



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:34 AM UTC

PDB ID : 2CEA / pdb_00002cea
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

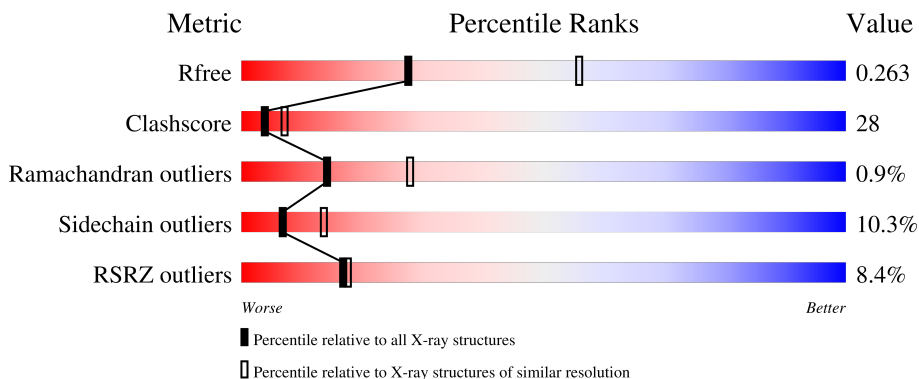
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	476	
1	B	476	
1	C	476	
1	D	476	
1	E	476	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	476	

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

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...

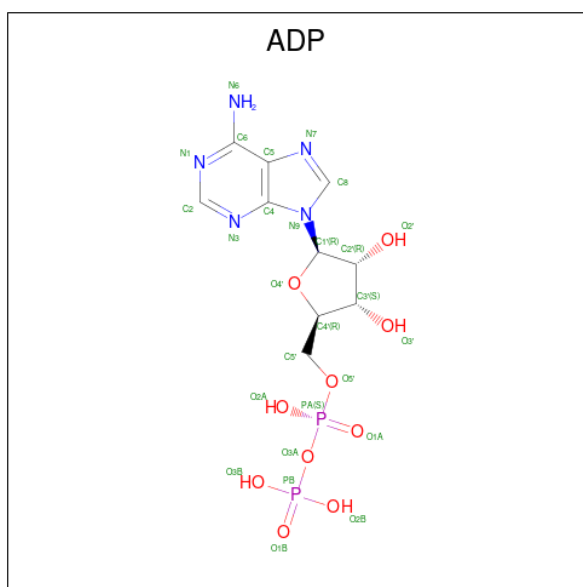
Continued from previous page...

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 (CCD ID: 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 (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
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		

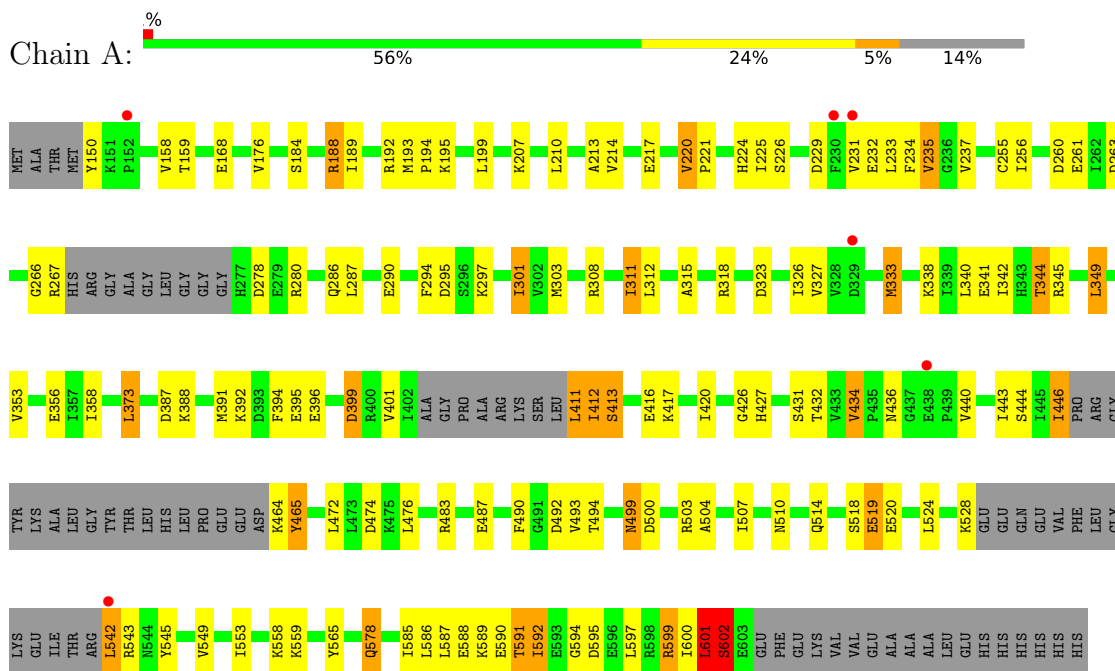
- Molecule 5 is water.

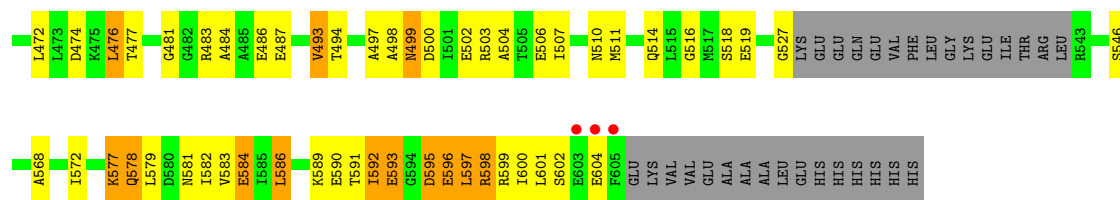
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	46	Total O 46 46	0	0
5	B	35	Total O 35 35	0	0
5	C	26	Total O 26 26	0	0
5	D	34	Total O 34 34	0	0
5	E	34	Total O 34 34	0	0
5	F	24	Total O 24 24	0	0

3 Residue-property plots

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





4 Data and refinement statistics

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 25.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.75) 97.4 (25.00-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.75Å)	Xtrriage
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	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 76.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19564	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.02	3/3202 (0.1%)	0.85	0/4314
1	B	0.96	2/3233 (0.1%)	0.84	3/4356 (0.1%)
1	C	0.77	0/3328	0.79	0/4488
1	D	0.89	0/3256	0.81	1/4388 (0.0%)
1	E	0.94	1/3185 (0.0%)	0.82	3/4291 (0.1%)
1	F	0.73	0/3248	0.77	2/4376 (0.0%)
All	All	0.89	6/19452 (0.0%)	0.81	9/26213 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	602	SER	C-N	-6.96	1.23	1.33
1	A	602	SER	C-N	-6.77	1.23	1.33
1	B	572	ILE	CA-CB	-6.30	1.47	1.54
1	A	440	VAL	CA-CB	-6.03	1.47	1.54
1	B	434	VAL	CA-CB	-5.70	1.46	1.54
1	A	504	ALA	CA-CB	-5.29	1.45	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	PRO	N-CA-CB	7.21	110.93	103.00
1	F	413	SER	CA-C-N	6.76	128.29	119.84
1	F	413	SER	C-N-CA	6.76	128.29	119.84
1	E	511	MET	N-CA-C	-5.64	105.13	111.28
1	E	592	ILE	N-CA-C	5.63	116.48	108.42
1	B	202	PRO	CA-C-N	5.10	125.01	119.76
1	B	202	PRO	C-N-CA	5.10	125.01	119.76
1	D	321	ARG	CB-CA-C	-5.09	109.10	116.54
1	E	445	ILE	N-CA-C	-5.03	107.03	113.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3160	0	3240	128	0
1	B	3191	0	3261	150	0
1	C	3280	0	3346	207	0
1	D	3212	0	3283	128	0
1	E	3144	0	3231	181	0
1	F	3204	0	3270	316	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	10	0
All	All	19564	0	19703	1108	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 28.

All (1108) 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:F:291:MET:HE2	1:F:294:PHE:CE2	1.80	1.15
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:E:291:MET:HE1	1:E:302:VAL:HG21	1.32	1.12
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:F:291:MET:HE2	1:F:294:PHE:HE2	1.02	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:F:447:PRO:C	1:F:450:TYR:CE1	2.37	1.03
1:D:291:MET:HE1	1:D:302:VAL:HG21	1.34	1.02
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:E:231:VAL:C	1:E:232:GLU:HG2	1.86	1.00
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:F:391:MET:HE3	1:F:395:GLU:OE2	1.63	0.99
1:F:447:PRO:C	1:F:450:TYR:HE1	1.71	0.98
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:308:ARG:HG2	1:F:311:ILE:HD12	1.45	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:446:ILE:C	1:A:446:ILE:HD12	1.97	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:E:231:VAL:HG12	1:E:232:GLU:CD	1.97	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:E:157:ARG:HH21	1:E:216:GLY:C	1.82	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:380:LEU:HA	1:D:383:ARG:HH12	1.38	0.86
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:A:373:LEU:HD12	1:A:373:LEU:C	2.00	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: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: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: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:B:479:LEU:HD11	1:B:503:ARG:HG2	1.63	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:307:ASN:HD22	1:D:307:ASN:C	1.88	0.81
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: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:E:246:PHE:HZ	1:E:291:MET:HE3	1.48	0.78
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:F:357:ILE:HG21	1:F:391:MET:HE1	1.64	0.78
1:D:438:GLU:OE2	1:D:439:PRO:HD2	1.84	0.78
1:F:591:THR:C	1:F:592:ILE:HD12	2.09	0.77
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: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:F:308:ARG:CG	1:F:311:ILE:HD12	2.14	0.76
1:D:291:MET:HE1	1:D:302:VAL:CG2	2.15	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:LEU:C	1:C:287:LEU:HD23	2.11	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:D:224:HIS:C	1:D:225:ILE:HD13	2.11	0.75
1:E:220:VAL:HG13	1:E:255:CYS:HA	1.66	0.75
1:E:231:VAL:C	1:E:232:GLU:CG	2.56	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:A:220:VAL:HG11	1:A:255:CYS:HA	1.67	0.75
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:F:162:ASP:C	1:F:342:ILE:HD13	2.13	0.74
1:F:287:LEU:C	1:F:287:LEU:CD2	2.60	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:C:373:LEU:HD23	1:C:373:LEU:C	2.13	0.74
1:D:225:ILE:HD13	1:D:225:ILE:N	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:E:291:MET:HE1	1:E:302:VAL:CG2	2.16	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:291:MET:HE1	1:C:302:VAL:HG11	1.70	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:B:542:LEU:C	1:B:542:LEU:HD23	2.14	0.72
1:E:469:ARG:NH1	1:E:517:MET:O	2.22	0.72
1:D:291:MET:CE	1:D:302:VAL:HG21	2.16	0.72
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:F:287:LEU:HD23	1:F:287:LEU:C	2.14	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: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: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:235:VAL:O	1:C:235:VAL:HG12	1.89	0.71
1:F:333:MET:HG3	1:F:334:LEU:HD23	1.70	0.71
1:C:444:SER:C	1:C:445:ILE:HD13	2.15	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:450:TYR:C	1:D:450:TYR:CD2	2.69	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:MET:CE	1:E:302:VAL:HG21	2.15	0.70
1:C:231:VAL:O	1:C:232:GLU:CB	2.39	0.70
1:C:291:MET:HA	1:C:291:MET:HE2	1.74	0.70
1:D:310:ASP:OD2	1:D:310:ASP:N	2.24	0.70
1:F:391:MET:CE	1:F:395:GLU:OE2	2.38	0.70
1:D:294:PHE:CD1	1:D:294:PHE:C	2.69	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:E:246:PHE:CZ	1:E:291:MET:HE3	2.25	0.70
1:C:593:GLU:C	5:C:2024:HOH:O	2.21	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
1:D:486:GLU:OE1	5:D:2020:HOH:O	2.10	0.69
1:D:195:LYS:HD2	1:D:320:GLY:O	1.93	0.69
1:C:224:HIS:C	1:C:224:HIS:CD2	2.71	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:F:197:ILE:HD12	1:F:303:MET:HE2	1.74	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:F:182:ASP:OD1	1:F:184:SER:OG	2.12	0.68
1:B:466:LEU:CD2	1:B:466:LEU:C	2.67	0.68
1:C:192:ARG:O	1:C:192:ARG:HG3	1.92	0.68
1:D:298:GLU:O	1:D:298:GLU: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:C:519:GLU:C	5:C:2018:HOH:O	2.30	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ASN:ND2	1:B:357:ILE:HD12	2.09	0.67
1:B:207:LYS:HZ2	3:B:1607:ADP:PB	2.17	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: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
1:A:446:ILE:C	1:A:446:ILE:CD1	2.68	0.66
1:B:570:GLU:HG2	5:B:2031:HOH:O	1.95	0.66
1:F:166:ALA:O	1:F:170:ILE:HG13	1.95	0.66
1:F:597:LEU:HD12	1:F:597:LEU:C	2.21	0.66
1:C:220:VAL:HG13	1:C:221:PRO:CD	2.26	0.66
1:C:287:LEU:C	1:C:287:LEU:CD2	2.69	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:A:510:ASN:ND2	1:A:514:GLN:CD	2.54	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: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:C:284:LEU:HD12	1:C:284:LEU:C	2.21	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:465:TYR:C	5:F:2008:HOH:O	2.41	0.64
1:F:527:GLY:O	5:F:2018:HOH:O	2.15	0.64
1:B:279:GLU:O	1:B:283:THR:OG1	2.15	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:594:GLY:C	1:B:596:GLU:N	2.56	0.64
1:F:180:LEU:CD2	1:F:301:ILE:HD11	2.27	0.63
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:499:ASN:ND2	1:B:500:ASP:N	2.47	0.63
1:B:577:LYS:HB2	1:B:577:LYS:HZ2	1.64	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:B:224:HIS:C	1:B:225:ILE:HD13	2.24	0.63
1:B:594:GLY:C	1:B:596:GLU:H	2.07	0.63
1:C:225:ILE:HG13	1:C:245:LEU:CD1	2.28	0.63
1:E:287:LEU:C	1:E:287:LEU:CD2	2.72	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:E:354:ASN:C	1:E:354:ASN:HD22	2.07	0.63
1:F:307:ASN:OD1	1:F:307:ASN:O	2.17	0.63
1:F:391:MET:HG3	1:F:395:GLU:CD	2.24	0.63
1:F:413:SER:OG	1:F:416:GLU:CD	2.41	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:591:THR:C	1:E:592:ILE:CG2	2.73	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:E:287:LEU:C	1:E:287:LEU:HD23	2.24	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:E:591:THR:C	1:E:592:ILE:HG22	2.26	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
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:B:483:ARG:NH1	1:B:493:VAL:HG11	2.16	0.60
1:C:291:MET:HE2	1:C:294:PHE:HE2	1.67	0.60
1:A:231:VAL:O	1:A:232:GLU:HB2	2.02	0.60
1:A:600:ILE:C	1:A:602:SER:H	2.09	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:267:ARG:O	1:E:268:HIS:C	2.45	0.60
1:E:594:GLY:C	1:E:596:GLU:N	2.58	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:A:599:ARG:O	1:A:602:SER:N	2.35	0.59
1:C:333:MET:C	1:C:333:MET:SD	2.84	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: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:E:594:GLY:C	1:E:596:GLU:H	2.10	0.59
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:F:416:GLU:O	1:F:417:LYS:C	2.46	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:C:445:ILE:HG22	1:C:445:ILE:O	2.03	0.58
1:F:286:GLN:HA	1:F:286:GLN:NE2	2.19	0.58
1:E:402:ILE:O	1:E:403:ALA:HB2	2.04	0.58
1:B:333:MET:HE2	1:B:589:LYS:O	2.04	0.58
1:E:490:PHE:C	1:E:492:ASP:H	2.12	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:PHE:O	1:B:233:LEU:HG	2.03	0.58
1:C:464:LYS:NZ	1:C:471:GLU:CD	2.62	0.58
1:E:438:GLU:O	1:E:439:PRO:C	2.47	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:F:233:LEU:HD21	1:F:241:ARG:NH1	2.19	0.58
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'	2.39	0.57
3:D:1608:ADP:H8	3:D:1608:ADP:C5'	2.17	0.57
1:F:357:ILE:CG2	1:F:391:MET:HE1	2.32	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
1:A:333:MET:HE1	1:A:356:GLU:HG3	1.85	0.57
1:B:313:ASP:C	1:B:313:ASP:OD1	2.47	0.57
1:B:542:LEU:HD23	1:B:543:ARG:N	2.19	0.57
1:B:344:THR:O	1:B:345:ARG:C	2.48	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:A:601:LEU:O	1:A:602:SER:C	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:354:ASN:C	1:C:354:ASN:HD22	2.13	0.56
1:C:464:LYS:NZ	1:C:471:GLU:OE2	2.38	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: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:D:284:LEU:O	1:D:285:ASN:C	2.48	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:A:578:GLN:CD	1:A:578:GLN:H	2.14	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:LEU:C	1:B:466:LEU:HD23	2.31	0.54
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:A:340:LEU:O	1:A:341:GLU:C	2.51	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:F:391:MET:HE3	1:F:395:GLU:CD	2.32	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:D:589:LYS:C	1:D:591:THR:H	2.15	0.54
1:F:233:LEU:CD2	1:F:241:ARG:CZ	2.86	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: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
1:F:414:PRO:HA	1:F:417:LYS:HB2	1.90	0.53
1:A:373:LEU:C	1:A:373:LEU:CD1	2.74	0.53
1:B:168:GLU:OE1	1:B:168:GLU:N	2.40	0.53
1:F:233:LEU:CD1	1:F:238:GLY:CA	2.85	0.53
1:C:438:GLU:O	1:C:439:PRO:C	2.52	0.53
1:E:366:VAL:O	1:E:367:GLY:C	2.51	0.53
1:F:278:ASP:O	1:F:279:GLU:C	2.52	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:C:597:LEU:CD2	1:C:597:LEU:C	2.81	0.53
1:D:185:LYS:HZ2	1:D:188:ARG:HH22	1.56	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:434:VAL:HG13	1:B:474:ASP:CG	2.34	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
3:C:1608:ADP:H8	3:C:1608:ADP:H5'1	1.73	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:F:173:LEU:HD22	1:F:303:MET:HE1	1.91	0.53
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: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:391:MET:O	1:B:395:GLU:HG3	2.08	0.52
1:D:185:LYS:NZ	1:D:188:ARG:HH22	2.08	0.52
1:A:199:LEU:HD11	1:A:303:MET:CE	2.40	0.52
1:C:311:ILE:O	1:C:311:ILE:HG22	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:ARG:HH21	1:D:311:ILE:HD12	1.75	0.52
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:D:185:LYS:HD2	1:D:185:LYS:C	2.35	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:D:446:ILE:O	1:D:447:PRO:C	2.50	0.51
1:E:582:ILE:HD13	1:E:597:LEU:HD11	1.87	0.51
1:B:195:LYS:NZ	5:B:2003:HOH:O	2.44	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:F:260:ASP:O	1:F:261:GLU:C	2.53	0.51
1:D:188:ARG:HB3	1:D:188:ARG:HH11	1.76	0.51
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:E:523:PRO:C	1:E:524:LEU:HD12	2.36	0.50
1:A:434:VAL:HG13	1:A:474:ASP:HB3	1.89	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:168:GLU:H	1:A:168:GLU:CD	2.18	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:D:333:MET:HG3	1:D:334:LEU:N	2.27	0.50
1:C:430:VAL:HG11	1:C:477:THR:HG22	1.93	0.50
1:D:280:ARG:O	1:D:281:GLU:C	2.52	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:354:ASN:OD1	1:B:354:ASN:C	2.55	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:F:497:ALA:O	1:F:498:ALA:C	2.54	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:167:GLU:H	1:C:167:GLU:CD	2.15	0.49
1:C:518:SER:OG	1:C:521:LEU:HB2	2.11	0.49
1:E:160:PHE:C	1:E:162:ASP:H	2.18	0.49
1:E:295:ASP:OD1	1:E:295:ASP:C	2.52	0.49
1:F:160:PHE:CE1	1:F:217:GLU:HG2	2.47	0.49
1:F:182:ASP:OD2	1:F:185:LYS:CG	2.57	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:B:224:HIS:O	1:B:225:ILE:HD13	2.11	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:B:542:LEU:C	1:B:542:LEU:CD2	2.85	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:344:THR:O	1:A:345:ARG:C	2.56	0.49
1:C:156:LYS:H	1:C:156:LYS:HE3	1.76	0.49
1:F:228:SER:HB3	1:F:261:GLU:CD	2.37	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:E:291:MET:HE2	1:E:294:PHE:HE2	1.77	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:F:206:GLY:CA	3:F:1607:ADP:N7	2.76	0.48
1:C:195:LYS:HB3	1:C:294:PHE:CZ	2.48	0.48
1:D:246:PHE:HZ	1:D:291:MET:HE3	1.78	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
1:C:441:HIS:C	1:C:597:LEU:HD12	2.39	0.48
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: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:442:ARG:NH2	1:C:451:LYS:HZ3	2.12	0.48
1:C:499:ASN:ND2	1:C:500:ASP:N	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:246:PHE:CZ	1:D:291:MET:HE3	2.50	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:F:202:PRO:HA	1:F:307:ASN:HD22	1.75	0.47
1:F:332:ASP:C	1:F:332:ASP:OD1	2.57	0.47
1:A:338:LYS:O	1:A:342:ILE:HG13	2.14	0.47
1:D:344:THR:O	1:D:345:ARG:C	2.58	0.47
1:E:413:SER:O	1:E:414:PRO:C	2.56	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:A:594:GLY:O	1:A:595:ASP:C	2.58	0.47
1:B:266:GLY:HA2	1:B:284:LEU:HD13	1.96	0.47
1:C:226:SER:HB3	1:C:229:ASP:CG	2.39	0.47
1:D:230:PHE:N	1:D:230:PHE:HD1	2.13	0.47
1:E:260:ASP:O	1:E:261:GLU:C	2.57	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:B:523:PRO:C	1:B:524:LEU:HD12	2.40	0.47
1:C:479:LEU:HD23	1:C:479:LEU:HA	1.83	0.47
1:C:602:SER:O	1:C:606:GLU:HB2	2.15	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ASN:HD22	1:A:500:ASP:H	1.63	0.47
1:B:284:LEU:O	1:B:285:ASN:C	2.56	0.47
1:E:244:ASP:OD1	1:E:244:ASP:C	2.58	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:361:ARG:C	1:B:363:PRO:HD2	2.40	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:E:411:LEU:HD12	1:E:411:LEU:C	2.40	0.46
1:C:224:HIS:C	1:C:224:HIS:HD2	2.21	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:F:589:LYS:C	1:F:591:THR:H	2.23	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: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:353:VAL:O	1:E:353:VAL:HG12	2.14	0.46
1:F:220:VAL:HG11	1:F:254:PRO:C	2.41	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: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:F:358:ILE:O	1:F:359:ALA:C	2.58	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:E:594:GLY:O	1:E:595:ASP:C	2.59	0.46
1:F:598:ARG:O	1:F:599:ARG:C	2.59	0.46
1:B:231:VAL:O	1:B:232:GLU:CB	2.49	0.45
1:B:466:LEU:C	1:B:466:LEU:HD22	2.40	0.45
1:D:178:GLU:OE2	1:D:178:GLU:N	2.49	0.45
1:D:307:ASN:ND2	1:D:307:ASN:C	2.62	0.45
1:E:434:VAL:O	1:E:434:VAL:HG12	2.16	0.45
1:F:173:LEU:HD13	1:F:303:MET:HE1	1.99	0.45
1:F:344:THR:O	1:F:345:ARG:C	2.59	0.45
1:B:594:GLY:O	1:B:595:ASP:C	2.58	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: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:464:LYS:HZ3	1:C:471:GLU:CD	2.23	0.45
1:C:509:ARG:HD2	5:C:2016:HOH:O	2.15	0.45
1:D:424:GLU:CD	1:D:448:ARG:HG3	2.42	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: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: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:591:THR:C	1:A:592:ILE:CG2	2.90	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:A:235:VAL:O	1:A:235:VAL:HG12	2.16	0.45
1:A:260:ASP:O	1:A:261:GLU:C	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LYS:HE3	3:C:1608:ADP:PB	2.57	0.45
1:E:160:PHE:C	1:E:162:ASP:N	2.70	0.45
1:F:438:GLU:O	1:F:439:PRO:C	2.59	0.45
1:F:499:ASN:HD22	1:F:499:ASN:N	2.14	0.45
1:B:430:VAL:CG1	1:B:478:ALA:HA	2.47	0.45
1:C:176:VAL:HG22	1:C:193:MET:HE1	1.98	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:C:291:MET:HE1	1:C:302:VAL:CG1	2.44	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:A:199:LEU:HD23	1:A:326:ILE:HB	1.98	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:193:MET:HE3	1:B:194:PRO:HD2	2.00	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:F:446:ILE:C	1:F:450:TYR:HE1	2.25	0.44
1:A:391:MET:O	1:A:395:GLU:HG3	2.17	0.44
1:A:600:ILE:C	1:A:602:SER:N	2.75	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:291:MET:HE2	1:D:291:MET:HA	2.00	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
1:A:476:LEU:HD12	1:A:476:LEU:HA	1.82	0.44
1:A:490:PHE:C	1:A:492:ASP:H	2.26	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:F:366:VAL:O	1:F:367:GLY:C	2.59	0.44
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:D:434:VAL:HG23	1:D:567:ARG:NH2	2.34	0.43
1:E:598:ARG:O	1:E:599:ARG:C	2.58	0.43
1:F:225:ILE:HG13	1:F:245:LEU:CD2	2.35	0.43
1:F:244:ASP:OD1	1:F:244:ASP:C	2.61	0.43
1:F:441:HIS:O	1:F:593:GLU:HA	2.17	0.43
1:B:400:ARG:O	1:B:401:VAL:C	2.61	0.43
1:B:543:ARG:HB2	1:B:545:TYR:CZ	2.52	0.43
1:C:291:MET:HE2	1:C:294:PHE:CE2	2.50	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:E:490:PHE:C	1:E:492:ASP:N	2.76	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:373:LEU:C	1:C:373:LEU:CD2	2.84	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:294:PHE:CD1	1:B:294:PHE:C	2.96	0.43
1:B:413:SER:OG	1:B:416:GLU:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:GLN:O	1:B:582:ILE:HG13	2.18	0.43
1:C:183:PRO:O	1:C:187:ASN:CG	2.61	0.43
1:E:239:ALA:HB1	1:E:286:GLN:HE21	1.84	0.43
1:E:354:ASN:C	1:E:354:ASN:ND2	2.76	0.43
1:F:226:SER:O	1:F:230:PHE:CD1	2.72	0.43
1:F:356:GLU:O	1:F:357:ILE:C	2.62	0.43
1:A:578:GLN:CD	1:A:578:GLN:N	2.76	0.43
1:B:205:THR:HA	5:B:2004:HOH:O	2.19	0.43
1:B:333:MET:HE1	1:B:589:LYS:HA	2.00	0.43
1:D:220:VAL:HG22	1:D:254:PRO:O	2.18	0.43
1:D:286:GLN:O	1:D:287:LEU:C	2.61	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
1:F:499:ASN:ND2	1:F:499:ASN:N	2.67	0.43
1:F:511:MET:HE2	1:F:511:MET:HB3	1.86	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:E:253:ALA:HA	1:E:254:PRO:C	2.44	0.43
1:F:206:GLY:N	3:F:1607:ADP:N7	2.67	0.43
1:F:253:ALA:HA	1:F:254:PRO:C	2.44	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:B:438:GLU:O	1:B:439:PRO:C	2.59	0.42
1:B:543:ARG:HD2	1:B:545:TYR:CE1	2.54	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:B:577:LYS:HB2	1:B:577:LYS:HZ3	1.84	0.42
1:F:197:ILE:HD12	1:F:303:MET:CE	2.47	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:LEU:O	1:E:344:THR:HG23	2.19	0.42
1:A:199:LEU:HD11	1:A:303:MET:HE2	2.01	0.42
1:A:443:ILE:O	1:A:591:THR:HG22	2.19	0.42
1:B:467:VAL:HG22	1:B:468:SER:N	2.33	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:C:224:HIS:C	1:C:225:ILE:HD13	2.45	0.42
1:D:446:ILE:C	1:D:448:ARG:N	2.75	0.42
1:E:313:ASP:OD1	1:E:313:ASP:C	2.63	0.42
1:A:483:ARG:NH1	1:A:493:VAL:CG1	2.83	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:521:LEU:HD23	1:B:521:LEU:HA	1.80	0.42
1:E:578:GLN:CD	1:E:578:GLN:H	2.26	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:B:333:MET:CE	1:B:589:LYS:O	2.68	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:C:284:LEU:O	1:C:285:ASN:C	2.63	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:167:GLU:N	1:C:167:GLU:CD	2.73	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:A:426:GLY:O	1:A:427:HIS:C	2.62	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:D:523:PRO:C	1:D:524:LEU:HD12	2.45	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:409:SER:C	1:D:410:LEU:HD23	2.46	0.41
1:F:354:ASN:C	1:F:354:ASN:ND2	2.76	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
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: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:F:173:LEU:HD22	1:F:303:MET:CE	2.51	0.41
1:F:510:ASN:HD22	1:F:510:ASN:HA	1.73	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:193:MET:HE3	1:C:194:PRO:HD2	2.03	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:291:MET:HE1	1:F:294:PHE:CZ	2.56	0.41
1:F:311:ILE:O	1:F:311:ILE:HG23	2.21	0.41
1:F:599:ARG:O	1:F:602:SER:N	2.53	0.41

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: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: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:C:245:LEU:HD23	1:C:246:PHE:CE1	2.56	0.40
1:F:262:ILE:HD12	1:F:304:ALA:HB2	1.99	0.40
1:F:294:PHE:CD1	1:F:294:PHE:C	2.99	0.40
1:F:599:ARG:O	1:F:600:ILE:C	2.64	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
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:193:MET:HE3	1:C:193:MET:HB3	1.81	0.40
1:C:329:ASP:OD2	1:C:451:LYS:HE2	2.21	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:375:ASN:ND2	1:F:375:ASN:C	2.78	0.40
1:F:481:GLY:O	1:F:484:ALA:HB3	2.22	0.40
1:A:545:TYR:CD1	1:A:545:TYR:C	2.99	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: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:527:GLY:C	5:F:2018:HOH:O	2.63	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:VAL:CG1	1:C:221:PRO:N	2.82	0.40
1:C:549:VAL:O	1:C:550:ALA:C	2.64	0.40
1:E:157:ARG:NH2	1:E:216:GLY:C	2.63	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%)	9	18
1	B	401/476 (84%)	378 (94%)	20 (5%)	3 (1%)	18	34
1	C	413/476 (87%)	393 (95%)	18 (4%)	2 (0%)	24	43
1	D	403/476 (85%)	383 (95%)	19 (5%)	1 (0%)	43	64
1	E	396/476 (83%)	376 (95%)	13 (3%)	7 (2%)	6	13
1	F	402/476 (84%)	372 (92%)	26 (6%)	4 (1%)	12	24
All	All	2412/2856 (84%)	2281 (95%)	109 (4%)	22 (1%)	14	28

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	303 (90%)	34 (10%)	7 14
1	B	339/390 (87%)	308 (91%)	31 (9%)	9 17
1	C	349/390 (90%)	309 (88%)	40 (12%)	5 10
1	D	342/390 (88%)	311 (91%)	31 (9%)	9 17
1	E	335/390 (86%)	302 (90%)	33 (10%)	7 15
1	F	340/390 (87%)	299 (88%)	41 (12%)	5 8
All	All	2042/2340 (87%)	1832 (90%)	210 (10%)	7 13

All (210) 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	235	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	280	ARG
1	A	287	LEU
1	A	301	ILE
1	A	311	ILE
1	A	327	VAL
1	A	333	MET
1	A	344	THR
1	A	349	LEU
1	A	373	LEU
1	A	399	ASP
1	A	401	VAL
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	592	ILE
1	A	597	LEU
1	A	599	ARG
1	A	601	LEU
1	B	156	LYS
1	B	171	GLU
1	B	256	ILE
1	B	265	VAL
1	B	278	ASP
1	B	279	GLU
1	B	281	GLU
1	B	283	THR
1	B	287	LEU
1	B	291	MET
1	B	310	ASP
1	B	311	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	324	LYS
1	B	325	LYS
1	B	345	ARG
1	B	400	ARG
1	B	429	VAL
1	B	434	VAL
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	577	LYS
1	B	578	GLN
1	B	588	GLU
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	184	SER
1	C	186	PHE
1	C	189	ILE
1	C	219	ASN
1	C	220	VAL
1	C	231	VAL
1	C	235	VAL
1	C	244	ASP
1	C	265	VAL
1	C	284	LEU
1	C	287	LEU
1	C	333	MET
1	C	334	LEU
1	C	344	THR
1	C	372	ASN
1	C	373	LEU
1	C	374	VAL
1	C	387	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	434	VAL
1	C	442	ARG
1	C	448	ARG
1	C	451	LYS
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	590	GLU
1	C	597	LEU
1	D	171	GLU
1	D	172	GLU
1	D	178	GLU
1	D	220	VAL
1	D	225	ILE
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	311	ILE
1	D	325	LYS
1	D	333	MET
1	D	344	THR
1	D	361	ARG
1	D	388	LYS
1	D	410	LEU
1	D	411	LEU
1	D	434	VAL
1	D	440	VAL
1	D	442	ARG
1	D	450	TYR
1	D	465	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	483	ARG
1	D	503	ARG
1	D	578	GLN
1	D	591	THR
1	D	593	GLU
1	D	602	SER
1	E	156	LYS
1	E	220	VAL
1	E	225	ILE
1	E	230	PHE
1	E	268	HIS
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	398	ILE
1	E	399	ASP
1	E	402	ILE
1	E	410	LEU
1	E	412	ILE
1	E	416	GLU
1	E	434	VAL
1	E	440	VAL
1	E	441	HIS
1	E	445	ILE
1	E	476	LEU
1	E	499	ASN
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	198	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	210	LEU
1	F	217	GLU
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	311	ILE
1	F	333	MET
1	F	349	LEU
1	F	353	VAL
1	F	373	LEU
1	F	374	VAL
1	F	383	ARG
1	F	387	ASP
1	F	399	ASP
1	F	412	ILE
1	F	420	ILE
1	F	434	VAL
1	F	445	ILE
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	577	LYS
1	F	578	GLN
1	F	584	GLU
1	F	586	LEU
1	F	592	ILE
1	F	593	GLU
1	F	595	ASP
1	F	596	GLU
1	F	597	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) 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	219	ASN
1	B	307	ASN
1	B	499	ASN
1	B	514	GLN
1	B	578	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	219	ASN
1	D	224	HIS
1	D	307	ASN
1	D	372	ASN
1	D	441	HIS
1	D	510	ASN
1	E	252	HIS
1	E	286	GLN
1	E	307	ASN
1	E	354	ASN
1	E	372	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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	1607	4	28,29,29	1.49	6 (21%)	43,45,45	1.86	10 (23%)
3	ADP	C	1608	4	28,29,29	1.40	5 (17%)	43,45,45	1.83	10 (23%)
3	ADP	F	1607	4	28,29,29	1.45	5 (17%)	43,45,45	1.91	9 (20%)
3	ADP	E	1604	4	28,29,29	1.32	5 (17%)	43,45,45	1.84	11 (25%)
3	ADP	D	1608	4	28,29,29	1.40	4 (14%)	43,45,45	1.82	9 (20%)
3	ADP	A	1604	4	28,29,29	1.38	4 (14%)	43,45,45	1.91	9 (20%)

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	B	1607	4	-	3/16/32/32	0/3/3/3
3	ADP	C	1608	4	-	3/16/32/32	0/3/3/3
3	ADP	F	1607	4	-	4/16/32/32	0/3/3/3
3	ADP	E	1604	4	-	2/16/32/32	0/3/3/3
3	ADP	D	1608	4	-	4/16/32/32	0/3/3/3
3	ADP	A	1604	4	-	3/16/32/32	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1604	ADP	C5-C4	4.25	1.46	1.39
3	C	1608	ADP	C5-C4	4.23	1.46	1.39
3	F	1607	ADP	C5-C4	4.12	1.46	1.39
3	E	1604	ADP	C5-C4	3.45	1.45	1.39
3	B	1607	ADP	C4-N9	-3.35	1.30	1.37
3	D	1608	ADP	C5-C4	3.35	1.45	1.39
3	F	1607	ADP	PA-O3A	3.15	1.62	1.59
3	A	1604	ADP	C8-N7	3.09	1.37	1.31
3	B	1607	ADP	C5-C4	3.06	1.44	1.39
3	D	1608	ADP	C5-N7	-3.01	1.33	1.39
3	E	1604	ADP	C5-N7	-2.89	1.33	1.39
3	D	1608	ADP	C4-N9	-2.84	1.31	1.37
3	B	1607	ADP	C5-N7	-2.75	1.34	1.39
3	E	1604	ADP	C8-N7	2.67	1.36	1.31
3	F	1607	ADP	C5-C6	2.66	1.48	1.41
3	C	1608	ADP	C5-N7	-2.65	1.34	1.39
3	C	1608	ADP	C8-N7	2.64	1.36	1.31
3	F	1607	ADP	C8-N7	2.58	1.36	1.31
3	B	1607	ADP	C8-N7	2.52	1.36	1.31
3	B	1607	ADP	C8-N9	-2.49	1.33	1.37
3	B	1607	ADP	PA-O3A	2.46	1.62	1.59
3	D	1608	ADP	C8-N7	2.41	1.36	1.31
3	A	1604	ADP	C5-N7	-2.34	1.34	1.39
3	C	1608	ADP	PA-O3A	2.33	1.62	1.59
3	A	1604	ADP	C5-C6	2.32	1.47	1.41
3	F	1607	ADP	C5-N7	-2.27	1.34	1.39
3	E	1604	ADP	C4-N9	-2.27	1.33	1.37
3	E	1604	ADP	C5-C6	2.26	1.47	1.41
3	C	1608	ADP	C5-C6	2.17	1.47	1.41

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1607	ADP	C5-C4-N3	-5.93	118.55	126.72
3	C	1608	ADP	C5-C4-N3	-5.80	118.73	126.72
3	E	1604	ADP	C5-C4-N3	-5.76	118.79	126.72
3	A	1604	ADP	C5-C4-N3	-5.63	118.96	126.72
3	D	1608	ADP	C5-C4-N3	-5.32	119.39	126.72
3	B	1607	ADP	C5-C4-N3	-4.92	119.95	126.72
3	F	1607	ADP	N3-C4-N9	4.49	134.81	127.17
3	C	1608	ADP	N3-C4-N9	4.43	134.70	127.17
3	A	1604	ADP	N3-C4-N9	4.26	134.41	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1608	ADP	N3-C4-N9	4.13	134.19	127.17
3	B	1607	ADP	C4-N9-C8	3.99	109.92	105.74
3	E	1604	ADP	N3-C4-N9	3.98	133.93	127.17
3	D	1608	ADP	N3-C2-N1	-3.97	122.57	128.58
3	F	1607	ADP	C2-N3-C4	3.89	121.33	111.83
3	A	1604	ADP	N3-C2-N1	-3.86	122.73	128.58
3	B	1607	ADP	N3-C2-N1	-3.86	122.75	128.58
3	C	1608	ADP	N3-C2-N1	-3.85	122.76	128.58
3	E	1604	ADP	C2-N3-C4	3.80	121.10	111.83
3	B	1607	ADP	N3-C4-N9	3.79	133.61	127.17
3	A	1604	ADP	C2-N3-C4	3.76	121.02	111.83
3	F	1607	ADP	N3-C2-N1	-3.74	122.92	128.58
3	E	1604	ADP	N3-C2-N1	-3.72	122.95	128.58
3	C	1608	ADP	C2-N3-C4	3.70	120.86	111.83
3	E	1604	ADP	C4-C5-N7	-3.44	106.65	110.58
3	A	1604	ADP	C2'-C1'-N9	-3.37	104.93	113.30
3	D	1608	ADP	C2-N3-C4	3.36	120.04	111.83
3	B	1607	ADP	C2-N3-C4	3.36	120.03	111.83
3	F	1607	ADP	C4-C5-N7	-3.34	106.76	110.58
3	A	1604	ADP	C4-C5-N7	-3.22	106.90	110.58
3	B	1607	ADP	C4-C5-N7	-3.17	106.95	110.58
3	C	1608	ADP	C4-C5-N7	-3.08	107.06	110.58
3	D	1608	ADP	C4-N9-C8	3.05	108.94	105.74
3	B	1607	ADP	N9-C8-N7	-2.96	109.73	113.94
3	D	1608	ADP	C2'-C1'-N9	-2.95	105.97	113.30
3	A	1604	ADP	C4-N9-C8	2.86	108.74	105.74
3	F	1607	ADP	C5-N7-C8	2.80	107.85	103.45
3	D	1608	ADP	C4-C5-N7	-2.78	107.41	110.58
3	A	1604	ADP	N9-C8-N7	-2.70	110.11	113.94
3	A	1604	ADP	C5-N7-C8	2.65	107.61	103.45
3	C	1608	ADP	C5-N7-C8	2.62	107.56	103.45
3	E	1604	ADP	C5-N7-C8	2.57	107.49	103.45
3	F	1607	ADP	C4-N9-C8	2.56	108.43	105.74
3	F	1607	ADP	N9-C8-N7	-2.56	110.31	113.94
3	D	1608	ADP	N9-C8-N7	-2.53	110.34	113.94
3	B	1607	ADP	C2'-C1'-N9	-2.49	107.11	113.30
3	C	1608	ADP	C4-N9-C8	2.44	108.30	105.74
3	E	1604	ADP	N9-C8-N7	-2.43	110.48	113.94
3	F	1607	ADP	C3'-C2'-C1'	2.43	106.06	101.46
3	C	1608	ADP	N9-C8-N7	-2.42	110.50	113.94
3	C	1608	ADP	C2'-C1'-N9	-2.37	107.41	113.30
3	E	1604	ADP	C4-N9-C8	2.25	108.10	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1607	ADP	C5-N7-C8	2.23	106.95	103.45
3	E	1604	ADP	C2'-C1'-N9	-2.22	107.80	113.30
3	B	1607	ADP	O2A-PA-O1A	2.19	122.62	112.44
3	D	1608	ADP	C5-N7-C8	2.18	106.87	103.45
3	E	1604	ADP	O4'-C1'-N9	2.07	112.06	108.09
3	C	1608	ADP	C2-N1-C6	2.05	122.09	118.73
3	E	1604	ADP	C6-C5-N7	2.02	135.98	132.09

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	A	1604	ADP	C5'-O5'-PA-O3A
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	F	1607	ADP	C5'-O5'-PA-O3A
3	E	1604	ADP	C3'-C4'-C5'-O5'
3	C	1608	ADP	O4'-C4'-C5'-O5'
3	E	1604	ADP	O4'-C4'-C5'-O5'
3	C	1608	ADP	C3'-C4'-C5'-O5'
3	B	1607	ADP	O4'-C4'-C5'-O5'
3	B	1607	ADP	C3'-C4'-C5'-O5'
3	D	1608	ADP	PA-O3A-PB-O1B
3	B	1607	ADP	PA-O3A-PB-O1B
3	C	1608	ADP	PB-O3A-PA-O2A
3	D	1608	ADP	O4'-C4'-C5'-O5'
3	F	1607	ADP	PA-O3A-PB-O1B
3	D	1608	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 36 short contacts:

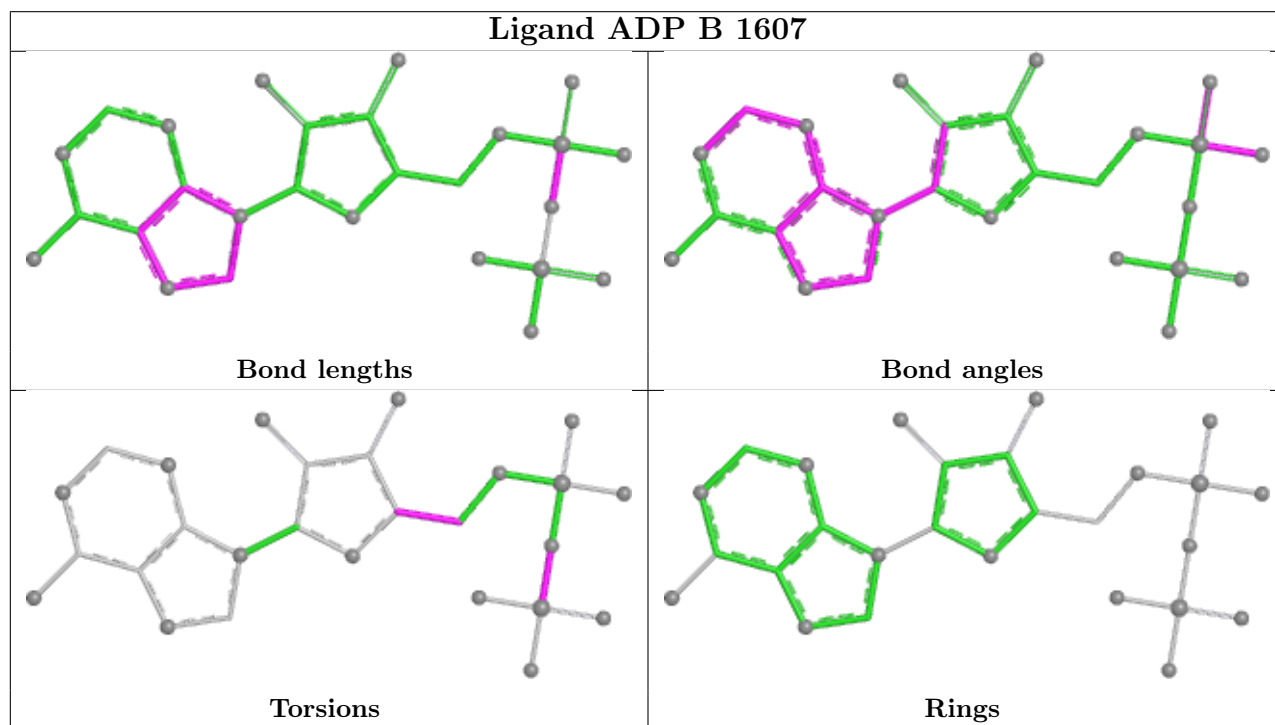
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1607	ADP	7	0
3	C	1608	ADP	10	0
3	F	1607	ADP	5	0
3	E	1604	ADP	7	0
3	D	1608	ADP	6	0

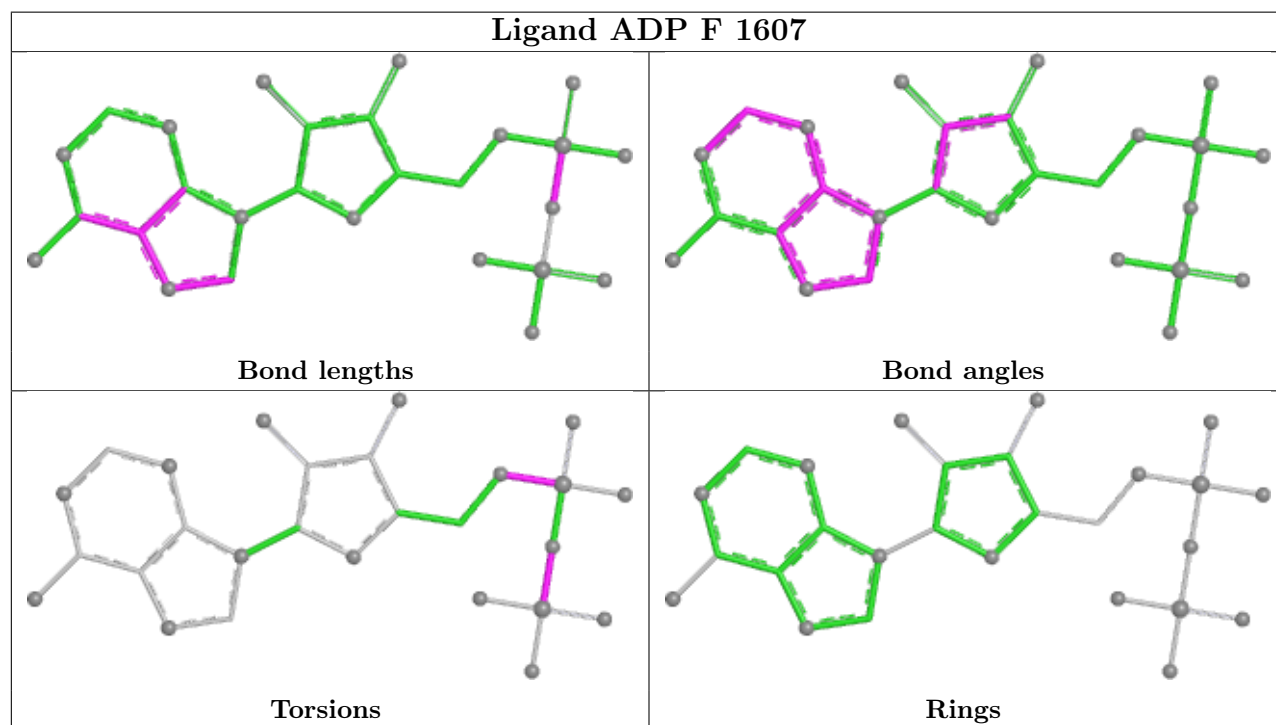
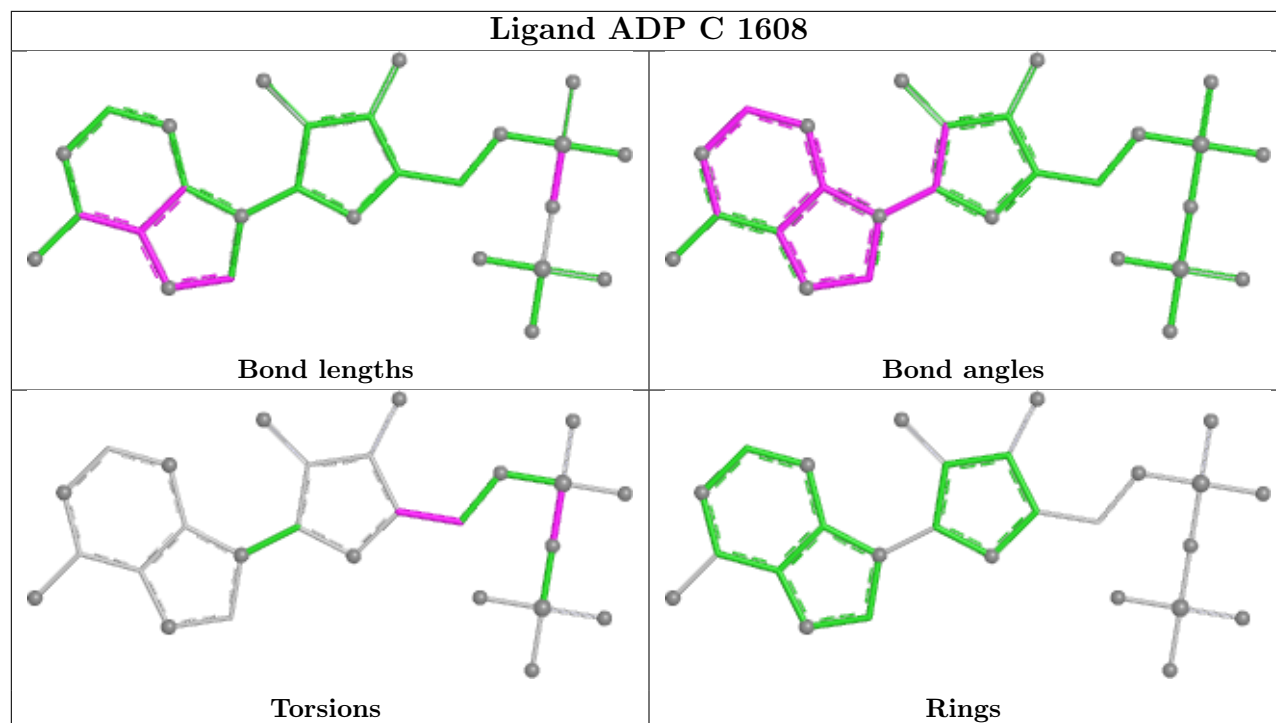
Continued on next page...

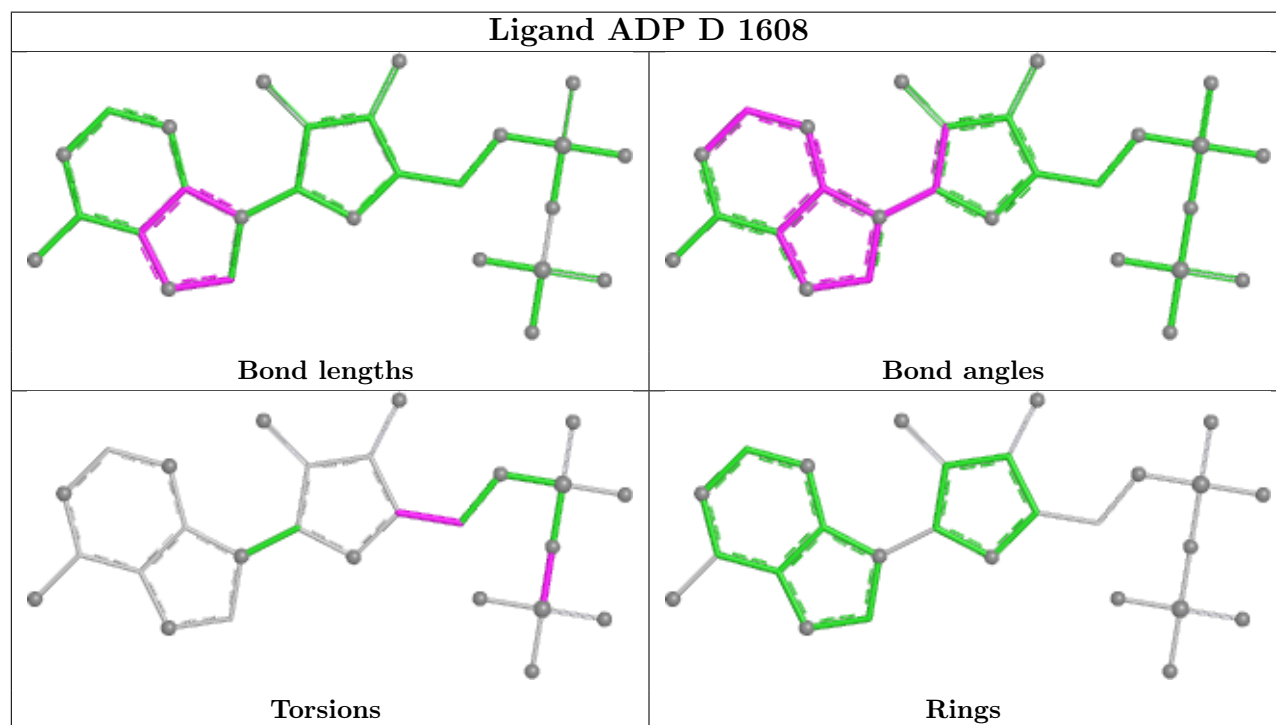
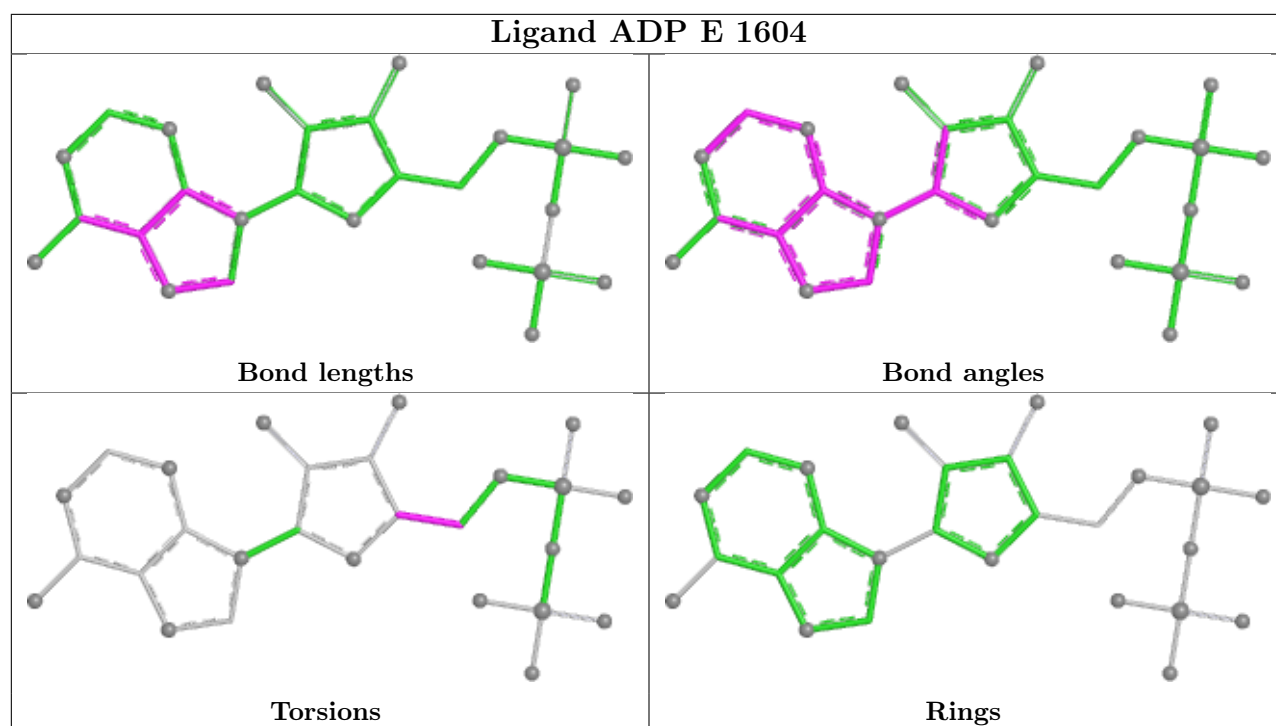
Continued from previous page...

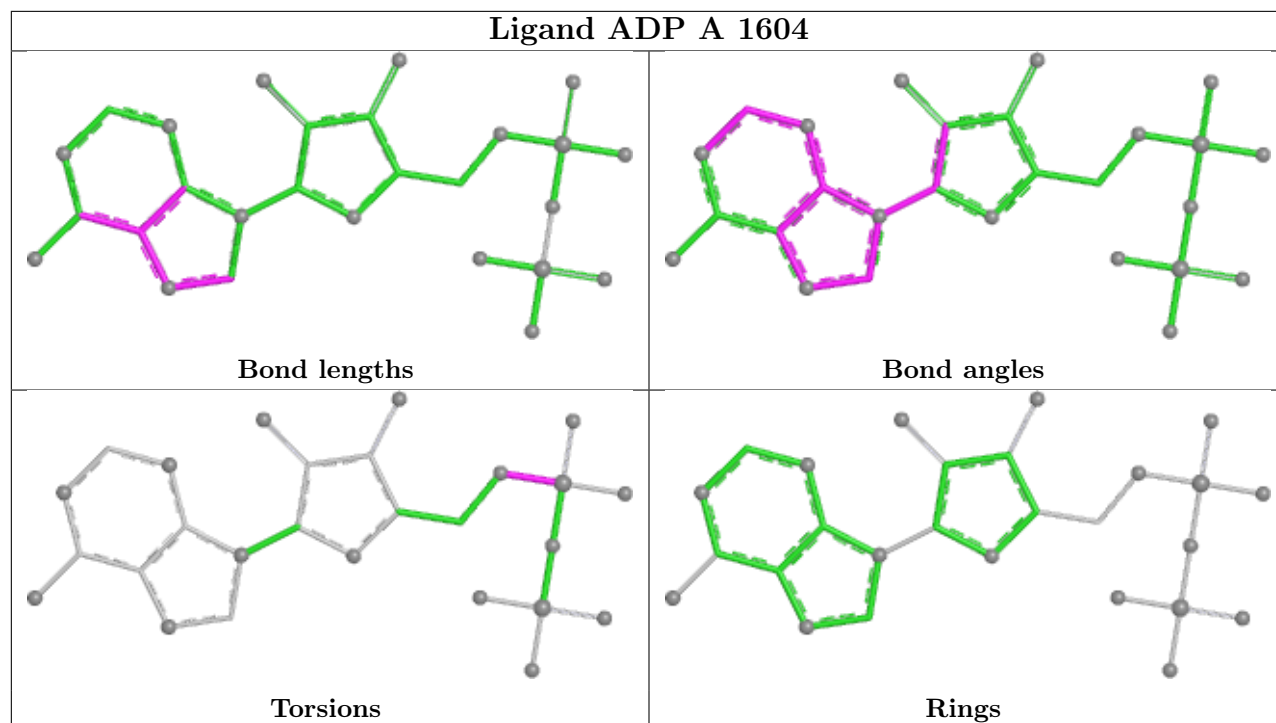
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1604	ADP	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	407/476 (85%)	0.10	6 (1%) 72 71	35, 44, 54, 66	0
1	B	411/476 (86%)	0.24	16 (3%) 43 40	34, 44, 54, 74	0
1	C	421/476 (88%)	0.50	19 (4%) 38 37	36, 43, 57, 86	0
1	D	413/476 (86%)	0.58	36 (8%) 16 16	35, 44, 56, 78	0
1	E	406/476 (85%)	0.43	22 (5%) 31 31	35, 44, 55, 84	0
1	F	412/476 (86%)	1.39	109 (26%) 1 1	34, 43, 56, 90	0
All	All	2470/2856 (86%)	0.54	208 (8%) 17 17	34, 43, 55, 90	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	231	VAL	7.9
1	F	245	LEU	6.9
1	F	230	PHE	6.8
1	F	234	PHE	6.7
1	F	152	PRO	5.6
1	F	389	ILE	5.3
1	F	205	THR	5.2
1	F	328	VAL	5.1
1	F	201	GLY	5.0
1	C	235	VAL	4.9
1	F	235	VAL	4.8
1	D	164	GLY	4.7
1	F	346	ASN	4.7
1	E	231	VAL	4.6
1	D	403	ALA	4.5
1	F	204	GLY	4.5
1	F	300	ILE	4.4
1	F	253	ALA	4.3
1	F	236	GLY	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	152	PRO	4.2
1	F	150	TYR	4.2
1	F	181	LYS	4.2
1	F	329	ASP	4.1
1	F	166	ALA	4.0
1	F	358	ILE	4.0
1	F	388	LYS	4.0
1	F	206	GLY	4.0
1	D	465	TYR	4.0
1	C	206	GLY	3.9
1	F	265	VAL	3.9
1	F	184	SER	3.9
1	D	542	LEU	3.8
1	F	327	VAL	3.8
1	C	328	VAL	3.8
1	F	301	ILE	3.7
1	F	158	VAL	3.7
1	D	165	GLY	3.7
1	F	255	CYS	3.7
1	F	449	GLY	3.7
1	F	203	PRO	3.7
1	D	156	LYS	3.6
1	E	185	LYS	3.6
1	D	163	VAL	3.6
1	E	232	GLU	3.6
1	B	329	ASP	3.6
1	E	190	GLY	3.5
1	D	161	LYS	3.5
1	C	234	PHE	3.5
1	F	401	VAL	3.5
1	C	236	GLY	3.5
1	E	410	LEU	3.5
1	F	200	VAL	3.4
1	D	206	GLY	3.4
1	F	191	ALA	3.4
1	F	605	PHE	3.4
1	F	208	THR	3.4
1	F	280	ARG	3.4
1	B	156	LYS	3.2
1	D	209	LEU	3.2
1	F	284	LEU	3.2
1	F	254	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	320	GLY	3.2
1	F	364	GLY	3.2
1	F	454	GLY	3.1
1	D	154	GLY	3.1
1	A	230	PHE	3.1
1	F	210	LEU	3.1
1	A	329	ASP	3.1
1	F	387	ASP	3.1
1	E	402	ILE	3.1
1	F	186	PHE	3.1
1	B	601	LEU	3.0
1	D	190	GLY	3.0
1	D	409	SER	3.0
1	F	257	VAL	3.0
1	F	228	SER	3.0
1	F	250	LYS	3.0
1	F	190	GLY	3.0
1	F	266	GLY	3.0
1	F	219	ASN	2.9
1	F	222	PHE	2.9
1	F	311	ILE	2.9
1	F	264	ALA	2.9
1	F	177	VAL	2.9
1	F	185	LYS	2.9
1	F	232	GLU	2.9
1	F	296	SER	2.9
1	C	243	ARG	2.9
1	F	213	ALA	2.9
1	D	231	VAL	2.9
1	E	191	ALA	2.8
1	F	258	PHE	2.8
1	F	326	ILE	2.8
1	D	191	ALA	2.8
1	F	156	LYS	2.8
1	D	205	THR	2.8
1	E	183	PRO	2.8
1	F	256	ILE	2.8
1	C	233	LEU	2.8
1	B	603	GLU	2.7
1	F	161	LYS	2.7
1	F	189	ILE	2.7
1	F	238	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	553	ILE	2.7
1	F	267	ARG	2.7
1	F	345	ARG	2.7
1	F	302	VAL	2.7
1	B	492	ASP	2.7
1	E	181	LYS	2.7
1	E	180	LEU	2.7
1	F	299	GLY	2.7
1	D	281	GLU	2.7
1	D	526	TRP	2.7
1	F	237	VAL	2.7
1	D	329	ASP	2.7
1	C	150	TYR	2.6
1	F	412	ILE	2.6
1	D	204	GLY	2.6
1	D	219	ASN	2.6
1	D	160	PHE	2.6
1	F	315	ALA	2.6
1	C	204	GLY	2.6
1	F	604	GLU	2.6
1	A	542	LEU	2.6
1	F	365	PHE	2.6
1	F	603	GLU	2.6
1	E	187	ASN	2.6
1	E	189	ILE	2.5
1	F	165	GLY	2.5
1	F	330	PRO	2.5
1	F	394	PHE	2.5
1	F	306	THR	2.5
1	F	179	PHE	2.5
1	B	209	LEU	2.5
1	B	206	GLY	2.5
1	C	191	ALA	2.5
1	C	209	LEU	2.5
1	D	402	ILE	2.5
1	E	152	PRO	2.5
1	F	347	LYS	2.4
1	F	375	ASN	2.4
1	D	188	ARG	2.4
1	F	370	LEU	2.4
1	F	199	LEU	2.4
1	C	544	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	295	ASP	2.4
1	C	181	LYS	2.4
1	B	188	ARG	2.4
1	F	239	ALA	2.4
1	A	438	GLU	2.4
1	D	237	VAL	2.4
1	C	329	ASP	2.3
1	E	188	ARG	2.3
1	F	188	ARG	2.3
1	B	150	TYR	2.3
1	D	551	SER	2.3
1	D	186	PHE	2.3
1	E	233	LEU	2.3
1	D	603	GLU	2.3
1	F	298	GLU	2.3
1	F	288	LEU	2.3
1	F	312	LEU	2.3
1	B	402	ILE	2.3
1	F	368	ALA	2.3
1	E	184	SER	2.3
1	F	348	PRO	2.2
1	E	329	ASP	2.2
1	F	229	ASP	2.2
1	F	313	ASP	2.2
1	B	154	GLY	2.2
1	F	366	VAL	2.2
1	F	382	ALA	2.2
1	F	281	GLU	2.2
1	C	448	ARG	2.2
1	F	202	PRO	2.2
1	B	165	GLY	2.2
1	D	153	SER	2.2
1	F	153	SER	2.2
1	E	235	VAL	2.2
1	C	218	ALA	2.2
1	D	588	GLU	2.2
1	D	159	THR	2.2
1	E	499	ASN	2.2
1	F	187	ASN	2.2
1	E	182	ASP	2.2
1	B	231	VAL	2.2
1	F	314	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	278	ASP	2.1
1	F	163	VAL	2.1
1	F	262	ILE	2.1
1	C	188	ARG	2.1
1	F	183	PRO	2.1
1	F	263	ASP	2.1
1	D	230	PHE	2.1
1	F	308	ARG	2.1
1	F	448	ARG	2.1
1	D	601	LEU	2.1
1	D	516	GLY	2.1
1	C	327	VAL	2.1
1	F	246	PHE	2.1
1	B	383	ARG	2.1
1	A	152	PRO	2.1
1	F	309	PRO	2.1
1	A	231	VAL	2.1
1	B	328	VAL	2.1
1	E	220	VAL	2.1
1	E	223	PHE	2.0
1	F	340	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
3	ADP	F	1607	27/27	0.73	0.12	72,79,80,81	0
4	MG	C	1609	1/1	0.80	0.10	60,60,60,60	0

Continued on next page...

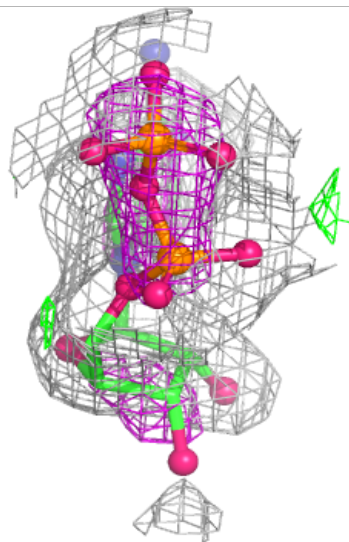
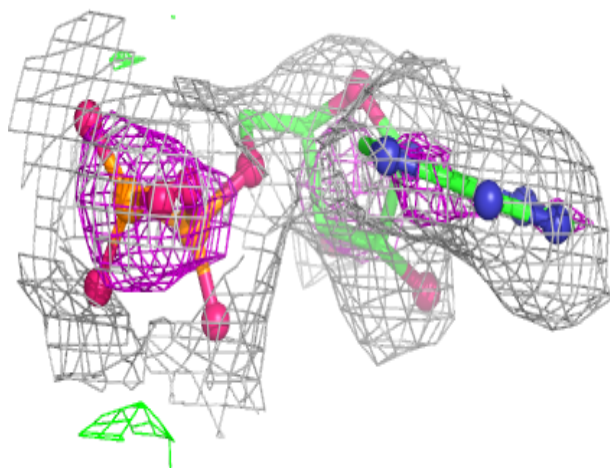
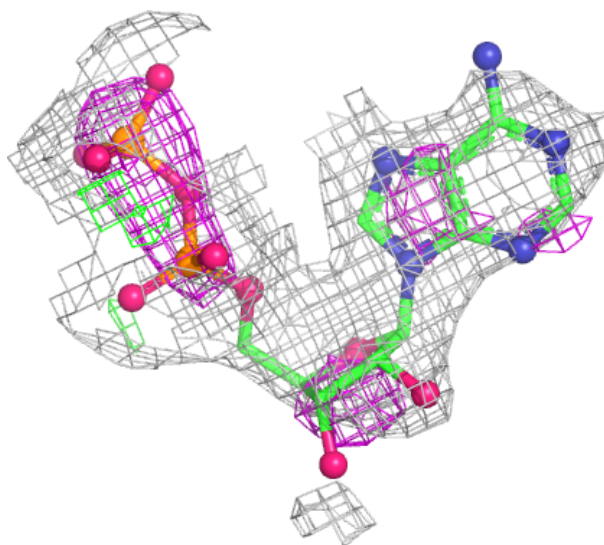
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADP	C	1608	27/27	0.85	0.11	54,57,59,61	0
4	MG	A	1605	1/1	0.86	0.09	47,47,47,47	0
4	MG	B	1608	1/1	0.89	0.12	44,44,44,44	0
4	MG	F	1608	1/1	0.90	0.10	68,68,68,68	0
4	MG	E	1605	1/1	0.93	0.08	53,53,53,53	0
3	ADP	A	1604	27/27	0.93	0.10	32,34,39,41	0
3	ADP	E	1604	27/27	0.94	0.09	34,38,42,48	0
4	MG	D	1609	1/1	0.94	0.10	41,41,41,41	0
3	ADP	B	1607	27/27	0.95	0.09	20,26,33,37	0
3	ADP	D	1608	27/27	0.95	0.09	21,25,30,31	0
2	ZN	E	1603	1/1	0.97	0.17	63,63,63,63	0
2	ZN	D	1607	1/1	0.98	0.27	79,79,79,79	0
2	ZN	A	1603	1/1	0.98	0.18	63,63,63,63	0
2	ZN	B	1606	1/1	0.99	0.20	64,64,64,64	0
2	ZN	C	1607	1/1	0.99	0.20	60,60,60,60	0
2	ZN	F	1606	1/1	1.00	0.17	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.

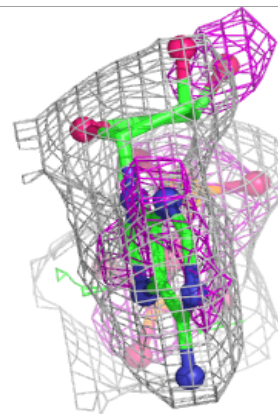
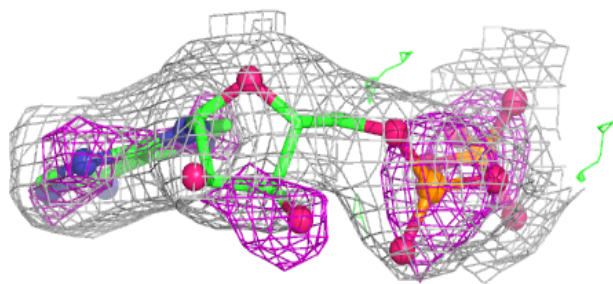
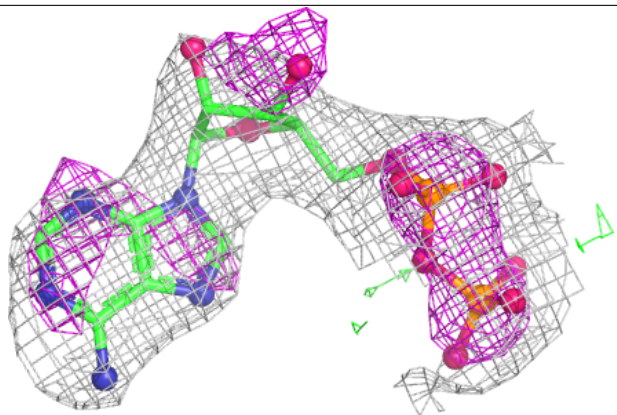
Electron density around ADP F 1607:

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



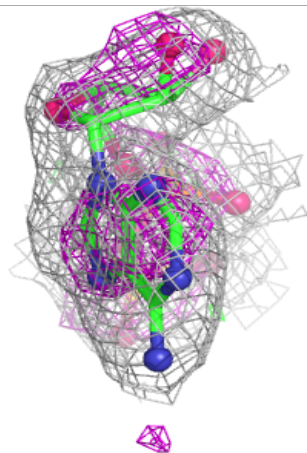
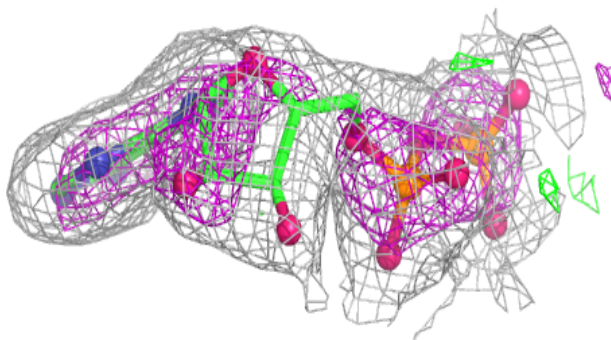
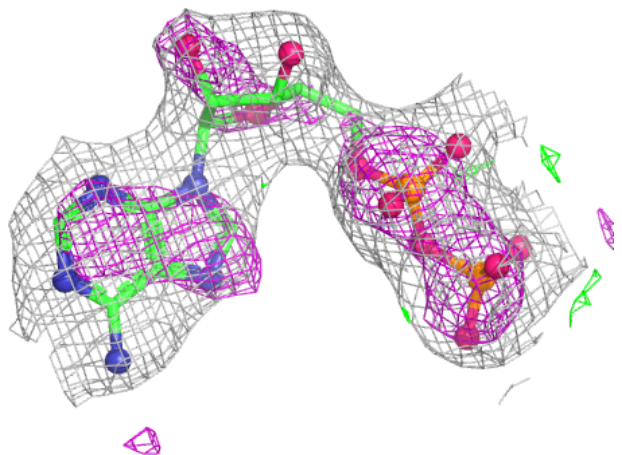
Electron density around ADP C 1608:

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



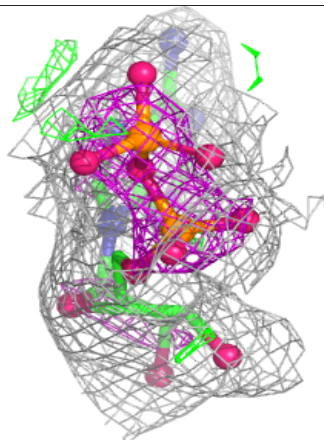
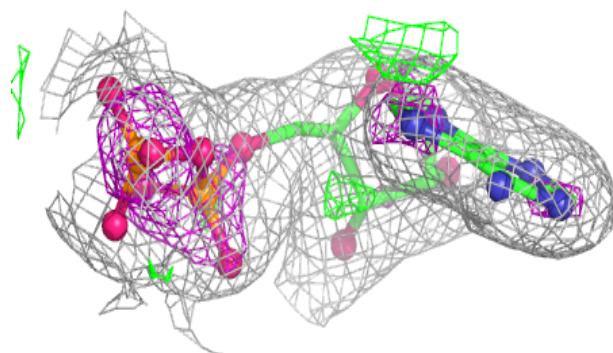
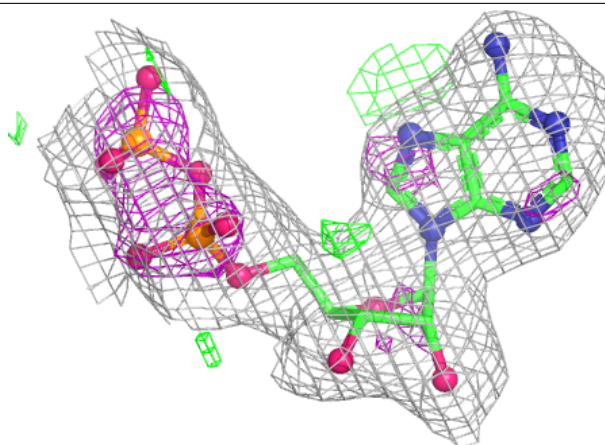
Electron density around ADP A 1604:

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

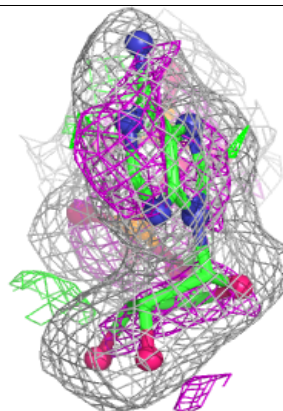
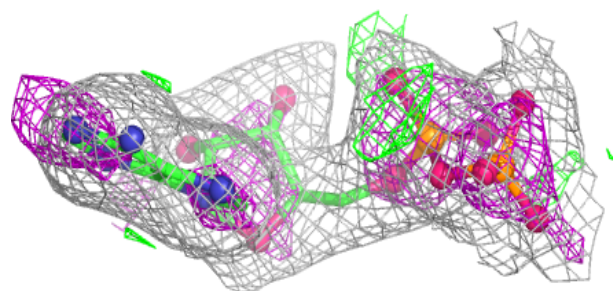
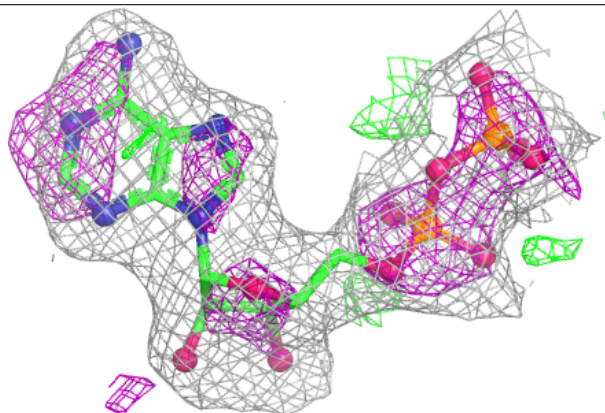


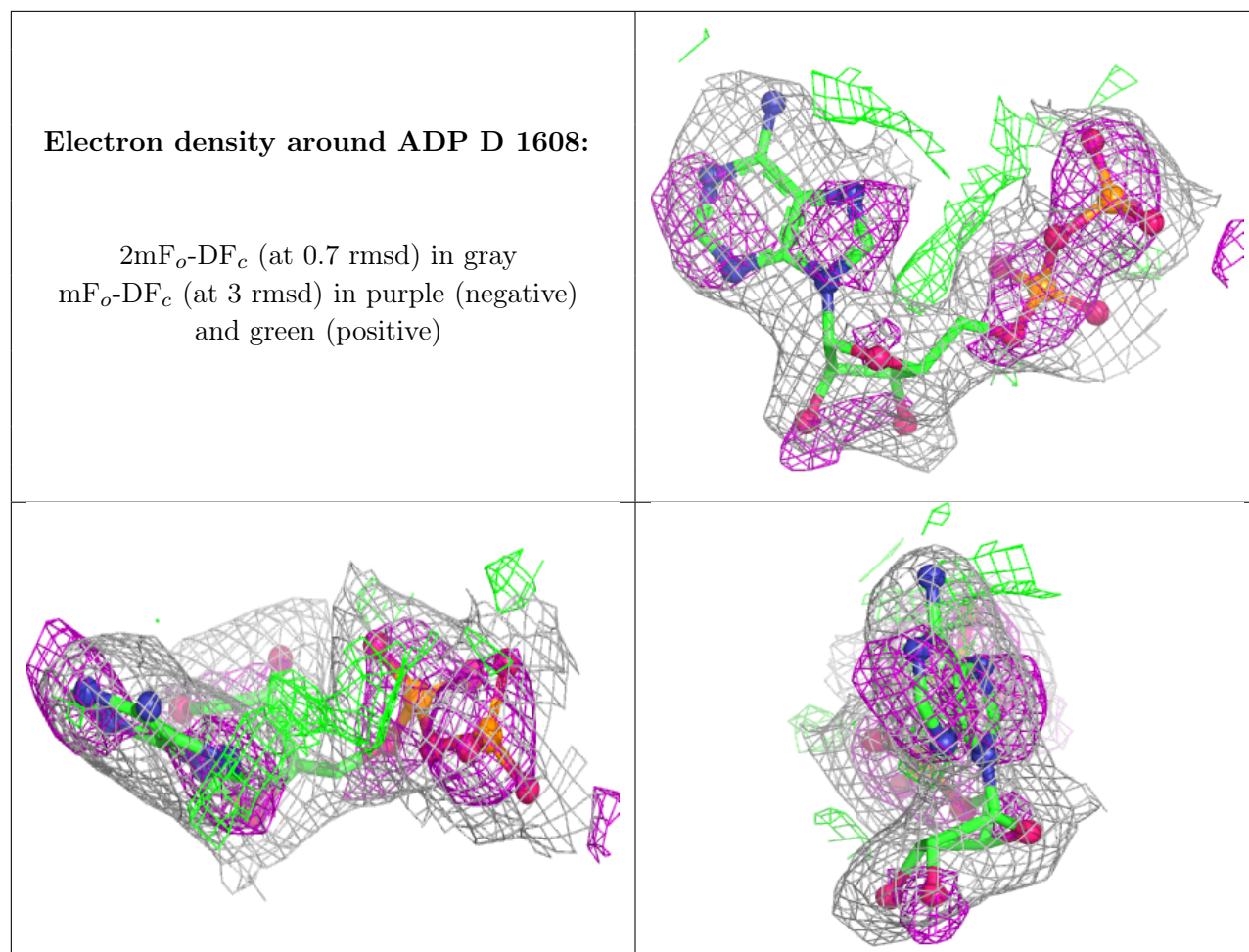
Electron density around ADP E 1604:

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

**Electron density around ADP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.