Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:36 pm BST

PDB ID	:	1BHN
Title	:	NUCLEOSIDE DIPHOSPHATE KINASE ISOFORM A FROM BOVINE RETINA
Authors	:	Ladner, J.E.; Abdulaev, N.G.; Kakuev, D.L.; Karaschuk, G.N.; Tordova, M.; Eisenstein, E.; Fujiwara, J.H.; Ridge, K.D.; Gilliland, G.L.
Deposited on	:	1998-06-10
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

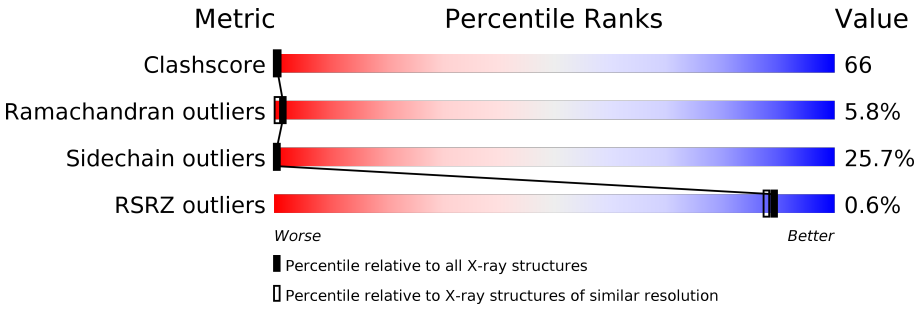
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	152	10% 36% 38% 15%
1	B	152	2% 9% 35% 39% 17%
1	C	152	12% 32% 38% 18%
1	D	152	11% 32% 43% 13%
1	E	152	14% 28% 44% 14%
1	F	152	% 9% 41% 38% 12%

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
2	35G	B	160	-	-	X	-
2	35G	F	160	-	-	X	-

2 Entry composition (i)

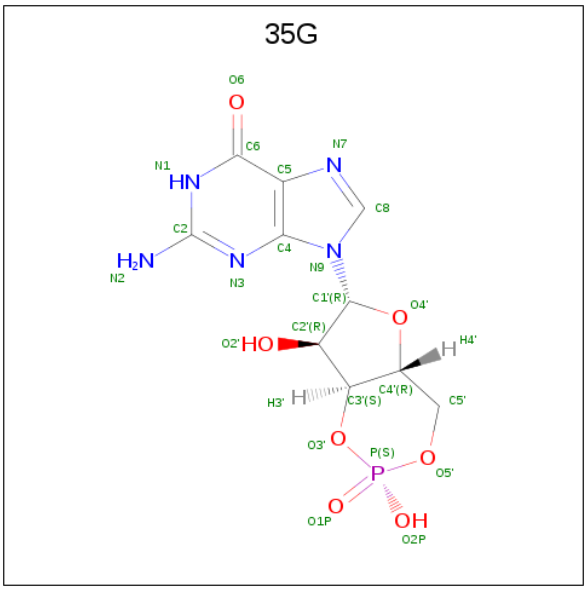
There are 4 unique types of molecules in this entry. The entry contains 7848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NUCLEOSIDE DIPHOSPHATE TRANSFERASE.

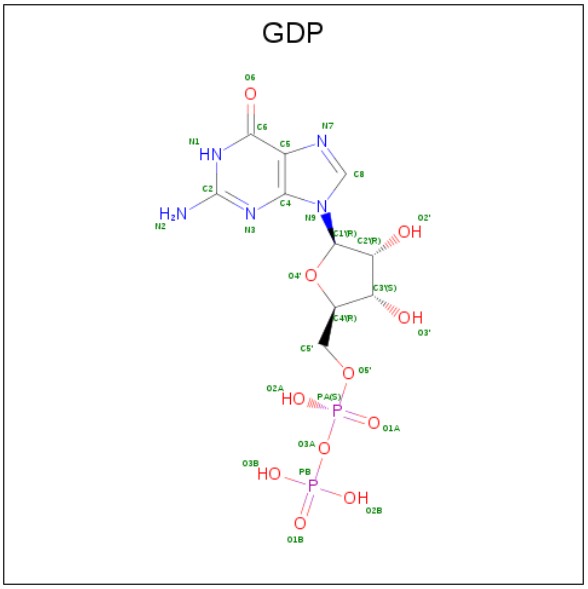
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1206	771	210	218	7			
1	B	151	Total	C	N	O	S	0	0	0
			1206	771	210	218	7			
1	C	151	Total	C	N	O	S	0	0	0
			1206	771	210	218	7			
1	D	151	Total	C	N	O	S	0	0	0
			1206	771	210	218	7			
1	E	151	Total	C	N	O	S	0	0	0
			1206	771	210	218	7			
1	F	151	Total	C	N	O	S	0	0	0
			1206	771	210	218	7			

- Molecule 2 is GUANOSINE-3',5'-MONOPHOSPHATE (three-letter code: 35G) (formula: $C_{10}H_{12}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	E	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is water.

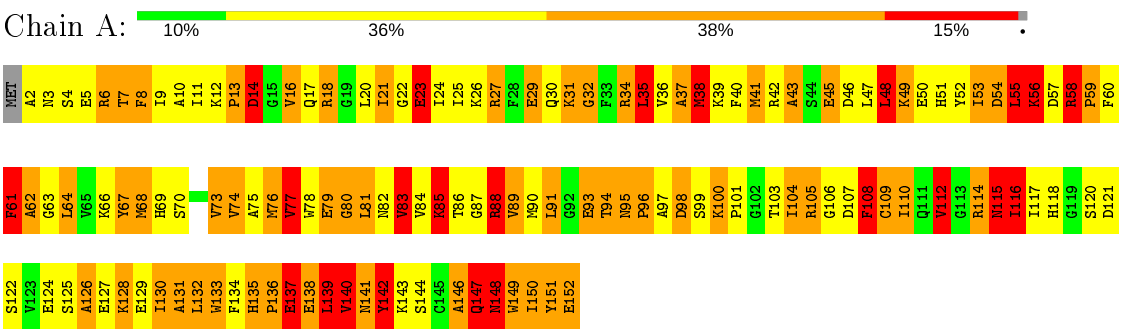
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O	0	0
			49	49		
4	B	49	Total	O	0	0
			49	49		
4	C	50	Total	O	0	0
			50	50		
4	D	40	Total	O	0	0
			40	40		
4	E	62	Total	O	0	0
			62	62		
4	F	56	Total	O	0	0
			56	56		

3 Residue-property plots (i)

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

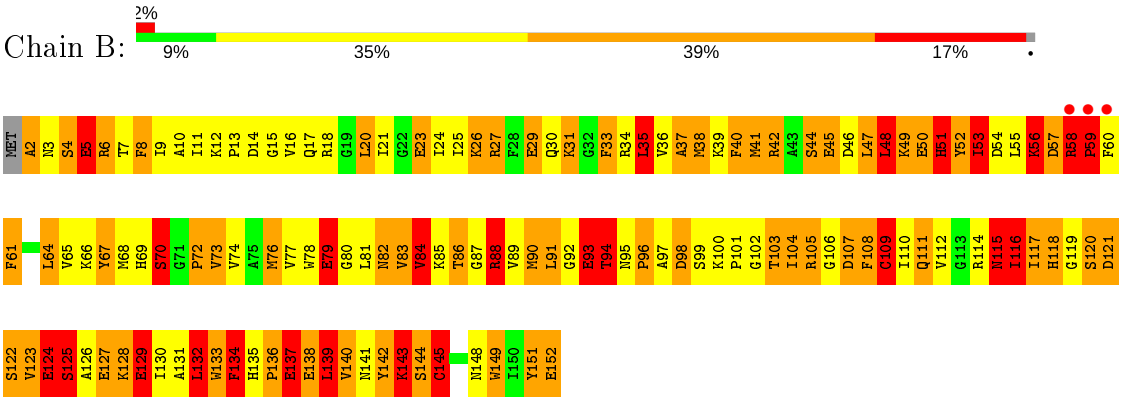
- Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

Chain A:



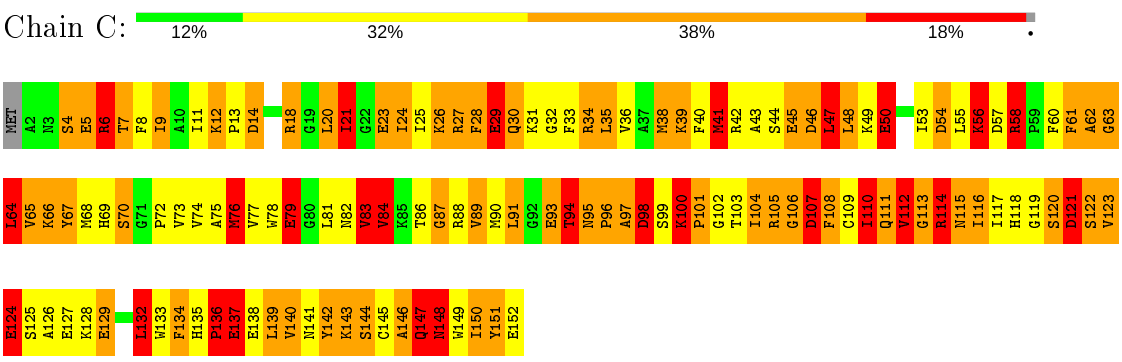
- Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

Chain B:



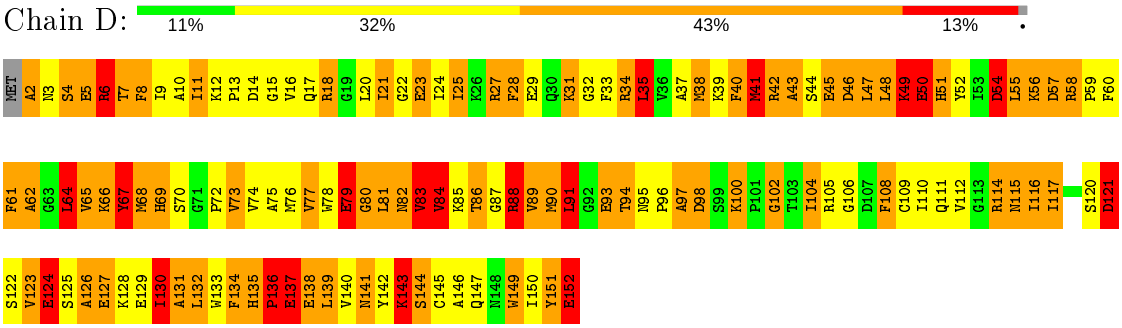
- Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

Chain C:



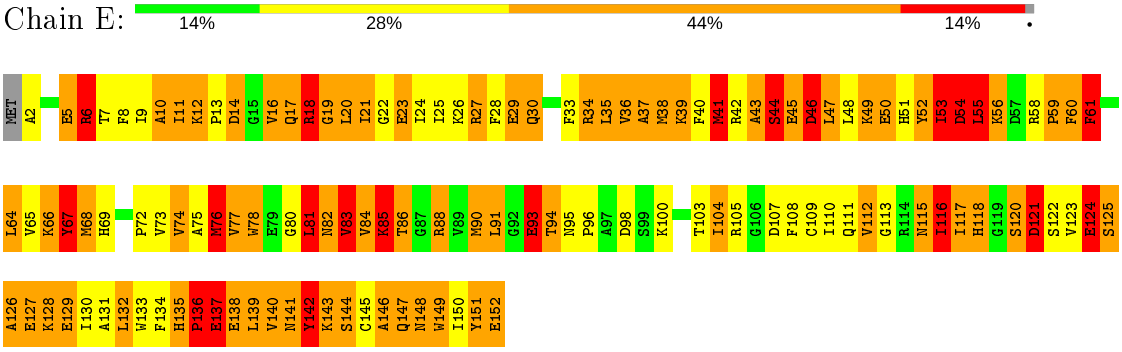
- Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

Chain D:



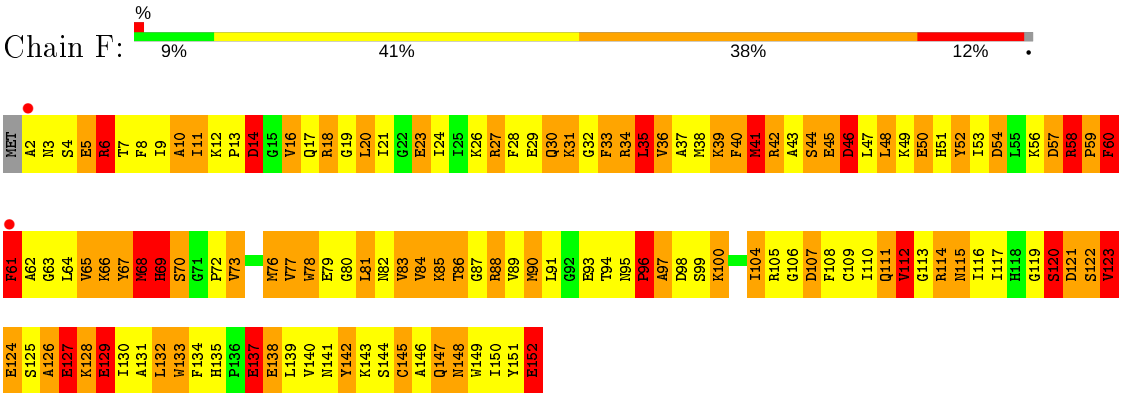
• Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

Chain E:



• Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.88Å 92.11Å 131.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 29.95 – 2.26	Depositor EDS
% Data completeness (in resolution range)	79.0 (20.00-2.40) 72.2 (29.95-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.26Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.200 , (Not available) 0.187 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.909	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 113.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7848	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: 35G, GDP

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	1.50	15/1233 (1.2%)	2.95	143/1659 (8.6%)
1	B	1.40	14/1233 (1.1%)	3.03	131/1659 (7.9%)
1	C	1.42	11/1233 (0.9%)	3.00	128/1659 (7.7%)
1	D	1.46	11/1233 (0.9%)	3.00	126/1659 (7.6%)
1	E	1.50	14/1233 (1.1%)	2.90	116/1659 (7.0%)
1	F	1.44	12/1233 (1.0%)	3.12	145/1659 (8.7%)
All	All	1.45	77/7398 (1.0%)	3.00	789/9954 (7.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	3	0
1	C	0	2
1	D	2	0
1	E	0	1
All	All	5	3

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	GLU	CD-OE2	11.47	1.38	1.25
1	F	29	GLU	CD-OE1	10.86	1.37	1.25
1	D	79	GLU	CD-OE2	10.70	1.37	1.25
1	B	5	GLU	CD-OE2	9.09	1.35	1.25
1	A	29	GLU	CD-OE1	8.83	1.35	1.25
1	D	129	GLU	CD-OE2	8.60	1.35	1.25
1	F	45	GLU	CD-OE2	8.44	1.34	1.25
1	A	79	GLU	CD-OE2	8.43	1.34	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	GLU	CD-OE2	8.33	1.34	1.25
1	D	152	GLU	CD-OE2	8.31	1.34	1.25
1	A	45	GLU	CD-OE1	8.25	1.34	1.25
1	F	138	GLU	CD-OE1	8.21	1.34	1.25
1	E	45	GLU	CD-OE1	8.11	1.34	1.25
1	C	5	GLU	CD-OE2	8.08	1.34	1.25
1	E	124	GLU	CD-OE1	7.87	1.34	1.25
1	C	129	GLU	CD-OE2	7.82	1.34	1.25
1	E	127	GLU	CD-OE2	7.61	1.34	1.25
1	A	5	GLU	CD-OE2	7.52	1.33	1.25
1	C	79	GLU	CD-OE2	7.49	1.33	1.25
1	F	5	GLU	CD-OE2	7.46	1.33	1.25
1	A	152	GLU	CD-OE1	7.45	1.33	1.25
1	A	23	GLU	CD-OE2	7.30	1.33	1.25
1	D	124	GLU	CD-OE1	7.30	1.33	1.25
1	C	93	GLU	CD-OE2	7.25	1.33	1.25
1	D	23	GLU	CD-OE1	7.21	1.33	1.25
1	C	124	GLU	CD-OE1	7.16	1.33	1.25
1	E	152	GLU	CD-OE2	7.03	1.33	1.25
1	E	138	GLU	CD-OE1	6.98	1.33	1.25
1	A	32	GLY	CA-C	6.97	1.63	1.51
1	C	152	GLU	CD-OE1	6.87	1.33	1.25
1	E	93	GLU	CD-OE1	6.87	1.33	1.25
1	C	50	GLU	CD-OE1	6.85	1.33	1.25
1	E	137	GLU	CD-OE2	6.78	1.33	1.25
1	F	79	GLU	CD-OE1	6.78	1.33	1.25
1	B	129	GLU	CD-OE2	6.76	1.33	1.25
1	D	45	GLU	CD-OE2	6.73	1.33	1.25
1	A	93	GLU	CD-OE1	6.63	1.32	1.25
1	D	137	GLU	CD-OE2	6.59	1.32	1.25
1	F	50	GLU	CD-OE1	6.56	1.32	1.25
1	A	138	GLU	CD-OE2	6.55	1.32	1.25
1	F	61	PHE	CB-CG	6.36	1.62	1.51
1	A	79	GLU	CD-OE1	-6.31	1.18	1.25
1	C	23	GLU	CD-OE2	6.30	1.32	1.25
1	B	124	GLU	CD-OE1	6.21	1.32	1.25
1	D	29	GLU	CD-OE1	-6.21	1.18	1.25
1	D	50	GLU	CD-OE1	6.17	1.32	1.25
1	F	152	GLU	CD-OE1	6.17	1.32	1.25
1	F	127	GLU	CD-OE2	6.15	1.32	1.25
1	B	23	GLU	CD-OE2	6.08	1.32	1.25
1	B	127	GLU	CD-OE2	6.06	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	ARG	NE-CZ	5.98	1.40	1.33
1	B	50	GLU	CD-OE1	5.93	1.32	1.25
1	A	50	GLU	CD-OE1	5.88	1.32	1.25
1	B	138	GLU	CD-OE2	5.88	1.32	1.25
1	A	127	GLU	CD-OE2	5.86	1.32	1.25
1	D	138	GLU	CD-OE1	5.85	1.32	1.25
1	E	129	GLU	CD-OE2	5.83	1.32	1.25
1	E	5	GLU	CD-OE2	5.56	1.31	1.25
1	E	50	GLU	CD-OE2	5.53	1.31	1.25
1	B	29	GLU	CD-OE1	5.52	1.31	1.25
1	C	137	GLU	CD-OE2	5.47	1.31	1.25
1	E	14	ASP	CG-OD2	5.46	1.38	1.25
1	C	127	GLU	CD-OE2	5.45	1.31	1.25
1	D	127	GLU	CD-OE2	5.43	1.31	1.25
1	B	56	LYS	C-N	-5.39	1.21	1.34
1	A	137	GLU	CD-OE2	5.26	1.31	1.25
1	F	124	GLU	CD-OE1	5.22	1.31	1.25
1	F	137	GLU	CD-OE2	5.21	1.31	1.25
1	F	23	GLU	CD-OE2	5.20	1.31	1.25
1	B	137	GLU	CD-OE2	5.20	1.31	1.25
1	B	93	GLU	CD-OE1	5.16	1.31	1.25
1	C	45	GLU	CD-OE1	5.15	1.31	1.25
1	E	29	GLU	CD-OE1	-5.15	1.20	1.25
1	E	42	ARG	NE-CZ	5.12	1.39	1.33
1	B	79	GLU	CD-OE2	5.09	1.31	1.25
1	B	55	LEU	CA-C	5.03	1.66	1.52
1	E	135	HIS	C-N	-5.01	1.24	1.34

All (789) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	98	ASP	CB-CG-OD2	-25.48	95.37	118.30
1	D	18	ARG	NE-CZ-NH2	22.93	131.76	120.30
1	F	67	TYR	CB-CG-CD2	-22.41	107.55	121.00
1	D	114	ARG	NE-CZ-NH1	20.97	130.78	120.30
1	A	88	ARG	NE-CZ-NH2	-20.26	110.17	120.30
1	E	27	ARG	NE-CZ-NH2	-19.90	110.35	120.30
1	C	88	ARG	CD-NE-CZ	-18.23	98.08	123.60
1	D	98	ASP	CB-CG-OD2	-17.74	102.33	118.30
1	F	61	PHE	CB-CG-CD2	17.61	133.13	120.80
1	B	98	ASP	CB-CG-OD1	17.43	133.99	118.30
1	F	58	ARG	NE-CZ-NH2	-17.01	111.80	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	58	ARG	NE-CZ-NH1	16.83	128.72	120.30
1	D	88	ARG	NE-CZ-NH2	-16.61	111.99	120.30
1	C	34	ARG	NE-CZ-NH1	16.21	128.41	120.30
1	F	114	ARG	NE-CZ-NH2	-15.42	112.59	120.30
1	C	58	ARG	NE-CZ-NH1	15.30	127.95	120.30
1	E	105	ARG	NE-CZ-NH1	14.80	127.70	120.30
1	D	27	ARG	NE-CZ-NH1	14.47	127.53	120.30
1	C	146	ALA	CB-CA-C	-14.24	88.74	110.10
1	A	27	ARG	NE-CZ-NH1	14.19	127.39	120.30
1	F	18	ARG	NE-CZ-NH2	-14.06	113.27	120.30
1	C	6	ARG	NE-CZ-NH2	-14.01	113.29	120.30
1	B	108	PHE	CB-CG-CD2	-13.90	111.07	120.80
1	B	8	PHE	CB-CG-CD1	-13.86	111.10	120.80
1	C	88	ARG	NE-CZ-NH1	-13.77	113.41	120.30
1	D	88	ARG	NE-CZ-NH1	13.62	127.11	120.30
1	A	88	ARG	NE-CZ-NH1	13.56	127.08	120.30
1	B	121	ASP	CB-CG-OD1	13.49	130.44	118.30
1	B	121	ASP	CB-CG-OD2	-13.48	106.17	118.30
1	C	14	ASP	CB-CG-OD1	13.37	130.33	118.30
1	A	114	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	F	41	MET	CG-SD-CE	13.27	121.42	100.20
1	B	151	TYR	CB-CG-CD1	13.21	128.93	121.00
1	C	58	ARG	NE-CZ-NH2	-13.20	113.70	120.30
1	F	38	MET	CG-SD-CE	-13.11	79.23	100.20
1	E	90	MET	CG-SD-CE	12.92	120.88	100.20
1	B	74	VAL	CA-CB-CG1	-12.87	91.59	110.90
1	F	67	TYR	CB-CG-CD1	12.77	128.66	121.00
1	D	114	ARG	NE-CZ-NH2	-12.66	113.97	120.30
1	A	112	VAL	CB-CA-C	-12.65	87.36	111.40
1	F	36	VAL	CA-CB-CG1	-12.63	91.96	110.90
1	E	42	ARG	NE-CZ-NH2	12.51	126.55	120.30
1	B	76	MET	CG-SD-CE	-12.50	80.20	100.20
1	D	41	MET	CG-SD-CE	-12.49	80.22	100.20
1	F	52	TYR	CB-CG-CD1	-12.49	113.51	121.00
1	F	42	ARG	NE-CZ-NH2	-12.44	114.08	120.30
1	F	105	ARG	NE-CZ-NH1	12.19	126.39	120.30
1	B	151	TYR	CB-CG-CD2	-12.14	113.71	121.00
1	A	8	PHE	CB-CG-CD1	-12.04	112.37	120.80
1	A	151	TYR	CB-CG-CD1	12.00	128.20	121.00
1	A	42	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	A	151	TYR	CB-CG-CD2	-11.94	113.84	121.00
1	B	105	ARG	NE-CZ-NH1	-11.85	114.38	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	35	LEU	CB-CG-CD2	11.78	131.03	111.00
1	D	58	ARG	NE-CZ-NH2	-11.71	114.44	120.30
1	A	34	ARG	NE-CZ-NH2	11.68	126.14	120.30
1	E	98	ASP	CB-CG-OD2	-11.56	107.90	118.30
1	E	36	VAL	CA-CB-CG1	-11.49	93.66	110.90
1	E	122	SER	N-CA-CB	11.47	127.70	110.50
1	C	67	TYR	CB-CG-CD2	-11.38	114.17	121.00
1	F	134	PHE	CB-CG-CD1	11.25	128.67	120.80
1	C	89	VAL	CG1-CB-CG2	11.15	128.75	110.90
1	E	54	ASP	CB-CG-OD1	-11.13	108.28	118.30
1	A	14	ASP	CB-CG-OD1	-11.06	108.35	118.30
1	C	97	ALA	CB-CA-C	-11.03	93.56	110.10
1	C	41	MET	CG-SD-CE	-10.98	82.63	100.20
1	D	67	TYR	CB-CG-CD1	10.90	127.54	121.00
1	F	34	ARG	NE-CZ-NH2	10.82	125.71	120.30
1	D	7	THR	CA-CB-CG2	-10.81	97.26	112.40
1	F	46	ASP	CB-CG-OD2	-10.78	108.60	118.30
1	B	7	THR	CA-CB-CG2	-10.73	97.38	112.40
1	F	151	TYR	CB-CG-CD2	-10.71	114.57	121.00
1	B	67	TYR	CB-CG-CD2	-10.67	114.60	121.00
1	C	27	ARG	NE-CZ-NH2	-10.49	115.06	120.30
1	E	67	TYR	CB-CG-CD1	10.49	127.29	121.00
1	D	6	ARG	NE-CZ-NH1	10.49	125.54	120.30
1	D	90	MET	CG-SD-CE	10.47	116.95	100.20
1	F	35	LEU	CB-CA-C	-10.41	90.42	110.20
1	E	6	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	B	151	TYR	N-CA-CB	10.29	129.11	110.60
1	F	132	LEU	CB-CG-CD1	-10.24	93.59	111.00
1	D	135	HIS	C-N-CD	-10.03	98.54	120.60
1	B	88	ARG	NE-CZ-NH1	-10.01	115.29	120.30
1	F	52	TYR	CB-CG-CD2	10.01	127.00	121.00
1	C	115	ASN	C-N-CA	9.97	146.64	121.70
1	B	8	PHE	CB-CG-CD2	9.94	127.76	120.80
1	A	54	ASP	CB-CG-OD1	9.93	127.24	118.30
1	C	67	TYR	CB-CG-CD1	9.92	126.95	121.00
1	C	14	ASP	CB-CG-OD2	-9.90	109.39	118.30
1	E	54	ASP	CA-CB-CG	-9.89	91.64	113.40
1	A	42	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	B	84	VAL	CA-CB-CG1	-9.81	96.18	110.90
1	E	67	TYR	CB-CG-CD2	-9.73	115.16	121.00
1	E	103	THR	CA-CB-CG2	9.65	125.92	112.40
1	E	76	MET	CG-SD-CE	-9.65	84.76	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	126	ALA	CB-CA-C	9.62	124.54	110.10
1	A	114	ARG	CG-CD-NE	-9.59	91.65	111.80
1	A	133	TRP	CD1-NE1-CE2	-9.56	100.39	109.00
1	A	24	ILE	CG1-CB-CG2	-9.48	90.54	111.40
1	D	114	ARG	CD-NE-CZ	9.46	136.85	123.60
1	C	21	ILE	CG1-CB-CG2	-9.44	90.64	111.40
1	D	5	GLU	CB-CA-C	-9.44	91.53	110.40
1	E	27	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	E	16	VAL	CG1-CB-CG2	-9.33	95.98	110.90
1	B	114	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	F	114	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	C	6	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	C	7	THR	CA-CB-CG2	-9.12	99.63	112.40
1	D	121	ASP	CB-CA-C	-9.09	92.22	110.40
1	F	132	LEU	CB-CG-CD2	9.05	126.39	111.00
1	B	48	LEU	CB-CG-CD1	9.04	126.36	111.00
1	E	35	LEU	CB-CG-CD2	8.98	126.26	111.00
1	C	95	ASN	CB-CA-C	-8.97	92.46	110.40
1	F	61	PHE	N-CA-CB	8.96	126.73	110.60
1	D	77	VAL	CA-CB-CG1	-8.95	97.48	110.90
1	B	120	SER	N-CA-CB	8.91	123.87	110.50
1	C	140	VAL	CG1-CB-CG2	8.90	125.14	110.90
1	F	122	SER	N-CA-CB	8.89	123.84	110.50
1	F	121	ASP	CB-CG-OD1	8.89	126.30	118.30
1	B	79	GLU	OE1-CD-OE2	-8.88	112.64	123.30
1	A	18	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	E	117	ILE	CA-CB-CG2	-8.78	93.33	110.90
1	D	34	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	D	38	MET	CG-SD-CE	-8.71	86.26	100.20
1	A	18	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	B	100	LYS	CB-CA-C	-8.58	93.24	110.40
1	C	6	ARG	CA-CB-CG	-8.55	94.58	113.40
1	F	69	HIS	CB-CA-C	8.55	127.50	110.40
1	F	27	ARG	NE-CZ-NH1	-8.50	116.05	120.30
1	E	10	ALA	CB-CA-C	-8.46	97.41	110.10
1	E	43	ALA	N-CA-CB	8.41	121.88	110.10
1	B	94	THR	CA-CB-CG2	-8.40	100.64	112.40
1	F	73	VAL	CG1-CB-CG2	8.39	124.33	110.90
1	F	62	ALA	CB-CA-C	8.39	122.69	110.10
1	E	105	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	B	37	ALA	CB-CA-C	-8.35	97.57	110.10
1	E	77	VAL	O-C-N	8.35	136.06	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	127	GLU	CG-CD-OE2	-8.34	101.63	118.30
1	C	132	LEU	CB-CG-CD1	-8.26	96.95	111.00
1	C	27	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	E	108	PHE	CB-CG-CD1	8.25	126.57	120.80
1	F	27	ARG	N-CA-CB	-8.25	95.76	110.60
1	D	67	TYR	CB-CG-CD2	-8.24	116.05	121.00
1	F	46	ASP	CB-CG-OD1	8.24	125.72	118.30
1	B	143	LYS	CB-CA-C	-8.22	93.95	110.40
1	C	54	ASP	CB-CG-OD1	-8.21	110.91	118.30
1	D	68	MET	CG-SD-CE	8.21	113.33	100.20
1	E	95	ASN	CB-CA-C	-8.19	94.03	110.40
1	C	67	TYR	N-CA-CB	-8.18	95.88	110.60
1	A	16	VAL	CA-CB-CG1	8.17	123.15	110.90
1	A	18	ARG	NH1-CZ-NH2	-8.16	110.42	119.40
1	E	123	VAL	CA-CB-CG2	-8.15	98.67	110.90
1	F	114	ARG	CA-CB-CG	-8.13	95.52	113.40
1	B	125	SER	CB-CA-C	8.06	125.42	110.10
1	F	152	GLU	N-CA-CB	-8.05	96.11	110.60
1	F	14	ASP	CB-CG-OD1	8.02	125.52	118.30
1	F	137	GLU	CG-CD-OE2	-8.02	102.26	118.30
1	B	67	TYR	CB-CG-CD1	8.01	125.81	121.00
1	F	88	ARG	CD-NE-CZ	8.00	134.80	123.60
1	C	18	ARG	N-CA-CB	-8.00	96.20	110.60
1	C	98	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	B	134	PHE	CB-CG-CD2	-7.97	115.22	120.80
1	B	30	GLN	CA-CB-CG	-7.96	95.90	113.40
1	C	46	ASP	CB-CG-OD2	7.93	125.44	118.30
1	F	77	VAL	CA-CB-CG2	-7.93	99.01	110.90
1	E	115	ASN	CA-CB-CG	-7.92	95.97	113.40
1	B	115	ASN	C-N-CA	7.91	141.49	121.70
1	E	93	GLU	N-CA-CB	7.90	124.83	110.60
1	B	103	THR	CA-CB-CG2	7.89	123.45	112.40
1	C	111	GLN	N-CA-CB	-7.87	96.43	110.60
1	E	136	PRO	N-CA-CB	-7.86	93.86	103.30
1	E	23	GLU	CG-CD-OE1	7.84	133.98	118.30
1	C	105	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	C	66	LYS	CD-CE-NZ	7.80	129.64	111.70
1	F	105	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	F	123	VAL	CG1-CB-CG2	-7.80	98.42	110.90
1	D	151	TYR	CB-CG-CD2	-7.73	116.36	121.00
1	B	132	LEU	CB-CA-C	-7.72	95.54	110.20
1	A	32	GLY	O-C-N	-7.70	110.38	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	28	PHE	CB-CG-CD1	7.67	126.17	120.80
1	C	134	PHE	CB-CA-C	-7.67	95.07	110.40
1	D	73	VAL	O-C-N	7.67	134.96	122.70
1	D	89	VAL	CA-CB-CG2	-7.67	99.40	110.90
1	A	50	GLU	N-CA-CB	-7.65	96.83	110.60
1	D	97	ALA	CB-CA-C	-7.64	98.64	110.10
1	A	83	VAL	CB-CA-C	-7.64	96.89	111.40
1	F	67	TYR	CG-CD1-CE1	-7.64	115.19	121.30
1	A	142	TYR	O-C-N	7.63	134.91	122.70
1	F	124	GLU	CB-CA-C	-7.63	95.14	110.40
1	B	33	PHE	N-CA-CB	-7.62	96.88	110.60
1	B	40	PHE	CG-CD2-CE2	7.62	129.18	120.80
1	A	67	TYR	CB-CG-CD2	-7.61	116.43	121.00
1	A	18	ARG	CA-CB-CG	-7.60	96.67	113.40
1	A	68	MET	CG-SD-CE	7.60	112.36	100.20
1	C	20	LEU	CB-CG-CD2	-7.57	98.13	111.00
1	F	61	PHE	CB-CG-CD1	-7.54	115.52	120.80
1	D	141	ASN	CB-CA-C	7.53	125.47	110.40
1	E	60	PHE	CB-CG-CD1	7.52	126.06	120.80
1	A	54	ASP	CB-CG-OD2	-7.52	111.54	118.30
1	C	70	SER	CB-CA-C	-7.51	95.82	110.10
1	B	105	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	A	38	MET	CG-SD-CE	-7.45	88.29	100.20
1	F	111	GLN	CG-CD-OE1	-7.43	106.74	121.60
1	D	18	ARG	NH1-CZ-NH2	-7.42	111.23	119.40
1	B	88	ARG	NH1-CZ-NH2	7.41	127.55	119.40
1	F	10	ALA	CB-CA-C	7.39	121.19	110.10
1	F	98	ASP	N-CA-CB	-7.39	97.30	110.60
1	D	35	LEU	CB-CA-C	-7.38	96.18	110.20
1	E	129	GLU	OE1-CD-OE2	-7.38	114.45	123.30
1	B	108	PHE	CB-CG-CD1	7.37	125.96	120.80
1	B	124	GLU	O-C-N	7.36	134.47	122.70
1	A	91	LEU	CB-CA-C	-7.35	96.23	110.20
1	A	134	PHE	N-CA-CB	-7.33	97.40	110.60
1	C	112	VAL	CA-CB-CG1	7.33	121.89	110.90
1	D	90	MET	CA-CB-CG	-7.31	100.86	113.30
1	A	99	SER	CB-CA-C	-7.31	96.21	110.10
1	A	115	ASN	N-CA-C	7.30	130.72	111.00
1	F	10	ALA	N-CA-CB	-7.28	99.90	110.10
1	A	13	PRO	N-CA-CB	7.27	112.03	103.30
1	A	132	LEU	CB-CG-CD1	7.26	123.35	111.00
1	D	11	ILE	O-C-N	7.25	134.29	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	103	THR	CA-CB-CG2	-7.24	102.27	112.40
1	A	61	PHE	CB-CG-CD1	7.22	125.86	120.80
1	C	57	ASP	CB-CG-OD1	-7.22	111.80	118.30
1	A	103	THR	OG1-CB-CG2	7.21	126.58	110.00
1	E	86	THR	CA-CB-CG2	-7.21	102.31	112.40
1	C	127	GLU	O-C-N	7.21	134.23	122.70
1	B	27	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	F	142	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	D	38	MET	O-C-N	7.19	134.21	122.70
1	F	20	LEU	CB-CG-CD1	-7.18	98.79	111.00
1	E	98	ASP	CB-CG-OD1	7.17	124.75	118.30
1	B	40	PHE	CB-CA-C	-7.16	96.07	110.40
1	C	120	SER	N-CA-CB	7.16	121.24	110.50
1	A	34	ARG	NH1-CZ-NH2	-7.12	111.56	119.40
1	A	27	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	F	14	ASP	CB-CG-OD2	-7.12	111.90	118.30
1	A	142	TYR	N-CA-CB	7.11	123.40	110.60
1	D	90	MET	C-N-CA	7.10	139.44	121.70
1	B	76	MET	O-C-N	7.09	134.04	122.70
1	D	152	GLU	CA-C-O	-7.08	105.23	120.10
1	D	133	TRP	CD1-NE1-CE2	-7.08	102.63	109.00
1	E	135	HIS	N-CA-CB	7.07	123.33	110.60
1	B	141	ASN	CB-CA-C	7.07	124.54	110.40
1	A	149	TRP	CH2-CZ2-CE2	-7.07	110.33	117.40
1	F	86	THR	CA-CB-CG2	-7.05	102.53	112.40
1	F	61	PHE	C-N-CA	-7.05	104.07	121.70
1	F	88	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	134	PHE	CA-C-N	-7.03	101.74	117.20
1	C	101	PRO	N-CA-CB	7.02	111.73	103.30
1	B	141	ASN	N-CA-CB	7.02	123.23	110.60
1	C	28	PHE	CA-CB-CG	-7.01	97.07	113.90
1	B	73	VAL	CA-CB-CG1	-7.01	100.39	110.90
1	A	61	PHE	CB-CG-CD2	-7.00	115.90	120.80
1	E	42	ARG	O-C-N	-7.00	111.51	122.70
1	A	2	ALA	O-C-N	6.98	133.86	122.70
1	D	35	LEU	CB-CG-CD2	6.97	122.85	111.00
1	A	121	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	D	69	HIS	O-C-N	6.96	133.83	122.70
1	F	44	SER	N-CA-CB	6.93	120.90	110.50
1	A	139	LEU	O-C-N	6.93	133.78	122.70
1	C	34	ARG	NH1-CZ-NH2	-6.92	111.78	119.40
1	C	84	VAL	CA-CB-CG2	-6.92	100.53	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	118	HIS	O-C-N	6.92	134.96	123.20
1	B	118	HIS	CB-CA-C	-6.92	96.57	110.40
1	F	60	PHE	CB-CG-CD1	-6.90	115.97	120.80
1	C	29	GLU	CG-CD-OE1	-6.87	104.57	118.30
1	A	21	ILE	CA-CB-CG2	6.86	124.62	110.90
1	E	2	ALA	N-CA-CB	6.84	119.67	110.10
1	B	124	GLU	CB-CA-C	-6.83	96.74	110.40
1	A	4	SER	CB-CA-C	6.81	123.04	110.10
1	D	143	LYS	CD-CE-NZ	6.81	127.35	111.70
1	C	42	ARG	CB-CA-C	-6.80	96.81	110.40
1	E	38	MET	CG-SD-CE	6.78	111.05	100.20
1	B	111	GLN	N-CA-CB	-6.77	98.41	110.60
1	C	63	GLY	O-C-N	6.76	133.52	122.70
1	D	139	LEU	CB-CG-CD2	-6.76	99.52	111.00
1	D	2	ALA	CB-CA-C	-6.75	99.97	110.10
1	B	54	ASP	CB-CG-OD1	-6.75	112.22	118.30
1	C	113	GLY	CA-C-O	6.74	132.74	120.60
1	A	85	LYS	N-CA-CB	-6.74	98.46	110.60
1	D	134	PHE	N-CA-CB	-6.74	98.47	110.60
1	C	136	PRO	CB-CA-C	-6.73	95.18	112.00
1	E	116	ILE	CA-CB-CG2	-6.71	97.48	110.90
1	A	3	ASN	CB-CA-C	-6.70	96.99	110.40
1	F	120	SER	N-CA-CB	6.70	120.55	110.50
1	E	88	ARG	CA-CB-CG	-6.69	98.68	113.40
1	B	134	PHE	N-CA-CB	6.68	122.62	110.60
1	E	18	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	55	LEU	N-CA-CB	-6.68	97.05	110.40
1	C	114	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	F	121	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	C	150	ILE	CA-CB-CG2	-6.67	97.57	110.90
1	D	10	ALA	N-CA-CB	6.67	119.43	110.10
1	C	151	TYR	CB-CG-CD1	6.66	125.00	121.00
1	F	77	VAL	CG1-CB-CG2	6.65	121.54	110.90
1	E	151	TYR	CG-CD2-CE2	-6.65	115.98	121.30
1	D	130	ILE	CB-CA-C	-6.64	98.32	111.60
1	A	67	TYR	CB-CA-C	6.64	123.67	110.40
1	C	151	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	C	139	LEU	CB-CG-CD2	-6.62	99.75	111.00
1	D	18	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	E	39	LYS	CD-CE-NZ	6.59	126.86	111.70
1	E	115	ASN	CB-CG-OD1	-6.59	108.43	121.60
1	C	83	VAL	CA-CB-CG2	6.58	120.78	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	77	VAL	N-CA-CB	6.58	125.98	111.50
1	E	17	GLN	CA-CB-CG	-6.57	98.95	113.40
1	A	140	VAL	CA-CB-CG2	6.56	120.74	110.90
1	C	93	GLU	CG-CD-OE2	-6.55	105.19	118.30
1	D	102	GLY	CA-C-O	6.55	132.40	120.60
1	A	151	TYR	O-C-N	6.54	133.17	122.70
1	B	148	ASN	CB-CA-C	-6.54	97.31	110.40
1	F	34	ARG	NH1-CZ-NH2	-6.53	112.21	119.40
1	D	47	LEU	CB-CG-CD1	-6.53	99.91	111.00
1	F	5	GLU	CG-CD-OE2	-6.52	105.26	118.30
1	B	140	VAL	CG1-CB-CG2	-6.51	100.48	110.90
1	F	40	PHE	CB-CA-C	-6.51	97.38	110.40
1	A	122	SER	N-CA-CB	6.51	120.26	110.50
1	E	34	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	D	81	LEU	CB-CG-CD2	-6.50	99.95	111.00
1	A	151	TYR	CA-C-N	-6.50	102.91	117.20
1	B	134	PHE	CB-CG-CD1	6.49	125.34	120.80
1	E	18	ARG	CD-NE-CZ	6.49	132.69	123.60
1	F	57	ASP	O-C-N	6.49	133.09	122.70
1	F	137	GLU	CG-CD-OE1	6.49	131.28	118.30
1	E	30	GLN	CA-CB-CG	-6.49	99.13	113.40
1	F	150	ILE	CA-C-N	-6.48	102.94	117.20
1	F	100	LYS	N-CA-CB	-6.48	98.94	110.60
1	A	37	ALA	CB-CA-C	-6.47	100.39	110.10
1	E	85	LYS	N-CA-CB	-6.45	98.99	110.60
1	D	42	ARG	C-N-CA	-6.44	105.59	121.70
1	D	90	MET	O-C-N	6.44	133.01	122.70
1	D	133	TRP	O-C-N	6.42	132.98	122.70
1	D	86	THR	CA-CB-CG2	-6.42	103.42	112.40
1	D	88	ARG	CD-NE-CZ	6.40	132.56	123.60
1	F	27	ARG	CG-CD-NE	6.40	125.23	111.80
1	D	117	ILE	CA-CB-CG1	6.38	123.12	111.00
1	C	124	GLU	CA-CB-CG	-6.37	99.39	113.40
1	F	67	TYR	CZ-CE2-CD2	-6.37	114.07	119.80
1	D	28	PHE	CE1-CZ-CE2	-6.36	108.55	120.00
1	B	59	PRO	CB-CA-C	-6.35	96.11	112.00
1	E	151	TYR	CZ-CE2-CD2	6.35	125.51	119.80
1	B	72	PRO	N-CD-CG	6.33	112.70	103.20
1	C	58	ARG	CD-NE-CZ	6.32	132.44	123.60
1	A	121	ASP	CB-CA-C	-6.32	97.77	110.40
1	B	88	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	A	114	ARG	NH1-CZ-NH2	6.30	126.33	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	65	VAL	CA-CB-CG2	-6.29	101.46	110.90
1	A	127	GLU	CA-CB-CG	-6.29	99.56	113.40
1	E	118	HIS	CA-C-N	-6.29	103.62	116.20
1	A	142	TYR	N-CA-C	-6.29	94.02	111.00
1	B	72	PRO	CA-N-CD	-6.29	102.70	111.50
1	C	132	LEU	N-CA-CB	-6.28	97.85	110.40
1	C	122	SER	CA-C-N	-6.27	103.40	117.20
1	A	133	TRP	O-C-N	6.27	132.73	122.70
1	E	37	ALA	CB-CA-C	-6.26	100.71	110.10
1	D	80	GLY	CA-C-O	6.26	131.86	120.60
1	E	107	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	C	146	ALA	N-CA-CB	-6.24	101.36	110.10
1	D	38	MET	CB-CA-C	-6.24	97.92	110.40
1	A	63	GLY	O-C-N	6.24	132.68	122.70
1	F	16	VAL	CA-CB-CG1	6.24	120.25	110.90
1	D	40	PHE	CB-CG-CD2	-6.23	116.44	120.80
1	F	78	TRP	O-C-N	6.22	132.66	122.70
1	C	29	GLU	N-CA-CB	6.22	121.79	110.60
1	D	133	TRP	CA-C-N	-6.21	103.53	117.20
1	A	136	PRO	O-C-N	-6.20	112.78	122.70
1	E	136	PRO	C-N-CA	-6.20	106.19	121.70
1	B	76	MET	CA-C-N	-6.19	103.59	117.20
1	C	91	LEU	N-CA-CB	-6.19	98.03	110.40
1	B	58	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	B	55	LEU	C-N-CA	6.18	137.14	121.70
1	D	83	VAL	CB-CA-C	-6.18	99.67	111.40
1	B	123	VAL	CB-CA-C	6.17	123.13	111.40
1	C	110	ILE	C-N-CA	-6.17	106.28	121.70
1	C	70	SER	O-C-N	6.16	133.67	123.20
1	F	31	LYS	N-CA-CB	-6.16	99.52	110.60
1	B	36	VAL	CA-CB-CG1	-6.16	101.67	110.90
1	E	81	LEU	CB-CG-CD1	6.15	121.46	111.00
1	F	144	SER	CB-CA-C	-6.14	98.43	110.10
1	D	102	GLY	O-C-N	-6.14	112.88	122.70
1	D	151	TYR	O-C-N	6.14	132.52	122.70
1	C	46	ASP	CB-CA-C	6.13	122.66	110.40
1	E	140	VAL	CA-CB-CG2	-6.12	101.71	110.90
1	E	61	PHE	N-CA-CB	6.12	121.62	110.60
1	B	112	VAL	CG1-CB-CG2	6.12	120.69	110.90
1	F	23	GLU	CB-CA-C	-6.12	98.17	110.40
1	C	39	LYS	O-C-N	6.11	132.48	122.70
1	C	108	PHE	C-N-CA	-6.11	106.43	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	137	GLU	CG-CD-OE2	-6.10	106.09	118.30
1	E	34	ARG	CB-CA-C	6.09	122.59	110.40
1	E	93	GLU	CA-C-O	6.09	132.88	120.10
1	E	115	ASN	O-C-N	6.08	132.43	122.70
1	A	98	ASP	CB-CA-C	6.08	122.56	110.40
1	D	74	VAL	CG1-CB-CG2	-6.07	101.18	110.90
1	B	138	GLU	OE1-CD-OE2	6.07	130.59	123.30
1	D	115	ASN	C-N-CA	6.07	136.88	121.70
1	F	4	SER	CB-CA-C	-6.06	98.59	110.10
1	B	131	ALA	O-C-N	6.05	132.39	122.70
1	E	77	VAL	CA-CB-CG2	-6.04	101.84	110.90
1	D	27	ARG	CG-CD-NE	6.04	124.48	111.80
1	D	143	LYS	CA-CB-CG	6.04	126.68	113.40
1	B	142	TYR	CB-CG-CD2	6.03	124.62	121.00
1	E	128	LYS	CB-CG-CD	6.03	127.28	111.60
1	F	37	ALA	O-C-N	-6.03	113.05	122.70
1	A	101	PRO	N-CA-CB	6.03	110.53	103.30
1	B	40	PHE	O-C-N	6.03	132.35	122.70
1	B	133	TRP	CB-CG-CD2	-6.03	118.76	126.60
1	C	86	THR	CA-CB-CG2	-6.02	103.97	112.40
1	D	55	LEU	CA-CB-CG	-6.02	101.46	115.30
1	B	11	ILE	CB-CA-C	-6.01	99.57	111.60
1	D	54	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	B	47	LEU	CB-CG-CD2	-5.99	100.82	111.00
1	B	122	SER	N-CA-CB	5.99	119.49	110.50
1	C	127	GLU	CG-CD-OE1	5.98	130.26	118.30
1	C	56	LYS	CB-CA-C	5.98	122.36	110.40
1	B	76	MET	N-CA-CB	5.97	121.35	110.60
1	B	26	LYS	O-C-N	-5.97	113.14	122.70
1	E	14	ASP	N-CA-CB	5.97	121.35	110.60
1	E	78	TRP	CE3-CZ3-CH2	-5.97	114.64	121.20
1	B	86	THR	CA-CB-CG2	-5.96	104.05	112.40
1	E	151	TYR	CG-CD1-CE1	5.96	126.07	121.30
1	C	57	ASP	CB-CG-OD2	5.96	123.67	118.30
1	D	127	GLU	CG-CD-OE1	5.95	130.21	118.30
1	A	27	ARG	CG-CD-NE	5.95	124.29	111.80
1	B	35	LEU	CD1-CG-CD2	5.95	128.35	110.50
1	B	123	VAL	CA-CB-CG1	5.95	119.82	110.90
1	B	134	PHE	O-C-N	5.95	132.22	122.70
1	E	21	ILE	CA-CB-CG2	5.95	122.79	110.90
1	D	149	TRP	CB-CG-CD2	-5.94	118.87	126.60
1	E	145	CYS	CA-C-N	-5.94	104.13	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	VAL	CA-CB-CG2	5.93	119.80	110.90
1	E	110	ILE	CB-CA-C	-5.93	99.74	111.60
1	B	60	PHE	O-C-N	5.92	132.17	122.70
1	B	58	ARG	O-C-N	5.91	132.33	121.10
1	B	37	ALA	N-CA-CB	-5.90	101.85	110.10
1	F	150	ILE	O-C-N	5.89	132.12	122.70
1	B	117	ILE	CG1-CB-CG2	-5.89	98.45	111.40
1	C	65	VAL	C-N-CA	-5.88	106.99	121.70
1	D	46	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	58	ARG	CA-CB-CG	-5.87	100.48	113.40
1	B	91	LEU	CA-C-N	-5.87	104.46	116.20
1	C	112	VAL	O-C-N	-5.87	113.22	123.20
1	C	34	ARG	CG-CD-NE	5.87	124.12	111.80
1	A	94	THR	CA-CB-CG2	-5.86	104.19	112.40
1	F	34	ARG	CB-CA-C	-5.86	98.69	110.40
1	B	42	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	B	116	ILE	CA-CB-CG1	-5.85	99.89	111.00
1	F	27	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	F	26	LYS	CB-CG-CD	-5.84	96.40	111.60
1	E	84	VAL	CG1-CB-CG2	5.84	120.25	110.90
1	B	91	LEU	C-N-CA	-5.84	110.03	122.30
1	A	107	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	100	LYS	N-CA-CB	-5.83	100.10	110.60
1	C	27	ARG	CG-CD-NE	5.83	124.03	111.80
1	D	93	GLU	CA-CB-CG	-5.83	100.58	113.40
1	E	44	SER	C-N-CA	-5.83	107.14	121.70
1	A	35	LEU	CB-CG-CD1	5.82	120.90	111.00
1	B	45	GLU	OE1-CD-OE2	5.81	130.27	123.30
1	D	126	ALA	CB-CA-C	5.81	118.81	110.10
1	D	115	ASN	CA-CB-CG	-5.80	100.63	113.40
1	E	78	TRP	CD2-CE2-CZ2	-5.80	115.33	122.30
1	E	65	VAL	CA-CB-CG2	5.80	119.60	110.90
1	F	29	GLU	CA-CB-CG	-5.80	100.65	113.40
1	C	76	MET	CB-CA-C	-5.79	98.81	110.40
1	F	42	ARG	NH1-CZ-NH2	5.79	125.77	119.40
1	A	31	LYS	N-CA-CB	5.79	121.02	110.60
1	D	6	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	26	LYS	O-C-N	-5.77	113.47	122.70
1	F	41	MET	CA-CB-CG	-5.77	103.50	113.30
1	A	64	LEU	CB-CA-C	5.77	121.16	110.20
1	A	34	ARG	CG-CD-NE	5.76	123.90	111.80
1	E	121	ASP	CB-CG-OD1	5.76	123.48	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	40	PHE	CZ-CE2-CD2	-5.76	113.19	120.10
1	F	107	ASP	N-CA-CB	-5.76	100.24	110.60
1	C	136	PRO	O-C-N	5.75	131.91	122.70
1	C	48	LEU	CB-CA-C	5.75	121.12	110.20
1	C	105	ARG	NH1-CZ-NH2	5.75	125.72	119.40
1	D	132	LEU	CB-CG-CD1	5.75	120.77	111.00
1	D	28	PHE	CZ-CE2-CD2	5.75	127.00	120.10
1	A	73	VAL	O-C-N	5.74	131.89	122.70
1	A	142	TYR	CA-C-N	-5.74	104.58	117.20
1	B	138	GLU	CG-CD-OE2	-5.73	106.83	118.30
1	D	108	PHE	C-N-CA	-5.73	107.37	121.70
1	C	50	GLU	CG-CD-OE1	-5.73	106.84	118.30
1	D	57	ASP	CB-CG-OD1	-5.73	113.14	118.30
1	D	134	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	F	93	GLU	CG-CD-OE2	-5.73	106.85	118.30
1	D	100	LYS	CA-C-O	5.73	132.12	120.10
1	B	129	GLU	CB-CA-C	-5.72	98.95	110.40
1	B	90	MET	O-C-N	5.72	131.86	122.70
1	B	152	GLU	N-CA-CB	5.71	120.88	110.60
1	A	88	ARG	CA-C-N	-5.70	104.65	117.20
1	E	68	MET	CA-CB-CG	-5.70	103.60	113.30
1	A	63	GLY	CA-C-N	-5.70	104.66	117.20
1	A	112	VAL	CA-CB-CG1	-5.69	102.36	110.90
1	C	108	PHE	CG-CD1-CE1	5.69	127.06	120.80
1	D	79	GLU	C-N-CA	-5.69	110.34	122.30
1	F	44	SER	O-C-N	5.69	131.81	122.70
1	C	87	GLY	C-N-CA	-5.69	107.48	121.70
1	A	35	LEU	N-CA-C	-5.68	95.66	111.00
1	D	8	PHE	O-C-N	5.68	131.78	122.70
1	E	38	MET	CA-C-O	5.67	132.02	120.10
1	E	122	SER	C-N-CA	-5.67	107.52	121.70
1	C	68	MET	CG-SD-CE	5.67	109.27	100.20
1	B	127	GLU	CG-CD-OE2	-5.67	106.97	118.30
1	C	84	VAL	O-C-N	5.67	131.76	122.70
1	A	98	ASP	N-CA-CB	5.66	120.79	110.60
1	E	55	LEU	N-CA-CB	5.66	121.72	110.40
1	A	147	GLN	N-CA-CB	-5.65	100.42	110.60
1	E	135	HIS	CA-C-O	5.65	131.97	120.10
1	E	88	ARG	O-C-N	5.65	131.74	122.70
1	B	46	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	51	HIS	CA-CB-CG	5.64	123.20	113.60
1	F	35	LEU	N-CA-CB	5.64	121.69	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	11	ILE	CB-CA-C	-5.64	100.32	111.60
1	C	65	VAL	O-C-N	-5.64	113.68	122.70
1	D	84	VAL	CA-CB-CG2	5.63	119.35	110.90
1	D	82	ASN	CA-CB-CG	5.63	125.79	113.40
1	C	107	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	108	PHE	CB-CA-C	-5.62	99.16	110.40
1	E	18	ARG	O-C-N	-5.62	113.64	123.20
1	F	122	SER	CA-C-N	-5.62	104.83	117.20
1	C	121	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	F	142	TYR	CB-CG-CD1	5.60	124.36	121.00
1	B	67	TYR	CB-CA-C	-5.59	99.22	110.40
1	A	29	GLU	CB-CA-C	-5.59	99.23	110.40
1	C	38	MET	CG-SD-CE	5.59	109.14	100.20
1	E	125	SER	CA-CB-OG	-5.58	96.12	111.20
1	B	79	GLU	CG-CD-OE1	5.58	129.47	118.30
1	E	149	TRP	CA-CB-CG	-5.58	103.09	113.70
1	A	48	LEU	C-N-CA	-5.58	107.75	121.70
1	C	28	PHE	CB-CG-CD1	5.58	124.70	120.80
1	B	121	ASP	O-C-N	-5.57	113.79	122.70
1	F	119	GLY	CA-C-O	-5.57	110.58	120.60
1	B	2	ALA	C-N-CA	5.57	135.62	121.70
1	D	79	GLU	N-CA-CB	5.57	120.62	110.60
1	D	89	VAL	CA-CB-CG1	5.57	119.25	110.90
1	E	65	VAL	CA-C-N	-5.56	104.97	117.20
1	D	8	PHE	CZ-CE2-CD2	5.55	126.77	120.10
1	B	31	LYS	CA-C-O	5.55	131.75	120.10
1	A	127	GLU	CA-C-N	-5.55	105.00	117.20
1	D	104	ILE	O-C-N	-5.54	113.83	122.70
1	F	52	TYR	CD1-CE1-CZ	-5.54	114.81	119.80
1	C	132	LEU	O-C-N	-5.53	113.85	122.70
1	A	98	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	108	PHE	N-CA-C	5.52	125.92	111.00
1	D	131	ALA	O-C-N	5.52	131.54	122.70
1	F	151	TYR	CG-CD2-CE2	-5.52	116.88	121.30
1	E	142	TYR	CG-CD2-CE2	5.52	125.72	121.30
1	B	115	ASN	N-CA-C	5.51	125.88	111.00
1	C	35	LEU	CB-CA-C	-5.51	99.73	110.20
1	C	93	GLU	CA-CB-CG	-5.51	101.28	113.40
1	D	58	ARG	CD-NE-CZ	5.51	131.32	123.60
1	D	91	LEU	C-N-CA	5.51	133.87	122.30
1	A	150	ILE	O-C-N	5.51	131.51	122.70
1	D	124	GLU	CA-C-O	5.51	131.67	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	97	ALA	O-C-N	5.50	131.50	122.70
1	C	121	ASP	CA-C-N	-5.50	105.10	117.20
1	E	146	ALA	N-CA-C	5.50	125.85	111.00
1	F	129	GLU	CG-CD-OE2	-5.50	107.31	118.30
1	C	24	ILE	CA-CB-CG2	-5.50	99.91	110.90
1	E	77	VAL	CA-C-N	-5.50	105.11	117.20
1	A	110	ILE	CA-CB-CG2	-5.49	99.91	110.90
1	B	134	PHE	CB-CA-C	-5.49	99.42	110.40
1	C	108	PHE	CB-CG-CD1	5.49	124.64	120.80
1	A	2	ALA	N-CA-CB	5.49	117.78	110.10
1	A	67	TYR	CG-CD2-CE2	-5.49	116.91	121.30
1	A	126	ALA	CB-CA-C	5.49	118.33	110.10
1	A	103	THR	CB-CA-C	-5.49	96.78	111.60
1	B	103	THR	CB-CA-C	-5.49	96.79	111.60
1	C	114	ARG	C-N-CA	-5.49	107.99	121.70
1	A	74	VAL	C-N-CA	-5.48	107.99	121.70
1	F	128	LYS	N-CA-CB	-5.48	100.74	110.60
1	A	26	LYS	CA-C-N	-5.47	105.17	117.20
1	A	46	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	123	VAL	CA-CB-CG2	5.47	119.11	110.90
1	D	98	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	146	ALA	N-CA-CB	-5.46	102.45	110.10
1	A	149	TRP	CD2-CE3-CZ3	-5.46	111.70	118.80
1	C	114	ARG	CG-CD-NE	-5.46	100.34	111.80
1	E	16	VAL	CA-CB-CG2	5.46	119.08	110.90
1	F	99	SER	CB-CA-C	-5.46	99.73	110.10
1	C	34	ARG	CD-NE-CZ	5.46	131.24	123.60
1	F	6	ARG	N-CA-CB	5.45	120.42	110.60
1	A	46	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	A	41	MET	CB-CA-C	-5.44	99.51	110.40
1	D	124	GLU	CA-C-N	-5.44	105.23	117.20
1	F	90	MET	O-C-N	5.44	131.41	122.70
1	C	114	ARG	CB-CG-CD	5.43	125.73	111.60
1	F	36	VAL	CA-CB-CG2	-5.43	102.75	110.90
1	C	62	ALA	CA-C-N	-5.43	105.34	116.20
1	A	48	LEU	CB-CA-C	-5.43	99.89	110.20
1	B	8	PHE	CB-CA-C	5.42	121.25	110.40
1	E	12	LYS	CD-CE-NZ	-5.42	99.23	111.70
1	D	130	ILE	CA-C-N	-5.42	105.28	117.20
1	F	89	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	A	135	HIS	N-CA-CB	5.41	120.34	110.60
1	B	127	GLU	CB-CA-C	-5.41	99.58	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	147	GLN	CA-C-N	-5.41	105.31	117.20
1	F	48	LEU	N-CA-CB	-5.40	99.60	110.40
1	F	111	GLN	O-C-N	5.40	131.33	122.70
1	C	34	ARG	N-CA-CB	5.39	120.31	110.60
1	A	133	TRP	N-CA-CB	5.39	120.31	110.60
1	F	138	GLU	CA-C-N	-5.39	105.35	117.20
1	A	43	ALA	CB-CA-C	-5.38	102.03	110.10
1	B	151	TYR	O-C-N	5.38	131.31	122.70
1	E	82	ASN	N-CA-CB	5.38	120.28	110.60
1	C	127	GLU	CB-CG-CD	5.38	128.71	114.20
1	D	98	ASP	O-C-N	5.38	131.30	122.70
1	D	14	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	F	93	GLU	CG-CD-OE1	5.37	129.04	118.30
1	B	77	VAL	CA-CB-CG1	-5.37	102.85	110.90
1	C	91	LEU	CA-C-O	5.37	131.37	120.10
1	E	118	HIS	CB-CA-C	-5.37	99.67	110.40
1	C	33	PHE	C-N-CA	-5.36	108.29	121.70
1	F	112	VAL	CB-CA-C	-5.36	101.22	111.40
1	F	61	PHE	CD1-CG-CD2	-5.36	111.33	118.30
1	A	35	LEU	O-C-N	5.35	131.27	122.70
1	D	49	LYS	O-C-N	5.35	131.26	122.70
1	D	74	VAL	CA-CB-CG1	-5.35	102.88	110.90
1	A	73	VAL	CA-CB-CG2	-5.34	102.89	110.90
1	F	88	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	F	104	ILE	CA-CB-CG2	-5.34	100.22	110.90
1	E	93	GLU	CA-CB-CG	-5.34	101.66	113.40
1	A	68	MET	CA-CB-CG	-5.34	104.23	113.30
1	E	55	LEU	O-C-N	5.33	131.23	122.70
1	A	76	MET	N-CA-CB	-5.33	101.01	110.60
1	F	40	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	E	20	LEU	N-CA-CB	-5.33	99.75	110.40
1	B	115	ASN	CA-CB-CG	-5.33	101.68	113.40
1	F	81	LEU	CB-CA-C	-5.33	100.08	110.20
1	F	145	CYS	CA-CB-SG	-5.32	104.42	114.00
1	F	104	ILE	CA-C-O	5.32	131.27	120.10
1	B	145	CYS	CB-CA-C	5.32	121.04	110.40
1	A	110	ILE	N-CA-CB	-5.31	98.59	110.80
1	F	6	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	47	LEU	CA-CB-CG	-5.31	103.09	115.30
1	C	88	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	E	42	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
1	F	112	VAL	CA-CB-CG1	5.31	118.86	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	98	ASP	N-CA-CB	-5.31	101.05	110.60
1	C	132	LEU	CB-CA-C	5.30	120.28	110.20
1	E	5	GLU	CG-CD-OE2	-5.30	107.69	118.30
1	B	107	ASP	CA-CB-CG	-5.30	101.74	113.40
1	D	65	VAL	CA-CB-CG2	-5.30	102.95	110.90
1	E	127	GLU	O-C-N	5.30	131.17	122.70
1	A	108	PHE	N-CA-C	5.29	125.29	111.00
1	C	94	THR	C-N-CA	5.29	134.93	121.70
1	C	79	GLU	CA-C-N	-5.29	105.63	116.20
1	F	126	ALA	CB-CA-C	-5.29	102.17	110.10
1	A	116	ILE	N-CA-C	5.29	125.27	111.00
1	A	3	ASN	N-CA-CB	5.27	120.09	110.60
1	C	27	ARG	CD-NE-CZ	5.27	130.98	123.60
1	A	142	TYR	CG-CD1-CE1	5.27	125.52	121.30
1	C	91	LEU	CB-CG-CD1	5.27	119.96	111.00
1	B	54	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	100	LYS	N-CA-C	5.27	125.22	111.00
1	F	68	MET	CA-CB-CG	-5.27	104.34	113.30
1	A	21	ILE	CA-C-O	-5.27	109.04	120.10
1	A	90	MET	N-CA-CB	5.26	120.08	110.60
1	D	48	LEU	CA-C-N	-5.26	105.62	117.20
1	E	74	VAL	N-CA-C	-5.26	96.80	111.00
1	E	81	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	F	148	ASN	N-CA-CB	5.25	120.06	110.60
1	C	60	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	D	25	ILE	CA-CB-CG1	5.25	120.97	111.00
1	D	51	HIS	CA-CB-CG	-5.25	104.68	113.60
1	B	107	ASP	O-C-N	5.25	131.09	122.70
1	E	46	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	6	ARG	CA-CB-CG	-5.24	101.87	113.40
1	D	62	ALA	N-CA-CB	5.24	117.44	110.10
1	D	136	PRO	N-CD-CG	-5.24	95.34	103.20
1	E	142	TYR	CB-CG-CD2	5.24	124.14	121.00
1	F	31	LYS	O-C-N	-5.24	114.29	123.20
1	F	107	ASP	CB-CG-OD1	5.24	123.02	118.30
1	C	87	GLY	CA-C-O	5.24	130.03	120.60
1	E	11	ILE	CB-CA-C	-5.24	101.12	111.60
1	A	149	TRP	CA-CB-CG	-5.23	103.75	113.70
1	B	82	ASN	O-C-N	-5.23	114.33	122.70
1	A	8	PHE	CG-CD1-CE1	-5.23	115.05	120.80
1	C	47	LEU	CA-C-N	-5.23	105.70	117.20
1	E	23	GLU	OE1-CD-OE2	-5.22	117.03	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	67	TYR	N-CA-CB	-5.22	101.21	110.60
1	A	38	MET	CA-CB-CG	5.21	122.16	113.30
1	A	42	ARG	CG-CD-NE	5.21	122.73	111.80
1	B	101	PRO	C-N-CA	-5.21	111.37	122.30
1	F	18	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	F	107	ASP	C-N-CA	-5.20	108.69	121.70
1	F	144	SER	O-C-N	5.20	131.02	122.70
1	E	60	PHE	CA-CB-CG	5.20	126.38	113.90
1	A	141	ASN	CB-CA-C	5.20	120.79	110.40
1	A	35	LEU	CB-CA-C	-5.19	100.34	110.20
1	F	66	LYS	CA-C-N	-5.18	105.79	117.20
1	F	108	PHE	N-CA-CB	-5.18	101.27	110.60
1	E	151	TYR	C-N-CA	-5.18	108.74	121.70
1	F	43	ALA	N-CA-CB	-5.18	102.84	110.10
1	B	72	PRO	N-CA-CB	5.18	109.52	103.30
1	A	96	PRO	CA-N-CD	-5.18	104.25	111.50
1	C	148	ASN	CA-CB-CG	-5.18	102.01	113.40
1	B	129	GLU	OE1-CD-OE2	5.18	129.51	123.30
1	E	104	ILE	CA-CB-CG1	5.18	120.84	111.00
1	E	52	TYR	CB-CG-CD2	5.18	124.11	121.00
1	F	152	GLU	CB-CA-C	5.18	120.75	110.40
1	F	126	ALA	C-N-CA	-5.17	108.78	121.70
1	F	132	LEU	O-C-N	-5.17	114.44	122.70
1	C	26	LYS	CA-C-O	5.16	130.94	120.10
1	A	108	PHE	C-N-CA	-5.16	108.80	121.70
1	F	67	TYR	CD1-CG-CD2	5.16	123.57	117.90
1	B	106	GLY	CA-C-O	5.15	129.88	120.60
1	D	5	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	D	27	ARG	NH1-CZ-NH2	-5.15	113.73	119.40
1	B	139	LEU	CD1-CG-CD2	-5.15	95.05	110.50
1	D	66	LYS	N-CA-CB	-5.15	101.34	110.60
1	B	55	LEU	N-CA-CB	-5.14	100.11	110.40
1	B	70	SER	CB-CA-C	-5.14	100.33	110.10
1	C	124	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	A	3	ASN	O-C-N	5.14	130.93	122.70
1	E	43	ALA	O-C-N	5.14	130.93	122.70
1	A	62	ALA	N-CA-CB	5.14	117.29	110.10
1	A	46	ASP	O-C-N	5.13	130.92	122.70
1	D	22	GLY	CA-C-O	5.13	129.84	120.60
1	E	34	ARG	CA-CB-CG	5.13	124.69	113.40
1	D	77	VAL	CB-CA-C	-5.13	101.65	111.40
1	A	105	ARG	CG-CD-NE	5.13	122.57	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	28	PHE	O-C-N	5.13	130.91	122.70
1	A	14	ASP	CB-CG-OD2	5.12	122.91	118.30
1	F	111	GLN	N-CA-CB	5.12	119.82	110.60
1	F	131	ALA	CB-CA-C	-5.12	102.42	110.10
1	F	33	PHE	N-CA-CB	-5.12	101.39	110.60
1	A	109	CYS	CA-CB-SG	-5.12	104.79	114.00
1	D	6	ARG	CA-CB-CG	-5.11	102.17	113.40
1	E	137	GLU	O-C-N	5.11	130.87	122.70
1	D	64	LEU	CB-CA-C	-5.10	100.51	110.20
1	D	149	TRP	CH2-CZ2-CE2	5.10	122.50	117.40
1	D	58	ARG	NH1-CZ-NH2	5.09	125.00	119.40
1	D	127	GLU	CB-CA-C	-5.09	100.21	110.40
1	F	86	THR	C-N-CA	-5.09	111.60	122.30
1	F	133	TRP	N-CA-CB	5.09	119.77	110.60
1	B	149	TRP	CA-CB-CG	-5.09	104.03	113.70
1	A	95	ASN	CB-CA-C	-5.09	100.22	110.40
1	A	89	VAL	O-C-N	5.09	130.84	122.70
1	B	86	THR	CA-CB-OG1	-5.09	98.32	109.00
1	F	77	VAL	CA-CB-CG1	5.09	118.53	110.90
1	C	142	TYR	CB-CG-CD2	5.08	124.05	121.00
1	C	27	ARG	O-C-N	5.08	130.83	122.70
1	B	106	GLY	CA-C-N	-5.08	106.02	117.20
1	A	27	ARG	CB-CG-CD	-5.08	98.39	111.60
1	D	40	PHE	CB-CA-C	-5.08	100.24	110.40
1	B	152	GLU	CA-C-O	-5.08	109.44	120.10
1	C	6	ARG	CB-CG-CD	5.08	124.81	111.60
1	B	109	CYS	N-CA-CB	-5.08	101.46	110.60
1	F	132	LEU	C-N-CA	-5.08	109.01	121.70
1	A	78	TRP	CG-CD2-CE3	-5.07	129.34	133.90
1	D	43	ALA	N-CA-CB	-5.07	103.00	110.10
1	A	133	TRP	NE1-CE2-CD2	5.07	112.37	107.30
1	C	106	GLY	O-C-N	-5.07	114.59	122.70
1	A	49	LYS	CA-CB-CG	-5.07	102.25	113.40
1	A	68	MET	N-CA-CB	-5.07	101.48	110.60
1	A	40	PHE	N-CA-CB	-5.07	101.48	110.60
1	A	148	ASN	CB-CA-C	5.07	120.53	110.40
1	D	5	GLU	CG-CD-OE1	5.06	128.43	118.30
1	E	139	LEU	O-C-N	5.06	130.80	122.70
1	A	131	ALA	CA-C-O	-5.06	109.48	120.10
1	D	47	LEU	CB-CA-C	-5.06	100.59	110.20
1	C	28	PHE	CA-C-O	5.06	130.72	120.10
1	C	101	PRO	O-C-N	5.05	131.79	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	D	23	GLU	CG-CD-OE1	-5.05	108.20	118.30
1	D	49	LYS	CA-C-N	-5.04	106.10	117.20
1	D	67	TYR	CD1-CE1-CZ	5.04	124.34	119.80
1	D	125	SER	N-CA-C	-5.04	97.38	111.00
1	E	41	MET	N-CA-CB	-5.04	101.52	110.60
1	F	133	TRP	CB-CA-C	-5.04	100.31	110.40
1	D	29	GLU	N-CA-CB	5.04	119.67	110.60
1	E	18	ARG	CA-C-O	5.04	130.68	120.10
1	F	35	LEU	CB-CG-CD2	5.04	119.56	111.00
1	B	8	PHE	CD1-CE1-CZ	-5.03	114.06	120.10
1	F	88	ARG	CA-C-N	-5.03	106.13	117.20
1	A	80	GLY	CA-C-O	5.03	129.65	120.60
1	F	115	ASN	CB-CA-C	5.03	120.45	110.40
1	E	2	ALA	CB-CA-C	5.03	117.64	110.10
1	C	64	LEU	CB-CG-CD2	5.02	119.54	111.00
1	F	76	MET	O-C-N	5.01	130.72	122.70
1	F	124	GLU	CA-CB-CG	-5.01	102.38	113.40
1	A	32	GLY	CA-C-N	5.00	128.21	117.20
1	F	137	GLU	C-N-CA	-5.00	109.19	121.70
1	B	23	GLU	CG-CD-OE1	5.00	128.31	118.30
1	E	85	LYS	CB-CA-C	-5.00	100.39	110.40

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	115	ASN	CA
1	B	141	ASN	CA
1	B	151	TYR	CA
1	D	140	VAL	CA
1	D	141	ASN	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	21	ILE	Mainchain
1	C	29	GLU	Sidechain
1	E	54	ASP	Sidechain

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	1206	0	1203	159	0
1	B	1206	0	1202	174	0
1	C	1206	0	1203	154	0
1	D	1206	0	1202	161	0
1	E	1206	0	1203	182	0
1	F	1206	0	1203	171	0
2	A	23	0	5	6	0
2	B	23	0	4	10	0
2	C	23	0	4	6	0
2	D	23	0	6	4	0
2	E	23	0	6	3	0
2	F	23	0	5	7	0
3	A	28	0	6	8	0
3	B	28	0	5	8	0
3	C	28	0	5	6	0
3	D	28	0	6	4	0
3	E	28	0	6	8	0
3	F	28	0	5	4	0
4	A	49	0	0	12	0
4	B	49	0	0	11	0
4	C	50	0	0	10	0
4	D	40	0	0	8	0
4	E	62	0	0	12	0
4	F	56	0	0	14	0
All	All	7848	0	7279	974	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 66.

All (974) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:35G:O5'	3:B:161:GDP:O3B	1.59	1.21
1:C:148:ASN:ND2	1:C:148:ASN:H	1.43	1.15
1:F:41:MET:HE3	1:F:133:TRP:HE3	1.12	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:160:35G:O5'	3:A:161:GDP:O3B	1.67	1.11
2:C:160:35G:O2P	3:C:161:GDP:O2B	1.70	1.09
2:B:160:35G:O5'	3:B:161:GDP:PB	2.13	1.06
1:C:72:PRO:HG3	1:F:140:VAL:HG11	1.31	1.06
2:C:160:35G:O2P	3:C:161:GDP:O3B	1.79	1.00
1:A:147:GLN:HE22	1:A:151:TYR:HD2	1.12	0.98
1:E:16:VAL:HG13	1:E:21:ILE:HD11	1.42	0.97
1:F:58:ARG:HH11	1:F:58:ARG:HG2	1.30	0.96
1:F:41:MET:HE3	1:F:133:TRP:CE3	2.01	0.96
1:C:148:ASN:N	1:C:148:ASN:HD22	1.64	0.95
1:A:37:ALA:HB3	1:A:77:VAL:HG13	1.46	0.94
1:B:37:ALA:HB2	1:B:139:LEU:HD12	1.49	0.94
1:D:136:PRO:HD2	1:D:137:GLU:HG3	1.48	0.93
1:B:58:ARG:HG3	1:B:59:PRO:HD2	1.46	0.93
1:A:13:PRO:HD3	1:A:73:VAL:HG12	1.48	0.93
1:C:140:VAL:HG11	1:F:72:PRO:HG3	1.51	0.92
1:D:127:GLU:HA	1:D:130:ILE:HG13	1.48	0.92
1:E:21:ILE:HG23	4:E:373:HOH:O	1.68	0.92
2:B:160:35G:C5'	3:B:161:GDP:PA	2.37	0.91
1:C:148:ASN:H	1:C:148:ASN:HD22	0.91	0.91
1:A:148:ASN:H	1:A:148:ASN:HD22	0.98	0.91
1:D:143:LYS:HB2	1:D:143:LYS:NZ	1.84	0.91
1:A:58:ARG:HG3	1:A:58:ARG:HH11	1.36	0.90
2:B:160:35G:O5'	3:B:161:GDP:O3A	1.89	0.89
1:C:43:ALA:HB1	1:C:47:LEU:HD13	1.53	0.89
1:B:48:LEU:HD21	1:B:68:MET:HB3	1.54	0.88
2:B:160:35G:C5'	3:B:161:GDP:O3A	2.21	0.88
2:E:160:35G:O2P	3:E:161:GDP:O3B	1.92	0.87
1:F:48:LEU:CD1	1:F:69:HIS:HB2	2.05	0.86
2:C:160:35G:O5'	3:C:161:GDP:O3B	1.93	0.86
1:A:37:ALA:HB2	1:A:139:LEU:HD12	1.59	0.85
2:C:160:35G:O2P	3:C:161:GDP:PB	2.33	0.85
1:C:72:PRO:HG3	1:F:140:VAL:CG1	2.05	0.85
2:C:160:35G:P	3:C:161:GDP:O3B	2.35	0.85
1:D:24:ILE:O	1:D:27:ARG:HB2	1.76	0.84
1:A:38:MET:HB2	1:A:76:MET:HG2	1.56	0.84
1:E:135:HIS:O	1:E:138:GLU:HB2	1.78	0.84
1:E:40:PHE:CE1	1:E:72:PRO:HB2	2.12	0.84
1:E:39:LYS:HE3	1:E:41:MET:CE	2.08	0.84
1:B:49:LYS:NZ	1:B:65:VAL:HG11	1.93	0.83
1:C:58:ARG:N	1:C:58:ARG:HD3	1.93	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:VAL:HG12	1:E:141:ASN:H	1.43	0.83
1:C:100:LYS:O	1:C:106:GLY:HA3	1.79	0.82
2:A:160:35G:P	3:A:161:GDP:O3B	2.37	0.82
1:C:82:ASN:O	1:C:83:VAL:C	2.18	0.82
1:A:148:ASN:H	1:A:148:ASN:ND2	1.72	0.81
1:E:54:ASP:HA	4:E:218:HOH:O	1.79	0.81
1:F:80:GLY:O	1:F:83:VAL:HG22	1.80	0.81
1:F:86:THR:O	1:F:90:MET:HG3	1.81	0.81
1:E:46:ASP:HA	1:E:49:LYS:HG3	1.62	0.80
1:D:138:GLU:C	1:D:139:LEU:HD12	2.01	0.80
1:B:39:LYS:HE3	1:B:41:MET:CE	2.11	0.80
1:E:140:VAL:HG12	1:E:141:ASN:N	1.97	0.80
1:B:45:GLU:O	1:B:49:LYS:HB2	1.81	0.79
1:C:93:GLU:N	1:C:99:SER:HB3	1.97	0.79
1:D:110:ILE:HD13	1:E:33:PHE:CE1	2.17	0.79
1:F:8:PHE:CZ	1:F:10:ALA:HB2	2.17	0.79
1:C:93:GLU:H	1:C:99:SER:HB3	1.48	0.79
1:B:13:PRO:HD3	1:B:73:VAL:CG1	2.14	0.78
1:F:52:TYR:CE1	2:F:160:35G:H5'2	2.19	0.78
1:E:18:ARG:O	1:E:20:LEU:HG	1.83	0.78
1:B:13:PRO:HD3	1:B:73:VAL:HG12	1.64	0.78
1:B:17:GLN:HG3	1:C:149:TRP:CE2	2.19	0.78
1:B:61:PHE:O	1:B:65:VAL:HG23	1.82	0.78
1:D:6:ARG:HA	1:D:83:VAL:HG21	1.65	0.77
1:F:61:PHE:O	1:F:65:VAL:HG23	1.84	0.77
1:E:25:ILE:O	1:E:29:GLU:HG3	1.85	0.77
1:A:25:ILE:HG21	1:E:21:ILE:HG22	1.67	0.77
1:D:128:LYS:O	1:D:131:ALA:HB3	1.85	0.77
1:E:93:GLU:O	1:E:94:THR:C	2.17	0.77
1:F:44:SER:O	1:F:47:LEU:N	2.18	0.77
1:A:148:ASN:N	1:A:148:ASN:HD22	1.78	0.77
1:F:58:ARG:HG2	1:F:58:ARG:NH1	1.96	0.76
1:D:139:LEU:HD12	1:D:139:LEU:N	2.00	0.76
1:E:143:LYS:HA	1:E:143:LYS:NZ	1.99	0.76
1:A:47:LEU:HD12	1:A:47:LEU:O	1.86	0.76
1:B:115:ASN:O	1:B:116:ILE:HG12	1.86	0.76
1:E:39:LYS:HE3	1:E:41:MET:HE2	1.68	0.76
1:A:31:LYS:HG3	1:A:31:LYS:O	1.86	0.76
1:E:143:LYS:HE2	4:E:472:HOH:O	1.85	0.76
1:F:48:LEU:HD11	1:F:68:MET:O	1.86	0.76
1:A:43:ALA:O	1:A:69:HIS:ND1	2.17	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LYS:HE3	1:C:109:CYS:O	1.85	0.75
1:A:45:GLU:O	1:A:49:LYS:HG2	1.87	0.75
1:F:88:ARG:HD2	1:F:121:ASP:HA	1.67	0.75
1:A:58:ARG:HG3	1:A:58:ARG:NH1	1.98	0.75
1:D:111:GLN:OE1	1:E:151:TYR:HA	1.87	0.75
1:F:39:LYS:HE3	1:F:41:MET:CE	2.16	0.75
1:A:36:VAL:HB	1:A:77:VAL:HG22	1.69	0.75
1:C:53:ILE:O	1:C:56:LYS:HB3	1.87	0.75
1:E:146:ALA:O	1:E:149:TRP:HB2	1.87	0.75
1:B:92:GLY:HA2	1:B:103:THR:HG21	1.69	0.74
1:C:11:ILE:HG13	1:C:76:MET:HE1	1.68	0.74
1:D:136:PRO:HD2	1:D:137:GLU:H	1.53	0.74
1:D:143:LYS:HE3	1:D:147:GLN:OE1	1.86	0.74
1:D:83:VAL:HG23	1:D:84:VAL:H	1.51	0.74
1:E:9:ILE:HG22	1:E:76:MET:HE3	1.70	0.74
1:D:52:TYR:HA	4:D:445:HOH:O	1.86	0.74
1:E:18:ARG:O	1:E:19:GLY:C	2.23	0.74
1:B:2:ALA:O	1:B:81:LEU:HA	1.88	0.74
1:C:23:GLU:HG2	4:C:435:HOH:O	1.87	0.73
1:B:135:HIS:N	1:B:138:GLU:OE2	2.20	0.73
1:A:131:ALA:HA	4:A:356:HOH:O	1.88	0.73
1:B:39:LYS:HE3	1:B:41:MET:HE2	1.69	0.73
1:E:46:ASP:HB2	4:E:381:HOH:O	1.89	0.73
1:D:46:ASP:HA	1:D:49:LYS:HD3	1.71	0.73
1:F:24:ILE:HD13	1:F:117:ILE:HD12	1.71	0.73
1:A:12:LYS:O	1:A:16:VAL:HG23	1.89	0.73
1:E:143:LYS:HA	1:E:143:LYS:HZ3	1.53	0.73
1:B:25:ILE:HG21	1:D:21:ILE:HG22	1.70	0.73
1:F:82:ASN:HB3	4:F:481:HOH:O	1.88	0.72
1:B:61:PHE:O	1:B:64:LEU:HB3	1.90	0.72
1:B:120:SER:OG	1:B:126:ALA:HA	1.89	0.72
1:E:138:GLU:C	1:E:139:LEU:HD12	2.09	0.72
1:E:80:GLY:N	1:E:83:VAL:HG22	2.05	0.72
1:B:135:HIS:O	1:B:137:GLU:N	2.23	0.72
1:B:135:HIS:O	1:B:138:GLU:HG3	1.88	0.72
1:C:78:TRP:O	1:C:83:VAL:HG11	1.90	0.72
1:F:41:MET:O	1:F:73:VAL:HG22	1.90	0.72
1:F:83:VAL:O	1:F:87:GLY:N	2.21	0.72
1:E:44:SER:O	1:E:45:GLU:C	2.21	0.71
1:B:14:ASP:O	1:B:18:ARG:HG3	1.90	0.71
1:A:17:GLN:HG3	1:B:149:TRP:CE2	2.25	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:PHE:CE1	1:B:83:VAL:HG13	2.25	0.71
1:D:3:ASN:HB3	1:D:81:LEU:HB2	1.71	0.71
1:A:7:THR:CB	1:A:84:VAL:HG22	2.20	0.71
1:A:144:SER:O	1:A:147:GLN:HB2	1.89	0.71
1:A:55:LEU:O	1:A:57:ASP:N	2.24	0.71
1:B:115:ASN:C	1:B:116:ILE:HG12	2.09	0.71
1:D:121:ASP:N	1:D:121:ASP:OD1	2.20	0.71
1:F:47:LEU:O	1:F:48:LEU:C	2.24	0.71
1:D:46:ASP:O	1:D:50:GLU:HB2	1.90	0.71
1:E:53:ILE:O	1:E:56:LYS:HB2	1.91	0.70
1:F:48:LEU:HD11	1:F:69:HIS:HB2	1.72	0.70
1:C:23:GLU:O	1:C:27:ARG:HG2	1.92	0.70
1:F:94:THR:O	1:F:96:PRO:HD3	1.90	0.70
1:F:33:PHE:CD1	1:F:83:VAL:HG13	2.27	0.70
1:D:45:GLU:HG2	1:D:65:VAL:HG12	1.73	0.70
1:D:78:TRP:O	1:D:83:VAL:HG11	1.91	0.70
1:A:81:LEU:HD12	1:A:82:ASN:HD22	1.55	0.70
1:A:7:THR:HB	1:A:84:VAL:HG22	1.74	0.70
1:B:37:ALA:HB2	1:B:139:LEU:CD1	2.20	0.70
1:B:139:LEU:N	1:B:139:LEU:HD13	2.07	0.70
1:C:12:LYS:HD2	1:C:117:ILE:N	2.06	0.70
1:B:136:PRO:C	1:B:137:GLU:HG3	2.12	0.69
1:B:87:GLY:O	1:B:88:ARG:C	2.29	0.69
1:B:45:GLU:O	1:B:49:LYS:NZ	2.23	0.69
1:B:88:ARG:HH21	1:B:121:ASP:HB2	1.57	0.69
1:E:80:GLY:H	1:E:83:VAL:CG2	2.06	0.69
1:C:39:LYS:HE2	1:C:134:PHE:CE1	2.28	0.69
1:E:115:ASN:O	1:E:116:ILE:HG12	1.92	0.69
1:F:52:TYR:OH	2:F:160:35G:O1P	2.11	0.69
1:E:148:ASN:H	1:E:148:ASN:HD22	1.40	0.69
1:B:126:ALA:O	1:B:130:ILE:HG12	1.92	0.69
1:E:11:ILE:HG13	1:E:76:MET:HE2	1.73	0.69
1:C:140:VAL:CG1	1:F:72:PRO:HG3	2.21	0.69
1:D:60:PHE:O	1:D:61:PHE:C	2.31	0.68
1:D:17:GLN:HG3	1:E:149:TRP:CE2	2.28	0.68
1:A:129:GLU:HA	4:A:382:HOH:O	1.93	0.68
1:C:148:ASN:ND2	1:C:148:ASN:N	2.17	0.68
2:A:160:35G:O2P	3:A:161:GDP:PB	2.51	0.68
1:E:44:SER:HB2	4:E:456:HOH:O	1.93	0.68
1:B:94:THR:HA	1:B:105:ARG:NH1	2.08	0.68
1:B:57:ASP:CG	1:B:58:ARG:H	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:MET:HG3	1:F:41:MET:O	1.94	0.68
1:D:143:LYS:HB2	1:D:143:LYS:HZ2	1.58	0.68
1:F:48:LEU:HD12	1:F:69:HIS:HB2	1.74	0.68
1:B:117:ILE:HG12	1:B:118:HIS:N	2.09	0.68
1:A:126:ALA:O	1:A:130:ILE:HG13	1.94	0.68
1:D:130:ILE:O	1:D:134:PHE:HB2	1.94	0.68
1:E:7:THR:OG1	1:E:120:SER:HB2	1.94	0.68
1:B:127:GLU:HA	1:B:130:ILE:HG13	1.75	0.67
1:C:143:LYS:HD3	1:C:147:GLN:OE1	1.94	0.67
1:E:61:PHE:O	1:E:64:LEU:HB3	1.94	0.67
1:E:86:THR:O	1:E:90:MET:HG3	1.93	0.67
1:C:91:LEU:HD11	1:C:117:ILE:HG12	1.76	0.67
1:C:146:ALA:O	1:C:149:TRP:HB2	1.95	0.67
1:A:135:HIS:N	1:A:138:GLU:OE2	2.27	0.67
1:E:39:LYS:HE3	1:E:41:MET:HE3	1.76	0.67
1:F:53:ILE:HG23	1:F:54:ASP:N	2.10	0.67
1:A:37:ALA:O	1:A:77:VAL:N	2.25	0.67
1:E:88:ARG:HB3	4:E:263:HOH:O	1.95	0.67
1:B:143:LYS:NZ	1:B:143:LYS:HA	2.10	0.67
1:B:88:ARG:O	1:B:91:LEU:HB2	1.94	0.66
1:D:52:TYR:CE1	2:D:160:35G:H5'2	2.30	0.66
1:B:34:ARG:NH2	1:B:79:GLU:OE2	2.27	0.66
1:D:95:ASN:O	1:D:98:ASP:N	2.26	0.66
1:C:95:ASN:HA	1:C:112:VAL:HG13	1.76	0.66
1:A:114:ARG:NH2	1:B:152:GLU:HB3	2.10	0.66
1:D:47:LEU:O	1:D:51:HIS:N	2.27	0.66
1:E:147:GLN:O	1:E:151:TYR:HB2	1.95	0.66
1:A:129:GLU:HG2	4:A:382:HOH:O	1.95	0.66
1:E:39:LYS:HG3	1:E:41:MET:HG2	1.77	0.66
1:A:81:LEU:CD1	1:A:82:ASN:HD22	2.09	0.66
1:C:139:LEU:N	1:C:139:LEU:HD12	2.11	0.66
1:E:27:ARG:HG3	1:E:104:ILE:CD1	2.26	0.66
1:D:151:TYR:HD1	1:F:111:GLN:HE21	1.43	0.66
1:F:30:GLN:NE2	4:F:331:HOH:O	2.29	0.66
1:D:135:HIS:O	1:D:138:GLU:N	2.27	0.65
1:F:123:VAL:O	1:F:126:ALA:N	2.29	0.65
1:A:47:LEU:C	1:A:47:LEU:HD12	2.16	0.65
1:C:128:LYS:O	1:C:132:LEU:HB2	1.95	0.65
1:A:7:THR:OG1	1:A:84:VAL:HG22	1.97	0.65
1:B:57:ASP:O	1:B:61:PHE:HB3	1.96	0.65
1:F:95:ASN:O	1:F:97:ALA:N	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:GLY:N	1:C:107:ASP:OD1	2.30	0.65
1:E:18:ARG:O	1:E:20:LEU:N	2.30	0.65
1:E:80:GLY:H	1:E:83:VAL:HG22	1.62	0.65
1:C:122:SER:O	1:C:126:ALA:N	2.19	0.65
4:A:256:HOH:O	1:E:21:ILE:HD12	1.96	0.65
1:D:58:ARG:O	1:D:59:PRO:C	2.33	0.65
1:E:55:LEU:H	1:E:55:LEU:HD23	1.62	0.65
2:B:160:35G:C5'	3:B:161:GDP:O3B	2.44	0.64
1:F:115:ASN:O	1:F:117:ILE:N	2.26	0.64
1:F:34:ARG:NH1	1:F:142:TYR:CE1	2.62	0.64
1:E:50:GLU:CG	1:E:132:LEU:HD21	2.26	0.64
1:A:114:ARG:O	1:A:116:ILE:N	2.30	0.64
1:B:58:ARG:HA	4:B:409:HOH:O	1.97	0.64
1:E:126:ALA:C	1:E:130:ILE:HD12	2.16	0.64
1:B:39:LYS:HE3	1:B:41:MET:HE3	1.79	0.64
1:B:95:ASN:O	1:B:97:ALA:N	2.31	0.64
1:D:17:GLN:HG3	1:E:149:TRP:CZ2	2.32	0.64
1:F:87:GLY:O	1:F:90:MET:HB2	1.97	0.64
1:B:88:ARG:HH21	1:B:121:ASP:CB	2.10	0.64
1:B:86:THR:HG23	4:B:357:HOH:O	1.98	0.64
1:C:144:SER:O	1:C:147:GLN:HB3	1.98	0.64
1:F:143:LYS:HD2	1:F:147:GLN:OE1	1.98	0.64
1:F:61:PHE:O	1:F:64:LEU:HB3	1.98	0.64
1:E:55:LEU:HD22	4:E:266:HOH:O	1.97	0.64
1:F:33:PHE:CD1	1:F:80:GLY:HA3	2.33	0.64
1:A:85:LYS:O	1:A:89:VAL:HG23	1.98	0.63
1:E:115:ASN:C	1:E:116:ILE:HG12	2.18	0.63
1:C:53:ILE:HG23	1:C:54:ASP:N	2.12	0.63
1:D:123:VAL:O	1:D:126:ALA:HB3	1.98	0.63
2:A:160:35G:O2P	3:A:161:GDP:O3B	2.16	0.63
1:B:142:TYR:HA	4:B:427:HOH:O	1.98	0.63
1:A:114:ARG:CZ	1:B:152:GLU:HB3	2.29	0.63
1:A:13:PRO:HD3	1:A:73:VAL:CG1	2.23	0.63
1:C:67:TYR:HA	1:C:70:SER:OG	1.98	0.63
1:E:118:HIS:ND1	2:E:160:35G:O1P	2.30	0.63
1:B:80:GLY:O	1:B:83:VAL:HG22	1.97	0.63
1:D:3:ASN:HA	1:D:81:LEU:HA	1.80	0.62
1:B:48:LEU:O	1:B:51:HIS:N	2.31	0.62
1:C:115:ASN:N	1:C:115:ASN:OD1	2.27	0.62
1:E:12:LYS:HE3	1:E:117:ILE:O	2.00	0.62
1:F:84:VAL:O	1:F:85:LYS:C	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:SER:OG	1:B:125:SER:HB3	1.98	0.62
1:F:113:GLY:C	1:F:114:ARG:HG2	2.12	0.62
1:F:14:ASP:O	1:F:18:ARG:HG3	2.00	0.62
1:A:23:GLU:O	1:A:27:ARG:HG2	1.99	0.62
1:C:43:ALA:CB	1:C:47:LEU:HD13	2.29	0.62
1:D:122:SER:O	1:D:126:ALA:N	2.30	0.62
1:D:23:GLU:O	1:D:27:ARG:HG2	1.99	0.62
1:E:10:ALA:N	1:E:118:HIS:O	2.31	0.62
2:F:160:35G:O5'	3:F:161:GDP:O3A	2.17	0.62
1:A:34:ARG:NH1	1:A:142:TYR:CE1	2.68	0.62
1:A:147:GLN:NE2	1:A:151:TYR:HD2	1.90	0.62
1:B:44:SER:OG	1:B:47:LEU:HB2	1.99	0.62
1:F:88:ARG:HD2	1:F:120:SER:O	2.00	0.62
1:E:39:LYS:NZ	1:E:133:TRP:O	2.31	0.62
1:E:113:GLY:HA3	1:F:152:GLU:OE1	1.99	0.62
1:B:139:LEU:N	1:B:139:LEU:HD22	2.14	0.62
1:C:113:GLY:O	1:C:114:ARG:HG2	1.99	0.62
1:A:36:VAL:N	1:A:77:VAL:O	2.29	0.62
1:B:51:HIS:HB2	1:B:132:LEU:CD1	2.30	0.62
1:C:12:LYS:HB3	1:C:13:PRO:CD	2.30	0.62
1:C:144:SER:OG	1:C:147:GLN:HB2	1.99	0.62
1:A:135:HIS:O	1:A:138:GLU:HG3	1.99	0.61
2:B:160:35G:H5'2	4:B:503:HOH:O	2.00	0.61
1:C:111:GLN:O	1:C:114:ARG:N	2.29	0.61
1:E:127:GLU:HA	1:E:130:ILE:HD12	1.81	0.61
1:A:80:GLY:O	1:A:83:VAL:HG22	1.99	0.61
1:A:96:PRO:HG3	1:A:115:ASN:HB3	1.83	0.61
1:A:11:ILE:HG13	1:A:76:MET:CE	2.30	0.61
1:C:123:VAL:O	1:C:126:ALA:HB3	2.01	0.61
1:C:101:PRO:HG3	4:C:302:HOH:O	2.01	0.61
1:C:54:ASP:HB3	4:C:358:HOH:O	1.99	0.61
2:D:160:35G:O2P	3:D:161:GDP:O3B	2.18	0.61
1:D:97:ALA:HA	4:D:239:HOH:O	2.00	0.61
1:A:64:LEU:O	1:A:68:MET:HG2	2.00	0.61
2:B:160:35G:P	3:B:161:GDP:O3B	2.59	0.61
1:D:93:GLU:O	1:D:105:ARG:HD2	2.00	0.61
1:F:85:LYS:HE3	4:F:481:HOH:O	2.00	0.61
1:A:96:PRO:HB3	1:A:105:ARG:HB3	1.82	0.61
1:E:150:ILE:HG22	1:E:150:ILE:O	2.01	0.61
1:D:15:GLY:N	1:D:116:ILE:HG22	2.15	0.61
1:D:9:ILE:N	1:D:76:MET:O	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:GLU:HG2	1:E:132:LEU:HD21	1.83	0.61
1:E:14:ASP:OD1	1:E:67:TYR:OH	2.14	0.60
1:F:91:LEU:HA	1:F:104:ILE:HG13	1.82	0.60
1:F:33:PHE:HD1	1:F:80:GLY:HA3	1.65	0.60
1:B:64:LEU:O	1:B:65:VAL:C	2.36	0.60
1:B:8:PHE:CZ	1:B:10:ALA:HB2	2.36	0.60
1:B:136:PRO:O	1:B:137:GLU:HG3	2.01	0.60
1:D:11:ILE:HG22	1:D:16:VAL:HG23	1.83	0.60
1:A:29:GLU:OE1	1:E:19:GLY:HA2	2.00	0.60
1:F:5:GLU:OE2	1:F:84:VAL:HG23	2.01	0.60
1:A:38:MET:HB2	1:A:76:MET:CG	2.31	0.60
2:B:160:35G:C5'	3:B:161:GDP:PB	2.89	0.60
1:B:42:ARG:HA	1:B:72:PRO:HA	1.84	0.60
1:D:45:GLU:O	1:D:48:LEU:HB2	2.02	0.60
1:A:41:MET:CE	1:A:133:TRP:CZ3	2.85	0.60
1:F:33:PHE:CE1	1:F:83:VAL:HG13	2.36	0.60
1:D:91:LEU:HD11	1:D:117:ILE:HD13	1.83	0.59
1:E:130:ILE:O	1:E:134:PHE:N	2.31	0.59
1:A:142:TYR:HA	4:A:389:HOH:O	2.01	0.59
1:B:41:MET:O	1:B:73:VAL:N	2.29	0.59
1:C:34:ARG:NH1	1:C:140:VAL:O	2.34	0.59
1:C:58:ARG:HD3	1:C:58:ARG:H	1.67	0.59
1:E:80:GLY:O	1:E:83:VAL:HG22	2.02	0.59
1:F:12:LYS:O	1:F:16:VAL:HG23	2.01	0.59
1:D:7:THR:HB	1:D:84:VAL:HA	1.84	0.59
1:E:81:LEU:CD1	1:E:82:ASN:HD22	2.15	0.59
1:B:6:ARG:HA	1:B:78:TRP:O	2.02	0.59
1:B:58:ARG:O	1:B:61:PHE:N	2.32	0.59
1:E:112:VAL:HG23	1:E:113:GLY:H	1.67	0.59
1:E:125:SER:O	1:E:129:GLU:HB2	2.03	0.59
2:A:160:35G:O5'	3:A:161:GDP:PB	2.60	0.59
1:B:38:MET:HG3	1:B:76:MET:HB3	1.85	0.59
1:D:45:GLU:HG2	1:D:65:VAL:CG1	2.32	0.59
1:B:125:SER:O	1:B:126:ALA:C	2.39	0.58
1:B:59:PRO:HD3	4:B:409:HOH:O	2.04	0.58
1:B:6:ARG:HG3	1:B:79:GLU:HB2	1.84	0.58
1:B:40:PHE:CE1	1:B:72:PRO:HB2	2.38	0.58
1:F:129:GLU:O	1:F:133:TRP:HD1	1.86	0.58
1:F:86:THR:O	1:F:87:GLY:C	2.36	0.58
1:D:64:LEU:HD12	1:D:64:LEU:O	2.02	0.58
1:F:67:TYR:O	1:F:70:SER:OG	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ARG:CG	1:B:59:PRO:HD2	2.27	0.58
1:B:49:LYS:HZ2	1:B:65:VAL:HG11	1.66	0.58
1:D:33:PHE:N	4:D:352:HOH:O	2.36	0.58
1:D:32:GLY:O	1:F:110:ILE:CD1	2.51	0.58
1:B:87:GLY:O	1:B:90:MET:N	2.37	0.58
1:A:97:ALA:N	4:A:249:HOH:O	2.30	0.58
1:D:52:TYR:O	1:D:61:PHE:HE1	1.86	0.58
1:B:143:LYS:HZ3	1:B:143:LYS:HA	1.68	0.58
1:B:40:PHE:HB2	1:D:38:MET:HB3	1.85	0.58
1:D:35:LEU:HD21	1:D:38:MET:HB2	1.86	0.58
1:B:140:VAL:HG11	1:D:72:PRO:HG3	1.86	0.58
1:E:80:GLY:N	1:E:83:VAL:CG2	2.66	0.58
1:F:14:ASP:OD1	1:F:67:TYR:OH	2.21	0.58
1:A:87:GLY:O	1:A:91:LEU:HD13	2.03	0.58
1:A:115:ASN:O	1:A:117:ILE:N	2.31	0.57
1:D:60:PHE:O	1:D:61:PHE:O	2.22	0.57
1:F:143:LYS:HZ3	1:F:147:GLN:CD	2.07	0.57
1:E:47:LEU:N	4:E:456:HOH:O	2.37	0.57
1:F:44:SER:O	1:F:47:LEU:HB3	2.03	0.57
1:B:89:VAL:O	1:B:103:THR:HG22	2.04	0.57
1:B:20:LEU:O	1:B:24:ILE:HG13	2.04	0.57
1:E:139:LEU:N	1:E:139:LEU:HD12	2.17	0.57
1:D:44:SER:OG	1:D:47:LEU:HB2	2.04	0.57
1:D:81:LEU:O	1:D:82:ASN:HB2	2.02	0.57
1:F:120:SER:OG	1:F:126:ALA:HA	2.05	0.57
1:D:100:LYS:O	1:D:106:GLY:HA3	2.04	0.57
1:E:55:LEU:HD13	4:E:266:HOH:O	2.03	0.57
1:C:140:VAL:HG11	1:F:72:PRO:CG	2.30	0.57
1:D:32:GLY:O	1:F:110:ILE:HD11	2.03	0.57
1:B:140:VAL:HG11	1:D:72:PRO:HB3	1.86	0.57
1:D:147:GLN:O	1:D:147:GLN:HG3	2.04	0.57
1:B:51:HIS:O	1:B:53:ILE:HG22	2.04	0.56
1:B:80:GLY:N	1:B:83:VAL:HG22	2.20	0.56
1:E:12:LYS:HB3	1:E:13:PRO:CD	2.34	0.56
1:F:8:PHE:HD2	1:F:129:GLU:OE1	1.88	0.56
1:A:43:ALA:HB3	1:A:48:LEU:HD21	1.87	0.56
1:D:80:GLY:HA2	4:D:446:HOH:O	2.05	0.56
1:E:47:LEU:HD12	1:E:47:LEU:O	2.05	0.56
1:F:39:LYS:HE3	1:F:41:MET:HE1	1.86	0.56
1:F:3:ASN:HA	1:F:81:LEU:HA	1.87	0.56
1:A:20:LEU:O	1:A:21:ILE:C	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LYS:O	1:B:27:ARG:C	2.42	0.56
1:E:20:LEU:O	1:E:24:ILE:HG13	2.05	0.56
1:C:105:ARG:HD3	1:C:115:ASN:HB2	1.87	0.56
1:F:100:LYS:HE3	4:F:364:HOH:O	2.06	0.56
1:F:123:VAL:O	1:F:124:GLU:C	2.43	0.56
1:F:126:ALA:O	1:F:130:ILE:HG13	2.05	0.56
1:D:44:SER:O	1:D:48:LEU:HD12	2.05	0.56
1:F:53:ILE:HG23	1:F:54:ASP:H	1.71	0.56
1:A:80:GLY:O	1:A:81:LEU:C	2.42	0.56
1:C:48:LEU:HD12	1:C:69:HIS:HB2	1.88	0.56
1:D:34:ARG:NH1	1:D:142:TYR:CD1	2.72	0.56
1:E:14:ASP:HA	1:F:149:TRP:CE3	2.41	0.56
1:B:138:GLU:C	1:B:139:LEU:HD13	2.26	0.56
1:C:135:HIS:O	1:C:138:GLU:HB2	2.06	0.56
1:E:6:ARG:HA	1:E:78:TRP:O	2.06	0.56
1:B:92:GLY:CA	1:B:103:THR:HG21	2.35	0.55
1:D:94:THR:OG1	3:D:161:GDP:O2B	2.22	0.55
1:F:72:PRO:HD2	4:F:233:HOH:O	2.06	0.55
1:D:46:ASP:O	1:D:47:LEU:C	2.44	0.55
1:D:28:PHE:CD1	1:D:90:MET:HE1	2.41	0.55
1:A:86:THR:O	1:A:89:VAL:HB	2.06	0.55
1:F:135:HIS:N	1:F:138:GLU:OE2	2.37	0.55
1:C:12:LYS:HE3	1:C:117:ILE:O	2.07	0.55
1:C:25:ILE:O	1:C:28:PHE:HB2	2.07	0.55
1:C:8:PHE:HE1	1:C:75:ALA:HB1	1.70	0.55
1:E:43:ALA:HB3	1:E:48:LEU:HD21	1.89	0.55
1:D:83:VAL:O	1:D:84:VAL:C	2.44	0.55
1:E:12:LYS:HG3	1:E:117:ILE:HA	1.88	0.55
1:B:123:VAL:O	1:B:124:GLU:C	2.43	0.55
1:B:45:GLU:HG3	1:B:69:HIS:CD2	2.42	0.55
1:C:147:GLN:O	1:C:147:GLN:HG3	1.89	0.55
1:D:2:ALA:O	1:D:4:SER:N	2.39	0.55
1:A:47:LEU:HD13	1:A:132:LEU:CD2	2.37	0.55
1:D:130:ILE:HG22	1:D:130:ILE:O	2.06	0.55
1:F:88:ARG:NH1	1:F:121:ASP:HB3	2.21	0.55
1:A:79:GLU:HG2	1:A:79:GLU:O	2.04	0.55
1:B:12:LYS:HE3	1:B:117:ILE:O	2.06	0.55
1:D:127:GLU:O	1:D:131:ALA:HB2	2.07	0.55
1:A:80:GLY:N	1:A:83:VAL:HG22	2.22	0.54
1:D:5:GLU:O	1:D:79:GLU:HB2	2.07	0.54
1:E:54:ASP:C	1:E:56:LYS:H	2.09	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:HG12	1:A:118:HIS:H	1.72	0.54
1:D:38:MET:HA	1:D:75:ALA:O	2.08	0.54
1:A:130:ILE:O	1:A:133:TRP:N	2.34	0.54
1:B:145:CYS:SG	1:E:146:ALA:HB2	2.47	0.54
1:C:83:VAL:O	1:C:84:VAL:C	2.45	0.54
1:D:83:VAL:HG23	1:D:84:VAL:N	2.22	0.54
1:E:24:ILE:HG21	1:E:117:ILE:HD12	1.89	0.54
1:C:29:GLU:OE2	1:F:19:GLY:HA2	2.07	0.54
1:C:95:ASN:HB3	1:C:98:ASP:HB2	1.89	0.54
1:D:132:LEU:HD23	1:D:132:LEU:O	2.07	0.54
1:F:6:ARG:HB3	1:F:77:VAL:HG12	1.88	0.54
1:B:49:LYS:HB2	1:B:49:LYS:HZ3	1.73	0.54
1:B:51:HIS:C	1:B:53:ILE:H	2.10	0.54
1:E:111:GLN:OE1	1:F:152:GLU:HB3	2.07	0.54
1:C:67:TYR:O	1:C:70:SER:OG	2.24	0.54
1:E:88:ARG:HH22	3:E:161:GDP:PB	2.31	0.54
1:A:41:MET:HE2	1:A:133:TRP:CZ3	2.43	0.54
1:D:16:VAL:HG22	1:D:21:ILE:HD11	1.90	0.54
1:A:96:PRO:HD3	1:A:112:VAL:HA	1.89	0.54
1:F:143:LYS:HE3	4:F:369:HOH:O	2.08	0.54
1:A:104:ILE:HG13	4:A:306:HOH:O	2.08	0.54
1:B:117:ILE:CG1	1:B:118:HIS:N	2.70	0.54
1:B:49:LYS:HB2	1:B:49:LYS:NZ	2.22	0.54
1:C:140:VAL:HG12	1:C:142:TYR:HD1	1.73	0.54
1:A:41:MET:CE	1:A:133:TRP:HZ3	2.21	0.54
1:B:108:PHE:HE1	1:C:30:GLN:NE2	2.06	0.54
1:D:115:ASN:C	1:D:117:ILE:H	2.10	0.53
1:A:152:GLU:HB3	1:C:111:GLN:CD	2.27	0.53
1:D:15:GLY:CA	1:D:116:ILE:HG22	2.38	0.53
1:D:11:ILE:O	1:D:73:VAL:HB	2.08	0.53
1:A:6:ARG:HG2	1:A:79:GLU:HB2	1.90	0.53
1:B:117:ILE:HG12	1:B:118:HIS:H	1.74	0.53
1:C:136:PRO:HG2	1:C:137:GLU:HG3	1.90	0.53
1:D:114:ARG:CZ	1:E:152:GLU:HB3	2.38	0.53
1:F:45:GLU:O	1:F:49:LYS:HG3	2.08	0.53
1:D:4:SER:HA	1:D:79:GLU:HG3	1.90	0.53
1:E:125:SER:O	1:E:126:ALA:C	2.46	0.53
2:F:160:35G:O5'	3:F:161:GDP:PB	2.66	0.53
1:B:88:ARG:HE	1:B:121:ASP:HA	1.73	0.53
1:B:51:HIS:O	1:B:53:ILE:N	2.41	0.53
1:C:138:GLU:C	1:C:139:LEU:HD12	2.28	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:ARG:HG2	4:F:326:HOH:O	2.08	0.53
1:B:52:TYR:OH	2:B:160:35G:O1P	2.25	0.53
1:E:81:LEU:HD11	1:E:82:ASN:HD22	1.73	0.53
1:B:108:PHE:HA	1:C:31:LYS:HA	1.91	0.53
1:B:117:ILE:CG1	1:B:118:HIS:H	2.22	0.53
1:D:3:ASN:HA	1:D:81:LEU:CA	2.38	0.53
1:D:6:ARG:CA	1:D:83:VAL:HG21	2.38	0.53
1:A:125:SER:O	1:A:129:GLU:HB2	2.09	0.53
1:A:11:ILE:HG13	1:A:76:MET:HE2	1.91	0.53
1:A:80:GLY:H	1:A:83:VAL:CG2	2.21	0.53
1:B:33:PHE:CZ	1:B:83:VAL:HG13	2.43	0.53
1:B:79:GLU:HA	1:B:83:VAL:HG21	1.89	0.53
1:C:121:ASP:N	1:C:121:ASP:OD1	2.31	0.53
1:C:38:MET:HG3	1:C:76:MET:HG3	1.90	0.53
1:D:34:ARG:NH1	1:D:140:VAL:O	2.31	0.53
1:A:139:LEU:N	1:A:139:LEU:HD13	2.24	0.53
1:B:27:ARG:NH2	1:B:107:ASP:OD2	2.31	0.53
1:B:95:ASN:C	1:B:97:ALA:H	2.12	0.53
1:D:139:LEU:N	1:D:139:LEU:CD1	2.71	0.53
1:A:105:ARG:HE	1:A:115:ASN:HB2	1.73	0.53
1:A:128:LYS:HG2	1:A:129:GLU:N	2.24	0.53
1:D:85:LYS:O	1:D:88:ARG:HB2	2.09	0.53
1:E:120:SER:OG	1:E:126:ALA:HA	2.09	0.53
1:E:58:ARG:HG3	1:E:59:PRO:HD2	1.91	0.53
1:F:34:ARG:NH1	1:F:142:TYR:CD1	2.77	0.53
1:C:14:ASP:OD1	1:C:67:TYR:OH	2.24	0.52
2:F:160:35G:H3'	3:F:161:GDP:O3A	2.08	0.52
1:F:35:LEU:HD21	1:F:76:MET:HG2	1.89	0.52
1:A:38:MET:HA	1:A:75:ALA:O	2.09	0.52
1:C:12:LYS:HD2	1:C:116:ILE:C	2.28	0.52
1:F:96:PRO:HD2	1:F:112:VAL:HA	1.90	0.52
1:F:11:ILE:HG12	1:F:24:ILE:HD12	1.91	0.52
1:F:58:ARG:CG	1:F:58:ARG:HH11	2.14	0.52
1:A:22:GLY:HA2	1:E:22:GLY:HA2	1.91	0.52
1:F:67:TYR:C	1:F:69:HIS:H	2.13	0.52
1:A:9:ILE:O	1:A:76:MET:N	2.39	0.52
1:F:88:ARG:CD	1:F:121:ASP:HA	2.38	0.52
1:B:23:GLU:O	1:B:26:LYS:HB3	2.09	0.52
3:A:161:GDP:O1A	3:A:161:GDP:O1B	2.28	0.52
1:C:12:LYS:HD2	1:C:117:ILE:CA	2.38	0.52
1:E:115:ASN:N	1:E:115:ASN:OD1	2.28	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:HD21	1:B:38:MET:HE2	1.91	0.52
1:C:143:LYS:NZ	1:C:143:LYS:HA	2.25	0.52
1:A:100:LYS:O	1:A:106:GLY:HA3	2.10	0.52
1:A:147:GLN:NE2	1:A:151:TYR:HB2	2.25	0.52
1:D:108:PHE:HD2	1:E:30:GLN:HB2	1.75	0.52
1:D:17:GLN:HA	1:D:17:GLN:OE1	2.10	0.52
1:E:135:HIS:O	1:E:137:GLU:N	2.42	0.52
1:A:110:ILE:HG22	1:A:110:ILE:O	2.09	0.52
1:A:53:ILE:O	1:A:56:LYS:HB2	2.10	0.52
1:B:84:VAL:O	1:B:88:ARG:HG2	2.10	0.52
1:C:113:GLY:C	1:C:114:ARG:HG2	2.30	0.52
1:F:31:LYS:HG3	1:F:31:LYS:O	2.08	0.52
1:C:53:ILE:CG2	1:C:54:ASP:N	2.73	0.51
1:C:87:GLY:O	1:C:91:LEU:HB2	2.10	0.51
3:D:161:GDP:O1A	3:D:161:GDP:O1B	2.29	0.51
1:E:34:ARG:NH1	1:E:36:VAL:HG22	2.26	0.51
1:B:51:HIS:HB2	1:B:132:LEU:HD11	1.91	0.51
1:B:85:LYS:O	1:B:89:VAL:HG23	2.10	0.51
1:C:123:VAL:CG2	1:C:124:GLU:N	2.74	0.51
1:E:117:ILE:HG12	1:E:118:HIS:N	2.25	0.51
1:D:54:ASP:N	1:D:54:ASP:OD1	2.44	0.51
1:E:50:GLU:HG3	1:E:132:LEU:HD21	1.90	0.51
1:F:122:SER:O	1:F:126:ALA:N	2.42	0.51
1:F:51:HIS:O	1:F:53:ILE:HG22	2.10	0.51
1:C:67:TYR:HA	1:C:70:SER:HG	1.75	0.51
1:D:42:ARG:HD3	1:D:69:HIS:CE1	2.45	0.51
1:D:9:ILE:O	1:D:76:MET:N	2.40	0.51
1:F:127:GLU:HB3	4:F:496:HOH:O	2.11	0.51
1:F:61:PHE:CE1	1:F:65:VAL:HG21	2.44	0.51
1:C:104:ILE:O	1:C:108:PHE:HD2	1.94	0.51
1:E:34:ARG:HH12	1:E:36:VAL:HG22	1.75	0.51
1:A:38:MET:HA	1:A:76:MET:HA	1.92	0.51
1:B:5:GLU:HB3	1:B:80:GLY:O	2.10	0.51
1:D:150:ILE:HG22	1:D:150:ILE:O	2.10	0.51
1:E:140:VAL:CG1	1:E:141:ASN:H	2.18	0.51
1:E:25:ILE:HD11	4:E:373:HOH:O	2.11	0.51
1:E:60:PHE:O	1:E:61:PHE:C	2.49	0.51
1:F:129:GLU:O	1:F:133:TRP:N	2.43	0.51
1:C:113:GLY:O	1:C:114:ARG:NE	2.39	0.51
1:D:123:VAL:HA	1:D:126:ALA:HB3	1.93	0.51
1:C:72:PRO:CG	1:F:140:VAL:HG11	2.23	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:LYS:HG2	1:D:68:MET:SD	2.50	0.51
1:E:11:ILE:HD12	1:E:74:VAL:HB	1.92	0.51
1:F:20:LEU:O	1:F:24:ILE:HG13	2.11	0.51
1:F:56:LYS:HD2	4:F:297:HOH:O	2.10	0.51
1:F:5:GLU:HG2	1:F:83:VAL:HG23	1.92	0.51
1:C:137:GLU:OE1	1:C:137:GLU:O	2.30	0.50
1:D:6:ARG:O	1:D:84:VAL:HG23	2.12	0.50
1:E:140:VAL:CG1	1:E:141:ASN:N	2.69	0.50
1:A:148:ASN:N	1:A:148:ASN:ND2	2.39	0.50
1:E:142:TYR:N	1:E:142:TYR:CD1	2.80	0.50
1:A:23:GLU:OE1	1:E:26:LYS:NZ	2.36	0.50
1:C:12:LYS:HB3	1:C:13:PRO:HD2	1.94	0.50
1:D:2:ALA:C	1:D:4:SER:H	2.15	0.50
1:F:122:SER:O	1:F:125:SER:HB2	2.11	0.50
1:F:32:GLY:HA2	4:F:252:HOH:O	2.11	0.50
1:F:64:LEU:O	1:F:65:VAL:C	2.48	0.50
1:C:39:LYS:HE2	1:C:134:PHE:CD1	2.46	0.50
1:D:110:ILE:HD13	1:E:33:PHE:CD1	2.46	0.50
1:F:6:ARG:HB3	1:F:77:VAL:CG1	2.41	0.50
1:E:88:ARG:CZ	1:E:121:ASP:HB2	2.41	0.50
1:F:39:LYS:HE3	1:F:41:MET:HE2	1.92	0.50
1:A:130:ILE:HG22	1:A:131:ALA:N	2.26	0.50
1:A:94:THR:HG23	1:A:95:ASN:N	2.25	0.50
1:B:39:LYS:HG3	1:B:41:MET:HG2	1.94	0.50
1:E:127:GLU:CA	1:E:130:ILE:HD12	2.42	0.50
1:A:139:LEU:CD1	1:A:139:LEU:N	2.74	0.50
1:A:30:GLN:NE2	4:A:325:HOH:O	2.43	0.49
1:F:135:HIS:O	1:F:138:GLU:HG3	2.10	0.49
1:B:33:PHE:CD1	1:B:83:VAL:HG13	2.47	0.49
1:C:45:GLU:HA	1:C:48:LEU:HB2	1.94	0.49
1:D:28:PHE:HD1	1:D:90:MET:HE1	1.77	0.49
1:A:14:ASP:OD2	1:A:114:ARG:O	2.29	0.49
1:C:99:SER:O	1:C:106:GLY:HA2	2.12	0.49
1:E:139:LEU:N	1:E:139:LEU:CD1	2.75	0.49
1:E:60:PHE:CZ	3:E:161:GDP:C8	2.99	0.49
1:A:110:ILE:HG23	4:B:399:HOH:O	2.12	0.49
1:E:33:PHE:CE1	1:E:83:VAL:HG13	2.48	0.49
1:A:112:VAL:O	1:A:112:VAL:HG12	2.12	0.49
1:A:22:GLY:O	1:E:22:GLY:HA3	2.12	0.49
1:E:140:VAL:HG22	4:E:375:HOH:O	2.12	0.49
1:E:50:GLU:O	1:E:53:ILE:HG22	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PHE:O	1:A:62:ALA:C	2.51	0.49
1:C:129:GLU:O	1:C:133:TRP:N	2.46	0.49
1:C:143:LYS:CE	1:C:143:LYS:HA	2.42	0.49
1:E:60:PHE:HE2	3:E:161:GDP:O4'	1.96	0.49
1:A:85:LYS:HB2	4:A:396:HOH:O	2.12	0.49
1:C:14:ASP:O	1:C:18:ARG:HB2	2.12	0.49
1:A:47:LEU:CD1	1:A:132:LEU:HD22	2.42	0.49
1:C:139:LEU:N	1:C:139:LEU:CD1	2.74	0.49
1:D:47:LEU:HD11	1:D:132:LEU:CD2	2.43	0.49
1:F:40:PHE:CE1	1:F:72:PRO:HB2	2.47	0.49
1:C:134:PHE:HD1	1:C:138:GLU:OE1	1.96	0.49
1:B:102:GLY:N	4:B:415:HOH:O	2.45	0.48
1:D:64:LEU:HD12	1:D:64:LEU:C	2.33	0.48
1:F:96:PRO:HB2	1:F:110:ILE:O	2.13	0.48
1:B:14:ASP:OD1	1:B:67:TYR:OH	2.30	0.48
1:B:93:GLU:N	1:B:99:SER:OG	2.45	0.48
1:D:135:HIS:O	1:D:137:GLU:N	2.46	0.48
1:D:152:GLU:HG3	1:D:152:GLU:OXT	2.13	0.48
1:E:14:ASP:HA	1:F:149:TRP:HE3	1.78	0.48
1:C:46:ASP:O	1:C:50:GLU:HB2	2.13	0.48
1:C:74:VAL:HG12	1:C:74:VAL:O	2.14	0.48
1:D:140:VAL:CG1	1:D:141:ASN:N	2.76	0.48
1:F:9:ILE:O	1:F:76:MET:HB2	2.13	0.48
1:B:4:SER:O	1:B:5:GLU:C	2.52	0.48
1:D:77:VAL:HG12	1:D:78:TRP:N	2.27	0.48
1:E:43:ALA:O	1:E:69:HIS:ND1	2.29	0.48
1:F:42:ARG:HA	1:F:72:PRO:HA	1.94	0.48
1:C:96:PRO:HA	1:C:99:SER:OG	2.13	0.48
1:F:11:ILE:HD13	1:F:21:ILE:HA	1.96	0.48
1:B:109:CYS:HB3	1:B:116:ILE:HD13	1.95	0.48
1:B:48:LEU:CB	1:B:65:VAL:HG13	2.44	0.48
1:C:150:ILE:HG22	1:C:150:ILE:O	2.10	0.48
1:D:52:TYR:OH	2:D:160:35G:O1P	2.24	0.48
1:D:87:GLY:O	1:D:90:MET:HB2	2.12	0.48
1:E:81:LEU:HG	1:E:81:LEU:O	2.14	0.48
1:E:88:ARG:O	1:E:91:LEU:HB2	2.13	0.48
1:B:49:LYS:HZ1	1:B:65:VAL:HG11	1.73	0.48
1:D:143:LYS:HB2	1:D:143:LYS:HZ3	1.74	0.48
1:D:46:ASP:HA	1:D:49:LYS:CD	2.43	0.48
1:D:86:THR:O	1:D:87:GLY:C	2.51	0.48
1:A:56:LYS:HD2	1:A:57:ASP:OD1	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:THR:CB	1:C:84:VAL:HG22	2.44	0.48
1:C:5:GLU:O	1:C:83:VAL:HG22	2.13	0.48
1:D:110:ILE:CD1	1:E:33:PHE:CD1	2.96	0.48
1:B:118:HIS:CG	1:B:119:GLY:N	2.80	0.48
1:B:2:ALA:O	1:B:5:GLU:HB2	2.13	0.48
1:E:67:TYR:O	1:E:68:MET:C	2.49	0.48
1:F:87:GLY:O	1:F:91:LEU:HD13	2.14	0.48
1:A:41:MET:HE2	1:A:133:TRP:HZ3	1.78	0.48
1:B:128:LYS:HG2	1:B:129:GLU:N	2.29	0.48
1:C:6:ARG:HG3	1:C:6:ARG:H	1.22	0.48
1:E:33:PHE:CD1	1:E:83:VAL:HG13	2.48	0.48
1:F:95:ASN:C	1:F:97:ALA:H	2.17	0.48
1:A:17:GLN:HG3	1:B:149:TRP:CZ2	2.49	0.47
1:A:34:ARG:NH2	1:A:36:VAL:HG22	2.29	0.47
1:D:27:ARG:NH1	1:D:102:GLY:O	2.46	0.47
1:E:143:LYS:HA	1:E:143:LYS:HZ2	1.77	0.47
1:E:38:MET:HA	1:E:75:ALA:O	2.14	0.47
1:A:35:LEU:O	1:A:142:TYR:OH	2.27	0.47
1:C:118:HIS:CG	1:C:119:GLY:N	2.82	0.47
1:C:25:ILE:HG21	1:C:25:ILE:HD13	1.69	0.47
1:E:34:ARG:O	1:E:78:TRP:HA	2.13	0.47
1:A:11:ILE:HA	1:A:117:ILE:HG13	1.95	0.47
1:C:145:CYS:HB2	1:D:145:CYS:O	2.14	0.47
1:F:124:GLU:HB2	4:F:485:HOH:O	2.15	0.47
1:F:141:ASN:OD1	1:F:141:ASN:N	2.46	0.47
1:B:133:TRP:CD1	1:B:133:TRP:N	2.83	0.47
1:C:24:ILE:O	1:C:27:ARG:HB2	2.14	0.47
1:C:83:VAL:HG23	1:C:84:VAL:H	1.79	0.47
1:D:51:HIS:HD2	1:D:52:TYR:CD2	2.32	0.47
1:F:123:VAL:HB	1:F:124:GLU:H	1.48	0.47
1:C:40:PHE:CE2	1:F:140:VAL:HB	2.49	0.47
1:F:67:TYR:O	1:F:69:HIS:N	2.46	0.47
1:E:127:GLU:N	1:E:130:ILE:HD12	2.29	0.47
1:C:111:GLN:N	4:C:209:HOH:O	2.30	0.47
1:E:129:GLU:O	1:E:133:TRP:HD1	1.98	0.47
1:B:59:PRO:N	4:B:365:HOH:O	2.47	0.47
1:E:124:GLU:O	1:E:127:GLU:N	2.48	0.47
1:A:80:GLY:H	1:A:83:VAL:HG22	1.79	0.47
1:C:26:LYS:O	1:C:27:ARG:C	2.53	0.47
1:C:95:ASN:C	1:C:97:ALA:H	2.18	0.47
1:A:135:HIS:HB3	1:A:137:GLU:OE2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:SER:HB3	4:D:303:HOH:O	2.15	0.47
1:E:85:LYS:HB3	4:E:354:HOH:O	2.14	0.47
1:F:113:GLY:O	1:F:114:ARG:NE	2.48	0.47
1:F:143:LYS:HZ3	1:F:147:GLN:NE2	2.12	0.47
1:A:118:HIS:HA	4:A:502:HOH:O	2.14	0.47
1:F:145:CYS:O	1:F:147:GLN:N	2.48	0.47
1:A:60:PHE:N	1:A:60:PHE:CD1	2.81	0.47
1:B:64:LEU:O	1:B:67:TYR:HB3	2.15	0.47
1:E:40:PHE:CZ	1:E:72:PRO:HB2	2.49	0.47
1:B:24:ILE:O	1:B:25:ILE:C	2.52	0.46
1:B:88:ARG:HH11	1:B:88:ARG:HD2	1.54	0.46
4:A:232:HOH:O	1:E:144:SER:HB3	2.13	0.46
1:F:12:LYS:HB3	1:F:13:PRO:CD	2.45	0.46
1:D:114:ARG:NH2	4:D:226:HOH:O	2.48	0.46
1:F:45:GLU:O	1:F:46:ASP:C	2.50	0.46
1:C:54:ASP:C	1:C:55:LEU:HD12	2.36	0.46
1:E:135:HIS:HB3	1:E:137:GLU:OE2	2.16	0.46
1:E:22:GLY:O	1:E:26:LYS:HB2	2.14	0.46
1:E:66:LYS:HE3	1:E:67:TYR:N	2.31	0.46
1:F:49:LYS:HA	1:F:61:PHE:HZ	1.80	0.46
1:B:48:LEU:CD2	1:B:68:MET:HB3	2.35	0.46
1:D:126:ALA:O	1:D:130:ILE:HG13	2.16	0.46
1:D:40:PHE:CZ	1:D:72:PRO:HG2	2.51	0.46
1:A:51:HIS:ND1	1:A:133:TRP:NE1	2.62	0.46
1:B:40:PHE:CZ	1:B:72:PRO:HB2	2.49	0.46
1:B:47:LEU:O	1:B:48:LEU:C	2.54	0.46
1:C:55:LEU:HD12	1:C:55:LEU:N	2.29	0.46
1:E:126:ALA:O	1:E:130:ILE:HD12	2.16	0.46
1:F:58:ARG:O	1:F:59:PRO:C	2.53	0.46
1:C:18:ARG:NH1	1:C:108:PHE:O	2.47	0.46
2:C:160:35G:P	3:C:161:GDP:PB	3.11	0.46
1:C:45:GLU:HB3	1:C:49:LYS:HE2	1.97	0.46
1:D:81:LEU:HG	1:D:81:LEU:O	2.15	0.46
1:F:36:VAL:HB	1:F:77:VAL:HB	1.96	0.46
1:A:58:ARG:CG	1:A:58:ARG:NH1	2.76	0.46
1:B:53:ILE:CG2	1:B:128:LYS:NZ	2.79	0.46
1:D:34:ARG:CG	1:D:142:TYR:CZ	2.98	0.46
1:F:65:VAL:HG23	1:F:65:VAL:H	1.40	0.46
1:C:89:VAL:HG12	1:C:90:MET:N	2.30	0.46
1:F:53:ILE:CG2	1:F:54:ASP:N	2.78	0.46
1:A:81:LEU:HD12	1:A:82:ASN:N	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:LEU:HA	1:F:48:LEU:HD23	1.72	0.46
1:B:128:LYS:CG	1:B:129:GLU:N	2.80	0.45
1:B:139:LEU:HD22	1:B:139:LEU:H	1.80	0.45
1:C:41:MET:O	1:C:73:VAL:HG22	2.16	0.45
1:D:108:PHE:CD2	1:E:30:GLN:HB2	2.52	0.45
1:D:134:PHE:HD1	1:D:138:GLU:OE1	1.98	0.45
1:D:56:LYS:NZ	1:D:57:ASP:OD2	2.49	0.45
1:F:127:GLU:O	1:F:128:LYS:C	2.53	0.45
1:D:42:ARG:O	1:D:43:ALA:C	2.52	0.45
1:E:109:CYS:HB3	1:E:116:ILE:HD13	1.98	0.45
1:E:134:PHE:O	1:E:136:PRO:HD3	2.16	0.45
1:E:81:LEU:HD12	1:E:81:LEU:C	2.35	0.45
1:F:111:GLN:C	1:F:113:GLY:H	2.19	0.45
1:F:67:TYR:C	1:F:69:HIS:N	2.70	0.45
1:D:67:TYR:O	1:D:70:SER:HB2	2.17	0.45
1:F:51:HIS:C	1:F:53:ILE:H	2.18	0.45
1:C:6:ARG:HA	1:C:83:VAL:HG21	1.97	0.45
1:D:44:SER:O	1:D:48:LEU:HB2	2.16	0.45
1:D:61:PHE:O	1:D:62:ALA:HB3	2.16	0.45
1:F:137:GLU:H	1:F:137:GLU:HG3	1.39	0.45
1:A:10:ALA:HA	1:A:74:VAL:O	2.17	0.45
2:A:160:35G:P	3:A:161:GDP:PB	3.15	0.45
1:B:12:LYS:HD2	4:B:404:HOH:O	2.16	0.45
1:C:26:LYS:O	1:C:30:GLN:HG2	2.16	0.45
1:E:64:LEU:O	1:E:68:MET:HG2	2.16	0.45
1:F:88:ARG:NH1	1:F:121:ASP:CB	2.79	0.45
3:F:161:GDP:O6	4:F:377:HOH:O	2.20	0.45
1:A:110:ILE:HD11	1:B:31:LYS:O	2.17	0.45
1:B:80:GLY:N	1:B:83:VAL:CG2	2.79	0.45
1:C:21:ILE:HG21	1:C:21:ILE:HD13	1.71	0.45
1:C:27:ARG:HD3	4:C:247:HOH:O	2.16	0.45
1:E:60:PHE:CE2	3:E:161:GDP:N9	2.85	0.45
1:A:129:GLU:O	1:A:130:ILE:C	2.55	0.45
1:B:38:MET:HB3	1:B:38:MET:HE3	1.74	0.45
1:B:48:LEU:O	1:B:49:LYS:C	2.55	0.45
1:D:12:LYS:O	1:D:13:PRO:C	2.53	0.45
1:F:6:ARG:HA	1:F:78:TRP:O	2.17	0.45
1:F:85:LYS:HB3	1:F:85:LYS:HE3	1.62	0.45
1:B:129:GLU:O	1:B:133:TRP:HD1	2.00	0.45
1:B:35:LEU:N	1:B:78:TRP:CE3	2.85	0.45
1:B:5:GLU:OE2	1:B:82:ASN:HA	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:PHE:HD1	1:E:73:VAL:O	2.00	0.45
1:A:55:LEU:HA	1:A:55:LEU:HD13	1.37	0.45
1:F:145:CYS:C	1:F:147:GLN:H	2.20	0.45
1:C:4:SER:HA	1:C:79:GLU:HG3	1.99	0.44
1:C:55:LEU:CD1	1:C:55:LEU:N	2.80	0.44
1:D:91:LEU:HA	1:D:91:LEU:HD12	1.71	0.44
1:B:12:LYS:HD3	1:B:68:MET:SD	2.57	0.44
1:B:94:THR:O	1:B:96:PRO:HD3	2.17	0.44
1:D:94:THR:HA	1:D:105:ARG:NH1	2.31	0.44
1:D:136:PRO:CD	1:D:137:GLU:H	2.26	0.44
1:E:14:ASP:OD2	1:E:116:ILE:HG22	2.18	0.44
1:E:5:GLU:OE2	1:E:84:VAL:HG23	2.17	0.44
1:D:6:ARG:NH1	4:D:294:HOH:O	2.50	0.44
1:E:47:LEU:HD12	1:E:47:LEU:C	2.38	0.44
1:F:23:GLU:O	1:F:24:ILE:C	2.53	0.44
1:F:70:SER:H	1:F:70:SER:HG	1.59	0.44
1:A:84:VAL:HG13	1:A:120:SER:O	2.16	0.44
1:C:8:PHE:C	1:C:9:ILE:HG12	2.36	0.44
1:C:91:LEU:HD11	1:C:117:ILE:CG1	2.46	0.44
1:D:47:LEU:O	1:D:50:GLU:HB2	2.18	0.44
1:E:135:HIS:C	1:E:137:GLU:N	2.70	0.44
1:F:8:PHE:CE2	1:F:10:ALA:HB2	2.52	0.44
1:F:5:GLU:O	1:F:83:VAL:HG21	2.18	0.44
1:A:129:GLU:O	1:A:133:TRP:HD1	1.99	0.44
1:A:47:LEU:CD1	1:A:132:LEU:CD2	2.95	0.44
1:A:14:ASP:O	1:A:18:ARG:HG3	2.18	0.44
1:B:91:LEU:O	1:B:105:ARG:HG3	2.17	0.44
1:A:132:LEU:HD23	1:A:132:LEU:O	2.18	0.44
1:A:38:MET:HG3	1:A:74:VAL:CG1	2.48	0.44
1:A:48:LEU:HD13	1:A:48:LEU:HA	1.53	0.44
1:A:59:PRO:O	1:A:60:PHE:C	2.56	0.44
1:A:39:LYS:N	1:A:75:ALA:O	2.43	0.44
1:C:8:PHE:CE1	1:C:75:ALA:HB1	2.50	0.44
1:E:30:GLN:HG2	1:E:30:GLN:H	1.49	0.44
1:E:8:PHE:HE1	1:E:75:ALA:HB1	1.83	0.44
1:F:47:LEU:O	1:F:48:LEU:O	2.34	0.44
1:A:140:VAL:HG12	1:A:141:ASN:H	1.82	0.44
1:A:31:LYS:HE2	1:C:110:ILE:HG23	2.00	0.44
1:F:100:LYS:O	1:F:106:GLY:HA3	2.17	0.44
1:A:37:ALA:HB2	1:A:139:LEU:CD1	2.40	0.44
1:C:6:ARG:HD2	4:C:380:HOH:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:SER:O	1:E:47:LEU:HB3	2.18	0.44
1:A:7:THR:HB	1:A:84:VAL:CG2	2.46	0.44
1:C:77:VAL:HG23	1:C:134:PHE:CE2	2.53	0.44
1:D:28:PHE:CD1	1:D:90:MET:CE	3.01	0.44
1:E:48:LEU:CD1	1:E:69:HIS:HB2	2.47	0.44
1:E:52:TYR:O	1:E:53:ILE:C	2.56	0.44
1:B:125:SER:HB3	4:B:422:HOH:O	2.18	0.43
1:B:134:PHE:HB3	1:B:138:GLU:OE2	2.18	0.43
1:B:29:GLU:OE2	1:D:21:ILE:HB	2.18	0.43
1:B:42:ARG:NH1	4:B:257:HOH:O	2.50	0.43
1:C:44:SER:O	1:C:48:LEU:N	2.43	0.43
1:E:60:PHE:CE2	3:E:161:GDP:O4'	2.70	0.43
1:A:31:LYS:CG	1:A:31:LYS:O	2.62	0.43
1:C:40:PHE:HE2	1:F:140:VAL:HB	1.83	0.43
1:D:108:PHE:O	1:D:109:CYS:HB3	2.17	0.43
1:E:117:ILE:HG12	1:E:118:HIS:H	1.82	0.43
1:F:69:HIS:O	1:F:69:HIS:CD2	2.71	0.43
1:C:29:GLU:OE2	4:C:321:HOH:O	2.21	0.43
1:D:8:PHE:HB3	1:D:120:SER:OG	2.18	0.43
1:D:37:ALA:O	1:D:76:MET:HA	2.18	0.43
1:F:88:ARG:O	1:F:91:LEU:HB2	2.19	0.43
1:A:41:MET:CE	1:A:133:TRP:CE3	3.01	0.43
1:C:104:ILE:O	1:C:108:PHE:CD2	2.71	0.43
1:D:47:LEU:HD11	1:D:132:LEU:HD22	2.01	0.43
1:E:12:LYS:HB3	1:E:13:PRO:HD2	2.01	0.43
1:F:60:PHE:CD1	1:F:60:PHE:N	2.80	0.43
1:F:85:LYS:HB2	4:F:280:HOH:O	2.19	0.43
1:D:41:MET:HB2	1:D:41:MET:HE2	1.62	0.43
1:F:27:ARG:NH2	1:F:107:ASP:OD2	2.48	0.43
1:A:37:ALA:O	1:A:76:MET:HA	2.19	0.43
1:B:122:SER:OG	1:B:124:GLU:HG3	2.17	0.43
1:D:144:SER:C	1:D:146:ALA:H	2.22	0.43
1:D:18:ARG:NH1	4:D:473:HOH:O	2.38	0.43
1:D:89:VAL:H	1:D:89:VAL:HG23	1.55	0.43
1:E:58:ARG:HA	1:E:59:PRO:HD3	1.78	0.43
1:E:37:ALA:O	1:E:76:MET:HA	2.18	0.43
1:A:108:PHE:O	1:A:109:CYS:HB3	2.19	0.43
1:A:117:ILE:HG12	1:A:118:HIS:N	2.33	0.43
1:A:7:THR:OG1	4:A:397:HOH:O	2.20	0.43
1:B:109:CYS:CB	1:B:116:ILE:HD13	2.49	0.43
1:B:45:GLU:HG3	1:B:69:HIS:HD2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASN:O	1:B:98:ASP:N	2.40	0.43
1:C:100:LYS:HD3	4:C:348:HOH:O	2.17	0.43
1:D:124:GLU:O	1:D:128:LYS:HB2	2.19	0.43
1:D:48:LEU:O	1:D:52:TYR:N	2.51	0.43
1:A:14:ASP:OD1	1:A:67:TYR:OH	2.23	0.43
1:A:14:ASP:OD2	1:A:116:ILE:N	2.51	0.43
1:C:61:PHE:O	1:C:63:GLY:N	2.51	0.43
1:D:149:TRP:O	1:F:114:ARG:HB3	2.18	0.43
1:E:12:LYS:HG3	1:E:117:ILE:CA	2.48	0.43
1:F:12:LYS:NZ	2:F:160:35G:O3'	2.48	0.43
1:A:80:GLY:O	1:A:83:VAL:CG2	2.66	0.43
1:B:117:ILE:HG21	1:B:117:ILE:HD13	1.57	0.43
1:C:40:PHE:HD1	1:C:74:VAL:HG22	1.84	0.43
1:C:7:THR:HB	1:C:84:VAL:HG22	2.01	0.43
1:E:80:GLY:O	1:E:83:VAL:CG2	2.66	0.43
1:A:12:LYS:HE3	1:A:117:ILE:O	2.19	0.43
1:A:152:GLU:HB3	1:C:111:GLN:OE1	2.19	0.43
1:C:125:SER:O	1:C:126:ALA:C	2.57	0.43
1:F:152:GLU:HG2	1:F:152:GLU:O	2.18	0.43
1:F:53:ILE:O	1:F:56:LYS:HB2	2.19	0.43
1:A:14:ASP:OD2	1:A:116:ILE:HA	2.19	0.42
1:E:40:PHE:O	1:E:41:MET:HB3	2.19	0.42
1:F:2:ALA:O	1:F:81:LEU:HA	2.19	0.42
1:F:44:SER:O	1:F:48:LEU:N	2.47	0.42
1:A:136:PRO:C	1:A:138:GLU:H	2.19	0.42
1:A:11:ILE:HG13	1:A:76:MET:HE1	2.00	0.42
1:B:16:VAL:HG13	1:B:21:ILE:HD11	2.01	0.42
1:C:20:LEU:O	1:C:24:ILE:HG13	2.19	0.42
1:C:65:VAL:H	1:C:65:VAL:HG23	1.62	0.42
1:D:11:ILE:HG21	1:D:11:ILE:HD13	1.46	0.42
1:D:25:ILE:HD13	1:D:25:ILE:HG21	1.80	0.42
1:F:3:ASN:HA	1:F:81:LEU:CA	2.48	0.42
1:A:82:ASN:O	1:A:83:VAL:C	2.57	0.42
1:A:9:ILE:HG23	1:A:9:ILE:HD12	1.71	0.42
1:B:93:GLU:O	1:B:99:SER:OG	2.38	0.42
1:C:18:ARG:NH1	4:C:264:HOH:O	2.28	0.42
1:E:45:GLU:O	1:E:48:LEU:HB2	2.19	0.42
1:A:30:GLN:C	1:A:32:GLY:H	2.23	0.42
1:B:127:GLU:O	1:B:128:LYS:C	2.51	0.42
1:C:118:HIS:CD2	1:C:119:GLY:N	2.88	0.42
1:D:136:PRO:HD2	1:D:137:GLU:CG	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:THR:O	1:E:77:VAL:HA	2.20	0.42
1:F:95:ASN:C	1:F:97:ALA:N	2.73	0.42
1:B:104:ILE:O	1:B:105:ARG:C	2.57	0.42
1:B:15:GLY:O	1:B:16:VAL:C	2.57	0.42
1:C:12:LYS:CB	1:C:13:PRO:CD	2.94	0.42
1:D:149:TRP:CE2	1:F:17:GLN:HG3	2.55	0.42
1:F:143:LYS:NZ	1:F:147:GLN:OE1	2.47	0.42
1:F:95:ASN:HA	1:F:112:VAL:HG13	2.01	0.42
1:B:110:ILE:HD11	1:C:32:GLY:C	2.39	0.42
1:B:135:HIS:HA	1:B:136:PRO:HD2	1.79	0.42
1:F:45:GLU:O	1:F:49:LYS:HB2	2.19	0.42
1:B:115:ASN:C	1:B:117:ILE:H	2.23	0.42
1:D:94:THR:O	1:D:96:PRO:HD3	2.19	0.42
1:E:26:LYS:O	1:E:26:LYS:HG2	2.19	0.42
1:E:53:ILE:HD11	1:E:56:LYS:NZ	2.35	0.42
1:D:56:LYS:HB3	1:D:56:LYS:NZ	2.34	0.42
1:E:135:HIS:HA	1:E:136:PRO:HD2	1.46	0.42
3:E:161:GDP:O1B	3:E:161:GDP:O1A	2.38	0.42
1:E:45:GLU:O	1:E:49:LYS:HG2	2.20	0.42
1:F:100:LYS:HA	1:F:100:LYS:HD3	1.95	0.42
1:D:31:LYS:HE2	1:F:109:CYS:O	2.19	0.42
1:F:49:LYS:HG2	1:F:61:PHE:HZ	1.85	0.42
1:B:127:GLU:HA	1:B:130:ILE:CG1	2.45	0.42
2:D:160:35G:O2P	3:D:161:GDP:PB	2.78	0.42
1:E:124:GLU:O	1:E:127:GLU:HB2	2.20	0.42
1:A:41:MET:HE1	1:A:133:TRP:CE3	2.55	0.41
1:A:36:VAL:HG23	1:A:79:GLU:HB3	2.02	0.41
1:B:29:GLU:HG3	1:B:78:TRP:HH2	1.85	0.41
1:B:39:LYS:CE	1:B:41:MET:HE3	2.49	0.41
1:B:58:ARG:O	1:B:61:PHE:CB	2.68	0.41
1:C:61:PHE:O	1:C:62:ALA:C	2.57	0.41
1:D:15:GLY:HA2	1:D:116:ILE:HG22	2.02	0.41
1:D:135:HIS:O	1:D:138:GLU:HB2	2.19	0.41
1:E:128:LYS:O	1:E:131:ALA:HB3	2.19	0.41
1:C:81:LEU:HB3	1:C:151:TYR:CE1	2.55	0.41
1:C:93:GLU:H	1:C:99:SER:CB	2.25	0.41
1:C:53:ILE:HG23	1:C:54:ASP:H	1.84	0.41
1:D:47:LEU:HA	1:D:47:LEU:HD12	1.57	0.41
1:E:58:ARG:HG3	1:E:59:PRO:CD	2.50	0.41
1:B:129:GLU:H	1:B:129:GLU:HG2	1.53	0.41
1:C:14:ASP:OD2	1:C:116:ILE:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:LEU:HD13	1:C:64:LEU:HA	1.71	0.41
1:F:123:VAL:HG23	4:F:485:HOH:O	2.19	0.41
1:B:126:ALA:O	1:B:127:GLU:C	2.57	0.41
1:E:9:ILE:HG22	1:E:76:MET:CE	2.46	0.41
1:F:46:ASP:O	1:F:49:LYS:HB2	2.21	0.41
1:A:140:VAL:HG12	1:A:141:ASN:N	2.36	0.41
1:B:129:GLU:O	1:B:133:TRP:CD1	2.74	0.41
1:C:28:PHE:O	1:C:29:GLU:C	2.58	0.41
1:D:135:HIS:O	1:D:136:PRO:C	2.59	0.41
1:E:132:LEU:HB3	1:E:133:TRP:CD1	2.56	0.41
1:E:8:PHE:H	1:E:120:SER:HB2	1.85	0.41
1:A:100:LYS:HD2	1:A:100:LYS:HA	1.93	0.41
1:A:142:TYR:N	1:A:142:TYR:CD1	2.88	0.41
1:A:146:ALA:O	1:A:149:TRP:N	2.48	0.41
1:C:146:ALA:C	1:C:148:ASN:N	2.74	0.41
1:E:17:GLN:HG3	1:F:149:TRP:CE2	2.56	0.41
1:E:45:GLU:HB3	1:E:49:LYS:HE2	2.03	0.41
1:F:60:PHE:O	1:F:63:GLY:N	2.29	0.41
1:A:135:HIS:O	1:A:138:GLU:HB2	2.21	0.41
1:B:81:LEU:O	1:B:82:ASN:C	2.59	0.41
1:F:12:LYS:HZ1	2:F:160:35G:P	2.43	0.41
1:A:8:PHE:HD2	1:A:129:GLU:OE1	2.03	0.41
1:A:88:ARG:NH2	3:A:161:GDP:O1B	2.46	0.41
1:B:67:TYR:HA	1:B:70:SER:HG	1.85	0.41
1:C:140:VAL:HG12	1:C:142:TYR:CD1	2.54	0.41
1:A:17:GLN:NE2	1:E:142:TYR:HD2	2.19	0.41
1:D:24:ILE:HA	1:D:27:ARG:HG3	2.03	0.41
2:E:160:35G:C5'	3:E:161:GDP:PA	2.84	0.41
1:F:67:TYR:C	1:F:67:TYR:CD1	2.89	0.41
1:A:112:VAL:HG12	1:A:115:ASN:ND2	2.36	0.41
1:A:83:VAL:O	1:A:84:VAL:C	2.57	0.41
1:B:140:VAL:HG11	1:D:72:PRO:CB	2.51	0.41
1:B:4:SER:C	1:B:79:GLU:HG3	2.42	0.41
1:B:111:GLN:OE1	1:C:151:TYR:HD1	2.04	0.41
1:D:41:MET:O	1:D:72:PRO:HA	2.21	0.41
1:E:48:LEU:O	1:E:49:LYS:C	2.56	0.41
1:F:123:VAL:C	1:F:125:SER:N	2.72	0.41
1:B:140:VAL:HG11	1:D:72:PRO:CG	2.50	0.40
1:B:86:THR:O	1:B:87:GLY:C	2.60	0.40
1:C:94:THR:HG22	4:C:499:HOH:O	2.20	0.40
1:D:84:VAL:HG21	1:D:123:VAL:HA	2.01	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:VAL:HG23	1:E:113:GLY:N	2.33	0.40
1:E:137:GLU:HG3	1:E:137:GLU:H	1.29	0.40
1:E:23:GLU:O	1:E:27:ARG:HG2	2.21	0.40
1:E:39:LYS:CE	1:E:41:MET:HE3	2.48	0.40
1:E:94:THR:O	1:E:96:PRO:HD3	2.21	0.40
1:F:53:ILE:CG2	1:F:54:ASP:H	2.34	0.40
1:C:100:LYS:HA	1:C:101:PRO:HD3	1.89	0.40
1:C:149:TRP:CE3	1:C:149:TRP:HA	2.57	0.40
1:C:45:GLU:O	1:C:48:LEU:N	2.55	0.40
1:D:47:LEU:CD1	1:D:132:LEU:CD2	2.99	0.40
1:E:81:LEU:HD12	1:E:82:ASN:HD22	1.85	0.40
1:A:6:ARG:HD2	1:A:36:VAL:HG21	2.03	0.40
1:B:93:GLU:O	1:B:95:ASN:N	2.54	0.40
1:A:152:GLU:N	1:C:111:GLN:OE1	2.31	0.40
1:C:34:ARG:NH1	1:C:36:VAL:HG22	2.36	0.40
1:C:9:ILE:O	1:C:76:MET:HE2	2.21	0.40
1:E:12:LYS:HB3	1:E:13:PRO:HD3	2.03	0.40
1:F:46:ASP:O	1:F:50:GLU:HB2	2.20	0.40
1:F:48:LEU:O	1:F:51:HIS:HB3	2.21	0.40
1:A:47:LEU:HD13	1:A:132:LEU:HD21	2.03	0.40
1:B:123:VAL:O	1:B:126:ALA:N	2.55	0.40
1:D:55:LEU:HA	1:D:55:LEU:HD23	1.48	0.40
1:E:51:HIS:ND1	1:E:133:TRP:NE1	2.63	0.40
1:E:64:LEU:HD12	1:E:64:LEU:O	2.22	0.40
1:B:9:ILE:HD13	1:B:9:ILE:HA	1.79	0.40
1:D:84:VAL:HG12	1:D:85:LYS:N	2.37	0.40
1:E:72:PRO:C	1:E:73:VAL:HG13	2.41	0.40
1:E:40:PHE:HE1	1:E:72:PRO:HB2	1.80	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	149/152 (98%)	126 (85%)	16 (11%)	7 (5%)	2 1
1	B	149/152 (98%)	118 (79%)	17 (11%)	14 (9%)	0 0
1	C	149/152 (98%)	122 (82%)	18 (12%)	9 (6%)	1 0
1	D	149/152 (98%)	119 (80%)	25 (17%)	5 (3%)	3 3
1	E	149/152 (98%)	122 (82%)	21 (14%)	6 (4%)	3 2
1	F	149/152 (98%)	117 (78%)	21 (14%)	11 (7%)	1 0
All	All	894/912 (98%)	724 (81%)	118 (13%)	52 (6%)	1 0

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	59	PRO
1	A	61	PHE
1	A	115	ASN
1	A	116	ILE
1	B	56	LYS
1	B	58	ARG
1	B	59	PRO
1	B	96	PRO
1	B	116	ILE
1	C	83	VAL
1	C	100	LYS
1	C	116	ILE
1	D	61	PHE
1	D	116	ILE
1	E	116	ILE
1	F	58	ARG
1	F	61	PHE
1	F	84	VAL
1	F	116	ILE
1	A	104	ILE
1	A	130	ILE
1	B	52	TYR
1	B	53	ILE
1	B	61	PHE
1	B	94	THR
1	B	136	PRO
1	C	84	VAL
1	C	147	GLN
1	E	19	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	59	PRO
1	E	61	PHE
1	F	68	MET
1	B	5	GLU
1	F	59	PRO
1	F	146	ALA
1	C	112	VAL
1	E	53	ILE
1	C	61	PHE
1	C	96	PRO
1	C	136	PRO
1	F	96	PRO
1	F	120	SER
1	B	48	LEU
1	B	104	ILE
1	B	84	VAL
1	D	21	ILE
1	E	83	VAL
1	F	123	VAL
1	D	84	VAL
1	D	136	PRO
1	F	112	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	128/129 (99%)	95 (74%)	33 (26%)	0	0
1	B	128/129 (99%)	91 (71%)	37 (29%)	0	0
1	C	128/129 (99%)	93 (73%)	35 (27%)	0	0
1	D	128/129 (99%)	100 (78%)	28 (22%)	1	1
1	E	128/129 (99%)	93 (73%)	35 (27%)	0	0
1	F	128/129 (99%)	99 (77%)	29 (23%)	1	1
All	All	768/774 (99%)	571 (74%)	197 (26%)	0	0

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	14	ASP
1	A	23	GLU
1	A	35	LEU
1	A	38	MET
1	A	48	LEU
1	A	53	ILE
1	A	54	ASP
1	A	55	LEU
1	A	56	LYS
1	A	58	ARG
1	A	66	LYS
1	A	70	SER
1	A	77	VAL
1	A	81	LEU
1	A	83	VAL
1	A	85	LYS
1	A	88	ARG
1	A	93	GLU
1	A	98	ASP
1	A	100	LYS
1	A	108	PHE
1	A	112	VAL
1	A	116	ILE
1	A	128	LYS
1	A	137	GLU
1	A	139	LEU
1	A	140	VAL
1	A	142	TYR
1	A	143	LYS
1	A	147	GLN
1	A	148	ASN
1	A	150	ILE
1	B	3	ASN
1	B	4	SER
1	B	6	ARG
1	B	20	LEU
1	B	35	LEU
1	B	38	MET
1	B	41	MET
1	B	44	SER
1	B	48	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	49	LYS
1	B	50	GLU
1	B	51	HIS
1	B	53	ILE
1	B	56	LYS
1	B	57	ASP
1	B	64	LEU
1	B	66	LYS
1	B	70	SER
1	B	79	GLU
1	B	83	VAL
1	B	88	ARG
1	B	93	GLU
1	B	109	CYS
1	B	115	ASN
1	B	116	ILE
1	B	124	GLU
1	B	125	SER
1	B	128	LYS
1	B	129	GLU
1	B	132	LEU
1	B	134	PHE
1	B	137	GLU
1	B	139	LEU
1	B	143	LYS
1	B	144	SER
1	B	145	CYS
1	B	151	TYR
1	C	4	SER
1	C	6	ARG
1	C	9	ILE
1	C	12	LYS
1	C	30	GLN
1	C	35	LEU
1	C	41	MET
1	C	47	LEU
1	C	50	GLU
1	C	56	LYS
1	C	58	ARG
1	C	64	LEU
1	C	66	LYS
1	C	76	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	79	GLU
1	C	83	VAL
1	C	94	THR
1	C	98	ASP
1	C	100	LYS
1	C	104	ILE
1	C	107	ASP
1	C	110	ILE
1	C	112	VAL
1	C	114	ARG
1	C	120	SER
1	C	121	ASP
1	C	123	VAL
1	C	124	GLU
1	C	132	LEU
1	C	137	GLU
1	C	141	ASN
1	C	143	LYS
1	C	144	SER
1	C	147	GLN
1	C	148	ASN
1	D	4	SER
1	D	6	ARG
1	D	20	LEU
1	D	31	LYS
1	D	35	LEU
1	D	39	LYS
1	D	41	MET
1	D	49	LYS
1	D	50	GLU
1	D	54	ASP
1	D	56	LYS
1	D	64	LEU
1	D	66	LYS
1	D	67	TYR
1	D	79	GLU
1	D	83	VAL
1	D	88	ARG
1	D	91	LEU
1	D	94	THR
1	D	104	ILE
1	D	112	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	121	ASP
1	D	124	GLU
1	D	130	ILE
1	D	137	GLU
1	D	143	LYS
1	D	144	SER
1	D	152	GLU
1	E	6	ARG
1	E	18	ARG
1	E	35	LEU
1	E	41	MET
1	E	44	SER
1	E	46	ASP
1	E	47	LEU
1	E	49	LYS
1	E	53	ILE
1	E	55	LEU
1	E	56	LYS
1	E	64	LEU
1	E	66	LYS
1	E	67	TYR
1	E	76	MET
1	E	81	LEU
1	E	83	VAL
1	E	85	LYS
1	E	91	LEU
1	E	93	GLU
1	E	94	THR
1	E	100	LYS
1	E	112	VAL
1	E	120	SER
1	E	121	ASP
1	E	124	GLU
1	E	132	LEU
1	E	136	PRO
1	E	137	GLU
1	E	141	ASN
1	E	142	TYR
1	E	143	LYS
1	E	144	SER
1	E	147	GLN
1	E	148	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	6	ARG
1	F	7	THR
1	F	14	ASP
1	F	30	GLN
1	F	35	LEU
1	F	39	LYS
1	F	41	MET
1	F	46	ASP
1	F	54	ASP
1	F	57	ASP
1	F	58	ARG
1	F	60	PHE
1	F	66	LYS
1	F	69	HIS
1	F	70	SER
1	F	83	VAL
1	F	85	LYS
1	F	96	PRO
1	F	112	VAL
1	F	120	SER
1	F	123	VAL
1	F	127	GLU
1	F	129	GLU
1	F	132	LEU
1	F	137	GLU
1	F	139	LEU
1	F	147	GLN
1	F	148	ASN
1	F	152	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	82	ASN
1	A	141	ASN
1	A	147	GLN
1	A	148	ASN
1	B	30	GLN
1	B	69	HIS
1	C	30	GLN
1	C	51	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	148	ASN
1	D	141	ASN
1	E	30	GLN
1	E	82	ASN
1	E	148	ASN
1	F	30	GLN
1	F	69	HIS
1	F	135	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	35G	B	160	-	22,26,26	2.04	4 (18%)	26,41,41	3.19	10 (38%)
2	35G	A	160	-	22,26,26	2.17	5 (22%)	26,41,41	4.58	10 (38%)
2	35G	F	160	-	22,26,26	2.47	7 (31%)	26,41,41	3.30	10 (38%)
2	35G	E	160	-	22,26,26	1.77	4 (18%)	26,41,41	3.87	9 (34%)
2	35G	D	160	-	22,26,26	1.97	4 (18%)	26,41,41	4.17	9 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GDP	B	161	-	24,30,30	1.29	2 (8%)	31,47,47	2.23	5 (16%)
3	GDP	F	161	-	24,30,30	1.17	2 (8%)	31,47,47	2.86	8 (25%)
3	GDP	D	161	-	24,30,30	1.20	2 (8%)	31,47,47	3.55	10 (32%)
3	GDP	C	161	-	24,30,30	1.44	3 (12%)	31,47,47	2.75	9 (29%)
3	GDP	A	161	-	24,30,30	1.31	2 (8%)	31,47,47	2.43	8 (25%)
3	GDP	E	161	-	24,30,30	1.36	3 (12%)	31,47,47	3.26	13 (41%)
2	35G	C	160	-	22,26,26	2.32	6 (27%)	26,41,41	4.21	10 (38%)

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
2	35G	B	160	-	-	0/0/31/31	0/4/4/4
2	35G	A	160	-	-	0/0/31/31	0/4/4/4
2	35G	F	160	-	-	0/0/31/31	0/4/4/4
2	35G	E	160	-	-	0/0/31/31	0/4/4/4
2	35G	D	160	-	-	0/0/31/31	0/4/4/4
3	GDP	B	161	-	-	0/12/32/32	0/3/3/3
3	GDP	F	161	-	-	3/12/32/32	0/3/3/3
3	GDP	D	161	-	-	2/12/32/32	0/3/3/3
3	GDP	C	161	-	-	0/12/32/32	0/3/3/3
3	GDP	A	161	-	-	2/12/32/32	0/3/3/3
3	GDP	E	161	-	-	1/12/32/32	0/3/3/3
2	35G	C	160	-	-	0/0/31/31	0/4/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	160	35G	P-O5'	-6.67	1.50	1.57
2	C	160	35G	P-O5'	-6.37	1.50	1.57
2	B	160	35G	P-O5'	-6.09	1.50	1.57
2	A	160	35G	P-O5'	-5.97	1.50	1.57
2	D	160	35G	P-O5'	-5.89	1.51	1.57
2	F	160	35G	P-O3'	-5.85	1.48	1.57
2	C	160	35G	C6-N1	4.85	1.41	1.33
3	C	161	GDP	C6-N1	4.74	1.41	1.33
2	A	160	35G	P-O3'	-4.56	1.50	1.57
3	E	161	GDP	C6-N1	4.55	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	160	35G	P-O5'	-4.52	1.52	1.57
2	B	160	35G	P-O3'	-4.49	1.50	1.57
3	A	161	GDP	C6-N1	4.45	1.40	1.33
2	A	160	35G	C6-N1	4.44	1.40	1.33
2	B	160	35G	C6-N1	4.35	1.40	1.33
2	D	160	35G	C6-N1	4.32	1.40	1.33
2	F	160	35G	C6-N1	4.31	1.40	1.33
2	E	160	35G	C6-N1	4.27	1.40	1.33
2	C	160	35G	P-O3'	-4.08	1.51	1.57
3	B	161	GDP	C6-N1	4.02	1.40	1.33
3	D	161	GDP	C6-N1	3.94	1.39	1.33
2	E	160	35G	P-O3'	-3.87	1.51	1.57
2	C	160	35G	C2-N1	3.75	1.42	1.35
2	D	160	35G	P-O3'	-3.73	1.51	1.57
3	F	161	GDP	C6-N1	3.55	1.39	1.33
2	F	160	35G	O3'-C3'	-2.99	1.39	1.44
2	A	160	35G	C2-N1	2.93	1.40	1.35
2	C	160	35G	O5'-C5'	-2.67	1.42	1.46
3	B	161	GDP	PA-O5'	-2.64	1.48	1.59
3	C	161	GDP	PA-O5'	-2.63	1.48	1.59
2	F	160	35G	C2-N1	2.56	1.39	1.35
2	C	160	35G	C8-N7	-2.44	1.30	1.34
3	F	161	GDP	PA-O5'	-2.44	1.49	1.59
3	A	161	GDP	PA-O5'	-2.40	1.49	1.59
2	F	160	35G	O4'-C1'	2.30	1.44	1.41
2	E	160	35G	C8-N7	-2.28	1.30	1.34
2	A	160	35G	O5'-C5'	-2.27	1.42	1.46
3	D	161	GDP	PA-O5'	-2.25	1.50	1.59
3	C	161	GDP	C8-N7	-2.21	1.30	1.34
3	E	161	GDP	C8-N7	-2.13	1.30	1.34
2	D	160	35G	C2-N1	2.12	1.39	1.35
2	F	160	35G	O5'-C5'	-2.11	1.43	1.46
2	B	160	35G	C2-N1	2.08	1.39	1.35
3	E	161	GDP	PA-O5'	-2.07	1.50	1.59

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	160	35G	C1'-N9-C4	-16.67	97.36	126.64
2	A	160	35G	C1'-N9-C4	-16.29	98.01	126.64
2	E	160	35G	C1'-N9-C4	-13.90	102.21	126.64
2	C	160	35G	C1'-N9-C4	-12.86	104.04	126.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	161	GDP	C5-C6-N1	-9.56	110.36	123.43
3	F	161	GDP	O3B-PB-O2B	9.55	144.13	107.64
2	A	160	35G	C5-C6-N1	-9.41	110.55	123.43
3	E	161	GDP	O3B-PB-O1B	9.19	146.66	110.68
3	D	161	GDP	C1'-N9-C4	-9.16	110.54	126.64
3	D	161	GDP	O3B-PB-O1B	9.04	146.09	110.68
2	F	160	35G	C5-C6-N1	-9.00	111.13	123.43
2	D	160	35G	C5-C6-N1	-8.61	111.65	123.43
3	B	161	GDP	C5-C6-N1	-8.59	111.69	123.43
2	A	160	35G	O3'-C3'-C4'	-8.53	104.27	110.71
2	B	160	35G	C5-C6-N1	-8.26	112.14	123.43
3	D	161	GDP	C5-C6-N1	-8.18	112.24	123.43
3	D	161	GDP	O3B-PB-O2B	-8.09	76.72	107.64
2	E	160	35G	C5-C6-N1	-7.95	112.56	123.43
3	A	161	GDP	C5-C6-N1	-7.94	112.58	123.43
2	F	160	35G	O5'-P-O3'	7.93	116.60	105.68
2	B	160	35G	O3'-C3'-C2'	7.77	123.23	115.61
2	C	160	35G	C5-C6-N1	-7.51	113.16	123.43
3	E	161	GDP	C5-C6-N1	-7.48	113.19	123.43
3	E	161	GDP	O3B-PB-O2B	-7.08	80.59	107.64
3	F	161	GDP	C5-C6-N1	-6.98	113.88	123.43
2	B	160	35G	C1'-N9-C4	-6.60	115.04	126.64
2	A	160	35G	C6-N1-C2	6.47	126.22	115.93
2	C	160	35G	C6-N1-C2	6.46	126.20	115.93
3	C	161	GDP	C6-N1-C2	6.36	126.04	115.93
3	F	161	GDP	O3B-PB-O1B	-6.31	85.96	110.68
2	C	160	35G	O5'-P-O3'	6.27	114.31	105.68
2	C	160	35G	N2-C2-N1	6.09	126.72	117.25
3	E	161	GDP	C6-N1-C2	6.03	125.52	115.93
2	C	160	35G	O3'-C3'-C4'	-6.03	106.16	110.71
3	A	161	GDP	C6-N1-C2	5.97	125.42	115.93
2	F	160	35G	C6-N1-C2	5.96	125.40	115.93
2	C	160	35G	N3-C2-N1	-5.92	119.32	127.22
2	E	160	35G	C6-N1-C2	5.67	124.94	115.93
3	D	161	GDP	C6-N1-C2	5.48	124.63	115.93
2	D	160	35G	C6-N1-C2	5.43	124.56	115.93
2	F	160	35G	O3'-P-O1P	-5.34	98.95	110.39
2	E	160	35G	O5'-P-O3'	5.34	113.03	105.68
3	B	161	GDP	C6-N1-C2	5.30	124.35	115.93
2	A	160	35G	O5'-P-O3'	5.18	112.81	105.68
2	D	160	35G	O3'-C3'-C2'	5.14	120.64	115.61
3	C	161	GDP	C1'-N9-C4	-5.11	117.66	126.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	160	35G	C6-N1-C2	5.09	124.03	115.93
3	F	161	GDP	C6-N1-C2	4.60	123.24	115.93
3	E	161	GDP	N3-C2-N1	-4.53	121.18	127.22
2	E	160	35G	O3'-C3'-C4'	-4.49	107.32	110.71
3	A	161	GDP	O3B-PB-O2B	4.41	124.49	107.64
2	F	160	35G	O3'-C3'-C2'	-4.23	111.45	115.61
3	C	161	GDP	O3B-PB-O1B	4.20	127.14	110.68
2	C	160	35G	C2'-C3'-C4'	-4.20	95.77	103.22
2	C	160	35G	C6-C5-C4	-4.18	116.81	120.80
3	E	161	GDP	PA-O3A-PB	-4.15	118.59	132.83
3	F	161	GDP	C1'-N9-C4	-4.13	119.39	126.64
2	F	160	35G	C1'-N9-C4	-4.10	119.43	126.64
2	B	160	35G	O5'-P-O3'	3.85	110.98	105.68
2	B	160	35G	O2'-C2'-C3'	3.79	121.94	111.17
3	A	161	GDP	C6-C5-C4	-3.76	117.21	120.80
3	C	161	GDP	C2-N3-C4	-3.68	111.15	115.36
3	D	161	GDP	O2B-PB-O3A	-3.49	92.94	104.64
2	A	160	35G	C2-N3-C4	-3.31	111.58	115.36
2	A	160	35G	N3-C2-N1	-3.30	122.82	127.22
2	D	160	35G	O2P-P-O3'	3.24	114.59	107.04
3	B	161	GDP	C2-N3-C4	-3.24	111.66	115.36
3	A	161	GDP	N3-C2-N1	-3.20	122.95	127.22
3	E	161	GDP	C6-C5-C4	-3.19	117.75	120.80
2	F	160	35G	O3'-C3'-C4'	-3.16	108.33	110.71
3	B	161	GDP	C1'-N9-C4	-3.14	121.12	126.64
3	C	161	GDP	O3B-PB-O2B	-3.13	95.68	107.64
2	E	160	35G	C2-N3-C4	-2.99	111.94	115.36
2	E	160	35G	N3-C2-N1	-2.91	123.34	127.22
3	A	161	GDP	O3B-PB-O1B	-2.88	99.42	110.68
3	A	161	GDP	C4-C5-N7	2.86	112.38	109.40
2	E	160	35G	C6-C5-C4	-2.86	118.06	120.80
3	B	161	GDP	O3B-PB-O1B	2.83	121.76	110.68
3	E	161	GDP	C4-C5-N7	2.80	112.32	109.40
3	D	161	GDP	C2-N3-C4	-2.79	112.18	115.36
3	C	161	GDP	PA-O3A-PB	-2.73	123.44	132.83
3	E	161	GDP	C1'-N9-C4	-2.73	121.84	126.64
3	D	161	GDP	PA-O3A-PB	-2.73	123.47	132.83
3	E	161	GDP	C3'-C2'-C1'	2.72	105.08	100.98
2	F	160	35G	C2-N3-C4	-2.71	112.27	115.36
3	A	161	GDP	C2-N3-C4	-2.68	112.30	115.36
2	E	160	35G	C4-C5-N7	2.60	112.11	109.40
3	D	161	GDP	O2A-PA-O1A	2.56	124.91	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	161	GDP	N3-C2-N1	-2.54	123.84	127.22
2	F	160	35G	N3-C2-N1	-2.51	123.88	127.22
2	D	160	35G	O5'-P-O1P	-2.50	104.68	110.44
2	C	160	35G	N2-C2-N3	-2.48	113.75	117.79
3	F	161	GDP	C6-C5-C4	-2.43	118.47	120.80
2	D	160	35G	C2-N3-C4	-2.40	112.62	115.36
2	D	160	35G	N3-C2-N1	-2.36	124.08	127.22
2	A	160	35G	O3'-C3'-C2'	2.36	117.92	115.61
3	E	161	GDP	N2-C2-N3	2.35	121.62	117.79
2	D	160	35G	O5'-P-O3'	2.33	108.89	105.68
2	B	160	35G	N3-C2-N1	-2.33	124.12	127.22
2	B	160	35G	C2-N3-C4	-2.30	112.73	115.36
3	E	161	GDP	O5'-C5'-C4'	2.19	116.54	108.99
3	F	161	GDP	O5'-C5'-C4'	2.16	116.42	108.99
3	E	161	GDP	O2'-C2'-C3'	2.15	118.76	111.82
3	D	161	GDP	N3-C2-N1	-2.11	124.41	127.22
3	F	161	GDP	C2-N3-C4	-2.10	112.96	115.36
2	F	160	35G	O4'-C4'-C3'	-2.09	100.40	104.87
3	C	161	GDP	C4-C5-N7	2.06	111.55	109.40
2	B	160	35G	C5'-C4'-C3'	-2.03	108.37	112.49
2	A	160	35G	C6-C5-C4	-2.03	118.86	120.80
2	B	160	35G	C6-C5-C4	-2.00	118.88	120.80
2	A	160	35G	N2-C2-N1	2.00	120.37	117.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	161	GDP	C5'-O5'-PA-O3A
3	F	161	GDP	C5'-O5'-PA-O1A
3	D	161	GDP	PA-O3A-PB-O2B
3	A	161	GDP	C5'-O5'-PA-O3A
3	D	161	GDP	PB-O3A-PA-O1A
3	E	161	GDP	PA-O3A-PB-O2B
3	A	161	GDP	PB-O3A-PA-O2A
3	F	161	GDP	C4'-C5'-O5'-PA

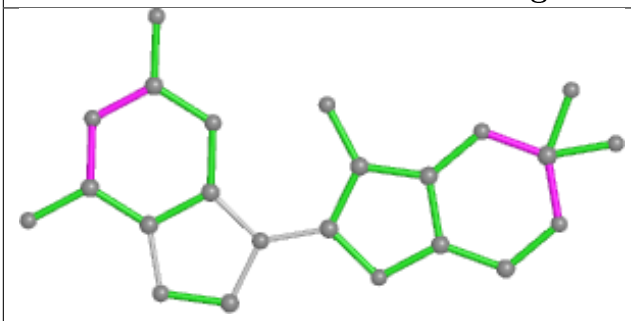
There are no ring outliers.

12 monomers are involved in 47 short contacts:

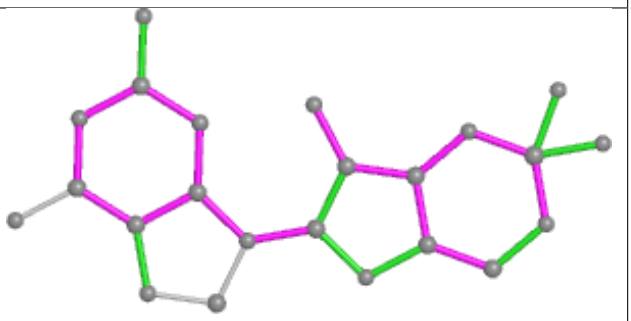
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	160	35G	10	0
2	A	160	35G	6	0
2	F	160	35G	7	0
2	E	160	35G	3	0
2	D	160	35G	4	0
3	B	161	GDP	8	0
3	F	161	GDP	4	0
3	D	161	GDP	4	0
3	C	161	GDP	6	0
3	A	161	GDP	8	0
3	E	161	GDP	8	0
2	C	160	35G	6	0

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.

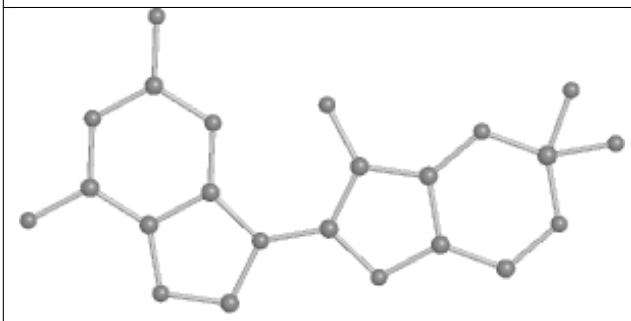
Ligand 35G B 160



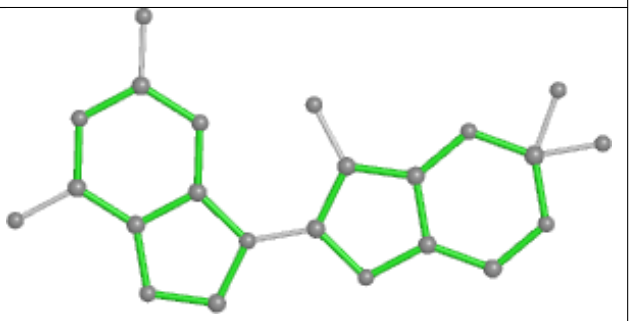
Bond lengths



Bond angles

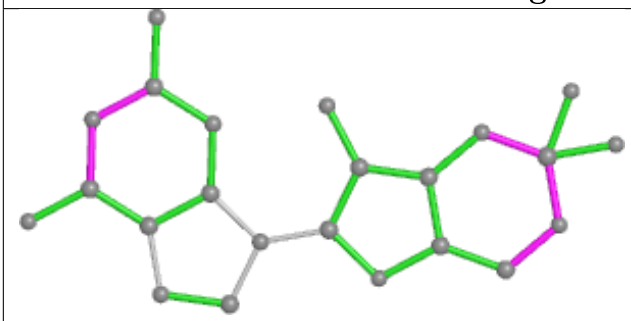


Torsions

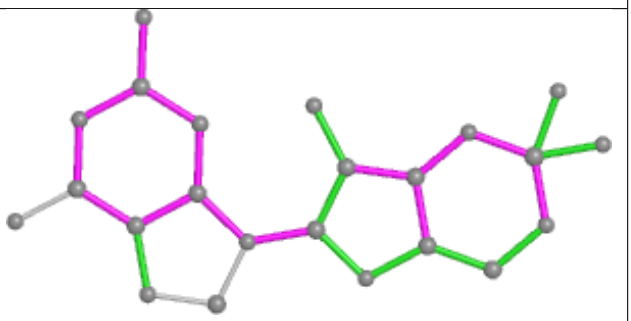


Rings

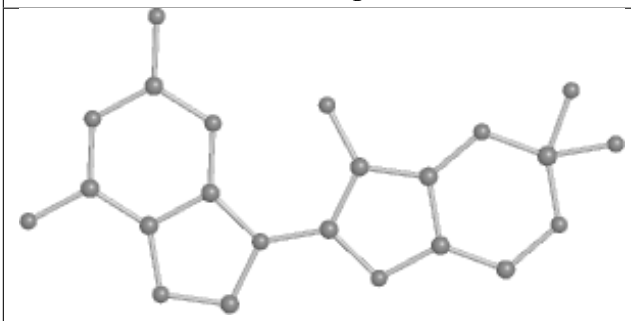
Ligand 35G A 160



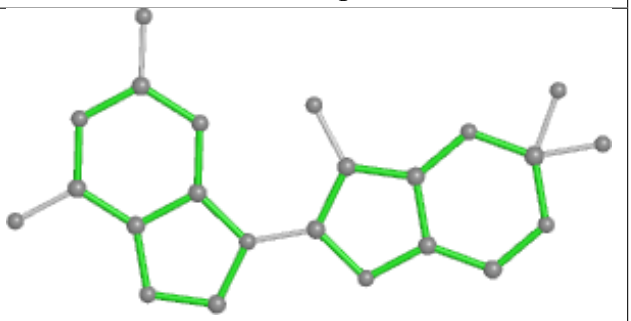
Bond lengths



Bond angles

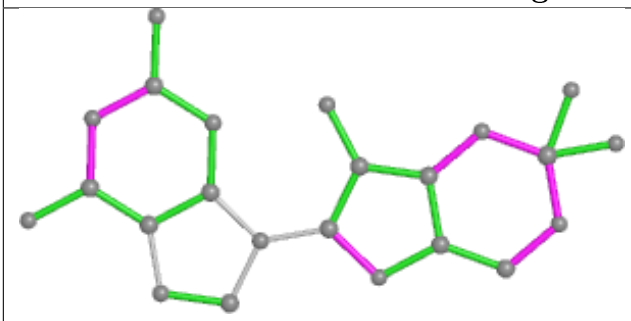


Torsions

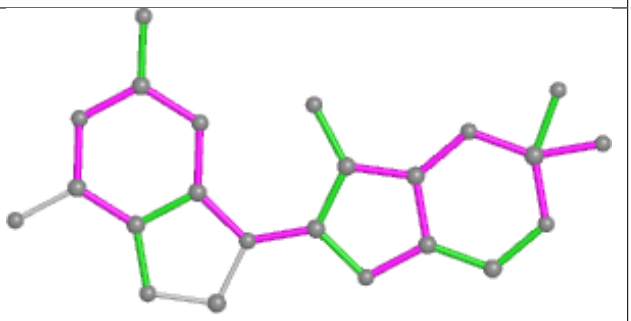


Rings

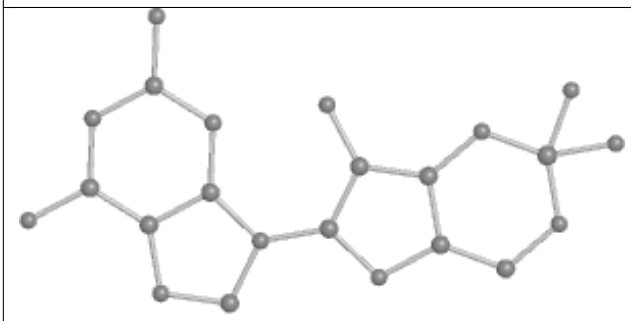
Ligand 35G F 160



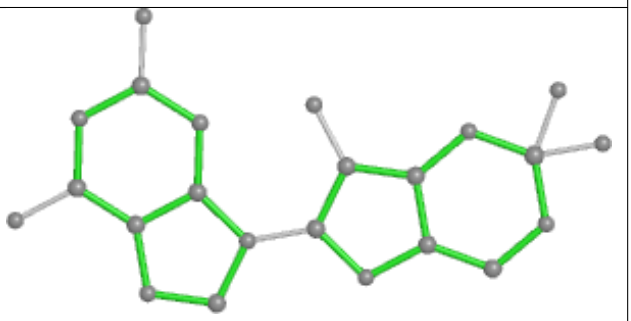
Bond lengths



Bond angles

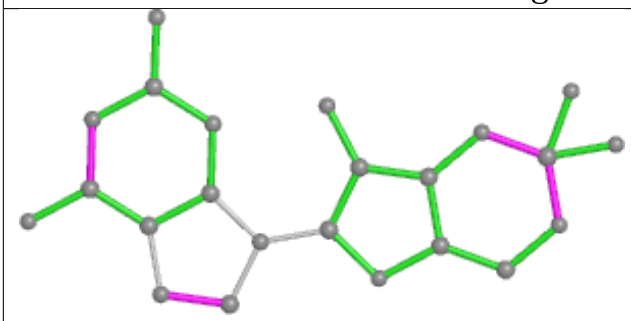


Torsions

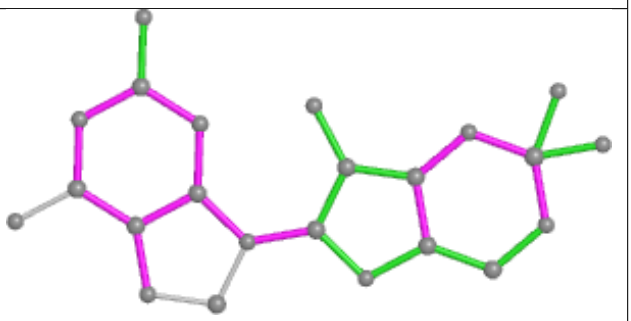


Rings

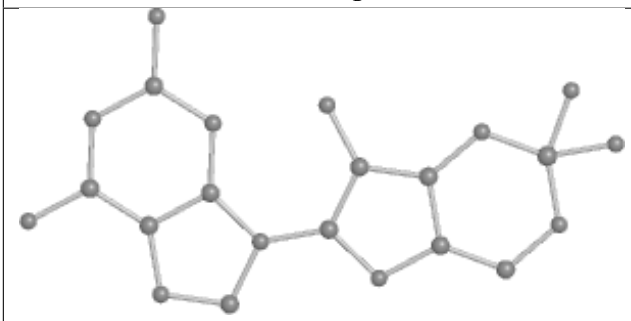
Ligand 35G E 160



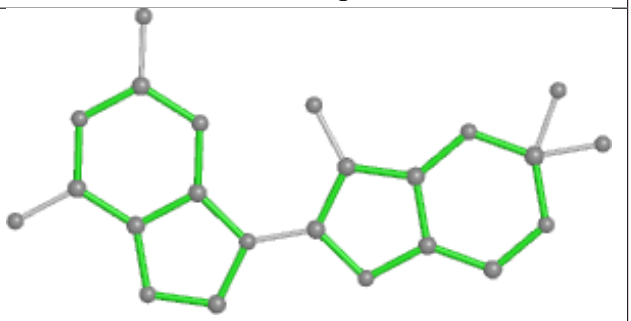
Bond lengths



Bond angles

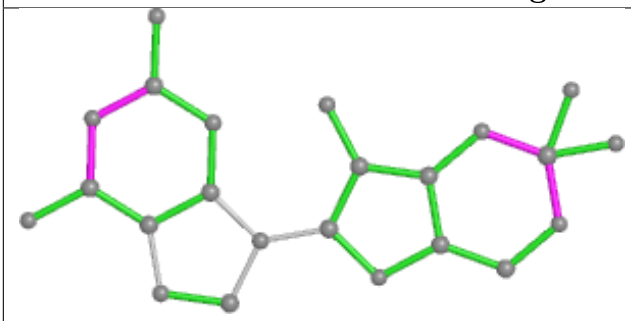


Torsions

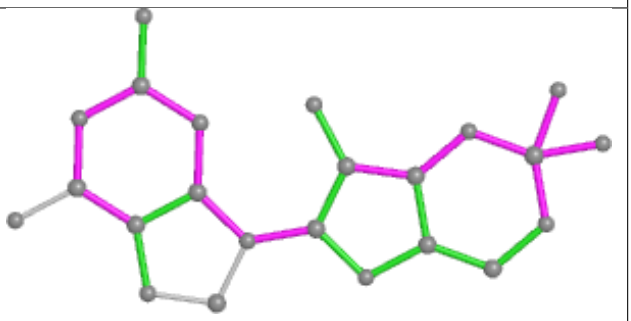


Rings

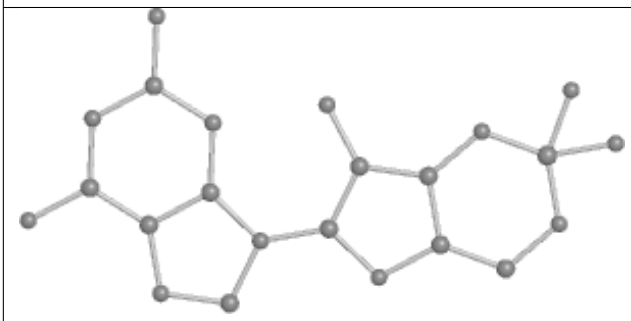
Ligand 35G D 160



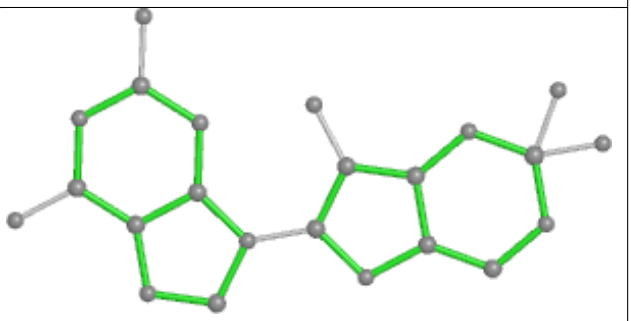
Bond lengths



Bond angles

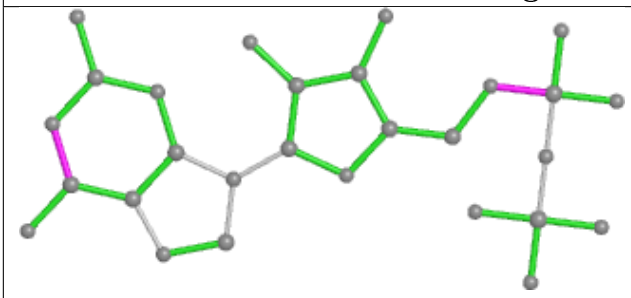


Torsions

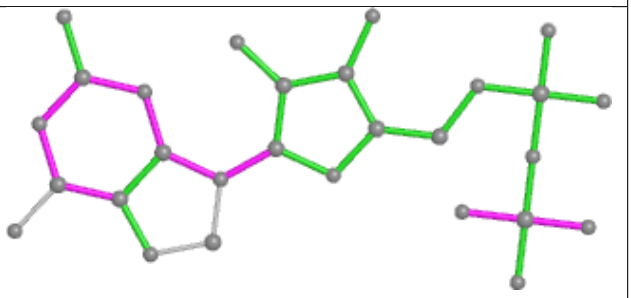


Rings

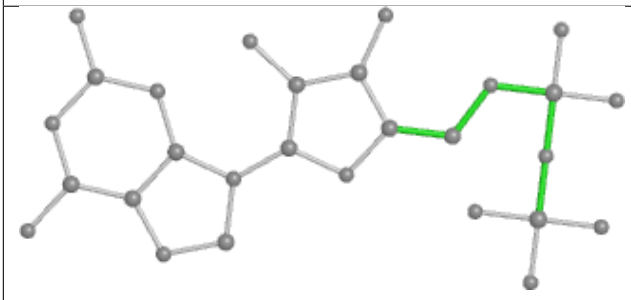
Ligand GDP B 161



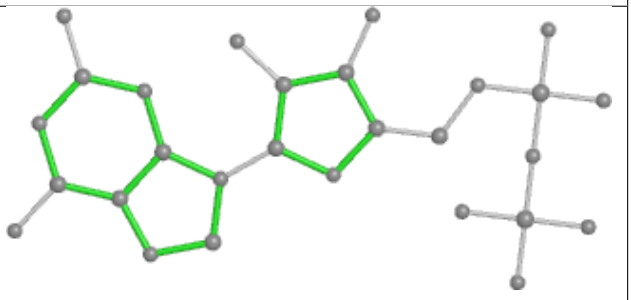
Bond lengths



Bond angles

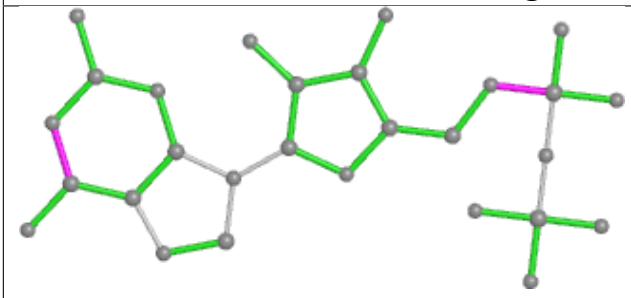


Torsions

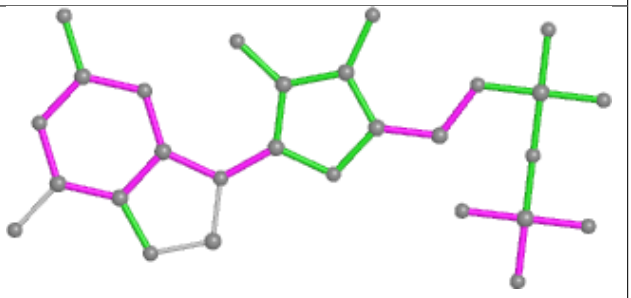


Rings

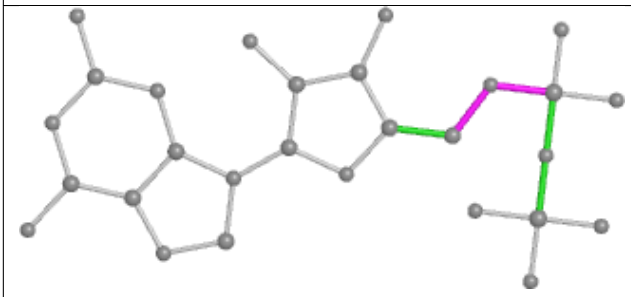
Ligand GDP F 161



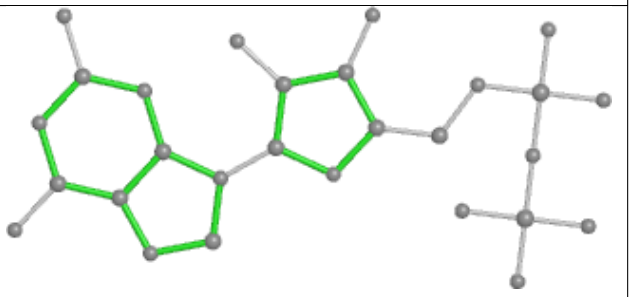
Bond lengths



Bond angles

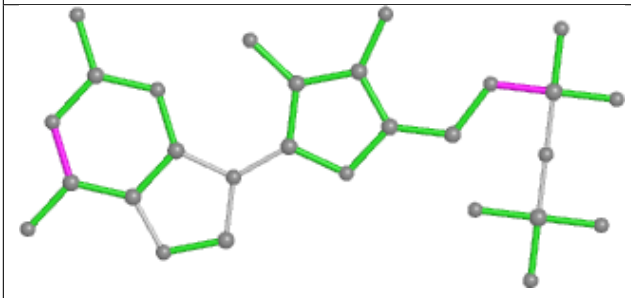


Torsions

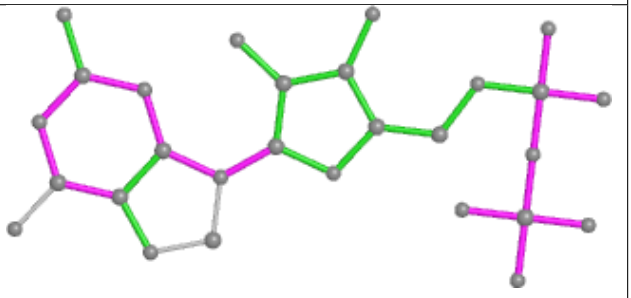


Rings

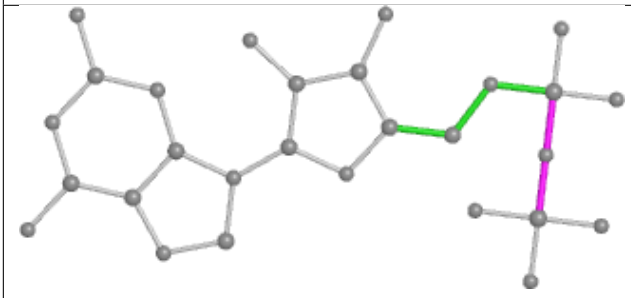
Ligand GDP D 161



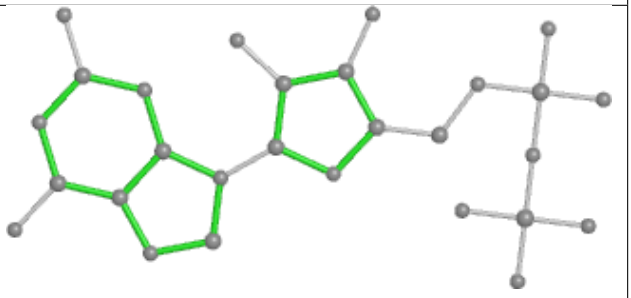
Bond lengths



Bond angles

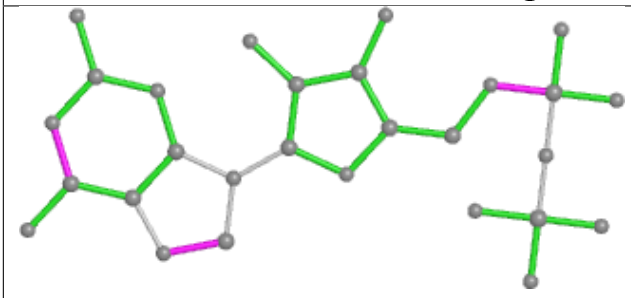


Torsions

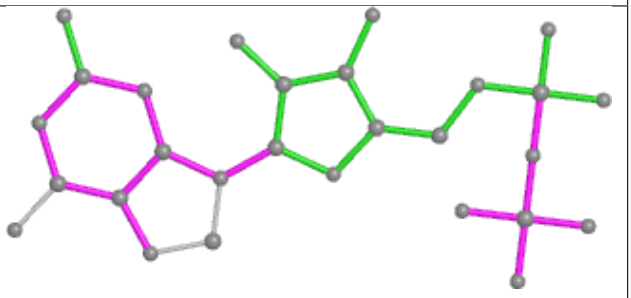


Rings

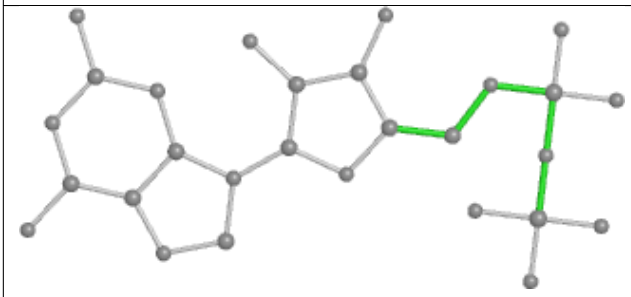
Ligand GDP C 161



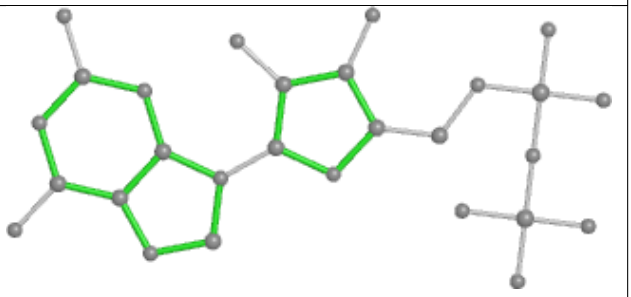
Bond lengths



Bond angles

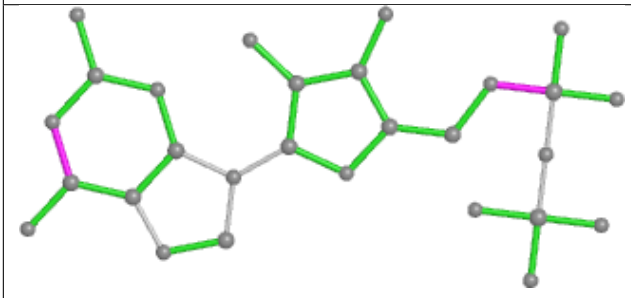


Torsions

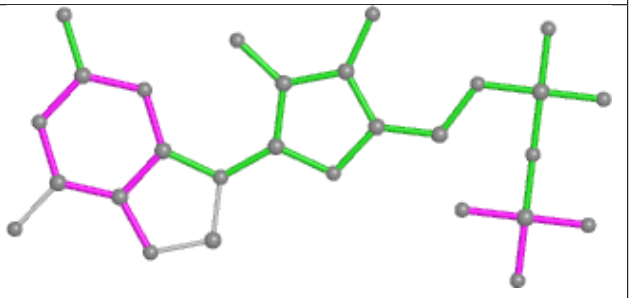


Rings

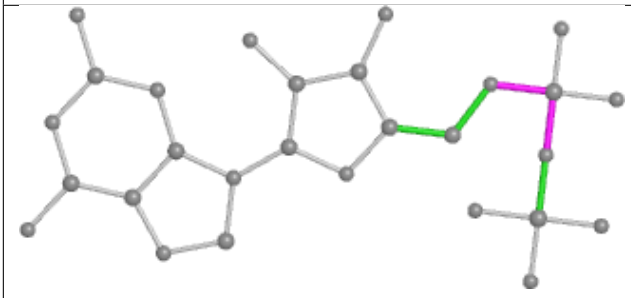
Ligand GDP A 161



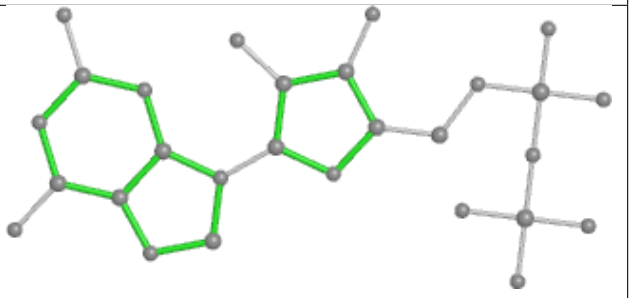
Bond lengths



Bond angles

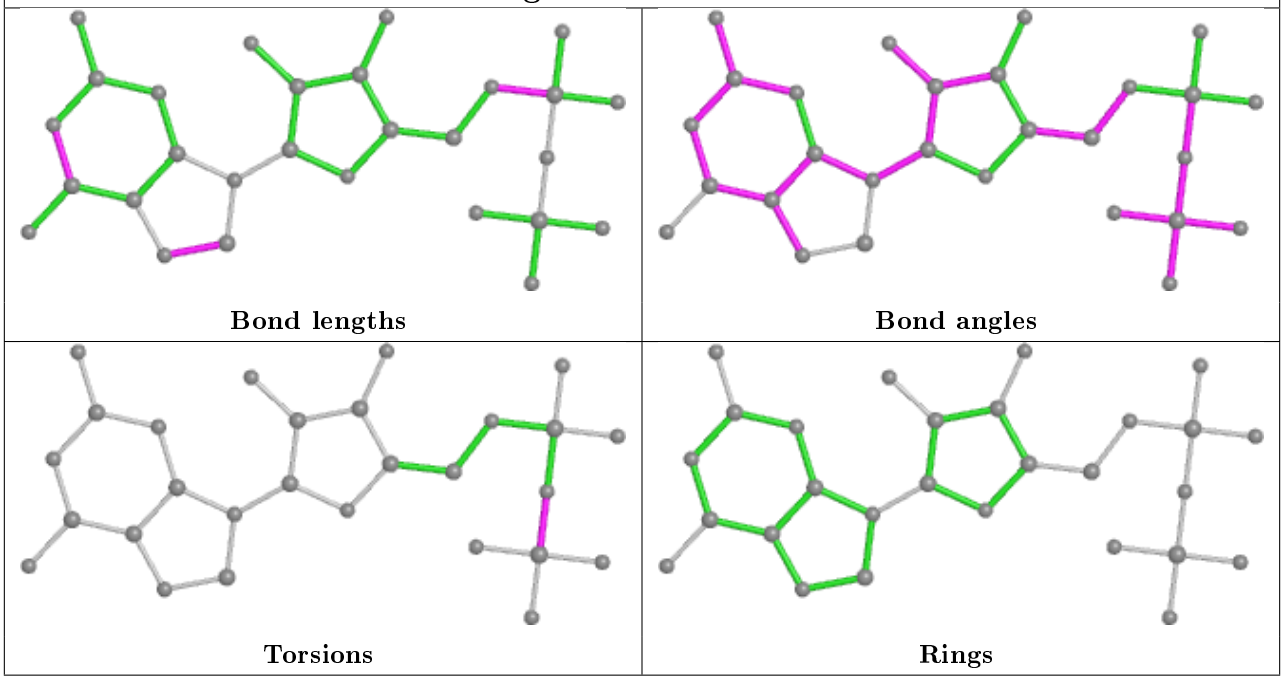


Torsions

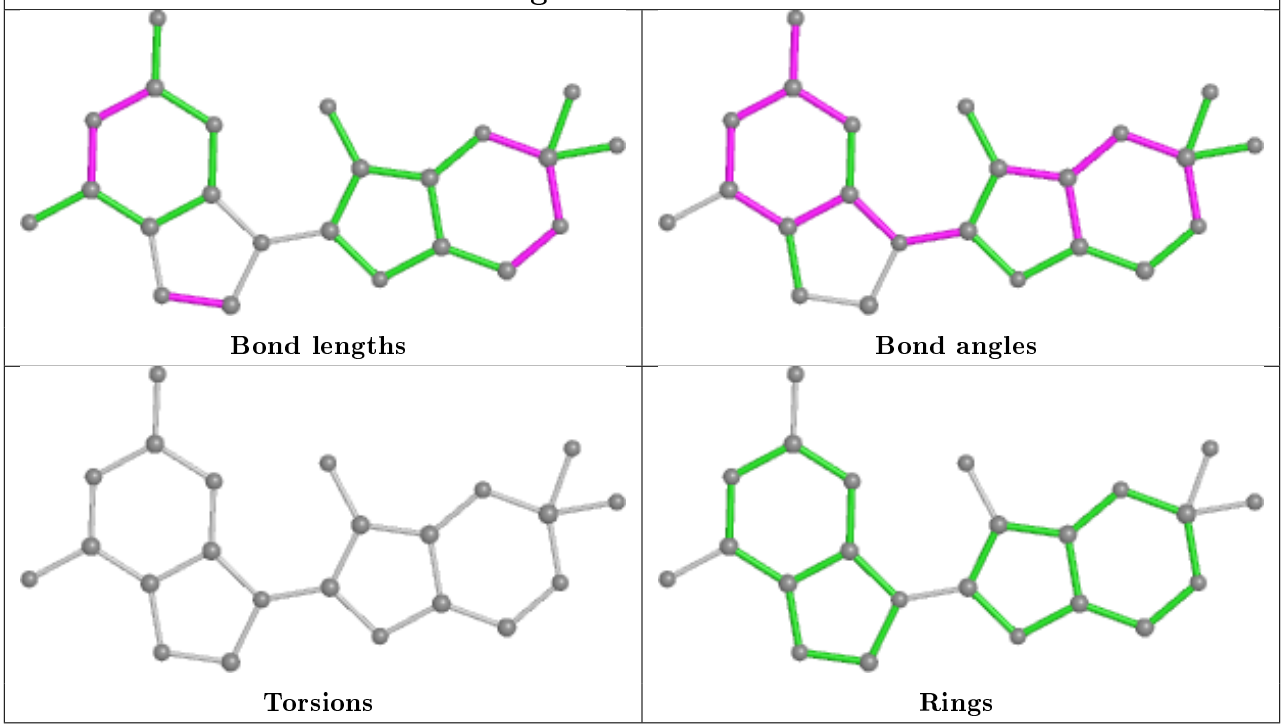


Rings

Ligand GDP E 161



Ligand 35G C 160



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	151/152 (99%)	-0.69	0 100 100	7, 25, 54, 76	0
1	B	151/152 (99%)	-0.50	3 (1%) 65 63	13, 28, 67, 81	0
1	C	151/152 (99%)	-0.77	0 100 100	12, 25, 55, 71	0
1	D	151/152 (99%)	-0.73	0 100 100	7, 26, 55, 70	0
1	E	151/152 (99%)	-0.66	0 100 100	11, 24, 58, 92	0
1	F	151/152 (99%)	-0.65	2 (1%) 77 75	10, 25, 61, 75	0
All	All	906/912 (99%)	-0.67	5 (0%) 89 88	7, 26, 60, 92	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	61	PHE	4.7
1	F	2	ALA	3.4
1	B	59	PRO	3.3
1	B	60	PHE	2.7
1	B	58	ARG	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands (i)

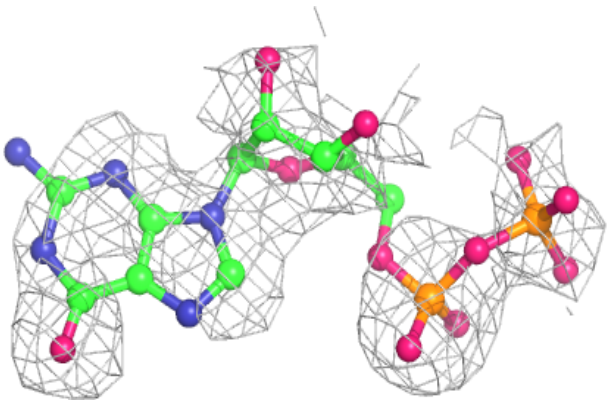
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

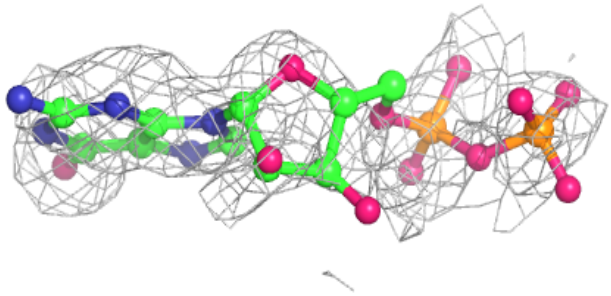
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GDP	B	161	28/28	0.76	0.26	23,99,99,99	28
2	35G	B	160	23/23	0.77	0.25	13,99,99,99	23
3	GDP	E	161	28/28	0.83	0.19	16,79,99,99	28
3	GDP	F	161	28/28	0.85	0.23	2,99,99,99	28
3	GDP	A	161	28/28	0.88	0.18	9,78,99,99	28
2	35G	F	160	23/23	0.88	0.17	11,52,99,99	23
2	35G	E	160	23/23	0.89	0.17	12,53,99,99	23
2	35G	A	160	23/23	0.90	0.16	6,70,99,99	23
3	GDP	D	161	28/28	0.91	0.15	4,38,99,99	28
3	GDP	C	161	28/28	0.91	0.15	5,32,99,99	28
2	35G	C	160	23/23	0.92	0.14	1,39,99,99	23
2	35G	D	160	23/23	0.93	0.16	1,69,99,99	23

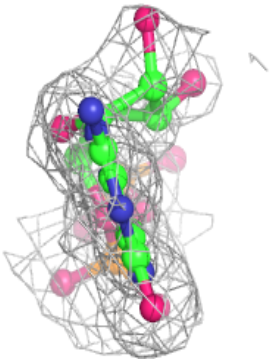
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP B 161:

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

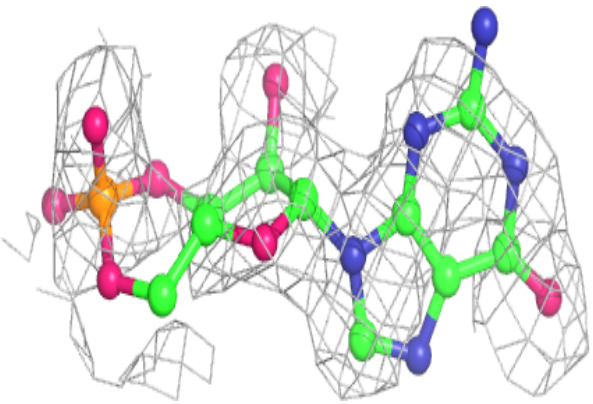


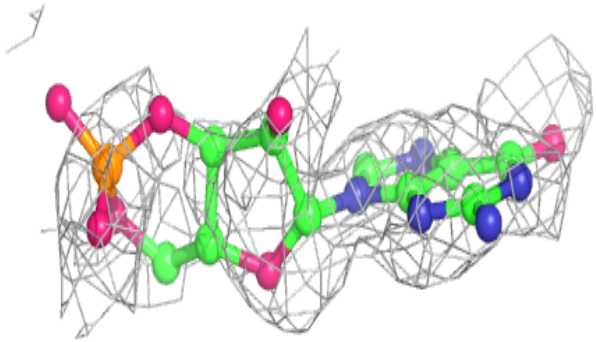


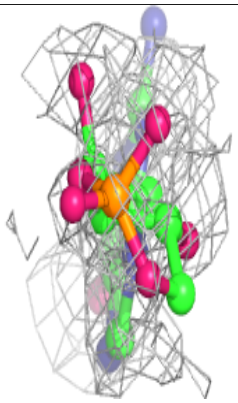


Electron density around 35G B 160:

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

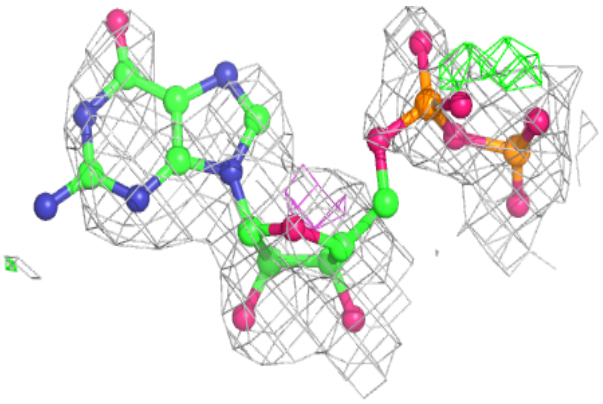


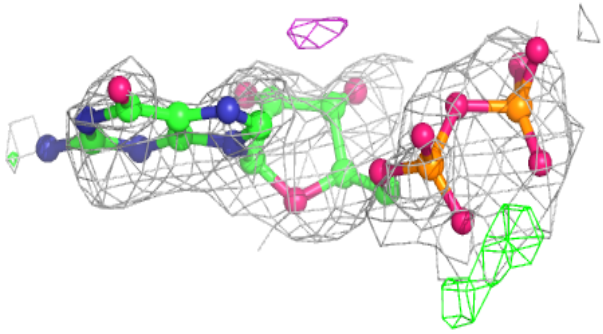


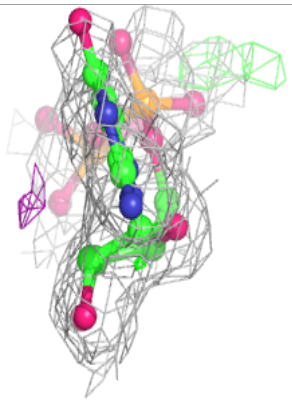


Electron density around GDP E 161:

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

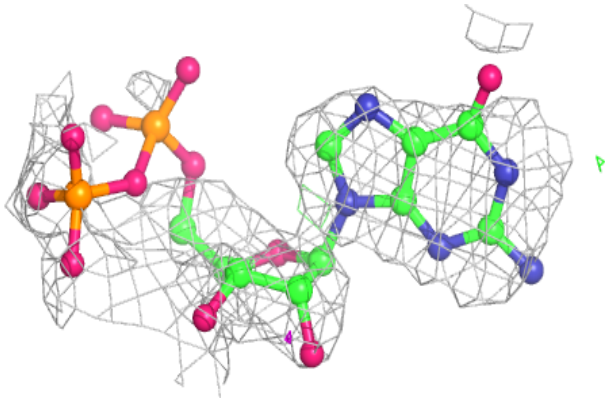


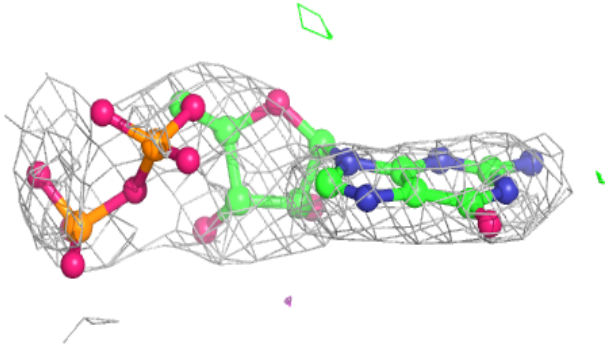


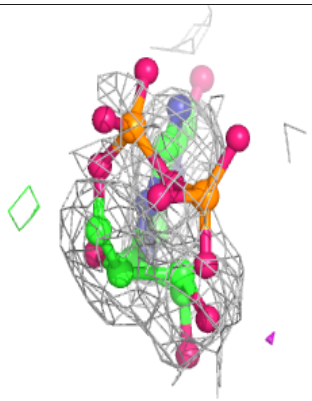


Electron density around GDP F 161:

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

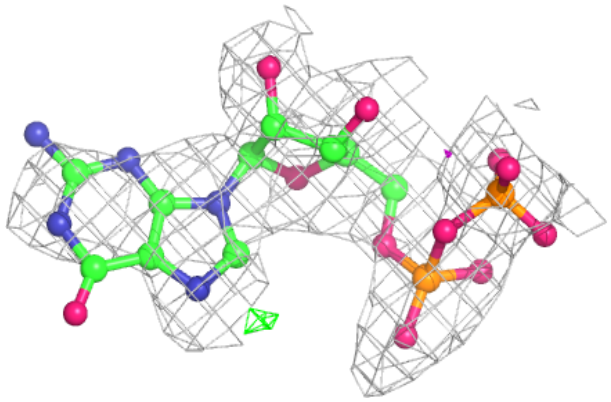


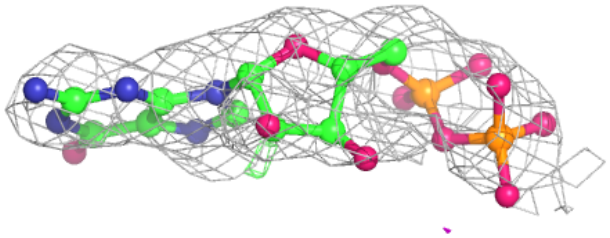


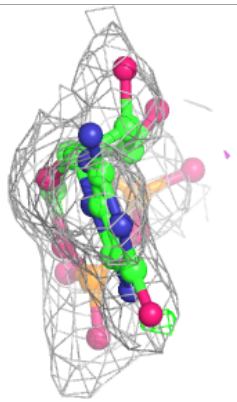


Electron density around GDP A 161:

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

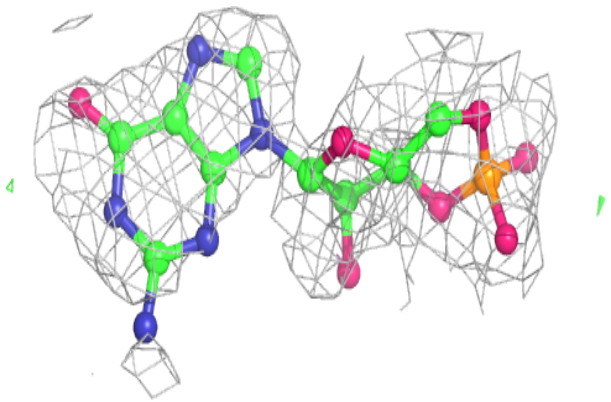


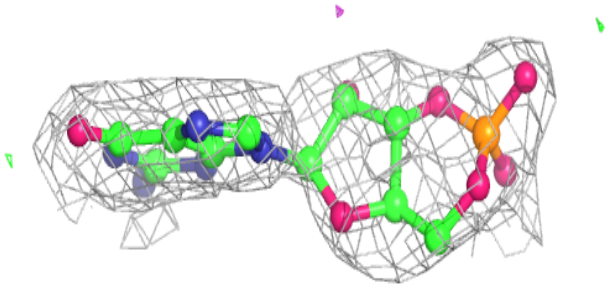


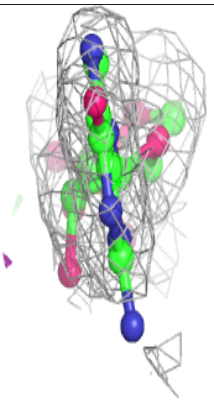


Electron density around 35G F 160:

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

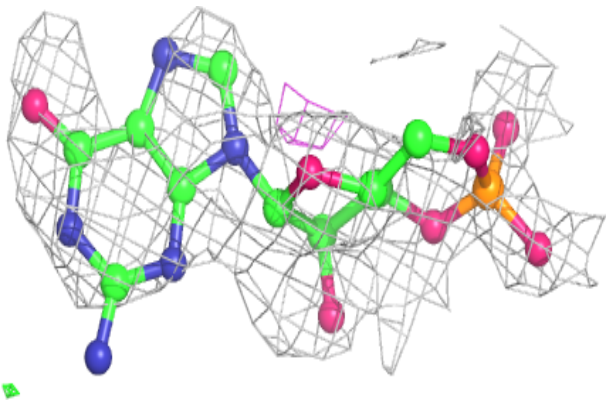


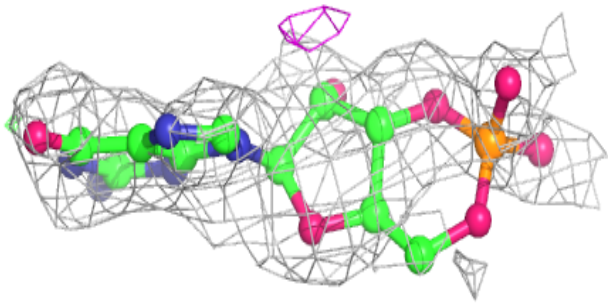


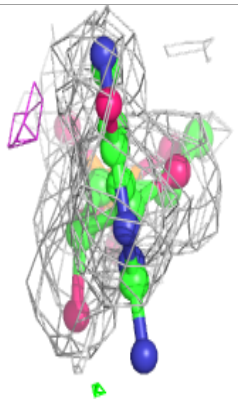


Electron density around 35G E 160:

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

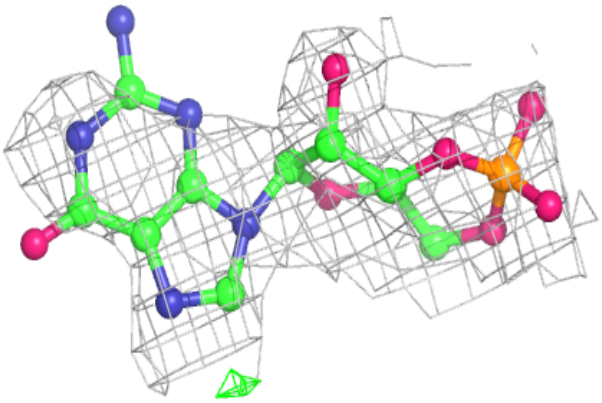


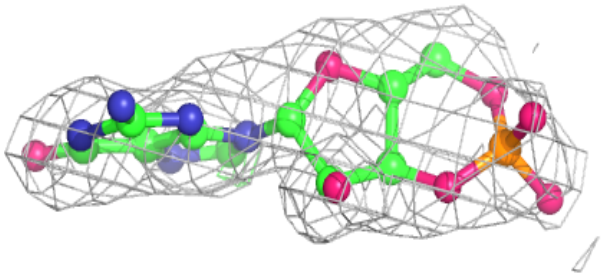


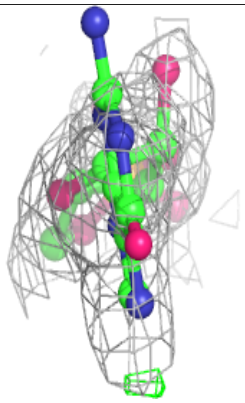


Electron density around 35G A 160:

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

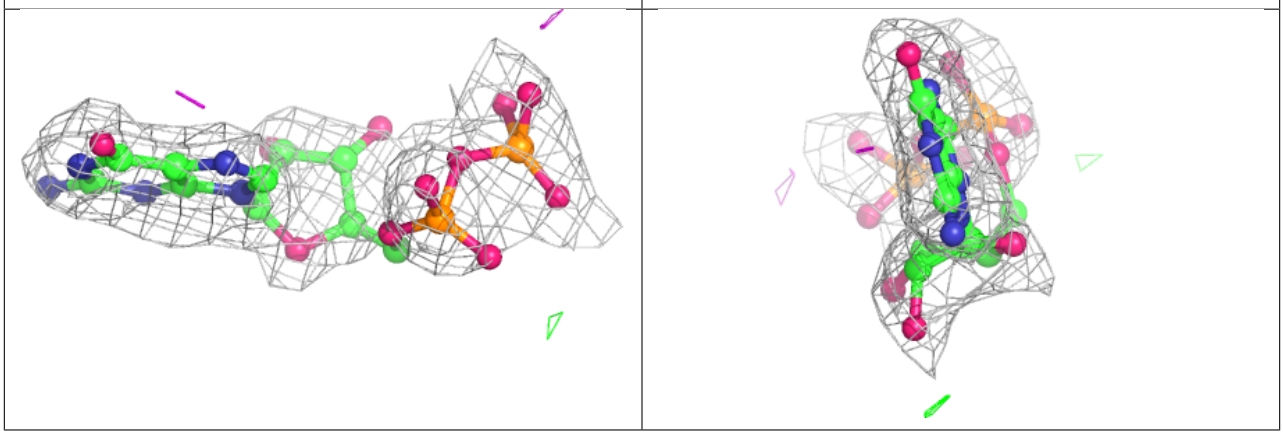






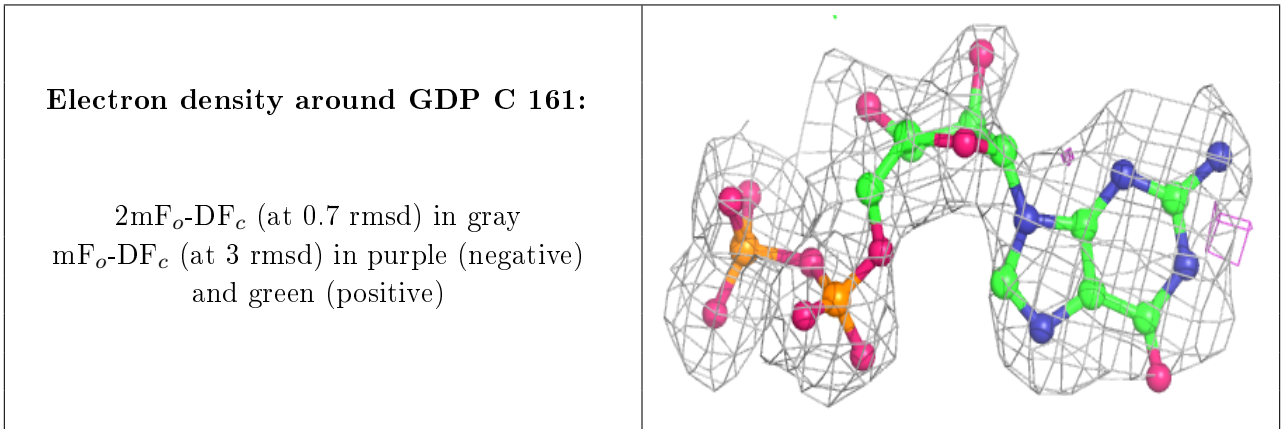
Electron density around GDP D 161:

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



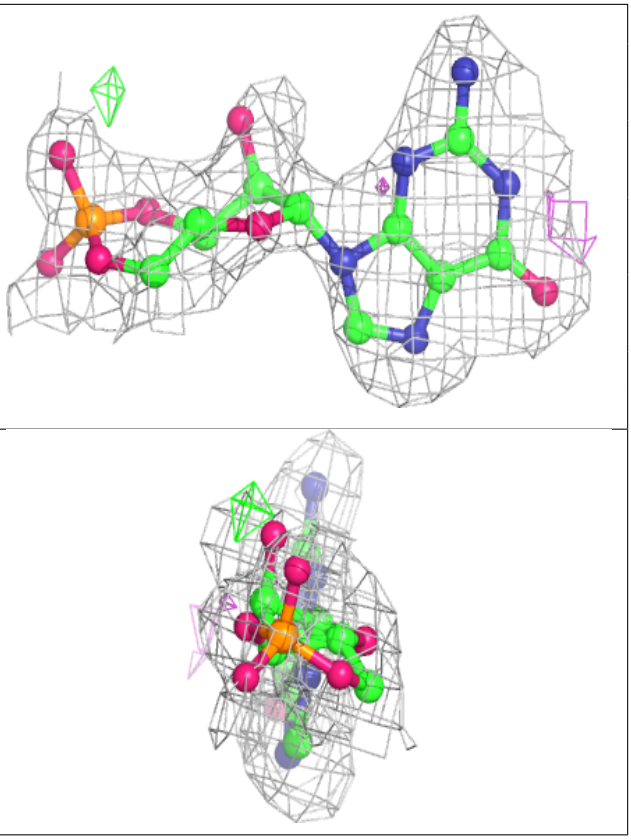
Electron density around GDP C 161:

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



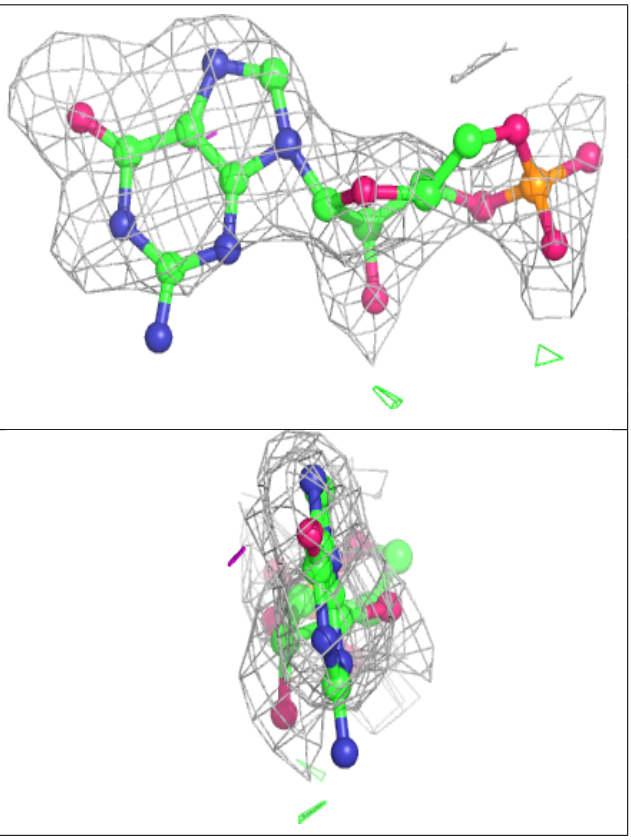
Electron density around 35G C 160:

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



Electron density around 35G D 160:

$2mF_o$-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.