Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2024 – 05:29 pm BST

PDB ID	:	2CEA
Title	:	CELL DIVISION PROTEIN FTSH
Authors	:	Bieniossek, C.; Baumann, U.
Deposited on	:	2006-02-03
Resolution	:	2.75 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

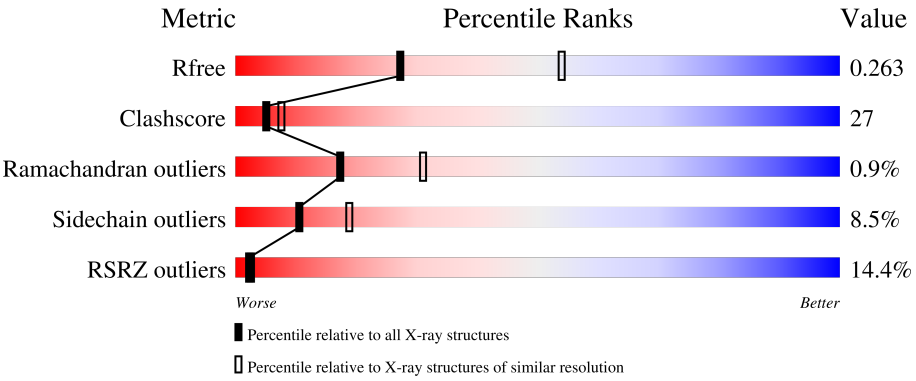
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 of 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 <=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	476	4% 59% 22% · 14%
1	B	476	7% 56% 27% · 14%
1	C	476	15% 50% 33% 6% 12%
1	D	476	8% 63% 21% · 13%
1	E	476	7% 55% 26% · 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	476	35% 41% 39% 5% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	C	1608	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19564 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 CELL DIVISION PROTEIN FTSH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	1
			3160	1996	559	595	10			
1	B	411	Total	C	N	O	S	0	0	0
			3191	2017	560	604	10			
1	C	421	Total	C	N	O	S	0	0	0
			3280	2076	573	621	10			
1	D	413	Total	C	N	O	S	0	0	0
			3212	2032	562	608	10			
1	E	406	Total	C	N	O	S	0	0	1
			3144	1986	557	591	10			
1	F	412	Total	C	N	O	S	0	0	0
			3204	2024	564	606	10			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	MET	-	expression tag	UNP Q9WZ49
A	611	ALA	-	expression tag	UNP Q9WZ49
A	612	ALA	-	expression tag	UNP Q9WZ49
A	613	ALA	-	expression tag	UNP Q9WZ49
A	614	LEU	-	expression tag	UNP Q9WZ49
A	615	GLU	-	expression tag	UNP Q9WZ49
A	616	HIS	-	expression tag	UNP Q9WZ49
A	617	HIS	-	expression tag	UNP Q9WZ49
A	618	HIS	-	expression tag	UNP Q9WZ49
A	619	HIS	-	expression tag	UNP Q9WZ49
A	620	HIS	-	expression tag	UNP Q9WZ49
A	621	HIS	-	expression tag	UNP Q9WZ49
A	410	LEU	LYS	engineered mutation	UNP Q9WZ49
A	415	ALA	LYS	engineered mutation	UNP Q9WZ49
B	146	MET	-	expression tag	UNP Q9WZ49
B	611	ALA	-	expression tag	UNP Q9WZ49
B	612	ALA	-	expression tag	UNP Q9WZ49

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	613	ALA	-	expression tag	UNP Q9WZ49
B	614	LEU	-	expression tag	UNP Q9WZ49
B	615	GLU	-	expression tag	UNP Q9WZ49
B	616	HIS	-	expression tag	UNP Q9WZ49
B	617	HIS	-	expression tag	UNP Q9WZ49
B	618	HIS	-	expression tag	UNP Q9WZ49
B	619	HIS	-	expression tag	UNP Q9WZ49
B	620	HIS	-	expression tag	UNP Q9WZ49
B	621	HIS	-	expression tag	UNP Q9WZ49
B	410	LEU	LYS	engineered mutation	UNP Q9WZ49
B	415	ALA	LYS	engineered mutation	UNP Q9WZ49
C	146	MET	-	expression tag	UNP Q9WZ49
C	611	ALA	-	expression tag	UNP Q9WZ49
C	612	ALA	-	expression tag	UNP Q9WZ49
C	613	ALA	-	expression tag	UNP Q9WZ49
C	614	LEU	-	expression tag	UNP Q9WZ49
C	615	GLU	-	expression tag	UNP Q9WZ49
C	616	HIS	-	expression tag	UNP Q9WZ49
C	617	HIS	-	expression tag	UNP Q9WZ49
C	618	HIS	-	expression tag	UNP Q9WZ49
C	619	HIS	-	expression tag	UNP Q9WZ49
C	620	HIS	-	expression tag	UNP Q9WZ49
C	621	HIS	-	expression tag	UNP Q9WZ49
C	410	LEU	LYS	engineered mutation	UNP Q9WZ49
C	415	ALA	LYS	engineered mutation	UNP Q9WZ49
D	146	MET	-	expression tag	UNP Q9WZ49
D	611	ALA	-	expression tag	UNP Q9WZ49
D	612	ALA	-	expression tag	UNP Q9WZ49
D	613	ALA	-	expression tag	UNP Q9WZ49
D	614	LEU	-	expression tag	UNP Q9WZ49
D	615	GLU	-	expression tag	UNP Q9WZ49
D	616	HIS	-	expression tag	UNP Q9WZ49
D	617	HIS	-	expression tag	UNP Q9WZ49
D	618	HIS	-	expression tag	UNP Q9WZ49
D	619	HIS	-	expression tag	UNP Q9WZ49
D	620	HIS	-	expression tag	UNP Q9WZ49
D	621	HIS	-	expression tag	UNP Q9WZ49
D	410	LEU	LYS	engineered mutation	UNP Q9WZ49
D	415	ALA	LYS	engineered mutation	UNP Q9WZ49
E	146	MET	-	expression tag	UNP Q9WZ49
E	611	ALA	-	expression tag	UNP Q9WZ49
E	612	ALA	-	expression tag	UNP Q9WZ49

Continued on next page...

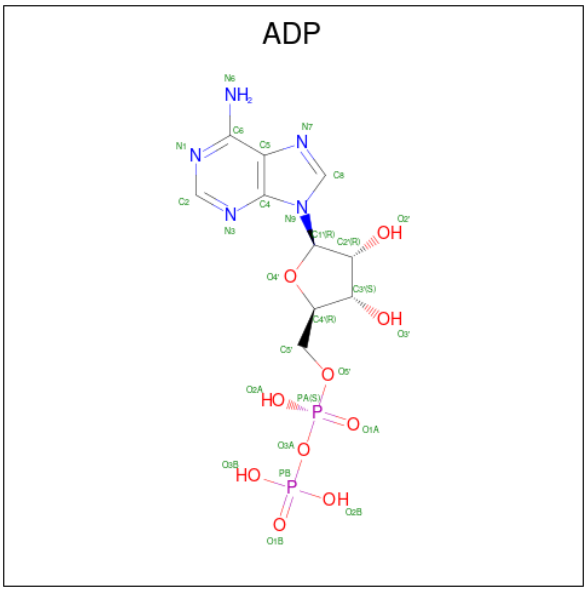
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	613	ALA	-	expression tag	UNP Q9WZ49
E	614	LEU	-	expression tag	UNP Q9WZ49
E	615	GLU	-	expression tag	UNP Q9WZ49
E	616	HIS	-	expression tag	UNP Q9WZ49
E	617	HIS	-	expression tag	UNP Q9WZ49
E	618	HIS	-	expression tag	UNP Q9WZ49
E	619	HIS	-	expression tag	UNP Q9WZ49
E	620	HIS	-	expression tag	UNP Q9WZ49
E	621	HIS	-	expression tag	UNP Q9WZ49
E	410	LEU	LYS	engineered mutation	UNP Q9WZ49
E	415	ALA	LYS	engineered mutation	UNP Q9WZ49
F	146	MET	-	expression tag	UNP Q9WZ49
F	611	ALA	-	expression tag	UNP Q9WZ49
F	612	ALA	-	expression tag	UNP Q9WZ49
F	613	ALA	-	expression tag	UNP Q9WZ49
F	614	LEU	-	expression tag	UNP Q9WZ49
F	615	GLU	-	expression tag	UNP Q9WZ49
F	616	HIS	-	expression tag	UNP Q9WZ49
F	617	HIS	-	expression tag	UNP Q9WZ49
F	618	HIS	-	expression tag	UNP Q9WZ49
F	619	HIS	-	expression tag	UNP Q9WZ49
F	620	HIS	-	expression tag	UNP Q9WZ49
F	621	HIS	-	expression tag	UNP Q9WZ49

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- 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	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

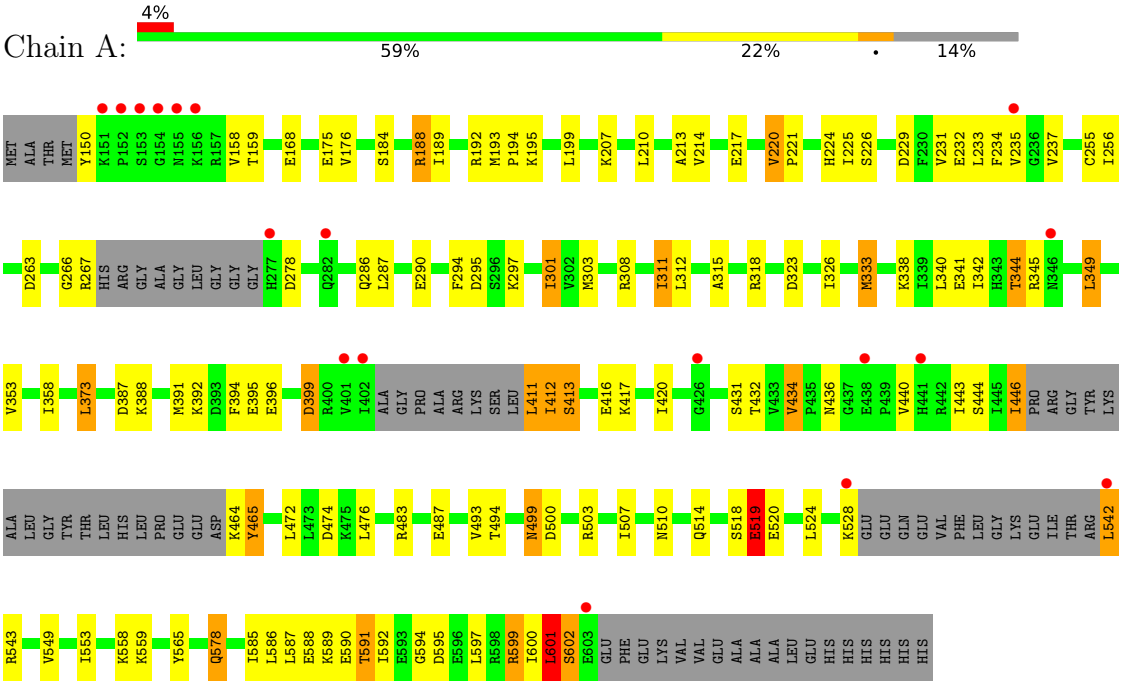
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	46	Total O 46 46	0	0
5	B	35	Total O 35 35	0	0
5	C	26	Total O 26 26	0	0
5	D	34	Total O 34 34	0	0
5	E	34	Total O 34 34	0	0
5	F	24	Total O 24 24	0	0

3 Residue-property plots (i)

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.

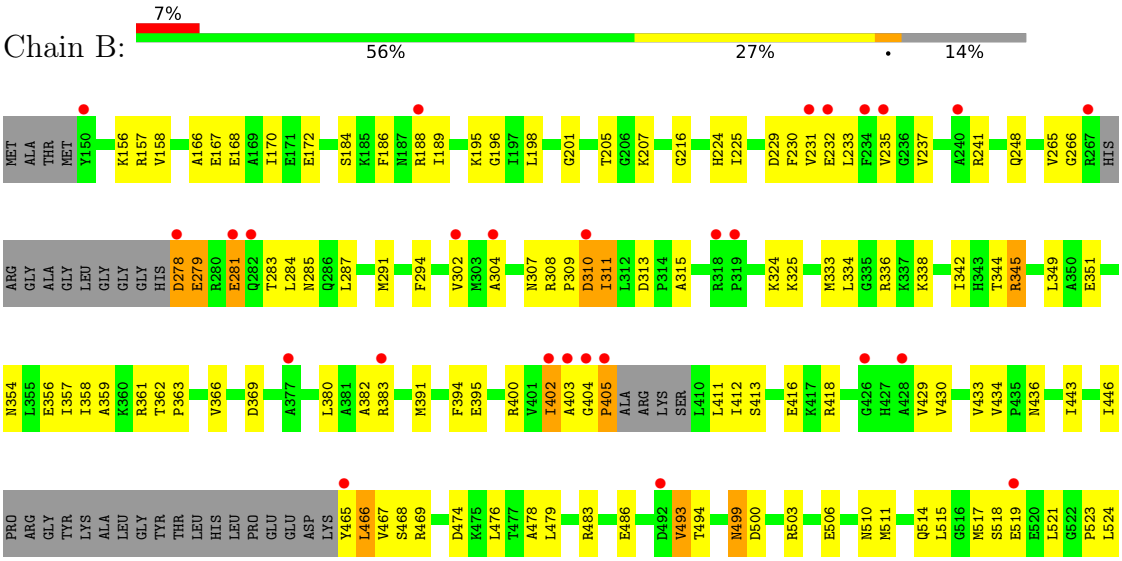
• Molecule 1: CELL DIVISION PROTEIN FTSH

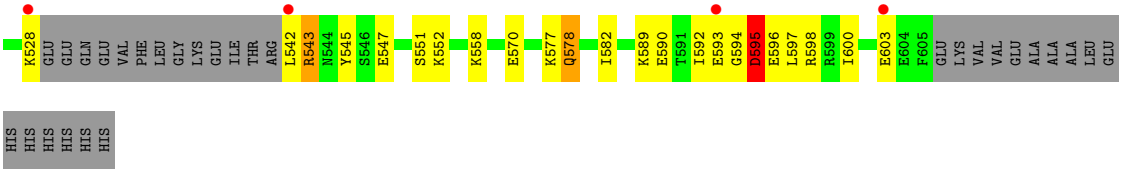
Chain A:



• Molecule 1: CELL DIVISION PROTEIN FTSH

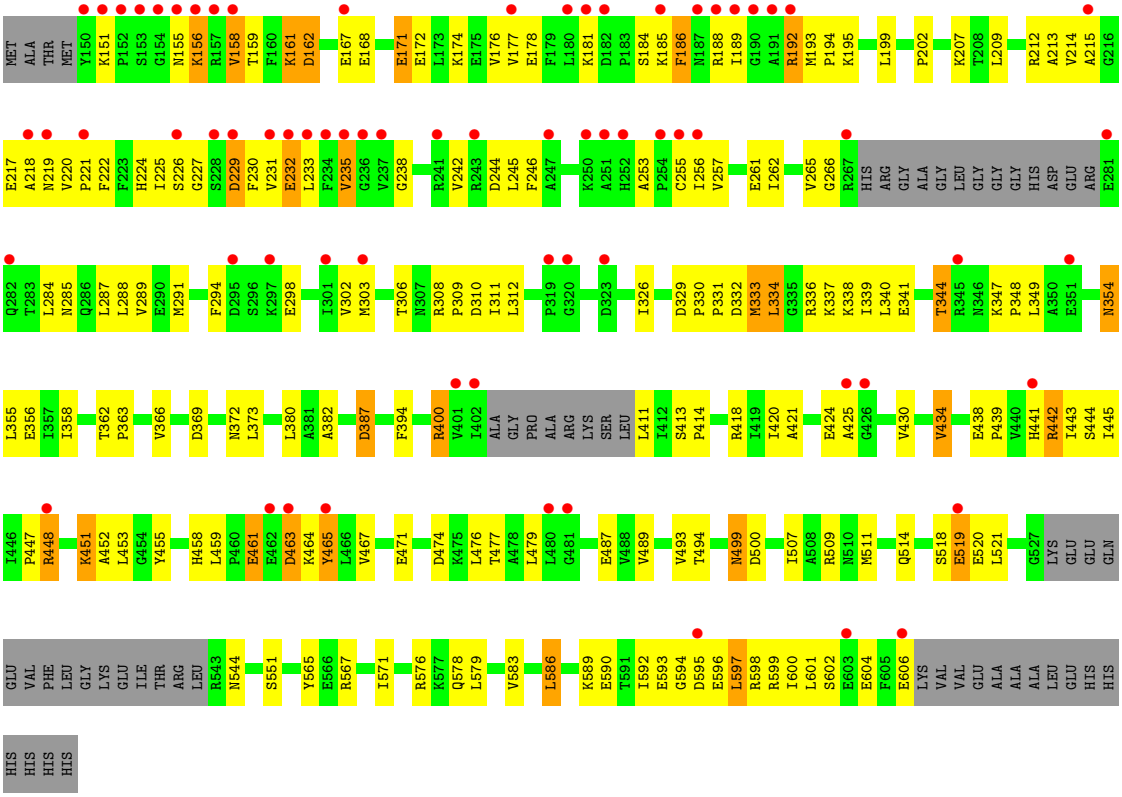
Chain B:





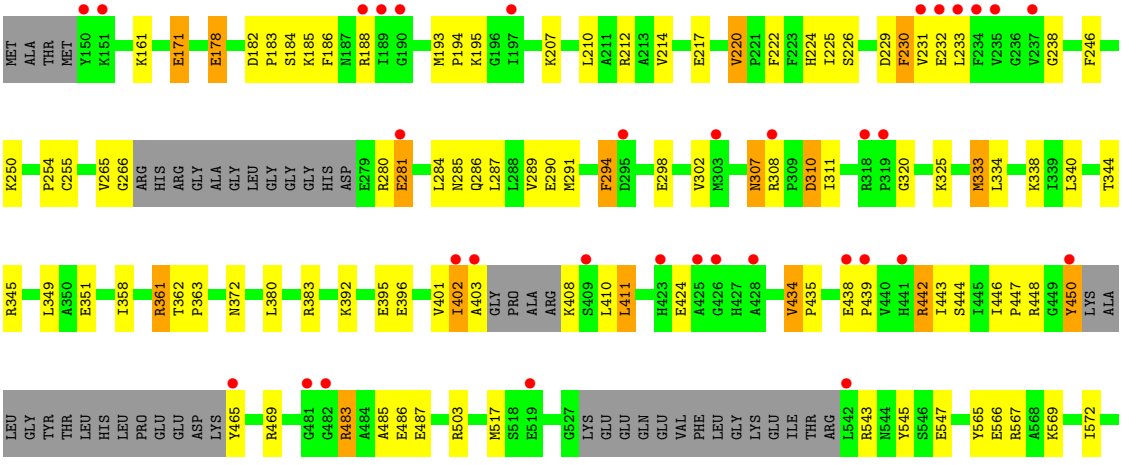
• Molecule 1: CELL DIVISION PROTEIN FTSH

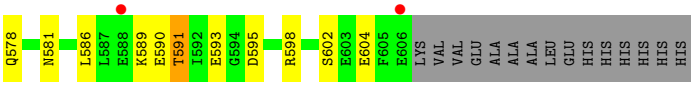
Chain C:



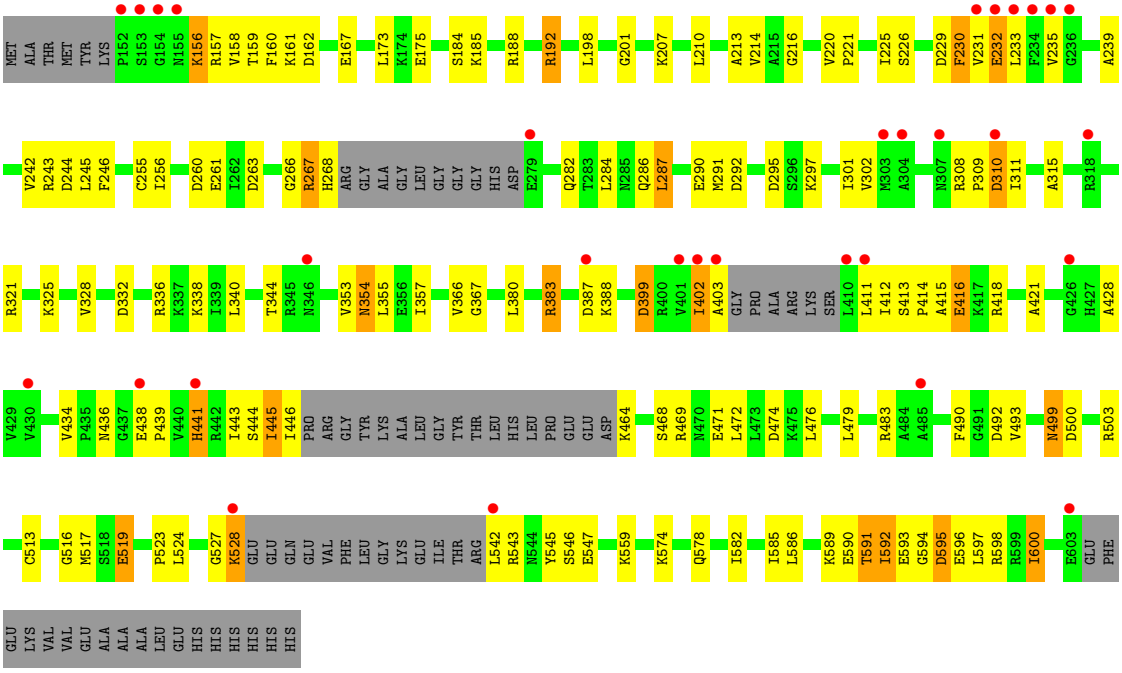
• Molecule 1: CELL DIVISION PROTEIN FTSH

Chain D:

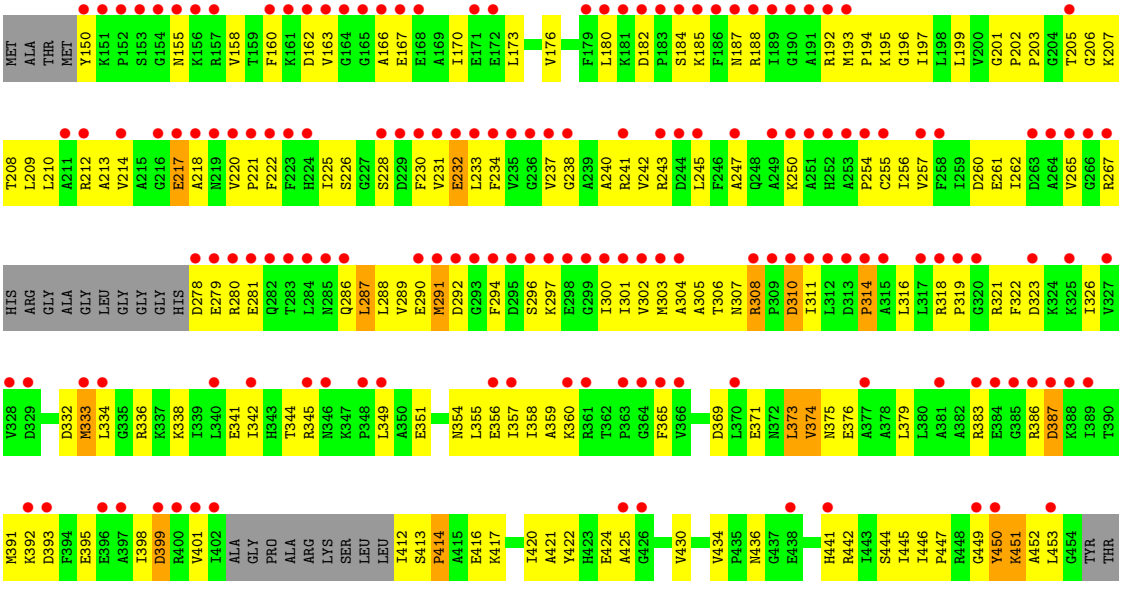


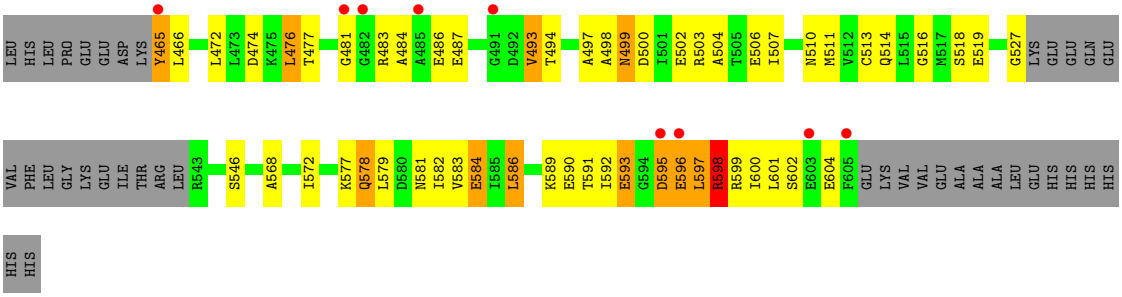


• Molecule 1: CELL DIVISION PROTEIN FTSH



• Molecule 1: CELL DIVISION PROTEIN FTSH




LEU HIS LEU PRO GLU GLU ASP LYS Y465 L466 L472 L473 D474 K475 L476 T477 G481 G482 R483 A484 A485 E486 E487 G491 D492 V493 T494 A497 A498 N499 D500 I501 E502 R503 A504 T505 E506 I507 N510 M511 V512 C513 Q514 L515 G516 M517 S518 E519 G527 LYS GLU GLU GLN GLU
VAL PHE LEU GLY LYS GLU ILE THR ARG LEU R543 S546 A568 I572 K577 Q578 L579 D580 N581 I582 V583 E584 I585 L586 K589 E590 T591 I592 E593 G594 D595 E596 L597 R598 R599 I600 L601 S602 E603 E604 F605 GLU LYS VAL VAL GLU ALA ALA ALA LEU GLU HIS HIS HIS
HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	165.32Å 165.32Å 234.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.75 19.98 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.75) 97.8 (19.98-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.262 0.215 , 0.263	Depositor DCC
R_{free} test set	1283 reflections (1.55%)	wwPDB-VP
Wilson B-factor (Å^2)	56.7	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 77.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19564	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, ADP, ZN

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	0.79	2/3202 (0.1%)	0.57	0/4314
1	B	0.76	2/3233 (0.1%)	0.56	1/4356 (0.0%)
1	C	0.59	0/3328	0.49	0/4488
1	D	0.68	0/3256	0.52	0/4388
1	E	0.72	1/3185 (0.0%)	0.54	0/4291
1	F	0.55	1/3248 (0.0%)	0.47	0/4376
All	All	0.68	6/19452 (0.0%)	0.53	1/26213 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	513	CYS	CB-SG	-7.17	1.70	1.82
1	A	519	GLU	CG-CD	6.13	1.61	1.51
1	F	513	CYS	CB-SG	-6.08	1.72	1.82
1	B	506	GLU	CG-CD	5.75	1.60	1.51
1	B	172	GLU	CG-CD	5.48	1.60	1.51
1	A	175	GLU	CG-CD	5.24	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	405	PRO	N-CA-CB	6.36	110.93	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3160	0	3240	119	0
1	B	3191	0	3261	143	0
1	C	3280	0	3346	199	0
1	D	3212	0	3283	121	0
1	E	3144	0	3231	172	0
1	F	3204	0	3270	301	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	7	0
3	C	27	0	12	10	0
3	D	27	0	12	6	0
3	E	27	0	12	7	0
3	F	27	0	12	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	46	0	0	5	0
5	B	35	0	0	13	0
5	C	26	0	0	9	0
5	D	34	0	0	11	0
5	E	34	0	0	6	0
5	F	24	0	0	9	0
All	All	19564	0	19703	1053	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 27.

All (1053) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:GLU:HA	5:C:2018:HOH:O	1.15	1.27
1:E:231:VAL:HG12	1:E:232:GLU:OE2	1.11	1.27
1:E:231:VAL:CG1	1:E:232:GLU:OE2	1.84	1.24
1:C:340:LEU:O	1:C:344:THR:HG22	1.38	1.20
1:C:594:GLY:N	5:C:2024:HOH:O	1.74	1.19
1:F:291:MET:CE	1:F:294:PHE:HE2	1.56	1.19
1:F:413:SER:OG	1:F:416:GLU:OE1	1.60	1.18
1:A:446:ILE:HG22	5:A:2025:HOH:O	1.02	1.16
1:E:231:VAL:O	1:E:232:GLU:HG2	1.46	1.15
1:F:203:PRO:HD3	1:F:307:ASN:HD22	1.03	1.14
1:F:187:ASN:HD21	1:F:297:LYS:HB3	1.14	1.12
1:C:334:LEU:HD22	1:C:338:LYS:HE2	1.20	1.12
1:F:291:MET:HE2	1:F:294:PHE:CE2	1.84	1.11
1:B:466:LEU:HD21	1:C:494:THR:HB	1.29	1.11
1:F:446:ILE:O	1:F:450:TYR:CE1	2.03	1.10
1:F:180:LEU:HD21	1:F:301:ILE:CD1	1.81	1.10
1:A:214:VAL:HG12	1:A:256:ILE:HD11	1.31	1.08
1:A:214:VAL:CG1	1:A:256:ILE:HD11	1.84	1.07
1:F:579:LEU:O	1:F:583:VAL:HG23	1.55	1.05
1:F:291:MET:CE	1:F:294:PHE:CE2	2.40	1.04
1:E:446:ILE:O	5:E:2019:HOH:O	1.74	1.04
1:D:402:ILE:HG22	1:D:403:ALA:N	1.69	1.03
1:C:177:VAL:O	1:C:181:LYS:HG3	1.59	1.02
1:F:187:ASN:ND2	1:F:297:LYS:HB3	1.75	1.01
1:F:446:ILE:O	1:F:450:TYR:CD1	2.14	1.01
1:F:288:LEU:HD22	1:F:321:ARG:HH11	1.19	1.00
1:C:334:LEU:HD22	1:C:338:LYS:CE	1.90	1.00
1:E:156:LYS:HZ2	1:E:156:LYS:HB2	1.26	0.99
1:C:334:LEU:CD2	1:C:338:LYS:HE2	1.93	0.98
1:F:314:PRO:HB2	1:F:318:ARG:HH21	1.28	0.98
1:F:447:PRO:C	1:F:450:TYR:CE1	2.37	0.97
1:F:308:ARG:HG2	1:F:311:ILE:HD12	1.45	0.97
1:E:582:ILE:HD11	1:E:597:LEU:CD1	1.95	0.97
1:D:402:ILE:HG22	1:D:403:ALA:H	1.27	0.96
1:F:499:ASN:HD22	1:F:500:ASP:H	1.03	0.95
1:E:231:VAL:C	1:E:232:GLU:HG2	1.86	0.95
1:E:582:ILE:CD1	1:E:597:LEU:CD1	2.44	0.95
1:E:402:ILE:HG22	1:E:403:ALA:N	1.80	0.95
1:F:354:ASN:OD1	1:F:357:ILE:HG13	1.67	0.95
1:F:578:GLN:H	1:F:578:GLN:HE21	0.97	0.95
1:F:250:LYS:NZ	1:F:294:PHE:HB2	1.82	0.94
1:A:220:VAL:CG1	1:A:255:CYS:HA	1.97	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:HG12	1:A:256:ILE:CD1	1.97	0.94
1:F:225:ILE:CD1	1:F:245:LEU:HD11	1.98	0.94
1:E:157:ARG:NH2	1:E:216:GLY:O	1.99	0.93
1:F:447:PRO:C	1:F:450:TYR:HE1	1.71	0.93
1:C:220:VAL:CG1	1:C:255:CYS:HA	1.99	0.93
1:F:225:ILE:HG13	1:F:245:LEU:HD21	1.51	0.93
1:D:487:GLU:OE1	1:D:565:TYR:OH	1.85	0.93
1:C:441:HIS:O	1:C:593:GLU:O	1.86	0.93
1:E:156:LYS:NZ	1:E:156:LYS:CB	2.32	0.93
1:F:371:GLU:O	1:F:374:VAL:HG12	1.67	0.92
1:A:483:ARG:CZ	1:A:493:VAL:HG11	2.00	0.92
1:A:588:GLU:OE2	5:A:2039:HOH:O	1.88	0.92
1:F:202:PRO:HA	1:F:307:ASN:ND2	1.85	0.92
1:F:499:ASN:HD22	1:F:500:ASP:N	1.66	0.92
1:E:600:ILE:O	1:E:600:ILE:HD12	1.69	0.91
1:D:344:THR:HG21	1:D:349:LEU:HD11	1.50	0.91
1:F:176:VAL:HG13	1:F:301:ILE:HD13	1.53	0.91
1:C:578:GLN:OE1	1:C:578:GLN:N	2.02	0.91
1:D:307:ASN:ND2	1:D:308:ARG:HG2	1.84	0.91
1:F:578:GLN:H	1:F:578:GLN:NE2	1.69	0.91
1:D:380:LEU:HA	1:D:383:ARG:NH1	1.84	0.90
1:D:185:LYS:HB3	5:D:2003:HOH:O	1.69	0.90
1:F:203:PRO:HD3	1:F:307:ASN:ND2	1.87	0.90
1:F:225:ILE:HD12	1:F:245:LEU:HD11	1.53	0.89
1:E:156:LYS:HB2	1:E:156:LYS:NZ	1.85	0.89
1:F:288:LEU:HD22	1:F:321:ARG:NH1	1.86	0.89
1:E:231:VAL:O	1:E:232:GLU:CG	2.20	0.89
1:A:373:LEU:HD12	1:A:373:LEU:O	1.73	0.88
1:F:291:MET:HE2	1:F:294:PHE:HE2	1.20	0.88
1:B:157:ARG:HD2	1:B:216:GLY:HA2	1.53	0.88
1:C:340:LEU:O	1:C:344:THR:CG2	2.21	0.88
1:B:231:VAL:O	1:B:232:GLU:HB2	1.71	0.88
1:F:465:TYR:HA	5:F:2008:HOH:O	1.73	0.88
1:A:434:VAL:HG11	1:A:474:ASP:HB3	1.55	0.88
1:E:446:ILE:O	1:E:446:ILE:HG22	1.71	0.87
1:D:182:ASP:HB3	5:D:2003:HOH:O	1.72	0.87
1:F:447:PRO:O	1:F:450:TYR:CE1	2.28	0.87
1:E:499:ASN:HD22	1:E:500:ASP:H	1.23	0.86
1:E:243:ARG:HH11	1:E:286:GLN:NE2	1.73	0.86
1:F:357:ILE:HG21	1:F:391:MET:HE1	1.55	0.86
1:D:380:LEU:HA	1:D:383:ARG:HH12	1.38	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ASN:HB3	1:C:212:ARG:NH2	1.91	0.86
1:A:434:VAL:CG1	1:A:474:ASP:HB3	2.06	0.86
1:B:207:LYS:NZ	3:B:1607:ADP:O1B	2.08	0.86
1:C:499:ASN:HD22	1:C:500:ASP:N	1.74	0.86
1:F:257:VAL:HB	1:F:302:VAL:HG22	1.58	0.85
1:F:231:VAL:O	1:F:232:GLU:HB2	1.74	0.85
1:B:466:LEU:HD21	1:C:494:THR:CB	2.07	0.85
1:A:184:SER:O	1:A:188:ARG:HG3	1.76	0.85
1:D:380:LEU:HD23	1:D:383:ARG:NH1	1.91	0.84
1:B:265:VAL:O	5:B:2007:HOH:O	1.95	0.84
1:E:499:ASN:HD22	1:E:500:ASP:N	1.75	0.84
1:A:446:ILE:C	1:A:446:ILE:HD12	1.97	0.84
1:F:452:ALA:HA	5:F:2007:HOH:O	1.76	0.84
1:B:184:SER:O	1:B:188:ARG:HG3	1.77	0.84
1:F:182:ASP:OD2	1:F:185:LYS:HG2	1.78	0.84
1:E:231:VAL:HG12	1:E:232:GLU:CD	1.97	0.83
1:C:499:ASN:HD22	1:C:500:ASP:H	1.26	0.83
1:D:195:LYS:NZ	1:D:294:PHE:O	2.10	0.83
1:E:157:ARG:HH21	1:E:216:GLY:C	1.82	0.83
1:F:220:VAL:CG1	1:F:254:PRO:O	2.26	0.83
1:E:308:ARG:HE	1:F:289:VAL:HG21	1.39	0.83
1:C:220:VAL:HG13	1:C:221:PRO:HD2	1.60	0.83
1:E:586:LEU:CD1	1:E:592:ILE:HG23	2.09	0.83
1:F:180:LEU:HD21	1:F:301:ILE:HD12	1.59	0.83
1:F:341:GLU:O	1:F:344:THR:HG22	1.78	0.83
1:B:230:PHE:HA	1:B:233:LEU:HD11	1.60	0.83
1:C:231:VAL:O	1:C:232:GLU:HB2	1.78	0.82
1:F:499:ASN:ND2	1:F:500:ASP:H	1.78	0.82
1:F:586:LEU:HD13	1:F:592:ILE:HD13	1.61	0.82
1:D:231:VAL:O	1:D:232:GLU:HB2	1.79	0.82
1:B:358:ILE:CD1	1:B:394:PHE:HB3	2.10	0.82
1:B:499:ASN:HD22	1:B:500:ASP:H	1.25	0.82
1:F:262:ILE:HD12	1:F:304:ALA:CB	2.10	0.82
1:F:291:MET:HE3	1:F:294:PHE:HE2	1.45	0.82
1:E:291:MET:HE1	1:E:302:VAL:HG21	1.62	0.81
1:B:479:LEU:HD11	1:B:503:ARG:HG2	1.63	0.81
1:D:307:ASN:HD22	1:D:308:ARG:HG2	1.43	0.81
1:F:578:GLN:HE21	1:F:578:GLN:N	1.76	0.81
1:C:174:LYS:O	1:C:178:GLU:HG2	1.81	0.81
1:F:238:GLY:O	1:F:242:VAL:HG23	1.80	0.81
1:A:487:GLU:OE2	1:A:565:TYR:OH	1.99	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:355:LEU:HA	1:F:358:ILE:HD12	1.60	0.81
1:F:451:LYS:HG2	1:F:453:LEU:HD12	1.63	0.81
1:F:187:ASN:HD21	1:F:297:LYS:CB	1.94	0.80
1:B:594:GLY:O	1:B:596:GLU:N	2.15	0.80
1:A:373:LEU:HD12	1:A:373:LEU:C	2.00	0.80
1:F:262:ILE:HD12	1:F:304:ALA:HB1	1.63	0.80
1:F:597:LEU:HD12	1:F:597:LEU:O	1.81	0.80
1:C:220:VAL:HG11	1:C:255:CYS:HA	1.61	0.80
1:C:592:ILE:HG23	1:C:596:GLU:OE2	1.80	0.80
1:A:176:VAL:HG13	1:A:301:ILE:HD13	1.64	0.80
1:C:195:LYS:O	1:C:302:VAL:HG22	1.81	0.80
1:E:483:ARG:NE	1:E:493:VAL:HG21	1.97	0.80
1:F:150:TYR:N	1:F:245:LEU:CD1	2.45	0.79
1:F:292:ASP:OD2	1:F:321:ARG:NH2	2.15	0.79
1:F:150:TYR:N	1:F:245:LEU:HD12	1.98	0.79
1:F:413:SER:O	1:F:416:GLU:N	2.16	0.79
1:F:233:LEU:HB2	1:F:279:GLU:OE2	1.82	0.78
1:F:354:ASN:HB3	1:F:357:ILE:HD12	1.65	0.78
1:F:373:LEU:HD12	1:F:401:VAL:HG21	1.65	0.78
1:C:156:LYS:H	1:C:156:LYS:CE	1.97	0.78
1:B:499:ASN:HD22	1:B:500:ASP:N	1.79	0.78
1:F:180:LEU:HD21	1:F:301:ILE:HD11	1.65	0.78
1:B:358:ILE:HD13	1:B:394:PHE:HB3	1.64	0.78
1:F:584:GLU:OE2	5:F:2023:HOH:O	2.01	0.78
1:A:413:SER:OG	1:A:416:GLU:HB2	1.84	0.78
1:B:483:ARG:CZ	1:B:493:VAL:HG11	2.14	0.78
1:D:438:GLU:OE2	1:D:439:PRO:HD2	1.84	0.78
1:F:220:VAL:HG12	1:F:221:PRO:HD2	1.65	0.77
1:F:237:VAL:O	1:F:241:ARG:HG3	1.85	0.77
1:E:291:MET:CE	1:E:302:VAL:HG21	2.15	0.77
1:B:595:ASP:OD2	1:B:595:ASP:N	2.19	0.76
1:E:582:ILE:HD11	1:E:597:LEU:HD12	1.65	0.76
1:D:307:ASN:HD22	1:D:307:ASN:C	1.88	0.76
1:F:308:ARG:CG	1:F:311:ILE:HD12	2.14	0.76
1:E:230:PHE:O	1:E:233:LEU:HG	1.85	0.76
1:A:214:VAL:CG1	1:A:256:ILE:CD1	2.59	0.76
1:E:220:VAL:HG13	1:E:255:CYS:HA	1.66	0.75
1:B:510:ASN:OD1	1:B:514:GLN:NE2	2.18	0.75
1:C:420:ILE:CG2	1:C:445:ILE:HG23	2.17	0.75
1:F:391:MET:HE2	1:F:395:GLU:OE2	1.87	0.75
1:A:220:VAL:HG11	1:A:255:CYS:HA	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:589:LYS:O	1:E:590:GLU:HB2	1.87	0.75
1:A:207:LYS:HE3	3:A:1604:ADP:O1B	1.86	0.75
1:C:487:GLU:OE1	1:C:565:TYR:OH	2.04	0.75
1:F:578:GLN:O	1:F:582:ILE:HG13	1.87	0.75
1:A:220:VAL:HG13	1:A:255:CYS:HA	1.68	0.75
1:D:383:ARG:NH2	1:E:175:GLU:OE2	2.20	0.75
1:F:446:ILE:O	1:F:450:TYR:HE1	1.65	0.75
1:F:586:LEU:CD1	1:F:592:ILE:HD13	2.15	0.75
1:F:373:LEU:HD11	1:F:398:ILE:HA	1.69	0.75
1:F:592:ILE:HD12	1:F:592:ILE:N	2.02	0.75
1:B:466:LEU:CD2	1:C:494:THR:HB	2.15	0.74
1:A:464:LYS:O	1:A:465:TYR:HB2	1.84	0.74
1:C:167:GLU:OE1	1:C:167:GLU:N	2.16	0.74
1:C:465:TYR:CD1	1:C:465:TYR:N	2.52	0.74
1:F:465:TYR:CA	5:F:2008:HOH:O	2.31	0.74
1:D:185:LYS:HD2	1:D:188:ARG:HH12	1.52	0.74
1:D:402:ILE:CG2	1:D:403:ALA:N	2.44	0.74
1:F:287:LEU:HD23	1:F:287:LEU:O	1.87	0.74
1:E:310:ASP:OD2	1:E:310:ASP:N	2.18	0.74
1:E:582:ILE:CD1	1:E:597:LEU:HD11	2.18	0.74
1:D:291:MET:CE	1:D:302:VAL:HG21	2.16	0.74
1:E:483:ARG:CZ	1:E:493:VAL:HG21	2.17	0.74
1:F:499:ASN:ND2	1:F:500:ASP:N	2.34	0.74
1:B:446:ILE:O	5:B:2019:HOH:O	2.06	0.74
1:F:332:ASP:O	1:F:336:ARG:HG3	1.88	0.74
1:F:442:ARG:HB2	1:F:593:GLU:HB2	1.69	0.74
1:D:225:ILE:N	1:D:225:ILE:HD13	2.01	0.74
1:B:358:ILE:CD1	1:B:394:PHE:CB	2.65	0.73
3:D:1608:ADP:C8	3:D:1608:ADP:H5'1	2.22	0.73
1:F:155:ASN:HD22	1:F:212:ARG:NH2	1.85	0.73
1:D:595:ASP:HA	1:D:598:ARG:HG3	1.70	0.73
1:E:226:SER:HB3	1:E:229:ASP:OD2	1.88	0.73
1:B:333:MET:HE2	1:B:589:LYS:O	1.89	0.73
1:C:156:LYS:H	1:C:156:LYS:HE2	1.52	0.73
1:B:577:LYS:HB2	1:B:577:LYS:NZ	2.03	0.73
1:A:214:VAL:HG11	1:A:256:ILE:HD11	1.70	0.73
1:C:465:TYR:N	1:C:465:TYR:HD1	1.84	0.73
1:F:476:LEU:HD21	1:F:504:ALA:HB1	1.71	0.73
1:E:464:LYS:N	5:E:2020:HOH:O	2.22	0.72
1:F:163:VAL:HG13	1:F:209:LEU:HD23	1.71	0.72
1:E:469:ARG:NH1	1:E:517:MET:O	2.22	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:LEU:CD1	1:A:592:ILE:HG23	2.19	0.72
1:E:156:LYS:CB	1:E:156:LYS:HZ3	2.02	0.72
1:A:499:ASN:N	1:A:499:ASN:HD22	1.86	0.72
1:C:225:ILE:HG13	1:C:245:LEU:HD13	1.71	0.72
1:C:344:THR:OG1	1:C:349:LEU:HD11	1.90	0.72
1:F:591:THR:C	1:F:592:ILE:HD12	2.09	0.72
1:E:402:ILE:CG2	1:E:403:ALA:N	2.52	0.72
1:F:447:PRO:CA	1:F:450:TYR:HE1	2.02	0.72
1:C:355:LEU:HA	1:C:358:ILE:HD12	1.72	0.72
1:D:604:GLU:OE1	1:D:604:GLU:HA	1.90	0.72
1:F:391:MET:CE	1:F:395:GLU:OE2	2.38	0.72
1:E:582:ILE:HD13	1:E:597:LEU:CD1	2.19	0.71
1:C:226:SER:HB3	1:C:229:ASP:OD1	1.89	0.71
1:C:230:PHE:HA	1:C:233:LEU:CD1	2.19	0.71
1:C:287:LEU:C	1:C:287:LEU:HD23	2.11	0.71
1:C:235:VAL:O	1:C:235:VAL:HG12	1.89	0.71
1:E:231:VAL:C	1:E:232:GLU:CG	2.56	0.71
1:F:333:MET:HG3	1:F:334:LEU:HD23	1.70	0.71
1:C:578:GLN:HG3	1:C:604:GLU:HG3	1.72	0.71
1:D:442:ARG:HB3	1:D:593:GLU:OE2	1.90	0.71
1:B:404:GLY:O	1:B:405:PRO:CB	2.38	0.71
1:C:231:VAL:HG12	1:C:232:GLU:HG2	1.71	0.71
1:D:224:HIS:C	1:D:225:ILE:HD13	2.11	0.71
1:F:155:ASN:HD22	1:F:212:ARG:CZ	2.04	0.71
1:F:376:GLU:HA	1:F:379:LEU:HD12	1.73	0.71
1:A:231:VAL:HG12	1:A:232:GLU:HG2	1.72	0.71
1:C:284:LEU:O	1:C:284:LEU:HD12	1.91	0.71
1:F:250:LYS:NZ	1:F:294:PHE:CB	2.54	0.70
1:E:220:VAL:CG1	1:E:255:CYS:HA	2.21	0.70
1:C:231:VAL:O	1:C:232:GLU:CB	2.39	0.70
1:D:310:ASP:OD2	1:D:310:ASP:N	2.24	0.70
1:A:184:SER:O	1:A:188:ARG:CG	2.40	0.70
1:B:443:ILE:HG13	1:B:597:LEU:HD11	1.73	0.70
1:D:298:GLU:O	1:D:298:GLU:HG3	1.92	0.70
1:B:434:VAL:HG11	1:B:474:ASP:HB3	1.74	0.69
1:D:230:PHE:O	1:D:233:LEU:HG	1.92	0.69
1:C:171:GLU:HA	1:C:171:GLU:OE2	1.91	0.69
1:D:220:VAL:HG13	1:D:255:CYS:HA	1.74	0.69
1:A:464:LYS:O	1:A:465:TYR:CB	2.39	0.69
1:D:185:LYS:HD2	1:D:185:LYS:O	1.92	0.69
1:E:600:ILE:O	1:E:600:ILE:CD1	2.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:ASP:C	1:F:342:ILE:HD13	2.13	0.69
1:F:287:LEU:C	1:F:287:LEU:CD2	2.60	0.69
1:D:486:GLU:OE1	5:D:2020:HOH:O	2.10	0.69
1:C:373:LEU:HD23	1:C:373:LEU:C	2.13	0.69
1:D:195:LYS:HD2	1:D:320:GLY:O	1.93	0.69
1:D:443:ILE:HG21	1:D:586:LEU:HD22	1.75	0.69
1:F:220:VAL:CG1	1:F:221:PRO:HD2	2.23	0.69
1:F:231:VAL:O	1:F:232:GLU:CB	2.41	0.69
1:F:483:ARG:HD2	1:F:493:VAL:CG2	2.23	0.69
1:D:217:GLU:HG3	5:D:2005:HOH:O	1.91	0.69
1:D:469:ARG:NH1	1:D:517:MET:O	2.26	0.69
1:E:214:VAL:HG12	1:E:256:ILE:HD11	1.75	0.69
1:C:334:LEU:O	1:C:338:LYS:HG2	1.93	0.69
1:E:586:LEU:HD12	1:E:592:ILE:HG23	1.75	0.69
1:E:156:LYS:HZ3	1:E:156:LYS:HB3	1.56	0.68
3:D:1608:ADP:H5'1	3:D:1608:ADP:H8	1.57	0.68
1:F:425:ALA:HB1	1:F:579:LEU:HD12	1.74	0.68
1:B:542:LEU:C	1:B:542:LEU:HD23	2.14	0.68
1:C:192:ARG:O	1:C:192:ARG:HG3	1.92	0.68
1:E:380:LEU:HD23	1:E:383:ARG:HH21	1.59	0.68
1:A:476:LEU:HD11	1:A:507:ILE:HB	1.75	0.68
1:B:429:VAL:O	1:B:433:VAL:HG23	1.93	0.68
1:B:207:LYS:HZ2	3:B:1607:ADP:PB	2.17	0.67
1:B:354:ASN:ND2	1:B:357:ILE:HD12	2.09	0.67
1:F:287:LEU:HD23	1:F:287:LEU:C	2.14	0.67
1:A:559:LYS:HD3	5:A:2031:HOH:O	1.93	0.67
1:C:519:GLU:CA	5:C:2018:HOH:O	1.93	0.67
1:B:594:GLY:O	1:B:597:LEU:N	2.27	0.67
1:E:483:ARG:HD2	1:E:493:VAL:CG2	2.24	0.67
1:F:180:LEU:CD2	1:F:301:ILE:CD1	2.69	0.67
1:C:519:GLU:O	5:C:2018:HOH:O	2.12	0.67
1:C:266:GLY:O	1:C:312:LEU:HA	1.94	0.67
1:E:188:ARG:NH1	5:E:2006:HOH:O	2.04	0.67
1:F:182:ASP:OD1	1:F:184:SER:OG	2.12	0.67
1:C:291:MET:HA	1:C:291:MET:HE2	1.77	0.66
1:C:593:GLU:C	5:C:2024:HOH:O	2.21	0.66
1:D:450:TYR:C	1:D:450:TYR:CD2	2.69	0.66
1:F:597:LEU:O	1:F:601:LEU:HG	1.95	0.66
1:B:207:LYS:NZ	3:B:1607:ADP:PB	2.68	0.66
1:E:594:GLY:O	1:E:596:GLU:N	2.28	0.66
1:F:387:ASP:OD1	1:F:387:ASP:N	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:GLU:HG2	5:B:2031:HOH:O	1.95	0.66
1:B:577:LYS:HB2	1:B:577:LYS:HZ2	1.61	0.66
1:F:166:ALA:O	1:F:170:ILE:HG13	1.95	0.66
1:C:220:VAL:HG13	1:C:221:PRO:CD	2.26	0.66
1:C:420:ILE:HG22	1:C:445:ILE:HG23	1.76	0.66
1:C:434:VAL:HG22	1:C:567:ARG:NH2	2.11	0.66
1:D:408:LYS:O	5:D:2016:HOH:O	2.13	0.66
1:A:340:LEU:O	1:A:344:THR:HB	1.96	0.66
1:B:237:VAL:O	1:B:241:ARG:HG3	1.94	0.65
1:F:374:VAL:CG1	1:F:375:ASN:N	2.59	0.65
1:C:444:SER:C	1:C:445:ILE:HD13	2.15	0.65
1:D:291:MET:HE3	1:D:302:VAL:HG21	1.77	0.65
1:A:542:LEU:HD13	1:A:543:ARG:H	1.60	0.65
1:D:446:ILE:HB	1:D:447:PRO:HD3	1.79	0.65
1:E:231:VAL:O	1:E:232:GLU:CB	2.43	0.65
1:F:233:LEU:HD21	1:F:241:ARG:CZ	2.26	0.65
1:D:294:PHE:CD1	1:D:294:PHE:C	2.69	0.65
1:C:287:LEU:HD23	1:C:287:LEU:O	1.97	0.65
1:F:225:ILE:HD11	1:F:245:LEU:HD11	1.78	0.65
1:F:334:LEU:O	1:F:338:LYS:HG2	1.97	0.65
1:E:543:ARG:HD2	1:E:545:TYR:CE1	2.32	0.65
1:D:443:ILE:HG21	1:D:586:LEU:CD2	2.27	0.65
1:E:402:ILE:HG22	1:E:403:ALA:H	1.62	0.64
1:F:527:GLY:O	5:F:2018:HOH:O	2.15	0.64
1:E:230:PHE:N	1:E:230:PHE:HD1	1.96	0.64
1:E:267:ARG:NH1	1:F:243:ARG:HD2	2.12	0.64
1:D:286:GLN:NE2	1:D:290:GLU:OE2	2.31	0.64
3:E:1604:ADP:C5'	3:E:1604:ADP:C8	2.81	0.64
1:F:442:ARG:CB	1:F:593:GLU:HB2	2.27	0.64
1:B:342:ILE:O	1:B:345:ARG:CD	2.46	0.64
1:C:224:HIS:C	1:C:224:HIS:CD2	2.71	0.64
1:E:231:VAL:HG11	1:E:232:GLU:OE2	1.92	0.64
1:E:243:ARG:NH1	1:E:286:GLN:NE2	2.45	0.64
1:E:582:ILE:HD11	1:E:597:LEU:HD11	1.73	0.64
1:F:220:VAL:HG13	1:F:254:PRO:O	1.98	0.64
1:E:263:ASP:O	1:E:267:ARG:HG2	1.97	0.64
1:C:291:MET:SD	1:C:302:VAL:HG21	2.38	0.64
1:E:421:ALA:HA	1:E:445:ILE:HD11	1.80	0.64
1:F:430:VAL:HG11	1:F:477:THR:HG22	1.80	0.64
1:F:452:ALA:HB2	5:F:2003:HOH:O	1.97	0.64
1:F:180:LEU:CD2	1:F:301:ILE:HD11	2.27	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:586:LEU:CD1	1:F:592:ILE:CD1	2.76	0.63
1:B:547:GLU:OE1	5:B:2026:HOH:O	2.15	0.63
1:D:226:SER:HB3	1:D:229:ASP:OD2	1.98	0.63
1:E:483:ARG:NH2	1:F:516:GLY:O	2.31	0.63
1:D:483:ARG:NH2	1:E:516:GLY:O	2.31	0.63
1:E:332:ASP:O	1:E:336:ARG:HG3	1.98	0.63
1:F:150:TYR:N	1:F:245:LEU:HD11	2.13	0.63
1:B:466:LEU:CD2	1:B:466:LEU:C	2.67	0.63
1:B:499:ASN:ND2	1:B:500:ASP:N	2.47	0.63
1:A:499:ASN:HD22	1:A:499:ASN:H	1.46	0.63
1:A:586:LEU:HD13	1:A:592:ILE:HG23	1.81	0.63
1:C:225:ILE:HG13	1:C:245:LEU:CD1	2.28	0.63
1:F:176:VAL:HG13	1:F:301:ILE:CD1	2.28	0.63
1:B:308:ARG:N	1:B:309:PRO:CD	2.62	0.63
1:F:208:THR:O	1:F:212:ARG:HG3	1.97	0.63
1:F:424:GLU:OE1	1:F:424:GLU:HA	1.97	0.63
1:D:231:VAL:O	1:D:232:GLU:CB	2.46	0.63
1:F:307:ASN:OD1	1:F:307:ASN:O	2.17	0.63
1:C:284:LEU:HD11	1:C:288:LEU:HG	1.81	0.62
1:B:362:THR:N	1:B:363:PRO:CD	2.62	0.62
1:C:202:PRO:HB2	1:C:448:ARG:HH21	1.64	0.62
1:C:222:PHE:HE2	1:C:224:HIS:HB2	1.64	0.62
1:D:185:LYS:CB	5:D:2003:HOH:O	2.39	0.62
1:A:483:ARG:NE	1:A:493:VAL:HG11	2.13	0.62
1:A:267:ARG:HG3	1:A:311:ILE:HG23	1.81	0.62
1:D:442:ARG:HB2	1:D:593:GLU:HG2	1.82	0.62
1:F:386:ARG:NH2	1:F:393:ASP:OD2	2.31	0.62
1:B:466:LEU:HD23	1:B:467:VAL:N	2.15	0.62
1:F:226:SER:O	1:F:230:PHE:CE1	2.52	0.62
1:C:597:LEU:CD2	1:C:597:LEU:O	2.48	0.62
1:B:334:LEU:O	1:B:338:LYS:HG2	2.00	0.61
1:F:595:ASP:OD1	1:F:595:ASP:N	2.30	0.61
1:C:214:VAL:HG12	1:C:256:ILE:HD11	1.82	0.61
1:C:230:PHE:HA	1:C:233:LEU:HD12	1.81	0.61
1:E:586:LEU:CD1	1:E:592:ILE:CG2	2.79	0.61
1:C:507:ILE:O	1:C:511:MET:HG3	2.00	0.61
3:E:1604:ADP:C8	3:E:1604:ADP:H5'1	2.35	0.61
1:F:220:VAL:CG1	1:F:255:CYS:HA	2.30	0.61
1:C:287:LEU:C	1:C:287:LEU:CD2	2.69	0.61
1:F:202:PRO:HG2	1:F:205:THR:CG2	2.30	0.61
1:D:361:ARG:NH2	1:D:395:GLU:OE2	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:ILE:HD11	1:D:411:LEU:HD12	1.81	0.61
1:F:176:VAL:CG1	1:F:301:ILE:HD13	2.29	0.61
1:E:591:THR:O	1:E:592:ILE:HG22	2.00	0.61
1:A:392:LYS:O	1:A:396:GLU:HG3	2.00	0.60
1:D:291:MET:HE1	1:D:302:VAL:HG21	1.82	0.60
1:B:483:ARG:NH1	1:B:493:VAL:HG11	2.16	0.60
1:A:231:VAL:O	1:A:232:GLU:HB2	2.02	0.60
1:A:510:ASN:ND2	1:A:514:GLN:CD	2.54	0.60
1:C:444:SER:O	1:C:445:ILE:HD13	2.01	0.60
1:E:230:PHE:N	1:E:230:PHE:CD1	2.66	0.60
1:B:230:PHE:HA	1:B:233:LEU:CD1	2.29	0.60
1:B:595:ASP:HA	1:B:598:ARG:HB2	1.83	0.60
1:B:411:LEU:HD12	1:B:412:ILE:H	1.67	0.60
1:D:547:GLU:OE2	1:E:546:SER:HB2	2.02	0.60
1:F:586:LEU:HD13	1:F:592:ILE:CD1	2.30	0.60
1:B:418:ARG:NH2	5:B:2018:HOH:O	2.34	0.60
1:D:220:VAL:CG1	1:D:255:CYS:HA	2.31	0.60
1:F:357:ILE:HG21	1:F:391:MET:CE	2.30	0.60
1:C:489:VAL:HG22	1:C:576:ARG:CZ	2.31	0.60
1:F:250:LYS:HZ3	1:F:294:PHE:CB	2.13	0.60
1:C:284:LEU:HD12	1:C:284:LEU:C	2.21	0.60
1:F:180:LEU:HD21	1:F:301:ILE:CG1	2.32	0.60
3:C:1608:ADP:H8	3:C:1608:ADP:C5'	2.15	0.60
1:D:188:ARG:NH1	1:D:188:ARG:HB3	2.17	0.59
1:F:572:ILE:HG23	1:F:579:LEU:HD22	1.84	0.59
1:F:465:TYR:C	5:F:2008:HOH:O	2.41	0.59
1:A:599:ARG:O	1:A:602:SER:N	2.35	0.59
1:E:499:ASN:ND2	1:E:500:ASP:N	2.49	0.59
1:F:476:LEU:CD2	1:F:504:ALA:HB1	2.32	0.59
1:F:210:LEU:O	1:F:214:VAL:HG23	2.03	0.59
1:F:230:PHE:O	1:F:233:LEU:HG	2.03	0.59
1:A:189:ILE:HD11	1:B:382:ALA:HB2	1.84	0.59
1:F:311:ILE:O	1:F:311:ILE:CG2	2.50	0.59
1:F:354:ASN:OD1	1:F:357:ILE:CG1	2.48	0.59
1:A:585:ILE:CD1	1:A:600:ILE:HD11	2.32	0.59
1:C:220:VAL:HG13	1:C:255:CYS:HA	1.83	0.59
1:B:279:GLU:O	1:B:283:THR:OG1	2.15	0.59
1:B:291:MET:HE3	1:B:302:VAL:HG21	1.84	0.59
1:C:341:GLU:HA	1:C:344:THR:CG2	2.33	0.59
1:D:178:GLU:OE2	1:D:178:GLU:CA	2.51	0.59
1:B:594:GLY:C	1:B:596:GLU:N	2.56	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:PHE:CD1	1:C:186:PHE:N	2.70	0.59
1:A:499:ASN:H	1:A:499:ASN:ND2	2.00	0.59
1:A:510:ASN:HD21	1:A:514:GLN:NE2	2.01	0.58
1:C:445:ILE:HG22	1:C:445:ILE:O	2.03	0.58
3:E:1604:ADP:C5'	3:E:1604:ADP:H8	2.16	0.58
1:A:589:LYS:O	1:A:590:GLU:HB2	2.03	0.58
1:E:586:LEU:HD12	1:E:592:ILE:CG2	2.33	0.58
1:C:159:THR:HB	1:C:217:GLU:OE1	2.03	0.58
1:F:286:GLN:HA	1:F:286:GLN:NE2	2.19	0.58
1:B:224:HIS:C	1:B:225:ILE:HD13	2.24	0.58
1:E:402:ILE:O	1:E:403:ALA:HB2	2.04	0.58
1:E:287:LEU:C	1:E:287:LEU:CD2	2.72	0.58
1:F:163:VAL:HG22	1:F:209:LEU:CD2	2.33	0.58
1:C:285:ASN:O	1:C:289:VAL:HG23	2.03	0.58
1:E:167:GLU:N	1:E:167:GLU:OE1	2.37	0.58
1:E:354:ASN:C	1:E:354:ASN:HD22	2.07	0.58
1:F:391:MET:HG3	1:F:395:GLU:CD	2.24	0.58
1:F:413:SER:OG	1:F:416:GLU:CD	2.41	0.58
1:B:230:PHE:O	1:B:233:LEU:HG	2.03	0.58
1:C:207:LYS:HE3	3:C:1608:ADP:O1B	2.04	0.58
1:A:308:ARG:HG2	1:A:311:ILE:HD12	1.86	0.58
1:B:358:ILE:HD11	1:B:394:PHE:HB2	1.86	0.58
1:B:547:GLU:HB2	5:B:2026:HOH:O	2.02	0.58
1:E:287:LEU:C	1:E:287:LEU:HD23	2.24	0.58
1:E:591:THR:C	1:E:592:ILE:CG2	2.73	0.58
1:F:233:LEU:HD21	1:F:241:ARG:NH1	2.19	0.58
1:B:594:GLY:C	1:B:596:GLU:H	2.07	0.57
1:C:257:VAL:HB	1:C:302:VAL:HG12	1.86	0.57
1:D:334:LEU:O	1:D:338:LYS:HG2	2.03	0.57
1:F:212:ARG:HG2	1:F:222:PHE:CZ	2.39	0.57
1:D:444:SER:HB3	1:D:591:THR:HG23	1.86	0.57
1:D:450:TYR:HD2	1:D:450:TYR:O	1.86	0.57
1:A:233:LEU:HD13	1:A:237:VAL:HG12	1.86	0.57
3:B:1607:ADP:C8	3:B:1607:ADP:H5'1	2.39	0.57
3:D:1608:ADP:H8	3:D:1608:ADP:C5'	2.17	0.57
1:B:479:LEU:CD1	1:B:503:ARG:HG2	2.33	0.57
1:C:230:PHE:HA	1:C:233:LEU:HD11	1.86	0.57
1:F:207:LYS:HE3	3:F:1607:ADP:O1B	2.04	0.57
1:F:226:SER:O	1:F:230:PHE:HE1	1.87	0.57
1:A:499:ASN:N	1:A:499:ASN:ND2	2.53	0.57
1:F:351:GLU:HA	1:F:351:GLU:OE2	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:LEU:HD23	1:B:543:ARG:N	2.19	0.57
1:E:184:SER:O	1:E:188:ARG:HB2	2.05	0.57
1:B:189:ILE:O	1:C:347:LYS:HE2	2.04	0.57
1:B:483:ARG:NH1	1:B:493:VAL:CG1	2.68	0.57
1:C:339:ILE:HG23	3:C:1608:ADP:C2	2.40	0.57
1:E:585:ILE:HG23	1:E:589:LYS:HD3	1.85	0.57
1:C:589:LYS:O	1:C:590:GLU:HB2	2.04	0.57
1:E:399:ASP:OD1	1:E:399:ASP:N	2.37	0.57
1:F:176:VAL:O	1:F:180:LEU:HG	2.05	0.57
1:D:442:ARG:CB	1:D:593:GLU:OE2	2.53	0.56
1:D:444:SER:CB	1:D:591:THR:HG23	2.35	0.56
1:B:196:GLY:HA2	1:B:302:VAL:O	2.06	0.56
1:E:192:ARG:HH11	1:E:192:ARG:HG2	1.71	0.56
1:E:527:GLY:O	1:E:528:LYS:HB2	2.05	0.56
1:C:181:LYS:HE3	1:C:218:ALA:HA	1.86	0.56
1:C:579:LEU:O	1:C:583:VAL:HG23	2.05	0.56
1:E:591:THR:C	1:E:592:ILE:HG22	2.26	0.56
1:C:291:MET:CE	1:C:294:PHE:HE2	2.18	0.56
1:C:597:LEU:O	1:C:597:LEU:HD23	2.06	0.56
1:F:442:ARG:HA	1:F:592:ILE:O	2.06	0.56
1:F:233:LEU:CD1	1:F:238:GLY:HA2	2.35	0.56
1:F:265:VAL:HA	1:F:280:ARG:HD2	1.86	0.56
1:C:464:LYS:NZ	1:C:471:GLU:OE1	2.38	0.56
1:E:308:ARG:NE	1:F:289:VAL:HG21	2.14	0.56
1:B:189:ILE:HG22	1:C:348:PRO:HG3	1.87	0.56
1:A:549:VAL:O	1:A:553:ILE:HG13	2.06	0.55
1:A:600:ILE:C	1:A:602:SER:H	2.09	0.55
1:D:246:PHE:O	1:D:250:LYS:HG3	2.06	0.55
1:E:434:VAL:CG1	1:E:474:ASP:HB3	2.36	0.55
1:B:310:ASP:OD2	1:B:310:ASP:N	2.37	0.55
1:D:171:GLU:OE2	1:D:171:GLU:HA	2.05	0.55
1:F:288:LEU:HD21	1:F:316:LEU:HD23	1.87	0.55
1:A:416:GLU:O	1:A:420:ILE:HD12	2.07	0.55
1:D:207:LYS:HE3	3:D:1608:ADP:O1B	2.07	0.55
1:D:372:ASN:ND2	1:D:401:VAL:HG12	2.22	0.55
1:E:434:VAL:HG11	1:E:474:ASP:HB3	1.89	0.55
1:F:225:ILE:HD12	1:F:245:LEU:CD1	2.31	0.55
1:F:452:ALA:CB	5:F:2003:HOH:O	2.52	0.55
1:F:483:ARG:HD2	1:F:493:VAL:HG21	1.88	0.55
1:C:593:GLU:N	5:C:2024:HOH:O	2.39	0.55
1:E:267:ARG:O	1:E:268:HIS:C	2.45	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:594:GLY:C	1:E:596:GLU:N	2.58	0.55
1:A:399:ASP:OD1	1:A:399:ASP:N	2.39	0.55
1:B:589:LYS:O	1:B:590:GLU:HB2	2.06	0.55
1:C:184:SER:O	1:C:188:ARG:HG3	2.06	0.55
1:E:547:GLU:OE2	1:F:546:SER:HB2	2.06	0.55
1:F:507:ILE:O	1:F:511:MET:HG3	2.06	0.55
1:F:446:ILE:O	1:F:450:TYR:HD1	1.86	0.55
1:F:220:VAL:HG12	1:F:255:CYS:HA	1.88	0.55
1:F:412:ILE:O	1:F:412:ILE:HG22	2.06	0.55
1:C:333:MET:C	1:C:333:MET:SD	2.84	0.55
1:C:366:VAL:HG22	1:C:369:ASP:OD2	2.07	0.55
1:D:380:LEU:HD23	1:D:383:ARG:HH12	1.69	0.55
1:D:380:LEU:CA	1:D:383:ARG:HH12	2.17	0.55
1:F:288:LEU:CD2	1:F:316:LEU:HD23	2.37	0.55
1:F:578:GLN:NE2	1:F:578:GLN:N	2.44	0.55
1:F:333:MET:HG3	1:F:334:LEU:N	2.22	0.54
1:D:446:ILE:O	1:D:448:ARG:N	2.40	0.54
1:F:202:PRO:HD2	1:F:205:THR:HG21	1.89	0.54
1:A:586:LEU:HD12	1:A:592:ILE:HG23	1.89	0.54
1:C:155:ASN:HB3	1:C:212:ARG:HH22	1.68	0.54
1:E:593:GLU:HA	1:E:593:GLU:OE1	2.07	0.54
1:B:278:ASP:OD2	1:B:278:ASP:N	2.40	0.54
1:D:402:ILE:CG2	1:D:403:ALA:H	2.01	0.54
1:E:582:ILE:CD1	1:E:597:LEU:HD13	2.37	0.54
1:B:186:PHE:CD1	1:C:382:ALA:HB1	2.42	0.54
1:A:476:LEU:CD1	1:A:507:ILE:HB	2.37	0.54
1:D:210:LEU:O	1:D:214:VAL:HG23	2.07	0.54
1:D:362:THR:N	1:D:363:PRO:CD	2.70	0.54
1:E:157:ARG:HH21	1:E:216:GLY:CA	2.20	0.54
1:C:464:LYS:NZ	1:C:471:GLU:OE2	2.38	0.54
1:F:233:LEU:CD2	1:F:241:ARG:CZ	2.86	0.54
1:F:416:GLU:O	1:F:417:LYS:C	2.46	0.54
1:F:577:LYS:HB3	1:F:578:GLN:NE2	2.23	0.54
1:E:185:LYS:HE3	5:E:2005:HOH:O	2.07	0.54
1:E:468:SER:OG	1:E:471:GLU:HG3	2.08	0.54
1:F:445:ILE:HD11	1:F:586:LEU:O	2.08	0.54
1:B:313:ASP:C	1:B:313:ASP:OD1	2.47	0.54
1:D:161:LYS:O	1:D:345:ARG:NH2	2.37	0.54
1:E:207:LYS:NZ	3:E:1604:ADP:O1B	2.34	0.53
1:F:220:VAL:HG12	1:F:221:PRO:CD	2.35	0.53
1:F:374:VAL:HG13	1:F:375:ASN:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:414:PRO:HA	1:F:417:LYS:HB2	1.90	0.53
1:B:168:GLU:OE1	1:B:168:GLU:N	2.40	0.53
1:E:490:PHE:C	1:E:492:ASP:H	2.12	0.53
1:F:233:LEU:CD1	1:F:238:GLY:CA	2.85	0.53
1:E:438:GLU:O	1:E:439:PRO:C	2.47	0.53
1:B:342:ILE:O	1:B:345:ARG:HD3	2.07	0.53
1:E:413:SER:O	1:E:416:GLU:N	2.42	0.53
1:C:421:ALA:HB1	1:C:583:VAL:HG13	1.91	0.53
1:F:202:PRO:O	1:F:205:THR:HG23	2.08	0.53
1:B:469:ARG:NH2	1:B:517:MET:O	2.42	0.53
1:C:309:PRO:HB2	1:C:459:LEU:HD21	1.90	0.53
1:C:380:LEU:HD21	1:C:400:ARG:HH21	1.73	0.53
1:E:188:ARG:HD3	5:E:2006:HOH:O	2.07	0.53
1:F:444:SER:HA	1:F:590:GLU:O	2.09	0.53
1:A:446:ILE:CG2	5:A:2025:HOH:O	1.89	0.53
1:B:201:GLY:O	1:B:307:ASN:HB3	2.09	0.53
1:F:305:ALA:O	1:F:306:THR:HB	2.08	0.53
1:C:420:ILE:HG21	1:C:445:ILE:HG23	1.88	0.53
1:C:425:ALA:HB1	1:C:579:LEU:HD12	1.90	0.53
1:C:464:LYS:NZ	1:C:471:GLU:CD	2.62	0.53
3:C:1608:ADP:H8	3:C:1608:ADP:H5'1	1.73	0.53
1:E:594:GLY:C	1:E:596:GLU:H	2.10	0.53
1:C:594:GLY:O	1:C:598:ARG:HG3	2.08	0.53
1:F:162:ASP:O	1:F:342:ILE:HD13	2.08	0.53
1:A:446:ILE:C	1:A:446:ILE:CD1	2.68	0.52
1:C:235:VAL:O	1:C:235:VAL:CG1	2.57	0.52
1:E:328:VAL:HG12	1:E:328:VAL:O	2.09	0.52
1:F:176:VAL:CG1	1:F:301:ILE:CD1	2.87	0.52
1:B:235:VAL:HG22	1:B:279:GLU:OE1	2.09	0.52
1:C:199:LEU:HD11	1:C:303:MET:CE	2.39	0.52
1:D:333:MET:HB3	1:D:590:GLU:OE1	2.10	0.52
1:F:291:MET:HE2	1:F:294:PHE:CZ	2.41	0.52
1:F:447:PRO:O	1:F:450:TYR:CZ	2.62	0.52
1:B:351:GLU:HG2	5:B:2015:HOH:O	2.09	0.52
1:B:597:LEU:O	1:B:597:LEU:HD23	2.10	0.52
1:F:357:ILE:O	1:F:360:LYS:HB2	2.09	0.52
1:F:592:ILE:N	1:F:592:ILE:CD1	2.71	0.52
1:F:318:ARG:HB3	1:F:319:PRO:HD2	1.92	0.52
1:F:444:SER:HB2	1:F:591:THR:HG23	1.90	0.52
1:B:344:THR:O	1:B:345:ARG:C	2.48	0.52
1:B:391:MET:O	1:B:395:GLU:HG3	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LYS:NZ	1:D:188:ARG:HH22	2.08	0.52
1:E:246:PHE:HZ	1:E:291:MET:HE3	1.75	0.52
1:A:199:LEU:HD11	1:A:303:MET:CE	2.40	0.52
1:C:311:ILE:HG22	1:C:311:ILE:O	2.09	0.52
1:F:233:LEU:HD13	1:F:238:GLY:CA	2.40	0.52
1:A:443:ILE:O	1:A:591:THR:CG2	2.58	0.52
1:B:313:ASP:OD1	1:B:315:ALA:N	2.35	0.52
1:F:217:GLU:HA	1:F:217:GLU:OE2	2.10	0.52
1:A:193:MET:HB3	1:A:194:PRO:HD2	1.90	0.52
1:A:601:LEU:O	1:A:602:SER:C	2.48	0.52
1:C:593:GLU:HG3	1:C:594:GLY:N	2.24	0.52
3:E:1604:ADP:H8	3:E:1604:ADP:H5'2	1.74	0.52
1:F:192:ARG:O	1:F:192:ARG:HG3	2.09	0.52
1:F:357:ILE:CG2	1:F:391:MET:HE1	2.35	0.52
1:C:195:LYS:O	1:C:302:VAL:CG2	2.57	0.52
1:D:207:LYS:HE3	3:D:1608:ADP:PB	2.50	0.52
1:D:308:ARG:HH21	1:D:311:ILE:HD12	1.75	0.52
1:C:354:ASN:C	1:C:354:ASN:HD22	2.13	0.51
1:D:344:THR:CG2	1:D:349:LEU:HD11	2.32	0.51
1:D:443:ILE:CG2	1:D:586:LEU:HD21	2.40	0.51
1:E:287:LEU:HD23	1:E:287:LEU:O	2.09	0.51
1:F:250:LYS:HA	1:F:300:ILE:HD11	1.91	0.51
1:B:358:ILE:HD11	1:B:394:PHE:CB	2.40	0.51
1:F:319:PRO:HA	1:F:323:ASP:HB3	1.92	0.51
1:C:186:PHE:HD1	1:C:186:PHE:H	1.58	0.51
1:C:222:PHE:CE2	1:C:224:HIS:HB2	2.43	0.51
1:D:233:LEU:HD12	1:D:238:GLY:CA	2.40	0.51
1:A:220:VAL:HG13	1:A:221:PRO:HD2	1.91	0.51
1:A:411:LEU:N	1:A:411:LEU:HD12	2.26	0.51
1:C:595:ASP:HA	1:C:598:ARG:HD3	1.93	0.51
1:A:483:ARG:HD2	1:A:493:VAL:HG13	1.92	0.51
1:B:354:ASN:HD22	1:B:357:ILE:HD12	1.74	0.51
1:D:217:GLU:CG	5:D:2005:HOH:O	2.56	0.51
1:E:582:ILE:HD13	1:E:597:LEU:HD11	1.87	0.51
1:F:160:PHE:CD1	1:F:217:GLU:HG2	2.45	0.51
1:F:237:VAL:HG12	1:F:241:ARG:HE	1.75	0.51
1:B:229:ASP:O	1:B:233:LEU:HD21	2.11	0.51
1:F:442:ARG:O	1:F:442:ARG:HG2	2.09	0.51
1:D:401:VAL:HG11	5:D:2013:HOH:O	2.10	0.51
1:D:188:ARG:HB3	1:D:188:ARG:HH11	1.76	0.51
1:D:284:LEU:O	1:D:285:ASN:C	2.48	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:VAL:CG1	1:E:256:ILE:HD11	2.41	0.51
1:F:208:THR:HB	3:F:1607:ADP:O1A	2.10	0.51
1:A:585:ILE:HD12	1:A:600:ILE:HD11	1.92	0.51
1:C:430:VAL:CG1	1:C:477:THR:HG22	2.40	0.51
1:E:266:GLY:HA2	1:E:284:LEU:HD13	1.93	0.51
1:F:262:ILE:CD1	1:F:304:ALA:HB1	2.39	0.51
1:F:338:LYS:O	1:F:342:ILE:HG13	2.11	0.51
1:D:333:MET:HG3	1:D:334:LEU:N	2.27	0.50
1:A:434:VAL:HG13	1:A:474:ASP:HB3	1.89	0.50
1:A:578:GLN:CD	1:A:578:GLN:H	2.14	0.50
3:B:1607:ADP:H5'1	3:B:1607:ADP:H8	1.74	0.50
1:C:284:LEU:CD1	1:C:288:LEU:HG	2.42	0.50
1:C:597:LEU:O	1:C:597:LEU:HD22	2.12	0.50
1:D:230:PHE:N	1:D:230:PHE:CD1	2.79	0.50
1:E:201:GLY:O	1:E:207:LYS:HE3	2.11	0.50
1:E:446:ILE:O	1:E:446:ILE:CG2	2.45	0.50
1:F:267:ARG:HB3	1:F:280:ARG:HE	1.75	0.50
1:B:158:VAL:O	1:B:216:GLY:HA3	2.11	0.50
1:B:166:ALA:O	1:B:170:ILE:HG13	2.12	0.50
1:A:224:HIS:O	1:A:225:ILE:HD13	2.11	0.50
1:C:207:LYS:HB2	3:C:1608:ADP:O3B	2.11	0.50
1:C:221:PRO:HG2	1:C:255:CYS:HB3	1.93	0.50
1:C:430:VAL:HG11	1:C:477:THR:HG22	1.93	0.50
1:D:543:ARG:HG3	1:D:545:TYR:CZ	2.47	0.50
1:E:220:VAL:HG13	1:E:221:PRO:HD2	1.93	0.50
1:B:224:HIS:O	1:B:225:ILE:HD13	2.11	0.50
1:B:466:LEU:C	1:B:466:LEU:HD23	2.31	0.50
1:D:358:ILE:O	1:D:362:THR:HG23	2.12	0.50
1:D:565:TYR:CE2	1:D:569:LYS:HE2	2.46	0.50
3:D:1608:ADP:C8	3:D:1608:ADP:C5'	2.91	0.50
1:F:262:ILE:HG22	1:F:306:THR:HB	1.94	0.50
1:C:291:MET:HE1	1:C:302:VAL:HG11	1.93	0.50
1:C:442:ARG:NH2	1:C:451:LYS:NZ	2.60	0.50
1:C:595:ASP:O	1:C:599:ARG:HG3	2.12	0.50
1:E:436:ASN:HB2	1:E:474:ASP:OD2	2.12	0.50
1:E:582:ILE:HD13	1:E:597:LEU:HD13	1.92	0.50
1:C:158:VAL:HG23	1:C:213:ALA:HA	1.93	0.50
1:F:250:LYS:HZ2	1:F:294:PHE:HB2	1.71	0.50
1:A:234:PHE:CG	1:A:235:VAL:N	2.79	0.49
1:C:518:SER:OG	1:C:521:LEU:HB2	2.11	0.49
1:F:160:PHE:CE1	1:F:217:GLU:HG2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:ASP:OD2	1:F:185:LYS:CG	2.57	0.49
1:A:340:LEU:O	1:A:341:GLU:C	2.51	0.49
1:E:292:ASP:HA	5:E:2009:HOH:O	2.11	0.49
1:F:430:VAL:CG1	1:F:477:THR:HG22	2.42	0.49
1:D:569:LYS:NZ	5:D:2028:HOH:O	2.17	0.49
1:E:367:GLY:HA3	3:E:1604:ADP:C8	2.48	0.49
1:F:451:LYS:O	1:F:451:LYS:CD	2.60	0.49
1:B:235:VAL:O	1:B:235:VAL:HG12	2.12	0.49
1:B:356:GLU:O	1:B:359:ALA:HB3	2.12	0.49
1:D:589:LYS:C	1:D:591:THR:H	2.15	0.49
1:F:240:ALA:HA	1:F:243:ARG:NH2	2.27	0.49
1:E:242:VAL:HG12	1:E:290:GLU:HG3	1.95	0.49
1:E:594:GLY:O	1:E:597:LEU:N	2.45	0.49
1:F:187:ASN:OD1	1:F:297:LYS:HG2	2.11	0.49
1:F:391:MET:HG3	1:F:395:GLU:OE2	2.11	0.49
1:C:156:LYS:H	1:C:156:LYS:HE3	1.76	0.49
1:C:597:LEU:CD2	1:C:597:LEU:C	2.81	0.49
1:F:267:ARG:CZ	1:F:311:ILE:HD13	2.42	0.49
1:A:476:LEU:HD13	1:A:507:ILE:HG21	1.93	0.49
1:B:499:ASN:ND2	1:B:500:ASP:H	2.00	0.49
1:C:202:PRO:O	1:C:207:LYS:HE2	2.12	0.49
1:D:178:GLU:OE2	1:D:178:GLU:HA	2.13	0.49
1:A:585:ILE:HD12	1:A:600:ILE:CD1	2.42	0.49
1:C:162:ASP:OD2	1:C:162:ASP:N	2.45	0.49
1:E:185:LYS:HE2	1:E:188:ARG:HH22	1.78	0.49
1:E:354:ASN:ND2	1:E:357:ILE:H	2.11	0.49
1:E:415:ALA:O	1:E:418:ARG:HB2	2.13	0.49
1:A:358:ILE:HD13	1:A:394:PHE:CD2	2.48	0.49
3:B:1607:ADP:H8	3:B:1607:ADP:C5'	2.26	0.48
1:F:197:ILE:HB	1:F:303:MET:HG2	1.95	0.48
1:C:438:GLU:O	1:C:439:PRO:C	2.52	0.48
1:D:307:ASN:ND2	1:D:307:ASN:C	2.62	0.48
1:E:366:VAL:O	1:E:367:GLY:C	2.51	0.48
1:F:206:GLY:CA	3:F:1607:ADP:N7	2.76	0.48
1:F:278:ASP:O	1:F:279:GLU:C	2.52	0.48
1:C:195:LYS:HB3	1:C:294:PHE:CZ	2.48	0.48
1:D:485:ALA:HB2	1:D:572:ILE:HD12	1.95	0.48
1:F:188:ARG:HB2	1:F:188:ARG:NH1	2.29	0.48
1:F:344:THR:OG1	1:F:349:LEU:HD21	2.13	0.48
1:F:349:LEU:N	1:F:349:LEU:HD23	2.28	0.48
1:B:486:GLU:OE1	1:B:494:THR:OG1	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:LYS:O	1:D:396:GLU:HG3	2.14	0.48
1:A:483:ARG:CZ	1:A:493:VAL:CG1	2.83	0.48
1:B:434:VAL:HG13	1:B:474:ASP:CG	2.34	0.48
1:B:499:ASN:HD22	1:B:499:ASN:N	2.10	0.48
1:B:596:GLU:O	1:B:600:ILE:HD12	2.13	0.48
3:C:1608:ADP:H5'1	3:C:1608:ADP:C8	2.48	0.48
1:C:311:ILE:O	1:C:311:ILE:CG2	2.61	0.48
1:E:243:ARG:NH1	1:E:286:GLN:HE21	2.12	0.48
1:F:412:ILE:O	1:F:412:ILE:CG2	2.62	0.48
1:C:499:ASN:ND2	1:C:500:ASP:N	2.53	0.48
1:B:167:GLU:OE1	1:B:167:GLU:N	2.26	0.47
3:C:1608:ADP:C5'	3:C:1608:ADP:C8	2.97	0.47
1:F:155:ASN:HB3	1:F:212:ARG:NH2	2.29	0.47
1:F:220:VAL:HG11	1:F:255:CYS:HA	1.95	0.47
1:A:315:ALA:HA	1:A:318:ARG:HG3	1.96	0.47
1:B:308:ARG:CZ	1:B:311:ILE:HD12	2.43	0.47
1:E:315:ALA:O	1:E:321:ARG:HD3	2.13	0.47
1:F:310:ASP:OD1	1:F:310:ASP:N	2.41	0.47
1:F:510:ASN:ND2	1:F:514:GLN:OE1	2.47	0.47
1:B:189:ILE:HG22	1:C:348:PRO:CG	2.44	0.47
1:B:366:VAL:HG22	1:B:369:ASP:OD2	2.13	0.47
1:C:442:ARG:HH21	1:C:451:LYS:NZ	2.11	0.47
1:F:163:VAL:HG22	1:F:209:LEU:HD21	1.96	0.47
1:F:436:ASN:HB2	1:F:474:ASP:OD2	2.15	0.47
1:E:353:VAL:O	1:E:353:VAL:HG12	2.14	0.47
1:F:202:PRO:HA	1:F:307:ASN:HD22	1.75	0.47
1:A:338:LYS:O	1:A:342:ILE:HG13	2.14	0.47
1:F:202:PRO:HG2	1:F:205:THR:HG21	1.96	0.47
1:F:449:GLY:O	1:F:450:TYR:O	2.33	0.47
1:F:486:GLU:OE1	1:F:494:THR:HG23	2.15	0.47
1:A:510:ASN:ND2	1:A:514:GLN:NE2	2.62	0.47
1:E:192:ARG:HG2	1:E:192:ARG:NH1	2.29	0.47
1:E:229:ASP:O	1:E:233:LEU:HD21	2.14	0.47
1:E:595:ASP:N	1:E:598:ARG:NH2	2.62	0.47
1:F:425:ALA:CB	1:F:579:LEU:HD12	2.44	0.47
1:B:266:GLY:HA2	1:B:284:LEU:HD13	1.96	0.47
1:C:519:GLU:C	5:C:2018:HOH:O	2.30	0.47
1:D:230:PHE:N	1:D:230:PHE:HD1	2.13	0.47
1:F:199:LEU:HD23	1:F:326:ILE:HB	1.97	0.47
1:F:465:TYR:N	1:F:465:TYR:CD1	2.81	0.47
1:C:479:LEU:HD23	1:C:479:LEU:HA	1.83	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:SER:O	1:C:606:GLU:HB2	2.15	0.47
1:D:185:LYS:HD2	1:D:185:LYS:C	2.35	0.47
1:F:286:GLN:O	1:F:290:GLU:HG2	2.14	0.47
1:A:263:ASP:HB2	1:A:311:ILE:HG21	1.95	0.47
1:A:444:SER:HB2	1:A:591:THR:HG23	1.97	0.47
1:A:499:ASN:HD22	1:A:500:ASP:H	1.63	0.47
1:E:336:ARG:NH2	1:E:590:GLU:OE2	2.42	0.47
1:F:599:ARG:HG3	1:F:600:ILE:H	1.80	0.47
1:B:342:ILE:O	1:B:345:ARG:HD2	2.15	0.46
1:B:402:ILE:HG22	1:B:403:ALA:N	2.30	0.46
1:B:411:LEU:HD12	1:B:412:ILE:N	2.30	0.46
1:D:446:ILE:O	1:D:447:PRO:C	2.50	0.46
1:F:220:VAL:CG1	1:F:221:PRO:CD	2.92	0.46
1:F:233:LEU:HD13	1:F:238:GLY:HA2	1.97	0.46
1:F:392:LYS:HB3	1:F:392:LYS:HE2	1.71	0.46
1:C:336:ARG:NE	1:C:362:THR:O	2.48	0.46
1:C:337:LYS:O	1:C:341:GLU:HG3	2.15	0.46
1:D:182:ASP:N	1:D:183:PRO:HD3	2.30	0.46
1:E:483:ARG:HD2	1:E:493:VAL:HG23	1.97	0.46
1:F:314:PRO:HB2	1:F:318:ARG:NH2	2.11	0.46
1:F:421:ALA:HB1	1:F:583:VAL:HG13	1.96	0.46
1:A:195:LYS:HE3	1:A:294:PHE:O	2.15	0.46
1:B:436:ASN:HB2	1:B:474:ASP:OD2	2.15	0.46
1:C:332:ASP:O	1:C:336:ARG:HG3	2.15	0.46
1:C:434:VAL:CG1	1:C:474:ASP:HB3	2.45	0.46
1:C:567:ARG:O	1:C:571:ILE:HG13	2.15	0.46
1:E:309:PRO:HD2	1:E:310:ASP:OD2	2.15	0.46
1:F:193:MET:SD	1:F:194:PRO:HD2	2.55	0.46
1:F:267:ARG:NH2	1:F:311:ILE:CD1	2.78	0.46
1:F:502:GLU:O	1:F:506:GLU:HG3	2.15	0.46
1:A:524:LEU:HD21	1:B:558:LYS:HA	1.97	0.46
1:E:595:ASP:OD1	1:E:598:ARG:NH2	2.41	0.46
1:F:260:ASP:O	1:F:261:GLU:C	2.53	0.46
1:E:596:GLU:O	1:E:600:ILE:HG22	2.15	0.46
1:B:308:ARG:N	1:B:309:PRO:HD3	2.31	0.46
1:B:570:GLU:HA	5:B:2031:HOH:O	2.16	0.46
1:A:225:ILE:HG22	1:A:226:SER:N	2.31	0.46
1:E:523:PRO:C	1:E:524:LEU:HD12	2.36	0.46
1:F:568:ALA:O	1:F:572:ILE:HG12	2.15	0.46
1:C:339:ILE:HD13	3:C:1608:ADP:C6	2.51	0.46
1:C:340:LEU:HD11	1:C:358:ILE:HG22	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:PHE:C	1:E:162:ASP:N	2.70	0.46
1:E:443:ILE:HG22	1:E:444:SER:N	2.31	0.46
1:E:483:ARG:CD	1:E:493:VAL:CG2	2.92	0.46
1:C:159:THR:OG1	1:C:161:LYS:HB3	2.16	0.46
1:C:238:GLY:O	1:C:242:VAL:HG23	2.15	0.46
1:D:184:SER:O	1:D:188:ARG:HB2	2.16	0.46
1:A:168:GLU:H	1:A:168:GLU:CD	2.18	0.45
1:B:231:VAL:O	1:B:232:GLU:CB	2.49	0.45
1:D:178:GLU:OE2	1:D:178:GLU:N	2.49	0.45
1:D:280:ARG:O	1:D:281:GLU:C	2.52	0.45
1:E:434:VAL:O	1:E:434:VAL:HG12	2.16	0.45
1:B:354:ASN:OD1	1:B:354:ASN:C	2.55	0.45
1:E:295:ASP:OD1	1:E:295:ASP:C	2.52	0.45
1:B:195:LYS:NZ	5:B:2003:HOH:O	2.44	0.45
1:C:336:ARG:NH2	1:C:363:PRO:HA	2.31	0.45
1:D:363:PRO:HD2	1:D:411:LEU:HD21	1.98	0.45
1:E:597:LEU:O	1:E:600:ILE:HG23	2.17	0.45
1:F:202:PRO:CD	1:F:205:THR:HG21	2.46	0.45
1:F:497:ALA:O	1:F:498:ALA:C	2.54	0.45
1:B:434:VAL:CG1	1:B:474:ASP:HB3	2.44	0.45
1:C:242:VAL:O	1:C:246:PHE:HD1	1.99	0.45
1:C:509:ARG:HD2	5:C:2016:HOH:O	2.15	0.45
1:E:472:LEU:HD23	1:E:472:LEU:HA	1.74	0.45
1:E:586:LEU:HD12	1:E:586:LEU:HA	1.83	0.45
1:E:600:ILE:O	1:E:600:ILE:CG1	2.65	0.45
1:A:150:TYR:CE2	1:A:225:ILE:HD12	2.52	0.45
1:A:323:ASP:OD1	5:A:2016:HOH:O	2.20	0.45
1:E:158:VAL:HG23	1:E:213:ALA:HA	1.97	0.45
1:E:160:PHE:C	1:E:162:ASP:H	2.18	0.45
1:F:365:PHE:CD1	1:F:369:ASP:HB3	2.52	0.45
1:A:226:SER:HB3	1:A:229:ASP:OD1	2.16	0.45
1:A:519:GLU:OE1	1:E:559:LYS:HD3	2.17	0.45
1:C:167:GLU:H	1:C:167:GLU:CD	2.15	0.45
1:C:209:LEU:HD12	1:C:209:LEU:HA	1.73	0.45
1:C:373:LEU:HD21	1:C:394:PHE:HD2	1.80	0.45
1:A:235:VAL:O	1:A:235:VAL:HG12	2.16	0.45
1:D:566:GLU:OE2	1:D:569:LYS:NZ	2.46	0.45
1:F:195:LYS:HG2	1:F:296:SER:HB3	1.98	0.45
1:F:197:ILE:HD12	1:F:303:MET:CE	2.47	0.45
1:C:207:LYS:HE3	3:C:1608:ADP:PB	2.57	0.45
1:F:499:ASN:HD22	1:F:499:ASN:N	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:VAL:CG1	1:B:478:ALA:HA	2.47	0.45
1:C:291:MET:CE	1:C:302:VAL:HG11	2.47	0.45
1:D:351:GLU:OE1	1:D:351:GLU:N	2.38	0.45
1:C:461:GLU:OE1	1:C:463:ASP:OD2	2.35	0.44
1:C:151:LYS:HE3	1:C:151:LYS:HB2	1.84	0.44
1:D:424:GLU:OE2	5:D:2031:HOH:O	2.21	0.44
1:D:444:SER:OG	1:D:447:PRO:HD2	2.17	0.44
1:F:228:SER:HB3	1:F:261:GLU:CD	2.37	0.44
1:A:199:LEU:HD23	1:A:326:ILE:HB	1.98	0.44
1:A:344:THR:O	1:A:345:ARG:C	2.56	0.44
1:B:552:LYS:NZ	5:B:2028:HOH:O	2.48	0.44
1:C:227:GLY:HA3	1:C:261:GLU:O	2.17	0.44
1:C:467:VAL:HG23	1:C:471:GLU:OE2	2.17	0.44
1:E:267:ARG:HH11	1:F:243:ARG:HD2	1.82	0.44
1:E:295:ASP:OD1	1:E:297:LYS:N	2.44	0.44
1:F:212:ARG:HA	1:F:222:PHE:CE1	2.52	0.44
1:F:596:GLU:O	1:F:600:ILE:HG13	2.17	0.44
1:A:159:THR:HB	1:A:217:GLU:OE1	2.18	0.44
1:B:248:GLN:OE1	1:B:248:GLN:HA	2.17	0.44
1:C:298:GLU:O	1:C:298:GLU:HG3	2.18	0.44
1:E:483:ARG:CD	1:E:493:VAL:HG21	2.47	0.44
1:F:213:ALA:O	1:F:217:GLU:HB2	2.18	0.44
1:B:198:LEU:HD12	1:B:304:ALA:O	2.17	0.44
1:B:281:GLU:CA	1:B:281:GLU:OE1	2.66	0.44
1:C:387:ASP:OD2	1:C:387:ASP:N	2.46	0.44
1:F:180:LEU:HD21	1:F:301:ILE:HG13	1.98	0.44
1:A:391:MET:O	1:A:395:GLU:HG3	2.17	0.44
1:C:310:ASP:OD1	1:C:310:ASP:N	2.50	0.44
1:E:585:ILE:CG2	1:E:589:LYS:HD3	2.48	0.44
1:E:591:THR:HG23	1:E:592:ILE:N	2.31	0.44
1:F:197:ILE:HD12	1:F:303:MET:HE2	1.99	0.44
1:B:542:LEU:C	1:B:542:LEU:CD2	2.85	0.44
3:B:1607:ADP:C8	3:B:1607:ADP:C5'	3.00	0.44
1:D:581:ASN:HB3	1:D:604:GLU:OE2	2.17	0.44
1:E:367:GLY:HA3	3:E:1604:ADP:N7	2.33	0.44
1:F:218:ALA:O	1:F:220:VAL:HG23	2.17	0.44
1:F:250:LYS:NZ	1:F:294:PHE:HA	2.33	0.44
1:F:291:MET:CE	1:F:294:PHE:CZ	2.97	0.44
1:F:375:ASN:O	1:F:375:ASN:ND2	2.50	0.44
1:D:434:VAL:HG22	1:D:435:PRO:HD2	1.98	0.44
1:E:159:THR:O	1:E:162:ASP:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LEU:HD12	1:A:476:LEU:HA	1.82	0.44
1:A:587:LEU:HD23	1:A:587:LEU:HA	1.86	0.44
1:B:518:SER:HB3	5:B:2024:HOH:O	2.17	0.44
1:C:172:GLU:OE1	1:C:326:ILE:HG23	2.18	0.44
1:C:354:ASN:ND2	1:C:356:GLU:HB3	2.33	0.44
1:C:193:MET:HE3	1:C:194:PRO:HD2	2.00	0.43
1:C:441:HIS:C	1:C:597:LEU:HD12	2.39	0.43
1:D:212:ARG:HG2	1:D:222:PHE:CE2	2.53	0.43
1:D:308:ARG:NH2	1:D:311:ILE:HD12	2.33	0.43
1:A:510:ASN:ND2	1:A:514:GLN:OE1	2.45	0.43
1:C:224:HIS:C	1:C:224:HIS:HD2	2.21	0.43
1:D:434:VAL:HG23	1:D:567:ARG:NH2	2.34	0.43
1:F:225:ILE:HG13	1:F:245:LEU:CD2	2.35	0.43
1:F:441:HIS:O	1:F:593:GLU:HA	2.17	0.43
1:B:543:ARG:HB2	1:B:545:TYR:CZ	2.52	0.43
1:D:285:ASN:O	1:D:289:VAL:HG23	2.18	0.43
1:E:445:ILE:HA	1:E:445:ILE:HD12	1.53	0.43
1:F:354:ASN:HD21	1:F:356:GLU:HB3	1.82	0.43
1:C:168:GLU:O	1:C:171:GLU:HB2	2.18	0.43
1:C:452:ALA:HB3	1:C:455:TYR:HD1	1.82	0.43
1:F:483:ARG:CD	1:F:493:VAL:HG21	2.48	0.43
1:F:599:ARG:HG2	1:F:599:ARG:HH11	1.83	0.43
1:B:291:MET:HE2	1:B:294:PHE:HE2	1.83	0.43
1:C:262:ILE:HG22	1:C:306:THR:HB	2.01	0.43
1:C:418:ARG:O	1:C:421:ALA:HB3	2.19	0.43
1:F:247:ALA:N	5:F:2002:HOH:O	2.51	0.43
1:F:287:LEU:HD21	1:F:291:MET:HG3	2.01	0.43
1:F:483:ARG:HD2	1:F:493:VAL:HG22	1.97	0.43
1:A:601:LEU:HD12	1:A:601:LEU:HA	1.82	0.43
1:B:413:SER:OG	1:B:416:GLU:HG3	2.19	0.43
1:B:578:GLN:O	1:B:582:ILE:HG13	2.18	0.43
1:E:239:ALA:HB1	1:E:286:GLN:HE21	1.84	0.43
1:F:226:SER:O	1:F:230:PHE:CD1	2.72	0.43
1:B:205:THR:HA	5:B:2004:HOH:O	2.19	0.43
1:D:220:VAL:HG22	1:D:254:PRO:O	2.18	0.43
1:F:173:LEU:HD13	1:F:214:VAL:HG21	2.01	0.43
1:F:233:LEU:HD13	1:F:238:GLY:N	2.34	0.43
1:F:260:ASP:OD2	1:F:261:GLU:N	2.52	0.43
1:F:595:ASP:O	1:F:599:ARG:HG2	2.18	0.43
1:C:600:ILE:O	1:C:604:GLU:HB2	2.19	0.43
1:E:338:LYS:HA	1:E:338:LYS:HD3	1.79	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:499:ASN:ND2	1:F:499:ASN:N	2.67	0.43
1:A:412:ILE:O	1:A:412:ILE:HG22	2.18	0.43
1:C:155:ASN:HB3	1:C:212:ARG:HH21	1.77	0.43
1:F:206:GLY:N	3:F:1607:ADP:N7	2.67	0.43
1:D:186:PHE:CD1	1:D:186:PHE:N	2.86	0.43
1:D:443:ILE:CG2	1:D:586:LEU:CD2	2.93	0.43
1:E:441:HIS:CD2	1:E:441:HIS:N	2.87	0.43
1:F:196:GLY:HA2	1:F:302:VAL:O	2.19	0.43
1:F:243:ARG:HG2	1:F:290:GLU:OE2	2.19	0.43
1:F:373:LEU:HD21	1:F:398:ILE:HG13	2.01	0.43
1:A:440:VAL:O	1:A:440:VAL:HG12	2.18	0.42
1:B:543:ARG:HD2	1:B:545:TYR:CE1	2.54	0.42
1:F:332:ASP:C	1:F:332:ASP:OD1	2.57	0.42
1:F:338:LYS:O	1:F:341:GLU:HB2	2.19	0.42
1:F:391:MET:CG	1:F:395:GLU:OE2	2.67	0.42
1:D:344:THR:O	1:D:345:ARG:C	2.58	0.42
1:E:413:SER:O	1:E:414:PRO:C	2.56	0.42
1:B:592:ILE:O	1:B:597:LEU:HD12	2.18	0.42
1:C:308:ARG:N	1:C:309:PRO:CD	2.82	0.42
1:B:380:LEU:O	1:B:383:ARG:HG2	2.20	0.42
1:C:253:ALA:HB1	1:C:298:GLU:O	2.20	0.42
1:D:340:LEU:O	1:D:344:THR:HB	2.18	0.42
1:E:260:ASP:O	1:E:261:GLU:C	2.57	0.42
1:E:340:LEU:O	1:E:344:THR:HG23	2.19	0.42
1:A:443:ILE:O	1:A:591:THR:HG22	2.19	0.42
1:A:594:GLY:O	1:A:595:ASP:C	2.58	0.42
1:B:467:VAL:HG22	1:B:468:SER:N	2.33	0.42
1:C:291:MET:HE1	1:C:294:PHE:HE2	1.85	0.42
1:B:284:LEU:O	1:B:285:ASN:C	2.56	0.42
1:B:523:PRO:C	1:B:524:LEU:HD12	2.40	0.42
1:C:220:VAL:CG1	1:C:221:PRO:N	2.82	0.42
1:C:333:MET:HG3	1:C:334:LEU:N	2.33	0.42
1:C:209:LEU:HD22	3:C:1608:ADP:H2'	2.00	0.42
1:A:483:ARG:NH1	1:A:493:VAL:CG1	2.83	0.42
1:E:244:ASP:OD1	1:E:244:ASP:C	2.58	0.42
1:F:240:ALA:HA	1:F:243:ARG:CZ	2.49	0.42
1:F:579:LEU:O	1:F:583:VAL:CG2	2.46	0.42
1:A:443:ILE:O	1:A:591:THR:HG23	2.20	0.42
1:B:344:THR:HG21	1:B:349:LEU:HD11	2.01	0.42
1:B:361:ARG:C	1:B:363:PRO:HD2	2.40	0.42
1:B:521:LEU:HD23	1:B:521:LEU:HA	1.80	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:411:LEU:HD12	1:E:411:LEU:C	2.40	0.42
1:F:173:LEU:HD22	1:F:176:VAL:HG21	2.02	0.42
1:F:316:LEU:O	1:F:322:PHE:HB2	2.20	0.42
1:C:226:SER:HB3	1:C:229:ASP:CG	2.39	0.42
1:F:422:TYR:CE2	1:F:583:VAL:HG21	2.55	0.42
1:A:436:ASN:HB2	1:A:474:ASP:OD2	2.19	0.41
1:F:420:ILE:H	1:F:420:ILE:HG13	1.63	0.41
1:A:266:GLY:O	1:A:312:LEU:HA	2.20	0.41
1:C:341:GLU:CA	1:C:344:THR:CG2	2.98	0.41
1:D:443:ILE:HG22	1:D:444:SER:N	2.35	0.41
1:E:173:LEU:HD12	1:E:210:LEU:HD22	2.01	0.41
1:F:311:ILE:O	1:F:311:ILE:HG22	2.20	0.41
1:F:589:LYS:C	1:F:591:THR:H	2.23	0.41
1:A:493:VAL:CG1	1:A:494:THR:N	2.83	0.41
1:B:279:GLU:N	1:B:279:GLU:OE2	2.53	0.41
1:C:363:PRO:HG2	1:C:411:LEU:HD13	2.02	0.41
1:C:455:TYR:O	1:C:458:HIS:HB2	2.20	0.41
1:D:193:MET:HB3	1:D:194:PRO:HD2	2.02	0.41
1:E:220:VAL:HG13	1:E:221:PRO:CD	2.51	0.41
1:E:428:ALA:HB1	1:E:597:LEU:CD2	2.50	0.41
1:F:233:LEU:CD2	1:F:241:ARG:NH2	2.84	0.41
1:F:465:TYR:HB2	1:F:466:LEU:H	1.37	0.41
3:F:1607:ADP:H8	3:F:1607:ADP:O5'	2.03	0.41
1:A:349:LEU:HD13	1:A:353:VAL:HG11	2.02	0.41
1:D:401:VAL:CG1	5:D:2013:HOH:O	2.68	0.41
1:E:225:ILE:HG13	1:E:245:LEU:HD22	2.01	0.41
1:F:447:PRO:CA	1:F:450:TYR:CE1	2.90	0.41
1:A:472:LEU:HD22	1:A:507:ILE:HG23	2.02	0.41
1:B:336:ARG:NH2	1:B:590:GLU:OE2	2.50	0.41
1:D:450:TYR:CD2	1:D:450:TYR:O	2.67	0.41
1:F:425:ALA:CB	1:F:579:LEU:CD1	2.99	0.41
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.85	0.41
1:A:220:VAL:HG13	1:A:221:PRO:CD	2.50	0.41
1:B:344:THR:O	1:B:344:THR:CG2	2.68	0.41
1:B:595:ASP:HA	1:B:598:ARG:CB	2.49	0.41
1:C:225:ILE:CG1	1:C:245:LEU:CD1	2.98	0.41
1:C:434:VAL:HG13	1:C:474:ASP:HB3	2.03	0.41
1:A:286:GLN:NE2	1:A:290:GLU:OE2	2.53	0.41
1:B:543:ARG:HB2	1:B:545:TYR:CE2	2.55	0.41
1:C:215:ALA:HB2	1:C:256:ILE:HD12	2.01	0.41
1:C:424:GLU:OE2	1:C:453:LEU:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:LEU:HA	1:E:479:LEU:HD23	1.72	0.41
1:F:201:GLY:O	1:F:307:ASN:HB2	2.20	0.41
1:F:358:ILE:O	1:F:359:ALA:C	2.58	0.41
1:B:499:ASN:ND2	1:B:499:ASN:N	2.68	0.41
1:C:443:ILE:HD12	1:C:586:LEU:CD2	2.51	0.41
1:D:333:MET:N	1:D:590:GLU:OE1	2.52	0.41
1:E:387:ASP:OD2	1:E:387:ASP:N	2.54	0.41
1:E:594:GLY:O	1:E:595:ASP:C	2.59	0.41
1:F:173:LEU:HD22	1:F:303:MET:CE	2.51	0.41
1:F:220:VAL:HG11	1:F:254:PRO:C	2.41	0.41
1:F:510:ASN:HD22	1:F:510:ASN:HA	1.73	0.41
1:F:598:ARG:O	1:F:599:ARG:C	2.59	0.41
1:A:158:VAL:HG23	1:A:213:ALA:HA	2.02	0.41
1:A:417:LYS:HE2	1:A:587:LEU:HD22	2.03	0.41
1:A:432:THR:HG21	1:A:601:LEU:HD23	2.03	0.41
1:A:599:ARG:HE	1:A:599:ARG:HB2	1.58	0.41
1:C:168:GLU:O	1:C:172:GLU:HG3	2.21	0.41
1:C:459:LEU:HD23	1:C:459:LEU:HA	1.93	0.41
1:E:340:LEU:HB3	1:E:355:LEU:HD22	2.03	0.41
1:E:355:LEU:HD23	1:E:355:LEU:HA	1.81	0.41
1:E:428:ALA:HB1	1:E:597:LEU:HD22	2.03	0.41
1:F:267:ARG:CZ	1:F:311:ILE:CD1	2.99	0.41
1:F:311:ILE:O	1:F:311:ILE:HG23	2.21	0.41
1:F:344:THR:O	1:F:345:ARG:C	2.59	0.41
1:F:599:ARG:O	1:F:602:SER:N	2.53	0.41
1:A:476:LEU:HD12	1:A:507:ILE:HD12	2.03	0.41
1:C:185:LYS:HD3	1:C:185:LYS:HA	1.83	0.41
1:C:441:HIS:O	1:C:597:LEU:HD12	2.20	0.41
1:E:441:HIS:CD2	1:E:441:HIS:H	2.39	0.41
1:A:195:LYS:CE	1:A:294:PHE:O	2.69	0.40
1:A:333:MET:HG2	1:A:589:LYS:HA	2.02	0.40
1:B:362:THR:N	1:B:363:PRO:HD2	2.36	0.40
1:B:466:LEU:C	1:B:466:LEU:HD22	2.40	0.40
1:B:483:ARG:NE	5:B:2021:HOH:O	2.34	0.40
1:B:511:MET:HA	1:B:515:LEU:HD12	2.03	0.40
1:B:594:GLY:O	1:B:595:ASP:C	2.58	0.40
1:C:245:LEU:HD23	1:C:246:PHE:CE1	2.56	0.40
1:E:291:MET:HE3	1:E:302:VAL:HG21	1.96	0.40
1:F:262:ILE:HD12	1:F:304:ALA:HB2	1.99	0.40
1:B:230:PHE:O	1:B:233:LEU:CG	2.69	0.40
1:C:413:SER:HB2	1:C:414:PRO:HD2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:GLU:CD	1:D:448:ARG:HG3	2.42	0.40
1:E:198:LEU:O	1:E:325:LYS:HA	2.21	0.40
1:E:483:ARG:CZ	1:E:493:VAL:CG2	2.95	0.40
1:F:581:ASN:CB	1:F:604:GLU:OE2	2.69	0.40
1:A:295:ASP:OD1	1:A:297:LYS:HB2	2.21	0.40
1:A:387:ASP:OD2	1:A:388:LYS:HG3	2.21	0.40
1:B:515:LEU:HB2	1:B:517:MET:HG3	2.03	0.40
1:C:291:MET:HA	1:C:291:MET:CE	2.49	0.40
1:C:329:ASP:OD2	1:C:451:LYS:HE2	2.21	0.40
1:C:445:ILE:HD13	1:C:445:ILE:N	2.36	0.40
1:C:596:GLU:HG3	1:C:599:ARG:HH12	1.87	0.40
1:C:597:LEU:CD2	1:C:601:LEU:HG	2.51	0.40
1:E:413:SER:HA	1:E:414:PRO:HD2	1.95	0.40
1:F:481:GLY:O	1:F:484:ALA:HB3	2.22	0.40
1:B:430:VAL:HG11	1:B:478:ALA:HA	2.02	0.40
1:B:593:GLU:O	1:B:596:GLU:HB3	2.21	0.40
1:C:176:VAL:HG22	1:C:193:MET:HE1	2.03	0.40
1:C:330:PRO:HA	1:C:331:PRO:HD3	1.90	0.40
1:C:589:LYS:O	1:C:590:GLU:CB	2.69	0.40
1:C:593:GLU:CA	5:C:2024:HOH:O	2.64	0.40
1:D:266:GLY:HA2	1:D:284:LEU:HD22	2.04	0.40
1:F:173:LEU:HD12	1:F:210:LEU:HD22	2.03	0.40
1:F:399:ASP:OD1	1:F:399:ASP:N	2.53	0.40
1:F:472:LEU:HD23	1:F:472:LEU:HA	1.94	0.40
1:F:597:LEU:HD13	1:F:597:LEU:HA	1.76	0.40
1:A:586:LEU:HD12	1:A:586:LEU:HA	1.92	0.40
1:E:207:LYS:NZ	1:E:207:LYS:HB2	2.37	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	397/476 (83%)	379 (96%)	13 (3%)	5 (1%)	12 21
1	B	401/476 (84%)	378 (94%)	20 (5%)	3 (1%)	22 39
1	C	413/476 (87%)	393 (95%)	18 (4%)	2 (0%)	29 47
1	D	403/476 (85%)	383 (95%)	19 (5%)	1 (0%)	47 69
1	E	396/476 (83%)	376 (95%)	13 (3%)	7 (2%)	8 15
1	F	402/476 (84%)	372 (92%)	26 (6%)	4 (1%)	15 27
All	All	2412/2856 (84%)	2281 (95%)	109 (4%)	22 (1%)	17 31

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	TYR
1	A	602	SER
1	B	595	ASP
1	D	402	ILE
1	F	450	TYR
1	A	519	GLU
1	F	232	GLU
1	E	267	ARG
1	F	598	ARG
1	A	278	ASP
1	A	601	LEU
1	B	519	GLU
1	C	232	GLU
1	E	161	LYS
1	E	595	ASP
1	E	232	GLU
1	E	519	GLU
1	C	447	PRO
1	E	235	VAL
1	E	402	ILE
1	F	414	PRO
1	B	402	ILE

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	337/390 (86%)	308 (91%)	29 (9%)	10 18
1	B	339/390 (87%)	317 (94%)	22 (6%)	17 30
1	C	349/390 (90%)	312 (89%)	37 (11%)	6 11
1	D	342/390 (88%)	318 (93%)	24 (7%)	15 26
1	E	335/390 (86%)	308 (92%)	27 (8%)	11 21
1	F	340/390 (87%)	305 (90%)	35 (10%)	7 12
All	All	2042/2340 (87%)	1868 (92%)	174 (8%)	10 19

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	ARG
1	A	192	ARG
1	A	220	VAL
1	A	287	LEU
1	A	301	ILE
1	A	311	ILE
1	A	333	MET
1	A	344	THR
1	A	349	LEU
1	A	373	LEU
1	A	399	ASP
1	A	411	LEU
1	A	412	ILE
1	A	413	SER
1	A	431	SER
1	A	434	VAL
1	A	446	ILE
1	A	499	ASN
1	A	503	ARG
1	A	518	SER
1	A	520	GLU
1	A	528	LYS
1	A	542	LEU
1	A	558	LYS
1	A	578	GLN
1	A	591	THR
1	A	597	LEU
1	A	599	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	601	LEU
1	B	156	LYS
1	B	278	ASP
1	B	279	GLU
1	B	281	GLU
1	B	287	LEU
1	B	310	ASP
1	B	311	ILE
1	B	324	LYS
1	B	325	LYS
1	B	345	ARG
1	B	400	ARG
1	B	465	TYR
1	B	466	LEU
1	B	476	LEU
1	B	493	VAL
1	B	499	ASN
1	B	528	LYS
1	B	543	ARG
1	B	551	SER
1	B	578	GLN
1	B	595	ASP
1	B	603	GLU
1	C	156	LYS
1	C	158	VAL
1	C	161	LYS
1	C	162	ASP
1	C	171	GLU
1	C	186	PHE
1	C	189	ILE
1	C	192	ARG
1	C	219	ASN
1	C	229	ASP
1	C	235	VAL
1	C	244	ASP
1	C	265	VAL
1	C	333	MET
1	C	334	LEU
1	C	344	THR
1	C	354	ASN
1	C	372	ASN
1	C	387	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	400	ARG
1	C	434	VAL
1	C	442	ARG
1	C	448	ARG
1	C	451	LYS
1	C	461	GLU
1	C	463	ASP
1	C	465	TYR
1	C	476	LEU
1	C	493	VAL
1	C	499	ASN
1	C	514	GLN
1	C	519	GLU
1	C	520	GLU
1	C	544	ASN
1	C	551	SER
1	C	586	LEU
1	C	597	LEU
1	D	171	GLU
1	D	178	GLU
1	D	220	VAL
1	D	230	PHE
1	D	265	VAL
1	D	281	GLU
1	D	287	LEU
1	D	294	PHE
1	D	307	ASN
1	D	310	ASP
1	D	325	LYS
1	D	333	MET
1	D	361	ARG
1	D	410	LEU
1	D	411	LEU
1	D	434	VAL
1	D	442	ARG
1	D	450	TYR
1	D	465	TYR
1	D	483	ARG
1	D	503	ARG
1	D	578	GLN
1	D	591	THR
1	D	602	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	156	LYS
1	E	192	ARG
1	E	230	PHE
1	E	282	GLN
1	E	287	LEU
1	E	301	ILE
1	E	310	ASP
1	E	311	ILE
1	E	354	ASN
1	E	383	ARG
1	E	388	LYS
1	E	399	ASP
1	E	412	ILE
1	E	416	GLU
1	E	441	HIS
1	E	445	ILE
1	E	476	LEU
1	E	499	ASN
1	E	503	ARG
1	E	519	GLU
1	E	528	LYS
1	E	542	LEU
1	E	574	LYS
1	E	578	GLN
1	E	591	THR
1	E	592	ILE
1	E	600	ILE
1	F	158	VAL
1	F	167	GLU
1	F	217	GLU
1	F	234	PHE
1	F	256	ILE
1	F	281	GLU
1	F	287	LEU
1	F	291	MET
1	F	308	ARG
1	F	310	ASP
1	F	314	PRO
1	F	333	MET
1	F	373	LEU
1	F	374	VAL
1	F	383	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	387	ASP
1	F	399	ASP
1	F	434	VAL
1	F	451	LYS
1	F	465	TYR
1	F	476	LEU
1	F	487	GLU
1	F	493	VAL
1	F	499	ASN
1	F	503	ARG
1	F	518	SER
1	F	519	GLU
1	F	578	GLN
1	F	584	GLU
1	F	586	LEU
1	F	593	GLU
1	F	595	ASP
1	F	596	GLU
1	F	597	LEU
1	F	598	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	HIS
1	A	375	ASN
1	A	499	ASN
1	A	510	ASN
1	B	499	ASN
1	B	514	GLN
1	C	224	HIS
1	C	286	GLN
1	C	354	ASN
1	C	499	ASN
1	C	510	ASN
1	C	514	GLN
1	C	544	ASN
1	D	224	HIS
1	D	307	ASN
1	D	372	ASN
1	D	499	ASN
1	D	510	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	578	GLN
1	E	224	HIS
1	E	286	GLN
1	E	354	ASN
1	E	441	HIS
1	E	499	ASN
1	E	514	GLN
1	F	187	ASN
1	F	307	ASN
1	F	375	ASN
1	F	499	ASN
1	F	510	ASN
1	F	514	GLN
1	F	578	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	$\#\|Z\|>2$
3	ADP	F	1607	4	24,29,29	1.06	3 (12%)	29,45,45	1.42	4 (13%)
3	ADP	D	1608	4	24,29,29	1.11	2 (8%)	29,45,45	1.44	2 (6%)
3	ADP	E	1604	4	24,29,29	1.01	1 (4%)	29,45,45	1.68	4 (13%)
3	ADP	B	1607	4	24,29,29	0.99	0	29,45,45	1.54	5 (17%)
3	ADP	C	1608	4	24,29,29	1.06	3 (12%)	29,45,45	1.42	4 (13%)
3	ADP	A	1604	4	24,29,29	1.10	3 (12%)	29,45,45	1.44	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	F	1607	4	-	4/12/32/32	0/3/3/3
3	ADP	D	1608	4	-	4/12/32/32	0/3/3/3
3	ADP	E	1604	4	-	2/12/32/32	0/3/3/3
3	ADP	B	1607	4	-	3/12/32/32	0/3/3/3
3	ADP	C	1608	4	-	3/12/32/32	0/3/3/3
3	ADP	A	1604	4	-	3/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1604	ADP	O4'-C1'	2.75	1.44	1.41
3	F	1607	ADP	O4'-C1'	2.71	1.44	1.41
3	D	1608	ADP	C2'-C1'	-2.55	1.49	1.53
3	D	1608	ADP	C2-N3	2.49	1.36	1.32
3	E	1604	ADP	C2-N3	2.37	1.35	1.32
3	F	1607	ADP	C2-N3	2.37	1.35	1.32
3	C	1608	ADP	O4'-C1'	2.36	1.44	1.41
3	C	1608	ADP	C2-N3	2.25	1.35	1.32
3	A	1604	ADP	C5-C4	2.17	1.46	1.40
3	C	1608	ADP	C5-C4	2.16	1.46	1.40
3	A	1604	ADP	C2-N3	2.13	1.35	1.32
3	F	1607	ADP	C5-C4	2.08	1.46	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1604	ADP	PA-O3A-PB	-5.79	112.97	132.83
3	A	1604	ADP	PA-O3A-PB	-3.95	119.29	132.83
3	D	1608	ADP	N3-C2-N1	-3.91	122.57	128.68
3	A	1604	ADP	N3-C2-N1	-3.80	122.73	128.68
3	B	1607	ADP	N3-C2-N1	-3.80	122.75	128.68
3	C	1608	ADP	N3-C2-N1	-3.79	122.76	128.68
3	F	1607	ADP	N3-C2-N1	-3.68	122.92	128.68
3	E	1604	ADP	N3-C2-N1	-3.66	122.95	128.68
3	B	1607	ADP	PA-O3A-PB	-3.65	120.30	132.83
3	C	1608	ADP	PA-O3A-PB	-3.63	120.35	132.83
3	D	1608	ADP	PA-O3A-PB	-3.57	120.58	132.83
3	F	1607	ADP	C3'-C2'-C1'	3.38	106.06	100.98
3	E	1604	ADP	C4-C5-N7	-2.64	106.65	109.40
3	F	1607	ADP	C4-C5-N7	-2.53	106.76	109.40
3	A	1604	ADP	C4-C5-N7	-2.40	106.90	109.40
3	E	1604	ADP	O4'-C1'-C2'	-2.37	103.46	106.93
3	B	1607	ADP	C4-C5-N7	-2.35	106.95	109.40
3	B	1607	ADP	C1'-N9-C4	-2.28	122.63	126.64
3	A	1604	ADP	C3'-C2'-C1'	2.25	104.37	100.98
3	C	1608	ADP	C4-C5-N7	-2.24	107.06	109.40
3	F	1607	ADP	PA-O3A-PB	-2.22	125.21	132.83
3	B	1607	ADP	O2A-PA-O1A	2.10	122.62	112.24
3	C	1608	ADP	C3'-C2'-C1'	2.01	104.00	100.98

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1604	ADP	C5'-O5'-PA-O1A
3	A	1604	ADP	C5'-O5'-PA-O2A
3	C	1608	ADP	O4'-C4'-C5'-O5'
3	D	1608	ADP	PA-O3A-PB-O3B
3	F	1607	ADP	C5'-O5'-PA-O1A
3	F	1607	ADP	C5'-O5'-PA-O2A
3	E	1604	ADP	O4'-C4'-C5'-O5'
3	E	1604	ADP	C3'-C4'-C5'-O5'
3	B	1607	ADP	O4'-C4'-C5'-O5'
3	C	1608	ADP	C3'-C4'-C5'-O5'
3	B	1607	ADP	C3'-C4'-C5'-O5'
3	D	1608	ADP	PA-O3A-PB-O1B
3	D	1608	ADP	O4'-C4'-C5'-O5'
3	B	1607	ADP	PA-O3A-PB-O1B
3	C	1608	ADP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	1608	ADP	C3'-C4'-C5'-O5'
3	F	1607	ADP	PA-O3A-PB-O1B
3	A	1604	ADP	C5'-O5'-PA-O3A
3	F	1607	ADP	C5'-O5'-PA-O3A

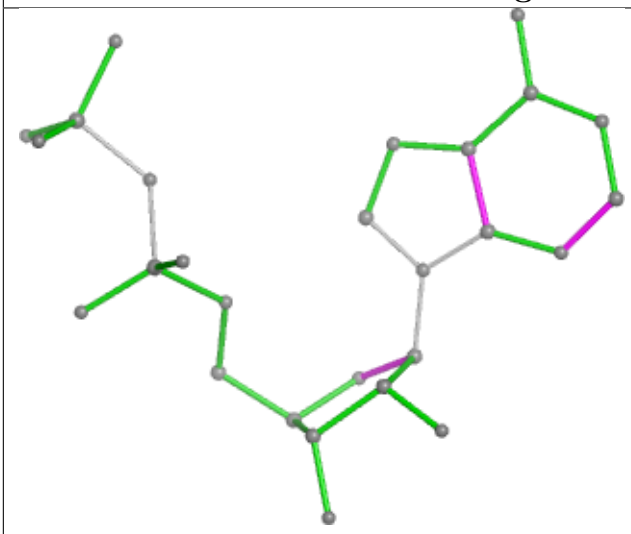
There are no ring outliers.

6 monomers are involved in 36 short contacts:

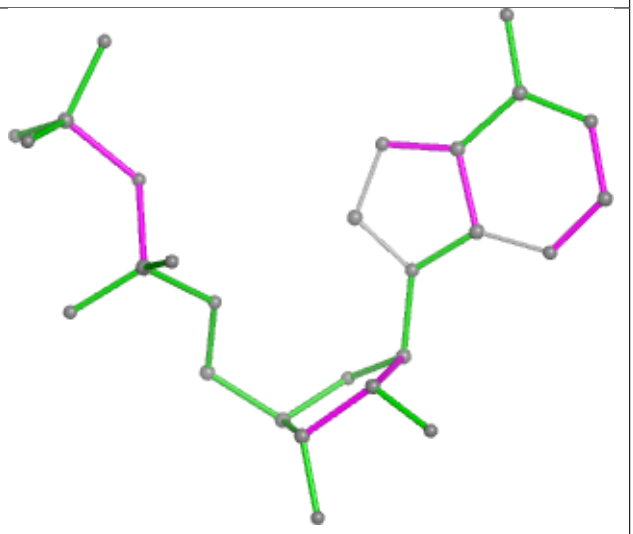
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1607	ADP	5	0
3	D	1608	ADP	6	0
3	E	1604	ADP	7	0
3	B	1607	ADP	7	0
3	C	1608	ADP	10	0
3	A	1604	ADP	1	0

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 then 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.

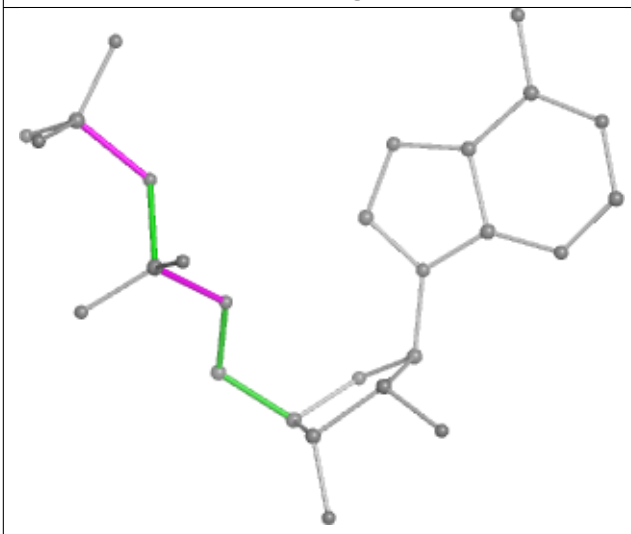
Ligand ADP F 1607



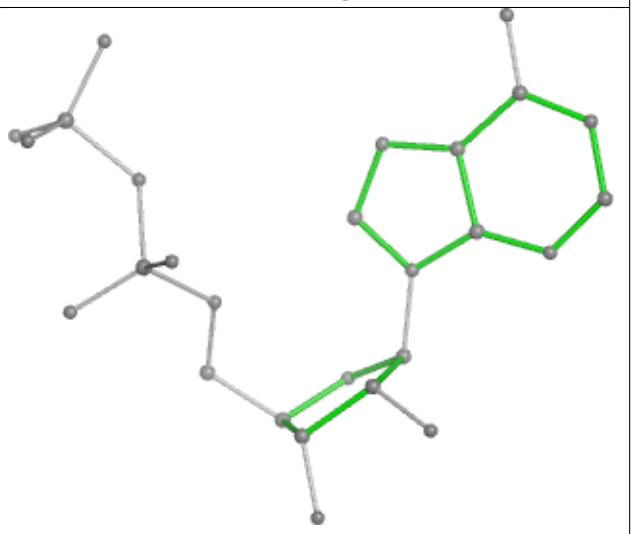
Bond lengths



Bond angles

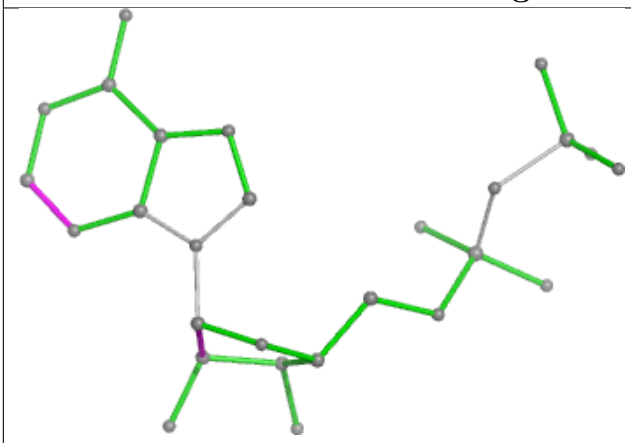


Torsions

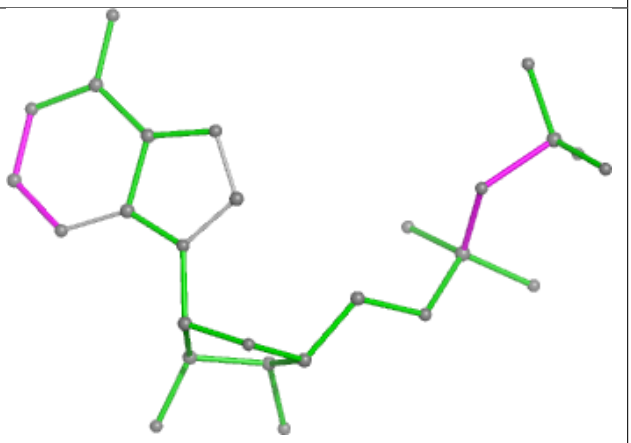


Rings

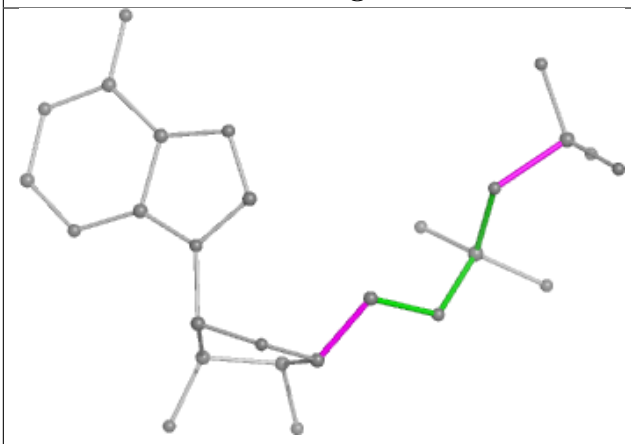
Ligand ADP D 1608



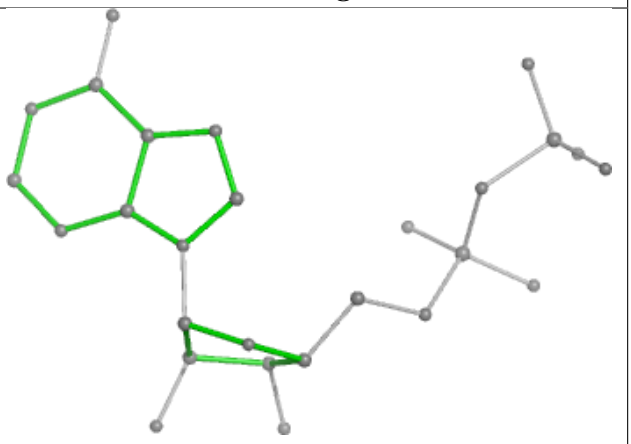
Bond lengths



Bond angles

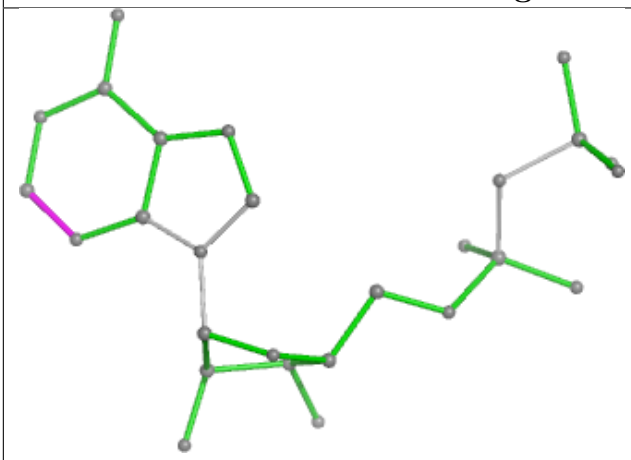


Torsions

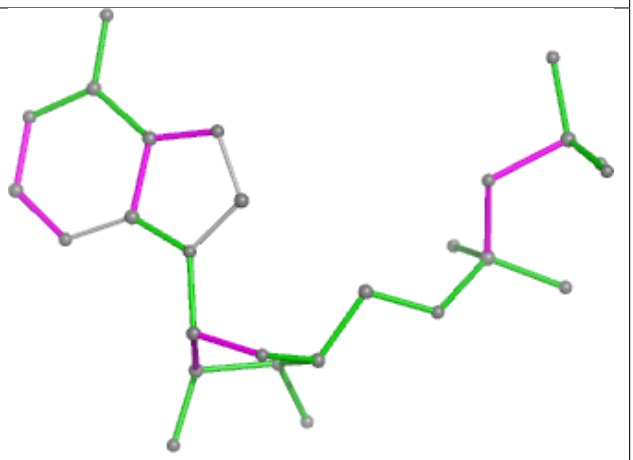


Rings

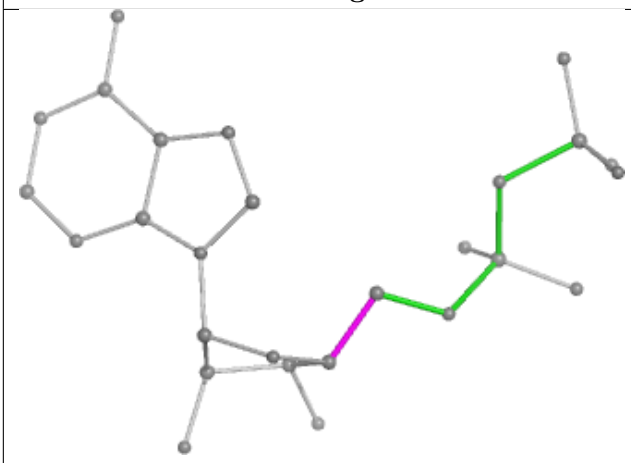
Ligand ADP E 1604



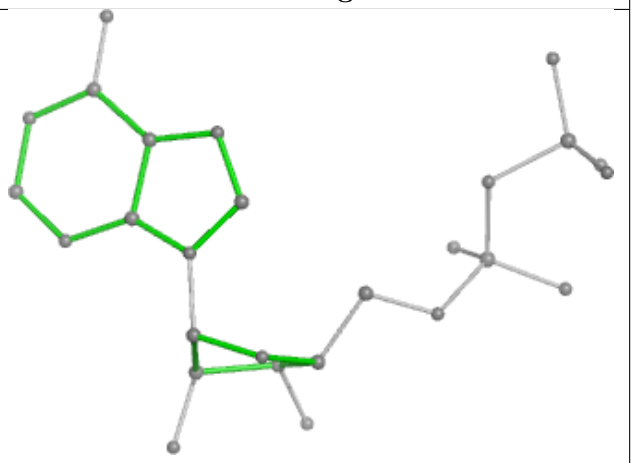
Bond lengths



Bond angles

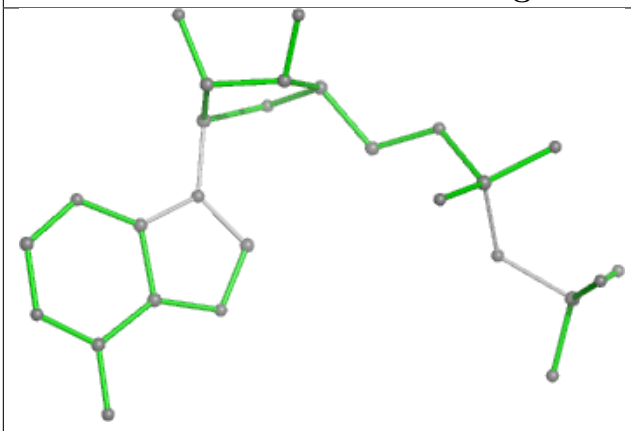


Torsions

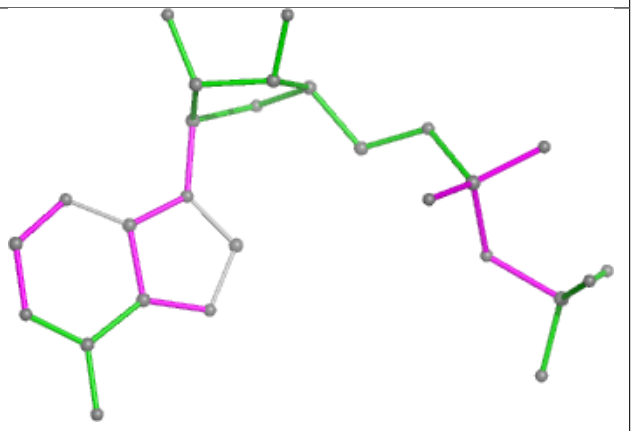


Rings

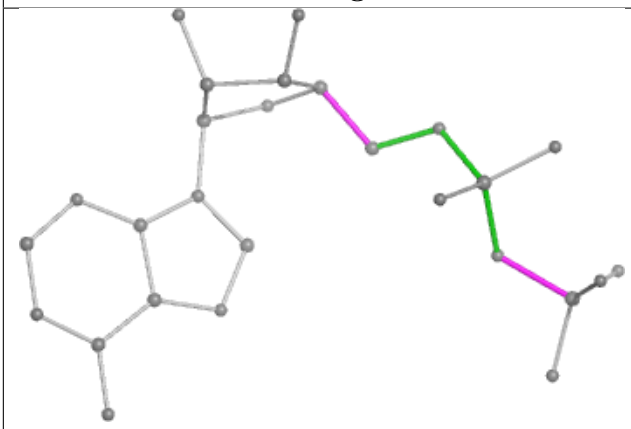
Ligand ADP B 1607



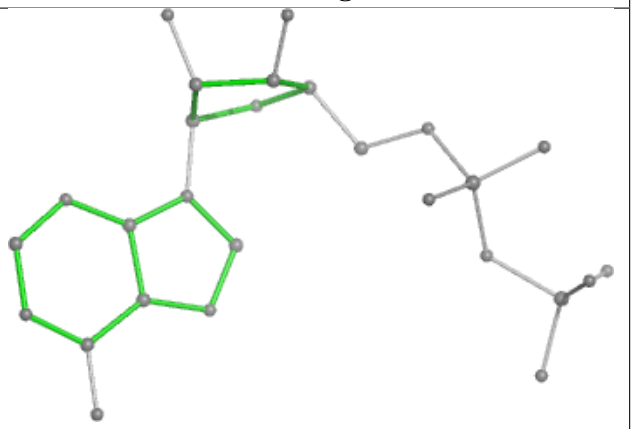
Bond lengths



Bond angles

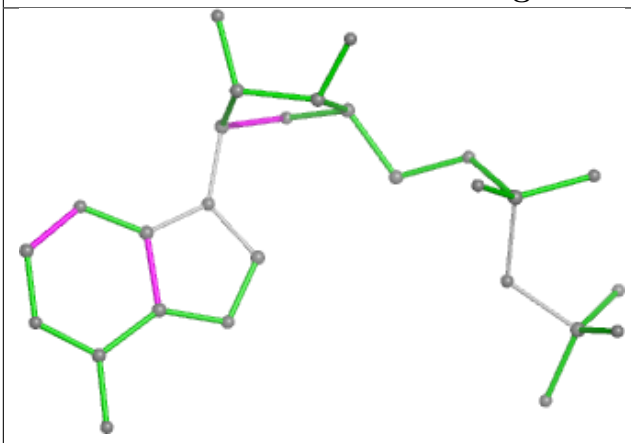


Torsions

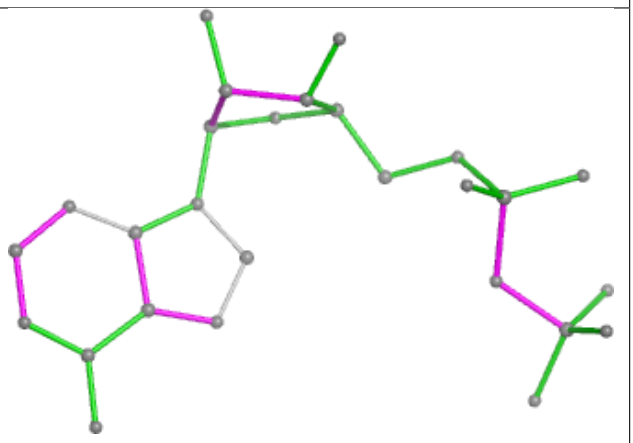


Rings

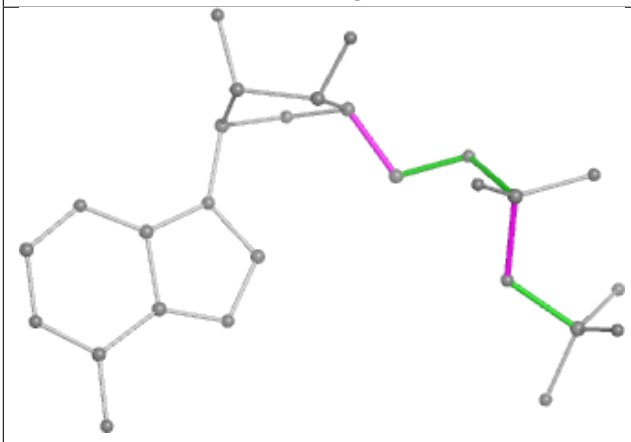
Ligand ADP C 1608



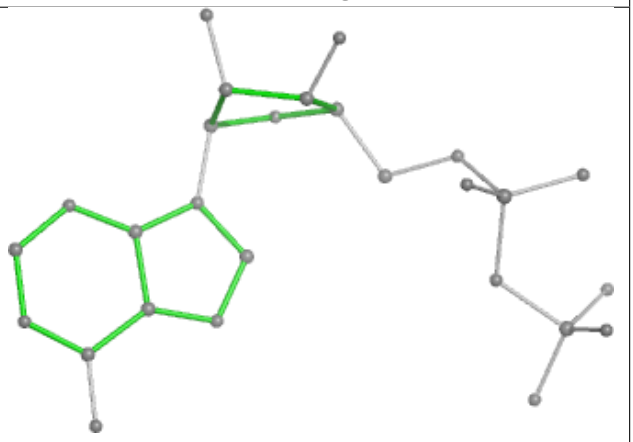
Bond lengths



Bond angles

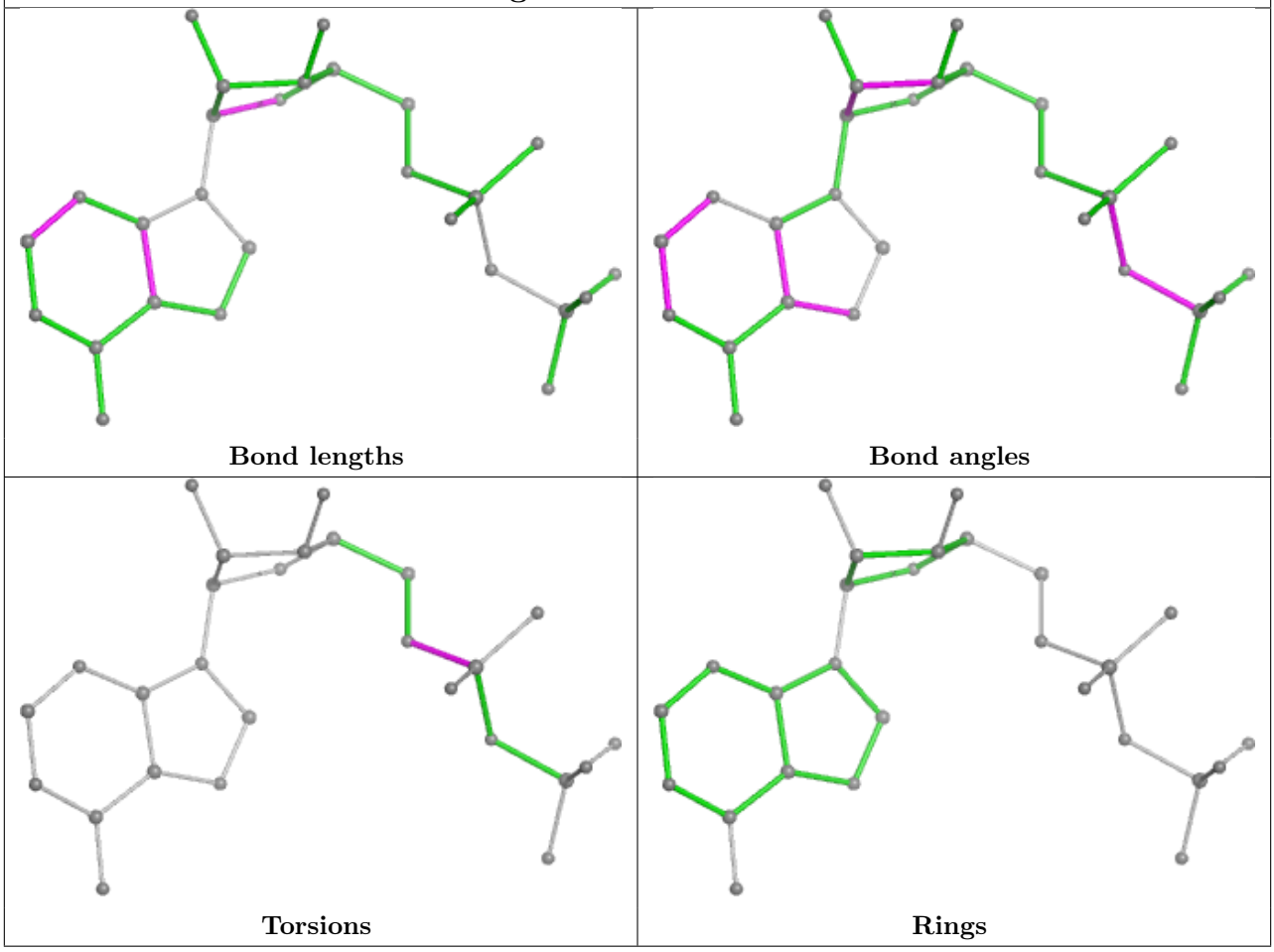


Torsions



Rings

Ligand ADP A 1604



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	407/476 (85%)	0.34	18 (4%) 34 41	35, 44, 54, 66	0
1	B	411/476 (86%)	0.40	31 (7%) 14 17	34, 44, 54, 74	0
1	C	421/476 (88%)	0.95	71 (16%) 1 1	36, 43, 57, 86	0
1	D	413/476 (86%)	0.51	36 (8%) 10 12	35, 44, 56, 78	0
1	E	406/476 (85%)	0.40	31 (7%) 13 16	35, 44, 55, 84	0
1	F	412/476 (86%)	2.31	168 (40%) 0 0	34, 43, 56, 90	0
All	All	2470/2856 (86%)	0.82	355 (14%) 2 2	34, 43, 55, 90	0

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	236	GLY	27.5
1	F	235	VAL	20.7
1	F	230	PHE	14.9
1	C	235	VAL	11.6
1	C	234	PHE	11.0
1	F	153	SER	11.0
1	F	190	GLY	10.8
1	F	299	GLY	10.3
1	F	278	ASP	10.3
1	F	231	VAL	9.6
1	F	251	ALA	9.3
1	C	154	GLY	9.1
1	F	181	LYS	8.7
1	F	219	ASN	8.6
1	F	152	PRO	8.2
1	F	254	PRO	8.2
1	F	237	VAL	8.2
1	F	300	ILE	8.1
1	F	298	GLU	8.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	154	GLY	8.0
1	F	189	ILE	7.9
1	F	232	GLU	7.9
1	F	184	SER	7.8
1	F	228	SER	7.8
1	F	157	ARG	7.7
1	F	182	ASP	7.7
1	C	188	ARG	7.7
1	F	188	ARG	7.7
1	C	236	GLY	7.6
1	F	302	VAL	7.6
1	F	318	ARG	7.3
1	F	222	PHE	7.2
1	C	233	LEU	7.2
1	F	319	PRO	7.1
1	F	161	LYS	7.0
1	F	365	PHE	6.9
1	C	182	ASP	6.9
1	F	186	PHE	6.9
1	F	320	GLY	6.9
1	E	235	VAL	6.7
1	F	313	ASP	6.7
1	B	465	TYR	6.6
1	F	245	LEU	6.5
1	E	232	GLU	6.5
1	E	410	LEU	6.4
1	F	388	LYS	6.4
1	F	238	GLY	6.3
1	F	301	ILE	6.3
1	D	403	ALA	6.2
1	F	253	ALA	6.2
1	F	257	VAL	6.2
1	F	385	GLY	6.2
1	F	164	GLY	6.1
1	F	150	TYR	6.1
1	C	153	SER	5.9
1	F	315	ALA	5.9
1	F	185	LYS	5.9
1	E	155	ASN	5.8
1	F	183	PRO	5.8
1	C	152	PRO	5.8
1	F	255	CYS	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	449	GLY	5.7
1	F	191	ALA	5.6
1	F	229	ASP	5.6
1	C	156	LYS	5.6
1	F	364	GLY	5.6
1	D	465	TYR	5.5
1	C	192	ARG	5.5
1	C	232	GLU	5.5
1	D	441	HIS	5.3
1	F	265	VAL	5.2
1	A	156	LYS	5.2
1	F	233	LEU	5.2
1	E	231	VAL	5.1
1	F	155	ASN	5.0
1	B	402	ILE	5.0
1	B	542	LEU	5.0
1	C	155	ASN	4.9
1	E	154	GLY	4.9
1	F	168	GLU	4.9
1	F	266	GLY	4.8
1	F	357	ILE	4.8
1	B	234	PHE	4.7
1	E	402	ILE	4.7
1	D	319	PRO	4.7
1	F	360	LYS	4.6
1	E	234	PHE	4.5
1	F	304	ALA	4.5
1	D	231	VAL	4.5
1	F	314	PRO	4.4
1	C	250	LYS	4.4
1	F	156	LYS	4.4
1	F	441	HIS	4.4
1	F	310	ASP	4.4
1	F	279	GLU	4.4
1	F	258	PHE	4.3
1	C	150	TYR	4.3
1	F	160	PHE	4.2
1	F	165	GLY	4.2
1	F	192	ARG	4.1
1	F	234	PHE	4.1
1	C	254	PRO	4.1
1	F	334	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	345	ARG	4.1
1	F	387	ASP	4.1
1	D	318	ARG	4.1
1	F	295	ASP	4.0
1	C	157	ARG	4.0
1	F	312	LEU	4.0
1	F	250	LYS	3.9
1	F	281	GLU	3.9
1	F	267	ARG	3.9
1	C	237	VAL	3.9
1	F	264	ALA	3.9
1	C	219	ASN	3.9
1	E	403	ALA	3.9
1	C	228	SER	3.9
1	F	241	ARG	3.8
1	D	450	TYR	3.8
1	F	180	LEU	3.8
1	C	426	GLY	3.8
1	F	401	VAL	3.8
1	C	241	ARG	3.8
1	F	303	MET	3.8
1	C	229	ASP	3.8
1	A	528	LYS	3.8
1	F	167	GLU	3.7
1	F	356	GLU	3.7
1	A	438	GLU	3.7
1	F	293	GLY	3.7
1	D	409	SER	3.7
1	C	448	ARG	3.7
1	F	221	PRO	3.7
1	F	361	ARG	3.6
1	C	181	LYS	3.6
1	B	426	GLY	3.6
1	C	301	ILE	3.6
1	D	281	GLU	3.6
1	B	278	ASP	3.6
1	F	280	ARG	3.6
1	C	191	ALA	3.6
1	F	309	PRO	3.6
1	F	283	THR	3.6
1	A	154	GLY	3.6
1	F	252	HIS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	218	ALA	3.6
1	D	232	GLU	3.5
1	A	153	SER	3.5
1	C	185	LYS	3.5
1	F	151	LYS	3.5
1	F	323	ASP	3.5
1	E	153	SER	3.4
1	D	295	ASP	3.4
1	F	311	ILE	3.4
1	B	404	GLY	3.4
1	B	403	ALA	3.4
1	D	425	ALA	3.4
1	F	329	ASP	3.4
1	F	399	ASP	3.4
1	C	247	ALA	3.4
1	E	528	LYS	3.4
1	C	319	PRO	3.4
1	A	155	ASN	3.3
1	F	381	ALA	3.3
1	C	281	GLU	3.3
1	F	294	PHE	3.3
1	F	363	PRO	3.3
1	F	396	GLU	3.3
1	F	389	ILE	3.3
1	B	405	PRO	3.3
1	C	606	GLU	3.3
1	F	450	TYR	3.3
1	A	426	GLY	3.3
1	F	171	GLU	3.3
1	F	333	MET	3.3
1	F	340	LEU	3.3
1	D	234	PHE	3.2
1	F	247	ALA	3.2
1	F	393	ASP	3.2
1	F	348	PRO	3.2
1	A	402	ILE	3.2
1	D	402	ILE	3.2
1	F	291	MET	3.2
1	E	603	GLU	3.2
1	C	595	ASP	3.1
1	F	327	VAL	3.1
1	C	190	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	425	ALA	3.1
1	C	189	ILE	3.1
1	C	251	ALA	3.1
1	C	465	TYR	3.1
1	A	542	LEU	3.1
1	B	603	GLU	3.1
1	F	224	HIS	3.0
1	C	345	ARG	3.0
1	F	402	ILE	3.0
1	B	235	VAL	3.0
1	F	603	GLU	3.0
1	E	441	HIS	3.0
1	F	223	PHE	3.0
1	B	282	GLN	3.0
1	C	401	VAL	3.0
1	C	441	HIS	3.0
1	C	151	LYS	3.0
1	B	231	VAL	3.0
1	F	308	ARG	3.0
1	F	383	ARG	2.9
1	F	166	ALA	2.9
1	F	292	ASP	2.9
1	D	588	GLU	2.9
1	B	267	ARG	2.8
1	F	465	TYR	2.8
1	F	453	LEU	2.8
1	F	163	VAL	2.8
1	F	595	ASP	2.8
1	F	377	ALA	2.8
1	F	370	LEU	2.8
1	C	320	GLY	2.8
1	F	297	LYS	2.8
1	D	426	GLY	2.8
1	F	214	VAL	2.8
1	B	593	GLU	2.8
1	C	481	GLY	2.8
1	F	342	ILE	2.8
1	F	426	GLY	2.8
1	C	187	ASN	2.7
1	F	296	SER	2.7
1	E	401	VAL	2.7
1	F	211	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	606	GLU	2.7
1	A	282	GLN	2.7
1	C	402	ILE	2.7
1	C	463	ASP	2.7
1	A	346	ASN	2.7
1	C	158	VAL	2.7
1	F	282	GLN	2.7
1	E	236	GLY	2.7
1	F	284	LEU	2.7
1	E	426	GLY	2.6
1	F	328	VAL	2.6
1	B	281	GLU	2.6
1	F	605	PHE	2.6
1	D	519	GLU	2.6
1	F	193	MET	2.6
1	D	542	LEU	2.6
1	F	349	LEU	2.6
1	C	177	VAL	2.6
1	F	286	GLN	2.6
1	E	279	GLU	2.6
1	C	180	LEU	2.6
1	F	425	ALA	2.6
1	C	231	VAL	2.6
1	B	310	ASP	2.6
1	E	387	ASP	2.6
1	D	481	GLY	2.6
1	E	318	ARG	2.6
1	F	162	ASP	2.5
1	B	318	ARG	2.5
1	F	317	LEU	2.5
1	C	226	SER	2.5
1	D	439	PRO	2.5
1	A	603	GLU	2.5
1	C	255	CYS	2.5
1	F	366	VAL	2.5
1	E	304	ALA	2.5
1	F	485	ALA	2.5
1	D	150	TYR	2.5
1	F	179	PHE	2.5
1	F	244	ASP	2.5
1	E	438	GLU	2.4
1	F	217	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	290	GLU	2.4
1	F	438	GLU	2.4
1	B	528	LYS	2.4
1	D	197	ILE	2.4
1	E	542	LEU	2.4
1	D	235	VAL	2.4
1	C	267	ARG	2.4
1	C	167	GLU	2.4
1	C	351	GLU	2.4
1	A	441	HIS	2.4
1	C	243	ARG	2.4
1	D	233	LEU	2.4
1	B	492	ASP	2.4
1	C	295	ASP	2.4
1	F	481	GLY	2.4
1	C	218	ALA	2.3
1	F	249	ALA	2.3
1	D	190	GLY	2.3
1	F	216	GLY	2.3
1	D	188	ARG	2.3
1	F	386	ARG	2.3
1	A	152	PRO	2.3
1	F	205	THR	2.3
1	F	243	ARG	2.3
1	D	237	VAL	2.3
1	B	319	PRO	2.3
1	C	282	GLN	2.3
1	D	438	GLU	2.3
1	F	220	VAL	2.3
1	F	384	GLU	2.3
1	E	346	ASN	2.3
1	B	428	ALA	2.3
1	B	240	ALA	2.3
1	C	323	ASP	2.3
1	C	252	HIS	2.2
1	A	151	LYS	2.2
1	F	491	GLY	2.2
1	B	519	GLU	2.2
1	E	411	LEU	2.2
1	D	308	ARG	2.2
1	F	392	LYS	2.2
1	F	346	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	152	PRO	2.2
1	D	428	ALA	2.2
1	A	235	VAL	2.2
1	E	307	ASN	2.2
1	F	285	ASN	2.2
1	D	423	HIS	2.2
1	C	215	ALA	2.2
1	D	303	MET	2.2
1	B	232	GLU	2.2
1	F	325	LYS	2.2
1	A	277	HIS	2.2
1	E	303	MET	2.2
1	C	603	GLU	2.2
1	F	400	ARG	2.1
1	E	430	VAL	2.1
1	E	233	LEU	2.1
1	B	383	ARG	2.1
1	D	151	LYS	2.1
1	C	221	PRO	2.1
1	F	482	GLY	2.1
1	B	304	ALA	2.1
1	B	150	TYR	2.1
1	E	310	ASP	2.1
1	F	212	ARG	2.1
1	F	172	GLU	2.1
1	B	377	ALA	2.1
1	D	482	GLY	2.1
1	C	462	GLU	2.1
1	C	303	MET	2.1
1	F	263	ASP	2.1
1	B	302	VAL	2.1
1	C	480	LEU	2.1
1	D	189	ILE	2.1
1	C	297	LYS	2.1
1	E	485	ALA	2.1
1	A	401	VAL	2.0
1	C	256	ILE	2.0
1	F	596	GLU	2.0
1	F	187	ASN	2.0
1	F	397	ALA	2.0
1	B	188	ARG	2.0
1	C	519	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

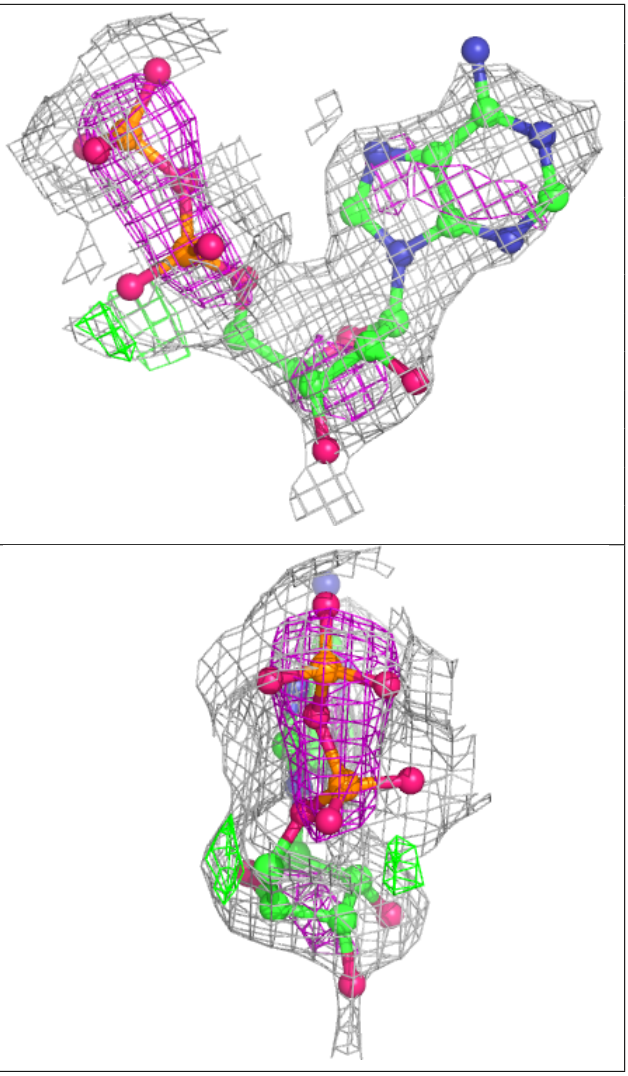
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

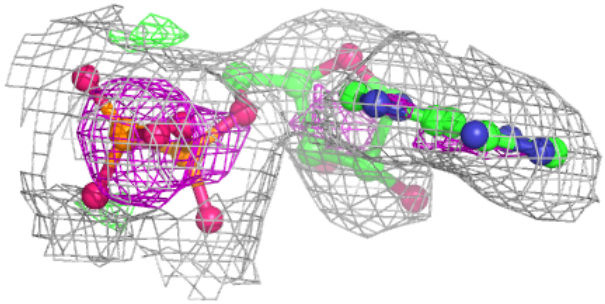
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	C	1609	1/1	0.67	0.14	60,60,60,60	0
4	MG	B	1608	1/1	0.88	0.16	44,44,44,44	0
4	MG	D	1609	1/1	0.90	0.20	41,41,41,41	0
4	MG	E	1605	1/1	0.90	0.20	53,53,53,53	0
3	ADP	F	1607	27/27	0.92	0.23	72,79,80,81	0
3	ADP	C	1608	27/27	0.93	0.24	54,57,59,61	0
4	MG	A	1605	1/1	0.93	0.12	47,47,47,47	0
4	MG	F	1608	1/1	0.95	0.10	68,68,68,68	0
3	ADP	E	1604	27/27	0.97	0.14	34,38,42,48	0
2	ZN	B	1606	1/1	0.97	0.23	64,64,64,64	0
2	ZN	C	1607	1/1	0.97	0.15	60,60,60,60	0
2	ZN	D	1607	1/1	0.97	0.27	79,79,79,79	0
3	ADP	A	1604	27/27	0.97	0.19	32,34,39,41	0
3	ADP	B	1607	27/27	0.97	0.14	20,26,33,37	0
2	ZN	A	1603	1/1	0.97	0.16	63,63,63,63	0
3	ADP	D	1608	27/27	0.97	0.14	21,25,30,31	0
2	ZN	E	1603	1/1	0.98	0.15	63,63,63,63	0
2	ZN	F	1606	1/1	0.98	0.13	69,69,69,69	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 F 1607:

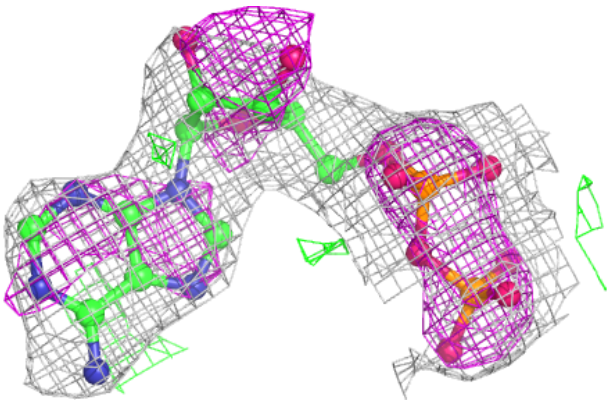
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

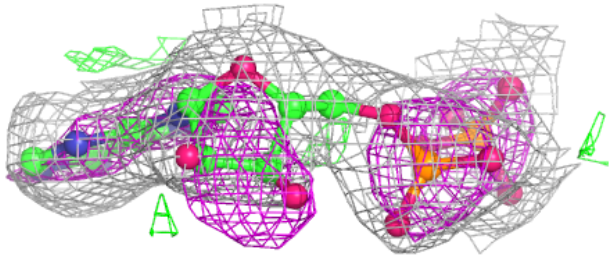


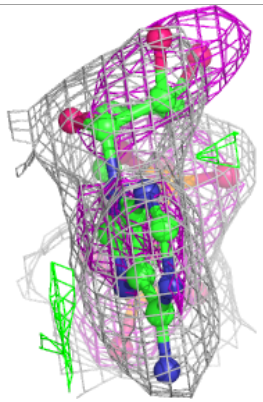


Electron density around ADP C 1608:

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

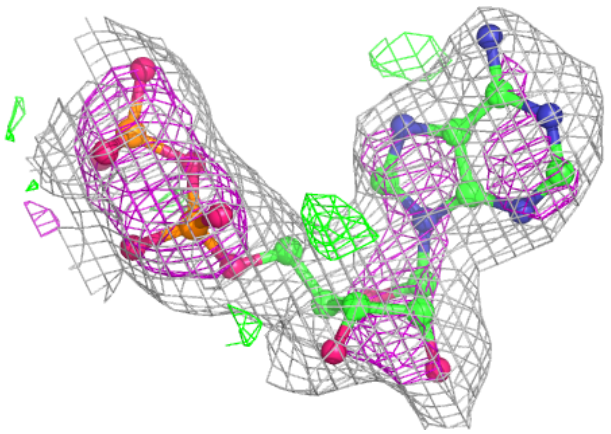


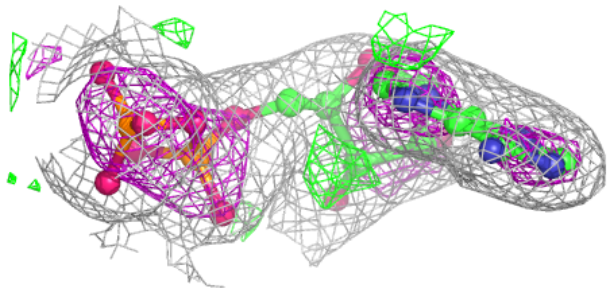


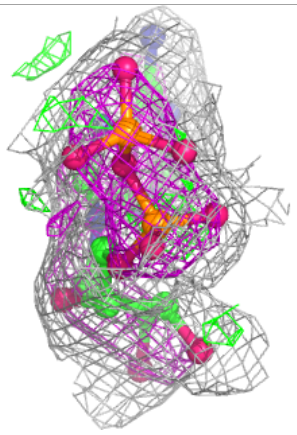


Electron density around ADP E 1604:

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

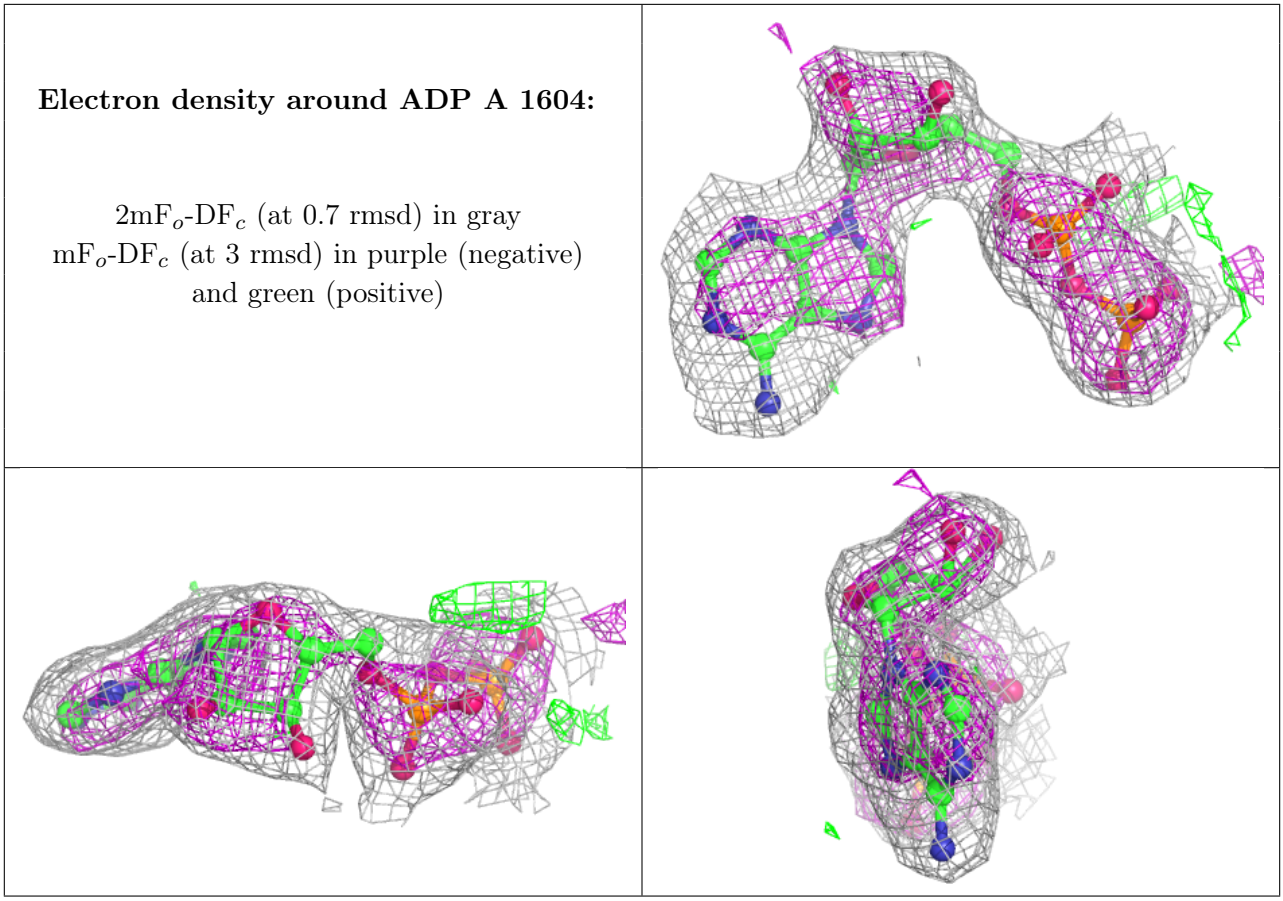






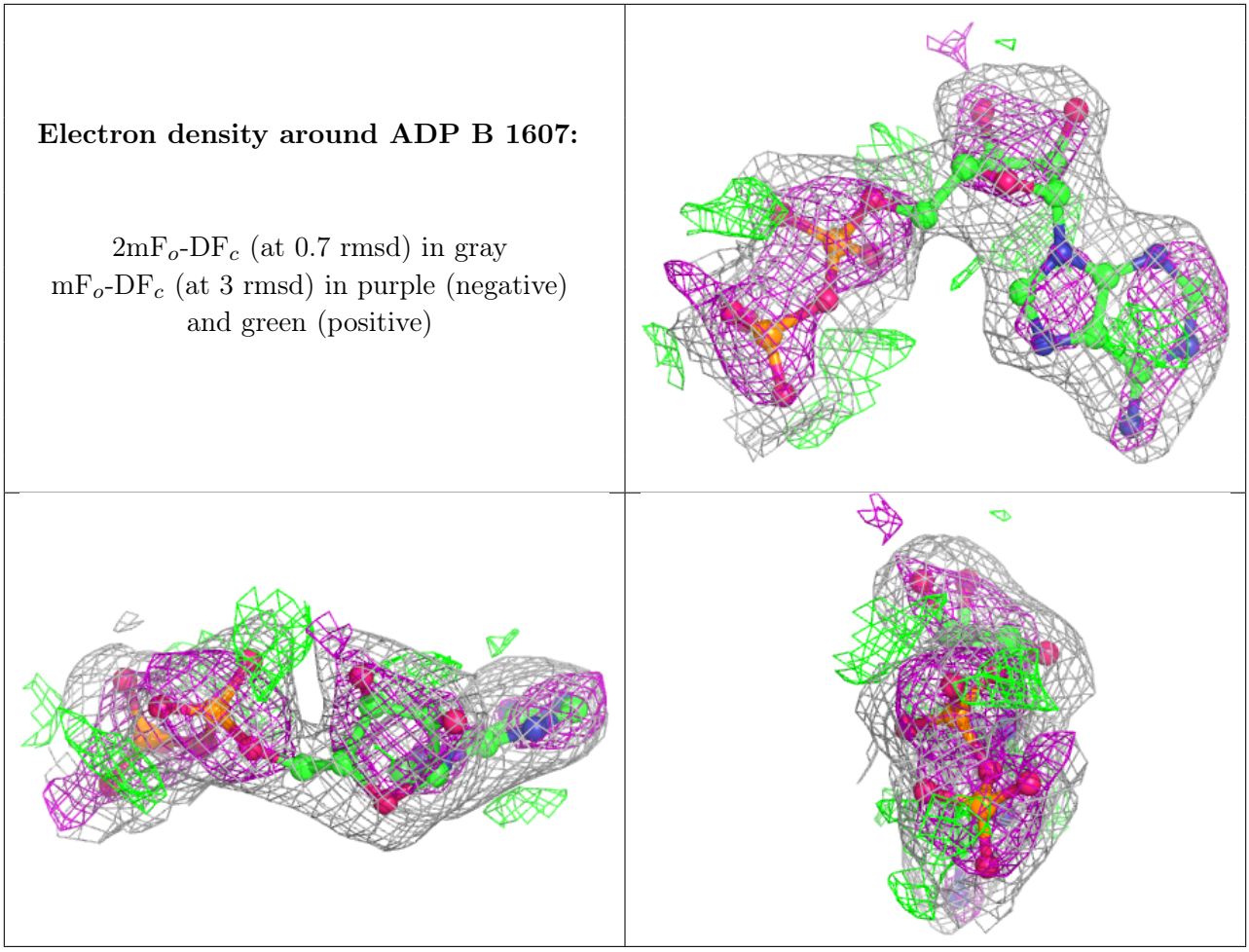
Electron density around ADP A 1604:

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



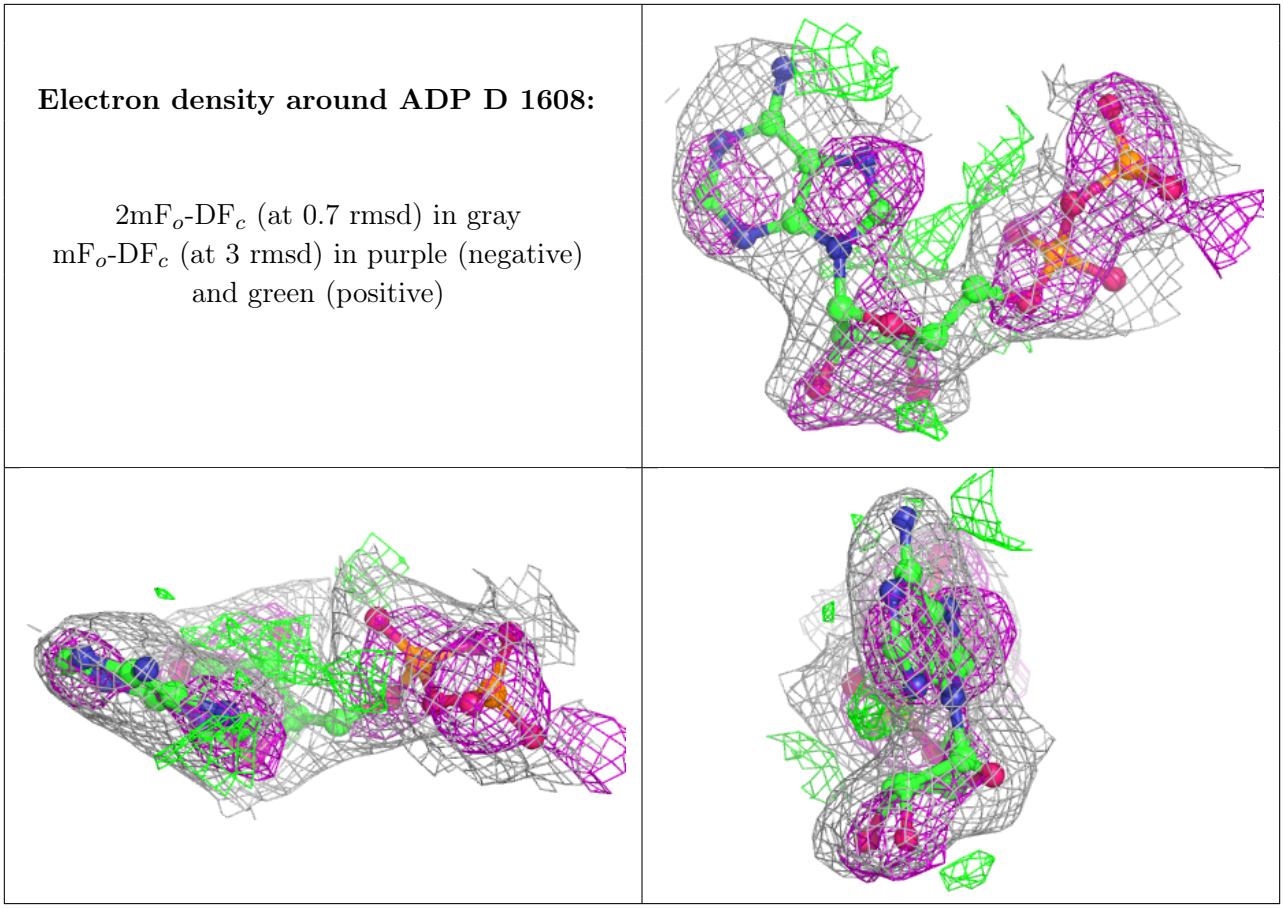
Electron density around ADP B 1607:

$2mF_o$-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 D 1608:

$2mF_o$-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

There are no such residues in this entry.