



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:41 pm BST

PDB ID : 5B0O
Title : Structure of the FliH-FliI complex
Authors : Imada, K.; Uchida, Y.; Kinoshita, M.; Namba, K.; Minamino, T.
Deposited on : 2015-11-02
Resolution : 3.00 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

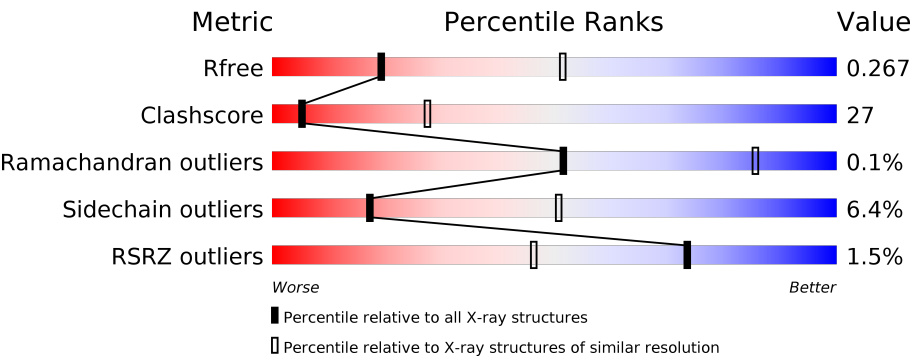
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 ≥ 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	456	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>55%40%..</div></div>
1	B	456	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>62%34%. .</div></div>
1	C	456	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>51%42%..</div></div>
1	D	456	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>59%37%. .</div></div>
2	E	140	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>62%33%..</div></div>
2	F	140	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>42%44%. 10%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	140	<div><div><div>%</div><div><div></div><div>48%</div><div>44%</div><div>6%</div></div><div></div></div></div>
2	H	140	<div><div><div>4%</div><div><div></div><div>43%</div><div>50%</div><div></div></div><div></div></div></div>
2	I	140	<div><div><div></div><div><div></div><div>61%</div><div>33%</div><div>5%</div></div><div></div></div></div>
2	J	140	<div><div><div>6%</div><div><div></div><div>41%</div><div>49%</div><div>5%</div></div><div></div></div></div>
2	K	140	<div><div><div></div><div><div></div><div>52%</div><div>42%</div><div>5%</div></div><div></div></div></div>
2	L	140	<div><div><div>3%</div><div><div></div><div>44%</div><div>43%</div><div>9%</div></div><div></div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21982 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 Flagellum-specific ATP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3391	2148	607	625	11			
1	B	455	Total	C	N	O	S	0	0	0
			3460	2187	621	641	11			
1	C	445	Total	C	N	O	S	0	0	0
			3395	2151	607	626	11			
1	D	454	Total	C	N	O	S	0	0	0
			3452	2182	620	639	11			

- Molecule 2 is a protein called Flagellar assembly protein FliH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	135	Total	C	N	O	S	0	0	0
			1040	645	193	196	6			
2	F	126	Total	C	N	O	S	0	0	0
			966	599	177	185	5			
2	G	136	Total	C	N	O	S	0	0	0
			1048	651	194	197	6			
2	H	136	Total	C	N	O	S	0	0	0
			1049	651	194	198	6			
2	I	133	Total	C	N	O	S	0	0	0
			1029	638	191	194	6			
2	J	133	Total	C	N	O	S	0	0	0
			1029	638	191	194	6			
2	K	133	Total	C	N	O	S	0	0	0
			1029	638	191	194	6			
2	L	127	Total	C	N	O	S	0	0	0
			986	612	185	183	6			

There are 24 discrepancies between the modelled and reference sequences:

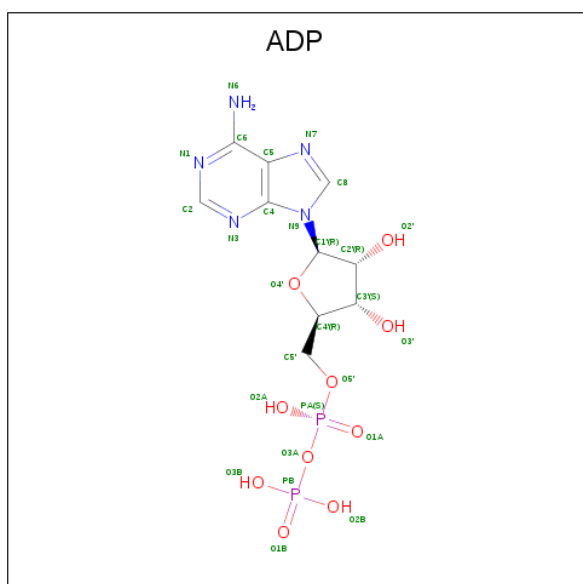
Chain	Residue	Modelled	Actual	Comment	Reference
E	96	GLY	-	expression tag	UNP P15934

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	97	SER	-	expression tag	UNP P15934
E	98	HIS	-	expression tag	UNP P15934
F	96	GLY	-	expression tag	UNP P15934
F	97	SER	-	expression tag	UNP P15934
F	98	HIS	-	expression tag	UNP P15934
G	96	GLY	-	expression tag	UNP P15934
G	97	SER	-	expression tag	UNP P15934
G	98	HIS	-	expression tag	UNP P15934
H	96	GLY	-	expression tag	UNP P15934
H	97	SER	-	expression tag	UNP P15934
H	98	HIS	-	expression tag	UNP P15934
I	96	GLY	-	expression tag	UNP P15934
I	97	SER	-	expression tag	UNP P15934
I	98	HIS	-	expression tag	UNP P15934
J	96	GLY	-	expression tag	UNP P15934
J	97	SER	-	expression tag	UNP P15934
J	98	HIS	-	expression tag	UNP P15934
K	96	GLY	-	expression tag	UNP P15934
K	97	SER	-	expression tag	UNP P15934
K	98	HIS	-	expression tag	UNP P15934
L	96	GLY	-	expression tag	UNP P15934
L	97	SER	-	expression tag	UNP P15934
L	98	HIS	-	expression tag	UNP P15934

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

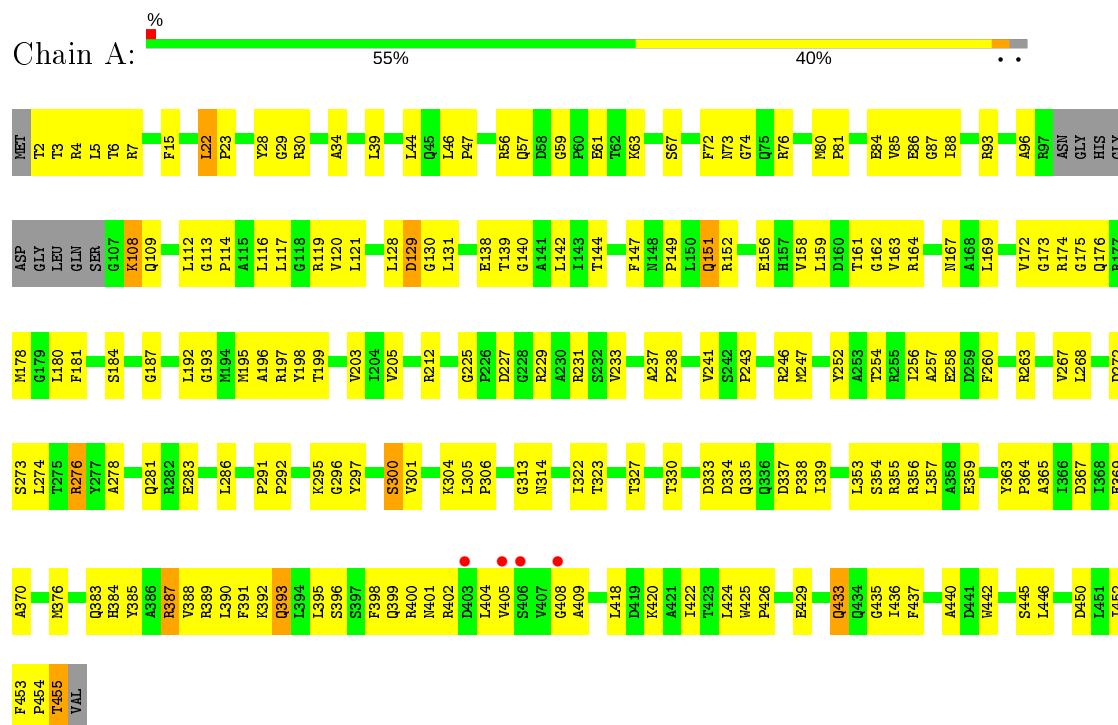


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

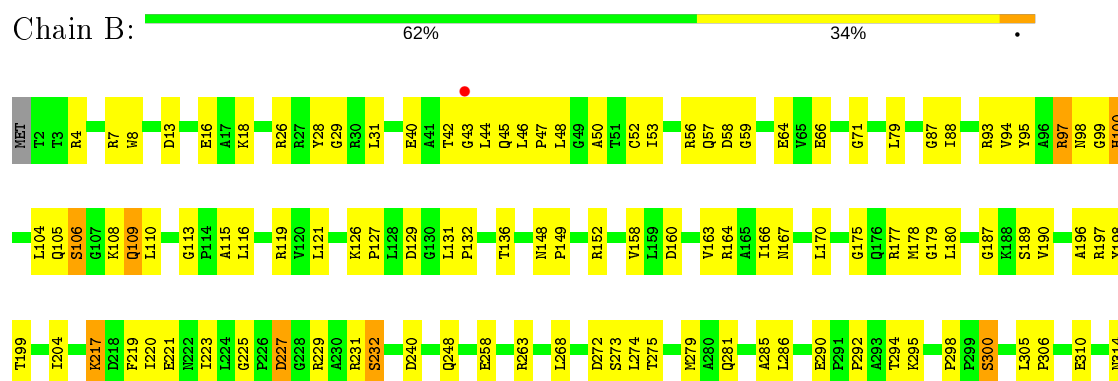
3 Residue-property plots [i](#)

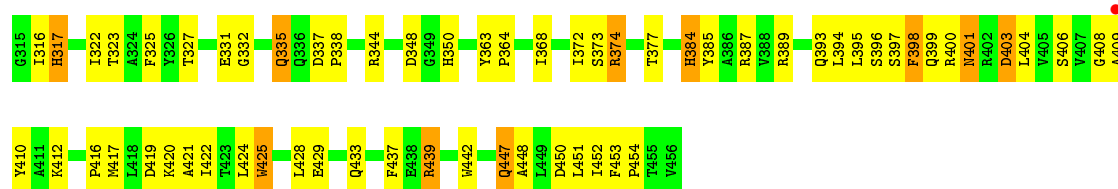
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Flagellum-specific ATP synthase

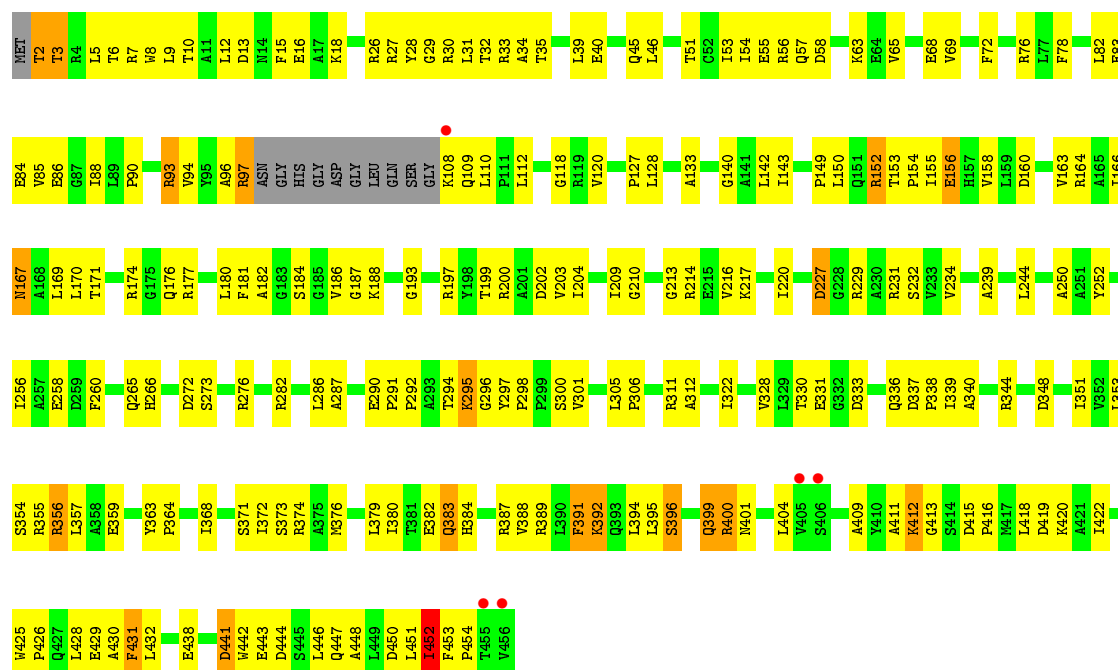


• Molecule 1: Flagellum-specific ATP synthase

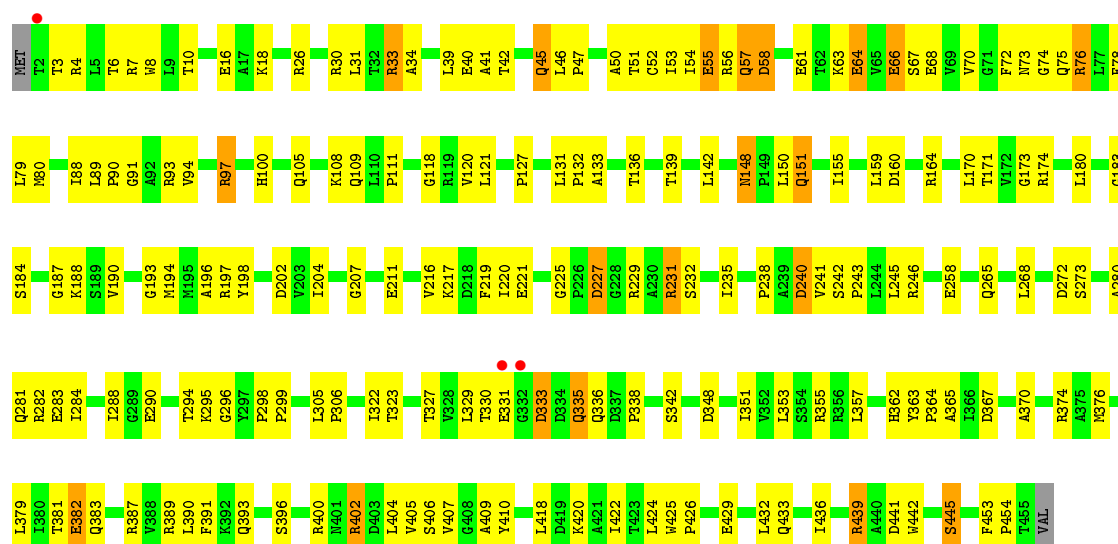




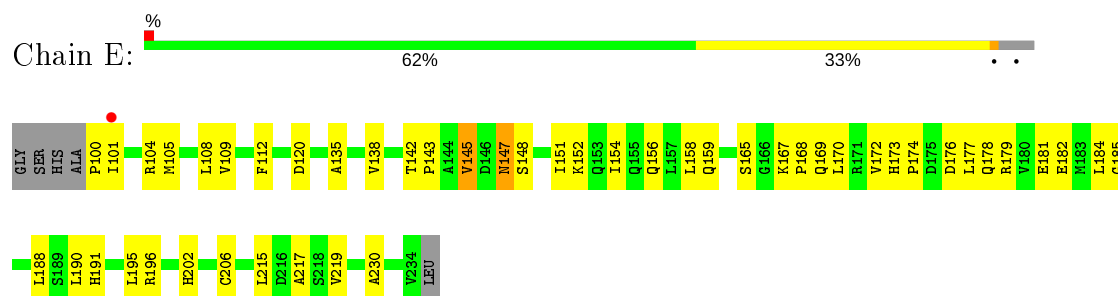
• Molecule 1: Flagellum-specific ATP synthase



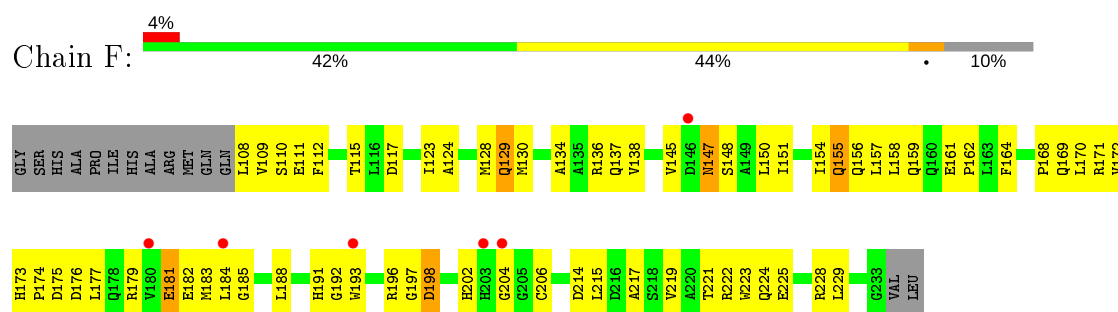
• Molecule 1: Flagellum-specific ATP synthase



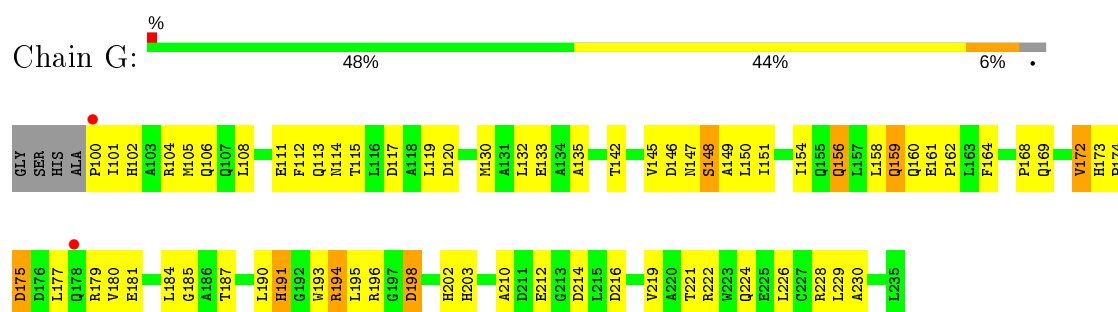
- Molecule 2: Flagellar assembly protein FliH



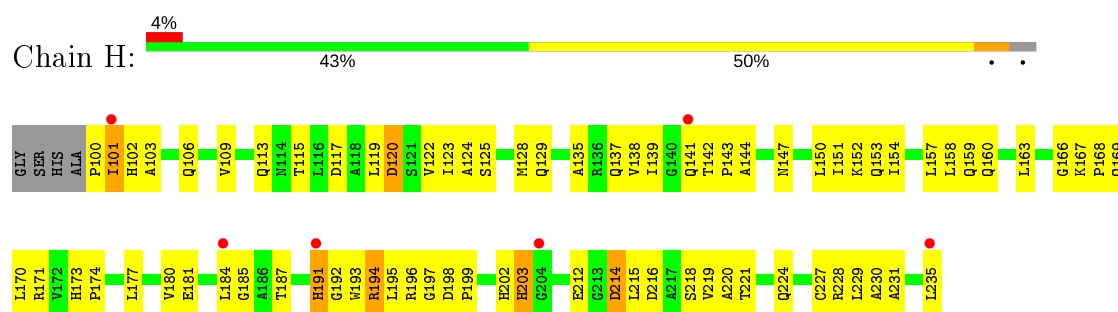
- Molecule 2: Flagellar assembly protein FliH



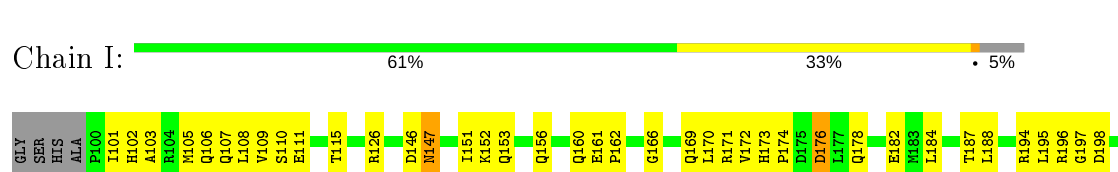
- Molecule 2: Flagellar assembly protein FliH

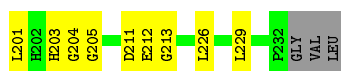


- Molecule 2: Flagellar assembly protein FliH

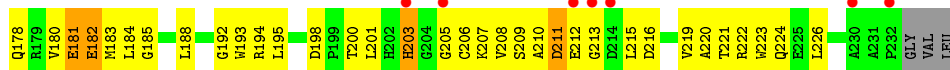


- Molecule 2: Flagellar assembly protein FliH

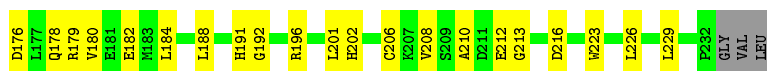




• Molecule 2: Flagellar assembly protein FliH



• Molecule 2: Flagellar assembly protein FliH



• Molecule 2: Flagellar assembly protein FliH



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.66Å 147.31Å 164.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.31 – 3.00 51.32 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (51.31-3.00) 99.2 (51.32-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.218 , 0.270 0.214 , 0.267	Depositor DCC
R_{free} test set	3293 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21982	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ADP

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	0.30	0/3452	0.54	0/4683
1	B	0.28	0/3523	0.52	0/4779
1	C	0.27	0/3456	0.50	0/4688
1	D	0.30	0/3515	0.53	0/4769
2	E	0.28	0/1057	0.48	0/1432
2	F	0.24	0/981	0.46	0/1330
2	G	0.26	0/1065	0.48	0/1443
2	H	0.26	0/1066	0.52	0/1443
2	I	0.25	0/1046	0.44	0/1417
2	J	0.24	0/1046	0.46	0/1417
2	K	0.24	0/1046	0.46	0/1417
2	L	0.26	0/1000	0.49	0/1350
All	All	0.28	0/22253	0.50	0/30168

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	ASP	Peptide
1	C	452	ILE	Peptide

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	3391	0	3464	169	1
1	B	3460	0	3524	164	3
1	C	3395	0	3470	205	0
1	D	3452	0	3515	166	0
2	E	1040	0	1043	40	0
2	F	966	0	965	67	0
2	G	1048	0	1054	87	0
2	H	1049	0	1054	109	0
2	I	1029	0	1031	56	0
2	J	1029	0	1031	91	1
2	K	1029	0	1031	57	2
2	L	986	0	991	78	3
3	A	27	0	12	5	0
3	B	27	0	12	7	0
3	C	27	0	12	3	0
3	D	27	0	12	4	0
All	All	21982	0	22221	1172	5

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 27.

All (1172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:231:ALA:HB1	2:L:232:PRO:HD2	1.23	1.18
1:A:450:ASP:HA	1:A:454:PRO:HD2	1.40	1.04
1:C:387:ARG:NH1	1:C:450:ASP:OD1	1.93	1.01
1:B:450:ASP:HA	1:B:454:PRO:HG2	1.42	1.00
2:I:194:ARG:NH1	2:I:211:ASP:OD2	1.94	1.00
1:A:196:ALA:O	1:A:231:ARG:NH1	1.96	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:VAL:O	1:B:167:ASN:ND2	1.97	0.97
2:J:172:VAL:HG12	2:J:173:HIS:H	1.27	0.96
1:B:439:ARG:HG3	1:B:439:ARG:HH11	1.27	0.96
2:G:172:VAL:O	2:G:198:ASP:N	2.01	0.94
1:C:163:VAL:O	1:C:167:ASN:ND2	2.01	0.93
1:A:197:ARG:NH2	1:A:436:ILE:O	2.01	0.93
1:B:47:PRO:HG2	1:B:50:ALA:HB2	1.51	0.93
1:A:387:ARG:HE	1:A:454:PRO:HG3	1.30	0.93
1:D:148:ASN:HB2	1:D:151:GLN:HB3	1.50	0.92
1:D:204:ILE:HB	1:D:232:SER:HB3	1.50	0.92
1:D:4:ARG:NH2	2:H:117:ASP:OD1	2.03	0.91
1:D:131:LEU:HG	1:D:132:PRO:HD2	1.48	0.91
1:A:56:ARG:HH22	1:A:63:LYS:HD3	1.36	0.91
1:C:412:LYS:HD2	1:C:413:GLY:H	1.37	0.88
1:C:452:ILE:HG23	1:C:453:PHE:H	1.39	0.88
2:J:173:HIS:CD2	2:J:175:ASP:H	1.91	0.88
1:C:453:PHE:N	1:C:454:PRO:HD3	1.88	0.87
2:F:196:ARG:HG2	2:F:197:GLY:H	1.37	0.87
1:A:114:PRO:HD3	1:A:263:ARG:HH12	1.38	0.86
2:G:102:HIS:HA	2:K:179:ARG:HH22	1.40	0.86
1:D:7:ARG:NH1	2:H:120:ASP:OD2	2.09	0.86
2:J:201:LEU:HD13	2:J:206:CYS:HA	1.58	0.86
1:C:186:VAL:HG11	1:C:353:LEU:HB3	1.58	0.86
2:G:113:GLN:OE1	2:K:104:ARG:NH1	2.08	0.86
2:F:154:ILE:O	2:F:158:LEU:HD13	1.75	0.85
2:L:126:ARG:NH1	2:L:129:GLN:OE1	2.10	0.84
2:H:173:HIS:HE1	2:L:232:PRO:HB3	1.40	0.84
1:D:188:LYS:NZ	1:D:272:ASP:OD2	2.11	0.84
2:I:173:HIS:ND1	2:I:174:PRO:HD2	1.92	0.84
2:F:222:ARG:NH1	2:J:138:VAL:O	2.11	0.83
1:C:216:VAL:O	1:C:220:ILE:HG12	1.78	0.83
1:D:333:ASP:O	1:D:335:GLN:NE2	2.11	0.83
1:D:57:GLN:HE21	1:D:57:GLN:HA	1.41	0.83
1:C:58:ASP:HB2	1:C:63:LYS:HD2	1.61	0.83
2:H:173:HIS:CD2	2:H:174:PRO:HD2	2.13	0.82
2:H:139:ILE:HG12	2:L:138:VAL:HG21	1.60	0.82
2:K:184:LEU:HD23	2:K:188:LEU:HD21	1.60	0.82
1:A:387:ARG:NE	1:A:454:PRO:HG3	1.93	0.82
2:F:137:GLN:OE1	2:J:153:GLN:NE2	2.13	0.82
1:C:127:PRO:HG3	1:C:133:ALA:HA	1.60	0.82
1:B:119:ARG:NH2	1:B:132:PRO:O	2.13	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:147:ASN:HB2	2:E:151:ILE:HG12	1.63	0.81
2:G:177:LEU:O	2:G:180:VAL:HG12	1.79	0.81
1:D:294:THR:HG22	1:D:295:LYS:H	1.45	0.81
2:G:222:ARG:NH1	2:K:138:VAL:O	2.14	0.81
1:D:53:ILE:HD11	1:D:97:ARG:HD3	1.62	0.81
2:J:171:ARG:NH2	2:J:213:GLY:O	2.14	0.80
1:A:149:PRO:HA	1:A:152:ARG:HD2	1.63	0.80
1:B:44:LEU:HD13	1:B:46:LEU:HD13	1.64	0.80
1:A:7:ARG:NH1	2:E:120:ASP:OD2	2.14	0.80
2:J:172:VAL:HG12	2:J:173:HIS:N	1.96	0.80
1:C:368:ILE:H	1:C:368:ILE:HD12	1.46	0.79
1:D:294:THR:HG21	1:D:338:PRO:HG2	1.63	0.79
1:D:53:ILE:HG21	1:D:64:GLU:HB3	1.63	0.79
1:D:387:ARG:HH21	1:D:454:PRO:HB3	1.48	0.79
2:E:173:HIS:CD2	2:E:174:PRO:HD2	2.18	0.79
1:C:184:SER:O	1:C:355:ARG:NH2	2.15	0.79
2:G:169:GLN:HE21	2:G:196:ARG:HB2	1.45	0.78
1:A:225:GLY:O	1:A:229:ARG:HB2	1.82	0.78
1:C:16:GLU:OE1	2:K:126:ARG:NH1	2.14	0.78
1:B:13:ASP:OD1	2:J:126:ARG:NH2	2.17	0.78
2:I:172:VAL:HG22	2:I:173:HIS:H	1.47	0.78
1:A:175:GLY:HA3	1:A:314:ASN:ND2	1.99	0.77
1:C:295:LYS:HE3	1:C:338:PRO:HG3	1.63	0.77
2:H:129:GLN:HE21	2:L:223:TRP:HD1	1.31	0.77
1:D:418:LEU:O	1:D:422:ILE:HG13	1.83	0.77
1:C:450:ASP:O	1:C:454:PRO:HD2	1.85	0.77
1:D:66:GLU:OE1	1:D:97:ARG:NH1	2.19	0.76
2:L:106:GLN:NE2	2:L:183:MET:SD	2.58	0.76
2:F:154:ILE:HD12	2:F:170:LEU:HD11	1.67	0.76
1:B:28:TYR:HB2	2:F:214:ASP:HB2	1.66	0.76
1:A:330:THR:HB	1:A:334:ASP:OD2	1.86	0.76
1:A:450:ASP:HA	1:A:454:PRO:CD	2.15	0.76
1:C:356:ARG:NH1	1:C:357:LEU:HD13	2.02	0.75
2:F:161:GLU:HG2	2:F:162:PRO:HA	1.68	0.75
2:H:173:HIS:CE1	2:L:232:PRO:HB3	2.21	0.75
1:B:295:LYS:HB3	1:B:338:PRO:HG3	1.68	0.75
1:A:383:GLN:HG3	1:A:387:ARG:HH22	1.51	0.75
1:B:113:GLY:HA2	1:B:263:ARG:NH2	2.01	0.75
1:C:149:PRO:HA	1:C:152:ARG:HD2	1.66	0.75
1:B:316:ILE:HG22	1:B:317:HIS:H	1.50	0.75
1:D:241:VAL:HG22	1:D:242:SER:H	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:111:GLU:HG2	2:J:205:GLY:HA2	1.69	0.75
2:J:184:LEU:HD22	2:J:188:LEU:HD13	1.69	0.75
1:C:152:ARG:NH2	1:C:312:ALA:O	2.20	0.75
1:B:44:LEU:HD21	1:B:94:VAL:HG23	1.68	0.74
2:F:173:HIS:CG	2:F:174:PRO:HD2	2.21	0.74
2:J:174:PRO:HA	2:J:177:LEU:HD23	1.69	0.74
2:G:147:ASN:HB2	2:G:151:ILE:HG12	1.69	0.74
2:L:231:ALA:CB	2:L:232:PRO:HD2	2.09	0.74
1:C:54:ILE:HG21	1:C:88:ILE:HD13	1.69	0.74
1:C:447:GLN:HA	1:C:450:ASP:OD2	1.88	0.74
2:H:212:GLU:OE1	2:H:212:GLU:N	2.19	0.74
2:F:108:LEU:HA	2:F:111:GLU:HB3	1.69	0.74
1:B:115:ALA:HB3	1:B:136:THR:HG22	1.70	0.73
1:B:408:GLY:HA3	1:C:389:ARG:CZ	2.17	0.73
2:H:101:ILE:HB	2:L:179:ARG:HE	1.53	0.73
1:C:400:ARG:HH11	1:C:400:ARG:HG2	1.53	0.73
1:D:89:LEU:HD12	1:D:91:GLY:H	1.54	0.73
1:A:454:PRO:HB2	1:A:455:THR:HG23	1.68	0.73
2:H:142:THR:HG22	2:H:143:PRO:O	1.89	0.73
1:C:441:ASP:OD2	1:C:443:GLU:N	2.22	0.73
2:L:231:ALA:HB1	2:L:232:PRO:CD	2.12	0.73
1:C:400:ARG:NH1	1:C:400:ARG:HG2	2.04	0.73
1:B:397:SER:O	1:B:401:ASN:ND2	2.22	0.72
1:C:112:LEU:HD12	1:C:140:GLY:HA3	1.71	0.72
2:G:105:MET:HA	2:G:108:LEU:HD12	1.71	0.72
1:A:114:PRO:HD3	1:A:263:ARG:NH1	2.04	0.72
2:I:173:HIS:HB3	2:I:176:ASP:OD2	1.88	0.72
1:C:170:LEU:HD23	1:C:351:ILE:HG22	1.72	0.72
2:E:142:THR:HG22	2:E:143:PRO:O	1.90	0.72
2:H:158:LEU:HD21	2:H:191:HIS:NE2	2.05	0.72
2:L:105:MET:HG2	2:L:184:LEU:HD21	1.69	0.72
1:B:295:LYS:CB	1:B:338:PRO:HG3	2.19	0.72
2:J:171:ARG:HH11	2:J:171:ARG:HG3	1.55	0.71
2:F:173:HIS:ND1	2:F:174:PRO:HD2	2.06	0.71
2:K:118:ALA:O	2:K:122:VAL:HG12	1.90	0.71
2:F:150:LEU:O	2:F:154:ILE:HG12	1.90	0.71
2:J:173:HIS:HD2	2:J:174:PRO:N	1.87	0.71
2:G:169:GLN:HB2	2:G:194:ARG:HD3	1.70	0.71
2:K:104:ARG:O	2:K:108:LEU:N	2.20	0.71
1:B:450:ASP:HA	1:B:454:PRO:CG	2.21	0.71
1:C:453:PHE:H	1:C:454:PRO:HD3	1.54	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:PHE:HB3	1:D:454:PRO:HA	1.73	0.71
2:H:196:ARG:HG2	2:H:197:GLY:N	2.06	0.71
1:B:177:ARG:NH1	1:B:310:GLU:HA	2.05	0.71
2:J:173:HIS:HD2	2:J:175:ASP:H	1.34	0.71
1:B:348:ASP:C	1:B:374:ARG:HG3	2.11	0.71
1:C:356:ARG:HH11	1:C:356:ARG:HG3	1.53	0.71
2:I:195:LEU:HD23	2:I:196:ARG:N	2.06	0.71
1:A:159:LEU:HD13	1:A:174:ARG:HG2	1.72	0.70
2:H:227:CYS:O	2:L:223:TRP:HH2	1.73	0.70
1:D:127:PRO:HG3	1:D:133:ALA:HA	1.73	0.70
1:B:439:ARG:CG	1:B:439:ARG:HH11	2.03	0.70
1:B:348:ASP:O	1:B:374:ARG:HG3	1.92	0.70
1:C:412:LYS:HD2	1:C:413:GLY:N	2.07	0.70
1:C:160:ASP:OD2	1:C:442:TRP:N	2.24	0.70
2:H:180:VAL:HG23	2:H:195:LEU:HD22	1.74	0.70
1:A:84:GLU:HA	1:A:84:GLU:OE1	1.91	0.70
2:F:196:ARG:HG2	2:F:197:GLY:N	2.05	0.70
2:J:125:SER:O	2:J:128:MET:HG2	1.92	0.69
2:J:172:VAL:CG1	2:J:173:HIS:H	2.03	0.69
1:A:357:LEU:HB2	1:A:365:ALA:HB1	1.74	0.69
1:A:454:PRO:CB	1:A:455:THR:HA	2.22	0.69
1:C:27:ARG:HH21	2:G:162:PRO:HD2	1.55	0.69
2:H:196:ARG:HG2	2:H:197:GLY:H	1.58	0.69
2:K:156:GLN:NE2	2:K:160:GLN:OE1	2.25	0.69
1:B:286:LEU:HD21	1:B:292:PRO:HG3	1.74	0.69
1:C:382:GLU:N	1:C:382:GLU:OE1	2.23	0.69
2:E:178:GLN:O	2:E:182:GLU:HG3	1.92	0.69
2:H:137:GLN:O	2:H:141:GLN:HB3	1.93	0.69
1:B:416:PRO:HA	1:B:419:ASP:HB2	1.75	0.69
1:B:97:ARG:NH1	1:B:99:GLY:HA3	2.08	0.69
1:A:396:SER:O	1:A:400:ARG:HG2	1.93	0.69
1:A:453:PHE:HB2	1:A:454:PRO:HD3	1.74	0.69
2:L:220:ALA:HA	2:L:223:TRP:HB2	1.75	0.69
2:K:133:GLU:O	2:K:137:GLN:HG2	1.93	0.68
1:C:167:ASN:O	1:C:171:THR:OG1	2.07	0.68
2:F:181:GLU:HG2	2:F:185:GLY:HA3	1.76	0.68
1:B:16:GLU:OE2	2:J:126:ARG:NH1	2.27	0.68
1:C:260:PHE:HB3	1:C:265:GLN:HB2	1.74	0.68
2:F:147:ASN:HD21	2:F:179:ARG:NH2	1.92	0.68
1:C:395:LEU:HD12	1:C:425:TRP:HZ3	1.59	0.68
1:A:295:LYS:HD2	1:A:338:PRO:HD3	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ARG:O	1:C:286:LEU:HD13	1.92	0.67
1:D:18:LYS:HD3	2:H:229:LEU:HD22	1.76	0.67
2:J:188:LEU:O	2:J:192:GLY:N	2.27	0.67
2:G:117:ASP:HA	2:G:120:ASP:OD2	1.95	0.67
2:I:194:ARG:HB3	2:I:196:ARG:HH12	1.58	0.67
1:A:354:SER:HB3	1:A:357:LEU:HD12	1.76	0.67
1:D:348:ASP:O	1:D:374:ARG:HG3	1.94	0.67
2:L:156:GLN:O	2:L:160:GLN:NE2	2.25	0.67
1:D:188:LYS:HD2	1:D:327:THR:HG21	1.77	0.67
1:B:401:ASN:HB2	1:B:404:LEU:HD22	1.76	0.66
2:H:230:ALA:HB3	2:L:223:TRP:HZ2	1.60	0.66
2:G:161:GLU:HA	2:G:162:PRO:C	2.14	0.66
1:B:403:ASP:HA	1:B:406:SER:HB3	1.77	0.66
1:C:164:ARG:HD2	1:C:431:PHE:CD1	2.30	0.66
2:G:219:VAL:HG13	2:K:138:VAL:HG12	1.76	0.66
1:B:398:PHE:CD2	1:B:398:PHE:C	2.69	0.66
1:A:424:LEU:HD22	1:A:452:ILE:HG23	1.78	0.66
2:K:169:GLN:OE1	2:K:196:ARG:HD2	1.95	0.66
1:B:363:TYR:HB3	3:B:601:ADP:C6	2.29	0.66
1:D:407:VAL:HG13	1:D:409:ALA:H	1.61	0.66
2:L:159:GLN:O	2:L:165:SER:OG	2.13	0.66
1:A:450:ASP:CA	1:A:454:PRO:HD2	2.22	0.66
1:A:57:GLN:NE2	1:A:61:GLU:O	2.29	0.66
1:B:196:ALA:O	1:B:231:ARG:NH1	2.29	0.66
1:D:294:THR:HG21	1:D:338:PRO:CG	2.26	0.66
1:C:193:GLY:O	1:C:197:ARG:HG3	1.95	0.66
2:G:145:VAL:O	2:G:179:ARG:NH2	2.28	0.66
1:C:452:ILE:HG22	1:C:454:PRO:HD3	1.77	0.65
1:C:452:ILE:HG23	1:C:453:PHE:N	2.11	0.65
1:D:357:LEU:HB2	1:D:365:ALA:HB1	1.79	0.65
2:F:147:ASN:HD21	2:F:179:ARG:HH21	1.45	0.65
1:A:454:PRO:HB2	1:A:455:THR:HA	1.77	0.65
2:F:173:HIS:HA	2:F:198:ASP:O	1.95	0.65
2:F:219:VAL:HG13	2:J:138:VAL:HG12	1.79	0.65
2:I:169:GLN:HB2	2:I:211:ASP:HB2	1.78	0.65
1:B:56:ARG:HD2	1:B:87:GLY:HA3	1.78	0.65
1:A:187:GLY:HA2	3:A:601:ADP:H5'2	1.78	0.65
1:C:65:VAL:HG13	1:C:83:GLU:HB2	1.79	0.65
2:F:172:VAL:HG11	2:F:176:ASP:HB2	1.78	0.65
2:J:153:GLN:O	2:J:157:LEU:HD13	1.96	0.65
2:K:173:HIS:ND1	2:K:174:PRO:HD2	2.12	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:VAL:HG12	1:C:186:VAL:O	1.97	0.64
2:G:145:VAL:O	2:G:145:VAL:HG22	1.97	0.64
1:A:56:ARG:NH2	1:A:63:LYS:HD3	2.08	0.64
2:H:230:ALA:HB3	2:L:223:TRP:CZ2	2.32	0.64
1:D:155:ILE:HG22	1:D:379:LEU:HD21	1.79	0.64
2:H:169:GLN:OE1	2:H:194:ARG:NH1	2.31	0.64
2:H:187:THR:O	2:H:191:HIS:HB2	1.97	0.64
1:A:295:LYS:HB2	1:A:338:PRO:HG2	1.80	0.64
1:A:199:THR:HG21	1:A:268:LEU:HD22	1.80	0.64
2:J:173:HIS:CD2	2:J:174:PRO:N	2.66	0.64
1:A:241:VAL:O	1:A:246:ARG:NH1	2.31	0.64
1:A:85:VAL:HB	1:A:88:ILE:HD12	1.80	0.64
2:G:130:MET:SD	2:K:158:LEU:HD23	2.38	0.64
1:B:190:VAL:HG21	3:B:601:ADP:H3'	1.80	0.63
1:B:187:GLY:N	3:B:601:ADP:O1A	2.28	0.63
2:G:102:HIS:HA	2:K:179:ARG:NH2	2.12	0.63
1:C:356:ARG:NH1	1:C:356:ARG:HG3	2.11	0.63
1:C:163:VAL:HG21	1:C:166:ILE:HD12	1.80	0.63
1:C:446:LEU:HD23	1:C:450:ASP:OD2	1.96	0.63
1:C:58:ASP:CB	1:C:63:LYS:HD2	2.28	0.63
2:I:172:VAL:HG22	2:I:173:HIS:N	2.12	0.63
1:B:131:LEU:HB3	1:B:132:PRO:HD2	1.80	0.63
1:C:127:PRO:CG	1:C:133:ALA:HA	2.28	0.63
2:L:178:GLN:OE1	2:L:178:GLN:N	2.31	0.63
2:J:173:HIS:C	2:J:173:HIS:CD2	2.70	0.63
1:B:57:GLN:NE2	1:B:59:GLY:O	2.32	0.63
1:C:348:ASP:O	1:C:374:ARG:HG2	1.98	0.63
1:D:381:THR:HG22	1:D:383:GLN:H	1.64	0.63
2:F:221:THR:O	2:F:224:GLN:HG2	1.99	0.63
1:B:316:ILE:HG22	1:B:317:HIS:N	2.13	0.62
1:C:169:LEU:O	1:C:376:MET:SD	2.57	0.62
2:H:147:ASN:O	2:H:150:LEU:HG	1.98	0.62
2:H:174:PRO:HD3	2:H:197:GLY:O	1.98	0.62
1:D:31:LEU:HD12	1:D:41:ALA:HB2	1.79	0.62
2:I:172:VAL:O	2:I:197:GLY:HA2	2.00	0.62
1:B:305:LEU:HB2	1:B:306:PRO:HD3	1.81	0.62
2:H:173:HIS:HD2	2:H:199:PRO:HA	1.64	0.62
2:H:202:HIS:HB2	2:H:219:VAL:CG1	2.29	0.62
1:C:452:ILE:CG2	1:C:454:PRO:HD3	2.28	0.62
2:L:138:VAL:HG23	2:L:139:ILE:N	2.14	0.62
1:C:229:ARG:HA	1:C:232:SER:OG	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:TYR:HE1	1:B:389:ARG:HE	1.47	0.62
2:K:105:MET:SD	2:K:184:LEU:HD11	2.40	0.62
1:C:400:ARG:HH11	1:C:400:ARG:CG	2.12	0.61
2:H:167:LYS:N	2:H:168:PRO:HD3	2.15	0.61
1:C:174:ARG:NH1	1:C:266:HIS:CE1	2.67	0.61
1:C:443:GLU:O	1:C:447:GLN:N	2.21	0.61
2:H:115:THR:HB	2:L:207:LYS:CD	2.31	0.61
2:J:169:GLN:NE2	2:J:194:ARG:HD2	2.16	0.61
2:J:172:VAL:O	2:J:198:ASP:N	2.20	0.61
2:J:102:HIS:CD2	2:J:183:MET:HG2	2.36	0.61
2:J:171:ARG:NH1	2:J:171:ARG:HG3	2.15	0.61
1:A:159:LEU:H	1:A:173:GLY:HA2	1.64	0.61
1:B:419:ASP:O	1:B:422:ILE:HG13	2.01	0.61
1:B:439:ARG:HG3	1:B:439:ARG:NH1	2.08	0.61
2:J:128:MET:HG3	2:J:129:GLN:N	2.15	0.61
1:A:174:ARG:O	1:A:314:ASN:ND2	2.28	0.61
1:B:105:GLN:O	1:B:108:LYS:HG2	2.00	0.61
1:C:199:THR:O	1:C:231:ARG:NH2	2.27	0.61
2:G:224:GLN:OE1	2:G:228:ARG:NH2	2.34	0.61
2:E:202:HIS:HB2	2:E:219:VAL:CG2	2.31	0.61
2:H:173:HIS:HD2	2:H:174:PRO:HD2	1.65	0.61
2:J:113:GLN:OE1	2:J:193:TRP:NE1	2.24	0.61
2:F:225:GLU:O	2:F:229:LEU:N	2.32	0.60
2:G:164:PHE:HB3	2:G:168:PRO:HG3	1.82	0.60
1:C:152:ARG:HH12	1:C:177:ARG:HH22	1.49	0.60
1:C:217:LYS:HD3	1:D:150:LEU:HA	1.83	0.60
1:A:295:LYS:HD2	1:A:338:PRO:CD	2.30	0.60
1:A:450:ASP:OD1	1:A:454:PRO:HG2	2.02	0.60
1:D:184:SER:O	1:D:355:ARG:NH2	2.34	0.60
2:E:105:MET:O	2:E:109:VAL:HG23	2.01	0.60
2:F:188:LEU:O	2:F:192:GLY:N	2.34	0.60
2:G:104:ARG:NE	2:K:176:ASP:OD1	2.34	0.60
1:B:403:ASP:OD1	1:B:403:ASP:N	2.31	0.60
2:F:108:LEU:HD23	2:F:109:VAL:H	1.66	0.60
1:B:97:ARG:HG3	1:B:97:ARG:O	2.00	0.60
1:D:197:ARG:NH2	1:D:436:ILE:O	2.35	0.60
1:A:334:ASP:O	1:A:335:GLN:HB2	2.00	0.60
2:K:162:PRO:HB2	2:K:210:ALA:HB1	1.84	0.60
1:B:453:PHE:N	1:B:454:PRO:HD3	2.17	0.59
1:C:167:ASN:H	1:C:167:ASN:ND2	2.00	0.59
2:H:139:ILE:HG12	2:L:138:VAL:CG2	2.30	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:108:LEU:HD21	2:I:176:ASP:HB2	1.83	0.59
1:A:109:GLN:HB3	1:A:139:THR:HB	1.83	0.59
1:C:6:THR:O	1:C:10:THR:HG22	2.03	0.59
1:C:330:THR:HB	1:C:333:ASP:HA	1.83	0.59
1:A:454:PRO:HB2	1:A:455:THR:CA	2.31	0.59
1:B:18:LYS:HE2	2:F:229:LEU:HD11	1.84	0.59
2:I:184:LEU:HD22	2:I:187:THR:HG21	1.84	0.59
2:L:173:HIS:HD2	2:L:201:LEU:O	1.85	0.59
2:I:184:LEU:HB3	2:I:188:LEU:HG	1.84	0.59
1:A:2:THR:HA	1:A:5:LEU:HB3	1.85	0.59
2:J:188:LEU:HD22	2:J:195:LEU:HD23	1.83	0.59
1:D:268:LEU:HD12	1:D:323:THR:O	2.03	0.59
2:G:180:VAL:HG21	2:G:195:LEU:HD11	1.84	0.59
2:H:230:ALA:CB	2:L:223:TRP:HZ2	2.16	0.59
1:B:26:ARG:HD3	1:B:28:TYR:CZ	2.38	0.58
2:J:209:SER:OG	2:J:210:ALA:N	2.36	0.58
1:C:15:PHE:HE2	2:G:132:LEU:HD11	1.67	0.58
1:D:151:GLN:NE2	1:D:151:GLN:O	2.36	0.58
2:H:135:ALA:O	2:H:139:ILE:HD12	2.02	0.58
1:C:388:VAL:O	1:C:392:LYS:HG2	2.02	0.58
1:C:187:GLY:HA2	3:C:601:ADP:O1A	2.02	0.58
1:A:130:GLY:C	1:A:131:LEU:HD12	2.24	0.58
1:A:297:TYR:CZ	1:A:339:ILE:HD11	2.37	0.58
2:E:173:HIS:HD2	2:E:174:PRO:HD2	1.65	0.58
2:I:229:LEU:HD12	2:I:229:LEU:O	2.03	0.58
1:B:189:SER:OG	3:B:601:ADP:O2B	2.19	0.58
2:H:180:VAL:HA	2:H:184:LEU:HB2	1.85	0.58
1:B:401:ASN:H	1:B:401:ASN:HD22	1.51	0.58
2:H:154:ILE:HA	2:H:157:LEU:HG	1.86	0.58
1:B:64:GLU:OE2	1:B:95:TYR:OH	2.22	0.58
1:D:217:LYS:HE3	1:D:221:GLU:OE1	2.04	0.58
2:H:180:VAL:O	2:H:184:LEU:HB2	2.03	0.58
2:J:172:VAL:HA	2:J:201:LEU:HD12	1.84	0.58
2:E:108:LEU:HD11	2:I:204:GLY:HA2	1.85	0.58
2:F:172:VAL:CG1	2:F:176:ASP:HB2	2.33	0.58
2:G:169:GLN:NE2	2:G:196:ARG:HB2	2.16	0.58
1:D:294:THR:HG22	1:D:295:LYS:N	2.17	0.57
1:B:53:ILE:HD13	1:B:64:GLU:HB3	1.85	0.57
1:D:164:ARG:HG3	1:D:445:SER:HB3	1.86	0.57
2:F:182:GLU:OE1	2:F:183:MET:HG3	2.04	0.57
2:F:202:HIS:HB2	2:F:219:VAL:HB	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:112:PHE:HD2	2:I:108:LEU:HD12	1.70	0.57
2:I:109:VAL:HG11	2:I:188:LEU:HD23	1.85	0.57
2:L:153:GLN:O	2:L:157:LEU:HD13	2.04	0.57
1:A:376:MET:HE2	1:A:388:VAL:HG21	1.84	0.57
2:J:198:ASP:OD1	2:J:200:THR:OG1	2.18	0.57
1:A:387:ARG:HD2	1:A:453:PHE:HB2	1.84	0.57
1:B:428:LEU:HD12	1:B:429:GLU:N	2.19	0.57
2:L:113:GLN:HG2	2:L:191:HIS:HB3	1.87	0.57
1:A:383:GLN:HG3	1:A:387:ARG:NH2	2.18	0.57
1:B:4:ARG:HA	1:B:7:ARG:HG3	1.86	0.57
2:H:138:VAL:O	2:H:142:THR:HB	2.05	0.57
2:I:172:VAL:O	2:I:198:ASP:N	2.32	0.57
2:K:172:VAL:HG12	2:K:173:HIS:N	2.20	0.57
1:A:109:GLN:HB3	1:A:139:THR:CB	2.35	0.57
1:B:198:TYR:OH	1:B:437:PHE:HA	2.03	0.57
1:C:2:THR:HG23	1:C:5:LEU:HB3	1.85	0.57
2:F:206:CYS:SG	2:F:217:ALA:HB3	2.44	0.57
2:L:129:GLN:HG3	2:L:130:MET:N	2.19	0.57
1:B:100:HIS:N	1:B:100:HIS:ND1	2.51	0.57
1:C:376:MET:O	1:C:380:ILE:HG12	2.05	0.57
2:F:171:ARG:HD3	2:F:198:ASP:HB2	1.85	0.57
2:H:214:ASP:O	2:H:215:LEU:HD12	2.04	0.57
1:B:225:GLY:O	1:B:229:ARG:HB3	2.05	0.57
1:B:398:PHE:HD2	1:B:398:PHE:C	2.07	0.57
1:C:118:GLY:HA2	1:C:229:ARG:O	2.05	0.57
2:F:161:GLU:HG2	2:F:162:PRO:CA	2.35	0.57
1:B:398:PHE:HB2	1:B:421:ALA:HB1	1.87	0.56
1:C:452:ILE:CG2	1:C:453:PHE:H	2.13	0.56
2:G:173:HIS:ND1	2:G:174:PRO:HD2	2.20	0.56
2:G:147:ASN:ND2	2:G:179:ARG:HD3	2.20	0.56
2:H:166:GLY:O	2:H:167:LYS:HG2	2.04	0.56
1:C:28:TYR:CD2	1:C:93:ARG:HB2	2.40	0.56
2:G:173:HIS:CD2	2:G:175:ASP:HB2	2.40	0.56
2:L:138:VAL:HG23	2:L:139:ILE:H	1.71	0.56
1:A:203:VAL:HB	1:A:267:VAL:HG12	1.86	0.56
1:A:355:ARG:O	1:A:359:GLU:HG3	2.05	0.56
2:G:177:LEU:HD12	2:G:180:VAL:HG11	1.87	0.56
1:A:429:GLU:HG2	1:A:433:GLN:HE22	1.70	0.56
1:B:447:GLN:O	1:B:451:LEU:HG	2.05	0.56
1:B:8:TRP:CG	2:F:123:ILE:HD11	2.40	0.56
1:C:209:ILE:HG13	1:C:250:ALA:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:VAL:CG1	1:C:353:LEU:HB3	2.32	0.56
2:H:174:PRO:HA	2:H:177:LEU:HB2	1.87	0.56
1:A:292:PRO:HB2	1:A:296:GLY:HA2	1.87	0.56
1:D:305:LEU:HB2	1:D:306:PRO:HD3	1.88	0.56
1:D:171:THR:HB	1:D:376:MET:HG3	1.86	0.56
1:B:8:TRP:CD2	2:F:123:ILE:HD11	2.40	0.56
1:A:163:VAL:O	1:A:167:ASN:ND2	2.38	0.56
1:C:256:ILE:O	1:C:260:PHE:HD2	1.88	0.56
1:C:415:ASP:HB2	1:C:418:LEU:HD12	1.87	0.56
2:J:162:PRO:HB2	2:J:210:ALA:HB3	1.88	0.56
1:B:204:ILE:HB	1:B:232:SER:HB3	1.86	0.56
1:C:356:ARG:CZ	1:C:357:LEU:HD13	2.35	0.56
2:H:180:VAL:CG2	2:H:195:LEU:HD22	2.34	0.56
2:H:219:VAL:HG13	2:H:220:ALA:N	2.21	0.56
2:J:174:PRO:CA	2:J:177:LEU:HD23	2.36	0.56
2:H:109:VAL:HA	2:L:105:MET:HE3	1.88	0.56
1:A:353:LEU:HA	1:A:365:ALA:O	2.05	0.56
1:B:273:SER:HB2	1:B:327:THR:O	2.06	0.56
2:G:164:PHE:CD1	2:G:210:ALA:HB3	2.41	0.56
1:A:73:ASN:O	1:A:76:ARG:N	2.39	0.56
1:D:120:VAL:C	1:D:121:LEU:HD12	2.26	0.56
2:H:101:ILE:HB	2:L:179:ARG:HH21	1.71	0.56
1:D:100:HIS:CD2	2:H:235:LEU:HD11	2.41	0.56
2:K:180:VAL:HG13	2:K:184:LEU:HD13	1.86	0.56
1:B:363:TYR:HA	1:B:364:PRO:C	2.25	0.55
1:B:52:CYS:SG	1:B:79:LEU:HD22	2.47	0.55
1:C:187:GLY:HA2	3:C:601:ADP:PA	2.45	0.55
1:D:196:ALA:O	1:D:231:ARG:NH1	2.39	0.55
1:D:290:GLU:HG2	1:D:298:PRO:HB3	1.87	0.55
2:H:180:VAL:HG23	2:H:184:LEU:HB3	1.89	0.55
2:G:101:ILE:O	2:K:179:ARG:NH2	2.39	0.55
2:H:202:HIS:HB2	2:H:219:VAL:HG11	1.87	0.55
2:I:156:GLN:O	2:I:160:GLN:HG3	2.07	0.55
1:C:53:ILE:N	1:C:53:ILE:HD12	2.22	0.55
2:E:195:LEU:HD23	2:E:196:ARG:N	2.21	0.55
2:K:173:HIS:ND1	2:K:175:ASP:OD2	2.39	0.55
1:C:227:ASP:N	1:C:227:ASP:OD2	2.38	0.55
1:D:441:ASP:O	1:D:445:SER:OG	2.23	0.55
2:H:203:HIS:ND1	2:H:203:HIS:N	2.54	0.55
1:B:197:ARG:NH1	1:B:223:ILE:O	2.39	0.55
1:C:143:ILE:HG22	1:C:143:ILE:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LEU:CG	1:D:132:PRO:HD2	2.29	0.55
1:D:329:LEU:CD2	1:D:331:GLU:HG2	2.37	0.55
1:D:53:ILE:HD11	1:D:97:ARG:CD	2.36	0.55
2:F:115:THR:HG21	2:J:207:LYS:HA	1.88	0.55
1:B:337:ASP:OD1	1:B:338:PRO:HD2	2.06	0.55
1:D:89:LEU:HD12	1:D:91:GLY:N	2.18	0.55
2:G:202:HIS:HB2	2:G:219:VAL:HB	1.88	0.55
2:J:161:GLU:CD	2:J:162:PRO:HD2	2.26	0.55
1:C:5:LEU:HB2	2:K:115:THR:HG23	1.88	0.55
1:A:243:PRO:O	1:A:247:MET:HG3	2.07	0.55
1:B:119:ARG:NH1	1:B:129:ASP:OD1	2.39	0.55
1:B:166:ILE:O	1:B:170:LEU:O	2.25	0.55
1:C:110:LEU:HD12	1:C:142:LEU:HD21	1.89	0.55
1:C:337:ASP:OD2	1:C:339:ILE:N	2.40	0.55
1:C:68:GLU:HG3	1:C:69:VAL:N	2.22	0.55
1:D:387:ARG:HH21	1:D:454:PRO:CB	2.20	0.55
1:D:75:GLN:H	1:D:75:GLN:CD	2.10	0.55
1:A:408:GLY:O	1:C:404:LEU:HD21	2.07	0.54
2:E:145:VAL:C	2:E:179:ARG:HH12	2.11	0.54
2:G:156:GLN:HA	2:G:159:GLN:HB3	1.88	0.54
2:H:196:ARG:CG	2:H:197:GLY:H	2.20	0.54
2:J:123:ILE:HG23	2:J:124:ALA:N	2.22	0.54
1:A:435:GLY:HA2	3:A:601:ADP:HN62	1.72	0.54
1:D:284:ILE:O	1:D:288:ILE:HG12	2.07	0.54
2:G:180:VAL:HG13	2:G:181:GLU:N	2.21	0.54
2:L:180:VAL:HG13	2:L:184:LEU:HD12	1.89	0.54
1:C:368:ILE:N	1:C:368:ILE:HD12	2.19	0.54
1:D:160:ASP:OD2	1:D:442:TRP:N	2.40	0.54
1:D:78:PHE:C	1:D:79:LEU:HD12	2.28	0.54
2:I:184:LEU:O	2:I:188:LEU:HG	2.08	0.54
1:C:252:TYR:CZ	1:C:256:ILE:HD11	2.43	0.54
1:C:46:LEU:HD11	1:C:96:ALA:HB2	1.89	0.54
2:L:184:LEU:O	2:L:188:LEU:HG	2.08	0.54
2:E:109:VAL:HG22	2:I:105:MET:SD	2.47	0.54
1:C:15:PHE:CE2	2:G:132:LEU:HD11	2.43	0.54
2:L:102:HIS:O	2:L:106:GLN:HG3	2.07	0.54
1:A:22:LEU:C	1:A:22:LEU:HD12	2.29	0.54
1:B:281:GLN:HE21	1:B:300:SER:HB2	1.71	0.54
1:A:418:LEU:O	1:A:418:LEU:HD23	2.07	0.54
1:C:292:PRO:HA	1:C:298:PRO:HB3	1.90	0.54
1:D:56:ARG:HB3	1:D:63:LYS:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:181:GLU:O	2:E:185:GLY:HA3	2.08	0.54
1:A:187:GLY:HA2	3:A:601:ADP:O1A	2.08	0.54
1:D:280:ALA:O	1:D:284:ILE:HD12	2.08	0.53
1:D:284:ILE:H	1:D:284:ILE:HD12	1.72	0.53
2:G:169:GLN:HE21	2:G:196:ARG:CB	2.20	0.53
2:L:176:ASP:O	2:L:180:VAL:HG23	2.08	0.53
1:A:46:LEU:HD11	1:A:96:ALA:HB2	1.89	0.53
1:B:290:GLU:OE1	1:B:300:SER:OG	2.26	0.53
1:B:42:THR:HG22	1:B:43:GLY:N	2.23	0.53
1:A:4:ARG:NH1	2:E:120:ASP:OD1	2.38	0.53
2:F:196:ARG:CG	2:F:197:GLY:H	2.18	0.53
2:L:122:VAL:HG12	2:L:122:VAL:O	2.07	0.53
1:D:363:TYR:HB3	3:D:601:ADP:C6	2.44	0.53
1:D:367:ASP:HB3	1:D:370:ALA:HB3	1.89	0.53
2:J:159:GLN:HG2	2:J:165:SER:HB2	1.90	0.53
1:B:180:LEU:HB3	1:B:327:THR:HG22	1.90	0.53
1:D:453:PHE:HB3	1:D:454:PRO:CA	2.38	0.53
2:H:173:HIS:HA	2:H:198:ASP:O	2.09	0.53
1:A:159:LEU:N	1:A:173:GLY:HA2	2.23	0.53
1:A:384:HIS:O	1:A:388:VAL:HG23	2.09	0.53
1:C:40:GLU:HG2	1:C:78:PHE:CD2	2.44	0.53
1:D:240:ASP:N	1:D:240:ASP:OD1	2.41	0.53
2:K:173:HIS:HD2	2:K:201:LEU:O	1.92	0.53
2:J:148:SER:O	2:J:151:ILE:HG22	2.09	0.53
2:L:129:GLN:HG3	2:L:130:MET:H	1.74	0.53
1:A:198:TYR:OH	1:A:437:PHE:HA	2.08	0.53
2:H:109:VAL:HG12	2:L:104:ARG:NH2	2.24	0.53
2:H:158:LEU:HD11	2:H:191:HIS:CE1	2.43	0.53
2:I:196:ARG:HH11	2:I:196:ARG:HG3	1.74	0.53
1:B:217:LYS:HE3	1:B:221:GLU:CD	2.30	0.53
1:D:188:LYS:HD2	1:D:327:THR:CG2	2.39	0.53
1:D:357:LEU:HD23	1:D:362:HIS:ND1	2.24	0.53
1:D:404:LEU:HG	1:D:410:TYR:HB2	1.91	0.53
1:D:190:VAL:HG11	1:D:436:ILE:HG12	1.91	0.53
1:A:180:LEU:HD23	1:A:327:THR:HG22	1.91	0.52
2:E:172:VAL:CG1	2:E:176:ASP:HB2	2.39	0.52
1:B:45:GLN:HG3	2:F:162:PRO:HD3	1.91	0.52
2:J:104:ARG:O	2:J:108:LEU:HG	2.09	0.52
1:B:108:LYS:HD2	1:B:248:GLN:NE2	2.24	0.52
1:C:28:TYR:HB2	2:G:214:ASP:HB2	1.91	0.52
2:E:145:VAL:O	2:E:179:ARG:NH1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:100:PRO:HD2	2:G:102:HIS:H	1.74	0.52
1:C:295:LYS:HG3	1:C:296:GLY:H	1.73	0.52
1:D:198:TYR:CG	1:D:439:ARG:HB2	2.45	0.52
1:A:176:GLN:HG2	1:A:178:MET:HG2	1.92	0.52
1:B:18:LYS:HB3	2:F:229:LEU:HD21	1.92	0.52
1:C:256:ILE:HG22	1:C:260:PHE:HE2	1.74	0.52
2:K:212:GLU:HG2	2:K:213:GLY:O	2.10	0.52
1:C:203:VAL:HG21	1:C:260:PHE:CD1	2.45	0.52
2:G:112:PHE:HA	2:K:206:CYS:SG	2.49	0.52
1:A:254:THR:O	1:A:258:GLU:HG3	2.10	0.52
2:I:176:ASP:N	2:I:176:ASP:OD2	2.40	0.52
2:I:172:VAL:HG23	2:I:205:GLY:O	2.09	0.52
1:D:159:LEU:H	1:D:173:GLY:HA2	1.75	0.52
1:D:188:LYS:HB3	3:D:601:ADP:O1B	2.09	0.52
2:H:119:LEU:HB3	2:H:123:ILE:HG13	1.92	0.52
1:A:405:VAL:HG11	1:A:422:ILE:HD11	1.91	0.52
1:D:241:VAL:O	1:D:246:ARG:NH1	2.43	0.52
1:A:120:VAL:C	1:A:121:LEU:HD12	2.30	0.52
1:C:174:ARG:HH12	1:C:266:HIS:CE1	2.28	0.52
2:F:145:VAL:O	2:F:145:VAL:HG22	2.10	0.52
2:H:196:ARG:CG	2:H:197:GLY:N	2.73	0.52
1:C:3:THR:O	1:C:7:ARG:N	2.37	0.51
1:D:193:GLY:O	1:D:197:ARG:HG3	2.11	0.51
1:D:241:VAL:HG22	1:D:242:SER:N	2.21	0.51
1:D:281:GLN:HA	1:D:281:GLN:HE21	1.74	0.51
2:H:120:ASP:N	2:H:120:ASP:OD1	2.41	0.51
2:H:180:VAL:HA	2:H:184:LEU:HD22	1.92	0.51
1:B:425:TRP:HA	1:B:428:LEU:HG	1.92	0.51
1:C:429:GLU:HG3	1:C:430:ALA:N	2.25	0.51
2:G:146:ASP:HB3	2:G:148:SER:HB3	1.93	0.51
2:G:111:GLU:O	2:G:115:THR:HG23	2.10	0.51
1:C:453:PHE:N	1:C:454:PRO:CD	2.66	0.51
1:D:187:GLY:HA2	3:D:601:ADP:H5'1	1.91	0.51
1:B:448:ALA:O	1:B:452:ILE:HG13	2.11	0.51
1:C:220:ILE:CD1	1:C:234:VAL:HG11	2.39	0.51
1:A:181:PHE:CD2	1:A:181:PHE:N	2.78	0.51
1:C:155:ILE:HD13	1:C:176:GLN:HB2	1.91	0.51
1:C:391:PHE:C	1:C:391:PHE:CD2	2.84	0.51
2:H:147:ASN:O	2:H:151:ILE:HG12	2.10	0.51
1:D:100:HIS:HD2	2:H:235:LEU:HD11	1.76	0.51
2:H:219:VAL:HG23	2:L:138:VAL:HB	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HD11	1:A:140:GLY:HA3	1.92	0.51
1:B:429:GLU:O	1:B:433:GLN:HG3	2.10	0.51
1:C:65:VAL:HG13	1:C:83:GLU:CB	2.41	0.51
2:F:193:TRP:CD1	2:F:193:TRP:N	2.79	0.51
1:A:257:ALA:HB1	1:A:267:VAL:HG21	1.93	0.51
1:A:300:SER:O	1:A:304:LYS:HG2	2.10	0.51
1:C:169:LEU:HD13	1:C:368:ILE:HG12	1.92	0.51
2:J:173:HIS:CE1	2:J:203:HIS:CE1	2.99	0.51
2:K:173:HIS:CD2	2:K:201:LEU:O	2.64	0.51
1:B:160:ASP:OD2	1:B:442:TRP:N	2.44	0.51
1:D:111:PRO:HB3	1:D:136:THR:HG21	1.93	0.51
1:D:58:ASP:O	1:D:61:GLU:HB2	2.11	0.51
2:J:150:LEU:O	2:J:154:ILE:HG12	2.11	0.51
1:C:164:ARG:NH2	1:C:438:GLU:OE2	2.42	0.51
1:C:8:TRP:NE1	2:G:120:ASP:OD1	2.42	0.51
2:I:170:LEU:C	2:I:170:LEU:HD23	2.31	0.51
2:J:188:LEU:CD2	2:J:195:LEU:HD23	2.40	0.51
2:K:136:ARG:HG3	2:K:137:GLN:N	2.26	0.51
1:A:56:ARG:HH22	1:A:63:LYS:CD	2.16	0.50
1:B:227:ASP:N	1:B:227:ASP:OD2	2.37	0.50
1:D:273:SER:HB2	1:D:327:THR:O	2.11	0.50
1:D:335:GLN:NE2	1:D:335:GLN:H	2.09	0.50
1:D:390:LEU:HD22	1:D:453:PHE:CE1	2.46	0.50
2:E:206:CYS:SG	2:E:217:ALA:HB3	2.51	0.50
2:H:174:PRO:O	2:H:177:LEU:HB3	2.11	0.50
2:J:184:LEU:HD12	2:J:184:LEU:C	2.31	0.50
2:L:161:GLU:O	2:L:165:SER:N	2.27	0.50
1:A:268:LEU:HD12	1:A:323:THR:O	2.12	0.50
1:B:401:ASN:CB	1:B:404:LEU:HD22	2.41	0.50
1:C:220:ILE:HD12	1:C:234:VAL:HG11	1.93	0.50
2:E:172:VAL:HG12	2:E:173:HIS:N	2.25	0.50
2:L:174:PRO:HD3	2:L:198:ASP:O	2.11	0.50
1:D:425:TRP:HB3	1:D:426:PRO:HD3	1.94	0.50
2:F:124:ALA:O	2:F:128:MET:HG3	2.12	0.50
2:I:194:ARG:HB3	2:I:196:ARG:NH1	2.26	0.50
2:L:178:GLN:O	2:L:182:GLU:HG2	2.11	0.50
1:A:120:VAL:HG12	1:A:128:LEU:HB2	1.93	0.50
1:C:416:PRO:O	1:C:419:ASP:HB3	2.11	0.50
1:D:33:ARG:HH11	1:D:33:ARG:HG3	1.76	0.50
1:D:40:GLU:HG2	1:D:76:ARG:HG3	1.94	0.50
1:B:26:ARG:HD3	1:B:28:TYR:OH	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ARG:HD3	1:D:348:ASP:OD1	2.12	0.50
1:C:395:LEU:HD12	1:C:425:TRP:CZ3	2.43	0.50
1:D:357:LEU:CB	1:D:365:ALA:HB1	2.40	0.50
1:D:31:LEU:HA	1:D:41:ALA:HB2	1.94	0.50
1:A:147:PHE:HE1	1:A:152:ARG:HB3	1.77	0.50
1:A:387:ARG:HD3	1:D:407:VAL:HG21	1.93	0.50
1:A:383:GLN:CG	1:A:387:ARG:HH22	2.21	0.50
2:J:184:LEU:HB2	2:J:188:LEU:HB2	1.94	0.50
2:L:191:HIS:HB2	2:L:193:TRP:CD1	2.46	0.50
2:G:142:THR:HG23	2:G:142:THR:O	2.12	0.50
2:G:158:LEU:HD12	2:G:158:LEU:N	2.27	0.50
2:H:173:HIS:CD2	2:H:199:PRO:HA	2.46	0.50
2:K:184:LEU:HB3	2:K:188:LEU:HG	1.94	0.50
2:L:145:VAL:HG12	2:L:146:ASP:N	2.27	0.50
1:C:355:ARG:O	1:C:359:GLU:N	2.42	0.50
2:E:154:ILE:HD13	2:E:170:LEU:HD21	1.94	0.50
1:C:452:ILE:HG22	1:C:454:PRO:CD	2.40	0.50
1:D:3:THR:HG23	1:D:7:ARG:HE	1.77	0.50
2:E:135:ALA:O	2:E:138:VAL:HG22	2.11	0.50
2:E:167:LYS:N	2:E:168:PRO:HD3	2.27	0.50
2:J:169:GLN:N	2:J:209:SER:O	2.44	0.50
1:C:13:ASP:OD1	2:K:126:ARG:NH2	2.44	0.50
2:L:172:VAL:HG22	2:L:173:HIS:N	2.27	0.50
1:A:429:GLU:CG	1:A:433:GLN:HE22	2.25	0.49
1:C:150:LEU:N	1:C:150:LEU:HD23	2.27	0.49
1:C:355:ARG:O	1:C:359:GLU:HB2	2.11	0.49
1:D:127:PRO:CG	1:D:133:ALA:HA	2.40	0.49
1:D:329:LEU:HD23	1:D:329:LEU:C	2.31	0.49
1:C:90:PRO:HD3	1:D:46:LEU:O	2.11	0.49
2:I:173:HIS:CD2	2:I:203:HIS:HA	2.46	0.49
2:J:173:HIS:C	2:J:173:HIS:HD2	2.13	0.49
2:K:104:ARG:O	2:K:108:LEU:HG	2.13	0.49
2:G:154:ILE:O	2:G:158:LEU:HD13	2.12	0.49
2:G:173:HIS:CD2	2:G:203:HIS:CE1	3.00	0.49
2:I:194:ARG:HH12	2:I:213:GLY:HA2	1.77	0.49
1:A:387:ARG:HG3	1:A:453:PHE:CD2	2.48	0.49
1:C:18:LYS:HB3	2:G:229:LEU:HD11	1.93	0.49
2:K:123:ILE:HD12	2:K:126:ARG:HB3	1.95	0.49
2:L:231:ALA:O	2:L:232:PRO:C	2.50	0.49
1:A:389:ARG:O	1:A:393:GLN:HG3	2.13	0.49
1:B:29:GLY:O	1:B:93:ARG:HA	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ALA:HB2	1:C:39:LEU:HD22	1.94	0.49
1:C:391:PHE:C	1:C:391:PHE:HD2	2.15	0.49
1:C:411:ALA:O	1:C:412:LYS:HG3	2.12	0.49
1:C:418:LEU:O	1:C:422:ILE:HG22	2.12	0.49
2:E:172:VAL:HG12	2:E:176:ASP:HB2	1.95	0.49
2:G:212:GLU:OE1	2:G:212:GLU:N	2.43	0.49
2:J:177:LEU:HD12	2:J:178:GLN:N	2.27	0.49
1:C:401:ASN:O	1:C:404:LEU:HB2	2.12	0.49
1:D:70:VAL:HG11	1:D:80:MET:SD	2.51	0.49
2:G:198:ASP:OD2	2:H:159:GLN:NE2	2.45	0.49
2:I:103:ALA:O	2:I:107:GLN:HG2	2.12	0.49
2:J:212:GLU:OE1	2:J:213:GLY:N	2.45	0.49
1:D:220:ILE:O	1:D:229:ARG:HD2	2.12	0.49
1:A:420:LYS:HE3	1:D:409:ALA:HB1	1.94	0.49
2:G:106:GLN:OE1	2:K:101:ILE:HG12	2.13	0.49
1:A:398:PHE:HE1	1:A:422:ILE:HG13	1.77	0.49
1:C:425:TRP:N	1:C:426:PRO:HD2	2.27	0.49
1:C:431:PHE:CD2	1:C:432:LEU:N	2.81	0.49
1:A:295:LYS:HG2	1:A:295:LYS:O	2.13	0.49
1:A:5:LEU:HB2	2:I:115:THR:HG23	1.95	0.49
1:B:121:LEU:HD23	1:B:127:PRO:HA	1.94	0.49
1:D:420:LYS:HG2	1:D:424:LEU:HD12	1.95	0.49
2:F:184:LEU:O	2:F:188:LEU:HG	2.13	0.49
2:J:162:PRO:CB	2:J:210:ALA:HB3	2.43	0.49
1:B:410:TYR:CD2	1:B:412:LYS:HD2	2.47	0.49
1:D:105:GLN:O	1:D:108:LYS:HB2	2.12	0.49
1:D:335:GLN:NE2	1:D:335:GLN:N	2.61	0.49
1:D:57:GLN:NE2	1:D:57:GLN:HA	2.20	0.49
1:D:54:ILE:HG12	1:D:94:VAL:HG12	1.93	0.49
2:E:202:HIS:HB2	2:E:219:VAL:HG22	1.94	0.49
2:G:164:PHE:HB3	2:G:168:PRO:CG	2.43	0.49
1:D:363:TYR:HA	1:D:364:PRO:C	2.33	0.48
2:G:146:ASP:HB2	2:K:141:GLN:OE1	2.13	0.48
2:L:100:PRO:N	2:L:103:ALA:HB3	2.28	0.48
1:B:108:LYS:HD2	1:B:248:GLN:HE22	1.76	0.48
1:B:416:PRO:HA	1:B:419:ASP:CB	2.42	0.48
1:C:404:LEU:HB3	1:C:409:ALA:CB	2.43	0.48
2:G:119:LEU:HD11	2:K:208:VAL:HG13	1.95	0.48
2:L:216:ASP:OD1	2:L:217:ALA:N	2.43	0.48
1:A:429:GLU:O	1:A:433:GLN:NE2	2.46	0.48
1:A:442:TRP:CE2	1:A:446:LEU:HD11	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:GLY:O	1:C:216:VAL:HB	2.12	0.48
1:C:26:ARG:HD2	1:C:28:TYR:CE1	2.47	0.48
1:D:381:THR:HG22	1:D:382:GLU:N	2.29	0.48
2:H:125:SER:O	2:H:128:MET:HB3	2.14	0.48
1:A:34:ALA:HB2	1:A:39:LEU:HD22	1.95	0.48
1:B:220:ILE:HG22	1:B:229:ARG:HD2	1.95	0.48
1:D:272:ASP:OD1	1:D:272:ASP:C	2.51	0.48
1:C:256:ILE:O	1:C:260:PHE:CD2	2.66	0.48
1:B:408:GLY:HA3	1:C:389:ARG:NE	2.27	0.48
1:A:297:TYR:HD2	1:A:301:VAL:HG21	1.79	0.48
1:C:415:ASP:HB2	1:C:418:LEU:CD1	2.42	0.48
2:H:150:LEU:O	2:H:154:ILE:HB	2.13	0.48
2:E:112:PHE:CD2	2:I:108:LEU:HD12	2.49	0.48
2:J:215:LEU:C	2:J:215:LEU:HD12	2.34	0.48
2:J:221:THR:O	2:J:224:GLN:HG2	2.14	0.48
1:B:199:THR:HG21	1:B:268:LEU:HD22	1.95	0.48
1:D:41:ALA:O	1:D:42:THR:HG23	2.14	0.48
2:H:143:PRO:O	2:H:144:ALA:HB2	2.14	0.48
1:A:138:GLU:OE2	1:A:138:GLU:HA	2.12	0.48
2:H:158:LEU:HD21	2:H:191:HIS:CD2	2.49	0.48
2:K:119:LEU:O	2:K:123:ILE:HG22	2.13	0.48
2:G:146:ASP:HB2	2:K:141:GLN:CD	2.34	0.48
1:B:258:GLU:HA	1:B:322:ILE:HD11	1.96	0.48
1:B:453:PHE:N	1:B:454:PRO:CD	2.76	0.48
1:B:4:ARG:NH2	2:F:117:ASP:OD1	2.47	0.48
1:D:348:ASP:C	1:D:374:ARG:HG3	2.33	0.48
2:F:109:VAL:HG23	2:F:110:SER:H	1.78	0.48
2:F:157:LEU:CG	2:F:215:LEU:HD13	2.44	0.48
2:H:101:ILE:HB	2:L:179:ARG:NE	2.24	0.48
1:A:152:ARG:NH2	1:A:313:GLY:HA3	2.29	0.48
1:B:377:THR:HG22	1:B:385:TYR:CE2	2.49	0.48
1:C:448:ALA:O	1:C:451:LEU:HG	2.14	0.48
1:D:164:ARG:NH2	1:D:433:GLN:O	2.46	0.48
2:H:180:VAL:O	2:H:185:GLY:N	2.47	0.48
2:H:221:THR:O	2:H:224:GLN:HG2	2.13	0.48
1:A:425:TRP:HB3	1:A:426:PRO:HD3	1.95	0.47
1:C:31:LEU:HD11	1:C:39:LEU:HB3	1.96	0.47
2:J:134:ALA:O	2:J:138:VAL:HG23	2.13	0.47
1:A:15:PHE:CZ	2:E:230:ALA:HB2	2.49	0.47
2:H:115:THR:HB	2:L:207:LYS:HD2	1.96	0.47
2:H:139:ILE:HD11	2:L:135:ALA:HA	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:184:LEU:HD22	2:J:188:LEU:CD1	2.42	0.47
2:K:110:SER:HA	2:K:191:HIS:CE1	2.49	0.47
1:B:368:ILE:HB	1:B:395:LEU:CD2	2.44	0.47
1:C:181:PHE:CD2	1:C:328:VAL:HB	2.49	0.47
2:G:190:LEU:C	2:G:190:LEU:HD23	2.34	0.47
2:G:173:HIS:HA	2:G:198:ASP:O	2.13	0.47
1:A:117:LEU:HD23	1:A:233:VAL:HG23	1.95	0.47
1:B:219:PHE:HD2	1:B:223:ILE:HD12	1.79	0.47
1:B:295:LYS:HE3	1:B:338:PRO:HB3	1.97	0.47
1:C:120:VAL:HG12	1:C:128:LEU:HB2	1.97	0.47
2:J:112:PHE:CE2	2:J:116:LEU:HD11	2.50	0.47
2:K:171:ARG:O	2:K:206:CYS:HA	2.14	0.47
1:A:454:PRO:HB2	1:A:455:THR:CG2	2.39	0.47
1:B:337:ASP:HA	1:B:338:PRO:HD3	1.73	0.47
1:C:272:ASP:OD1	1:C:273:SER:HB3	2.14	0.47
1:B:409:ALA:HB2	1:C:392:LYS:CE	2.44	0.47
1:C:34:ALA:CB	1:C:39:LEU:HD22	2.44	0.47
1:A:57:GLN:NE2	1:A:59:GLY:O	2.47	0.47
1:B:87:GLY:H	1:B:88:ILE:HD12	1.79	0.47
1:C:180:LEU:HD13	1:C:351:ILE:HD11	1.96	0.47
1:D:109:GLN:HG3	1:D:139:THR:OG1	2.15	0.47
2:J:159:GLN:HA	2:J:165:SER:HB3	1.97	0.47
2:J:215:LEU:HD12	2:J:216:ASP:N	2.29	0.47
2:K:123:ILE:HG13	2:K:127:LEU:HG	1.96	0.47
1:B:439:ARG:NH1	1:B:439:ARG:CG	2.69	0.47
1:D:425:TRP:NE1	1:D:429:GLU:OE1	2.48	0.47
2:F:173:HIS:HD2	2:F:175:ASP:CG	2.18	0.47
1:A:272:ASP:HA	1:A:273:SER:HA	1.65	0.47
1:B:56:ARG:HD2	1:B:87:GLY:CA	2.42	0.47
1:D:55:GLU:OE1	1:D:93:ARG:HB2	2.15	0.47
2:F:173:HIS:HB3	2:F:175:ASP:OD1	2.15	0.47
2:G:111:GLU:HA	2:G:114:ASN:HB2	1.96	0.47
2:L:102:HIS:HB3	2:L:183:MET:HG2	1.96	0.47
2:L:198:ASP:HB3	2:L:201:LEU:HD13	1.96	0.47
2:L:210:ALA:O	2:L:211:ASP:CB	2.62	0.47
1:C:180:LEU:HD21	1:C:188:LYS:HB2	1.97	0.47
2:H:137:GLN:HB3	2:H:141:GLN:OE1	2.15	0.47
2:H:180:VAL:CA	2:H:184:LEU:HB2	2.45	0.47
2:I:151:ILE:HG23	2:I:152:LYS:HD3	1.97	0.47
2:J:170:LEU:HD21	2:J:172:VAL:HG23	1.97	0.47
2:J:171:ARG:NH1	2:J:207:LYS:HB2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:GLU:OE1	1:C:311:ARG:NH2	2.48	0.47
1:D:155:ILE:HG23	1:D:174:ARG:O	2.15	0.47
1:D:243:PRO:HB2	1:D:284:ILE:HD11	1.97	0.47
2:E:100:PRO:HG2	2:E:101:ILE:H	1.80	0.47
2:F:168:PRO:O	2:F:169:GLN:HG3	2.15	0.47
2:G:173:HIS:CD2	2:G:203:HIS:HE1	2.33	0.47
2:K:178:GLN:O	2:K:182:GLU:HG3	2.15	0.47
2:K:142:THR:HG23	2:K:143:PRO:HD2	1.97	0.46
1:A:108:LYS:HG3	1:A:108:LYS:H	1.45	0.46
1:D:75:GLN:HG3	1:D:76:ARG:NH1	2.31	0.46
2:K:110:SER:HA	2:K:191:HIS:NE2	2.30	0.46
1:A:295:LYS:CB	1:A:338:PRO:HG2	2.45	0.46
1:B:190:VAL:CG2	3:B:601:ADP:H5'1	2.46	0.46
1:C:294:THR:HG22	1:C:295:LYS:N	2.29	0.46
1:D:52:CYS:O	1:D:67:SER:N	2.48	0.46
1:D:72:PHE:CD2	1:D:72:PHE:C	2.88	0.46
2:F:185:GLY:HA2	2:F:188:LEU:HD12	1.98	0.46
2:F:136:ARG:NH1	2:J:226:LEU:HA	2.29	0.46
1:A:334:ASP:O	1:A:335:GLN:CB	2.64	0.46
1:A:367:ASP:HB3	1:A:370:ALA:HB3	1.98	0.46
1:A:212:ARG:NH2	1:B:344:ARG:O	2.38	0.46
1:B:394:LEU:HD12	1:B:453:PHE:HE1	1.79	0.46
1:B:396:SER:HB3	1:B:400:ARG:HH12	1.81	0.46
1:C:394:LEU:HD22	1:C:420:LYS:HB2	1.97	0.46
1:A:420:LYS:NZ	1:D:409:ALA:O	2.34	0.46
2:H:167:LYS:HG3	2:H:167:LYS:O	2.15	0.46
2:L:210:ALA:O	2:L:211:ASP:HB3	2.16	0.46
1:B:387:ARG:HE	1:B:454:PRO:HB3	1.80	0.46
1:C:363:TYR:HA	1:C:364:PRO:C	2.34	0.46
1:D:282:ARG:HD2	1:D:296:GLY:HA3	1.98	0.46
1:D:6:THR:O	1:D:10:THR:HG23	2.15	0.46
1:A:161:THR:HB	1:A:195:MET:HE2	1.97	0.46
1:A:376:MET:CE	1:A:388:VAL:HG11	2.46	0.46
1:A:86:GLU:OE1	1:B:106:SER:OG	2.34	0.46
1:C:294:THR:HB	1:C:297:TYR:O	2.14	0.46
1:C:441:ASP:OD2	1:C:442:TRP:N	2.49	0.46
1:D:216:VAL:O	1:D:220:ILE:HG13	2.16	0.46
2:H:177:LEU:O	2:H:180:VAL:HG12	2.16	0.46
2:J:173:HIS:CE1	2:J:203:HIS:HE1	2.33	0.46
2:L:161:GLU:HG3	2:L:163:LEU:HB3	1.98	0.46
1:A:22:LEU:HA	1:A:23:PRO:HD3	1.70	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLY:HA2	1:B:263:ARG:HH22	1.75	0.46
1:B:268:LEU:HD12	1:B:323:THR:O	2.15	0.46
1:B:178:MET:O	1:B:325:PHE:HA	2.15	0.46
1:C:337:ASP:HA	1:C:338:PRO:HD3	1.76	0.46
1:C:33:ARG:HE	1:C:35:THR:CG2	2.29	0.46
1:C:452:ILE:CG2	1:C:453:PHE:N	2.76	0.46
1:D:204:ILE:HB	1:D:232:SER:CB	2.35	0.46
1:D:238:PRO:O	1:D:241:VAL:HG12	2.16	0.46
2:G:221:THR:O	2:G:224:GLN:HB2	2.15	0.46
2:H:102:HIS:O	2:H:106:GLN:HG3	2.14	0.46
1:A:163:VAL:C	1:A:167:ASN:HD22	2.19	0.46
1:A:286:LEU:HD21	1:A:292:PRO:HG3	1.98	0.46
1:A:291:PRO:HA	1:A:292:PRO:HD3	1.68	0.46
1:B:116:LEU:HD22	1:B:121:LEU:CD1	2.45	0.46
1:C:163:VAL:C	1:C:167:ASN:HD21	2.16	0.46
1:C:291:PRO:HA	1:C:292:PRO:HD3	1.69	0.46
1:A:187:GLY:HA2	3:A:601:ADP:C5'	2.45	0.46
1:B:163:VAL:C	1:B:167:ASN:ND2	2.67	0.46
1:D:362:HIS:O	1:D:365:ALA:HB2	2.16	0.46
1:D:45:GLN:O	1:D:45:GLN:HG2	2.15	0.46
2:E:148:SER:O	2:E:152:LYS:HG3	2.16	0.46
2:G:104:ARG:O	2:G:108:LEU:HG	2.15	0.46
1:A:399:GLN:HA	1:A:402:ARG:NH1	2.31	0.46
1:A:162:GLY:HA2	1:A:440:ALA:O	2.16	0.46
1:B:56:ARG:NH2	1:B:58:ASP:OD2	2.49	0.46
1:C:383:GLN:O	1:C:387:ARG:HG3	2.15	0.46
2:F:157:LEU:HD11	2:F:215:LEU:HD13	1.97	0.46
2:G:187:THR:O	2:G:191:HIS:HB2	2.16	0.46
2:H:100:PRO:N	2:H:103:ALA:HB3	2.31	0.46
2:J:211:ASP:HB3	2:J:212:GLU:H	1.47	0.46
2:J:220:ALA:HA	2:J:223:TRP:CD1	2.50	0.46
1:B:177:ARG:HH11	1:B:310:GLU:HA	1.80	0.45
1:C:356:ARG:HH11	1:C:357:LEU:H	1.64	0.45
2:F:172:VAL:HG12	2:F:173:HIS:N	2.32	0.45
2:I:195:LEU:HD23	2:I:195:LEU:C	2.36	0.45
2:J:184:LEU:HD13	2:J:188:LEU:HB3	1.97	0.45
1:A:387:ARG:HH11	1:D:407:VAL:HG23	1.81	0.45
1:D:227:ASP:N	1:D:227:ASP:OD2	2.46	0.45
2:G:181:GLU:O	2:G:185:GLY:HA3	2.17	0.45
2:J:181:GLU:HG2	2:J:184:LEU:HD11	1.98	0.45
2:L:136:ARG:HG3	2:L:141:GLN:HG2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLY:HA2	3:B:601:ADP:H5'2	1.98	0.45
1:C:290:GLU:OE1	1:C:300:SER:OG	2.33	0.45
2:G:219:VAL:HG13	2:K:138:VAL:CG1	2.43	0.45
2:J:159:GLN:HG2	2:J:165:SER:CB	2.45	0.45
2:J:172:VAL:CG1	2:J:173:HIS:N	2.67	0.45
1:A:46:LEU:HB3	1:A:47:PRO:HD2	1.99	0.45
1:C:170:LEU:HD21	1:C:371:SER:HB2	1.98	0.45
1:C:411:ALA:C	1:C:412:LYS:HG3	2.36	0.45
1:D:387:ARG:NH2	1:D:454:PRO:HB3	2.26	0.45
2:F:130:MET:SD	2:J:158:LEU:HD23	2.57	0.45
2:L:173:HIS:ND1	2:L:174:PRO:HD2	2.31	0.45
1:A:144:THR:HG21	1:A:258:GLU:OE1	2.16	0.45
1:B:108:LYS:CD	1:B:248:GLN:HE22	2.30	0.45
1:B:152:ARG:HD3	1:B:314:ASN:O	2.16	0.45
1:D:8:TRP:O	2:H:124:ALA:HA	2.16	0.45
2:H:169:GLN:HE21	2:H:196:ARG:HB2	1.81	0.45
1:A:274:LEU:HD11	1:A:305:LEU:HD22	1.99	0.45
1:C:210:GLY:O	1:C:239:ALA:HB2	2.16	0.45
1:D:272:ASP:HA	1:D:273:SER:HA	1.51	0.45
1:A:387:ARG:NH1	1:D:407:VAL:HG23	2.31	0.45
2:H:192:GLY:C	2:H:193:TRP:HD1	2.20	0.45
2:I:107:GLN:O	2:I:111:GLU:HB3	2.16	0.45
2:J:150:LEU:O	2:J:153:GLN:HB3	2.17	0.45
1:B:372:ILE:HG12	1:B:373:SER:N	2.31	0.45
1:B:408:GLY:HA3	1:C:389:ARG:NH2	2.32	0.45
1:C:368:ILE:H	1:C:368:ILE:CD1	2.21	0.45
1:D:410:TYR:CZ	1:D:418:LEU:HD23	2.51	0.45
2:H:103:ALA:HA	2:H:106:GLN:CD	2.36	0.45
2:H:150:LEU:HD12	2:H:150:LEU:C	2.37	0.45
2:G:135:ALA:HB2	2:K:131:ALA:HA	1.99	0.45
1:B:368:ILE:HD12	1:B:368:ILE:N	2.32	0.45
1:B:158:VAL:HG11	1:B:442:TRP:CE3	2.52	0.45
1:D:405:VAL:HA	1:D:410:TYR:HB3	1.98	0.45
2:F:150:LEU:HB2	2:F:204:GLY:HA2	1.99	0.45
2:G:196:ARG:HE	2:H:159:GLN:HE21	1.64	0.45
2:I:107:GLN:HA	2:I:110:SER:HB3	1.98	0.45
2:I:172:VAL:CG2	2:I:173:HIS:H	2.23	0.45
1:A:237:ALA:CB	1:A:246:ARG:HA	2.47	0.45
1:A:187:GLY:CA	3:A:601:ADP:H5'2	2.45	0.45
1:B:31:LEU:HD12	1:B:40:GLU:O	2.16	0.45
1:D:118:GLY:HA2	1:D:229:ARG:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:ARG:O	1:D:393:GLN:HG3	2.17	0.45
2:H:180:VAL:HG13	2:H:181:GLU:N	2.32	0.45
2:I:173:HIS:HD2	2:I:203:HIS:HA	1.82	0.45
1:A:292:PRO:CB	1:A:296:GLY:HA2	2.47	0.45
2:H:171:ARG:HG2	2:H:196:ARG:HD2	1.98	0.45
1:D:26:ARG:HB3	2:H:216:ASP:HB3	1.98	0.45
1:A:116:LEU:O	1:A:119:ARG:HB2	2.17	0.44
1:A:389:ARG:HA	1:A:392:LYS:HE2	1.99	0.44
1:B:179:GLY:O	1:B:350:HIS:HA	2.17	0.44
2:F:108:LEU:HD23	2:F:109:VAL:N	2.29	0.44
2:F:109:VAL:HG23	2:F:110:SER:N	2.32	0.44
2:J:184:LEU:HD12	2:J:185:GLY:N	2.32	0.44
2:J:181:GLU:HA	2:J:184:LEU:HG	1.98	0.44
1:A:305:LEU:HB2	1:A:306:PRO:HD3	2.00	0.44
1:A:80:MET:HA	1:A:81:PRO:HD3	1.72	0.44
1:C:287:ALA:HA	1:D:299:PRO:HG3	1.99	0.44
1:C:29:GLY:N	1:C:94:VAL:O	2.41	0.44
1:D:51:THR:HG22	1:D:68:GLU:HG2	1.99	0.44
2:F:177:LEU:HD23	2:F:177:LEU:C	2.37	0.44
2:G:154:ILE:HG23	2:G:158:LEU:CD1	2.48	0.44
2:F:223:TRP:HE3	2:J:138:VAL:HG21	1.82	0.44
1:C:188:LYS:HG2	3:C:601:ADP:O1B	2.18	0.44
2:G:101:ILE:HG23	2:G:104:ARG:NH1	2.32	0.44
1:A:113:GLY:HA2	1:A:263:ARG:NH1	2.32	0.44
1:A:401:ASN:HB3	1:A:418:LEU:HD11	2.00	0.44
1:B:119:ARG:NH1	1:B:131:LEU:HB2	2.33	0.44
1:B:119:ARG:NH1	1:B:129:ASP:OD2	2.48	0.44
1:B:285:ALA:HB3	1:B:298:PRO:HG3	2.00	0.44
2:G:148:SER:OG	2:G:149:ALA:N	2.50	0.44
2:G:150:LEU:O	2:G:154:ILE:HD12	2.17	0.44
2:K:179:ARG:H	2:K:179:ARG:HG2	1.55	0.44
1:B:109:GLN:O	1:B:110:LEU:HD12	2.17	0.44
1:D:207:GLY:HA2	1:D:235:ILE:O	2.18	0.44
1:D:329:LEU:HD21	1:D:331:GLU:HG2	2.00	0.44
2:H:115:THR:HB	2:L:207:LYS:HD3	1.99	0.44
2:H:160:GLN:O	2:H:163:LEU:HD12	2.17	0.44
2:J:209:SER:OG	2:J:210:ALA:O	2.35	0.44
1:B:389:ARG:O	1:B:393:GLN:HG3	2.17	0.44
1:C:452:ILE:O	1:C:453:PHE:CD2	2.71	0.44
2:G:164:PHE:CE1	2:G:210:ALA:HB3	2.52	0.44
1:A:387:ARG:HD2	1:A:453:PHE:CB	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:HG2	1:B:28:TYR:CE1	2.51	0.44
1:C:244:LEU:HA	1:C:244:LEU:HD23	1.83	0.44
1:D:258:GLU:HA	1:D:322:ILE:HD11	2.00	0.44
1:D:47:PRO:HD2	1:D:50:ALA:HB2	1.99	0.44
2:F:157:LEU:HD21	2:F:215:LEU:HD13	2.00	0.44
2:K:223:TRP:CZ3	2:K:226:LEU:HD23	2.53	0.44
2:H:109:VAL:HG12	2:L:104:ARG:HH21	1.82	0.44
1:A:129:ASP:OD1	1:A:129:ASP:N	2.51	0.44
1:A:247:MET:CE	1:A:281:GLN:HE21	2.31	0.44
1:B:401:ASN:H	1:B:401:ASN:ND2	2.16	0.44
1:B:420:LYS:O	1:B:424:LEU:HD13	2.18	0.44
1:B:408:GLY:CA	1:C:389:ARG:CZ	2.92	0.44
1:C:404:LEU:CA	1:C:409:ALA:HB2	2.47	0.44
2:H:158:LEU:HD12	2:H:158:LEU:N	2.32	0.44
2:I:161:GLU:OE2	2:I:162:PRO:HD2	2.18	0.44
2:L:157:LEU:O	2:L:160:GLN:HB2	2.18	0.44
1:A:295:LYS:HB2	1:A:338:PRO:CG	2.48	0.44
1:A:433:GLN:HB2	1:A:433:GLN:HE21	1.61	0.44
1:C:297:TYR:HB3	1:C:301:VAL:HG21	1.99	0.44
1:D:418:LEU:O	1:D:422:ILE:N	2.49	0.44
2:G:111:GLU:OE1	2:K:202:HIS:HE1	2.01	0.44
2:L:201:LEU:H	2:L:201:LEU:HD12	1.83	0.44
1:C:186:VAL:CG1	1:C:186:VAL:O	2.64	0.43
1:C:388:VAL:HG12	1:C:392:LYS:HD3	2.00	0.43
1:D:241:VAL:CG2	1:D:245:LEU:HD12	2.48	0.43
1:D:381:THR:HG21	1:D:383:GLN:CG	2.48	0.43
1:D:432:LEU:HD23	1:D:432:LEU:HA	1.86	0.43
2:J:173:HIS:CD2	2:J:174:PRO:HD2	2.53	0.43
1:A:276:ARG:HA	1:A:276:ARG:HD2	1.44	0.43
1:B:175:GLY:HA3	1:B:314:ASN:OD1	2.18	0.43
1:C:163:VAL:CG2	1:C:166:ILE:HD12	2.47	0.43
1:C:401:ASN:OD1	1:C:404:LEU:HD12	2.18	0.43
1:D:46:LEU:HA	1:D:47:PRO:HD3	1.84	0.43
2:F:123:ILE:HD12	2:F:123:ILE:C	2.39	0.43
2:G:168:PRO:HG2	2:G:193:TRP:NE1	2.33	0.43
2:L:168:PRO:HG2	2:L:193:TRP:CH2	2.53	0.43
1:A:390:LEU:HA	1:A:393:GLN:HG3	2.00	0.43
1:C:40:GLU:HG2	1:C:78:PHE:CE2	2.53	0.43
2:E:177:LEU:HD23	2:E:177:LEU:C	2.39	0.43
2:H:129:GLN:NE2	2:L:219:VAL:HG13	2.33	0.43
2:K:212:GLU:N	2:K:212:GLU:OE1	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:111:GLU:HG2	2:L:112:PHE:N	2.33	0.43
1:D:353:LEU:HA	1:D:365:ALA:O	2.19	0.43
2:E:181:GLU:OE1	2:E:181:GLU:C	2.56	0.43
2:E:190:LEU:HD23	2:E:190:LEU:HA	1.80	0.43
2:G:104:ARG:CZ	2:K:176:ASP:OD1	2.67	0.43
1:A:172:VAL:HG12	1:A:173:GLY:N	2.33	0.43
1:A:278:ALA:HB2	1:A:305:LEU:HD21	1.99	0.43
2:E:151:ILE:HG23	2:E:184:LEU:HD11	2.01	0.43
2:E:109:VAL:HG13	2:I:105:MET:HG3	2.01	0.43
1:B:335:GLN:HG3	1:B:335:GLN:H	1.52	0.43
1:D:391:PHE:C	1:D:391:PHE:CD2	2.92	0.43
2:G:145:VAL:O	2:G:145:VAL:CG2	2.66	0.43
2:H:103:ALA:O	2:H:106:GLN:HB2	2.19	0.43
1:D:164:ARG:HG3	1:D:445:SER:CB	2.48	0.43
1:D:40:GLU:OE2	1:D:76:ARG:HG2	2.19	0.43
2:I:170:LEU:O	2:I:195:LEU:HA	2.19	0.43
2:J:107:GLN:O	2:J:111:GLU:HG3	2.18	0.43
1:A:73:ASN:O	1:A:74:GLY:C	2.57	0.43
1:B:295:LYS:HD2	1:B:338:PRO:HG3	2.01	0.43
1:B:316:ILE:CG2	1:B:317:HIS:N	2.82	0.43
1:B:88:ILE:N	1:B:88:ILE:HD12	2.33	0.43
1:C:153:THR:OG1	1:C:154:PRO:HD2	2.19	0.43
1:C:204:ILE:O	1:C:232:SER:HA	2.19	0.43
1:C:351:ILE:HA	1:C:371:SER:HB3	2.00	0.43
2:F:150:LEU:HD12	2:F:204:GLY:CA	2.48	0.43
2:I:198:ASP:HB3	2:I:201:LEU:HG	2.00	0.43
2:K:124:ALA:HB2	2:K:155:GLN:OE1	2.18	0.43
2:H:122:VAL:HG13	2:L:219:VAL:HG21	2.01	0.43
1:A:180:LEU:C	1:A:181:PHE:HD2	2.22	0.43
1:B:274:LEU:HD23	1:B:274:LEU:HA	1.90	0.43
1:C:384:HIS:O	1:C:388:VAL:HG23	2.19	0.43
1:C:394:LEU:HD21	1:C:420:LYS:HD3	2.00	0.43
1:C:56:ARG:O	1:C:63:LYS:N	2.36	0.43
1:D:180:LEU:CD1	1:D:351:ILE:HB	2.49	0.43
2:G:100:PRO:HD2	2:G:102:HIS:HB3	2.01	0.43
2:G:173:HIS:CD2	2:G:175:ASP:H	2.37	0.43
2:G:173:HIS:HD2	2:G:175:ASP:HB2	1.84	0.43
2:I:172:VAL:CG2	2:I:173:HIS:N	2.81	0.43
2:I:178:GLN:O	2:I:182:GLU:HG3	2.19	0.43
1:A:158:VAL:HG11	1:A:442:TRP:CZ3	2.54	0.42
1:A:181:PHE:N	1:A:181:PHE:HD2	2.16	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:PHE:H	1:B:454:PRO:HD3	1.80	0.42
1:B:8:TRP:N	1:B:8:TRP:CD1	2.86	0.42
1:C:51:THR:HG21	1:C:108:LYS:HD3	2.00	0.42
1:D:211:GLU:OE1	1:D:211:GLU:HA	2.19	0.42
1:C:431:PHE:C	1:C:431:PHE:CD2	2.93	0.42
1:D:31:LEU:O	1:D:90:PRO:O	2.37	0.42
2:I:226:LEU:HD23	2:I:226:LEU:O	2.19	0.42
2:J:102:HIS:CD2	2:J:102:HIS:N	2.86	0.42
2:J:155:GLN:O	2:J:158:LEU:HB2	2.19	0.42
2:L:168:PRO:HB2	2:L:193:TRP:CZ3	2.54	0.42
1:B:272:ASP:HA	1:B:273:SER:HA	1.62	0.42
2:G:196:ARG:HG2	2:H:159:GLN:NE2	2.33	0.42
2:L:171:ARG:HH21	2:L:209:SER:CB	2.33	0.42
1:A:404:LEU:HB3	1:A:409:ALA:HB3	2.00	0.42
1:B:397:SER:HB2	1:B:417:MET:CE	2.49	0.42
2:H:177:LEU:O	2:H:180:VAL:HB	2.19	0.42
2:I:101:ILE:HD12	2:I:101:ILE:C	2.39	0.42
1:A:151:GLN:O	1:A:151:GLN:HG3	2.19	0.42
1:A:164:ARG:HG3	1:A:445:SER:HA	2.02	0.42
1:A:337:ASP:HA	1:A:338:PRO:HD3	1.69	0.42
1:C:305:LEU:HB2	1:C:306:PRO:HD3	2.01	0.42
1:D:219:PHE:C	1:D:219:PHE:CD1	2.93	0.42
2:H:101:ILE:HD13	2:H:102:HIS:N	2.34	0.42
2:L:201:LEU:N	2:L:201:LEU:HD12	2.34	0.42
1:A:169:LEU:O	1:A:376:MET:HE1	2.20	0.42
1:C:372:ILE:HG13	1:C:373:SER:N	2.35	0.42
1:D:108:LYS:O	1:D:142:LEU:N	2.49	0.42
1:D:243:PRO:CB	1:D:284:ILE:HD11	2.50	0.42
2:G:229:LEU:C	2:G:229:LEU:HD23	2.40	0.42
2:L:229:LEU:HD12	2:L:230:ALA:H	1.84	0.42
1:C:182:ALA:HB2	1:C:353:LEU:HB2	2.01	0.42
1:D:73:ASN:OD1	1:D:74:GLY:N	2.47	0.42
2:E:108:LEU:HD21	2:I:176:ASP:CB	2.49	0.42
2:I:162:PRO:O	2:I:166:GLY:N	2.43	0.42
2:K:156:GLN:O	2:K:160:GLN:HG3	2.19	0.42
1:C:412:LYS:CD	1:C:413:GLY:H	2.21	0.42
2:E:188:LEU:HA	2:E:188:LEU:HD23	1.87	0.42
2:H:166:GLY:O	2:H:167:LYS:CG	2.66	0.42
2:L:170:LEU:O	2:L:195:LEU:HD12	2.20	0.42
1:A:28:TYR:CD2	1:A:93:ARG:HB3	2.54	0.42
1:B:397:SER:HB2	1:B:417:MET:HG2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ARG:HD3	1:B:8:TRP:CZ2	2.55	0.42
1:C:441:ASP:CG	1:C:444:ASP:H	2.21	0.42
2:J:176:ASP:O	2:J:180:VAL:HG23	2.19	0.42
2:L:171:ARG:HA	2:L:196:ARG:O	2.20	0.42
1:A:164:ARG:HB2	1:A:440:ALA:CB	2.50	0.42
1:A:363:TYR:HA	1:A:364:PRO:C	2.40	0.42
1:A:453:PHE:HB2	1:A:454:PRO:CD	2.46	0.42
1:C:82:LEU:N	1:C:82:LEU:HD12	2.35	0.42
1:D:194:MET:CE	3:D:601:ADP:N6	2.83	0.42
2:F:134:ALA:O	2:F:138:VAL:HG23	2.20	0.42
2:J:102:HIS:CE1	2:J:182:GLU:OE1	2.73	0.42
1:B:148:ASN:HA	1:B:149:PRO:HD3	1.85	0.41
1:B:450:ASP:O	1:B:454:PRO:HD2	2.20	0.41
1:D:31:LEU:HD21	1:D:39:LEU:HD23	2.02	0.41
2:G:196:ARG:HG2	2:H:159:GLN:HE22	1.84	0.41
2:I:106:GLN:HG2	2:I:187:THR:HG21	2.02	0.41
2:J:215:LEU:O	2:J:219:VAL:HG23	2.20	0.41
2:J:220:ALA:HA	2:J:223:TRP:HD1	1.84	0.41
1:A:454:PRO:CB	1:A:455:THR:CA	2.92	0.41
1:A:2:THR:CA	1:A:5:LEU:HB3	2.48	0.41
1:D:30:ARG:O	1:D:41:ALA:HB1	2.19	0.41
1:D:338:PRO:O	1:D:342:SER:HB2	2.19	0.41
2:H:180:VAL:HG23	2:H:184:LEU:CB	2.50	0.41
2:H:216:ASP:OD1	2:H:218:SER:HB3	2.20	0.41
2:I:171:ARG:HA	2:I:196:ARG:O	2.19	0.41
2:I:196:ARG:NH1	2:I:196:ARG:HG3	2.34	0.41
2:E:108:LEU:CD1	2:I:204:GLY:HA2	2.50	0.41
2:G:115:THR:HG21	2:K:206:CYS:O	2.20	0.41
1:A:149:PRO:CA	1:A:152:ARG:HD2	2.44	0.41
1:A:238:PRO:O	1:A:241:VAL:HG22	2.21	0.41
1:A:56:ARG:HG3	1:A:87:GLY:O	2.20	0.41
1:D:225:GLY:O	1:D:229:ARG:HG3	2.20	0.41
2:H:101:ILE:HB	2:L:179:ARG:NH2	2.35	0.41
2:K:173:HIS:CE1	2:K:175:ASP:OD2	2.72	0.41
1:B:50:ALA:HA	1:B:104:LEU:HD23	2.02	0.41
1:C:428:LEU:HD21	1:C:452:ILE:HD11	2.02	0.41
1:D:243:PRO:HG3	1:D:283:GLU:OE2	2.20	0.41
1:D:34:ALA:HB1	1:D:88:ILE:HG22	2.02	0.41
2:I:126:ARG:HA	2:I:126:ARG:HD2	1.80	0.41
2:I:178:GLN:NE2	2:I:182:GLU:OE2	2.53	0.41
2:J:188:LEU:HG	2:J:193:TRP:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:NH2	1:A:283:GLU:OE1	2.50	0.41
1:A:395:LEU:O	1:A:399:GLN:HG2	2.20	0.41
1:A:453:PHE:CB	1:A:454:PRO:HD3	2.43	0.41
1:B:109:GLN:C	1:B:110:LEU:HD12	2.41	0.41
1:C:15:PHE:CE1	2:G:230:ALA:HB2	2.56	0.41
1:C:158:VAL:HG23	1:C:171:THR:CG2	2.50	0.41
1:D:402:ARG:O	1:D:406:SER:N	2.25	0.41
2:F:112:PHE:HE1	2:J:208:VAL:CG2	2.34	0.41
2:L:101:ILE:HG23	2:L:102:HIS:N	2.36	0.41
1:A:192:LEU:HD11	1:A:327:THR:HG21	2.01	0.41
1:B:387:ARG:NE	1:B:454:PRO:HB3	2.35	0.41
1:C:336:GLN:HG3	1:C:336:GLN:H	1.67	0.41
1:C:56:ARG:HG2	1:C:57:GLN:N	2.35	0.41
2:H:113:GLN:O	2:H:117:ASP:N	2.37	0.41
2:J:101:ILE:HD11	2:J:183:MET:SD	2.60	0.41
2:J:169:GLN:HE21	2:J:194:ARG:HD2	1.85	0.41
1:C:84:GLU:HG2	1:C:86:GLU:H	1.86	0.41
2:F:154:ILE:CD1	2:F:170:LEU:HD11	2.45	0.41
2:J:109:VAL:HG13	2:J:193:TRP:CH2	2.55	0.41
2:G:226:LEU:HD21	2:K:134:ALA:HB1	2.02	0.41
2:L:100:PRO:HG2	2:L:101:ILE:H	1.86	0.41
2:H:135:ALA:HB2	2:L:131:ALA:HA	2.02	0.41
1:A:401:ASN:O	1:A:401:ASN:OD1	2.39	0.41
1:B:199:THR:HG21	1:B:268:LEU:CD2	2.50	0.41
1:B:437:PHE:N	1:B:437:PHE:CD1	2.88	0.41
1:B:394:LEU:CD1	1:B:453:PHE:HE1	2.33	0.41
1:B:48:LEU:CD2	1:B:71:GLY:HA2	2.51	0.41
1:C:354:SER:HB3	1:C:356:ARG:NH1	2.36	0.41
1:C:156:GLU:O	1:C:379:LEU:HD23	2.21	0.41
1:C:55:GLU:HB2	1:C:93:ARG:HG3	2.01	0.41
1:C:82:LEU:N	1:C:82:LEU:CD1	2.84	0.41
1:D:183:GLY:HA2	1:D:330:THR:O	2.21	0.41
1:A:29:GLY:N	1:A:44:LEU:HD23	2.36	0.41
1:B:363:TYR:HB3	3:B:601:ADP:C5	2.55	0.41
1:C:383:GLN:HG2	1:C:383:GLN:H	1.66	0.41
1:C:396:SER:O	1:C:399:GLN:HB3	2.20	0.41
2:E:215:LEU:HD23	2:E:215:LEU:HA	1.94	0.41
2:H:138:VAL:O	2:H:142:THR:CB	2.69	0.41
2:I:147:ASN:O	2:I:151:ILE:HG22	2.21	0.41
2:L:136:ARG:HA	2:L:141:GLN:H	1.86	0.41
1:A:193:GLY:O	1:A:197:ARG:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:THR:O	1:B:279:MET:HG3	2.21	0.41
1:B:177:ARG:HH12	1:B:310:GLU:HA	1.81	0.41
2:G:158:LEU:CD1	2:G:193:TRP:CZ3	3.04	0.41
2:H:214:ASP:OD1	2:H:214:ASP:N	2.54	0.41
2:J:164:PHE:N	2:J:164:PHE:CD2	2.89	0.41
1:A:252:TYR:O	1:A:256:ILE:HG13	2.21	0.41
1:C:354:SER:CB	1:C:356:ARG:NH1	2.84	0.41
2:E:158:LEU:HD22	2:E:191:HIS:CG	2.56	0.41
2:J:173:HIS:CD2	2:J:174:PRO:CD	3.03	0.41
2:J:188:LEU:HD21	2:J:193:TRP:O	2.20	0.41
2:L:162:PRO:HA	2:L:165:SER:HB2	2.02	0.41
1:A:205:VAL:HG21	1:A:257:ALA:HB2	2.02	0.40
1:D:396:SER:OG	1:D:400:ARG:NH2	2.54	0.40
2:F:224:GLN:HG3	2:F:225:GLU:N	2.36	0.40
2:H:158:LEU:H	2:H:158:LEU:CD1	2.35	0.40
2:I:102:HIS:H	2:I:102:HIS:CD2	2.39	0.40
2:J:123:ILE:HG13	2:J:127:LEU:HG	2.03	0.40
1:A:385:TYR:CD1	1:A:385:TYR:O	2.75	0.40
1:B:97:ARG:HH11	1:B:99:GLY:HA3	1.85	0.40
1:C:340:ALA:O	1:C:344:ARG:HB2	2.21	0.40
1:C:356:ARG:HH11	1:C:356:ARG:CG	2.26	0.40
1:C:40:GLU:HG2	1:C:78:PHE:HD2	1.86	0.40
1:D:4:ARG:HB2	1:D:7:ARG:NH2	2.37	0.40
2:G:161:GLU:HG2	2:G:162:PRO:HA	2.04	0.40
2:H:152:LYS:HB2	2:H:152:LYS:HE3	1.86	0.40
2:H:198:ASP:OD1	2:H:199:PRO:HD2	2.22	0.40
2:I:146:ASP:C	2:I:146:ASP:OD1	2.59	0.40
2:L:138:VAL:CG2	2:L:139:ILE:N	2.83	0.40
1:A:87:GLY:HA2	1:B:47:PRO:HB2	2.03	0.40
1:B:149:PRO:HA	1:B:152:ARG:HG3	2.02	0.40
1:C:200:ARG:HA	1:C:200:ARG:HD3	1.84	0.40
1:D:180:LEU:HD12	1:D:351:ILE:HB	2.04	0.40
1:D:294:THR:O	1:D:295:LYS:C	2.59	0.40
1:C:32:THR:O	1:D:74:GLY:HA2	2.21	0.40
2:F:148:SER:O	2:F:151:ILE:HB	2.22	0.40
2:G:101:ILE:O	2:G:101:ILE:HG22	2.22	0.40
2:G:194:ARG:H	2:G:194:ARG:HG3	1.50	0.40
2:H:153:GLN:HG3	2:H:154:ILE:N	2.37	0.40
2:E:104:ARG:NH2	2:I:203:HIS:O	2.55	0.40
2:K:188:LEU:O	2:K:192:GLY:N	2.43	0.40
2:H:231:ALA:HB2	2:L:223:TRP:CZ2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:HIS:C	1:B:384:HIS:HD1	2.24	0.40
1:B:404:LEU:HD12	1:B:404:LEU:N	2.35	0.40
1:C:202:ASP:N	1:C:202:ASP:OD2	2.55	0.40
1:C:276:ARG:HD3	1:C:276:ARG:HA	1.93	0.40
1:C:85:VAL:HB	1:C:88:ILE:HD12	2.03	0.40
1:C:53:ILE:HD11	1:C:97:ARG:HG2	2.03	0.40
2:G:174:PRO:O	2:G:177:LEU:HB3	2.21	0.40
1:A:267:VAL:CG2	1:A:322:ILE:HG12	2.50	0.40
1:B:316:ILE:CG2	1:B:317:HIS:H	2.25	0.40
1:C:12:LEU:HB3	2:K:130:MET:HE1	2.03	0.40
1:C:258:GLU:HA	1:C:322:ILE:HD11	2.03	0.40
1:D:202:ASP:HB2	1:D:265:GLN:HB3	2.03	0.40
2:F:129:GLN:HG2	2:J:222:ARG:HD2	2.03	0.40
2:F:151:ILE:O	2:F:155:GLN:N	2.43	0.40
2:F:193:TRP:HD1	2:F:193:TRP:N	2.19	0.40
2:G:151:ILE:HG23	2:G:184:LEU:HD22	2.04	0.40
2:H:170:LEU:HD23	2:H:170:LEU:C	2.42	0.40
2:K:161:GLU:HA	2:K:162:PRO:HD3	1.97	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:GLU:OE2	2:L:196:ARG:NH2[3_445]	2.08	0.12
1:B:13:ASP:OD2	2:K:121:SER:OG[1_655]	2.10	0.10
2:J:125:SER:O	2:K:125:SER:OG[1_655]	2.15	0.05
1:A:6:THR:OG1	2:L:114:ASN:OD1[1_655]	2.16	0.04
1:B:332:GLY:N	2:L:211:ASP:OD1[3_445]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/456 (97%)	429 (97%)	12 (3%)	0	100	100
1	B	453/456 (99%)	438 (97%)	13 (3%)	2 (0%)	34	72
1	C	441/456 (97%)	426 (97%)	13 (3%)	2 (0%)	29	68
1	D	452/456 (99%)	440 (97%)	12 (3%)	0	100	100
2	E	133/140 (95%)	131 (98%)	2 (2%)	0	100	100
2	F	124/140 (89%)	121 (98%)	3 (2%)	0	100	100
2	G	134/140 (96%)	124 (92%)	10 (8%)	0	100	100
2	H	134/140 (96%)	127 (95%)	7 (5%)	0	100	100
2	I	131/140 (94%)	127 (97%)	4 (3%)	0	100	100
2	J	131/140 (94%)	126 (96%)	5 (4%)	0	100	100
2	K	131/140 (94%)	129 (98%)	2 (2%)	0	100	100
2	L	121/140 (86%)	115 (95%)	6 (5%)	0	100	100
All	All	2826/2944 (96%)	2733 (97%)	89 (3%)	4 (0%)	51	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	294	THR
1	C	295	LYS
1	C	452	ILE
1	B	317	HIS

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	350/358 (98%)	328 (94%)	22 (6%)	18	51
1	B	357/358 (100%)	334 (94%)	23 (6%)	17	51
1	C	351/358 (98%)	326 (93%)	25 (7%)	14	46
1	D	356/358 (99%)	333 (94%)	23 (6%)	17	50
2	E	112/115 (97%)	106 (95%)	6 (5%)	22	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	104/115 (90%)	94 (90%)	10 (10%)	8	32
2	G	113/115 (98%)	102 (90%)	11 (10%)	8	31
2	H	113/115 (98%)	106 (94%)	7 (6%)	18	52
2	I	111/115 (96%)	107 (96%)	4 (4%)	35	70
2	J	111/115 (96%)	105 (95%)	6 (5%)	22	57
2	K	111/115 (96%)	106 (96%)	5 (4%)	27	64
2	L	106/115 (92%)	101 (95%)	5 (5%)	26	63
All	All	2295/2352 (98%)	2148 (94%)	147 (6%)	17	51

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	22	LEU
1	A	30	ARG
1	A	67	SER
1	A	72	PHE
1	A	108	LYS
1	A	129	ASP
1	A	142	LEU
1	A	151	GLN
1	A	156	GLU
1	A	184	SER
1	A	227	ASP
1	A	260	PHE
1	A	276	ARG
1	A	300	SER
1	A	356	ARG
1	A	369	GLU
1	A	387	ARG
1	A	391	PHE
1	A	393	GLN
1	A	433	GLN
1	A	455	THR
1	B	66	GLU
1	B	97	ARG
1	B	98	ASN
1	B	100	HIS
1	B	106	SER
1	B	109	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	126	LYS
1	B	164	ARG
1	B	217	LYS
1	B	227	ASP
1	B	232	SER
1	B	240	ASP
1	B	300	SER
1	B	335	GLN
1	B	374	ARG
1	B	384	HIS
1	B	398	PHE
1	B	399	GLN
1	B	401	ASN
1	B	403	ASP
1	B	425	TRP
1	B	439	ARG
1	B	447	GLN
1	C	2	THR
1	C	3	THR
1	C	9	LEU
1	C	30	ARG
1	C	45	GLN
1	C	72	PHE
1	C	76	ARG
1	C	93	ARG
1	C	97	ARG
1	C	109	GLN
1	C	152	ARG
1	C	156	GLU
1	C	167	ASN
1	C	227	ASP
1	C	331	GLU
1	C	356	ARG
1	C	383	GLN
1	C	391	PHE
1	C	392	LYS
1	C	396	SER
1	C	399	GLN
1	C	400	ARG
1	C	412	LYS
1	C	431	PHE
1	C	441	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	16	GLU
1	D	33	ARG
1	D	45	GLN
1	D	55	GLU
1	D	57	GLN
1	D	58	ASP
1	D	64	GLU
1	D	66	GLU
1	D	76	ARG
1	D	97	ARG
1	D	148	ASN
1	D	151	GLN
1	D	170	LEU
1	D	227	ASP
1	D	231	ARG
1	D	240	ASP
1	D	333	ASP
1	D	335	GLN
1	D	336	GLN
1	D	382	GLU
1	D	402	ARG
1	D	439	ARG
1	D	445	SER
2	E	145	VAL
2	E	147	ASN
2	E	156	GLN
2	E	159	GLN
2	E	165	SER
2	E	169	GLN
2	F	129	GLN
2	F	147	ASN
2	F	155	GLN
2	F	156	GLN
2	F	159	GLN
2	F	164	PHE
2	F	181	GLU
2	F	191	HIS
2	F	198	ASP
2	F	228	ARG
2	G	133	GLU
2	G	148	SER
2	G	156	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	159	GLN
2	G	160	GLN
2	G	172	VAL
2	G	175	ASP
2	G	191	HIS
2	G	194	ARG
2	G	198	ASP
2	G	216	ASP
2	H	101	ILE
2	H	120	ASP
2	H	191	HIS
2	H	194	ARG
2	H	203	HIS
2	H	214	ASP
2	H	228	ARG
2	I	147	ASN
2	I	153	GLN
2	I	176	ASP
2	I	212	GLU
2	J	171	ARG
2	J	173	HIS
2	J	181	GLU
2	J	182	GLU
2	J	203	HIS
2	J	211	ASP
2	K	106	GLN
2	K	153	GLN
2	K	175	ASP
2	K	216	ASP
2	K	229	LEU
2	L	129	GLN
2	L	160	GLN
2	L	171	ARG
2	L	196	ARG
2	L	223	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	281	GLN
1	A	433	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	167	ASN
1	B	248	GLN
1	B	401	ASN
1	D	57	GLN
1	D	100	HIS
1	D	281	GLN
2	F	137	GLN
2	G	169	GLN
2	G	173	HIS
2	G	203	HIS
2	H	159	GLN
2	H	173	HIS
2	I	102	HIS
2	I	169	GLN
2	J	102	HIS
2	J	153	GLN
2	J	169	GLN
2	J	173	HIS
2	J	203	HIS
2	L	173	HIS

5.3.3 RNA [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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
3	ADP	A	601	-	24,29,29	0.99	1 (4%)	29,45,45	1.52	4 (13%)
3	ADP	C	601	-	24,29,29	0.98	1 (4%)	29,45,45	1.49	4 (13%)
3	ADP	B	601	-	24,29,29	0.99	1 (4%)	29,45,45	1.51	4 (13%)
3	ADP	D	601	-	24,29,29	0.98	1 (4%)	29,45,45	1.42	4 (13%)

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
3	ADP	A	601	-	-	6/12/32/32	0/3/3/3
3	ADP	C	601	-	-	2/12/32/32	0/3/3/3
3	ADP	B	601	-	-	2/12/32/32	0/3/3/3
3	ADP	D	601	-	-	1/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	ADP	C5-C4	2.70	1.48	1.40
3	A	601	ADP	C5-C4	2.64	1.47	1.40
3	C	601	ADP	C5-C4	2.57	1.47	1.40
3	D	601	ADP	C5-C4	2.55	1.47	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	ADP	C3'-C2'-C1'	3.75	106.63	100.98
3	A	601	ADP	PA-O3A-PB	-3.68	120.21	132.83
3	C	601	ADP	C3'-C2'-C1'	3.65	106.47	100.98
3	A	601	ADP	C3'-C2'-C1'	3.65	106.47	100.98
3	B	601	ADP	PA-O3A-PB	-3.45	120.97	132.83
3	C	601	ADP	PA-O3A-PB	-3.25	121.66	132.83
3	D	601	ADP	C3'-C2'-C1'	3.20	105.80	100.98
3	C	601	ADP	N3-C2-N1	-3.14	123.78	128.68
3	B	601	ADP	N3-C2-N1	-3.09	123.84	128.68
3	D	601	ADP	N3-C2-N1	-3.04	123.93	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	ADP	PA-O3A-PB	-3.03	122.43	132.83
3	A	601	ADP	N3-C2-N1	-3.02	123.96	128.68
3	C	601	ADP	C4-C5-N7	-2.83	106.45	109.40
3	A	601	ADP	C4-C5-N7	-2.73	106.55	109.40
3	D	601	ADP	C4-C5-N7	-2.68	106.60	109.40
3	B	601	ADP	C4-C5-N7	-2.60	106.69	109.40

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ADP	PA-O3A-PB-O2B
3	A	601	ADP	PA-O3A-PB-O3B
3	A	601	ADP	C5'-O5'-PA-O1A
3	C	601	ADP	C5'-O5'-PA-O1A
3	C	601	ADP	C5'-O5'-PA-O3A
3	B	601	ADP	O4'-C4'-C5'-O5'
3	B	601	ADP	C3'-C4'-C5'-O5'
3	A	601	ADP	C5'-O5'-PA-O3A
3	A	601	ADP	C5'-O5'-PA-O2A
3	D	601	ADP	O4'-C4'-C5'-O5'
3	A	601	ADP	O4'-C4'-C5'-O5'

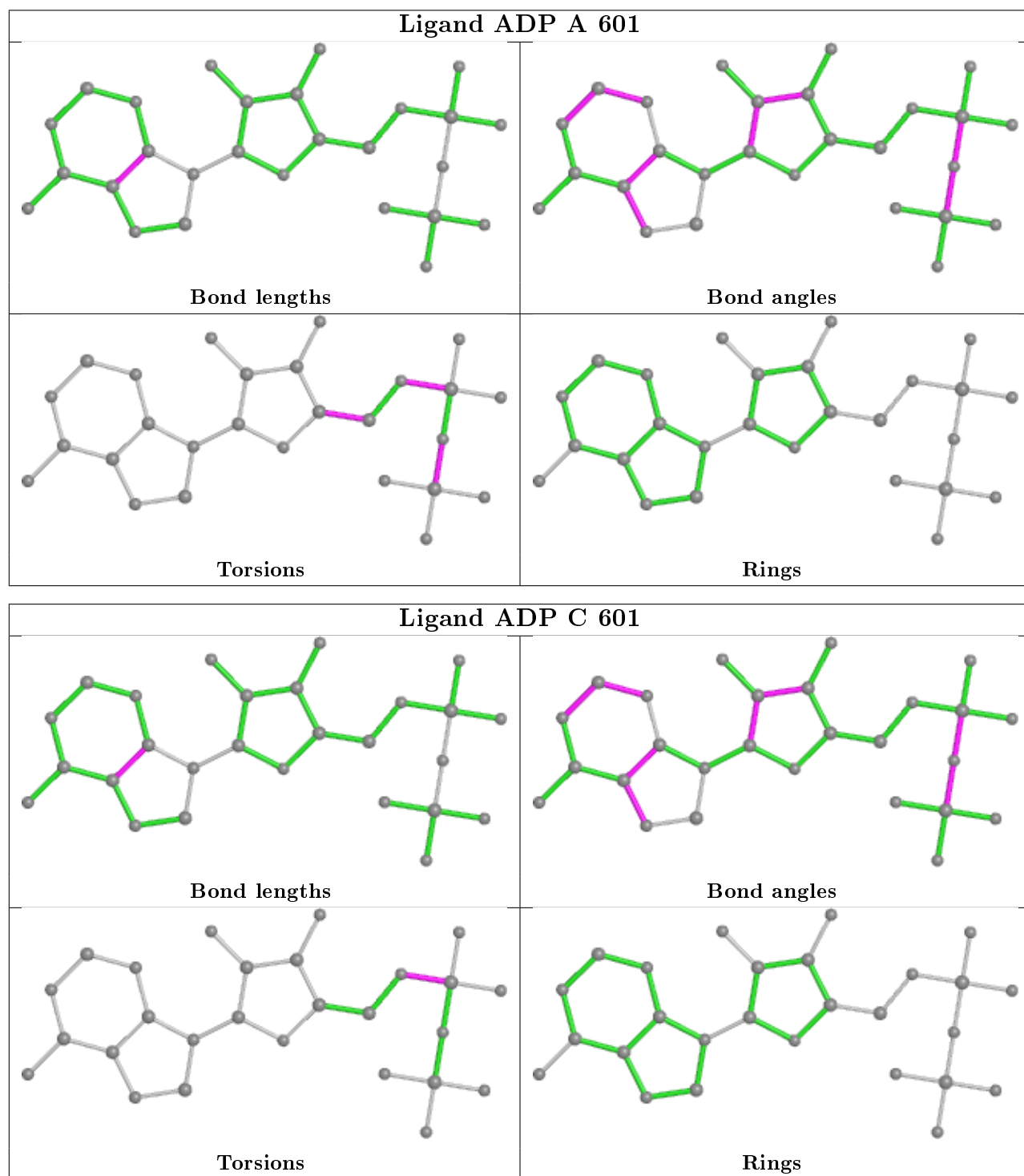
There are no ring outliers.

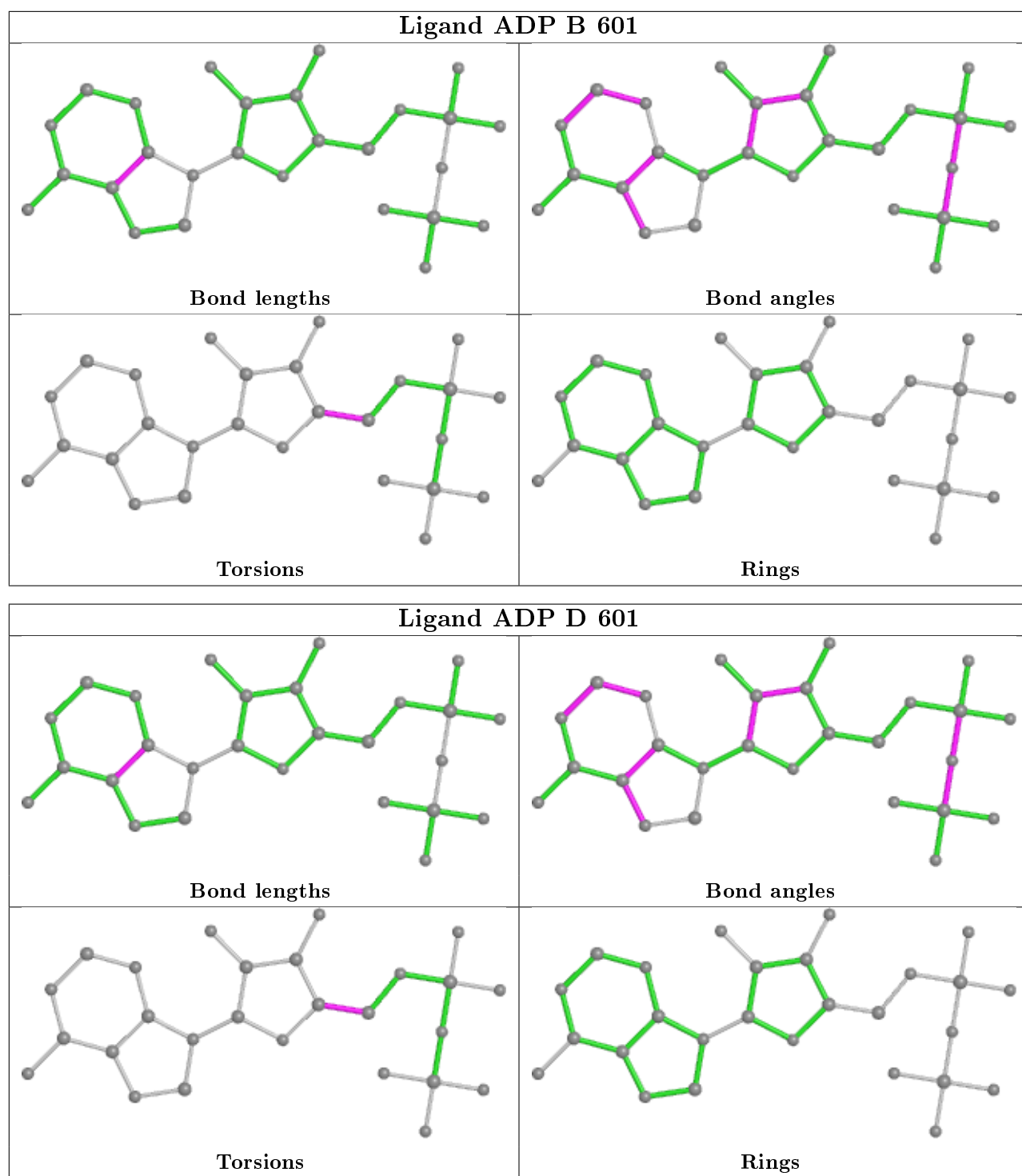
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ADP	5	0
3	C	601	ADP	3	0
3	B	601	ADP	7	0
3	D	601	ADP	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	445/456 (97%)	-0.51	4 (0%) 84 63	28, 50, 94, 139	0
1	B	455/456 (99%)	-0.51	2 (0%) 92 79	33, 59, 118, 147	0
1	C	445/456 (97%)	-0.34	5 (1%) 80 56	40, 71, 132, 157	0
1	D	454/456 (99%)	-0.55	3 (0%) 87 69	28, 49, 90, 134	0
2	E	135/140 (96%)	-0.48	1 (0%) 87 69	28, 45, 108, 138	0
2	F	126/140 (90%)	0.17	6 (4%) 30 11	63, 109, 133, 139	0
2	G	136/140 (97%)	-0.16	2 (1%) 73 46	54, 101, 136, 160	0
2	H	136/140 (97%)	0.23	6 (4%) 34 13	62, 107, 145, 148	0
2	I	133/140 (95%)	-0.36	0 100 100	32, 61, 105, 116	0
2	J	133/140 (95%)	0.08	9 (6%) 17 5	70, 108, 147, 158	0
2	K	133/140 (95%)	-0.31	0 100 100	39, 85, 116, 131	0
2	L	127/140 (90%)	0.10	4 (3%) 49 21	41, 89, 139, 147	1 (0%)
All	All	2858/2944 (97%)	-0.34	42 (1%) 73 46	28, 67, 130, 160	1 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	206	CYS	5.4
2	H	204	GLY	4.8
1	C	456	VAL	4.7
2	H	184	LEU	4.0
1	C	455	THR	3.9
1	C	405	VAL	3.7
2	F	193	TRP	3.6
2	G	100	PRO	3.5
1	D	2	THR	3.4
2	J	172	VAL	3.2
2	J	232	PRO	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	406	SER	2.9
2	H	141	GLN	2.9
2	F	184	LEU	2.9
2	F	203	HIS	2.9
2	L	209	SER	2.9
2	J	175	ASP	2.7
2	J	205	GLY	2.7
2	H	235	LEU	2.7
2	F	204	GLY	2.7
2	H	101	ILE	2.7
2	J	213	GLY	2.7
1	B	43	GLY	2.6
2	J	203	HIS	2.6
1	D	331	GLU	2.5
2	F	146	ASP	2.5
2	E	101	ILE	2.4
2	J	214	ASP	2.3
1	A	408	GLY	2.3
1	D	332	GLY	2.3
1	C	406	SER	2.3
1	A	403	ASP	2.2
2	H	191	HIS	2.2
2	G	178	GLN	2.2
2	J	212	GLU	2.2
2	L	102	HIS	2.2
1	B	409	ALA	2.1
1	C	108	LYS	2.1
1	A	405	VAL	2.1
2	L	219	VAL	2.1
2	F	180	VAL	2.1
2	J	230	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

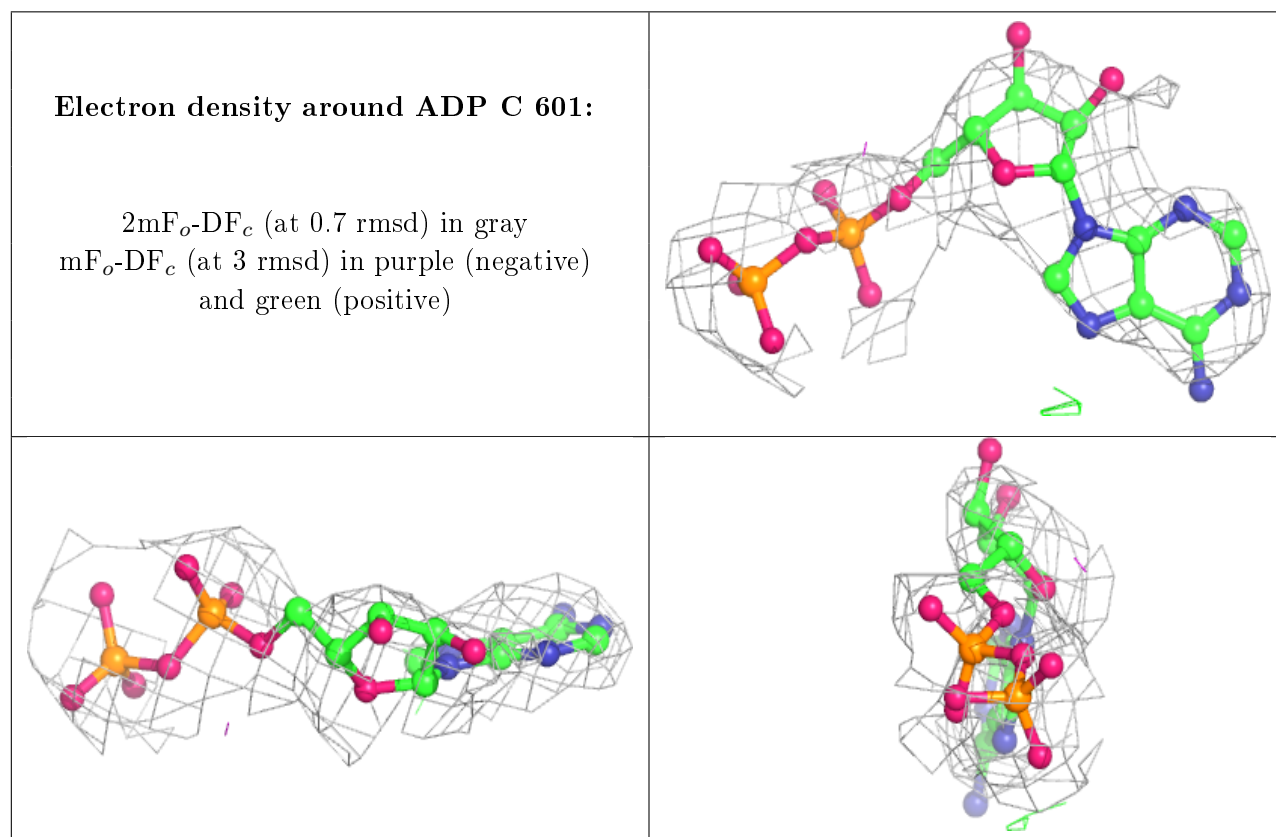
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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.

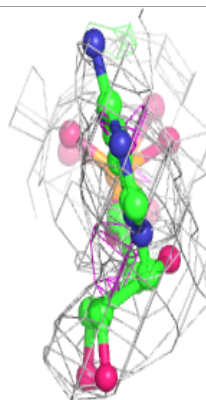
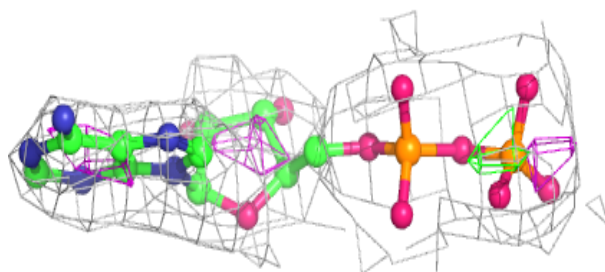
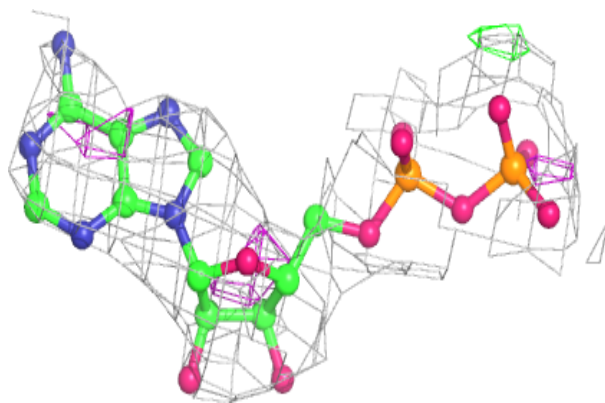
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADP	C	601	27/27	0.88	0.19	72,89,104,111	0
3	ADP	B	601	27/27	0.91	0.21	59,79,92,92	0
3	ADP	A	601	27/27	0.94	0.18	47,57,74,77	0
3	ADP	D	601	27/27	0.96	0.16	51,63,73,81	0

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.

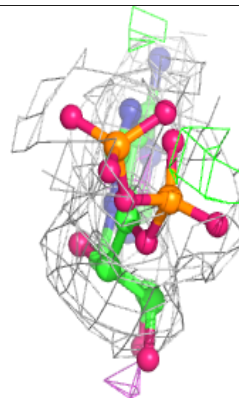
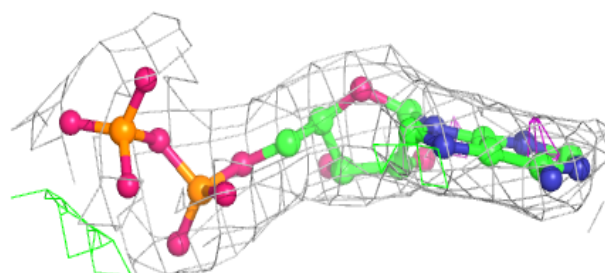
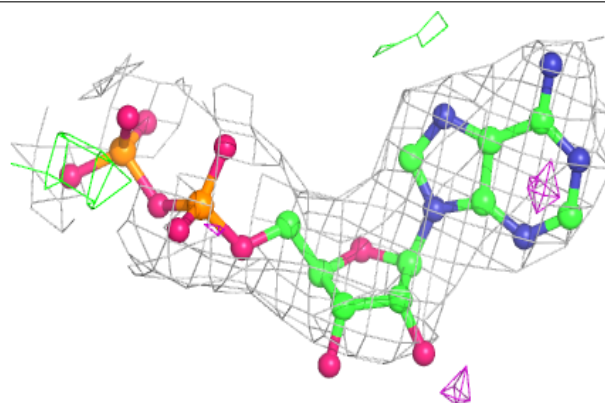


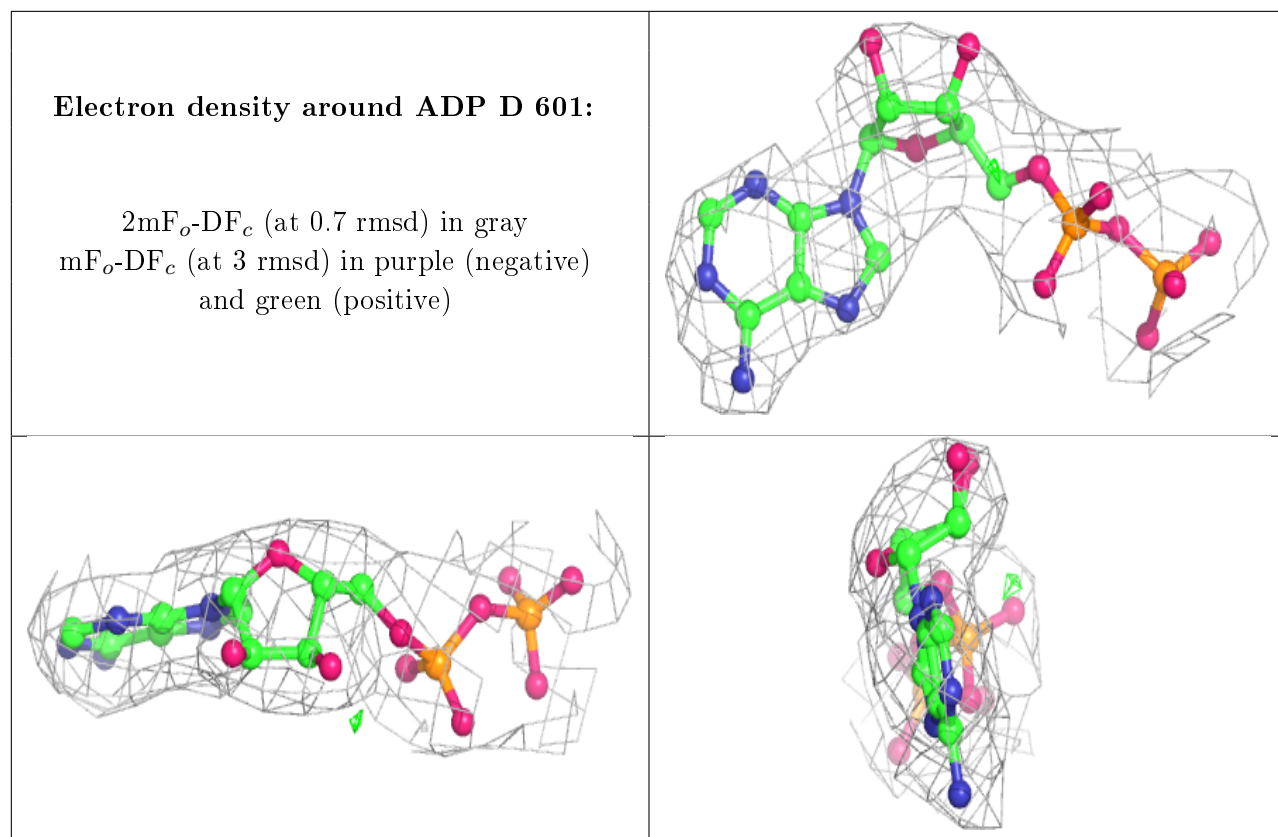
Electron density around ADP B 601:

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

**Electron density around ADP A 601:**

$2mF_o-DF_c$ (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.