B:353:GLU:HB2	1:B:356:LEU:HD12	2.01	0.42
2:E:155:PHE:N	2:E:155:PHE:CD1	2.87	0.42
1:H:32:LEU:HD11	1:H:42:HIS:HB2	2.02	0.42
1:H:26:GLU:HB3	1:H:46:ASN:ND2	2.35	0.42
1:C:168:ILE:HD11	1:C:339:PRO:HB3	2.01	0.42
2:D:52:HIS:CD2	2:D:58:VAL:HG12	2.55	0.42
1:H:166:LEU:HB3	1:H:349:GLN:HG3	2.01	0.42
1:H:335:SER:HB2	11:H:2137:HOH:O	2.20	0.42
1:J:362:ARG:HA	1:J:363:PRO:C	2.41	0.42
2:M:112:GLN:HG2	11:M:2053:HOH:O	2.20	0.42
1:H:137:ILE:N	1:H:138:PRO:CD	2.83	0.41
2:K:433:PRO:HG3	11:K:2159:HOH:O	2.18	0.41
1:A:108:VAL:HA	1:A:113:ASN:O	2.20	0.41
2:D:285:LEU:C	2:D:285:LEU:HD23	2.40	0.41
1:B:48:GLN:HB3	2:F:68:GLY:HA2	2.02	0.41
1:H:136:ILE:HD13	2:L:219:TYR:CD1	2.55	0.41
2:L:142:LEU:HD21	2:L:374:VAL:HG21	2.01	0.41
2:M:374:VAL:O	2:M:377:ILE:HG22	2.21	0.41
2:F:408:ARG:NE	2:F:454:GLU:OE1	2.36	0.41
2:E:253:LEU:O	2:E:306:SER:HA	2.20	0.41
2:K:200:MET:HE3	2:K:200:MET:HB2	2.00	0.41
2:M:141:ASP:HB3	2:M:434:LEU:HD13	2.03	0.41
1:A:99:VAL:HG22	1:A:253:MET:HA	2.01	0.41
1:C:163:GLN:HG3	1:C:347:ASP:HB2	2.02	0.41
2:D:200:MET:HB2	2:D:200:MET:HE2	1.87	0.41
1:H:410:LEU:HB2	1:H:415:GLN:HG3	2.02	0.41
1:I:158:PRO:O	1:I:375:GLY:HA3	2.21	0.41
1:J:44:LEU:O	2:K:71:ARG:NH2	2.53	0.41
2:K:181:SER:O	2:K:215:VAL:HA	2.20	0.41
2:L:218:VAL:HG21	2:L:236:GLY:HA2	2.01	0.41
3:N:6:ILE:HG21	3:N:250:PHE:HB2	2.02	0.41
1:C:164:ARG:N	1:C:164:ARG:HD3	2.36	0.41
2:E:31:PRO:HD2	2:E:34:ASN:ND2	2.36	0.41
3:G:206:GLU:N	11:G:2017:HOH:O	2.54	0.41
1:H:136:ILE:HD13	2:L:219:TYR:HD1	1.84	0.41
1:I:353:GLU:HB2	1:I:356:LEU:HD12	2.02	0.41
1:J:344:SER:HA	8:K:1478:AZI:N3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ARG:HD2	11:B:2133:HOH:O	2.21	0.41
1:B:438:ILE:O	1:B:442:VAL:HG12	2.20	0.41
2:D:142:LEU:HD21	2:D:374:VAL:HG21	2.01	0.41
2:F:153:GLY:HA3	2:F:329:LEU:HD13	2.03	0.41
2:D:264:ALA:O	2:D:267:GLU:HB2	2.21	0.41
2:F:112:GLN:H	2:F:112:GLN:HE21	1.69	0.41
1:H:213:VAL:O	1:H:216:LEU:HB3	2.21	0.41
1:J:263:HIS:HD2	1:J:320:SER:OG	2.04	0.41
2:M:13:ILE:HD12	2:M:73:GLN:HB3	2.03	0.41
1:A:152:ALA:HA	1:A:428:LEU:HD22	2.03	0.41
2:E:139:VAL:HG13	2:E:414:LEU:HD22	2.02	0.41
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.55	0.41
1:H:186:GLN:HG3	1:H:199:LEU:HD23	2.03	0.41
1:I:422:VAL:O	1:I:426:GLU:HG2	2.21	0.41
1:J:287:ARG:HA	1:J:288:PRO:HD3	1.92	0.41
2:M:440:GLY:O	2:M:444:ILE:HG13	2.21	0.41
1:A:172:GLN:HA	4:A:1511:ANP:N3B	2.36	0.41
1:A:26:GLU:HB3	1:A:46:ASN:ND2	2.36	0.41
1:B:130:GLY:HA2	6:B:1512:GOL:C3	2.50	0.41
1:I:268:TYR:HB2	1:I:325:PRO:HA	2.03	0.41
1:I:47:VAL:CG1	1:I:90:ARG:HG2	2.51	0.41
2:M:84:ILE:HD13	2:M:235:THR:HG23	2.03	0.41
1:A:74:VAL:HG22	11:A:2006:HOH:O	2.22	0.40
1:C:187:LYS:HE2	1:C:224:ASP:HB3	2.03	0.40
1:C:297:ASP:HA	2:D:267:GLU:HG2	2.02	0.40
2:M:327:ALA:HB3	11:M:2146:HOH:O	2.20	0.40
3:N:254:ARG:NH2	11:N:2027:HOH:O	2.53	0.40
1:I:288:PRO:HB3	2:M:276:PRO:HG3	2.03	0.40
2:K:163:THR:O	2:K:166:ILE:HG22	2.21	0.40
1:B:286:ARG:HA	2:E:275:ILE:HD12	2.02	0.40
2:E:132:ILE:HD11	2:E:363:VAL:CG1	2.50	0.40
2:L:97:VAL:HB	2:L:232:VAL:HG13	2.03	0.40
1:C:283:LEU:HD21	1:C:289:PRO:HB3	2.02	0.40
2:L:254:PHE:CD2	2:L:307:VAL:HB	2.56	0.40
2:L:97:VAL:HG13	2:L:98:ILE:HG23	2.03	0.40
2:D:387:ILE:CG2	3:G:19:ILE:HD13	2.47	0.40
1:H:246:ALA:HB3	1:H:247:PRO:HD3	2.04	0.40
1:J:456:LEU:HD23	1:J:461:ILE:HD13	2.03	0.40
2:L:32:ILE:O	2:L:33:LEU:HB2	2.21	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%)	469 (97%)	15 (3%)	1 (0%)	51	67
1	B	475/510 (93%)	458 (96%)	16 (3%)	1 (0%)	51	67
1	C	493/510 (97%)	481 (98%)	10 (2%)	2 (0%)	38	54
1	H	485/510 (95%)	469 (97%)	16 (3%)	0	100	100
1	I	475/510 (93%)	462 (97%)	12 (2%)	1 (0%)	51	67
1	J	493/510 (97%)	480 (97%)	10 (2%)	3 (1%)	28	41
2	D	465/482 (96%)	441 (95%)	23 (5%)	1 (0%)	51	67
2	E	464/482 (96%)	444 (96%)	17 (4%)	3 (1%)	28	41
2	F	464/482 (96%)	446 (96%)	18 (4%)	0	100	100
2	K	465/482 (96%)	442 (95%)	21 (4%)	2 (0%)	38	54
2	L	464/482 (96%)	446 (96%)	16 (3%)	2 (0%)	38	54
2	M	464/482 (96%)	445 (96%)	18 (4%)	1 (0%)	51	67
3	G	155/272 (57%)	152 (98%)	3 (2%)	0	100	100
3	N	155/272 (57%)	151 (97%)	4 (3%)	0	100	100
All	All	6002/6496 (92%)	5786 (96%)	199 (3%)	17 (0%)	44	60

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
1	J	407	GLY
1	C	409	ASP
1	J	409	ASP
1	A	385	GLN
2	D	385	GLN
2	K	385	GLN
1	B	35	GLY
1	J	337	TYR

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Mol	Chain	Res	Type
1	I	35	GLY
2	E	81	PRO
2	E	156	GLY
2	L	156	GLY
2	E	279	VAL
2	K	279	VAL
2	L	279	VAL
2	M	279	VAL

### 5.3.2 Protein sidechains [i](#)

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%)	379 (96%)	14 (4%)	40	60
1	B	389/413 (94%)	377 (97%)	12 (3%)	45	66
1	C	399/413 (97%)	384 (96%)	15 (4%)	38	58
1	H	393/413 (95%)	379 (96%)	14 (4%)	40	60
1	I	389/413 (94%)	377 (97%)	12 (3%)	45	66
1	J	399/413 (97%)	383 (96%)	16 (4%)	36	55
2	D	377/386 (98%)	372 (99%)	5 (1%)	73	87
2	E	376/386 (97%)	358 (95%)	18 (5%)	30	47
2	F	376/386 (97%)	364 (97%)	12 (3%)	44	65
2	K	377/386 (98%)	371 (98%)	6 (2%)	68	83
2	L	376/386 (97%)	360 (96%)	16 (4%)	33	52
2	M	376/386 (97%)	360 (96%)	16 (4%)	33	52
3	G	140/230 (61%)	126 (90%)	14 (10%)	9	13
3	N	140/230 (61%)	132 (94%)	8 (6%)	24	38
All	All	4900/5254 (93%)	4722 (96%)	178 (4%)	40	60

All (178) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	47	VAL
1	A	74	VAL
1	A	91	THR
1	A	94	ILE
1	A	99	VAL
1	A	102	GLU
1	A	136	ILE
1	A	157	VAL
1	A	164	ARG
1	A	355	GLU
1	A	403	PHE
1	A	410	LEU
1	A	479	LEU
1	A	496	LYS
1	B	47	VAL
1	B	57	SER
1	B	99	VAL
1	B	164	ARG
1	B	171	ARG
1	B	193	THR
1	B	217	VAL
1	B	349	GLN
1	B	371	VAL
1	B	418	LEU
1	B	442	VAL
1	B	503	ASN
1	C	74	VAL
1	C	99	VAL
1	C	123	SER
1	C	164	ARG
1	C	171	ARG
1	C	216	LEU
1	C	217	VAL
1	C	334	VAL
1	C	335	SER
1	C	406	PHE
1	C	409	ASP
1	C	475	GLN
1	C	479	LEU
1	C	482	LYS
1	C	505	LEU
2	D	89	GLU
2	D	97	VAL

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Mol	Chain	Res	Type
2	D	249	GLN
2	D	274	ARG
2	D	390	ILE
2	E	111	LYS
2	E	129	GLU
2	E	139	VAL
2	E	162	LYS
2	E	215	VAL
2	E	223	ASN
2	E	232	VAL
2	E	257	ASN
2	E	293	GLN
2	E	297	THR
2	E	310	ILE
2	E	337	ARG
2	E	352	ASP
2	E	358	MET
2	E	412	ARG
2	E	420	VAL
2	E	428	LEU
2	E	431	LEU
2	F	9	THR
2	F	27	GLU
2	F	112	GLN
2	F	199	GLU
2	F	223	ASN
2	F	232	VAL
2	F	237	LEU
2	F	247	GLU
2	F	249	GLN
2	F	274	ARG
2	F	279	VAL
2	F	403	THR
3	G	2	THR
3	G	8	ARG
3	G	87	LYS
3	G	88	GLN
3	G	110	ASP
3	G	113	ARG
3	G	137	THR
3	G	168	VAL
3	G	169	ILE

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Mol	Chain	Res	Type
3	G	218	LYS
3	G	226	SER
3	G	232	MET
3	G	240	SER
3	G	262	LEU
1	H	74	VAL
1	H	91	THR
1	H	94	ILE
1	H	102	GLU
1	H	141	SER
1	H	164	ARG
1	H	188	ARG
1	H	216	LEU
1	H	344	SER
1	H	403	PHE
1	H	409	ASP
1	H	419	SER
1	H	434	SER
1	H	479	LEU
1	I	63	SER
1	I	79	ASP
1	I	80	LYS
1	I	99	VAL
1	I	164	ARG
1	I	171	ARG
1	I	193	THR
1	I	335	SER
1	I	349	GLN
1	I	371	VAL
1	I	442	VAL
1	I	479	LEU
1	J	47	VAL
1	J	57	SER
1	J	63	SER
1	J	74	VAL
1	J	99	VAL
1	J	164	ARG
1	J	217	VAL
1	J	334	VAL
1	J	335	SER
1	J	406	PHE
1	J	409	ASP

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Mol	Chain	Res	Type
1	J	444	VAL
1	J	475	GLN
1	J	479	LEU
1	J	482	LYS
1	J	505	LEU
2	K	97	VAL
2	K	111	LYS
2	K	335	LEU
2	K	390	ILE
2	K	419	GLN
2	K	428	LEU
2	L	43	THR
2	L	76	LEU
2	L	111	LYS
2	L	139	VAL
2	L	162	LYS
2	L	215	VAL
2	L	223	ASN
2	L	232	VAL
2	L	257	ASN
2	L	293	GLN
2	L	310	ILE
2	L	358	MET
2	L	412	ARG
2	L	420	VAL
2	L	428	LEU
2	L	431	LEU
2	M	9	THR
2	M	27	GLU
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	237	LEU
2	M	247	GLU
2	M	249	GLN
2	M	266	SER
2	M	279	VAL
2	M	303	SER
2	M	399	GLU

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Mol	Chain	Res	Type
2	M	403	THR
3	N	8	ARG
3	N	87	LYS
3	N	110	ASP
3	N	113	ARG
3	N	168	VAL
3	N	218	LYS
3	N	240	SER
3	N	262	LEU

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

Mol	Chain	Res	Type
1	A	396	GLN
1	A	415	GLN
1	A	432	GLN
1	B	48	GLN
1	B	65	ASN
1	B	172	GLN
1	B	349	GLN
1	B	432	GLN
1	B	503	ASN
1	C	263	HIS
1	C	432	GLN
2	D	130	GLN
2	D	194	ASN
2	D	221	GLN
2	E	130	GLN
2	E	171	ASN
2	E	194	ASN
2	E	223	ASN
2	E	249	GLN
2	E	257	ASN
2	E	293	GLN
2	E	308	GLN
2	E	379	GLN
2	E	385	GLN
2	F	112	GLN
2	F	221	GLN
2	F	223	ASN
2	F	419	GLN
2	F	443	GLN

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Mol	Chain	Res	Type
3	G	15	ASN
3	G	88	GLN
3	G	211	ASN
1	H	396	GLN
1	H	432	GLN
1	H	476	HIS
1	I	48	GLN
1	I	113	ASN
1	I	349	GLN
1	I	503	ASN
1	J	263	HIS
1	J	416	GLN
1	J	432	GLN
2	K	130	GLN
2	K	194	ASN
2	K	221	GLN
2	L	130	GLN
2	L	223	ASN
2	L	249	GLN
2	L	257	ASN
2	L	293	GLN
2	L	308	GLN
2	L	361	ASN
2	L	379	GLN
2	L	385	GLN
2	M	112	GLN
2	M	221	GLN
2	M	223	ASN
2	M	249	GLN
2	M	419	GLN
2	M	443	GLN
3	N	88	GLN
3	N	211	ASN
3	N	225	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 10 are monoatomic - leaving 30 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	29,33,33	2.13	9 (31%)	28,52,52	2.21	6 (21%)
6	GOL	A	1513	-	5,5,5	0.33	0	5,5,5	0.52	0
6	GOL	A	1514	-	5,5,5	0.34	0	5,5,5	0.67	0
4	ANP	B	1510	5	29,33,33	2.11	9 (31%)	28,52,52	1.95	6 (21%)
6	GOL	B	1512	-	5,5,5	0.39	0	5,5,5	0.33	0
6	GOL	B	1513	-	5,5,5	0.32	0	5,5,5	0.43	0
4	ANP	C	1511	5	29,33,33	1.99	8 (27%)	28,52,52	2.13	6 (21%)
6	GOL	C	1513	-	5,5,5	0.36	0	5,5,5	0.20	0
7	ADP	D	1476	5	25,29,29	1.15	1 (4%)	24,45,45	1.50	2 (8%)
8	AZI	D	1478	-	0,2,2	0.00	-	0,1,1	0.00	-
6	GOL	D	1479	-	5,5,5	0.36	0	5,5,5	0.36	0
9	PO4	E	1475	-	4,4,4	0.77	0	6,6,6	0.36	0
4	ANP	F	1475	5	29,33,33	2.17	9 (31%)	28,52,52	2.26	7 (25%)
10	QUE	G	1273[A]	-	22,24,24	2.41	6 (27%)	27,36,36	1.52	3 (11%)
10	QUE	G	1273[B]	-	22,24,24	2.36	6 (27%)	27,36,36	1.42	3 (11%)
4	ANP	H	1511	5	29,33,33	2.00	7 (24%)	28,52,52	1.86	4 (14%)
6	GOL	H	1513	-	5,5,5	0.39	0	5,5,5	0.38	0
6	GOL	H	1514	-	5,5,5	0.38	0	5,5,5	0.36	0
4	ANP	I	1510	5	29,33,33	2.04	7 (24%)	28,52,52	2.36	5 (17%)
6	GOL	I	1512	-	5,5,5	0.39	0	5,5,5	0.33	0
4	ANP	J	1511	5	29,33,33	1.95	7 (24%)	28,52,52	2.04	6 (21%)
6	GOL	J	1513	-	5,5,5	0.38	0	5,5,5	0.43	0
7	ADP	K	1476	5	25,29,29	1.16	2 (8%)	24,45,45	1.64	3 (12%)
8	AZI	K	1478	-	0,2,2	0.00	-	0,1,1	0.00	-
6	GOL	K	1479	-	5,5,5	0.42	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	K	1480	-	5,5,5	0.32	0	5,5,5	0.37	0
9	PO4	L	1475	-	4,4,4	0.77	0	6,6,6	0.35	0
4	ANP	M	1475	5	29,33,33	2.09	10 (34%)	28,52,52	2.26	7 (25%)
10	QUE	N	1273[A]	-	22,24,24	2.42	6 (27%)	27,36,36	1.56	3 (11%)
10	QUE	N	1273[B]	-	22,24,24	2.37	6 (27%)	27,36,36	1.47	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	1511	5	-	0/13/38/38	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	-	0/13/38/38	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	-	0/13/38/38	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	-	0/13/38/38	0/3/3/3
10	QUE	G	1273[A]	-	-	0/4/4/4	0/3/3/3
10	QUE	G	1273[B]	-	-	0/4/4/4	0/3/3/3
4	ANP	H	1511	5	-	0/13/38/38	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	-	0/13/38/38	0/3/3/3
6	GOL	I	1512	-	-	0/4/4/4	0/0/0/0
4	ANP	J	1511	5	-	0/13/38/38	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	-	0/13/38/38	0/3/3/3
10	QUE	N	1273[A]	-	-	0/4/4/4	0/3/3/3
10	QUE	N	1273[B]	-	-	0/4/4/4	0/3/3/3



All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1511	ANP	PG-O2G	-2.80	1.49	1.56
4	A	1511	ANP	PG-O2G	-2.48	1.49	1.56
4	M	1475	ANP	PG-O3G	-2.33	1.50	1.56
4	B	1510	ANP	PG-O2G	-2.30	1.50	1.56
4	H	1511	ANP	PB-O2B	-2.29	1.50	1.56
4	B	1510	ANP	PB-O2B	-2.28	1.50	1.56
4	J	1511	ANP	PG-O2G	-2.28	1.50	1.56
4	I	1510	ANP	PB-O2B	-2.25	1.50	1.56
4	F	1475	ANP	PG-O3G	-2.17	1.50	1.56
4	A	1511	ANP	PB-O2B	-2.17	1.50	1.56
4	F	1475	ANP	PB-O2B	-2.16	1.50	1.56
4	M	1475	ANP	PG-O2G	-2.14	1.50	1.56
4	H	1511	ANP	PG-O2G	-2.12	1.50	1.56
4	I	1510	ANP	PG-O2G	-2.11	1.50	1.56
4	F	1475	ANP	PG-O2G	-2.05	1.51	1.56
4	C	1511	ANP	PG-O3G	-2.02	1.51	1.56
4	M	1475	ANP	PB-O2B	-2.01	1.51	1.56
4	B	1510	ANP	C2-N3	2.02	1.35	1.32
4	F	1475	ANP	O4'-C1'	2.02	1.44	1.41
4	B	1510	ANP	O4'-C1'	2.03	1.44	1.41
10	G	1273[B]	QUE	C14-C11	2.06	1.50	1.46
4	J	1511	ANP	PB-O3A	2.06	1.61	1.59
4	M	1475	ANP	O4'-C1'	2.08	1.44	1.41
4	C	1511	ANP	PB-O3A	2.08	1.61	1.59
10	G	1273[A]	QUE	C14-C11	2.10	1.50	1.46
10	N	1273[A]	QUE	C9-C10	2.13	1.48	1.41
7	K	1476	ADP	O4'-C1'	2.13	1.44	1.41
4	A	1511	ANP	O4'-C1'	2.14	1.44	1.41
10	N	1273[B]	QUE	C14-C11	2.18	1.50	1.46
4	M	1475	ANP	PB-O3A	2.21	1.61	1.59
10	N	1273[B]	QUE	C9-C10	2.28	1.48	1.41
10	G	1273[B]	QUE	C9-C10	2.33	1.49	1.41
10	N	1273[A]	QUE	C14-C11	2.33	1.50	1.46
10	G	1273[A]	QUE	C9-C10	2.33	1.49	1.41
4	A	1511	ANP	PB-O3A	2.89	1.62	1.59
4	F	1475	ANP	C5-C4	3.00	1.47	1.40
4	A	1511	ANP	C5-C4	3.03	1.47	1.40
4	M	1475	ANP	C5-C4	3.06	1.47	1.40
4	C	1511	ANP	C5-C4	3.14	1.47	1.40
4	I	1510	ANP	C5-C4	3.20	1.47	1.40
4	J	1511	ANP	C5-C4	3.24	1.47	1.40
10	N	1273[B]	QUE	C2-C3	3.26	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	1273[B]	QUE	C2-C3	3.26	1.49	1.43
4	H	1511	ANP	C5-C4	3.26	1.47	1.40
4	B	1510	ANP	C5-C4	3.36	1.48	1.40
10	N	1273[A]	QUE	C2-C3	3.37	1.49	1.43
7	K	1476	ADP	C5-C4	3.49	1.48	1.40
10	G	1273[A]	QUE	C2-C3	3.51	1.49	1.43
7	D	1476	ADP	C5-C4	3.59	1.48	1.40
4	H	1511	ANP	PB-O1B	3.74	1.50	1.46
4	C	1511	ANP	PG-N3B	3.77	1.73	1.63
4	A	1511	ANP	PB-N3B	3.83	1.73	1.63
4	J	1511	ANP	PG-N3B	3.93	1.73	1.63
4	I	1510	ANP	PG-N3B	3.95	1.73	1.63
4	A	1511	ANP	PG-N3B	3.99	1.73	1.63
4	F	1475	ANP	PB-N3B	4.08	1.74	1.63
4	B	1510	ANP	PG-N3B	4.12	1.74	1.63
4	M	1475	ANP	PG-N3B	4.12	1.74	1.63
4	C	1511	ANP	PB-N3B	4.13	1.74	1.63
4	H	1511	ANP	PG-N3B	4.14	1.74	1.63
4	M	1475	ANP	PB-N3B	4.15	1.74	1.63
4	C	1511	ANP	PB-O1B	4.18	1.50	1.46
4	I	1510	ANP	PB-N3B	4.22	1.74	1.63
4	J	1511	ANP	PB-O1B	4.25	1.50	1.46
4	J	1511	ANP	PB-N3B	4.31	1.74	1.63
4	B	1510	ANP	PB-N3B	4.36	1.74	1.63
4	J	1511	ANP	PG-O1G	4.37	1.51	1.46
4	F	1475	ANP	PG-N3B	4.37	1.74	1.63
4	H	1511	ANP	PB-N3B	4.47	1.75	1.63
4	I	1510	ANP	PB-O1B	4.57	1.51	1.46
4	B	1510	ANP	PG-O1G	4.60	1.51	1.46
4	F	1475	ANP	PG-O1G	4.63	1.51	1.46
4	M	1475	ANP	PG-O1G	4.76	1.51	1.46
4	H	1511	ANP	PG-O1G	4.76	1.51	1.46
4	C	1511	ANP	PG-O1G	4.84	1.51	1.46
4	I	1510	ANP	PG-O1G	4.95	1.51	1.46
4	A	1511	ANP	PB-O1B	4.97	1.51	1.46
4	M	1475	ANP	PB-O1B	5.03	1.51	1.46
4	B	1510	ANP	PB-O1B	5.16	1.52	1.46
4	A	1511	ANP	PG-O1G	5.32	1.52	1.46
10	G	1273[A]	QUE	C9-C3	5.42	1.49	1.41
10	N	1273[B]	QUE	C9-C3	5.43	1.49	1.41
10	N	1273[A]	QUE	C9-C3	5.46	1.49	1.41
10	G	1273[B]	QUE	C9-C3	5.47	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	1273[B]	QUE	C18-C17	5.54	1.49	1.40
10	G	1273[B]	QUE	C18-C17	5.55	1.49	1.40
10	G	1273[A]	QUE	C18-C17	5.70	1.49	1.40
10	N	1273[A]	QUE	C18-C17	5.75	1.49	1.40
10	G	1273[B]	QUE	C3-C4	5.76	1.49	1.41
10	N	1273[B]	QUE	C3-C4	5.80	1.49	1.41
10	N	1273[A]	QUE	C3-C4	5.94	1.49	1.41
10	G	1273[A]	QUE	C3-C4	5.94	1.49	1.41
4	F	1475	ANP	PB-O1B	6.17	1.53	1.46

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1475	ANP	O1G-PG-N3B	-7.43	100.67	111.79
4	C	1511	ANP	N3-C2-N1	-7.35	122.46	128.86
4	I	1510	ANP	O1G-PG-N3B	-7.22	101.00	111.79
4	M	1475	ANP	O1G-PG-N3B	-7.02	101.28	111.79
4	A	1511	ANP	N3-C2-N1	-6.65	123.07	128.86
4	H	1511	ANP	N3-C2-N1	-6.36	123.32	128.86
4	F	1475	ANP	N3-C2-N1	-6.03	123.61	128.86
4	I	1510	ANP	N3-C2-N1	-6.02	123.61	128.86
7	K	1476	ADP	N3-C2-N1	-5.88	123.73	128.86
4	B	1510	ANP	N3-C2-N1	-5.83	123.78	128.86
4	M	1475	ANP	N3-C2-N1	-5.81	123.80	128.86
4	A	1511	ANP	O1G-PG-N3B	-5.73	103.22	111.79
4	J	1511	ANP	N3-C2-N1	-5.63	123.96	128.86
4	J	1511	ANP	O1G-PG-N3B	-5.50	103.57	111.79
7	D	1476	ADP	N3-C2-N1	-5.26	124.28	128.86
4	C	1511	ANP	O1G-PG-N3B	-4.72	104.73	111.79
10	G	1273[A]	QUE	C5-C4-C3	-4.66	117.89	123.05
10	N	1273[A]	QUE	C5-C4-C3	-4.61	117.94	123.05
10	N	1273[B]	QUE	C5-C4-C3	-4.29	118.30	123.05
4	A	1511	ANP	C4-C5-N7	-4.12	105.43	109.41
10	G	1273[B]	QUE	C5-C4-C3	-4.11	118.50	123.05
4	B	1510	ANP	O1G-PG-N3B	-3.94	105.90	111.79
4	F	1475	ANP	C4-C5-N7	-3.49	106.03	109.41
4	F	1475	ANP	O1B-PB-N3B	-3.42	106.67	111.79
4	H	1511	ANP	C4-C5-N7	-3.38	106.15	109.41
4	I	1510	ANP	PA-O3A-PB	-3.37	120.48	132.38
7	K	1476	ADP	C4-C5-N7	-3.04	106.47	109.41
4	B	1510	ANP	PA-O3A-PB	-2.96	121.92	132.38
4	J	1511	ANP	C4-C5-N7	-2.94	106.57	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1475	ANP	C4-C5-N7	-2.92	106.58	109.41
4	B	1510	ANP	C4-C5-N7	-2.84	106.67	109.41
4	J	1511	ANP	PA-O3A-PB	-2.76	122.63	132.38
4	M	1475	ANP	O3A-PB-N3B	-2.74	98.98	106.59
4	A	1511	ANP	PA-O3A-PB	-2.72	122.78	132.38
4	I	1510	ANP	C4-C5-N7	-2.66	106.84	109.41
10	G	1273[B]	QUE	C10-C9-C3	-2.59	117.69	121.28
10	N	1273[B]	QUE	C10-C9-C3	-2.57	117.72	121.28
10	N	1273[A]	QUE	C10-C9-C3	-2.54	117.76	121.28
10	G	1273[A]	QUE	C10-C9-C3	-2.50	117.82	121.28
4	J	1511	ANP	O1B-PB-N3B	-2.38	108.23	111.79
7	D	1476	ADP	C4-C5-N7	-2.28	107.21	109.41
4	F	1475	ANP	PA-O3A-PB	-2.16	124.74	132.38
4	C	1511	ANP	O1B-PB-N3B	-2.14	108.58	111.79
4	C	1511	ANP	PA-O3A-PB	-2.14	124.83	132.38
4	M	1475	ANP	PA-O3A-PB	-2.08	125.05	132.38
4	M	1475	ANP	O3G-PG-O2G	2.06	113.45	107.69
7	K	1476	ADP	C2-N1-C6	2.16	122.55	118.77
4	B	1510	ANP	O3G-PG-O2G	2.19	113.83	107.69
4	F	1475	ANP	O3G-PG-O2G	2.21	113.89	107.69
4	C	1511	ANP	C2-N1-C6	2.28	122.76	118.77
4	A	1511	ANP	O3G-PG-O2G	2.38	114.36	107.69
4	F	1475	ANP	O2B-PB-O1B	2.58	115.24	109.87
4	H	1511	ANP	O3G-PG-O2G	2.67	115.17	107.69
4	C	1511	ANP	O2B-PB-O1B	3.66	117.48	109.87
4	H	1511	ANP	O2B-PB-O1B	3.72	117.60	109.87
4	A	1511	ANP	O2B-PB-O1B	3.79	117.75	109.87
10	G	1273[B]	QUE	O12-C4-C5	3.84	120.60	116.11
4	J	1511	ANP	O2B-PB-O1B	3.94	118.05	109.87
4	M	1475	ANP	O2B-PB-O1B	3.97	118.12	109.87
10	G	1273[A]	QUE	O12-C4-C5	4.03	120.83	116.11
4	B	1510	ANP	O2B-PB-O1B	4.06	118.31	109.87
10	N	1273[B]	QUE	O12-C4-C5	4.11	120.92	116.11
10	N	1273[A]	QUE	O12-C4-C5	4.48	121.35	116.11
4	I	1510	ANP	O2B-PB-O1B	4.55	119.33	109.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1511	ANP	1	0
6	A	1513	GOL	4	0
6	B	1512	GOL	1	0
6	B	1513	GOL	1	0
6	C	1513	GOL	2	0
10	G	1273[A]	QUE	3	0
10	G	1273[B]	QUE	1	0
6	J	1513	GOL	2	0
8	K	1478	AZI	1	0
4	M	1475	ANP	2	0
10	N	1273[A]	QUE	2	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%)	0.34	8 (1%) 72 70	19, 38, 62, 98	0
1	B	479/510 (93%)	0.34	24 (5%) 30 28	16, 37, 90, 105	0
1	C	495/510 (97%)	0.12	7 (1%) 75 74	14, 32, 54, 94	0
1	H	487/510 (95%)	0.33	11 (2%) 61 58	17, 38, 61, 100	0
1	I	479/510 (93%)	0.44	34 (7%) 17 15	16, 37, 90, 104	0
1	J	495/510 (97%)	0.06	8 (1%) 72 70	17, 32, 53, 94	0
2	D	467/482 (96%)	0.32	14 (2%) 51 49	16, 33, 65, 92	0
2	E	466/482 (96%)	0.62	36 (7%) 14 12	19, 46, 90, 117	0
2	F	466/482 (96%)	0.05	3 (0%) 89 87	13, 31, 57, 73	0
2	K	467/482 (96%)	0.34	12 (2%) 56 54	17, 33, 65, 92	0
2	L	466/482 (96%)	0.56	26 (5%) 25 24	20, 46, 89, 117	0
2	M	466/482 (96%)	0.09	6 (1%) 77 75	15, 30, 57, 74	0
3	G	167/272 (61%)	1.95	72 (43%) 0 0	16, 78, 123, 128	0
3	N	167/272 (61%)	1.75	65 (38%) 0 0	18, 76, 124, 129	0
All	All	6054/6496 (93%)	0.39	326 (5%) 26 25	13, 37, 87, 129	0

All (326) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	138	PHE	10.8
3	G	43	VAL	8.7
2	M	474	ALA	8.1
3	N	40	PRO	8.0
3	G	42	ARG	7.8
1	H	406	PHE	7.6
3	G	215	TYR	7.3
2	E	394	ASP	7.1

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Mol	Chain	Res	Type	RSRZ
2	K	390	ILE	7.0
3	N	161	ILE	7.0
3	G	212	ILE	6.8
1	B	193	THR	6.7
2	K	389	ALA	6.7
1	J	407	GLY	6.6
3	N	169	ILE	6.5
3	G	106	ILE	6.3
1	I	412	ALA	6.3
3	N	113	ARG	6.2
3	G	136	PRO	6.1
3	N	43	VAL	6.0
1	I	478	ALA	5.8
3	G	29	ALA	5.8
3	G	74	ASP	5.7
1	I	396	GLN	5.7
1	B	488	LYS	5.6
3	G	137	THR	5.5
3	G	87	LYS	5.5
3	G	168	VAL	5.3
3	N	134	ARG	5.3
2	E	395	GLU	5.3
2	K	394	ASP	5.2
3	G	109	GLY	5.2
3	G	169	ILE	5.2
3	G	46	VAL	5.1
3	G	214	TYR	5.1
3	G	132	GLY	5.0
3	G	133	ARG	5.0
3	N	42	ARG	5.0
1	J	409	ASP	4.9
1	I	509	GLU	4.9
1	A	94	ILE	4.9
2	E	393	MET	4.9
1	I	413	ALA	4.8
1	C	409	ASP	4.8
3	N	107	GLY	4.7
3	N	215	TYR	4.7
2	L	391	LEU	4.7
1	I	472	VAL	4.7
1	I	471	HIS	4.7
2	L	424	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
3	N	106	ILE	4.7
3	G	111	LYS	4.6
3	N	32	ALA	4.6
3	G	131	VAL	4.6
3	G	173	THR	4.6
1	I	392	LEU	4.6
2	L	394	ASP	4.6
3	N	108	VAL	4.5
3	N	130	GLU	4.5
3	N	216	SER	4.4
3	G	134	ARG	4.4
1	H	409	ASP	4.3
3	G	85	VAL	4.3
3	G	89	MET	4.3
3	G	39	LYS	4.3
3	N	212	ILE	4.2
2	D	394	ASP	4.2
3	G	32	ALA	4.2
3	N	135	PRO	4.2
3	N	38	LEU	4.2
3	G	216	SER	4.2
2	E	396	LEU	4.1
3	N	83	SER	4.1
3	N	76	GLY	4.1
1	H	405	GLN	4.1
1	C	406	PHE	4.1
2	L	425	THR	4.0
1	B	487	GLY	4.0
3	G	115	ILE	3.9
2	L	393	MET	3.9
3	G	31	TYR	3.9
3	N	89	MET	3.9
3	N	209	LEU	3.9
2	E	457	PHE	3.9
2	D	389	ALA	3.8
2	L	427	HIS	3.8
1	A	406	PHE	3.8
3	N	136	PRO	3.8
3	N	214	TYR	3.8
2	K	393	MET	3.7
3	G	113	ARG	3.7
2	L	474	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
3	N	74	ASP	3.7
1	B	497	LEU	3.7
2	L	396	LEU	3.7
3	G	223	SER	3.7
1	B	23	VAL	3.7
3	N	213	ILE	3.6
1	H	414	THR	3.6
2	E	424	PHE	3.6
3	G	161	ILE	3.6
3	N	29	ALA	3.6
3	N	173	THR	3.6
3	N	75	ARG	3.6
2	E	391	LEU	3.6
3	N	31	TYR	3.6
3	G	110	ASP	3.6
2	K	391	LEU	3.6
2	E	458	TYR	3.5
2	L	132	ILE	3.5
3	G	45	GLY	3.5
3	G	217	LEU	3.5
3	G	83	SER	3.4
2	D	390	ILE	3.4
2	D	396	LEU	3.4
2	M	178	GLY	3.4
3	G	213	ILE	3.4
3	N	45	GLY	3.4
3	G	108	VAL	3.4
3	G	76	GLY	3.3
1	B	469	LEU	3.3
2	D	386	ASP	3.3
2	K	396	LEU	3.3
3	G	162	PHE	3.3
1	C	405	GLN	3.3
3	N	131	VAL	3.3
1	I	473	ILE	3.3
2	D	475	GLU	3.3
2	K	426	GLY	3.3
2	E	388	ILE	3.2
2	M	27	GLU	3.2
2	L	457	PHE	3.2
3	N	133	ARG	3.2
2	E	473	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	L	470	ALA	3.2
3	N	211	ASN	3.2
1	I	508	PHE	3.2
2	E	387	ILE	3.2
3	G	33	ARG	3.2
3	N	39	LYS	3.2
3	N	221	THR	3.2
3	N	132	GLY	3.2
1	B	412	ALA	3.2
2	D	248	GLY	3.2
3	G	40	PRO	3.2
2	L	384	LEU	3.2
2	M	176	ALA	3.1
2	E	471	ASP	3.1
3	G	112	ILE	3.1
3	G	139	GLY	3.1
2	E	384	LEU	3.1
3	N	77	LEU	3.1
1	A	92	GLY	3.1
2	E	474	ALA	3.1
1	C	408	SER	3.1
2	L	390	ILE	3.1
3	N	140	ASP	3.0
1	B	393	GLU	3.0
2	D	387	ILE	3.0
2	E	428	LEU	3.0
3	G	211	ASN	3.0
3	G	218	LYS	3.0
3	N	166	ARG	3.0
2	L	388	ILE	2.9
1	B	460	LYS	2.9
3	G	221	THR	2.9
2	E	345	TYR	2.9
1	A	122	GLY	2.9
3	N	86	ALA	2.9
3	N	217	LEU	2.8
1	I	411	ASP	2.8
1	J	408	SER	2.8
2	E	435	LYS	2.8
1	J	405	GLN	2.8
1	C	412	ALA	2.8
1	I	485	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	L	451	HIS	2.8
1	I	488	LYS	2.8
3	G	167	SER	2.8
2	L	420	VAL	2.8
3	G	25	MET	2.8
1	B	489	ILE	2.8
3	N	227	ALA	2.8
3	N	129	LYS	2.8
3	N	139	GLY	2.7
1	J	406	PHE	2.7
3	N	171	TYR	2.7
2	E	390	ILE	2.7
3	G	230	THR	2.7
3	N	80	ALA	2.7
3	N	87	LYS	2.7
2	E	114	ALA	2.7
1	I	415	GLN	2.7
3	G	38	LEU	2.7
1	B	509	GLU	2.7
3	G	165	PHE	2.7
3	G	164	ARG	2.7
2	L	411	GLN	2.7
1	A	30	ARG	2.7
1	H	94	ILE	2.7
3	N	162	PHE	2.7
2	K	246	GLN	2.7
3	N	229	MET	2.6
1	I	479	LEU	2.6
3	G	36	ARG	2.6
3	N	170	SER	2.6
2	L	344	ILE	2.6
3	N	72	SER	2.6
3	N	163	ASN	2.6
1	B	392	LEU	2.6
1	H	415	GLN	2.6
3	G	170	SER	2.6
1	I	506	ALA	2.5
2	E	427	HIS	2.5
3	N	110	ASP	2.5
3	G	163	ASN	2.5
2	E	385	GLN	2.5
3	G	86	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	417	LEU	2.5
1	H	140	ILE	2.5
1	I	399	GLU	2.5
2	D	399	GLU	2.5
1	A	24	ASP	2.5
2	M	391	LEU	2.5
3	N	114	SER	2.5
1	B	475	GLN	2.4
2	E	300	LYS	2.4
2	L	395	GLU	2.4
3	G	75	ARG	2.4
3	G	166	ARG	2.4
1	J	193	THR	2.4
3	G	220	SER	2.4
3	N	35	GLU	2.4
3	N	223	SER	2.4
1	A	405	GLN	2.4
3	N	36	ARG	2.4
1	B	471	HIS	2.4
3	G	206	GLU	2.4
1	I	391	LYS	2.4
1	I	502	THR	2.4
1	I	421	GLY	2.4
3	G	27	ALA	2.4
3	G	47	GLY	2.4
3	G	107	GLY	2.4
3	G	44	TYR	2.4
3	N	206	GLU	2.4
3	G	28	ALA	2.3
1	B	455	LYS	2.3
2	E	317	LEU	2.3
2	E	423	VAL	2.3
1	I	483	ILE	2.3
2	D	388	ILE	2.3
2	E	425	THR	2.3
1	B	410	LEU	2.3
3	N	33	ARG	2.3
3	G	130	GLU	2.3
1	I	492	GLU	2.3
2	D	391	LEU	2.3
2	L	473	LEU	2.3
1	I	460	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	385	GLN	2.3
2	D	466	ALA	2.3
3	G	35	GLU	2.3
3	N	210	ALA	2.3
1	B	25	LEU	2.3
2	F	428	LEU	2.3
2	E	109	LYS	2.2
3	N	26	VAL	2.2
2	F	246	GLN	2.2
3	G	226	SER	2.2
3	N	81	ILE	2.2
2	K	475	GLU	2.2
1	I	469	LEU	2.2
2	E	386	ASP	2.2
1	I	491	GLU	2.2
1	I	455	LYS	2.2
3	N	138	PHE	2.2
1	C	17	LEU	2.2
3	N	225	GLN	2.2
1	I	36	ASP	2.2
2	E	402	LEU	2.2
2	E	193	GLY	2.2
3	G	207	TYR	2.2
3	N	115	ILE	2.2
1	B	35	GLY	2.2
2	E	453	PRO	2.2
1	B	30	ARG	2.2
2	E	12	ARG	2.2
2	E	472	LYS	2.1
1	I	501	VAL	2.1
2	L	398	GLU	2.1
1	H	25	LEU	2.1
1	J	17	LEU	2.1
2	M	12	ARG	2.1
1	A	93	ALA	2.1
2	K	472	LYS	2.1
2	D	473	LEU	2.1
3	G	171	TYR	2.1
2	D	384	LEU	2.1
2	E	445	LEU	2.1
2	L	383	SER	2.1
2	K	401	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	435	LYS	2.1
1	H	400	VAL	2.1
2	E	468	ALA	2.1
1	B	508	PHE	2.1
1	I	393	GLU	2.1
1	H	24	ASP	2.1
2	E	159	GLY	2.1
1	H	447	ALA	2.1
2	K	27	GLU	2.1
1	B	480	LEU	2.1
2	F	394	ASP	2.1
1	C	492	GLU	2.1
1	J	18	GLY	2.1
1	B	463	LYS	2.1
2	E	56	SER	2.0
3	G	88	GLN	2.0
1	B	473	ILE	2.0
1	I	25	LEU	2.0
2	L	410	ILE	2.0
1	B	413	ALA	2.0
1	I	30	ARG	2.0
2	L	406	ARG	2.0
1	I	505	LEU	2.0
1	I	194	ASP	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. 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( $\text{\AA}^2$ )	Q<0.9
8	AZI	D	1478	3/3	0.94	0.34	6.08	10,10,12,22	0
6	GOL	H	1514	6/6	0.92	0.32	5.87	36,45,46,53	0
6	GOL	B	1513	6/6	0.91	0.23	5.61	28,38,39,42	0
6	GOL	A	1514	6/6	0.88	0.35	5.09	32,38,46,54	0
6	GOL	C	1513	6/6	0.96	0.23	5.08	36,38,41,47	0
6	GOL	J	1513	6/6	0.91	0.23	3.81	31,33,37,37	0
6	GOL	A	1513	6/6	0.89	0.29	3.60	39,41,46,48	0
6	GOL	B	1512	6/6	0.96	0.22	3.44	20,23,24,31	0
10	QUE	N	1273[B]	22/22	0.86	0.23	3.33	49,51,51,51	22
10	QUE	N	1273[A]	22/22	0.86	0.23	3.23	34,42,44,45	22
6	GOL	K	1480	6/6	0.88	0.30	3.14	38,45,47,50	0
8	AZI	K	1478	3/3	0.95	0.24	3.09	6,6,12,18	0
10	QUE	G	1273[A]	22/22	0.89	0.21	2.06	37,41,43,43	22
10	QUE	G	1273[B]	22/22	0.89	0.21	1.99	65,65,66,66	22
6	GOL	H	1513	6/6	0.94	0.23	1.38	44,46,49,53	0
6	GOL	I	1512	6/6	0.94	0.16	0.58	19,27,28,37	0
9	PO4	L	1475	5/5	0.85	0.22	0.52	84,84,85,86	0
4	ANP	M	1475	31/31	0.97	0.16	0.41	18,25,30,33	0
6	GOL	D	1479	6/6	0.90	0.18	0.38	29,37,40,43	0
6	GOL	K	1479	6/6	0.90	0.17	0.31	38,41,44,49	0
4	ANP	I	1510	31/31	0.96	0.16	-0.38	20,37,44,52	0
9	PO4	E	1475	5/5	0.96	0.17	-0.48	70,70,71,71	0
7	ADP	D	1476	27/27	0.97	0.14	-0.67	13,25,29,29	0
7	ADP	K	1476	27/27	0.98	0.14	-0.77	20,26,29,30	0
4	ANP	J	1511	31/31	0.96	0.14	-0.86	14,26,28,30	0
4	ANP	A	1511	31/31	0.96	0.15	-0.93	18,25,32,33	0
4	ANP	C	1511	31/31	0.97	0.13	-1.37	18,24,32,34	0
5	MG	F	1476	1/1	0.95	0.12	-1.55	18,18,18,18	0
4	ANP	B	1510	31/31	0.95	0.14	-1.57	22,36,42,48	0
4	ANP	F	1475	31/31	0.98	0.13	-1.63	13,22,35,36	0
4	ANP	H	1511	31/31	0.96	0.13	-1.95	20,29,34,36	0
5	MG	K	1477	1/1	0.90	0.10	-2.86	22,22,22,22	0
5	MG	D	1477	1/1	0.97	0.09	-7.70	18,18,18,18	0
5	MG	M	1476	1/1	0.98	0.08	-8.29	16,16,16,16	0
5	MG	A	1512	1/1	0.95	0.06	-	28,28,28,28	0
5	MG	H	1512	1/1	0.95	0.04	-	25,25,25,25	0
5	MG	I	1511	1/1	0.98	0.16	-	29,29,29,29	0
5	MG	B	1511	1/1	0.92	0.12	-	29,29,29,29	0
5	MG	J	1512	1/1	0.97	0.07	-	18,18,18,18	0
5	MG	C	1512	1/1	0.96	0.12	-	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.