



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:18 AM BST

PDB ID : 3ZRY  
Title : Rotor architecture in the F(1)-c(10)-ring complex of the yeast F-ATP synthase  
Authors : Giraud, M.-F.; Dautant, A.  
Deposited on : 2011-06-21  
Resolution : 6.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

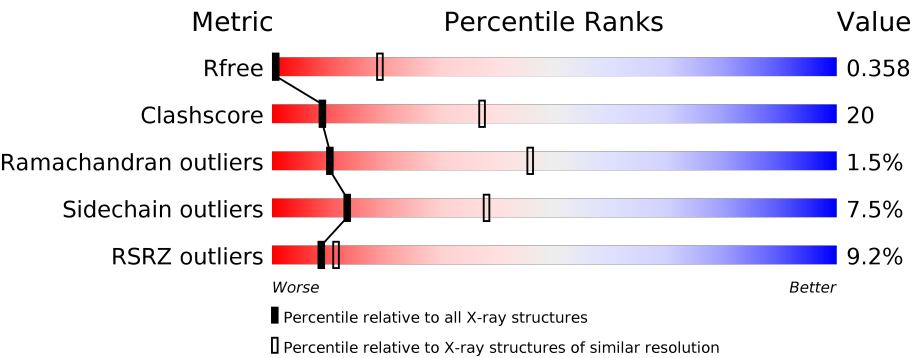
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)
RSRZ outliers	127900	1002 (9.00-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	510	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>63%30%5%</div></div>
1	B	510	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>57%33%5%5%</div></div>
1	C	510	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>64%30%5%</div></div>
2	D	478	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>69%27%..</div></div>
2	E	478	<div><div>10%</div><div><div></div><div></div><div></div><div></div></div><div>64%33%..</div></div>
2	F	478	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>60%37%..</div></div>

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Mol	Chain	Length	Quality of chain
3	G	278	
4	H	138	
5	I	61	
6	J	76	
6	K	76	
6	L	76	
6	M	76	
6	N	76	
6	O	76	
6	P	76	
6	Q	76	
6	R	76	
6	S	76	

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
7	ANP	A	600	X	-	-	-
7	ANP	B	600	X	-	-	-
7	ANP	C	600	X	-	-	X
7	ANP	D	600	X	-	-	-
7	ANP	F	600	X	-	X	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 30100 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, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	1
			3665	2314	649	699	3			
1	B	484	Total	C	N	O	S	0	0	1
			3670	2317	650	700	3			
1	C	485	Total	C	N	O	S	0	0	1
			3674	2319	651	701	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	SER	PRO	variant	UNP P07251
B	305	SER	PRO	variant	UNP P07251
C	305	SER	PRO	variant	UNP P07251

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	471	Total	C	N	O	S	0	0	1
			3550	2250	605	689	6			
2	E	469	Total	C	N	O	S	0	0	1
			3537	2243	603	685	6			
2	F	470	Total	C	N	O	S	0	0	1
			3544	2247	604	687	6			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	266	Total	C	N	O	S	0	0	1
			2022	1270	355	387	10			

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	119	Total	C	N	O	S	0	0	0
			747	468	132	145	2			

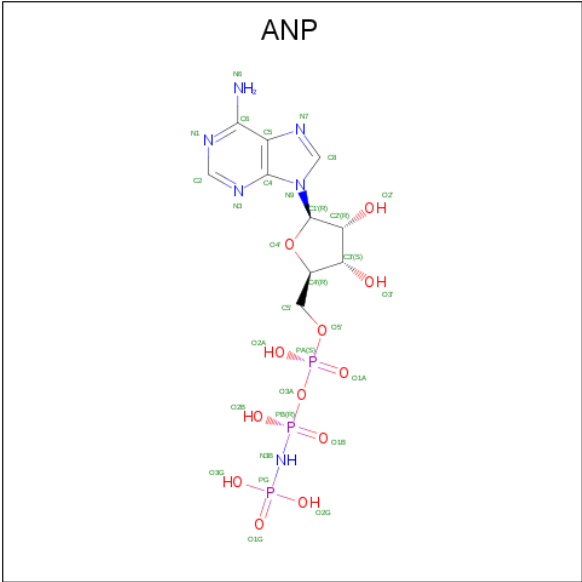
- Molecule 5 is a protein called ATP SYNTHASE CATALYTIC SECTOR F1 EPSILON SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	49	Total	C	N	O	S	0	0	1
			325	201	57	67				

- Molecule 6 is a protein called ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	73	Total	C	N	O	S	0	0	1
			515	343	81	88	3			
6	K	73	Total	C	N	O	S	0	0	1
			517	347	80	87	3			
6	L	72	Total	C	N	O	S	0	0	1
			507	337	80	87	3			
6	M	73	Total	C	N	O	S	0	0	1
			515	342	81	88	4			
6	N	73	Total	C	N	O	S	0	0	1
			515	342	81	88	4			
6	O	74	Total	C	N	O	S	0	0	1
			523	348	82	89	4			
6	P	75	Total	C	N	O	S	0	0	1
			534	357	83	90	4			
6	Q	75	Total	C	N	O	S	0	0	1
			534	357	83	90	4			
6	R	74	Total	C	N	O	S	0	0	1
			523	348	82	89	4			
6	S	74	Total	C	N	O	S	0	0	1
			523	348	82	89	4			

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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

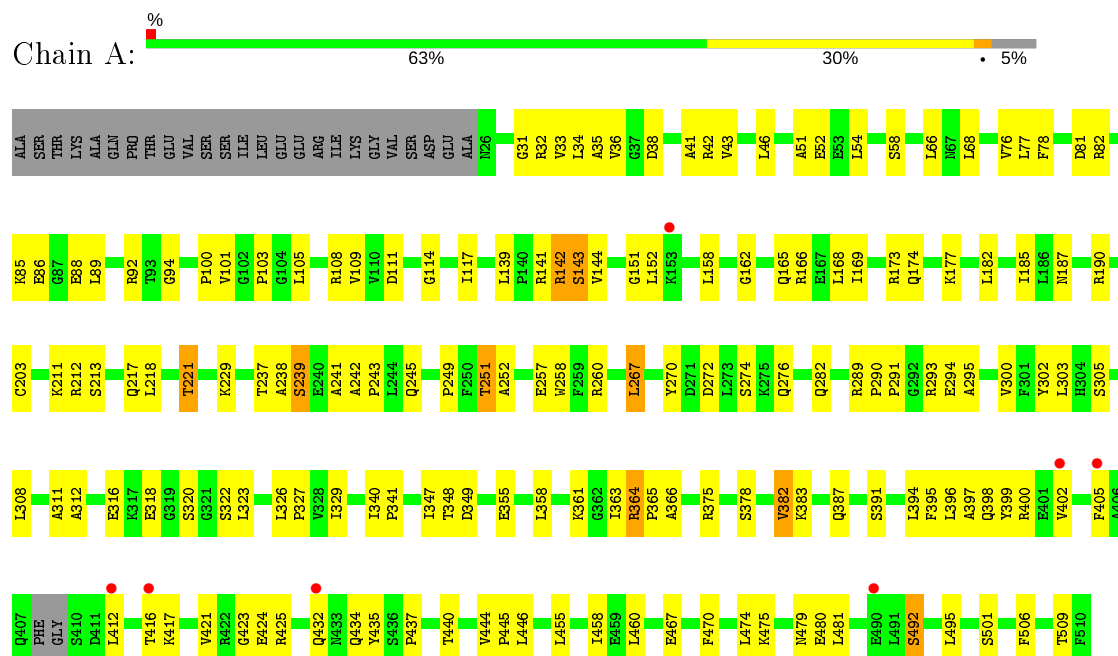
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mg	0	0
			1	1		
8	A	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		

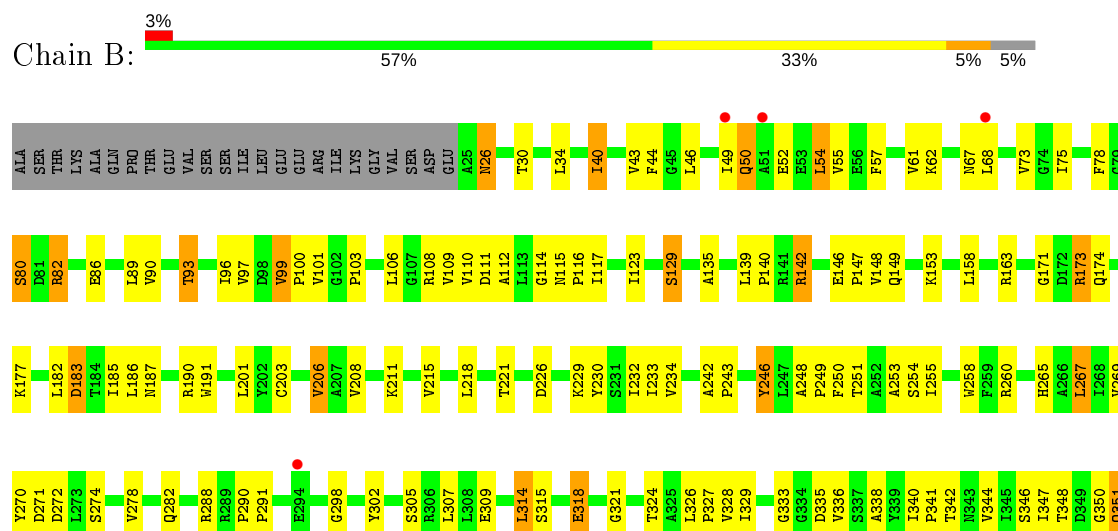
### 3 Residue-property plots

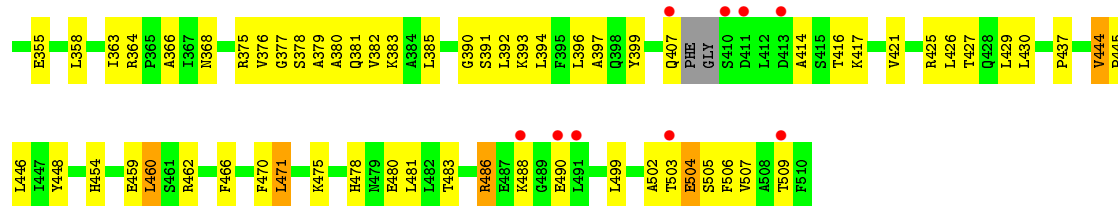
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

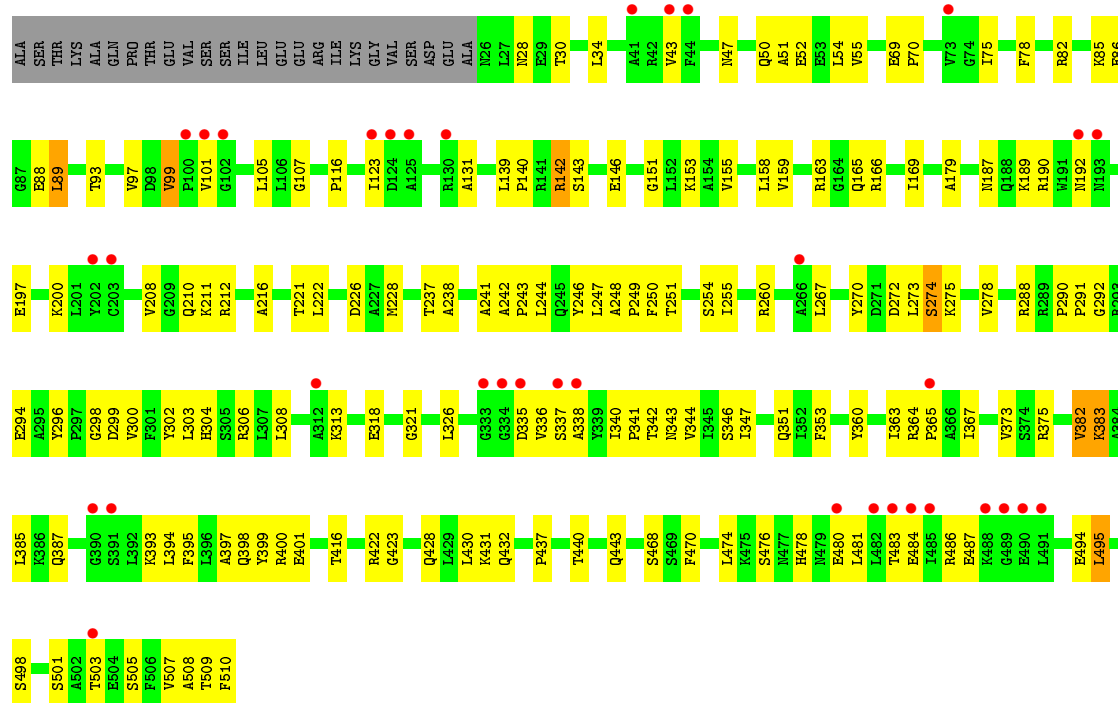


#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

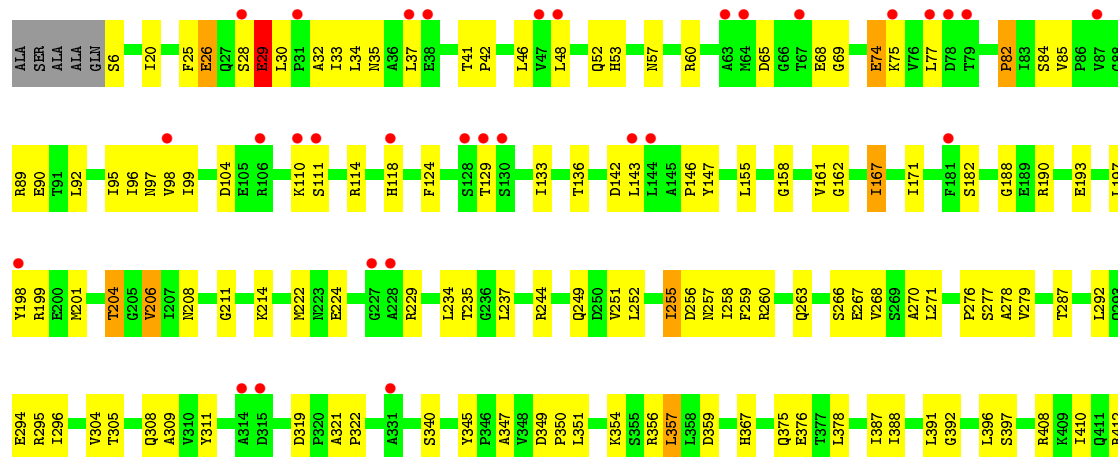




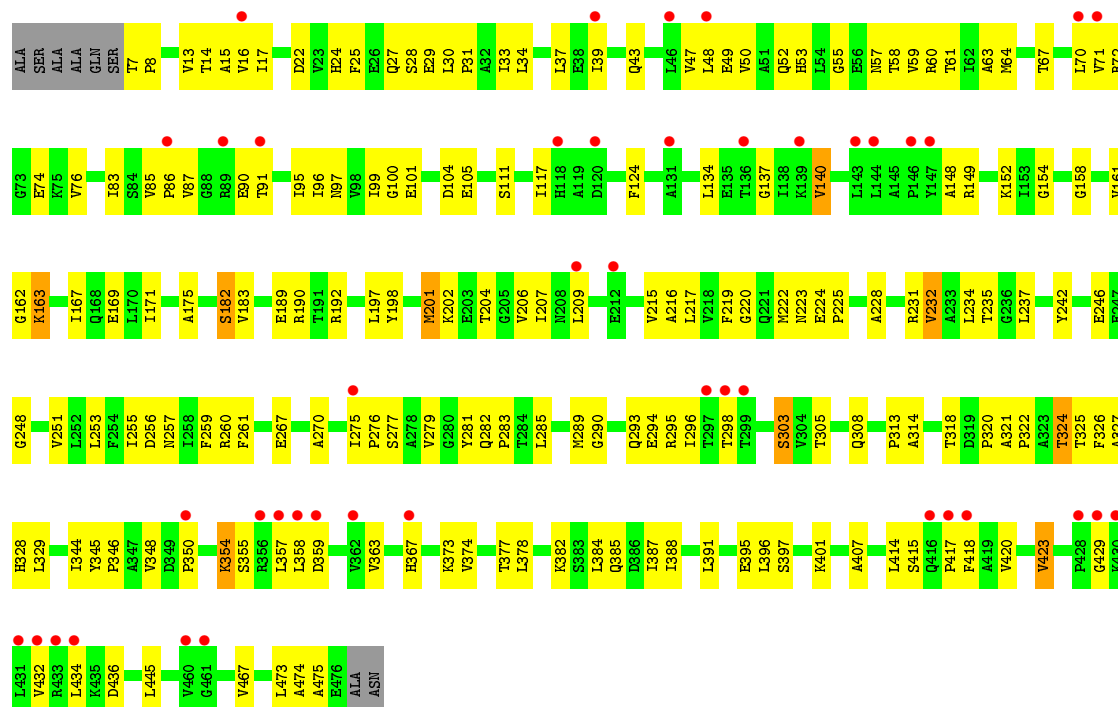
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL







Chain G:



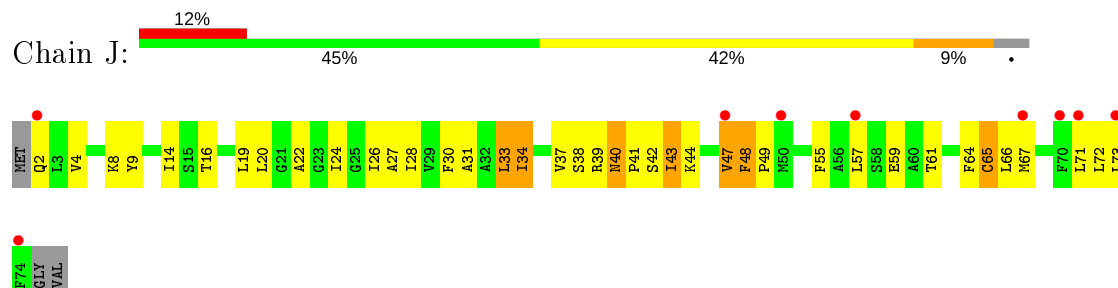
Chain H:



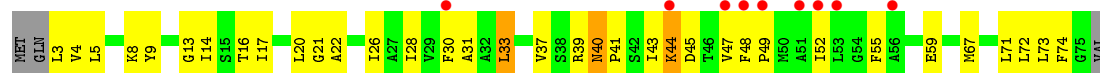
Chain I:



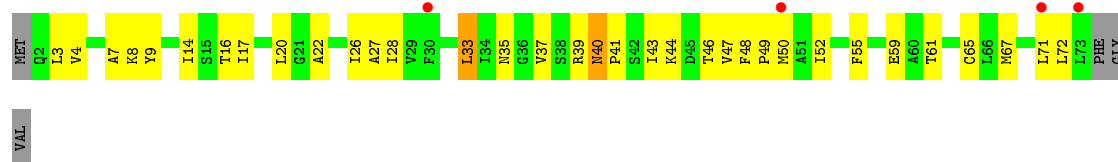
Chain J:



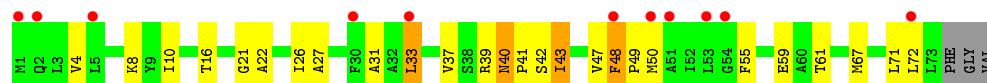
- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



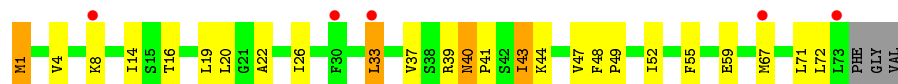
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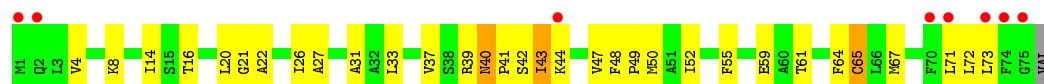
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- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

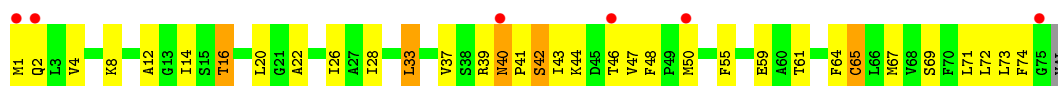


- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

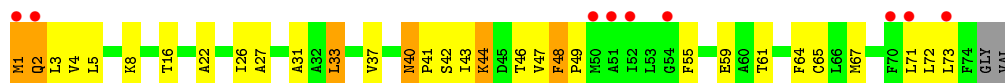


- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

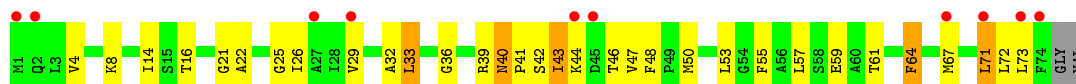




- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.69Å 174.91Å 164.26Å 90.00° 93.92° 90.00°	Depositor
Resolution (Å)	54.62 – 6.50 54.63 – 6.50	Depositor EDS
% Data completeness (in resolution range)	96.6 (54.62-6.50) 96.6 (54.63-6.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 6.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.317 , 0.339 0.307 , 0.358	Depositor DCC
$R_{free}$ test set	560 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	274.6	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 232.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.71	EDS
Total number of atoms	30100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	309.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: MG, 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	0.21	0/3719	0.46	0/5034
1	B	0.21	0/3724	0.46	0/5041
1	C	0.21	0/3729	0.47	0/5049
2	D	0.22	0/3606	0.47	0/4891
2	E	0.22	0/3593	0.46	1/4872 (0.0%)
2	F	0.21	0/3600	0.47	0/4883
3	G	0.24	0/2045	0.47	0/2752
4	H	0.22	0/755	0.47	0/1035
5	I	0.26	0/327	0.52	0/447
6	J	0.23	0/522	0.51	0/708
6	K	0.25	0/525	0.58	0/712
6	L	0.24	0/514	0.54	0/697
6	M	0.25	0/522	0.55	0/707
6	N	0.24	0/522	0.54	0/707
6	O	0.27	0/530	0.56	0/718
6	P	0.25	0/542	0.52	0/734
6	Q	0.25	0/542	0.51	0/734
6	R	0.25	0/530	0.54	0/718
6	S	0.27	0/530	0.61	0/718
All	All	0.22	0/30377	0.48	1/41157 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	391	LEU	CA-CB-CG	5.70	128.40	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	3665	0	3748	126	0
1	B	3670	0	3753	155	0
1	C	3674	0	3754	125	0
2	D	3550	0	3621	118	0
2	E	3537	0	3610	132	0
2	F	3544	0	3616	146	0
3	G	2022	0	2069	200	0
4	H	747	0	592	68	0
5	I	325	0	249	46	0
6	J	515	0	558	62	0
6	K	517	0	559	37	0
6	L	507	0	547	38	0
6	M	515	0	559	31	0
6	N	515	0	559	34	0
6	O	523	0	570	44	0
6	P	534	0	579	32	0
6	Q	534	0	579	37	0
6	R	523	0	570	35	0
6	S	523	0	570	51	0
7	A	31	0	13	1	0
7	B	31	0	13	2	0
7	C	31	0	13	5	0
7	D	31	0	13	6	0
7	F	31	0	13	10	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
All	All	30100	0	30727	1232	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 20.

All (1232) 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)
6:M:40:ASN:HB3	6:M:41:PRO:HA	1.20	1.15
1:C:291:PRO:HD2	3:G:273:GLY:CA	1.76	1.15
1:C:509:THR:HG23	1:C:510:PHE:N	1.54	1.14
2:E:390:ILE:HG21	3:G:28:SER:CB	1.76	1.14
3:G:191:SER:HB2	3:G:194:PHE:CB	1.77	1.12
1:C:291:PRO:CD	3:G:273:GLY:HA2	1.83	1.09
6:K:48:PHE:CZ	6:K:52:ILE:HD11	1.89	1.08
3:G:128:LEU:HD11	5:I:44:TYR:HB2	1.35	1.08
4:H:42:LEU:HB2	6:O:41:PRO:HG3	1.34	1.06
3:G:151:LEU:HD22	3:G:211:GLU:HG2	1.33	1.06
3:G:54:ASN:O	3:G:193:SER:HB2	1.55	1.05
2:E:391:LEU:HD23	3:G:32:SER:OG	1.57	1.05
4:H:42:LEU:CB	6:O:41:PRO:HG3	1.87	1.04
3:G:131:ASN:OD1	5:I:43:PHE:HB2	1.58	1.04
3:G:141:GLN:HG3	5:I:19:GLN:HE22	1.19	1.03
5:I:10:TYR:HA	5:I:13:TYR:HB2	1.38	1.03
6:Q:71:LEU:HD23	6:R:73:LEU:HD11	1.40	1.02
2:E:390:ILE:HD13	3:G:28:SER:HB2	1.43	1.00
2:F:7:THR:HB	2:F:8:PRO:HD2	1.43	0.99
6:S:40:ASN:HB3	6:S:41:PRO:HA	1.43	0.99
3:G:129:SER:O	5:I:44:TYR:HA	1.61	0.99
3:G:147:ALA:CB	3:G:215:ALA:HB2	1.94	0.97
6:Q:1:MET:N	6:R:2:GLN:HE22	1.62	0.97
2:E:390:ILE:HG21	3:G:28:SER:HB3	1.44	0.96
3:G:151:LEU:HD23	3:G:156:ALA:HB3	1.46	0.96
2:E:390:ILE:HG21	3:G:28:SER:HB2	1.47	0.95
4:H:29:GLN:HB2	4:H:42:LEU:HD11	1.43	0.95
3:G:185:ALA:HB1	3:G:206:PRO:HB2	1.49	0.92
6:M:50:MET:SD	6:N:33:LEU:HD11	2.10	0.92
6:Q:1:MET:H2	6:R:2:GLN:HE22	0.94	0.91
3:G:96:ARG:HE	3:G:121:THR:HG21	1.34	0.91
6:J:33:LEU:HD11	6:S:50:MET:SD	2.11	0.90
1:C:509:THR:CG2	1:C:510:PHE:N	2.30	0.88
6:J:19:LEU:HB3	6:S:61:THR:HG23	1.52	0.88
4:H:42:LEU:HD13	6:O:41:PRO:HG2	1.55	0.87
1:B:444:VAL:HG23	1:B:445:PRO:HD3	1.56	0.87
2:F:162:GLY:HA3	7:F:600:ANP:H8	1.57	0.87
3:G:130:ILE:HA	5:I:43:PHE:O	1.73	0.87
1:B:109:VAL:HG22	1:B:233:ILE:HB	1.56	0.87
1:C:508:ALA:O	1:C:509:THR:HG22	1.73	0.87
3:G:128:LEU:CD1	5:I:44:TYR:HB2	2.05	0.86
3:G:84:CYS:HB3	3:G:233:ARG:NH2	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:43:ILE:HD13	6:S:46:THR:HG23	1.57	0.86
3:G:55:ALA:O	3:G:192:PRO:HD2	1.75	0.86
1:B:407:GLN:HB3	3:G:239:ASN:OD1	1.75	0.85
1:C:291:PRO:HG2	3:G:272:THR:OG1	1.76	0.85
1:A:151:GLY:HA3	1:A:437:PRO:HB2	1.59	0.85
3:G:23:MET:HB3	3:G:237:MET:HG3	1.55	0.85
1:B:381:GLN:HG2	1:B:382:VAL:H	1.39	0.85
2:D:29:GLU:O	2:D:29:GLU:HG2	1.76	0.84
1:B:290:PRO:HD2	2:F:270:ALA:HB1	1.60	0.84
3:G:188:ILE:HD13	3:G:209:LEU:HD23	1.56	0.84
6:Q:73:LEU:O	6:Q:74:PHE:CD1	2.30	0.84
1:B:67:ASN:HB2	2:F:17:ILE:HG12	1.60	0.84
6:N:39:ARG:HH22	6:O:39:ARG:CG	1.92	0.82
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.60	0.82
3:G:141:GLN:HG3	5:I:19:GLN:NE2	1.92	0.82
6:Q:1:MET:H2	6:R:2:GLN:NE2	1.78	0.82
3:G:131:ASN:O	5:I:42:ALA:HA	1.79	0.82
1:C:142:ARG:HG2	1:C:143:SER:N	1.95	0.81
1:C:51:ALA:HB3	2:D:68:GLU:HA	1.63	0.81
3:G:96:ARG:NE	3:G:121:THR:HG21	1.95	0.81
3:G:140:PHE:HE2	3:G:216:ASN:HD21	1.26	0.81
6:J:40:ASN:HB3	6:J:41:PRO:HA	1.61	0.81
6:M:40:ASN:HB3	6:M:41:PRO:CA	2.03	0.81
3:G:151:LEU:CD2	3:G:211:GLU:HG2	2.10	0.81
2:E:20:ILE:HD11	2:E:271:LEU:HB3	1.60	0.80
3:G:54:ASN:CB	3:G:197:PHE:HE1	1.94	0.80
1:B:190:ARG:HH12	1:B:437:PRO:HB2	1.45	0.80
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.64	0.80
3:G:139:THR:HG21	5:I:37:ARG:HA	1.63	0.79
2:D:224:GLU:O	2:D:229:ARG:HD3	1.83	0.79
3:G:208:ASP:HB3	5:I:10:TYR:CD2	2.18	0.79
3:G:55:ALA:HB1	3:G:191:SER:CB	2.12	0.79
1:C:267:LEU:HD11	1:C:326:LEU:HD12	1.63	0.78
3:G:127:LYS:O	5:I:46:GLN:HA	1.82	0.78
2:F:162:GLY:CA	7:F:600:ANP:H8	2.14	0.78
6:N:40:ASN:HB3	6:N:41:PRO:HA	1.65	0.78
1:A:405:PHE:CE1	3:G:22:THR:HG23	2.18	0.78
6:L:48:PHE:CE2	6:L:52:ILE:HD11	2.19	0.78
1:C:288:ARG:O	3:G:276:SER:HB3	1.84	0.78
6:O:40:ASN:HB3	6:O:41:PRO:HA	1.65	0.78
4:H:31:ASN:HB3	4:H:38:ARG:HH21	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:42:LEU:HD13	6:O:41:PRO:CG	2.14	0.78
1:B:335:ASP:HB2	3:G:257:ARG:NH1	1.99	0.77
1:A:305:SER:HB2	2:E:222:MET:HB3	1.64	0.77
4:H:37:GLY:H	6:Q:39:ARG:HH21	1.32	0.77
6:N:39:ARG:HH22	6:O:39:ARG:HG3	1.48	0.77
2:E:390:ILE:HD11	3:G:25:ILE:HG23	1.67	0.77
4:H:46:VAL:HG11	6:N:39:ARG:HB3	1.65	0.76
6:L:40:ASN:HB3	6:L:41:PRO:HA	1.68	0.76
6:P:40:ASN:HB3	6:P:41:PRO:HA	1.67	0.76
6:O:40:ASN:CB	6:O:41:PRO:HA	2.15	0.76
2:F:182:SER:HB3	2:F:215:VAL:HG23	1.68	0.76
6:N:48:PHE:CZ	6:N:52:ILE:HD11	2.20	0.76
5:I:9:SER:O	5:I:13:TYR:CA	2.33	0.76
3:G:55:ALA:HB1	3:G:191:SER:HB3	1.68	0.75
6:R:40:ASN:HB3	6:R:41:PRO:HA	1.67	0.75
3:G:55:ALA:HB1	3:G:191:SER:OG	1.85	0.75
2:E:168:GLN:HA	2:E:171:ILE:HD12	1.68	0.75
6:M:37:VAL:HG13	6:M:43:ILE:HG22	1.69	0.75
4:H:42:LEU:CB	6:O:41:PRO:CG	2.64	0.75
6:J:40:ASN:CB	6:J:41:PRO:HA	2.17	0.74
1:B:376:VAL:HG11	2:F:192:ARG:HD2	1.69	0.74
1:C:299:ASP:HB3	2:D:267:GLU:HB3	1.68	0.74
2:D:345:TYR:HB3	7:D:600:ANP:N6	2.03	0.74
2:E:148:ALA:HB3	2:E:151:GLY:HA3	1.67	0.74
1:B:50:GLN:OE1	1:B:96:ILE:HD11	1.87	0.74
3:G:130:ILE:CG2	5:I:42:ALA:HB1	2.17	0.74
4:H:37:GLY:N	6:Q:39:ARG:HH21	1.86	0.74
6:S:40:ASN:HB3	6:S:41:PRO:CA	2.15	0.74
6:K:40:ASN:HB3	6:K:41:PRO:HA	1.70	0.74
1:B:335:ASP:OD2	3:G:257:ARG:HD3	1.88	0.73
5:I:9:SER:O	5:I:13:TYR:N	2.21	0.73
1:C:142:ARG:HG2	1:C:143:SER:H	1.52	0.73
1:C:365:PRO:HB2	1:C:367:ILE:HG13	1.71	0.73
6:N:40:ASN:CB	6:N:41:PRO:HA	2.18	0.73
6:O:8:LYS:HG2	6:O:72:LEU:O	1.88	0.73
6:J:43:ILE:CD1	6:S:46:THR:HG23	2.17	0.73
1:B:68:LEU:O	2:F:15:ALA:HA	1.88	0.72
2:F:52:GLN:HE21	2:F:60:ARG:HD2	1.53	0.72
2:F:391:LEU:HD22	2:F:395:GLU:HG3	1.70	0.72
3:G:95:VAL:O	3:G:99:LEU:HB2	1.89	0.72
3:G:143:SER:OG	3:G:219:LEU:HB2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:LEU:HD23	1:B:444:VAL:HG13	1.70	0.72
3:G:211:GLU:O	5:I:11:ALA:HB2	1.89	0.72
3:G:54:ASN:CB	3:G:197:PHE:CE1	2.72	0.72
3:G:182:ILE:HD11	3:G:217:GLN:HB2	1.72	0.71
2:F:189:GLU:O	2:F:222:MET:HG2	1.91	0.71
3:G:151:LEU:HD22	3:G:211:GLU:CG	2.15	0.71
6:K:21:GLY:HA3	6:L:20:LEU:HA	1.73	0.71
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.73	0.71
2:F:7:THR:HB	2:F:8:PRO:CD	2.20	0.71
1:C:291:PRO:HD2	3:G:273:GLY:HA2	0.87	0.71
6:S:40:ASN:CB	6:S:41:PRO:HA	2.21	0.71
2:F:33:ILE:O	2:F:34:LEU:HB2	1.90	0.70
2:F:345:TYR:HB3	7:F:600:ANP:N6	2.07	0.70
6:J:27:ALA:HA	6:S:29:VAL:CG2	2.20	0.70
1:C:97:VAL:HG11	1:C:247:LEU:HD21	1.74	0.70
6:J:55:PHE:CE1	6:S:57:LEU:HD13	2.27	0.70
6:N:43:ILE:HG23	6:N:44:LYS:H	1.55	0.70
1:B:333:GLY:O	3:G:253:ILE:HD13	1.92	0.70
1:C:290:PRO:HG3	3:G:276:SER:HB2	1.75	0.69
1:B:407:GLN:C	3:G:239:ASN:ND2	2.46	0.69
1:C:151:GLY:O	1:C:437:PRO:HA	1.92	0.69
6:R:40:ASN:CB	6:R:41:PRO:HA	2.23	0.69
2:F:388:ILE:HD12	2:F:396:LEU:HD11	1.72	0.69
3:G:147:ALA:HB2	3:G:215:ALA:HB2	1.72	0.69
6:O:40:ASN:HB3	6:O:41:PRO:CA	2.22	0.69
2:E:384:LEU:O	2:E:388:ILE:HG12	1.92	0.69
3:G:51:PHE:CD1	4:H:49:VAL:HG11	2.28	0.69
1:A:211:LYS:HE3	1:A:213:SER:OG	1.92	0.69
3:G:188:ILE:CD1	3:G:209:LEU:HD23	2.22	0.69
6:J:40:ASN:HB3	6:J:41:PRO:CA	2.23	0.69
6:L:40:ASN:CB	6:L:41:PRO:HA	2.23	0.69
6:Q:1:MET:N	6:R:2:GLN:NE2	2.38	0.69
6:P:40:ASN:CB	6:P:41:PRO:HA	2.22	0.68
1:B:425:ARG:HD3	1:B:460:LEU:HD13	1.74	0.68
1:C:179:ALA:CB	7:C:600:ANP:H8	2.23	0.68
1:B:381:GLN:HG2	1:B:382:VAL:N	2.06	0.68
2:D:133:ILE:HD11	2:D:146:PRO:HB2	1.74	0.68
2:D:142:ASP:HB3	2:D:434:LEU:HD12	1.75	0.68
3:G:43:LYS:NZ	4:H:12:LEU:O	2.25	0.68
6:J:42:SER:O	6:J:47:VAL:HG13	1.94	0.68
6:Q:69:SER:O	6:Q:73:LEU:HD12	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:97:ASN:HB2	2:F:101:GLU:H	1.59	0.68
2:D:162:GLY:HA2	7:D:600:ANP:H8	1.76	0.68
4:H:12:LEU:N	4:H:23:SER:HA	2.09	0.68
3:G:151:LEU:HD13	3:G:211:GLU:OE1	1.94	0.68
6:L:50:MET:SD	6:M:48:PHE:HE1	2.17	0.68
1:C:169:ILE:HD11	1:C:326:LEU:HD22	1.75	0.67
1:C:274:SER:O	1:C:278:VAL:HG23	1.95	0.67
6:K:40:ASN:CB	6:K:41:PRO:HA	2.24	0.67
6:Q:42:SER:HB2	6:Q:47:VAL:HG23	1.75	0.67
2:F:53:HIS:CD2	2:F:59:VAL:HG12	2.30	0.67
6:J:72:LEU:HD21	6:K:73:LEU:HD21	1.76	0.67
6:J:27:ALA:HA	6:S:29:VAL:HG22	1.77	0.67
2:D:33:ILE:HG22	2:D:34:LEU:HG	1.77	0.67
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.76	0.67
3:G:141:GLN:CG	5:I:19:GLN:HE22	2.03	0.67
6:P:43:ILE:HG23	6:P:44:LYS:H	1.58	0.67
2:E:139:LYS:HE2	2:E:432:VAL:HG21	1.76	0.66
2:F:384:LEU:O	2:F:388:ILE:HG12	1.95	0.66
2:D:197:LEU:O	2:D:201:MET:HG2	1.95	0.66
2:F:202:LYS:HE3	2:F:209:LEU:HD11	1.77	0.66
6:J:57:LEU:HD12	6:K:30:PHE:CZ	2.30	0.66
1:A:506:PHE:HA	1:A:509:THR:HG22	1.78	0.66
3:G:268:VAL:O	3:G:272:THR:HG23	1.95	0.66
3:G:54:ASN:O	3:G:193:SER:CB	2.39	0.66
6:P:48:PHE:CE2	6:P:52:ILE:HD11	2.30	0.66
1:B:272:ASP:HB2	1:B:328:VAL:O	1.96	0.66
4:H:42:LEU:HB3	6:O:41:PRO:HG3	1.76	0.66
1:A:185:ILE:HG12	1:A:203:CYS:SG	2.35	0.66
3:G:208:ASP:HB3	5:I:10:TYR:CE2	2.29	0.66
1:A:425:ARG:HG3	1:A:460:LEU:HD12	1.78	0.66
1:B:338:ALA:HB3	1:B:341:PRO:HG2	1.77	0.66
6:J:43:ILE:CG1	6:S:46:THR:HG23	2.25	0.66
1:B:242:ALA:HB2	1:B:282:GLN:NE2	2.11	0.66
2:F:137:GLY:HA2	2:F:432:VAL:O	1.96	0.66
4:H:46:VAL:HG12	6:N:39:ARG:O	1.96	0.65
1:B:206:VAL:HG23	1:B:269:VAL:O	1.96	0.65
4:H:29:GLN:HB2	4:H:42:LEU:CD1	2.24	0.65
2:E:391:LEU:HB3	2:E:395:GLU:HG3	1.78	0.65
6:S:43:ILE:HG23	6:S:44:LYS:H	1.61	0.65
3:G:151:LEU:HD11	5:I:11:ALA:HB2	1.77	0.65
1:A:182:LEU:HD23	1:A:435:TYR:HE1	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:127:LYS:O	5:I:46:GLN:HG3	1.96	0.65
3:G:185:ALA:O	3:G:187:THR:N	2.30	0.65
6:M:37:VAL:CG1	6:M:43:ILE:HG22	2.27	0.65
6:N:40:ASN:HB3	6:N:41:PRO:CA	2.26	0.65
5:I:9:SER:OG	5:I:10:TYR:N	2.30	0.65
6:K:14:ILE:HG21	6:L:14:ILE:HD13	1.79	0.64
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.78	0.64
4:H:88:ILE:HG22	4:H:89:GLU:HG2	1.78	0.64
6:K:48:PHE:CE1	6:K:52:ILE:HD11	2.32	0.64
2:D:98:VAL:HG13	2:D:99:ILE:HG23	1.79	0.64
3:G:162:ILE:HD13	3:G:210:PHE:CE1	2.31	0.64
1:C:483:THR:HG23	1:C:486:ARG:NH2	2.12	0.64
3:G:147:ALA:HB3	3:G:215:ALA:HB2	1.77	0.64
6:J:39:ARG:HD2	6:S:39:ARG:HH21	1.62	0.64
1:A:444:VAL:HG22	1:A:445:PRO:HD3	1.78	0.64
1:C:69:GLU:HB3	1:C:70:PRO:CD	2.27	0.64
1:B:67:ASN:HB2	2:F:17:ILE:CG1	2.27	0.64
2:E:390:ILE:CD1	3:G:25:ILE:HA	2.28	0.64
6:J:26:ILE:HD12	6:J:55:PHE:HD1	1.61	0.64
2:D:34:LEU:O	2:D:82:PRO:HA	1.97	0.64
2:E:241:GLU:OE2	2:E:295:ARG:HB3	1.97	0.64
2:F:48:LEU:HD23	2:F:63:ALA:HA	1.78	0.64
6:L:46:THR:CG2	6:M:43:ILE:HG21	2.27	0.64
2:E:243:PHE:HB2	2:E:251:VAL:HG21	1.80	0.64
2:F:197:LEU:O	2:F:201:MET:HG2	1.98	0.64
1:C:294:GLU:N	3:G:269:ASP:OD2	2.31	0.64
2:E:220:GLY:HA3	2:E:232:VAL:HG11	1.80	0.64
3:G:185:ALA:O	3:G:186:LYS:C	2.34	0.64
3:G:185:ALA:CB	3:G:206:PRO:HB2	2.24	0.64
6:J:55:PHE:CD1	6:S:57:LEU:HD13	2.33	0.64
2:D:351:LEU:HD23	2:D:375:GLN:HG2	1.80	0.63
6:L:40:ASN:HB3	6:L:41:PRO:CA	2.28	0.63
3:G:55:ALA:CB	3:G:191:SER:HB3	2.27	0.63
1:A:168:LEU:HB2	1:A:348:THR:HG21	1.80	0.63
1:C:290:PRO:CG	3:G:276:SER:HB2	2.29	0.63
2:D:340:SER:HB3	2:D:347:ALA:HB2	1.80	0.63
3:G:150:LEU:HD23	3:G:214:LEU:HD21	1.79	0.63
6:P:40:ASN:HB3	6:P:41:PRO:CA	2.27	0.63
1:A:35:ALA:HB3	1:A:42:ARG:NH1	2.13	0.63
1:A:282:GLN:OE1	2:D:287:THR:HG23	1.99	0.63
1:A:475:LYS:O	1:A:479:ASN:HB2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:222:MET:HA	2:D:229:ARG:HD2	1.80	0.63
2:F:158:GLY:O	2:F:161:VAL:HG22	1.98	0.63
6:O:42:SER:O	6:O:47:VAL:HB	1.99	0.63
1:A:143:SER:OG	2:E:199:ARG:NH2	2.32	0.63
1:C:241:ALA:HB3	1:C:244:LEU:HD12	1.80	0.63
6:K:40:ASN:HB3	6:K:41:PRO:CA	2.28	0.63
3:G:180:LYS:HZ1	3:G:220:THR:HB	1.64	0.62
1:C:290:PRO:HB2	2:D:270:ALA:HB1	1.79	0.62
2:E:391:LEU:HD13	2:E:395:GLU:HG3	1.82	0.62
1:B:290:PRO:HD2	2:F:270:ALA:CB	2.27	0.62
3:G:128:LEU:HD11	5:I:44:TYR:CB	2.20	0.62
4:H:29:GLN:HG2	4:H:60:MET:HG3	1.81	0.62
1:B:135:ALA:HB3	2:F:223:ASN:HD22	1.65	0.62
1:C:375:ARG:HD3	7:D:600:ANP:H5'2	1.81	0.62
1:B:329:ILE:HD11	1:B:344:VAL:HG21	1.81	0.62
1:A:166:ARG:HD3	1:A:308:LEU:O	1.99	0.62
1:B:269:VAL:HG22	1:B:326:LEU:HB2	1.81	0.62
2:E:98:VAL:HG13	2:E:99:ILE:HG23	1.80	0.62
3:G:184:ASN:HA	3:G:210:PHE:CD1	2.35	0.62
1:C:50:GLN:HG2	2:D:69:GLY:HA2	1.82	0.62
2:D:244:ARG:HD3	2:D:304:VAL:CG2	2.29	0.62
1:C:363:ILE:HG12	1:C:431:LYS:HE2	1.81	0.62
3:G:147:ALA:HB2	3:G:215:ALA:CB	2.30	0.62
2:E:166:PHE:HE1	2:E:170:LEU:HD11	1.65	0.62
3:G:173:LEU:HD23	3:G:235:ASN:OD1	1.99	0.62
1:A:316:GLU:HA	1:A:320:SER:OG	2.00	0.61
1:B:342:THR:HG21	2:F:314:ALA:HA	1.82	0.61
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.81	0.61
3:G:108:VAL:HG22	3:G:128:LEU:HB3	1.82	0.61
2:E:390:ILE:HD11	3:G:25:ILE:CA	2.30	0.61
6:O:50:MET:SD	6:P:33:LEU:HD11	2.40	0.61
1:A:151:GLY:HA3	1:A:437:PRO:CB	2.29	0.61
1:A:82:ARG:HG3	2:D:32:ALA:HB1	1.82	0.61
1:B:173:ARG:NH2	2:E:326:PHE:HD2	1.98	0.61
2:E:142:ASP:HB3	2:E:434:LEU:HD13	1.83	0.61
1:A:405:PHE:CZ	3:G:22:THR:HG23	2.36	0.61
2:E:390:ILE:HD11	3:G:25:ILE:HA	1.82	0.61
1:B:158:LEU:HD22	1:B:393:LYS:HD2	1.81	0.61
1:B:358:LEU:HB2	1:B:366:ALA:HB1	1.83	0.60
1:C:116:PRO:HD3	1:C:123:ILE:HG12	1.83	0.60
1:A:139:LEU:HD22	2:E:104:ASP:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:191:SER:CB	3:G:194:PHE:CB	2.68	0.60
4:H:46:VAL:CG1	6:N:39:ARG:HB3	2.32	0.60
6:R:40:ASN:HB3	6:R:41:PRO:CA	2.27	0.60
1:A:212:ARG:HG2	1:A:237:THR:HG21	1.83	0.60
3:G:150:LEU:HD22	3:G:218:MET:CE	2.30	0.60
1:C:494:GLU:H	1:C:494:GLU:CD	2.04	0.60
3:G:52:TYR:CD2	3:G:183:PHE:HD2	2.17	0.60
4:H:28:THR:O	4:H:42:LEU:HG	2.02	0.60
3:G:147:ALA:O	3:G:151:LEU:HG	2.02	0.60
3:G:147:ALA:HB2	3:G:215:ALA:CA	2.32	0.60
4:H:29:GLN:HA	4:H:42:LEU:HG	1.84	0.60
6:Q:73:LEU:O	6:Q:74:PHE:CG	2.54	0.60
2:D:391:LEU:CD2	3:G:83:LEU:HD11	2.31	0.60
2:E:423:VAL:HG23	2:E:424:PHE:HD1	1.67	0.60
2:E:390:ILE:CG2	3:G:28:SER:HB3	2.27	0.60
1:A:166:ARG:NH2	2:E:190:ARG:HD3	2.16	0.60
1:C:272:ASP:OD1	1:C:275:LYS:HD2	2.02	0.60
2:D:95:ILE:HD12	2:D:104:ASP:HB3	1.84	0.60
2:E:39:ILE:HD11	2:E:48:LEU:HD11	1.83	0.60
3:G:140:PHE:HA	3:G:219:LEU:HD12	1.84	0.60
1:C:290:PRO:HG3	3:G:277:LEU:N	2.16	0.59
1:C:336:VAL:HG11	1:C:353:PHE:CE1	2.37	0.59
2:F:255:ILE:HD12	2:F:308:GLN:HG2	1.84	0.59
1:A:349:ASP:HA	1:A:375:ARG:HD3	1.84	0.59
1:B:182:LEU:HA	1:B:185:ILE:HD12	1.83	0.59
1:C:260:ARG:O	1:C:321:GLY:HA3	2.01	0.59
6:J:14:ILE:HD13	6:S:14:ILE:HG21	1.83	0.59
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.83	0.59
3:G:205:VAL:HG13	3:G:206:PRO:HD3	1.84	0.59
1:B:290:PRO:HB3	2:F:276:PRO:HG3	1.84	0.59
4:H:42:LEU:HB3	6:O:41:PRO:CG	2.31	0.59
1:C:222:LEU:HB3	1:C:228:MET:HG2	1.84	0.59
1:C:290:PRO:CA	3:G:276:SER:HB2	2.33	0.59
1:B:67:ASN:CB	2:F:17:ILE:HG12	2.30	0.59
6:J:20:LEU:HG	6:S:21:GLY:CA	2.33	0.59
1:C:212:ARG:HG3	1:C:237:THR:HG21	1.85	0.59
2:F:152:LYS:NZ	2:F:293:GLN:HG3	2.18	0.59
6:J:14:ILE:HG22	6:K:13:GLY:O	2.03	0.59
1:C:248:ALA:HB3	1:C:249:PRO:HD3	1.85	0.59
2:F:134:LEU:HB2	2:F:149:ARG:HG2	1.85	0.59
3:G:47:ALA:HB3	4:H:86:THR:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:GLU:HB2	2:D:111:SER:HB3	1.85	0.59
1:A:361:LYS:O	2:D:376:GLU:HG2	2.03	0.59
3:G:151:LEU:HD21	3:G:211:GLU:HA	1.85	0.59
6:N:39:ARG:NH2	6:O:39:ARG:HG3	2.18	0.59
6:L:46:THR:HG23	6:M:43:ILE:HG21	1.85	0.58
1:B:270:TYR:CE1	1:B:307:LEU:HD21	2.39	0.58
2:E:30:LEU:HD21	2:E:57:ASN:HA	1.84	0.58
2:F:162:GLY:HA3	7:F:600:ANP:C8	2.32	0.58
2:E:166:PHE:CE1	2:E:170:LEU:HD11	2.38	0.58
1:B:173:ARG:HG2	1:B:174:GLN:HG2	1.85	0.58
1:B:185:ILE:HG23	1:B:203:CYS:SG	2.44	0.58
6:K:20:LEU:HD22	6:L:20:LEU:HD11	1.84	0.58
6:N:37:VAL:HG11	6:N:43:ILE:HD13	1.85	0.58
1:B:375:ARG:NH1	2:F:190:ARG:NH2	2.51	0.58
2:D:279:VAL:HG12	2:D:279:VAL:O	2.04	0.58
3:G:185:ALA:O	3:G:188:ILE:N	2.30	0.58
1:A:51:ALA:O	1:A:52:GLU:HB2	2.03	0.58
1:C:55:VAL:HG21	1:C:75:ILE:HD13	1.84	0.58
3:G:77:ILE:CG2	3:G:222:MET:HG2	2.34	0.58
1:B:55:VAL:HG21	1:B:75:ILE:HD13	1.84	0.58
2:E:33:ILE:O	2:E:34:LEU:HB2	2.03	0.58
2:E:102:PRO:HG3	2:E:108:PRO:HA	1.86	0.57
1:B:335:ASP:CB	3:G:257:ARG:NH1	2.67	0.57
1:A:383:LYS:O	1:A:387:GLN:HG3	2.03	0.57
1:B:267:LEU:HD12	1:B:324:THR:HB	1.87	0.57
1:C:375:ARG:HD3	7:D:600:ANP:C5'	2.34	0.57
4:H:14:PHE:CD1	4:H:85:VAL:HG23	2.38	0.57
4:H:29:GLN:O	4:H:60:MET:HB2	2.04	0.57
1:A:143:SER:N	2:E:199:ARG:HH12	2.02	0.57
1:A:364:ARG:HA	1:A:365:PRO:C	2.25	0.57
3:G:47:ALA:HB3	4:H:86:THR:CG2	2.34	0.57
2:E:359:ASP:O	2:E:363:VAL:HG22	2.04	0.57
2:F:473:LEU:C	2:F:475:ALA:H	2.07	0.57
5:I:9:SER:O	5:I:13:TYR:HA	2.04	0.57
3:G:211:GLU:O	5:I:11:ALA:CB	2.53	0.57
1:C:342:THR:HG22	2:D:311:TYR:OH	2.05	0.57
2:F:373:LYS:HB3	2:F:445:LEU:HD13	1.86	0.57
3:G:180:LYS:NZ	3:G:220:THR:HB	2.19	0.57
5:I:8:MET:N	5:I:12:ALA:O	2.38	0.57
6:S:42:SER:O	6:S:47:VAL:HB	2.04	0.57
6:J:43:ILE:HG23	6:J:44:LYS:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:252:LEU:HD23	2:D:305:THR:HB	1.86	0.57
6:Q:1:MET:O	6:Q:2:GLN:HB2	2.03	0.57
1:B:309:GLU:HG3	2:F:223:ASN:HB3	1.87	0.57
7:F:600:ANP:O5'	7:F:600:ANP:H1'	2.05	0.57
1:A:165:GLN:HG2	1:A:166:ARG:N	2.19	0.56
2:E:99:ILE:HG13	2:E:101:GLU:HG3	1.87	0.56
3:G:35:GLU:O	3:G:39:ILE:HG12	2.05	0.56
3:G:43:LYS:HG3	4:H:20:THR:HG21	1.86	0.56
6:N:39:ARG:HH22	6:O:39:ARG:HG2	1.67	0.56
6:Q:71:LEU:CD2	6:R:73:LEU:HD11	2.26	0.56
1:B:414:ALA:HA	1:B:417:LYS:HB3	1.87	0.56
1:B:407:GLN:C	3:G:239:ASN:CG	2.63	0.56
6:M:40:ASN:CB	6:M:41:PRO:HA	2.13	0.56
1:C:344:VAL:HA	1:C:347:ILE:HD12	1.85	0.56
6:Q:71:LEU:HD23	6:R:73:LEU:CD1	2.27	0.56
1:C:440:THR:HA	1:C:443:GLN:HE21	1.69	0.56
2:F:162:GLY:HA2	7:F:600:ANP:PA	2.46	0.56
3:G:14:LYS:HA	3:G:248:ILE:HD11	1.87	0.56
1:C:146:GLU:HB2	1:C:163:ARG:HB2	1.88	0.56
1:A:92:ARG:HH21	1:A:94:GLY:HA2	1.70	0.56
1:C:336:VAL:HG11	1:C:353:PHE:HE1	1.71	0.56
2:F:374:VAL:HG23	2:F:445:LEU:HD11	1.87	0.56
3:G:115:LYS:O	3:G:119:LEU:HB2	2.05	0.56
1:A:340:ILE:HB	1:A:341:PRO:HD3	1.88	0.56
1:A:152:LEU:HD23	1:A:432:GLN:NE2	2.21	0.56
3:G:166:TYR:HB3	3:G:221:ALA:HB1	1.86	0.56
5:I:12:ALA:O	5:I:15:ASN:N	2.29	0.56
6:O:39:ARG:HH22	6:P:39:ARG:HD2	1.70	0.56
6:J:20:LEU:HG	6:S:21:GLY:N	2.20	0.56
1:B:26:ASN:ND2	1:B:26:ASN:N	2.52	0.56
1:B:270:TYR:HB2	1:B:327:PRO:HA	1.88	0.56
2:D:391:LEU:HD22	3:G:83:LEU:HD11	1.88	0.56
1:A:302:TYR:HE1	2:E:223:ASN:O	1.88	0.56
1:B:26:ASN:HD22	1:B:26:ASN:N	2.03	0.55
3:G:115:LYS:HD3	3:G:129:SER:OG	2.05	0.55
1:A:424:GLU:HB3	1:A:460:LEU:HD21	1.88	0.55
1:B:106:LEU:HD23	1:B:230:TYR:HA	1.88	0.55
2:E:391:LEU:CB	2:E:395:GLU:HG3	2.36	0.55
3:G:112:ASP:OD1	3:G:131:ASN:HB3	2.05	0.55
3:G:84:CYS:HB3	3:G:233:ARG:CZ	2.36	0.55
3:G:141:GLN:HA	5:I:15:ASN:ND2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:130:ILE:HG22	5:I:42:ALA:HB1	1.88	0.55
2:E:319:ASP:O	2:E:322:PRO:HD2	2.06	0.55
1:B:314:LEU:HD22	1:B:318:GLU:HB2	1.89	0.55
1:C:373:VAL:HG12	1:C:393:LYS:NZ	2.21	0.55
2:D:188:GLY:O	2:D:260:ARG:HD2	2.06	0.55
1:B:248:ALA:HB3	1:B:249:PRO:HD3	1.88	0.55
2:E:39:ILE:HG12	2:E:76:VAL:HG22	1.88	0.55
2:F:290:GLY:O	2:F:294:GLU:HB2	2.07	0.55
3:G:140:PHE:HE2	3:G:216:ASN:ND2	2.01	0.55
6:J:30:PHE:CZ	6:S:53:LEU:HD22	2.41	0.55
1:B:444:VAL:CG2	1:B:445:PRO:HD3	2.33	0.55
2:F:215:VAL:HG22	2:F:216:ALA:H	1.71	0.55
1:B:290:PRO:CD	2:F:270:ALA:HB1	2.34	0.55
2:F:237:LEU:HD21	2:F:295:ARG:HB2	1.88	0.55
6:K:14:ILE:HG21	6:L:14:ILE:CD1	2.37	0.55
1:B:171:GLY:H	1:B:177:LYS:HD3	1.71	0.55
1:B:429:LEU:HD11	1:B:446:LEU:HB3	1.89	0.55
1:B:505:SER:O	1:B:509:THR:HG22	2.07	0.55
2:E:346:PRO:HD3	2:E:418:PHE:CZ	2.42	0.55
6:S:22:ALA:O	6:S:26:ILE:HG12	2.07	0.55
2:E:391:LEU:HB3	2:E:395:GLU:CG	2.36	0.55
1:C:290:PRO:CB	3:G:276:SER:HB2	2.37	0.55
6:M:26:ILE:HD12	6:M:55:PHE:HD1	1.70	0.55
6:R:46:THR:HG23	6:S:43:ILE:HD13	1.88	0.55
1:A:168:LEU:HD11	1:A:329:ILE:HB	1.89	0.55
1:C:398:GLN:O	1:C:401:GLU:HB3	2.07	0.55
1:A:141:ARG:O	2:E:195:ASN:ND2	2.40	0.55
3:G:40:SER:O	4:H:17:PRO:HA	2.06	0.55
6:O:39:ARG:NH2	6:P:39:ARG:HD2	2.22	0.55
1:A:446:LEU:HD11	1:A:467:GLU:HG3	1.88	0.54
6:J:61:THR:O	6:J:65:CYS:HB2	2.08	0.54
1:B:375:ARG:HH12	2:F:190:ARG:NH2	2.04	0.54
4:H:42:LEU:HD22	6:O:41:PRO:HG2	1.87	0.54
1:B:147:PRO:HG3	1:B:380:ALA:O	2.06	0.54
1:B:110:VAL:O	1:B:234:VAL:HA	2.06	0.54
2:E:390:ILE:HD11	3:G:25:ILE:CG2	2.36	0.54
6:K:22:ALA:O	6:K:26:ILE:HG12	2.06	0.54
1:B:340:ILE:HB	1:B:341:PRO:HD3	1.89	0.54
2:F:350:PRO:HB2	2:F:378:LEU:HD13	1.89	0.54
4:H:12:LEU:N	4:H:22:TYR:O	2.41	0.54
4:H:70:ILE:HG23	4:H:72:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:VAL:CG2	1:A:445:PRO:HD3	2.38	0.54
2:F:259:PHE:CZ	2:F:313:PRO:HG3	2.42	0.54
2:F:432:VAL:HG12	2:F:436:ASP:HB3	1.90	0.54
6:J:38:SER:HB3	6:S:36:GLY:O	2.08	0.54
6:P:61:THR:O	6:P:65:CYS:HB2	2.08	0.54
1:A:270:TYR:HB2	1:A:327:PRO:HA	1.90	0.54
1:B:142:ARG:HB2	1:B:315:SER:HA	1.90	0.54
1:C:211:LYS:HB2	2:F:294:GLU:OE1	2.08	0.54
2:E:126:GLU:HA	2:E:300:LYS:HE3	1.90	0.54
1:A:382:VAL:HG11	1:A:440:THR:HG21	1.90	0.54
1:B:483:THR:HA	1:B:486:ARG:NH2	2.22	0.54
1:B:211:LYS:O	1:B:215:VAL:HG23	2.08	0.54
6:R:22:ALA:O	6:R:26:ILE:HG12	2.08	0.54
1:B:101:VAL:HG12	1:B:255:ILE:HA	1.88	0.53
1:A:32:ARG:NH1	1:A:89:LEU:HB2	2.23	0.53
3:G:139:THR:HB	5:I:37:ARG:HG3	1.91	0.53
3:G:182:ILE:HD12	3:G:214:LEU:HA	1.90	0.53
4:H:41:VAL:HA	4:H:45:HIS:CD2	2.44	0.53
1:A:143:SER:H	2:E:199:ARG:HH12	1.56	0.53
6:J:22:ALA:O	6:J:26:ILE:HG12	2.08	0.53
6:Q:61:THR:O	6:Q:65:CYS:HB2	2.08	0.53
6:R:73:LEU:HD23	6:R:73:LEU:C	2.29	0.53
2:E:153:ILE:N	2:E:153:ILE:HD12	2.23	0.53
3:G:143:SER:O	3:G:215:ALA:HB1	2.08	0.53
6:Q:43:ILE:HG23	6:Q:44:LYS:H	1.74	0.53
6:R:71:LEU:HD23	6:S:73:LEU:HD11	1.89	0.53
1:C:494:GLU:CD	1:C:494:GLU:N	2.62	0.53
2:F:50:VAL:HA	2:F:61:THR:HG22	1.89	0.53
6:P:22:ALA:O	6:P:26:ILE:HG12	2.08	0.53
6:Q:33:LEU:HD22	6:Q:33:LEU:O	2.09	0.53
1:C:292:GLY:N	1:C:296:TYR:O	2.30	0.53
6:J:20:LEU:HA	6:S:21:GLY:HA3	1.90	0.53
6:L:8:LYS:HG2	6:L:72:LEU:O	2.09	0.53
6:O:22:ALA:O	6:O:26:ILE:HG12	2.09	0.53
7:B:600:ANP:H1'	7:B:600:ANP:O5'	2.08	0.53
2:F:53:HIS:HD2	2:F:59:VAL:HG12	1.74	0.53
2:F:281:TYR:CE2	2:F:320:PRO:HD2	2.44	0.53
4:H:28:THR:O	4:H:42:LEU:CD2	2.57	0.53
6:N:8:LYS:HG2	6:N:72:LEU:O	2.09	0.53
2:D:278:ALA:HA	3:G:270:ILE:HD11	1.91	0.53
2:D:46:LEU:CD1	2:D:65:ASP:HB3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:HIS:CE1	1:B:502:ALA:HB2	2.44	0.53
1:C:299:ASP:HA	2:D:267:GLU:OE2	2.08	0.53
2:F:47:VAL:HG21	2:F:99:ILE:HG21	1.90	0.53
2:E:398:GLU:HA	2:E:401:LYS:HE2	1.91	0.52
1:B:309:GLU:CG	2:F:223:ASN:HB3	2.39	0.52
1:A:103:PRO:HD3	1:A:258:TRP:CZ2	2.44	0.52
3:G:150:LEU:HD22	3:G:218:MET:HE1	1.92	0.52
6:L:26:ILE:HD12	6:L:55:PHE:HD1	1.73	0.52
2:F:281:TYR:HE2	2:F:320:PRO:HD2	1.74	0.52
1:B:335:ASP:HB2	3:G:257:ARG:HH11	1.73	0.52
4:H:57:VAL:HG12	4:H:58:GLU:N	2.23	0.52
6:L:67:MET:O	6:L:71:LEU:HB2	2.10	0.52
1:A:417:LYS:O	1:A:421:VAL:HG23	2.08	0.52
1:C:290:PRO:HG3	3:G:276:SER:C	2.30	0.52
1:C:346:SER:O	2:D:190:ARG:NH2	2.43	0.52
4:H:42:LEU:HB3	6:O:41:PRO:CB	2.40	0.52
1:A:289:ARG:HH21	2:E:17:ILE:HG23	1.73	0.52
2:F:382:LYS:HA	2:F:385:GLN:HG2	1.92	0.52
2:F:39:ILE:HG13	2:F:76:VAL:HG13	1.91	0.52
6:J:8:LYS:HG2	6:J:72:LEU:O	2.09	0.52
6:N:22:ALA:O	6:N:26:ILE:HG12	2.09	0.52
6:R:43:ILE:HG23	6:R:44:LYS:H	1.74	0.52
6:S:8:LYS:HG2	6:S:72:LEU:O	2.10	0.52
6:L:50:MET:SD	6:M:48:PHE:CE1	3.02	0.52
1:B:305:SER:O	1:B:309:GLU:HG2	2.10	0.52
2:E:197:LEU:HD23	2:E:219:PHE:HZ	1.75	0.52
3:G:52:TYR:HE2	3:G:183:PHE:HB2	1.75	0.52
6:J:26:ILE:HG21	6:S:57:LEU:HB2	1.92	0.52
6:Q:22:ALA:O	6:Q:26:ILE:HG12	2.10	0.52
1:A:399:TYR:CD1	1:A:423:GLY:HA3	2.44	0.52
2:D:434:LEU:O	2:D:438:VAL:HG23	2.10	0.52
1:C:343:ASN:O	1:C:347:ILE:HG13	2.10	0.52
2:D:85:VAL:CG1	2:D:235:THR:HG23	2.37	0.52
1:A:38:ASP:CG	2:D:52:GLN:HE21	2.13	0.52
6:P:67:MET:O	6:P:71:LEU:HB2	2.10	0.52
1:A:212:ARG:CG	1:A:237:THR:HG21	2.40	0.52
6:Q:42:SER:CB	6:Q:47:VAL:HG23	2.40	0.52
6:R:8:LYS:HG2	6:R:72:LEU:O	2.10	0.52
1:B:30:THR:HA	1:B:90:VAL:O	2.11	0.51
2:D:257:ASN:OD1	2:D:259:PHE:HB3	2.10	0.51
2:E:258:ILE:HG22	2:E:309:ALA:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:8:LYS:HG2	6:P:72:LEU:O	2.10	0.51
1:C:503:THR:O	1:C:507:VAL:HG23	2.10	0.51
2:F:134:LEU:HB2	2:F:149:ARG:CG	2.40	0.51
3:G:141:GLN:NE2	5:I:19:GLN:OE1	2.44	0.51
6:Q:8:LYS:HG2	6:Q:72:LEU:O	2.10	0.51
6:R:42:SER:OG	6:R:47:VAL:HG23	2.11	0.51
1:C:43:VAL:HG21	1:C:75:ILE:HD12	1.91	0.51
2:D:158:GLY:O	2:D:161:VAL:HG22	2.10	0.51
2:E:85:VAL:CG1	2:E:235:THR:HG23	2.41	0.51
2:F:377:THR:HG22	2:F:407:ALA:HB2	1.91	0.51
2:F:90:GLU:HG3	2:F:111:SER:HA	1.91	0.51
6:L:22:ALA:O	6:L:26:ILE:HG12	2.10	0.51
6:N:26:ILE:HD12	6:N:55:PHE:HD1	1.75	0.51
6:N:67:MET:O	6:N:71:LEU:HB2	2.10	0.51
1:C:373:VAL:HG12	1:C:393:LYS:HZ3	1.76	0.51
2:F:237:LEU:HD21	2:F:295:ARG:CB	2.40	0.51
1:C:290:PRO:HB3	3:G:273:GLY:O	2.10	0.51
5:I:12:ALA:O	5:I:13:TYR:C	2.49	0.51
1:C:242:ALA:HB3	1:C:243:PRO:HD3	1.92	0.51
1:A:141:ARG:HB2	2:E:195:ASN:CG	2.31	0.51
6:L:33:LEU:HD22	6:L:33:LEU:O	2.10	0.51
2:F:345:TYR:HA	2:F:346:PRO:C	2.30	0.51
6:K:67:MET:O	6:K:71:LEU:HB2	2.10	0.51
6:K:8:LYS:HG2	6:K:72:LEU:O	2.10	0.51
6:O:47:VAL:HG12	6:O:48:PHE:N	2.25	0.51
6:O:67:MET:O	6:O:71:LEU:HB2	2.10	0.51
6:R:67:MET:O	6:R:71:LEU:HB2	2.10	0.51
1:B:466:PHE:CZ	1:B:470:PHE:HB2	2.46	0.51
2:D:276:PRO:HG3	3:G:273:GLY:HA3	1.93	0.51
3:G:162:ILE:HD13	3:G:210:PHE:HE1	1.74	0.51
6:K:20:LEU:HB3	6:L:20:LEU:CD1	2.40	0.51
6:J:39:ARG:HD2	6:S:39:ARG:NH2	2.25	0.51
2:D:136:THR:HG21	2:D:147:TYR:CD2	2.45	0.51
2:D:263:GLN:O	2:D:266:SER:HB3	2.11	0.51
6:Q:67:MET:O	6:Q:71:LEU:HB2	2.10	0.51
1:A:169:ILE:HD11	1:A:326:LEU:HD13	1.92	0.51
1:C:51:ALA:O	1:C:52:GLU:HB2	2.10	0.51
2:D:408:ARG:O	2:D:412:ARG:HD2	2.11	0.51
1:B:46:LEU:O	2:F:72:ARG:NH2	2.44	0.51
2:F:96:ILE:HG22	2:F:97:ASN:N	2.26	0.51
6:O:26:ILE:HD12	6:O:55:PHE:HD1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:43:ILE:HG13	6:S:44:LYS:N	2.25	0.51
1:A:117:ILE:HD12	2:D:124:PHE:CG	2.46	0.50
2:F:298:THR:HG23	2:F:303:SER:HA	1.93	0.50
3:G:157:GLY:HA2	3:G:210:PHE:CE2	2.45	0.50
6:J:48:PHE:CZ	6:S:50:MET:HG2	2.46	0.50
2:E:67:THR:HB	2:E:70:LEU:HD12	1.93	0.50
1:B:298:GLY:O	2:F:267:GLU:HG2	2.11	0.50
6:K:8:LYS:HG3	6:L:9:TYR:HD2	1.75	0.50
6:M:67:MET:O	6:M:71:LEU:HB2	2.10	0.50
6:Q:37:VAL:C	6:Q:39:ARG:H	2.13	0.50
6:J:67:MET:O	6:J:71:LEU:HB2	2.11	0.50
6:M:8:LYS:HG2	6:M:72:LEU:O	2.11	0.50
1:A:36:VAL:HG13	2:D:53:HIS:HB2	1.93	0.50
1:B:201:LEU:HD21	1:B:267:LEU:HB2	1.93	0.50
1:A:282:GLN:OE1	2:D:287:THR:CG2	2.59	0.50
2:F:363:VAL:HB	2:F:367:HIS:ND1	2.26	0.50
3:G:147:ALA:HB2	3:G:215:ALA:HA	1.92	0.50
6:K:21:GLY:N	6:L:20:LEU:HG	2.27	0.50
1:A:470:PHE:CZ	1:A:474:LEU:HD11	2.47	0.50
2:F:345:TYR:HB3	7:F:600:ANP:C6	2.41	0.50
2:F:67:THR:HB	2:F:70:LEU:HD12	1.93	0.50
6:J:4:VAL:HG22	6:K:5:LEU:HB3	1.94	0.50
1:A:158:LEU:HD11	1:A:396:LEU:HD12	1.92	0.50
1:A:86:GLU:OE1	2:D:57:ASN:N	2.41	0.50
1:B:471:LEU:O	1:B:475:LYS:HG3	2.12	0.50
2:E:237:LEU:HD21	2:E:295:ARG:HB2	1.93	0.50
6:L:35:ASN:O	6:L:39:ARG:HD3	2.11	0.50
6:S:67:MET:O	6:S:71:LEU:HB2	2.11	0.50
1:A:141:ARG:NH1	1:A:312:ALA:HB2	2.27	0.50
1:C:208:VAL:O	1:C:275:LYS:HD3	2.12	0.50
2:D:90:GLU:HG3	2:D:110:LYS:O	2.12	0.50
2:E:169:GLU:OE1	2:E:420:VAL:HG22	2.12	0.50
2:F:152:LYS:HZ1	2:F:293:GLN:HG3	1.76	0.50
6:Q:26:ILE:HD12	6:Q:55:PHE:HD1	1.76	0.50
1:C:28:ASN:HA	1:C:47:ASN:HB2	1.93	0.50
2:F:13:VAL:CG2	2:F:74:GLU:HB3	2.41	0.50
3:G:143:SER:HB2	3:G:219:LEU:HD12	1.93	0.50
4:H:57:VAL:HG12	4:H:58:GLU:H	1.77	0.50
2:F:27:GLN:O	2:F:29:GLU:N	2.45	0.50
6:J:72:LEU:HD21	6:K:73:LEU:CD2	2.39	0.50
6:J:31:ALA:HB1	6:S:32:ALA:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:220:GLY:N	2:F:232:VAL:HG21	2.28	0.49
2:F:154:GLY:HA3	2:F:329:LEU:HD13	1.93	0.49
4:H:29:GLN:HB3	4:H:60:MET:CE	2.42	0.49
6:M:33:LEU:O	6:M:33:LEU:HD22	2.12	0.49
1:A:182:LEU:HD13	1:A:218:LEU:HD11	1.94	0.49
1:C:140:PRO:HB2	1:C:318:GLU:HG3	1.93	0.49
2:D:208:ASN:ND2	2:D:211:GLY:HA3	2.27	0.49
2:E:182:SER:O	2:E:215:VAL:HA	2.12	0.49
2:F:30:LEU:HD11	2:F:57:ASN:HA	1.94	0.49
4:H:41:VAL:HG12	4:H:42:LEU:H	1.77	0.49
6:K:44:LYS:O	6:K:45:ASP:HB2	2.13	0.49
6:M:22:ALA:O	6:M:26:ILE:HG12	2.12	0.49
1:B:158:LEU:HD22	1:B:393:LYS:CD	2.42	0.49
2:D:25:PHE:O	2:D:57:ASN:HB3	2.12	0.49
2:F:148:ALA:HB2	2:F:357:LEU:HG	1.95	0.49
2:F:47:VAL:HB	2:F:64:MET:HB2	1.93	0.49
2:F:37:LEU:HB2	2:F:48:LEU:HB2	1.94	0.49
4:H:76:THR:HG23	4:H:84:CYS:HB2	1.93	0.49
3:G:150:LEU:HD22	3:G:218:MET:HE2	1.94	0.49
2:D:133:ILE:HD11	2:D:146:PRO:CB	2.41	0.49
2:F:171:ILE:O	2:F:175:ALA:HB3	2.12	0.49
2:F:215:VAL:HG22	2:F:216:ALA:N	2.28	0.49
2:F:293:GLN:HG2	2:F:328:HIS:CG	2.47	0.49
6:P:65:CYS:SG	6:Q:16:THR:HG22	2.53	0.49
6:J:37:VAL:HG11	6:S:46:THR:CG2	2.43	0.49
6:J:30:PHE:HZ	6:S:53:LEU:HD22	1.77	0.49
1:B:57:PHE:HB2	1:B:61:VAL:HG13	1.94	0.49
2:D:391:LEU:HD22	3:G:83:LEU:CD1	2.43	0.49
2:D:162:GLY:CA	7:D:600:ANP:H8	2.40	0.49
2:E:168:GLN:HE21	2:E:201:MET:HG3	1.78	0.49
3:G:140:PHE:HA	3:G:219:LEU:CD1	2.42	0.49
4:H:29:GLN:OE1	4:H:42:LEU:CD1	2.60	0.49
3:G:141:GLN:HB2	5:I:37:ARG:O	2.13	0.49
1:C:395:PHE:CZ	1:C:422:ARG:HD2	2.47	0.49
3:G:167:ASN:O	3:G:225:GLY:HA2	2.12	0.49
1:C:187:ASN:OD1	1:C:190:ARG:NH1	2.43	0.49
1:C:290:PRO:CB	2:D:270:ALA:HB1	2.41	0.49
2:E:259:PHE:O	2:E:262:THR:HB	2.13	0.49
3:G:141:GLN:OE1	5:I:37:ARG:O	2.30	0.49
6:P:72:LEU:HD21	6:Q:73:LEU:HD21	1.94	0.49
1:C:397:ALA:HA	1:C:400:ARG:NH2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:201:MET:HA	2:E:204:THR:HG22	1.94	0.49
6:P:26:ILE:HD12	6:P:55:PHE:HD1	1.78	0.49
1:B:260:ARG:HG2	1:B:314:LEU:HD12	1.95	0.49
1:B:54:LEU:HB3	1:B:93:THR:OG1	2.13	0.49
6:O:33:LEU:HD22	6:O:33:LEU:O	2.13	0.49
1:A:272:ASP:OD2	1:A:274:SER:HB2	2.13	0.48
1:B:333:GLY:O	3:G:253:ILE:HG21	2.13	0.48
2:E:229:ARG:HH22	2:E:267:GLU:CD	2.16	0.48
1:C:216:ALA:N	2:F:124:PHE:HE1	2.11	0.48
2:F:242:TYR:CE1	2:F:246:GLU:HG3	2.48	0.48
3:G:76:ALA:HB3	3:G:109:THR:HG22	1.95	0.48
5:I:19:GLN:HA	5:I:22:ARG:CB	2.43	0.48
1:B:385:LEU:HD23	1:B:444:VAL:CG1	2.42	0.48
1:C:179:ALA:HB2	7:C:600:ANP:H8	1.94	0.48
1:C:85:LYS:HD3	2:F:30:LEU:O	2.14	0.48
1:B:82:ARG:NH1	2:E:33:ILE:O	2.45	0.48
2:F:231:ARG:HD3	2:F:234:LEU:HD12	1.95	0.48
3:G:188:ILE:HD13	3:G:209:LEU:CD2	2.35	0.48
6:L:33:LEU:HD23	6:L:47:VAL:HG12	1.93	0.48
1:A:105:LEU:O	1:A:108:ARG:HB2	2.13	0.48
1:C:270:TYR:O	1:C:272:ASP:HA	2.13	0.48
5:I:32:ALA:O	5:I:33:SER:C	2.52	0.48
6:J:47:VAL:CG2	6:J:48:PHE:N	2.76	0.48
1:A:242:ALA:N	1:A:243:PRO:CD	2.76	0.48
1:B:355:GLU:HB3	1:B:358:LEU:HD12	1.95	0.48
1:C:399:TYR:CD1	1:C:423:GLY:HA3	2.48	0.48
4:H:80:ASP:O	4:H:81:SER:HB3	2.13	0.48
1:C:34:LEU:O	1:C:86:GLU:HG3	2.13	0.48
1:C:364:ARG:O	1:C:432:GLN:O	2.31	0.48
2:D:95:ILE:HD11	2:D:198:TYR:CE1	2.48	0.48
2:D:26:GLU:HA	2:D:26:GLU:OE1	2.13	0.48
1:A:82:ARG:NH1	2:D:35:ASN:OD1	2.46	0.48
1:A:36:VAL:HG23	1:A:41:ALA:HB2	1.95	0.48
1:B:82:ARG:HB2	2:E:33:ILE:O	2.13	0.48
2:F:140:VAL:CG1	2:F:414:LEU:HD22	2.44	0.48
2:F:49:GLU:CD	2:F:231:ARG:HE	2.17	0.48
3:G:141:GLN:CB	5:I:37:ARG:O	2.62	0.48
3:G:51:PHE:HD1	4:H:49:VAL:HG11	1.74	0.48
6:R:26:ILE:HD12	6:R:55:PHE:HD1	1.78	0.48
1:A:77:LEU:HD13	1:A:81:ASP:HB3	1.95	0.48
1:B:99:VAL:HG11	1:B:251:THR:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:141:GLN:OE1	5:I:38:SER:C	2.52	0.48
2:E:390:ILE:HD11	3:G:25:ILE:CB	2.44	0.48
6:J:27:ALA:CB	6:S:25:GLY:O	2.61	0.48
1:C:383:LYS:O	1:C:387:GLN:HG3	2.14	0.48
2:E:345:TYR:HA	2:E:346:PRO:C	2.34	0.48
3:G:150:LEU:HB3	3:G:214:LEU:HD21	1.95	0.48
5:I:10:TYR:CA	5:I:13:TYR:HB2	2.27	0.48
6:J:19:LEU:HB3	6:S:61:THR:CG2	2.35	0.48
6:L:28:ILE:HG22	6:M:31:ALA:HB2	1.94	0.48
1:B:108:ARG:HH22	1:B:116:PRO:HB3	1.78	0.48
1:B:383:LYS:HD2	1:B:490:GLU:HG2	1.96	0.48
1:C:69:GLU:HB3	1:C:70:PRO:HD3	1.94	0.48
2:D:143:LEU:O	2:D:367:HIS:HE1	1.97	0.48
2:E:346:PRO:HB2	2:E:348:VAL:HG23	1.96	0.48
6:O:61:THR:O	6:O:65:CYS:HB2	2.14	0.48
1:A:355:GLU:HB2	1:A:358:LEU:HD12	1.96	0.48
1:B:173:ARG:O	1:B:174:GLN:HB2	2.13	0.48
1:B:249:PRO:HB3	1:B:270:TYR:CD1	2.49	0.48
1:A:68:LEU:HB3	2:E:72:ARG:HD3	1.95	0.48
3:G:144:ALA:HB1	5:I:12:ALA:HA	1.95	0.48
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.96	0.47
2:F:86:PRO:O	2:F:91:THR:HG21	2.14	0.47
3:G:157:GLY:N	3:G:210:PHE:CE2	2.82	0.47
6:M:33:LEU:O	6:M:37:VAL:HG23	2.13	0.47
7:A:600:ANP:O5'	7:A:600:ANP:H1'	2.14	0.47
1:C:166:ARG:HD3	1:C:308:LEU:O	2.13	0.47
2:F:169:GLU:HG2	2:F:418:PHE:CD1	2.49	0.47
6:N:33:LEU:HD23	6:N:47:VAL:HG12	1.95	0.47
6:N:37:VAL:C	6:N:39:ARG:H	2.18	0.47
1:B:100:PRO:HD2	1:B:114:GLY:HA3	1.96	0.47
1:B:43:VAL:CG2	1:B:75:ILE:HD12	2.45	0.47
2:E:257:ASN:OD1	2:E:259:PHE:HB3	2.14	0.47
2:F:242:TYR:CD1	2:F:246:GLU:HG3	2.48	0.47
6:M:26:ILE:HD12	6:M:55:PHE:CD1	2.49	0.47
1:A:182:LEU:HD21	1:A:221:THR:HG21	1.95	0.47
1:B:290:PRO:HA	1:B:291:PRO:HD3	1.71	0.47
1:C:189:LYS:HE3	1:C:226:ASP:HB3	1.97	0.47
1:C:478:HIS:HB3	1:C:481:LEU:HG	1.95	0.47
2:F:285:LEU:C	2:F:285:LEU:HD23	2.35	0.47
3:G:149:LYS:HA	3:G:152:SER:HB2	1.96	0.47
6:M:37:VAL:O	6:M:37:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:43:ILE:HG13	6:P:44:LYS:N	2.29	0.47
1:B:129:SER:HB3	1:B:254:SER:HB3	1.97	0.47
1:B:478:HIS:HB3	1:B:481:LEU:HG	1.97	0.47
1:C:34:LEU:O	2:F:55:GLY:HA2	2.14	0.47
2:D:34:LEU:HD13	2:D:118:HIS:CG	2.50	0.47
1:C:290:PRO:CG	2:D:270:ALA:HB1	2.44	0.47
2:D:20:ILE:HG13	2:D:271:LEU:HB3	1.97	0.47
2:E:138:ILE:HG22	2:E:140:VAL:HG23	1.97	0.47
2:E:407:ALA:HA	2:E:410:ILE:HD12	1.95	0.47
1:B:346:SER:HB2	2:F:260:ARG:NH2	2.30	0.47
6:K:26:ILE:HD12	6:K:55:PHE:HD1	1.78	0.47
6:S:26:ILE:HD12	6:S:55:PHE:HD1	1.79	0.47
7:B:600:ANP:O1A	7:B:600:ANP:N3B	2.48	0.47
6:J:28:ILE:HG22	6:K:31:ALA:HB2	1.96	0.47
1:A:241:ALA:HB1	1:A:243:PRO:HD2	1.96	0.47
2:E:26:GLU:HB2	2:E:29:GLU:OE1	2.15	0.47
6:J:55:PHE:CZ	6:S:57:LEU:HD22	2.50	0.47
6:Q:33:LEU:HD23	6:Q:47:VAL:HG12	1.95	0.47
1:A:54:LEU:HD11	1:A:78:PHE:HE2	1.80	0.47
1:C:107:GLY:HA2	1:C:228:MET:O	2.15	0.47
1:C:54:LEU:HD11	1:C:78:PHE:HE2	1.80	0.47
2:E:174:ILE:HG13	2:E:252:LEU:HG	1.97	0.47
6:J:26:ILE:HD12	6:J:55:PHE:CD1	2.47	0.47
6:Q:40:ASN:OD1	6:Q:41:PRO:HA	2.15	0.47
6:R:33:LEU:HD22	6:R:33:LEU:O	2.14	0.47
1:B:288:ARG:CZ	2:E:275:ILE:HD11	2.45	0.47
1:A:36:VAL:O	2:D:53:HIS:O	2.33	0.47
4:H:31:ASN:O	4:H:57:VAL:HG13	2.14	0.47
6:Q:12:ALA:HB1	6:Q:73:LEU:HD11	1.97	0.47
6:R:73:LEU:O	6:R:73:LEU:HD23	2.13	0.47
6:J:31:ALA:HB1	6:S:32:ALA:HB2	1.95	0.47
6:J:37:VAL:C	6:J:39:ARG:H	2.16	0.47
1:A:152:LEU:HA	1:A:432:GLN:HE22	1.79	0.47
1:C:54:LEU:O	1:C:93:THR:HB	2.15	0.47
2:D:96:ILE:HG22	2:D:97:ASN:O	2.15	0.47
3:G:77:ILE:HG23	3:G:222:MET:HG2	1.97	0.47
6:O:21:GLY:HA3	6:P:20:LEU:HA	1.97	0.46
1:B:110:VAL:CG1	1:B:123:ILE:HD11	2.45	0.46
1:C:155:VAL:HG23	1:C:367:ILE:HD11	1.98	0.46
2:D:29:GLU:CG	2:D:29:GLU:O	2.58	0.46
1:B:139:LEU:HD23	2:F:105:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:74:PHE:CD1	6:K:74:PHE:C	2.88	0.46
6:K:8:LYS:HG3	6:L:9:TYR:CD2	2.50	0.46
6:O:28:ILE:HB	6:P:27:ALA:HB1	1.97	0.46
3:G:133:ILE:HG22	3:G:134:GLY:N	2.31	0.46
3:G:271:ILE:N	3:G:271:ILE:HD13	2.30	0.46
1:B:73:VAL:HG12	1:B:75:ILE:HG13	1.96	0.46
2:E:391:LEU:CD2	3:G:32:SER:OG	2.46	0.46
1:A:249:PRO:HG2	1:A:276:GLN:HG3	1.97	0.46
2:D:237:LEU:HD22	2:D:292:LEU:HD12	1.97	0.46
2:F:277:SER:HB3	2:F:281:TYR:O	2.15	0.46
3:G:262:VAL:O	3:G:266:GLU:HG3	2.15	0.46
4:H:42:LEU:CD1	6:O:41:PRO:HG2	2.35	0.46
1:A:35:ALA:HB3	1:A:42:ARG:HH12	1.79	0.46
2:D:388:ILE:HA	2:D:392:GLY:O	2.16	0.46
2:E:344:ILE:HG23	2:E:415:SER:HB3	1.97	0.46
2:F:348:VAL:O	2:F:350:PRO:HD3	2.16	0.46
4:H:45:HIS:CD2	6:O:39:ARG:O	2.68	0.46
5:I:8:MET:O	5:I:9:SER:O	2.33	0.46
6:K:37:VAL:C	6:K:39:ARG:H	2.19	0.46
1:A:168:LEU:HD12	1:A:327:PRO:O	2.16	0.46
1:B:163:ARG:HH11	1:B:265:HIS:CD2	2.33	0.46
4:H:41:VAL:O	4:H:42:LEU:HB2	2.15	0.46
1:A:434:GLN:HG2	1:A:435:TYR:CD1	2.51	0.46
2:E:244:ARG:HD3	2:E:304:VAL:HG23	1.97	0.46
2:F:201:MET:HB2	2:F:207:ILE:HD12	1.97	0.46
6:M:21:GLY:HA3	6:N:20:LEU:HA	1.97	0.46
1:A:492:SER:HB2	1:A:495:LEU:H	1.79	0.46
2:D:41:THR:HB	2:D:42:PRO:HD2	1.98	0.46
6:R:61:THR:O	6:R:65:CYS:HB2	2.16	0.46
1:B:139:LEU:N	1:B:140:PRO:CD	2.78	0.46
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.45	0.46
2:F:256:ASP:HA	2:F:257:ASN:HA	1.67	0.46
2:F:95:ILE:HD11	2:F:198:TYR:CD1	2.51	0.46
4:H:70:ILE:HG23	4:H:71:SER:N	2.31	0.46
4:H:42:LEU:CD1	6:O:41:PRO:CG	2.91	0.46
1:A:103:PRO:C	1:A:105:LEU:H	2.18	0.45
1:B:109:VAL:O	1:B:117:ILE:HG13	2.16	0.45
2:D:425:THR:C	2:D:427:ILE:H	2.19	0.45
6:M:37:VAL:C	6:M:39:ARG:H	2.18	0.45
1:B:391:SER:O	1:B:393:LYS:N	2.49	0.45
1:B:425:ARG:HD3	1:B:460:LEU:CD1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:132:GLU:HG3	2:E:149:ARG:HB3	1.97	0.45
1:A:251:THR:HG22	1:A:252:ALA:N	2.31	0.45
1:A:402:VAL:HG13	1:A:405:PHE:CD2	2.51	0.45
1:B:103:PRO:HD3	1:B:258:TRP:CZ2	2.52	0.45
1:B:271:ASP:HA	1:B:272:ASP:HA	1.68	0.45
2:F:162:GLY:HA2	7:F:600:ANP:H8	1.94	0.45
1:B:183:ASP:HA	1:B:186:LEU:HD12	1.97	0.45
1:B:43:VAL:HG21	1:B:75:ILE:HD12	1.97	0.45
3:G:141:GLN:NE2	5:I:38:SER:O	2.46	0.45
6:K:17:ILE:HB	6:L:17:ILE:HG13	1.99	0.45
1:B:488:LYS:HB3	1:B:490:GLU:H	1.82	0.45
2:D:30:LEU:HD11	2:D:57:ASN:HA	1.97	0.45
6:J:48:PHE:N	6:J:49:PRO:CD	2.79	0.45
1:A:82:ARG:NH2	2:D:35:ASN:OD1	2.46	0.45
2:F:325:THR:O	2:F:326:PHE:C	2.55	0.45
3:G:43:LYS:HB3	4:H:15:ALA:CB	2.46	0.45
1:B:394:LEU:HA	1:B:397:ALA:HB3	1.98	0.45
2:D:356:ARG:CG	2:D:357:LEU:HD23	2.46	0.45
1:B:86:GLU:OE1	2:E:55:GLY:HA2	2.17	0.45
2:F:293:GLN:HG2	2:F:328:HIS:CB	2.47	0.45
2:F:357:LEU:O	2:F:359:ASP:N	2.49	0.45
3:G:93:LYS:HG2	3:G:97:ARG:HH12	1.81	0.45
6:L:61:THR:O	6:L:65:CYS:HB2	2.16	0.45
6:J:66:LEU:HD21	6:S:64:PHE:CE1	2.52	0.45
1:A:101:VAL:HG23	1:A:258:TRP:CD1	2.51	0.45
1:B:153:LYS:HE3	1:B:430:LEU:O	2.17	0.45
1:C:298:GLY:O	2:D:267:GLU:HG2	2.17	0.45
1:C:166:ARG:NH1	1:C:347:ILE:O	2.49	0.45
2:E:390:ILE:HG23	3:G:29:THR:N	2.32	0.45
3:G:157:GLY:N	3:G:210:PHE:HE2	2.14	0.45
6:O:4:VAL:O	6:O:8:LYS:HB2	2.17	0.45
2:D:349:ASP:HA	2:D:350:PRO:HD2	1.85	0.45
1:C:51:ALA:O	2:D:68:GLU:HB2	2.17	0.45
6:P:4:VAL:O	6:P:8:LYS:HB2	2.17	0.45
1:A:32:ARG:HH12	1:A:89:LEU:HB2	1.81	0.45
1:B:396:LEU:HA	1:B:399:TYR:HB3	1.99	0.45
1:B:499:LEU:HD12	1:B:502:ALA:HB3	1.99	0.45
1:C:179:ALA:CB	7:C:600:ANP:C8	2.93	0.45
2:E:256:ASP:HA	2:E:257:ASN:HA	1.60	0.45
2:E:457:PHE:CE1	2:E:466:VAL:HG11	2.52	0.45
7:F:600:ANP:O5'	7:F:600:ANP:Cl'	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:28:THR:O	4:H:42:LEU:HD21	2.16	0.45
6:M:37:VAL:CG1	6:M:43:ILE:CG2	2.94	0.45
1:B:503:THR:O	1:B:507:VAL:HG23	2.17	0.44
1:C:364:ARG:HA	1:C:365:PRO:C	2.37	0.44
2:D:26:GLU:CA	2:D:26:GLU:OE1	2.65	0.44
1:A:68:LEU:O	2:E:15:ALA:HA	2.17	0.44
2:E:237:LEU:HD21	2:E:295:ARG:HD3	1.99	0.44
2:F:282:GLN:HA	2:F:283:PRO:HD3	1.80	0.44
2:F:387:ILE:HG23	2:F:391:LEU:HD12	1.98	0.44
4:H:28:THR:O	4:H:42:LEU:CG	2.65	0.44
3:G:151:LEU:CD1	5:I:11:ALA:HB2	2.46	0.44
6:J:37:VAL:O	6:J:37:VAL:HG12	2.17	0.44
6:O:33:LEU:CD2	6:O:47:VAL:HG13	2.47	0.44
6:P:40:ASN:CB	6:P:41:PRO:CA	2.91	0.44
1:A:397:ALA:HA	1:A:400:ARG:NH2	2.32	0.44
2:D:387:ILE:HD12	2:D:387:ILE:H	1.81	0.44
3:G:31:LEU:O	3:G:35:GLU:HG2	2.17	0.44
5:I:13:TYR:O	5:I:16:VAL:HG12	2.17	0.44
6:J:4:VAL:HG13	6:K:9:TYR:CZ	2.53	0.44
6:J:4:VAL:O	6:J:8:LYS:HB2	2.17	0.44
6:K:33:LEU:HD22	6:K:33:LEU:O	2.17	0.44
6:S:4:VAL:O	6:S:8:LYS:HB2	2.17	0.44
1:B:139:LEU:HD22	2:F:104:ASP:HA	2.00	0.44
1:B:146:GLU:O	1:B:163:ARG:HG3	2.18	0.44
1:B:208:VAL:HG21	1:B:249:PRO:HG3	1.98	0.44
1:C:153:LYS:N	1:C:432:GLN:OE1	2.48	0.44
2:F:204:THR:OG1	2:F:206:VAL:HG23	2.17	0.44
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.99	0.44
6:K:4:VAL:O	6:K:8:LYS:HB2	2.17	0.44
6:M:4:VAL:O	6:M:8:LYS:HB2	2.17	0.44
6:P:42:SER:O	6:P:47:VAL:HG23	2.17	0.44
6:Q:4:VAL:O	6:Q:8:LYS:HB2	2.17	0.44
6:R:33:LEU:HD23	6:R:47:VAL:HG12	1.98	0.44
6:J:43:ILE:HG12	6:S:46:THR:HG23	1.97	0.44
1:A:391:SER:O	1:A:394:LEU:HB3	2.18	0.44
1:A:446:LEU:CD1	1:A:467:GLU:HG3	2.47	0.44
1:B:139:LEU:N	1:B:140:PRO:HD2	2.32	0.44
1:B:226:ASP:O	1:B:229:LYS:HG2	2.17	0.44
4:H:42:LEU:HD22	6:O:41:PRO:CG	2.47	0.44
1:A:294:GLU:O	1:A:295:ALA:HB3	2.18	0.44
1:B:34:LEU:HD11	1:B:44:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:208:ASP:HB3	5:I:10:TYR:CG	2.51	0.44
2:F:201:MET:HA	2:F:201:MET:HE2	1.99	0.44
6:N:1:MET:HG3	6:N:4:VAL:HB	1.99	0.44
6:N:4:VAL:O	6:N:8:LYS:HB2	2.17	0.44
1:A:109:VAL:HG12	1:A:117:ILE:CG1	2.47	0.44
1:A:142:ARG:HG2	1:A:143:SER:H	1.82	0.44
1:A:85:LYS:O	1:A:88:GLU:HB2	2.17	0.44
1:B:242:ALA:HB3	1:B:243:PRO:HD3	1.99	0.44
1:B:377:GLY:C	1:B:379:ALA:H	2.21	0.44
1:C:131:ALA:O	1:C:250:PHE:HB3	2.16	0.44
2:D:256:ASP:HA	2:D:257:ASN:HA	1.65	0.44
2:D:52:GLN:OE1	2:D:60:ARG:HD2	2.18	0.44
2:E:423:VAL:HG23	2:E:424:PHE:CD1	2.49	0.44
3:G:78:THR:OG1	3:G:114:ILE:HB	2.18	0.44
3:G:197:PHE:HA	4:H:47:PRO:O	2.18	0.44
6:J:38:SER:OG	6:S:36:GLY:CA	2.66	0.44
6:R:71:LEU:CD2	6:S:73:LEU:HD21	2.47	0.44
1:B:40:ILE:H	1:B:40:ILE:HG12	1.73	0.44
1:C:302:TYR:CZ	1:C:306:ARG:HD3	2.53	0.44
1:C:89:LEU:HD23	1:C:89:LEU:C	2.38	0.44
2:D:182:SER:OG	2:D:252:LEU:HB2	2.17	0.44
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.98	0.44
2:E:260:ARG:HA	2:E:263:GLN:HB2	1.99	0.44
2:E:277:SER:OG	2:E:278:ALA:N	2.44	0.44
2:E:410:ILE:HG23	2:E:441:PHE:HE1	1.83	0.44
2:F:201:MET:HA	2:F:201:MET:CE	2.47	0.44
2:F:217:LEU:HB3	2:F:219:PHE:HE2	1.83	0.44
2:F:397:SER:O	2:F:401:LYS:HB2	2.17	0.44
2:F:432:VAL:CG1	2:F:436:ASP:HB3	2.47	0.44
1:A:144:VAL:CG1	1:A:162:GLY:HA3	2.48	0.44
1:B:112:ALA:O	1:B:251:THR:HG21	2.18	0.44
2:D:271:LEU:HD23	2:D:271:LEU:HA	1.87	0.44
2:E:224:GLU:O	2:E:229:ARG:HD3	2.18	0.44
2:E:317:LEU:HA	2:E:317:LEU:HD23	1.89	0.44
3:G:186:LYS:O	3:G:189:GLU:N	2.51	0.44
3:G:77:ILE:HG21	3:G:222:MET:HG2	2.00	0.44
1:B:335:ASP:CG	3:G:257:ARG:NH1	2.72	0.44
6:L:28:ILE:HB	6:M:27:ALA:HB1	2.00	0.44
1:C:336:VAL:CG1	1:C:353:PHE:HE1	2.31	0.43
2:D:26:GLU:HB2	2:D:29:GLU:OE1	2.18	0.43
2:D:425:THR:C	2:D:427:ILE:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:26:ILE:HD12	6:L:55:PHE:CD1	2.50	0.43
6:N:26:ILE:HD12	6:N:55:PHE:CD1	2.52	0.43
6:Q:46:THR:HG23	6:R:43:ILE:HD13	2.00	0.43
6:S:42:SER:HB2	6:S:46:THR:HB	2.00	0.43
1:A:363:ILE:O	1:A:366:ALA:HA	2.18	0.43
7:C:600:ANP:H1'	7:C:600:ANP:O5'	2.18	0.43
2:E:168:GLN:HE21	2:E:201:MET:CG	2.31	0.43
2:E:184:PHE:HA	2:E:254:PHE:HB2	1.99	0.43
2:F:33:ILE:O	2:F:34:LEU:CB	2.64	0.43
3:G:74:ILE:HG23	3:G:165:PHE:HD2	1.83	0.43
4:H:42:LEU:O	4:H:43:ALA:C	2.57	0.43
6:P:33:LEU:HD22	6:P:33:LEU:O	2.18	0.43
1:A:405:PHE:CE1	3:G:22:THR:CG2	2.98	0.43
2:E:255:ILE:HB	2:E:308:GLN:HG2	1.98	0.43
1:B:302:TYR:CE1	2:F:225:PRO:HA	2.54	0.43
2:F:320:PRO:O	2:F:324:THR:OG1	2.32	0.43
2:F:417:PRO:HB2	2:F:429:GLY:HA2	2.01	0.43
3:G:185:ALA:HA	3:G:188:ILE:HD12	2.00	0.43
6:K:3:LEU:HD13	6:L:3:LEU:HD23	2.00	0.43
6:R:33:LEU:CD2	6:R:47:VAL:HG12	2.49	0.43
6:Q:50:MET:SD	6:R:33:LEU:HD11	2.57	0.43
6:R:4:VAL:O	6:R:8:LYS:HB2	2.17	0.43
1:A:187:ASN:O	1:A:190:ARG:HG3	2.19	0.43
1:C:290:PRO:HA	1:C:291:PRO:HD3	1.74	0.43
3:G:205:VAL:CG1	3:G:206:PRO:HD3	2.49	0.43
4:H:41:VAL:HG12	4:H:42:LEU:N	2.33	0.43
6:L:4:VAL:O	6:L:8:LYS:HB2	2.17	0.43
1:A:267:LEU:HD11	1:A:326:LEU:HG	1.98	0.43
1:A:77:LEU:CD1	1:A:81:ASP:HB3	2.48	0.43
1:B:111:ASP:OD2	1:B:115:ASN:HB2	2.18	0.43
1:B:62:LYS:O	1:B:78:PHE:HB2	2.18	0.43
2:D:234:LEU:HD23	2:D:234:LEU:N	2.33	0.43
2:D:257:ASN:HD21	2:D:311:TYR:N	2.16	0.43
2:E:150:GLY:HA2	2:E:304:VAL:O	2.19	0.43
2:E:366:GLU:O	2:E:370:VAL:HG23	2.18	0.43
2:F:96:ILE:CG2	2:F:97:ASN:N	2.81	0.43
3:G:205:VAL:N	3:G:206:PRO:CD	2.82	0.43
3:G:55:ALA:O	3:G:56:GLU:C	2.57	0.43
4:H:42:LEU:HB3	6:O:41:PRO:HB3	2.01	0.43
6:J:9:TYR:HB3	6:S:72:LEU:HD22	2.00	0.43
1:C:197:GLU:HA	1:C:200:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:VAL:O	1:C:303:LEU:HB3	2.19	0.43
2:E:221:GLN:HB2	2:E:223:ASN:OD1	2.18	0.43
6:O:28:ILE:HG22	6:P:31:ALA:HB2	1.99	0.43
1:B:344:VAL:HA	1:B:347:ILE:HD12	2.01	0.43
1:B:350:GLY:C	1:B:351:GLN:HG3	2.39	0.43
1:C:267:LEU:HD11	1:C:326:LEU:CD1	2.41	0.43
1:C:294:GLU:HB2	1:C:296:TYR:CD2	2.53	0.43
1:C:299:ASP:N	1:C:299:ASP:OD1	2.49	0.43
2:D:447:GLY:C	2:D:449:TYR:H	2.22	0.43
2:E:152:LYS:HE3	2:E:296:ILE:O	2.19	0.43
2:E:431:LEU:HD23	2:E:431:LEU:C	2.39	0.43
2:F:183:VAL:O	2:F:253:LEU:HD12	2.18	0.43
2:F:83:ILE:HB	2:F:117:ILE:HG12	2.00	0.43
6:O:72:LEU:HD21	6:P:73:LEU:HD21	2.00	0.43
6:Q:28:ILE:HG22	6:R:31:ALA:HB2	2.00	0.43
2:D:155:LEU:HB2	2:D:309:ALA:HA	2.01	0.43
3:G:182:ILE:HD11	3:G:217:GLN:CB	2.43	0.43
6:J:27:ALA:HB2	6:S:25:GLY:O	2.19	0.43
6:K:40:ASN:CB	6:K:41:PRO:CA	2.91	0.43
1:A:290:PRO:HA	1:A:291:PRO:HD3	1.88	0.43
1:A:402:VAL:HG12	1:A:402:VAL:O	2.17	0.43
1:C:375:ARG:HD3	7:D:600:ANP:O3'	2.19	0.43
1:B:335:ASP:CG	3:G:257:ARG:HD3	2.38	0.43
6:M:61:THR:HG23	6:N:19:LEU:HB3	2.01	0.43
1:A:165:GLN:HG2	1:A:166:ARG:H	1.82	0.43
1:A:177:LYS:HE2	1:A:177:LYS:HB2	1.64	0.43
1:B:187:ASN:OD1	1:B:437:PRO:HB3	2.18	0.43
2:D:199:ARG:HB3	2:D:199:ARG:CZ	2.49	0.43
2:E:133:ILE:HD12	2:E:146:PRO:HB2	2.00	0.43
2:F:224:GLU:HB3	2:F:228:ALA:HB3	2.00	0.43
2:F:275:ILE:O	2:F:283:PRO:HG3	2.18	0.43
2:F:326:PHE:C	2:F:328:HIS:H	2.22	0.43
3:G:162:ILE:HG21	3:G:214:LEU:HD13	2.00	0.43
6:J:27:ALA:CB	6:S:29:VAL:HG23	2.49	0.43
6:P:14:ILE:HG21	6:Q:14:ILE:HD13	2.01	0.43
1:B:80:SER:OG	1:B:82:ARG:HB3	2.19	0.42
2:E:95:ILE:HB	2:E:104:ASP:HB3	2.01	0.42
4:H:48:THR:H	4:H:77:VAL:HB	1.84	0.42
6:K:33:LEU:CD2	6:K:47:VAL:HG12	2.49	0.42
6:N:40:ASN:CB	6:N:41:PRO:CA	2.89	0.42
6:Q:28:ILE:HB	6:R:27:ALA:HB1	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:HA	1:B:123:ILE:HD13	1.91	0.42
1:C:192:ASN:HA	1:C:200:LYS:HG2	2.01	0.42
1:C:302:TYR:CE1	1:C:306:ARG:HD3	2.54	0.42
2:D:204:THR:HB	2:D:206:VAL:HG23	2.00	0.42
2:F:289:MET:CE	2:F:324:THR:HB	2.49	0.42
3:G:110:ILE:HG23	3:G:133:ILE:HG13	2.02	0.42
2:E:390:ILE:CD1	3:G:25:ILE:O	2.66	0.42
6:L:7:ALA:HB1	6:M:10:ILE:HG13	2.01	0.42
1:A:174:GLN:HB3	2:D:354:LYS:HD2	2.00	0.42
2:D:37:LEU:HB2	2:D:48:LEU:HB2	2.01	0.42
2:E:320:PRO:O	2:E:324:THR:OG1	2.36	0.42
6:O:37:VAL:C	6:O:39:ARG:H	2.20	0.42
1:A:311:ALA:HA	1:A:323:LEU:HD23	2.01	0.42
1:B:174:GLN:NE2	2:E:356:ARG:HD3	2.35	0.42
1:C:273:LEU:HD13	1:C:304:HIS:CD2	2.54	0.42
2:D:33:ILE:O	2:D:34:LEU:HB2	2.19	0.42
3:G:143:SER:OG	3:G:219:LEU:CB	2.63	0.42
3:G:3:LEU:HD21	3:G:255:TYR:CE1	2.54	0.42
6:N:48:PHE:CE2	6:N:52:ILE:HD11	2.53	0.42
6:P:21:GLY:HA3	6:Q:20:LEU:HA	2.00	0.42
1:B:139:LEU:HD23	2:F:105:GLU:HB2	2.01	0.42
1:B:390:GLY:O	1:B:391:SER:HB2	2.19	0.42
1:C:470:PHE:CZ	1:C:474:LEU:HD11	2.55	0.42
1:A:143:SER:HG	2:E:199:ARG:HH22	1.66	0.42
2:E:321:ALA:HB3	2:E:322:PRO:HD3	2.02	0.42
4:H:33:PRO:HD3	4:H:57:VAL:HG22	2.01	0.42
4:H:17:PRO:HD3	4:H:88:ILE:HA	2.01	0.42
1:B:368:ASN:C	1:B:368:ASN:OD1	2.58	0.42
1:B:454:HIS:HD2	1:B:504:GLU:HG3	1.85	0.42
2:E:50:VAL:HA	2:E:61:THR:HG22	2.01	0.42
2:F:192:ARG:NH1	2:F:192:ARG:HG2	2.34	0.42
3:G:216:ASN:HD22	3:G:216:ASN:HA	1.56	0.42
4:H:29:GLN:CB	4:H:42:LEU:HD11	2.32	0.42
6:J:48:PHE:HA	6:J:48:PHE:HD1	1.69	0.42
6:K:26:ILE:HD12	6:K:55:PHE:CD1	2.54	0.42
6:O:52:ILE:H	6:O:52:ILE:HG13	1.59	0.42
1:C:99:VAL:HG11	1:C:251:THR:HB	2.02	0.42
1:C:428:GLN:NE2	1:C:431:LYS:HD2	2.35	0.42
2:D:46:LEU:HD12	2:D:65:ASP:HB3	2.01	0.42
2:E:125:ALA:C	2:E:127:GLN:H	2.23	0.42
2:F:382:LYS:O	2:F:385:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:13:GLN:HB3	4:H:84:CYS:SG	2.59	0.42
6:N:14:ILE:HG21	6:O:14:ILE:HD13	2.01	0.42
1:B:305:SER:HA	1:B:347:ILE:HG21	2.02	0.42
1:C:85:LYS:O	1:C:88:GLU:HB3	2.18	0.42
1:C:50:GLN:CG	2:D:69:GLY:HA2	2.49	0.42
2:F:85:VAL:HG12	2:F:100:GLY:HA3	2.01	0.42
6:K:33:LEU:HD23	6:K:47:VAL:HG12	2.01	0.42
1:A:291:PRO:HB2	1:A:295:ALA:HA	2.01	0.42
1:A:300:VAL:O	1:A:303:LEU:HB3	2.19	0.42
1:B:190:ARG:HB2	1:B:191:TRP:CE3	2.55	0.42
1:C:158:LEU:HD11	1:C:430:LEU:CD1	2.49	0.42
2:D:167:ILE:O	2:D:171:ILE:HD12	2.20	0.42
2:D:190:ARG:HD2	2:D:193:GLU:OE2	2.20	0.42
2:E:148:ALA:CB	2:E:151:GLY:HA3	2.45	0.42
2:E:275:ILE:HA	2:E:276:PRO:HD2	1.91	0.42
2:F:293:GLN:HG2	2:F:328:HIS:HB3	2.01	0.42
3:G:168:ASP:HA	3:G:169:PRO:HD3	1.89	0.42
6:M:50:MET:SD	6:N:33:LEU:CD1	2.96	0.42
1:A:38:ASP:OD2	2:D:52:GLN:NE2	2.53	0.42
1:A:391:SER:O	1:A:395:PHE:HD1	2.03	0.42
1:A:54:LEU:HD11	1:A:78:PHE:CE2	2.55	0.42
2:D:142:ASP:HB3	2:D:434:LEU:CD1	2.45	0.42
2:D:256:ASP:OD1	2:D:257:ASN:HB2	2.20	0.42
2:D:357:LEU:N	2:D:357:LEU:HD23	2.35	0.42
2:E:143:LEU:HB2	2:E:437:THR:CG2	2.50	0.42
1:A:217:GLN:HB2	2:D:129:THR:HG21	2.02	0.41
1:A:257:GLU:HG2	1:A:260:ARG:NH1	2.35	0.41
1:A:58:SER:HB2	1:A:88:GLU:HG2	2.02	0.41
2:D:89:ARG:HG2	2:D:92:LEU:HD12	2.01	0.41
2:E:117:ILE:HA	2:E:238:THR:OG1	2.20	0.41
1:B:288:ARG:HG2	2:E:275:ILE:CD1	2.49	0.41
2:F:201:MET:CB	2:F:207:ILE:HD12	2.50	0.41
4:H:30:VAL:HG21	4:H:83:LEU:HD23	2.02	0.41
4:H:41:VAL:O	4:H:42:LEU:HD12	2.20	0.41
6:J:34:ILE:HD12	6:S:33:LEU:HA	2.01	0.41
6:Q:26:ILE:HD12	6:Q:55:PHE:CD1	2.55	0.41
6:R:1:MET:HE3	6:R:5:LEU:HD12	2.03	0.41
6:R:2:GLN:HG3	6:R:2:GLN:O	2.19	0.41
1:A:33:VAL:HA	1:A:43:VAL:HG22	2.02	0.41
1:A:66:LEU:HD12	1:A:76:VAL:HG11	2.02	0.41
1:B:488:LYS:HD3	1:B:490:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ARG:HA	2:F:33:ILE:HB	2.01	0.41
2:D:277:SER:OG	2:D:278:ALA:N	2.52	0.41
3:G:140:PHE:CE2	3:G:216:ASN:ND2	2.81	0.41
3:G:24:LYS:HG3	3:G:238:ASP:HB2	2.01	0.41
3:G:47:ALA:HA	4:H:84:CYS:HB3	2.03	0.41
6:L:43:ILE:HG23	6:L:44:LYS:H	1.83	0.41
6:P:50:MET:SD	6:Q:33:LEU:HD11	2.60	0.41
1:B:148:VAL:HG23	1:B:163:ARG:HG2	2.02	0.41
2:D:319:ASP:OD2	2:D:322:PRO:HD2	2.19	0.41
3:G:143:SER:CB	3:G:219:LEU:HD12	2.50	0.41
1:A:348:THR:O	2:E:190:ARG:NH2	2.48	0.41
1:B:67:ASN:HA	2:F:16:VAL:O	2.20	0.41
2:D:95:ILE:HD11	2:D:198:TYR:CD1	2.55	0.41
6:J:33:LEU:CD1	6:S:50:MET:SD	2.97	0.41
1:B:260:ARG:O	1:B:321:GLY:HA3	2.20	0.41
2:E:102:PRO:HD3	2:E:109:ILE:HD12	2.01	0.41
2:E:356:ARG:O	2:E:357:LEU:HD23	2.21	0.41
2:E:427:ILE:HA	2:E:428:PRO:HD2	1.86	0.41
2:F:14:THR:HG21	2:F:24:HIS:HB2	2.02	0.41
3:G:173:LEU:HD23	3:G:235:ASN:ND2	2.36	0.41
3:G:184:ASN:O	3:G:185:ALA:O	2.38	0.41
2:E:390:ILE:HG12	3:G:29:THR:CG2	2.50	0.41
6:L:33:LEU:O	6:L:37:VAL:HG23	2.20	0.41
6:J:24:ILE:HG13	6:S:21:GLY:O	2.21	0.41
1:B:250:PHE:O	1:B:253:ALA:HB3	2.21	0.41
1:B:52:GLU:O	1:B:97:VAL:HG23	2.20	0.41
2:E:388:ILE:HD12	2:E:393:MET:HG2	2.03	0.41
1:A:100:PRO:HD2	1:A:114:GLY:HA3	2.03	0.41
1:A:455:LEU:HD22	1:A:458:ILE:HD12	2.01	0.41
1:B:363:ILE:C	1:B:364:ARG:HG2	2.40	0.41
1:B:426:LEU:O	1:B:429:LEU:HB3	2.20	0.41
1:C:139:LEU:HA	1:C:139:LEU:HD12	1.87	0.41
2:D:258:ILE:HD11	2:D:292:LEU:HD21	2.02	0.41
2:D:84:SER:CB	2:D:114:ARG:HE	2.34	0.41
2:E:316:ASP:OD2	3:G:259:ARG:NH2	2.52	0.41
2:F:163:LYS:NZ	7:F:600:ANP:O3G	2.50	0.41
2:F:87:VAL:HG21	2:F:242:TYR:CD1	2.55	0.41
3:G:182:ILE:CD1	3:G:217:GLN:HB2	2.46	0.41
1:B:96:ILE:O	1:B:97:VAL:C	2.59	0.41
1:C:313:LYS:HG3	1:C:313:LYS:O	2.20	0.41
1:C:340:ILE:HB	1:C:341:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:433:ARG:HA	2:D:433:ARG:HD2	1.87	0.41
2:E:153:ILE:HA	2:E:331:ALA:O	2.20	0.41
2:E:275:ILE:HD12	2:E:275:ILE:H	1.85	0.41
6:J:42:SER:O	6:J:47:VAL:CG1	2.66	0.41
6:L:37:VAL:HG12	6:L:37:VAL:O	2.19	0.41
1:A:111:ASP:OD1	1:A:111:ASP:C	2.59	0.41
1:A:31:GLY:HA3	1:A:46:LEU:HG	2.03	0.41
1:B:171:GLY:N	1:B:177:LYS:HD3	2.34	0.41
1:C:101:VAL:HG12	1:C:255:ILE:HA	2.03	0.41
2:D:356:ARG:HG2	2:D:357:LEU:HD23	2.03	0.41
2:D:378:LEU:HD21	2:D:410:ILE:HG22	2.02	0.41
1:A:347:ILE:HA	2:E:222:MET:CE	2.50	0.41
1:C:360:TYR:OH	2:F:354:LYS:HD3	2.21	0.41
3:G:188:ILE:O	3:G:191:SER:OG	2.30	0.41
2:E:390:ILE:HD13	3:G:25:ILE:O	2.21	0.41
4:H:29:GLN:HB3	4:H:60:MET:HE2	2.03	0.41
6:L:33:LEU:CD2	6:L:47:VAL:HG12	2.51	0.41
6:N:33:LEU:HD22	6:N:33:LEU:O	2.20	0.41
1:A:34:LEU:O	1:A:86:GLU:HG3	2.21	0.41
2:D:255:ILE:HG13	2:D:308:GLN:HG2	2.02	0.41
1:A:347:ILE:HA	2:E:222:MET:HE1	2.03	0.41
2:F:25:PHE:CZ	2:F:31:PRO:HG3	2.56	0.41
2:F:13:VAL:HG21	2:F:74:GLU:HB3	2.02	0.41
6:M:50:MET:CE	6:N:43:ILE:HD11	2.51	0.41
6:R:3:LEU:HA	6:R:3:LEU:HD23	1.97	0.41
6:R:48:PHE:N	6:R:49:PRO:CD	2.84	0.41
3:G:173:LEU:HD23	3:G:235:ASN:HD21	1.85	0.41
3:G:139:THR:CG2	5:I:37:ARG:HG3	2.50	0.41
5:I:9:SER:O	5:I:13:TYR:CB	2.69	0.41
6:J:33:LEU:O	6:J:37:VAL:HG23	2.21	0.41
6:L:48:PHE:N	6:L:49:PRO:CD	2.84	0.41
6:P:37:VAL:HG11	6:P:43:ILE:HD13	2.03	0.41
1:A:329:ILE:HA	1:A:329:ILE:HD13	1.96	0.40
1:B:421:VAL:O	1:B:425:ARG:HG2	2.21	0.40
1:B:68:LEU:O	2:F:15:ALA:CA	2.63	0.40
2:D:244:ARG:HD3	2:D:304:VAL:HG23	2.03	0.40
2:D:90:GLU:HA	2:D:90:GLU:OE1	2.20	0.40
2:E:31:PRO:HG3	2:E:37:LEU:HD21	2.02	0.40
2:E:410:ILE:HG23	2:E:441:PHE:CE1	2.56	0.40
4:H:41:VAL:O	4:H:42:LEU:CB	2.69	0.40
6:J:43:ILE:HD13	6:S:46:THR:CG2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:37:VAL:HG11	6:M:43:ILE:CG2	2.51	0.40
6:M:48:PHE:N	6:M:49:PRO:CD	2.84	0.40
6:N:37:VAL:O	6:N:37:VAL:HG12	2.22	0.40
6:N:48:PHE:N	6:N:49:PRO:CD	2.84	0.40
6:O:14:ILE:HG21	6:P:14:ILE:HD13	2.03	0.40
6:P:37:VAL:O	6:P:37:VAL:HG12	2.21	0.40
1:C:382:VAL:HG12	1:C:385:LEU:H	1.86	0.40
1:C:470:PHE:CE2	1:C:474:LEU:HD11	2.56	0.40
2:E:128:SER:HB2	2:E:298:THR:HB	2.03	0.40
3:G:53:LYS:HA	3:G:53:LYS:HD3	1.90	0.40
4:H:12:LEU:HB2	4:H:23:SER:HA	2.03	0.40
6:M:33:LEU:HD23	6:M:47:VAL:HG12	2.03	0.40
1:A:394:LEU:HG	1:A:398:GLN:NE2	2.37	0.40
1:C:212:ARG:CG	1:C:237:THR:HG21	2.50	0.40
1:C:484:GLU:HG2	1:C:495:LEU:HD11	2.02	0.40
2:D:204:THR:HB	2:D:206:VAL:CG2	2.51	0.40
2:D:74:GLU:HG3	2:D:75:LYS:N	2.37	0.40
2:E:145:ALA:HA	2:E:355:SER:HB2	2.04	0.40
2:E:167:ILE:HG23	2:E:254:PHE:CE2	2.57	0.40
2:E:391:LEU:HD21	3:G:31:LEU:HD23	2.04	0.40
3:G:197:PHE:C	3:G:199:ILE:H	2.24	0.40
1:A:402:VAL:HG11	1:A:416:THR:HB	2.03	0.40
1:B:243:PRO:HA	1:B:246:TYR:HB3	2.03	0.40
1:C:335:ASP:OD2	1:C:338:ALA:HB2	2.22	0.40
1:A:239:SER:HB3	2:D:294:GLU:HG3	2.03	0.40
6:L:37:VAL:C	6:L:39:ARG:H	2.25	0.40
6:N:33:LEU:CD2	6:N:47:VAL:HG12	2.51	0.40
6:P:26:ILE:HD12	6:P:55:PHE:CD1	2.57	0.40
6:R:37:VAL:HG12	6:R:37:VAL:O	2.22	0.40
1:A:446:LEU:HD21	1:A:467:GLU:HA	2.03	0.40
1:B:459:GLU:H	1:B:462:ARG:NH2	2.19	0.40
1:C:179:ALA:HB3	7:C:600:ANP:H8	2.03	0.40
2:F:192:ARG:HG2	2:F:192:ARG:HH11	1.86	0.40
2:F:388:ILE:HD11	2:F:396:LEU:HD21	2.03	0.40
2:F:473:LEU:C	2:F:475:ALA:N	2.73	0.40
1:B:49:ILE:O	2:F:71:VAL:HG13	2.21	0.40
4:H:22:TYR:HE2	4:H:68:PHE:CZ	2.39	0.40
6:K:28:ILE:HB	6:L:27:ALA:HB1	2.03	0.40
6:K:48:PHE:N	6:K:49:PRO:CD	2.84	0.40
6:O:47:VAL:CG1	6:O:48:PHE:N	2.84	0.40
6:O:48:PHE:N	6:O:49:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:48:PHE:N	6:P:49:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	479/510 (94%)	430 (90%)	46 (10%)	3 (1%)	25	66
1	B	480/510 (94%)	433 (90%)	45 (9%)	2 (0%)	34	72
1	C	483/510 (95%)	445 (92%)	36 (8%)	2 (0%)	34	72
2	D	469/478 (98%)	429 (92%)	37 (8%)	3 (1%)	25	66
2	E	467/478 (98%)	425 (91%)	36 (8%)	6 (1%)	12	48
2	F	468/478 (98%)	419 (90%)	41 (9%)	8 (2%)	9	42
3	G	260/278 (94%)	225 (86%)	28 (11%)	7 (3%)	5	31
4	H	109/138 (79%)	88 (81%)	16 (15%)	5 (5%)	2	21
5	I	43/61 (70%)	27 (63%)	8 (19%)	8 (19%)	0	2
6	J	71/76 (93%)	64 (90%)	6 (8%)	1 (1%)	11	46
6	K	71/76 (93%)	65 (92%)	5 (7%)	1 (1%)	11	46
6	L	70/76 (92%)	65 (93%)	4 (6%)	1 (1%)	11	46
6	M	71/76 (93%)	66 (93%)	3 (4%)	2 (3%)	5	30
6	N	71/76 (93%)	66 (93%)	3 (4%)	2 (3%)	5	30
6	O	72/76 (95%)	67 (93%)	4 (6%)	1 (1%)	11	46
6	P	73/76 (96%)	67 (92%)	4 (6%)	2 (3%)	5	31
6	Q	73/76 (96%)	63 (86%)	9 (12%)	1 (1%)	11	46
6	R	72/76 (95%)	66 (92%)	5 (7%)	1 (1%)	11	46
6	S	72/76 (95%)	66 (92%)	4 (6%)	2 (3%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3974/4201 (95%)	3576 (90%)	340 (9%)	58 (2%)	10	46

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	29	GLU
2	F	28	SER
3	G	152	SER
3	G	185	ALA
3	G	186	LYS
3	G	202	ASP
3	G	204	ASN
4	H	43	ALA
5	I	9	SER
5	I	23	SER
5	I	33	SER
5	I	55	GLU
5	I	56	PRO
6	P	43	ILE
1	C	238	ALA
2	E	123	SER
2	E	474	ALA
2	F	43	GLN
2	F	358	LEU
2	F	423	VAL
3	G	203	ALA
4	H	14	PHE
5	I	32	ALA
6	M	40	ASN
6	N	43	ILE
6	O	40	ASN
1	B	392	LEU
2	D	28	SER
2	E	353	SER
6	J	40	ASN
6	K	40	ASN
6	L	40	ASN
6	N	40	ASN
6	P	40	ASN
6	R	40	ASN
6	S	40	ASN
1	A	229	LYS

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Mol	Chain	Res	Type
1	A	238	ALA
2	E	126	GLU
2	F	279	VAL
2	F	327	ALA
2	F	474	ALA
4	H	42	LEU
4	H	93	LEU
6	M	42	SER
1	B	448	TYR
3	G	78	THR
5	I	30	GLN
6	S	43	ILE
1	C	505	SER
5	I	11	ALA
2	E	461	GLY
4	H	33	PRO
2	D	82	PRO
2	F	248	GLY
6	Q	40	ASN
2	E	141	VAL
1	A	382	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	388/412 (94%)	370 (95%)	18 (5%)	27	52
1	B	388/412 (94%)	351 (90%)	37 (10%)	8	28
1	C	388/412 (94%)	363 (94%)	25 (6%)	17	42
2	D	380/384 (99%)	361 (95%)	19 (5%)	24	49
2	E	378/384 (98%)	359 (95%)	19 (5%)	24	49
2	F	379/384 (99%)	360 (95%)	19 (5%)	24	49
3	G	216/236 (92%)	190 (88%)	26 (12%)	5	20
4	H	53/112 (47%)	43 (81%)	10 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	23/48 (48%)	20 (87%)	3 (13%)	4	18
6	J	53/56 (95%)	42 (79%)	11 (21%)	1	7
6	K	53/56 (95%)	48 (91%)	5 (9%)	8	28
6	L	52/56 (93%)	49 (94%)	3 (6%)	20	45
6	M	53/56 (95%)	48 (91%)	5 (9%)	8	28
6	N	53/56 (95%)	49 (92%)	4 (8%)	13	38
6	O	54/56 (96%)	49 (91%)	5 (9%)	9	29
6	P	55/56 (98%)	51 (93%)	4 (7%)	14	39
6	Q	55/56 (98%)	48 (87%)	7 (13%)	4	19
6	R	54/56 (96%)	46 (85%)	8 (15%)	3	15
6	S	54/56 (96%)	48 (89%)	6 (11%)	6	22
All	All	3129/3344 (94%)	2895 (92%)	234 (8%)	13	38

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ARG
1	A	143	SER
1	A	173	ARG
1	A	221	THR
1	A	239	SER
1	A	245	GLN
1	A	251	THR
1	A	267	LEU
1	A	293	ARG
1	A	318	GLU
1	A	322	SER
1	A	364	ARG
1	A	378	SER
1	A	412	LEU
1	A	480	GLU
1	A	481	LEU
1	A	492	SER
1	A	501	SER
1	B	26	ASN
1	B	40	ILE
1	B	50	GLN
1	B	54	LEU

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Mol	Chain	Res	Type
1	B	80	SER
1	B	82	ARG
1	B	89	LEU
1	B	93	THR
1	B	99	VAL
1	B	129	SER
1	B	142	ARG
1	B	149	GLN
1	B	173	ARG
1	B	183	ASP
1	B	206	VAL
1	B	218	LEU
1	B	221	THR
1	B	232	ILE
1	B	246	TYR
1	B	267	LEU
1	B	274	SER
1	B	278	VAL
1	B	314	LEU
1	B	318	GLU
1	B	336	VAL
1	B	348	THR
1	B	351	GLN
1	B	378	SER
1	B	416	THR
1	B	427	THR
1	B	444	VAL
1	B	460	LEU
1	B	471	LEU
1	B	480	GLU
1	B	486	ARG
1	B	504	GLU
1	B	506	PHE
1	C	30	THR
1	C	89	LEU
1	C	99	VAL
1	C	105	LEU
1	C	142	ARG
1	C	159	VAL
1	C	165	GLN
1	C	210	GLN
1	C	221	THR

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Mol	Chain	Res	Type
1	C	246	TYR
1	C	254	SER
1	C	274	SER
1	C	337	SER
1	C	351	GLN
1	C	382	VAL
1	C	383	LYS
1	C	394	LEU
1	C	416	THR
1	C	468	SER
1	C	476	SER
1	C	480	GLU
1	C	487	GLU
1	C	495	LEU
1	C	498	SER
1	C	501	SER
2	D	6	SER
2	D	26	GLU
2	D	29	GLU
2	D	74	GLU
2	D	77	LEU
2	D	167	ILE
2	D	204	THR
2	D	206	VAL
2	D	214	LYS
2	D	249	GLN
2	D	251	VAL
2	D	255	ILE
2	D	268	VAL
2	D	357	LEU
2	D	359	ASP
2	D	396	LEU
2	D	397	SER
2	D	423	VAL
2	D	464	GLU
2	E	89	ARG
2	E	128	SER
2	E	129	THR
2	E	140	VAL
2	E	165	VAL
2	E	190	ARG
2	E	232	VAL

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Mol	Chain	Res	Type
2	E	298	THR
2	E	324	THR
2	E	352	ASP
2	E	359	ASP
2	E	376	GLU
2	E	380	THR
2	E	386	ASP
2	E	406	ARG
2	E	433	ARG
2	E	446	GLU
2	E	464	GLU
2	E	465	ASP
2	F	58	THR
2	F	140	VAL
2	F	163	LYS
2	F	167	ILE
2	F	182	SER
2	F	201	MET
2	F	232	VAL
2	F	251	VAL
2	F	261	PHE
2	F	303	SER
2	F	305	THR
2	F	318	THR
2	F	324	THR
2	F	354	LYS
2	F	355	SER
2	F	420	VAL
2	F	423	VAL
2	F	434	LEU
2	F	467	VAL
3	G	2	THR
3	G	3	LEU
3	G	4	LYS
3	G	9	ARG
3	G	17	GLU
3	G	19	ILE
3	G	80	ASP
3	G	106	ASP
3	G	121	THR
3	G	136	ASP
3	G	143	SER

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Mol	Chain	Res	Type
3	G	145	LEU
3	G	148	ASP
3	G	152	SER
3	G	164	ILE
3	G	216	ASN
3	G	218	MET
3	G	231	SER
3	G	234	ARG
3	G	235	ASN
3	G	247	MET
3	G	254	LEU
3	G	264	THR
3	G	269	ASP
3	G	272	THR
3	G	276	SER
4	H	12	LEU
4	H	19	GLU
4	H	29	GLN
4	H	30	VAL
4	H	42	LEU
4	H	49	VAL
4	H	60	MET
4	H	64	ASN
4	H	70	ILE
4	H	86	THR
5	I	14	LEU
5	I	27	THR
5	I	31	THR
6	J	2	GLN
6	J	16	THR
6	J	33	LEU
6	J	34	ILE
6	J	43	ILE
6	J	47	VAL
6	J	48	PHE
6	J	59	GLU
6	J	64	PHE
6	J	65	CYS
6	J	73	LEU
6	K	16	THR
6	K	33	LEU
6	K	43	ILE

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Mol	Chain	Res	Type
6	K	44	LYS
6	K	59	GLU
6	L	16	THR
6	L	33	LEU
6	L	59	GLU
6	M	16	THR
6	M	33	LEU
6	M	43	ILE
6	M	48	PHE
6	M	59	GLU
6	N	1	MET
6	N	16	THR
6	N	33	LEU
6	N	59	GLU
6	O	16	THR
6	O	33	LEU
6	O	52	ILE
6	O	59	GLU
6	O	64	PHE
6	P	16	THR
6	P	59	GLU
6	P	64	PHE
6	P	65	CYS
6	Q	16	THR
6	Q	33	LEU
6	Q	42	SER
6	Q	48	PHE
6	Q	59	GLU
6	Q	64	PHE
6	Q	65	CYS
6	R	1	MET
6	R	2	GLN
6	R	16	THR
6	R	33	LEU
6	R	44	LYS
6	R	48	PHE
6	R	59	GLU
6	R	64	PHE
6	S	16	THR
6	S	33	LEU
6	S	48	PHE
6	S	59	GLU

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Mol	Chain	Res	Type
6	S	64	PHE
6	S	71	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	398	GLN
1	A	407	GLN
1	A	418	GLN
1	B	26	ASN
1	B	47	ASN
1	B	149	GLN
1	B	174	GLN
1	B	282	GLN
1	B	351	GLN
1	B	454	HIS
1	B	477	ASN
1	C	210	GLN
1	C	225	HIS
1	C	407	GLN
1	C	452	ASN
2	D	195	ASN
2	D	367	HIS
2	E	43	GLN
2	E	168	GLN
2	F	52	GLN
3	G	90	GLN
3	G	216	ASN
5	I	15	ASN
5	I	30	GLN
6	J	2	GLN
6	M	2	GLN
6	R	2	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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$
7	ANP	D	600	8	29,33,33	2.76	9 (31%)	31,52,52	2.67	10 (32%)
7	ANP	F	600	8	29,33,33	2.79	8 (27%)	31,52,52	2.61	11 (35%)
7	ANP	A	600	8	29,33,33	2.74	8 (27%)	31,52,52	2.77	11 (35%)
7	ANP	C	600	8	29,33,33	2.76	8 (27%)	31,52,52	2.70	11 (35%)
7	ANP	B	600	8	29,33,33	2.74	8 (27%)	31,52,52	2.67	10 (32%)

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
7	ANP	D	600	8	2/2/7/8	7/14/38/38	0/3/3/3
7	ANP	F	600	8	2/2/7/8	7/14/38/38	0/3/3/3
7	ANP	A	600	8	2/2/7/8	8/14/38/38	0/3/3/3
7	ANP	C	600	8	2/2/7/8	9/14/38/38	0/3/3/3
7	ANP	B	600	8	2/2/7/8	3/14/38/38	0/3/3/3

All (41) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	600	ANP	PB-O3A	-10.59	1.45	1.59
7	C	600	ANP	PB-O3A	-10.37	1.46	1.59
7	B	600	ANP	PB-O3A	-10.25	1.46	1.59
7	A	600	ANP	PB-O3A	-10.20	1.46	1.59
7	D	600	ANP	PB-O3A	-10.18	1.46	1.59
7	D	600	ANP	PG-O1G	6.63	1.56	1.46
7	A	600	ANP	PG-O1G	6.55	1.56	1.46
7	C	600	ANP	PG-O1G	6.47	1.56	1.46
7	F	600	ANP	PG-O1G	6.44	1.56	1.46
7	B	600	ANP	PG-O1G	6.41	1.56	1.46
7	B	600	ANP	C2-N3	3.48	1.37	1.32
7	A	600	ANP	C2-N3	3.39	1.37	1.32
7	C	600	ANP	C2-N3	3.21	1.37	1.32
7	D	600	ANP	C2-N3	3.21	1.37	1.32
7	F	600	ANP	C2-N3	3.20	1.37	1.32
7	F	600	ANP	PA-O5'	-2.96	1.47	1.59
7	C	600	ANP	PA-O5'	-2.91	1.47	1.59
7	B	600	ANP	C6-N6	2.90	1.44	1.34
7	D	600	ANP	PA-O5'	-2.89	1.47	1.59
7	F	600	ANP	C6-N6	2.87	1.44	1.34
7	C	600	ANP	C6-N6	2.87	1.44	1.34
7	A	600	ANP	C6-N6	2.87	1.44	1.34
7	D	600	ANP	C6-N6	2.85	1.44	1.34
7	A	600	ANP	PA-O5'	-2.85	1.47	1.59
7	B	600	ANP	PA-O5'	-2.83	1.47	1.59
7	D	600	ANP	C2'-C1'	-2.71	1.49	1.53
7	F	600	ANP	PG-O2G	-2.67	1.49	1.56
7	C	600	ANP	PB-N3B	-2.64	1.56	1.63
7	F	600	ANP	C2'-C1'	-2.63	1.49	1.53
7	B	600	ANP	PG-O2G	-2.62	1.49	1.56
7	A	600	ANP	PB-N3B	-2.61	1.56	1.63
7	D	600	ANP	PG-O2G	-2.61	1.49	1.56
7	C	600	ANP	PG-O2G	-2.60	1.49	1.56
7	A	600	ANP	PG-O2G	-2.58	1.49	1.56
7	D	600	ANP	PB-N3B	-2.58	1.56	1.63
7	B	600	ANP	PB-N3B	-2.52	1.56	1.63
7	F	600	ANP	PB-N3B	-2.51	1.56	1.63
7	C	600	ANP	C2'-C1'	-2.24	1.50	1.53
7	A	600	ANP	C2'-C1'	-2.23	1.50	1.53
7	B	600	ANP	C2'-C1'	-2.16	1.50	1.53
7	D	600	ANP	C2'-C3'	-2.04	1.47	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	600	ANP	O1B-PB-N3B	-9.49	97.80	111.77
7	A	600	ANP	O1B-PB-N3B	-9.41	97.91	111.77
7	C	600	ANP	O1B-PB-N3B	-8.90	98.67	111.77
7	F	600	ANP	O1B-PB-N3B	-8.62	99.08	111.77
7	B	600	ANP	O1B-PB-N3B	-8.11	99.83	111.77
7	D	600	ANP	N3-C2-N1	-5.19	120.56	128.68
7	C	600	ANP	N3-C2-N1	-5.18	120.59	128.68
7	F	600	ANP	N3-C2-N1	-5.17	120.60	128.68
7	A	600	ANP	N3-C2-N1	-5.07	120.75	128.68
7	B	600	ANP	N3-C2-N1	-5.01	120.84	128.68
7	F	600	ANP	O2B-PB-O1B	4.98	120.37	109.92
7	C	600	ANP	O2B-PB-O1B	4.61	119.58	109.92
7	D	600	ANP	O2B-PB-O1B	4.59	119.53	109.92
7	B	600	ANP	O2B-PB-O1B	4.57	119.51	109.92
7	A	600	ANP	O2B-PB-O3A	4.50	119.67	104.64
7	A	600	ANP	O2B-PB-O1B	4.50	119.36	109.92
7	B	600	ANP	O2B-PB-O3A	4.49	119.63	104.64
7	C	600	ANP	O2B-PB-O3A	4.38	119.25	104.64
7	B	600	ANP	C1'-N9-C4	4.22	134.05	126.64
7	D	600	ANP	O2B-PB-O3A	4.13	118.42	104.64
7	C	600	ANP	O3A-PB-N3B	-4.04	95.38	106.59
7	B	600	ANP	O3A-PB-N3B	-4.01	95.48	106.59
7	A	600	ANP	C1'-N9-C4	3.85	133.40	126.64
7	F	600	ANP	O2B-PB-O3A	3.85	117.49	104.64
7	F	600	ANP	O3A-PB-N3B	-3.78	96.10	106.59
7	A	600	ANP	O3A-PB-N3B	-3.50	96.88	106.59
7	B	600	ANP	O5'-PA-O1A	-3.26	96.31	109.07
7	A	600	ANP	O5'-PA-O1A	-3.25	96.36	109.07
7	A	600	ANP	PA-O3A-PB	-3.20	121.33	132.62
7	C	600	ANP	O5'-PA-O1A	-3.20	96.57	109.07
7	B	600	ANP	PA-O3A-PB	-3.19	121.36	132.62
7	F	600	ANP	O5'-PA-O1A	-3.11	96.90	109.07
7	C	600	ANP	PA-O3A-PB	-2.99	122.08	132.62
7	D	600	ANP	O3A-PB-N3B	-2.98	98.32	106.59
7	D	600	ANP	O5'-PA-O1A	-2.94	97.59	109.07
7	F	600	ANP	C1'-N9-C4	2.85	131.65	126.64
7	F	600	ANP	PA-O3A-PB	-2.83	122.66	132.62
7	C	600	ANP	C1'-N9-C4	2.82	131.60	126.64
7	D	600	ANP	C1'-N9-C4	2.78	131.53	126.64
7	D	600	ANP	PA-O3A-PB	-2.76	122.89	132.62
7	D	600	ANP	O3G-PG-O1G	-2.55	107.04	113.45
7	B	600	ANP	O2A-PA-O5'	2.55	119.58	107.75
7	A	600	ANP	O2A-PA-O5'	2.53	119.51	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	600	ANP	O2A-PA-O5'	2.52	119.44	107.75
7	F	600	ANP	O2A-PA-O5'	2.51	119.42	107.75
7	C	600	ANP	O3G-PG-O1G	-2.48	107.23	113.45
7	A	600	ANP	O3G-PG-O1G	-2.38	107.46	113.45
7	D	600	ANP	O2A-PA-O5'	2.32	118.50	107.75
7	C	600	ANP	O1G-PG-N3B	-2.29	108.39	111.77
7	B	600	ANP	O3G-PG-O1G	-2.22	107.87	113.45
7	F	600	ANP	O3G-PG-O1G	-2.10	108.19	113.45
7	A	600	ANP	O1G-PG-N3B	-2.06	108.74	111.77
7	F	600	ANP	O1G-PG-N3B	-2.04	108.77	111.77

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	F	600	ANP	C3'
7	F	600	ANP	C1'
7	B	600	ANP	C3'
7	B	600	ANP	C1'
7	D	600	ANP	C3'
7	D	600	ANP	C1'
7	A	600	ANP	C3'
7	A	600	ANP	C1'
7	C	600	ANP	C3'
7	C	600	ANP	C1'

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	600	ANP	PB-N3B-PG-O1G
7	F	600	ANP	PG-N3B-PB-O1B
7	F	600	ANP	PG-N3B-PB-O3A
7	F	600	ANP	PA-O3A-PB-O1B
7	F	600	ANP	O4'-C4'-C5'-O5'
7	B	600	ANP	PB-N3B-PG-O1G
7	B	600	ANP	PG-N3B-PB-O1B
7	B	600	ANP	PA-O3A-PB-O1B
7	D	600	ANP	PB-N3B-PG-O1G
7	D	600	ANP	PG-N3B-PB-O1B
7	D	600	ANP	PG-N3B-PB-O3A
7	D	600	ANP	PA-O3A-PB-O1B
7	D	600	ANP	PA-O3A-PB-O2B
7	D	600	ANP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
7	D	600	ANP	C3'-C4'-C5'-O5'
7	A	600	ANP	PG-N3B-PB-O1B
7	A	600	ANP	PG-N3B-PB-O3A
7	A	600	ANP	PA-O3A-PB-O1B
7	A	600	ANP	C5'-O5'-PA-O1A
7	C	600	ANP	PG-N3B-PB-O1B
7	C	600	ANP	PG-N3B-PB-O3A
7	C	600	ANP	PA-O3A-PB-O1B
7	C	600	ANP	C5'-O5'-PA-O1A
7	C	600	ANP	O4'-C4'-C5'-O5'
7	C	600	ANP	C3'-C4'-C5'-O5'
7	F	600	ANP	C3'-C4'-C5'-O5'
7	A	600	ANP	C3'-C4'-C5'-O5'
7	A	600	ANP	O4'-C4'-C5'-O5'
7	C	600	ANP	C5'-O5'-PA-O3A
7	A	600	ANP	C5'-O5'-PA-O2A
7	C	600	ANP	C5'-O5'-PA-O2A
7	F	600	ANP	PA-O3A-PB-O2B
7	A	600	ANP	PA-O3A-PB-O2B
7	C	600	ANP	PA-O3A-PB-O2B

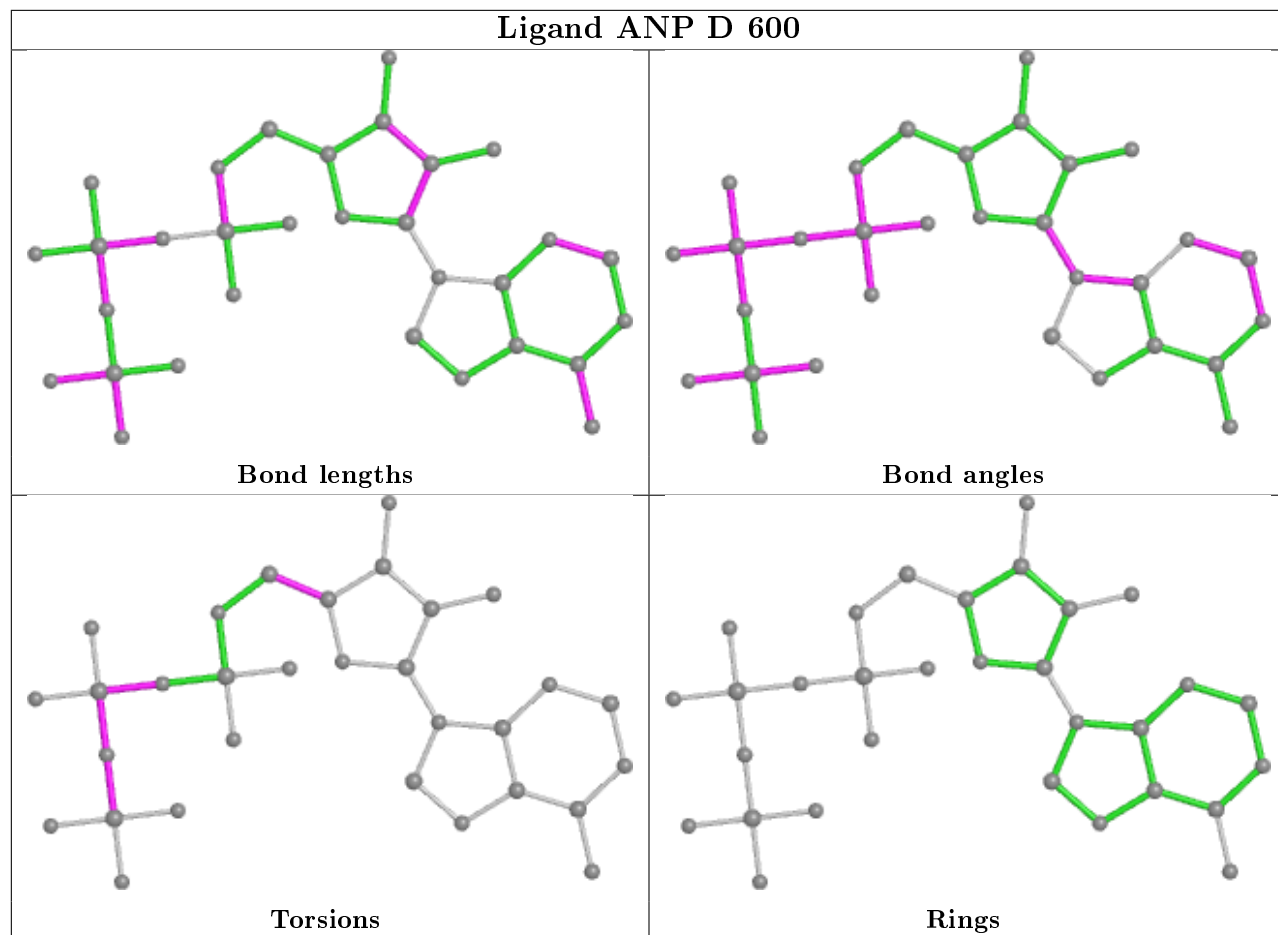
There are no ring outliers.

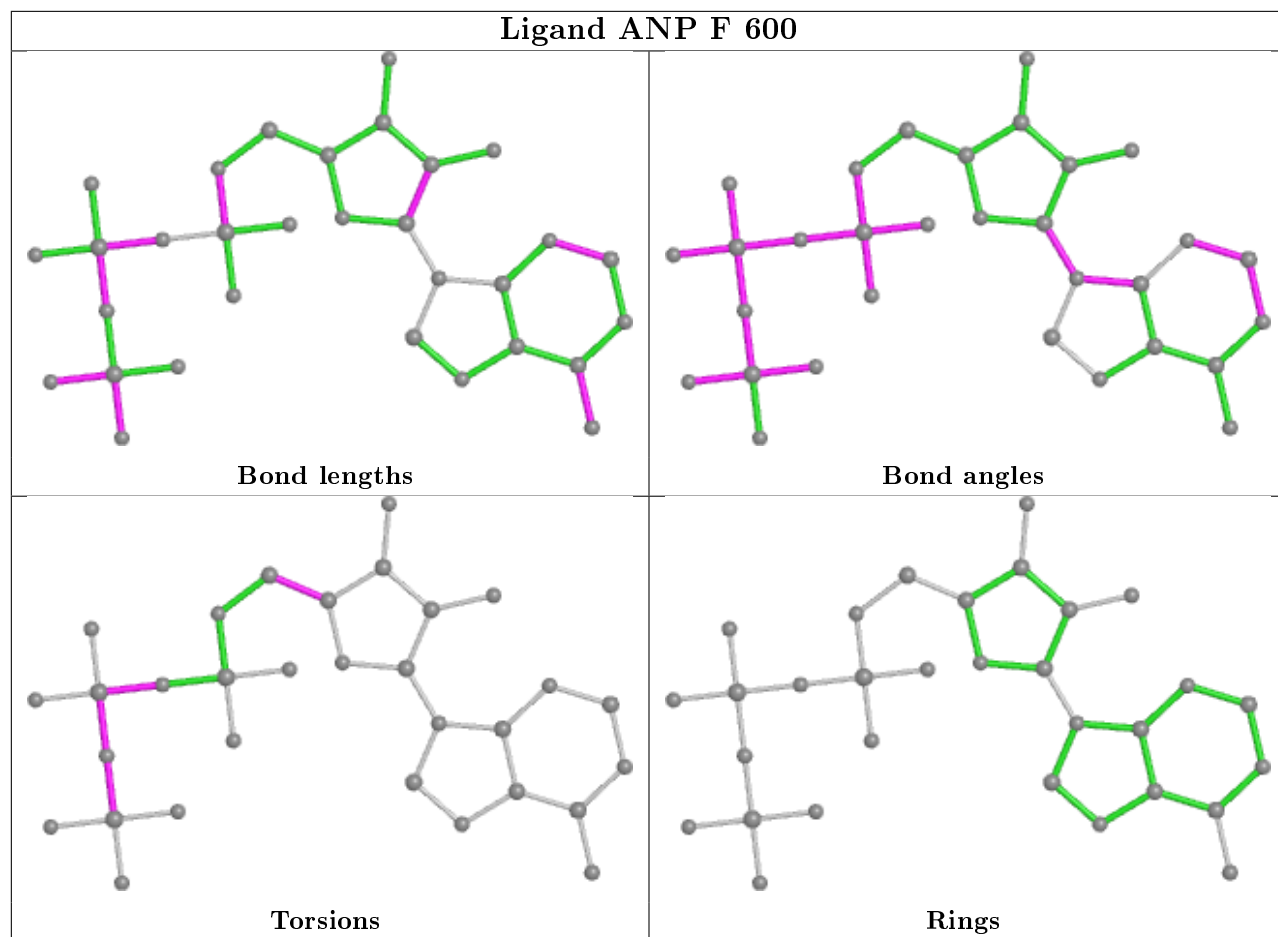
5 monomers are involved in 24 short contacts:

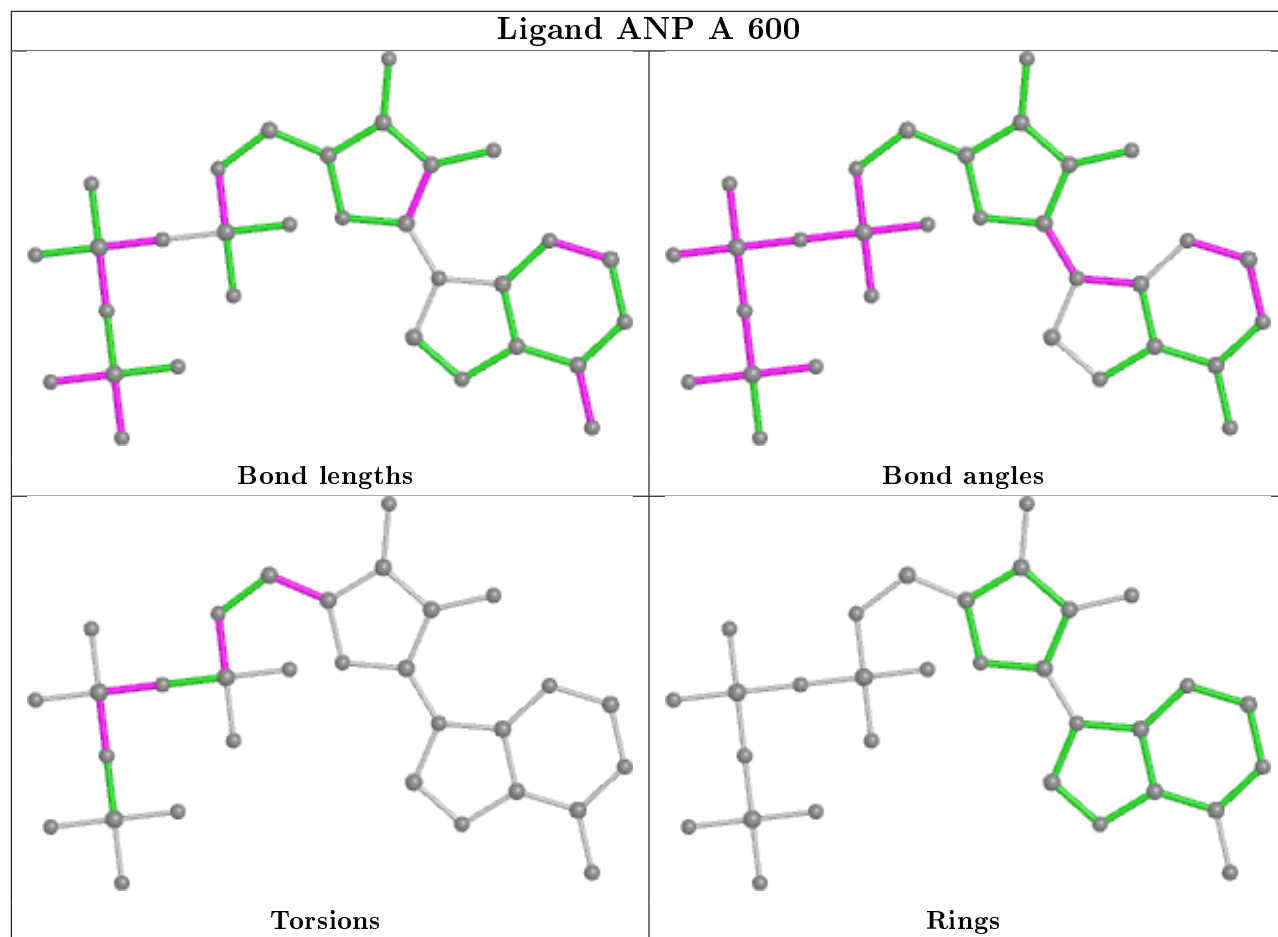
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	600	ANP	6	0
7	F	600	ANP	10	0
7	A	600	ANP	1	0
7	C	600	ANP	5	0
7	B	600	ANP	2	0

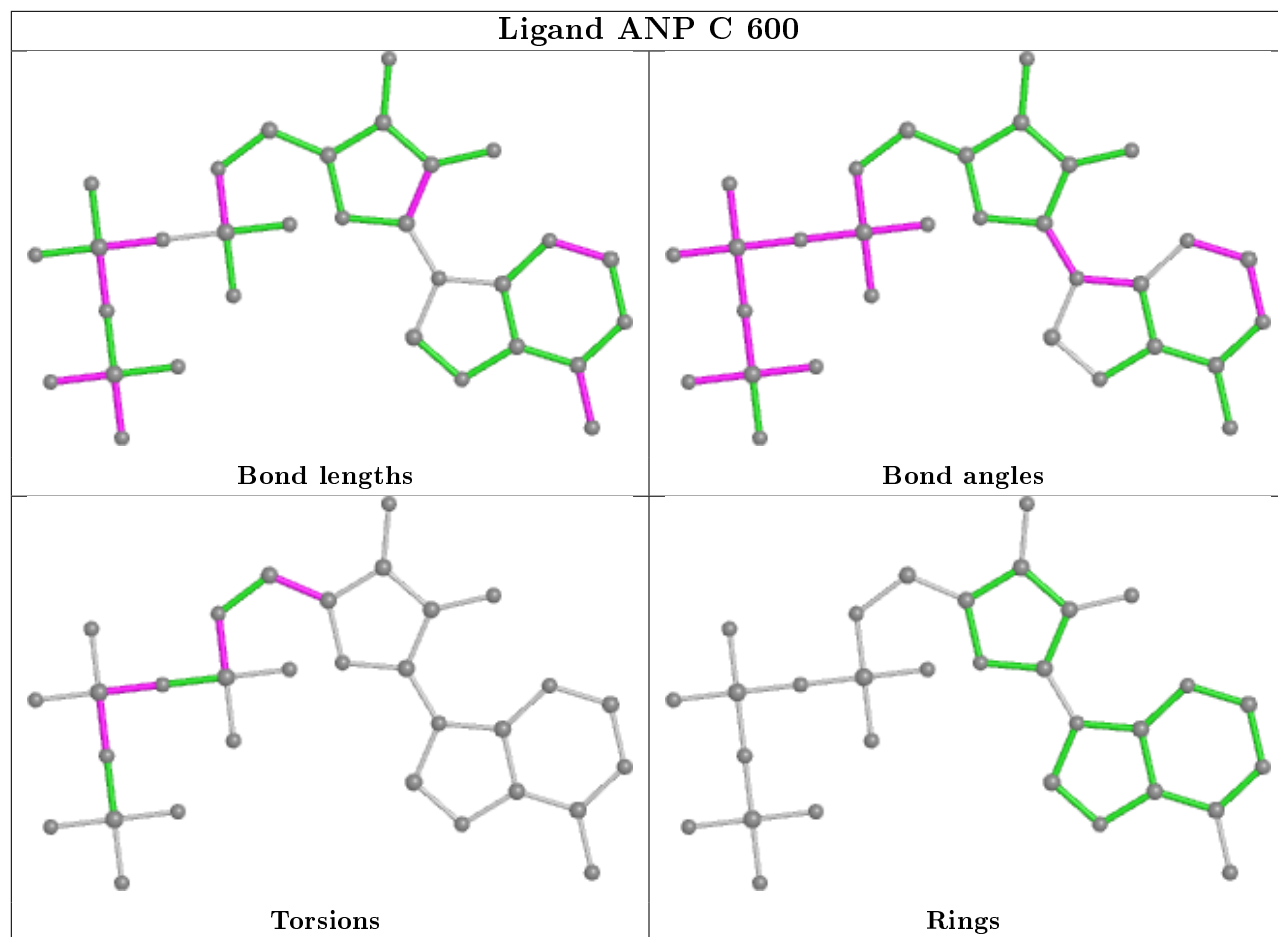
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

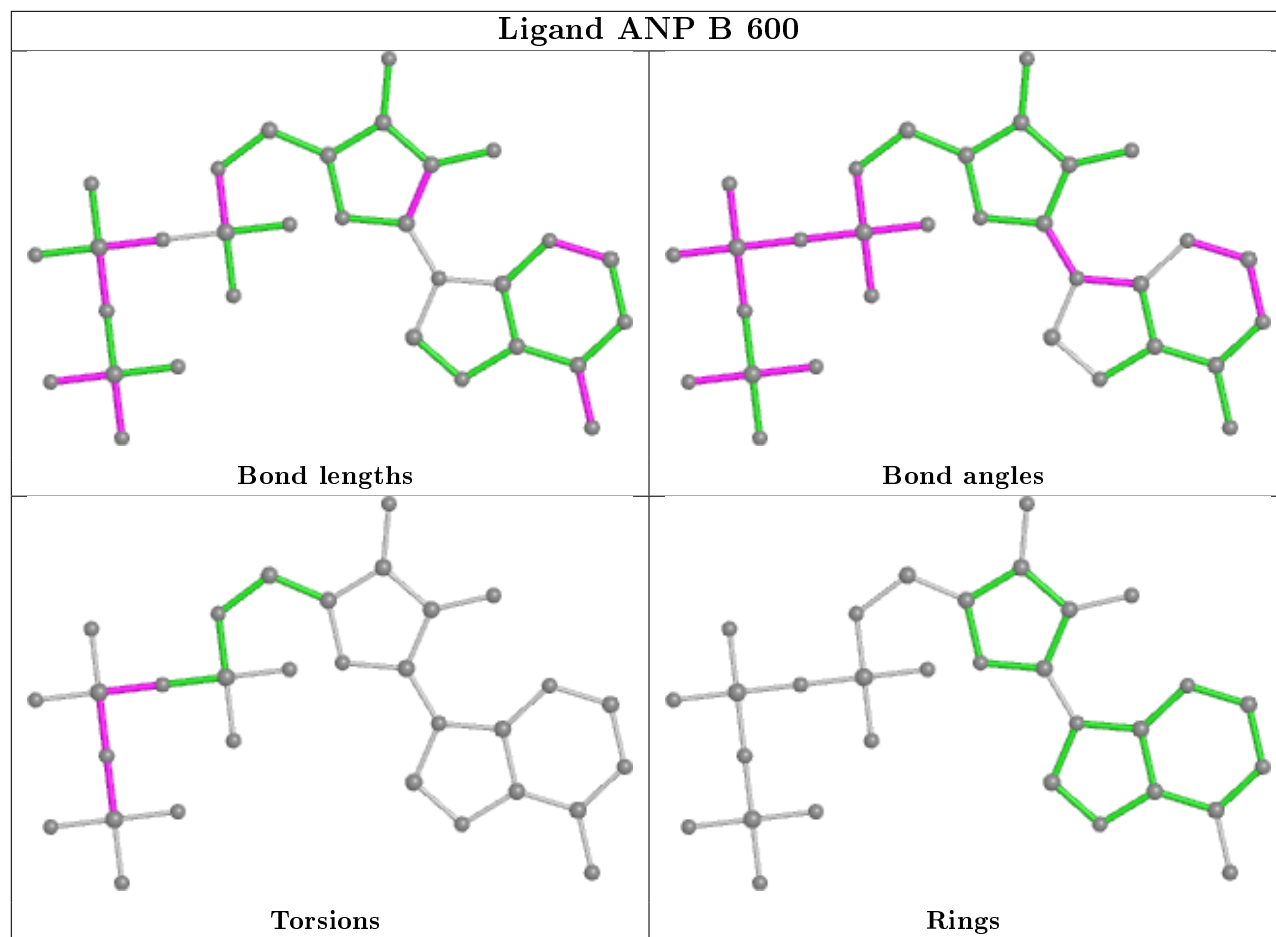












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	200:ASP	C	201:THR	N	3.99

## 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	483/510 (94%)	0.17	7 (1%) 75 66	190, 219, 279, 304	0
1	B	484/510 (94%)	0.27	13 (2%) 54 47	184, 237, 325, 351	0
1	C	485/510 (95%)	0.54	35 (7%) 15 16	255, 279, 425, 448	0
2	D	471/478 (98%)	0.48	35 (7%) 14 15	217, 250, 325, 361	0
2	E	469/478 (98%)	0.56	47 (10%) 7 10	215, 255, 301, 336	0
2	F	470/478 (98%)	0.62	43 (9%) 9 11	242, 287, 363, 404	0
3	G	266/278 (95%)	1.44	87 (32%) 0 2	315, 367, 397, 413	0
4	H	119/138 (86%)	1.19	23 (19%) 1 3	339, 382, 438, 476	0
5	I	49/61 (80%)	0.84	6 (12%) 4 8	298, 368, 423, 442	0
6	J	73/76 (96%)	0.84	9 (12%) 4 8	407, 446, 474, 482	0
6	K	73/76 (96%)	0.51	9 (12%) 4 8	414, 437, 478, 491	0
6	L	72/76 (94%)	0.33	4 (5%) 24 24	399, 482, 524, 524	0
6	M	73/76 (96%)	0.72	11 (15%) 2 5	424, 488, 520, 520	0
6	N	73/76 (96%)	0.50	5 (6%) 17 17	430, 526, 526, 526	0
6	O	74/76 (97%)	0.52	5 (6%) 17 17	420, 455, 487, 493	0
6	P	75/76 (98%)	0.57	8 (10%) 6 9	419, 452, 487, 506	0
6	Q	75/76 (98%)	0.75	6 (8%) 12 14	445, 458, 488, 517	0
6	R	74/76 (97%)	0.74	9 (12%) 4 8	414, 436, 466, 485	0
6	S	74/76 (97%)	0.88	10 (13%) 3 6	378, 432, 464, 480	0
All	All	4032/4201 (95%)	0.57	372 (9%) 9 11	184, 280, 466, 526	0

All (372) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	J	74	PHE	10.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	P	75	GLY	8.0
2	F	461	GLY	7.7
3	G	134	GLY	7.1
3	G	122	HIS	7.1
4	H	44	ASN	7.0
4	H	43	ALA	6.6
4	H	81	SER	6.6
4	H	42	LEU	6.0
3	G	103	PRO	6.0
6	J	73	LEU	5.9
3	G	104	ASN	5.8
3	G	125	ASN	5.8
2	F	357	LEU	5.5
2	F	430	LYS	5.4
3	G	105	ALA	5.4
6	Q	2	GLN	5.1
1	B	410	SER	5.0
2	F	358	LEU	5.0
6	P	74	PHE	4.9
3	G	138	PRO	4.8
6	J	2	GLN	4.7
3	G	124	ASN	4.7
1	C	488	LYS	4.7
1	C	483	THR	4.6
3	G	59	ASN	4.5
6	S	2	GLN	4.5
6	P	1	MET	4.5
6	Q	1	MET	4.5
3	G	71	LYS	4.5
4	H	28	THR	4.4
3	G	167	ASN	4.4
6	R	2	GLN	4.4
1	C	490	GLU	4.4
1	C	491	LEU	4.4
3	G	206	PRO	4.4
6	J	71	LEU	4.3
4	H	26	GLU	4.3
4	H	80	ASP	4.3
6	P	73	LEU	4.3
3	G	121	THR	4.3
4	H	82	GLN	4.3
6	S	1	MET	4.2

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Mol	Chain	Res	Type	RSRZ
6	P	71	LEU	4.2
1	A	402	VAL	4.2
6	J	70	PHE	4.2
1	B	411	ASP	4.2
3	G	106	ASP	4.1
3	G	87	ILE	4.1
2	F	143	LEU	4.1
3	G	211	GLU	4.1
2	D	31	PRO	4.1
6	Q	75	GLY	4.0
4	H	29	GLN	4.0
1	B	490	GLU	3.9
1	C	484	GLU	3.9
3	G	140	PHE	3.9
3	G	214	LEU	3.9
2	E	297	THR	3.9
2	F	299	THR	3.9
6	M	1	MET	3.9
2	D	429	GLY	3.8
1	C	101	VAL	3.8
6	L	73	LEU	3.8
2	D	63	ALA	3.8
4	H	68	PHE	3.8
6	R	54	GLY	3.8
3	G	102	GLN	3.8
1	C	124	ASP	3.8
6	M	50	MET	3.8
3	G	207	ARG	3.7
2	D	430	LYS	3.7
1	C	482	LEU	3.7
6	S	74	PHE	3.7
2	E	333	THR	3.7
4	H	41	VAL	3.7
6	R	73	LEU	3.7
3	G	1	ALA	3.6
6	N	30	PHE	3.6
3	G	99	LEU	3.6
3	G	232	ALA	3.6
4	H	40	GLY	3.6
3	G	191	SER	3.6
3	G	100	ASN	3.6
2	D	64	MET	3.6

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Mol	Chain	Res	Type	RSRZ
5	I	49	ASN	3.5
1	C	123	ILE	3.5
2	E	353	SER	3.5
2	F	16	VAL	3.5
2	D	315	ASP	3.5
1	C	100	PRO	3.5
3	G	123	PRO	3.5
6	M	51	ALA	3.5
3	G	224	GLN	3.5
1	B	488	LYS	3.5
1	C	73	VAL	3.5
2	E	391	LEU	3.5
1	C	485	ILE	3.4
4	H	30	VAL	3.4
3	G	168	ASP	3.4
5	I	28	GLU	3.4
3	G	37	ALA	3.4
2	D	461	GLY	3.4
4	H	27	VAL	3.4
2	D	48	LEU	3.4
2	E	395	GLU	3.3
3	G	133	ILE	3.3
6	K	48	PHE	3.3
6	S	67	MET	3.3
2	F	433	ARG	3.3
3	G	34	ALA	3.3
3	G	107	ILE	3.3
3	G	231	SER	3.3
6	S	73	LEU	3.3
6	K	47	VAL	3.3
5	I	27	THR	3.3
1	C	480	GLU	3.2
6	R	51	ALA	3.2
2	F	367	HIS	3.2
2	D	37	LEU	3.2
2	F	144	LEU	3.2
6	R	1	MET	3.2
6	O	41	PRO	3.2
1	A	432	GLN	3.1
6	M	2	GLN	3.1
2	D	38	GLU	3.1
1	C	202	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
3	G	101	ASP	3.1
1	C	125	ALA	3.1
6	N	33	LEU	3.1
1	C	335	ASP	3.0
3	G	273	GLY	3.0
3	G	276	SER	3.0
3	G	228	ALA	3.0
3	G	72	GLU	3.0
3	G	2	THR	3.0
2	D	78	ASP	3.0
2	E	350	PRO	3.0
2	F	362	VAL	3.0
2	F	39	ILE	3.0
3	G	230	ILE	3.0
3	G	79	SER	3.0
3	G	135	LYS	3.0
2	F	118	HIS	3.0
1	C	192	ASN	3.0
2	F	70	LEU	3.0
3	G	137	ALA	2.9
2	E	348	VAL	2.9
2	E	420	VAL	2.9
2	F	460	VAL	2.9
3	G	45	ASP	2.9
6	R	71	LEU	2.9
2	E	147	TYR	2.9
3	G	55	ALA	2.9
3	G	200	ASP	2.9
2	D	47	VAL	2.9
3	G	175	PHE	2.9
2	E	143	LEU	2.9
3	G	78	THR	2.9
6	P	70	PHE	2.9
3	G	44	MET	2.9
2	F	429	GLY	2.8
2	F	86	PRO	2.8
6	L	71	LEU	2.8
2	E	393	MET	2.8
6	Q	50	MET	2.8
2	E	86	PRO	2.8
2	E	296	ILE	2.8
2	F	139	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
6	K	44	LYS	2.8
2	F	136	THR	2.8
1	C	102	GLY	2.8
1	B	407	GLN	2.8
2	F	418	PHE	2.7
6	J	47	VAL	2.7
2	E	122	PRO	2.7
2	F	432	VAL	2.7
3	G	9	ARG	2.7
2	F	434	LEU	2.7
2	D	228	ALA	2.7
3	G	229	GLU	2.7
6	O	42	SER	2.7
2	E	298	THR	2.7
6	S	71	LEU	2.7
2	E	293	GLN	2.7
2	E	394	ASP	2.7
2	F	298	THR	2.7
2	E	181	PHE	2.7
6	J	67	MET	2.7
3	G	169	PRO	2.6
6	Q	46	THR	2.6
1	C	193	ASN	2.6
2	D	428	PRO	2.6
2	E	388	ILE	2.6
3	G	233	ARG	2.6
1	A	490	GLU	2.6
6	K	52	ILE	2.6
1	B	294	GLU	2.6
1	C	489	GLY	2.6
2	F	89	ARG	2.6
1	C	43	VAL	2.6
2	D	79	THR	2.6
2	F	212	GLU	2.6
3	G	275	SER	2.6
2	E	386	ASP	2.6
5	I	30	GLN	2.6
2	F	417	PRO	2.6
1	C	334	GLY	2.6
1	B	413	ASP	2.6
2	D	75	LYS	2.6
2	D	77	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	358	LEU	2.6
1	C	365	PRO	2.6
3	G	227	ALA	2.6
6	M	48	PHE	2.6
2	F	359	ASP	2.6
3	G	126	ILE	2.6
3	G	226	TYR	2.6
2	F	356	ARG	2.5
2	E	157	GLY	2.5
1	B	509	THR	2.5
3	G	222	MET	2.5
2	D	130	SER	2.5
2	D	143	LEU	2.5
2	D	110	LYS	2.5
2	E	367	HIS	2.5
3	G	80	ASP	2.5
2	F	131	ALA	2.5
2	E	53	HIS	2.5
4	H	36	SER	2.5
2	F	146	PRO	2.5
1	A	153	LYS	2.5
1	B	503	THR	2.5
1	B	49	ILE	2.5
2	D	118	HIS	2.5
3	G	28	SER	2.5
5	I	11	ALA	2.5
2	E	198	TYR	2.5
6	M	5	LEU	2.5
1	C	44	PHE	2.5
2	E	158	GLY	2.5
6	Q	40	ASN	2.5
3	G	84	CYS	2.4
2	E	389	ALA	2.4
1	A	405	PHE	2.4
1	C	333	GLY	2.4
2	E	387	ILE	2.4
4	H	14	PHE	2.4
2	F	416	GLN	2.4
6	L	50	MET	2.4
2	F	120	ASP	2.4
4	H	13	GLN	2.4
2	D	28	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	312	ALA	2.4
2	F	275	ILE	2.4
3	G	177	PRO	2.4
2	E	146	PRO	2.4
2	E	390	ILE	2.3
3	G	86	SER	2.3
3	G	88	HIS	2.3
6	R	70	PHE	2.3
2	F	209	LEU	2.3
2	E	392	GLY	2.3
3	G	204	ASN	2.3
2	E	404	VAL	2.3
2	F	297	THR	2.3
6	K	30	PHE	2.3
2	E	332	THR	2.3
4	H	45	HIS	2.3
6	K	53	LEU	2.3
3	G	6	VAL	2.3
3	G	38	LYS	2.3
3	G	81	LYS	2.3
2	E	346	PRO	2.3
2	E	418	PHE	2.3
2	E	429	GLY	2.3
2	D	198	TYR	2.3
2	D	87	VAL	2.3
2	F	431	LEU	2.3
1	C	391	SER	2.3
1	C	41	ALA	2.3
1	B	491	LEU	2.3
2	F	91	THR	2.3
2	E	31	PRO	2.3
6	K	51	ALA	2.3
6	M	54	GLY	2.3
1	C	503	THR	2.3
2	E	109	ILE	2.2
1	B	68	LEU	2.2
2	F	48	LEU	2.2
1	C	337	SER	2.2
3	G	47	ALA	2.2
6	M	53	LEU	2.2
6	L	30	PHE	2.2
2	E	59	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	G	74	ILE	2.2
5	I	42	ALA	2.2
2	D	129	THR	2.2
2	D	106	ARG	2.2
6	K	49	PRO	2.2
2	D	98	VAL	2.2
2	D	331	ALA	2.2
6	R	52	ILE	2.2
6	S	29	VAL	2.2
2	F	428	PRO	2.2
2	F	147	TYR	2.2
4	H	67	LYS	2.2
1	C	390	GLY	2.2
3	G	274	ALA	2.2
6	P	44	LYS	2.2
2	E	295	ARG	2.2
6	M	72	LEU	2.2
6	O	2	GLN	2.2
1	C	266	ALA	2.2
2	E	461	GLY	2.2
6	M	30	PHE	2.2
2	F	46	LEU	2.2
6	J	50	MET	2.2
2	F	350	PRO	2.2
3	G	30	ARG	2.2
3	G	139	THR	2.2
3	G	210	PHE	2.2
2	E	419	ALA	2.2
1	A	416	THR	2.2
6	R	50	MET	2.2
6	S	44	LYS	2.2
2	E	168	GLN	2.1
6	S	45	ASP	2.1
1	C	130	ARG	2.1
6	O	1	MET	2.1
2	E	204	THR	2.1
3	G	160	PRO	2.1
6	N	67	MET	2.1
1	C	338	ALA	2.1
6	M	33	LEU	2.1
1	C	203	CYS	2.1
4	H	62	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	314	ALA	2.1
3	G	176	GLU	2.1
4	H	83	LEU	2.1
2	E	106	ARG	2.1
3	G	198	GLU	2.1
4	H	66	LYS	2.1
6	S	27	ALA	2.1
1	B	51	ALA	2.1
3	G	201	THR	2.1
2	F	71	VAL	2.1
3	G	235	ASN	2.1
3	G	120	ARG	2.1
4	H	79	PRO	2.1
2	D	144	LEU	2.1
2	D	181	PHE	2.1
3	G	234	ARG	2.1
3	G	77	ILE	2.1
2	D	128	SER	2.1
3	G	27	ALA	2.1
6	O	50	MET	2.1
3	G	225	GLY	2.1
3	G	190	GLN	2.0
1	A	412	LEU	2.0
2	E	417	PRO	2.0
6	P	2	GLN	2.0
6	K	56	ALA	2.0
6	N	8	LYS	2.0
3	G	172	SER	2.0
2	D	67	THR	2.0
3	G	213	THR	2.0
2	D	227	GLY	2.0
2	E	334	VAL	2.0
6	N	73	LEU	2.0
6	J	57	LEU	2.0
2	D	111	SER	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 monosaccharides in this entry.

## 6.4 Ligands ⓘ

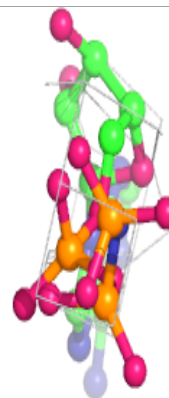
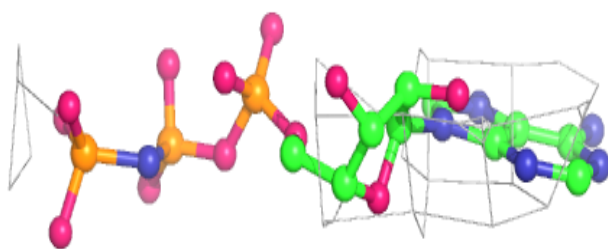
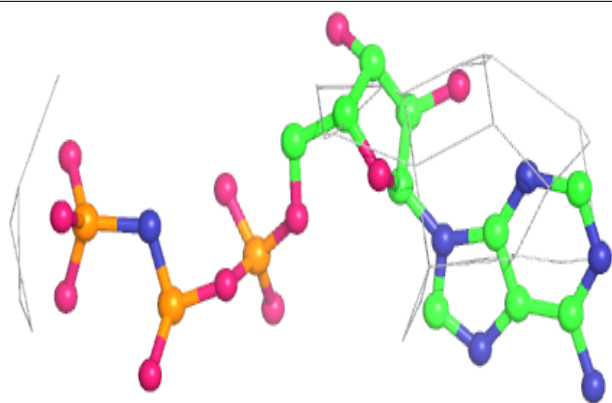
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	ANP	C	600	31/31	0.73	0.41	309,327,335,341	0
7	ANP	F	600	31/31	0.78	0.42	216,249,272,272	0
7	ANP	A	600	31/31	0.80	0.53	199,210,219,227	0
8	MG	B	700	1/1	0.80	0.89	410,410,410,410	0
7	ANP	B	600	31/31	0.81	0.41	190,214,226,227	0
8	MG	F	700	1/1	0.84	0.65	376,376,376,376	0
7	ANP	D	600	31/31	0.89	0.39	231,238,281,287	0
8	MG	C	700	1/1	0.90	0.74	405,405,405,405	0
8	MG	D	700	1/1	0.90	0.45	395,395,395,395	0
8	MG	A	700	1/1	0.95	0.74	394,394,394,394	0

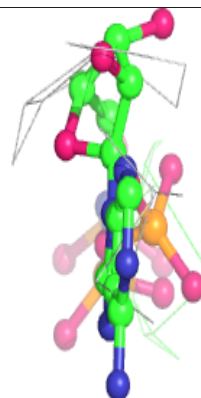
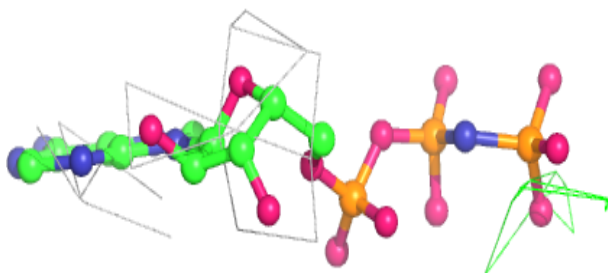
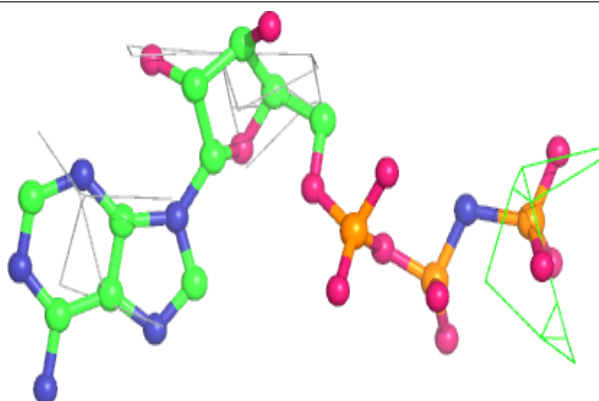
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ANP C 600:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

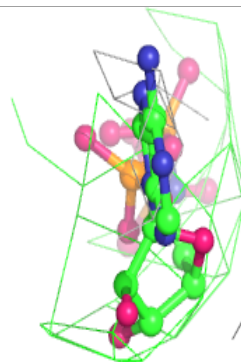
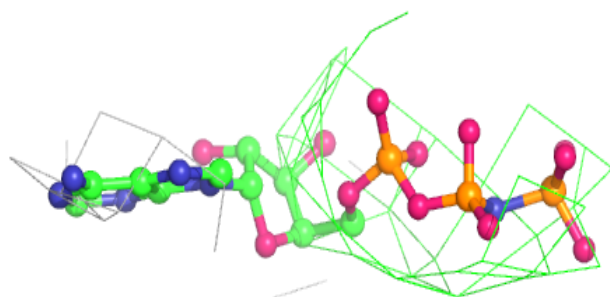
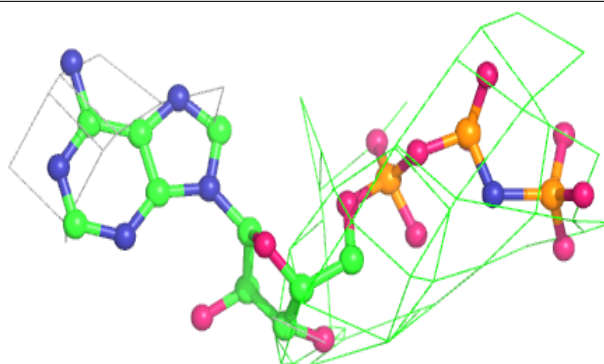
**Electron density around ANP F 600:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

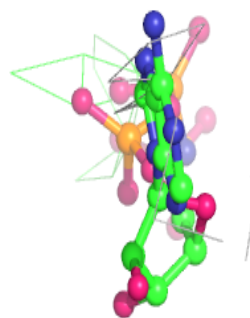
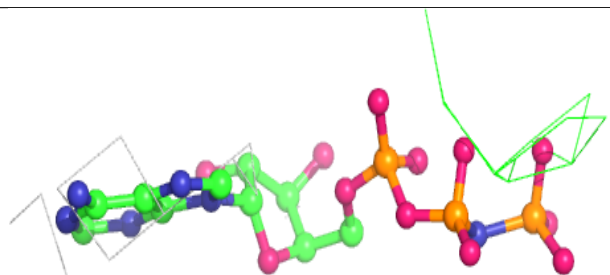
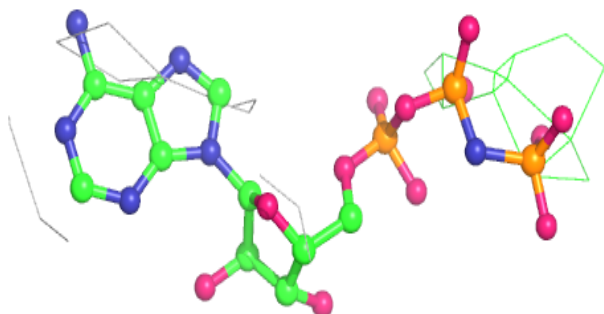


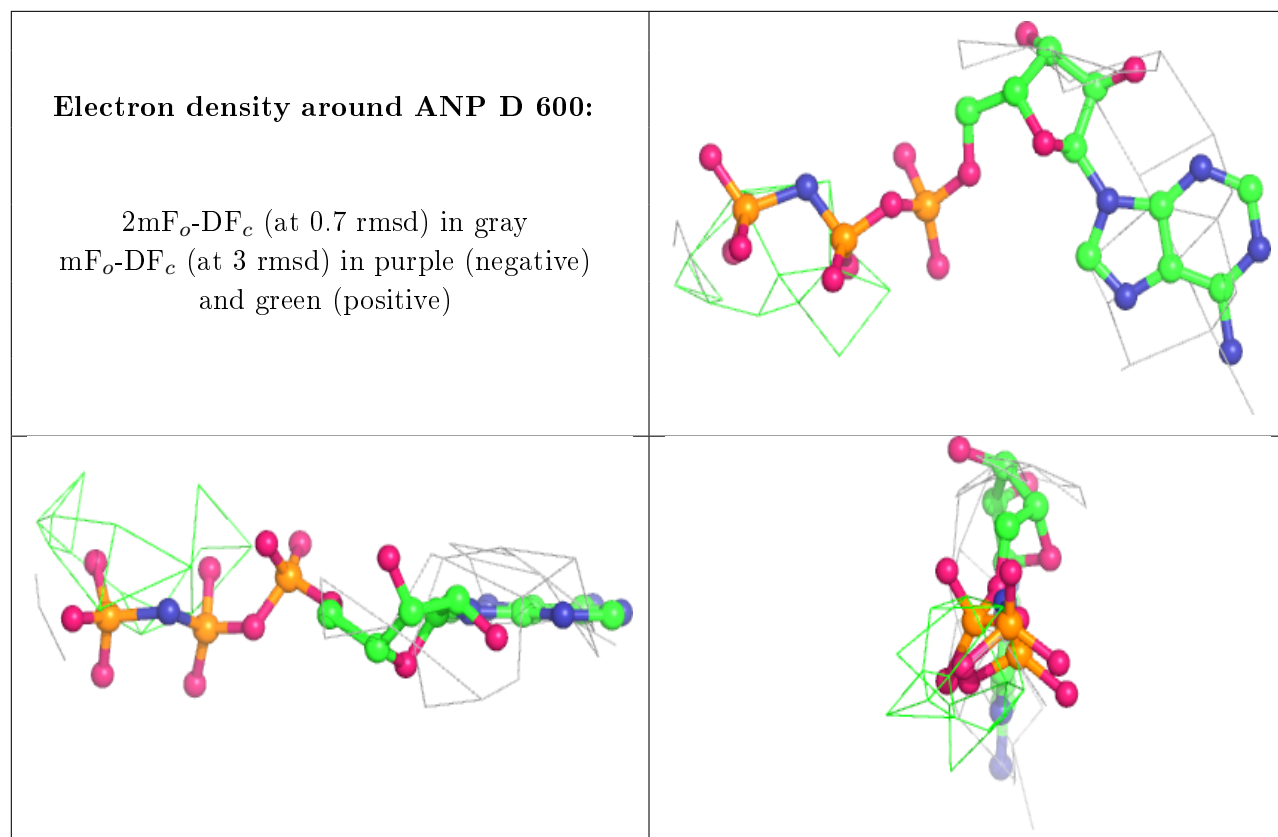
**Electron density around ANP A 600:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ANP B 600:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.