



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:22 AM UTC

PDB ID : 1WUU / pdb_00001wuu
Title : crystal structure of human galactokinase complexed with MgAMPPNP and galactose
Authors : Thoden, J.B.; Timson, D.J.; Reece, R.J.; Holden, H.M.
Deposited on : 2004-12-08
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

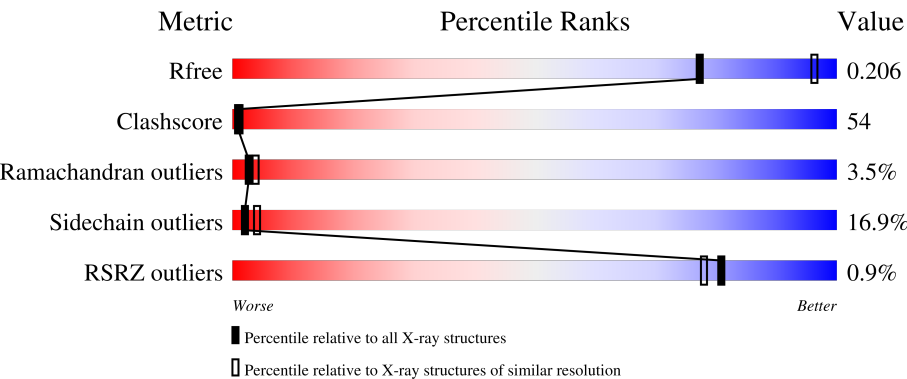
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	399	% 28%58%10%..
1	B	399	% 25%55%16%..
1	C	399	% 29%56%12%..
1	D	399	% 27%52%17%..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12358 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 Galactokinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	Se	0	0	0
			2960	1847	538	559	8	8			
1	B	390	Total	C	N	O	S	Se	0	0	0
			2942	1838	530	558	8	8			
1	C	390	Total	C	N	O	S	Se	0	0	0
			2944	1838	532	558	8	8			
1	D	390	Total	C	N	O	S	Se	0	1	0
			2952	1842	535	559	8	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MSE	-	expression tag	UNP P51570
A	-5	ALA	-	expression tag	UNP P51570
A	-4	HIS	-	expression tag	UNP P51570
A	-3	HIS	-	expression tag	UNP P51570
A	-2	HIS	-	expression tag	UNP P51570
A	-1	HIS	-	expression tag	UNP P51570
A	0	HIS	-	expression tag	UNP P51570
A	1	HIS	-	expression tag	UNP P51570
A	55	MSE	MET	modified residue	UNP P51570
A	60	MSE	MET	modified residue	UNP P51570
A	180	MSE	MET	modified residue	UNP P51570
A	185	MSE	MET	modified residue	UNP P51570
A	192	MSE	MET	modified residue	UNP P51570
A	307	MSE	MET	modified residue	UNP P51570
A	343	MSE	MET	modified residue	UNP P51570
A	365	MSE	MET	modified residue	UNP P51570
B	-6	MSE	-	expression tag	UNP P51570
B	-5	ALA	-	expression tag	UNP P51570
B	-4	HIS	-	expression tag	UNP P51570
B	-3	HIS	-	expression tag	UNP P51570
B	-2	HIS	-	expression tag	UNP P51570

Continued on next page...

Continued from previous page...

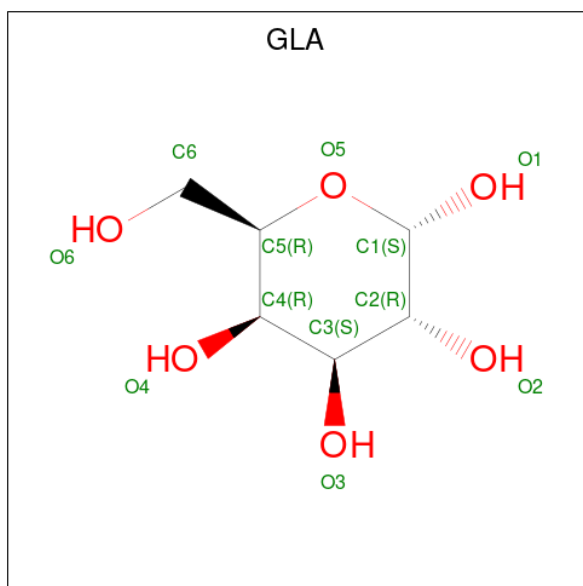
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	HIS	-	expression tag	UNP P51570
B	0	HIS	-	expression tag	UNP P51570
B	1	HIS	-	expression tag	UNP P51570
B	55	MSE	MET	modified residue	UNP P51570
B	60	MSE	MET	modified residue	UNP P51570
B	180	MSE	MET	modified residue	UNP P51570
B	185	MSE	MET	modified residue	UNP P51570
B	192	MSE	MET	modified residue	UNP P51570
B	307	MSE	MET	modified residue	UNP P51570
B	343	MSE	MET	modified residue	UNP P51570
B	365	MSE	MET	modified residue	UNP P51570
C	-6	MSE	-	expression tag	UNP P51570
C	-5	ALA	-	expression tag	UNP P51570
C	-4	HIS	-	expression tag	UNP P51570
C	-3	HIS	-	expression tag	UNP P51570
C	-2	HIS	-	expression tag	UNP P51570
C	-1	HIS	-	expression tag	UNP P51570
C	0	HIS	-	expression tag	UNP P51570
C	1	HIS	-	expression tag	UNP P51570
C	55	MSE	MET	modified residue	UNP P51570
C	60	MSE	MET	modified residue	UNP P51570
C	180	MSE	MET	modified residue	UNP P51570
C	185	MSE	MET	modified residue	UNP P51570
C	192	MSE	MET	modified residue	UNP P51570
C	307	MSE	MET	modified residue	UNP P51570
C	343	MSE	MET	modified residue	UNP P51570
C	365	MSE	MET	modified residue	UNP P51570
D	-6	MSE	-	expression tag	UNP P51570
D	-5	ALA	-	expression tag	UNP P51570
D	-4	HIS	-	expression tag	UNP P51570
D	-3	HIS	-	expression tag	UNP P51570
D	-2	HIS	-	expression tag	UNP P51570
D	-1	HIS	-	expression tag	UNP P51570
D	0	HIS	-	expression tag	UNP P51570
D	1	HIS	-	expression tag	UNP P51570
D	55	MSE	MET	modified residue	UNP P51570
D	60	MSE	MET	modified residue	UNP P51570
D	180	MSE	MET	modified residue	UNP P51570
D	185	MSE	MET	modified residue	UNP P51570
D	192	MSE	MET	modified residue	UNP P51570
D	307	MSE	MET	modified residue	UNP P51570
D	343	MSE	MET	modified residue	UNP P51570

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	365	MSE	MET	modified residue	UNP P51570

- Molecule 2 is alpha-D-galactopyranose (CCD ID: GLA) (formula: $C_6H_{12}O_6$).

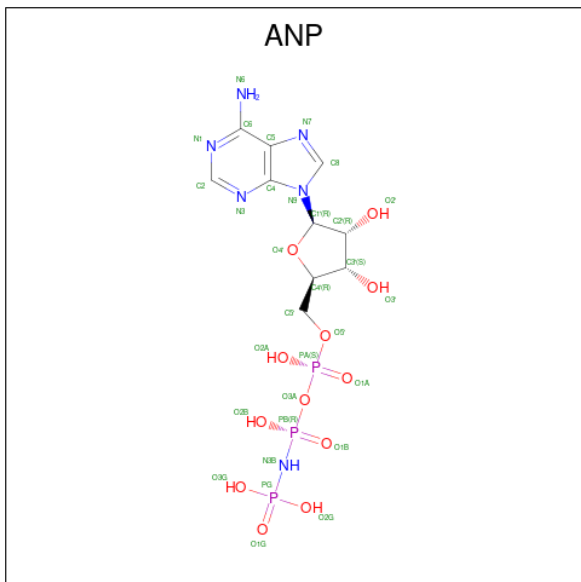


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).



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

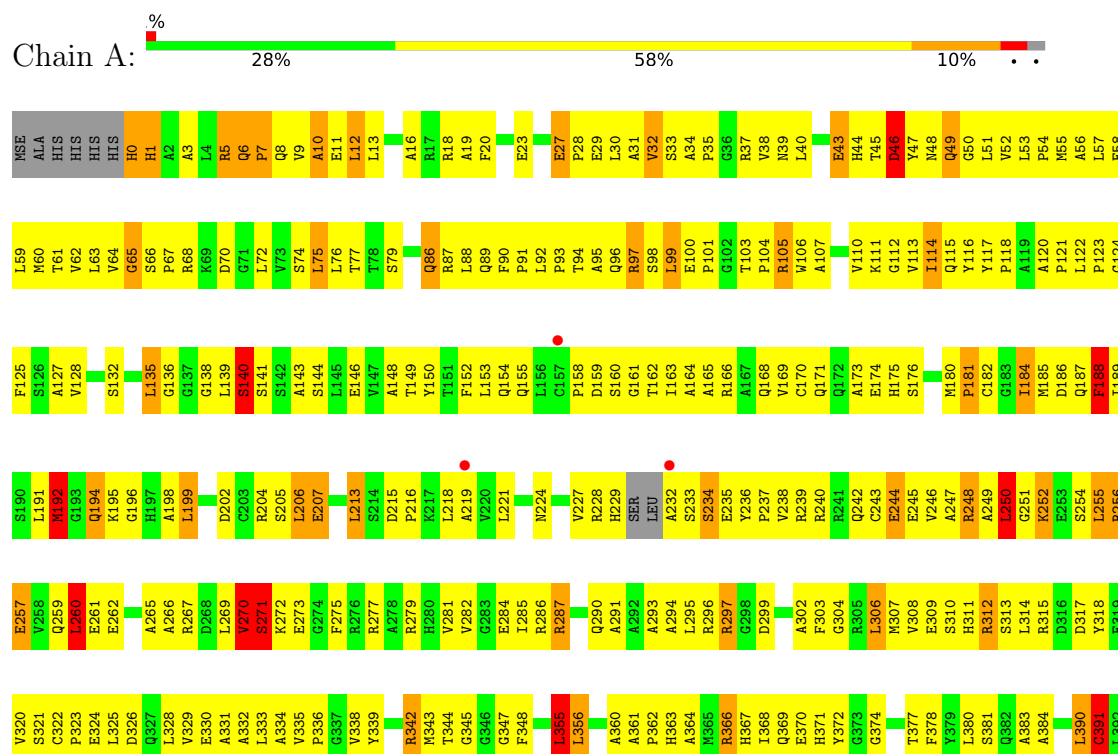
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	94	Total O 94 94	0	0
5	B	89	Total O 89 89	0	0
5	C	105	Total O 105 105	0	0
5	D	96	Total O 96 96	0	0

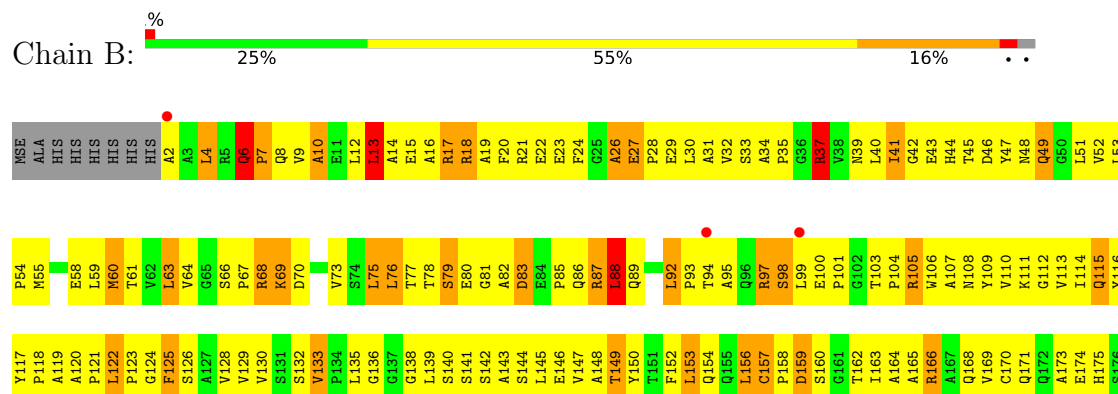
3 Residue-property plots

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

• Molecule 1: Galactokinase



• Molecule 1: Galactokinase





L325	R204	R264	R205	R206	E207	T208	S209	L210	V211	P212	L213	S214	D215	P216	K217	L218	A219	V220	L221	T222	T223	N224	S225	N226	V227	R228	H229	S230	LEU	ALA	S233	S234	E235	T236	P237	V238	R239	R240	R241	Q242	C243	R244	E245	V246	A247	R248	A249	L250	Q251	K252	E253	S254	L255	R256	E257	V258	Q259	L260	E261	E262	L263
D326	A265	A266	R267	D268	L269	V270	S271	K272	E273	G274	F275	R276	R277	A278	H280	V281	V282	G283	E284	T285	R286	R287	T288	A289	Q290	A291	A292	A293	A294	L295	R296	R297	Y300	R301	A302	F303	G304	R305	L306	M307	V308	E309	S310	H311	R312	S313	L314	R315	D316	D317	Y318	E319	V320	S321	C322	P323	E324				
Y339	G340	S341	R342	M343	T344	G345	G346	G347	F348	G349	G350	C351	T352	Y353	T354	L355	L356	E357	A358	S359	A360	A361	P362	H363	A364	M365	R366	H367	I368	Q369	E370	H371	Y372	G373	G374	T375	A376	T377	F378	Y379	L380	S381	Q382	D385	L392																

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.20Å 109.60Å 115.80Å 90.00° 95.90° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-2.50) 97.7 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.50Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.201 , 0.258 0.201 , 0.206	Depositor DCC
R_{free} test set	6099 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 151.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12358	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, ANP, MG

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	1.24	3/3007 (0.1%)	1.59	29/4062 (0.7%)
1	B	1.15	1/2987 (0.0%)	1.62	38/4036 (0.9%)
1	C	1.20	1/2990 (0.0%)	1.59	29/4040 (0.7%)
1	D	1.24	2/3002 (0.1%)	1.59	34/4055 (0.8%)
All	All	1.21	7/11986 (0.1%)	1.60	130/16193 (0.8%)

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	D	1	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	GLN	CA-CB	-10.31	1.36	1.53
1	B	320	VAL	CA-CB	-6.13	1.48	1.54
1	A	195	LYS	CA-C	-5.68	1.45	1.53
1	A	1	HIS	CB-CG	-5.17	1.43	1.50
1	C	189	ILE	N-CA	-5.07	1.40	1.46
1	D	24	PHE	CA-C	-5.05	1.46	1.52
1	D	77	THR	CA-C	-5.04	1.46	1.52

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	ASP	N-CA-CB	-14.32	86.29	110.49
1	B	70	ASP	CB-CA-C	13.28	136.85	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	VAL	N-CA-C	9.96	116.62	107.56
1	B	232	ALA	N-CA-C	-8.59	102.86	112.57
1	D	229	HIS	N-CA-C	8.44	122.00	108.41
1	B	371	HIS	CA-CB-CG	-8.28	105.52	113.80
1	D	371	HIS	CA-CB-CG	-8.01	105.80	113.80
1	C	311	HIS	CA-CB-CG	-7.89	105.91	113.80
1	A	234	SER	N-CA-C	-7.84	103.69	113.18
1	B	125	PHE	N-CA-C	7.63	120.12	108.52
1	D	157	CYS	C-N-CD	-7.62	93.76	125.00
1	D	229	HIS	N-CA-CB	7.43	122.03	110.21
1	D	69	LYS	N-CA-C	-7.40	103.98	113.16
1	A	46	ASP	CB-CA-C	-7.28	95.94	110.42
1	B	215	ASP	O-C-N	7.25	125.62	121.27
1	D	188	PHE	CA-CB-CG	-7.00	106.80	113.80
1	D	120	ALA	N-CA-C	6.82	114.27	108.13
1	A	391	CYS	N-CA-CB	6.81	120.50	109.95
1	A	194	GLN	CB-CG-CD	-6.78	101.07	112.60
1	A	1	HIS	CA-CB-CG	-6.75	107.05	113.80
1	B	351	CYS	N-CA-C	6.71	120.54	110.14
1	D	327	GLN	CA-C-N	6.62	129.45	120.38
1	D	327	GLN	C-N-CA	6.62	129.45	120.38
1	C	351	CYS	N-CA-C	6.52	120.52	110.42
1	D	280	HIS	CA-CB-CG	-6.47	107.33	113.80
1	D	248	ARG	N-CA-CB	6.45	119.71	110.16
1	D	77	THR	N-CA-CB	6.41	121.07	110.63
1	D	199	LEU	CA-C-N	-6.40	113.91	122.42
1	D	199	LEU	C-N-CA	-6.40	113.91	122.42
1	A	233	SER	N-CA-C	-6.36	105.16	113.17
1	A	345	GLY	CA-C-N	6.36	127.18	119.99
1	A	345	GLY	C-N-CA	6.36	127.18	119.99
1	C	183	GLY	CA-C-N	6.34	129.43	120.42
1	C	183	GLY	C-N-CA	6.34	129.43	120.42
1	A	7	PRO	N-CA-CB	6.33	108.97	103.27
1	B	391	CYS	N-CA-CB	6.32	120.72	110.43
1	B	6	GLN	CA-C-O	6.30	123.98	119.32
1	D	177	PHE	CA-CB-CG	-6.20	107.60	113.80
1	D	185	MSE	N-CA-C	6.18	118.53	111.11
1	A	378	PHE	CA-CB-CG	6.17	119.97	113.80
1	C	124	GLY	N-CA-C	-6.14	101.72	111.18
1	C	113	VAL	N-CA-C	-6.10	104.38	110.30
1	A	188	PHE	CB-CA-C	-6.08	101.33	110.88
1	B	37	ARG	N-CA-C	6.08	118.40	108.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	SER	N-CA-C	6.06	119.95	110.32
1	C	21	ARG	N-CA-C	-6.05	103.64	111.02
1	C	54	PRO	CB-CA-C	-6.04	101.59	111.56
1	B	381	SER	N-CA-C	6.00	119.16	110.28
1	C	211	VAL	N-CA-C	5.94	113.96	107.60
1	C	388	LYS	N-CA-C	5.94	118.20	109.24
1	C	69	LYS	CA-C-N	5.93	128.51	120.38
1	C	69	LYS	C-N-CA	5.93	128.51	120.38
1	D	35	PRO	CB-CA-C	-5.89	101.83	111.56
1	D	354	THR	N-CA-C	5.89	118.11	108.52
1	A	270	VAL	N-CA-C	5.88	116.33	108.27
1	A	355	LEU	CB-CA-C	-5.88	100.05	109.75
1	B	337	GLY	N-CA-C	-5.86	106.98	114.37
1	B	363	HIS	N-CA-CB	5.77	118.54	109.94
1	B	390	LEU	CA-C-N	-5.75	114.79	122.72
1	B	390	LEU	C-N-CA	-5.75	114.79	122.72
1	D	120	ALA	N-CA-CB	-5.74	105.87	111.27
1	B	7	PRO	N-CA-CB	5.74	108.14	103.32
1	C	128	VAL	CB-CA-C	-5.74	104.38	111.32
1	B	83	ASP	CA-CB-CG	-5.70	106.90	112.60
1	D	277	ARG	CA-CB-CG	-5.66	102.77	114.10
1	D	11	GLU	N-CA-CB	5.66	118.53	110.16
1	D	116	TYR	N-CA-C	5.64	119.86	112.92
1	C	90	PHE	O-C-N	5.64	125.32	121.71
1	C	176	SER	N-CA-C	5.61	117.84	111.11
1	B	88	LEU	N-CA-C	5.61	116.59	107.23
1	B	4	LEU	N-CA-C	-5.56	102.16	110.23
1	A	10	ALA	N-CA-C	-5.52	105.16	111.07
1	B	192	MSE	N-CA-C	5.50	118.03	111.71
1	B	48	ASN	CA-C-N	5.50	129.98	122.34
1	B	48	ASN	C-N-CA	5.50	129.98	122.34
1	C	48	ASN	CA-C-N	5.43	130.28	122.35
1	C	48	ASN	C-N-CA	5.43	130.28	122.35
1	B	157	CYS	CA-C-N	5.41	126.60	119.84
1	B	157	CYS	C-N-CA	5.41	126.60	119.84
1	A	27	GLU	CA-C-N	5.40	125.31	119.85
1	A	27	GLU	C-N-CA	5.40	125.31	119.85
1	B	133	VAL	CA-C-O	5.39	122.70	119.19
1	C	316	ASP	N-CA-C	5.39	117.97	111.40
1	B	69	LYS	N-CA-C	-5.38	105.52	111.71
1	C	68	ARG	N-CA-C	5.38	117.16	108.34
1	D	351	CYS	N-CA-C	5.37	118.74	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	PHE	CA-CB-CG	-5.34	108.45	113.80
1	C	16	ALA	CA-C-N	5.34	127.70	120.65
1	C	16	ALA	C-N-CA	5.34	127.70	120.65
1	A	192	MSE	N-CA-C	5.33	119.65	113.20
1	D	381	SER	N-CA-C	5.32	117.55	110.53
1	D	101	PRO	N-CA-CB	5.30	107.96	103.35
1	C	122	LEU	CA-C-N	5.30	126.46	119.84
1	C	122	LEU	C-N-CA	5.30	126.46	119.84
1	B	46	ASP	N-CA-C	5.29	116.73	111.07
1	B	334	ALA	CA-C-N	-5.29	118.78	122.59
1	B	334	ALA	C-N-CA	-5.29	118.78	122.59
1	D	45	THR	N-CA-C	-5.27	107.40	113.88
1	C	48	ASN	O-C-N	5.25	128.50	122.25
1	C	270	VAL	CB-CA-C	-5.25	103.05	110.82
1	A	158	PRO	N-CA-CB	5.24	107.97	103.31
1	A	255	LEU	N-CA-C	-5.24	106.66	113.16
1	A	160	SER	CA-C-N	5.24	131.67	121.41
1	A	160	SER	C-N-CA	5.24	131.67	121.41
1	B	60	MSE	CB-CA-C	-5.20	101.19	111.91
1	D	198	ALA	CA-C-N	-5.19	114.70	122.39
1	D	198	ALA	C-N-CA	-5.19	114.70	122.39
1	B	222	ILE	CB-CA-C	-5.18	103.89	110.98
1	D	133	VAL	N-CA-CB	5.17	115.32	109.99
1	A	260	LEU	CA-C-N	5.17	127.21	120.28
1	A	260	LEU	C-N-CA	5.17	127.21	120.28
1	B	367	HIS	CA-CB-CG	-5.17	108.63	113.80
1	A	256	ARG	N-CA-CB	5.16	118.25	110.30
1	D	119	ALA	N-CA-C	5.16	117.96	110.17
1	C	8	GLN	CB-CA-C	5.15	119.01	109.54
1	A	65	GLY	N-CA-C	5.12	118.02	110.80
1	A	90	PHE	O-C-N	5.12	125.83	121.83
1	D	78	THR	N-CA-CB	-5.12	102.90	110.53
1	A	114	ILE	CB-CA-C	-5.11	105.35	112.04
1	C	268	ASP	CA-CB-CG	-5.11	107.50	112.60
1	D	70	ASP	N-CA-C	5.09	118.65	112.23
1	D	378	PHE	N-CA-C	5.08	117.68	109.40
1	B	391	CYS	CB-CA-C	5.08	118.13	109.75
1	B	26	ALA	N-CA-C	5.07	116.51	108.96
1	B	237	PRO	N-CA-CB	5.07	108.86	103.39
1	C	381	SER	N-CA-C	5.04	117.96	110.14
1	A	140	SER	N-CA-C	5.04	118.57	111.52
1	D	270	VAL	N-CA-C	5.03	117.24	108.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	ASP	CA-C-N	5.02	126.12	119.84
1	B	215	ASP	C-N-CA	5.02	126.12	119.84

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	229	HIS	CA

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2960	0	2947	298	0
1	B	2942	0	2930	348	0
1	C	2944	0	2929	316	0
1	D	2952	0	2939	326	0
2	A	12	0	12	2	0
2	B	12	0	12	0	0
2	C	12	0	12	1	0
2	D	12	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	13	6	0
4	B	31	0	13	7	0
4	C	31	0	13	8	0
4	D	31	0	13	3	0
5	A	94	0	0	6	0
5	B	89	0	0	8	0
5	C	105	0	0	9	0
5	D	96	0	0	14	0
All	All	12358	0	11845	1281	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 54.

All (1281) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ILE:HG23	1:B:208:THR:HG22	1.24	1.18
1:B:250:LEU:HD21	1:B:266:ALA:HB2	1.20	1.16
1:A:266:ALA:HB1	1:A:269:LEU:HB2	1.29	1.14
1:A:307:MSE:HE1	1:A:355:LEU:HB2	1.30	1.13
1:A:246:VAL:HG22	1:A:270:VAL:HG11	1.27	1.12
1:A:304:GLY:HA2	1:A:307:MSE:HE3	1.22	1.10
1:B:259:GLN:HB2	1:B:262:GLU:HG3	1.33	1.09
1:B:153:LEU:HA	1:B:156:LEU:HD12	1.33	1.08
1:D:266:ALA:HA	1:D:269:LEU:HD12	1.35	1.08
1:C:97:ARG:HH11	1:C:97:ARG:HB2	1.22	1.04
1:D:77:THR:HG22	1:D:79:SER:H	1.23	1.04
1:B:2:ALA:HB2	1:D:334:ALA:HB1	1.35	1.03
1:D:198:ALA:HB2	1:D:213:LEU:HD11	1.44	0.99
1:B:150:TYR:HE2	1:B:166:ARG:HD3	1.26	0.99
1:A:98:SER:HB3	1:A:115:GLN:HE22	1.28	0.97
1:C:94:THR:HG22	1:C:96:GLN:H	1.27	0.97
1:C:135:LEU:HD22	4:C:395:ANP:H3'	1.48	0.96
1:D:88:LEU:HD12	1:D:89:GLN:H	1.27	0.95
1:A:100:GLU:HG3	1:A:101:PRO:HD2	1.50	0.93
1:C:188:PHE:CE2	1:C:192:MSE:HE3	2.04	0.93
1:A:188:PHE:CD2	1:A:192:MSE:HG3	2.05	0.92
1:B:14:ALA:HB1	1:B:18:ARG:NH1	1.84	0.91
1:C:113:VAL:HG11	1:C:149:THR:HG22	1.50	0.91
1:C:115:GLN:HG2	1:C:177:PHE:HZ	1.36	0.91
1:B:197:HIS:HD2	1:B:210:LEU:HB3	1.34	0.90
1:B:77:THR:HG22	1:B:79:SER:H	1.37	0.89
1:B:152:PHE:CD2	1:B:156:LEU:HD11	2.08	0.89
1:D:85:PRO:HD2	1:D:104:PRO:HG3	1.53	0.89
1:A:116:TYR:O	1:A:117:TYR:C	2.16	0.89
1:C:49:GLN:HE21	1:C:204:ARG:HG3	1.34	0.89
1:C:361:ALA:HB3	1:C:362:PRO:HD3	1.55	0.89
1:A:184:ILE:HD12	1:A:184:ILE:H	1.35	0.89
1:B:93:PRO:HA	1:B:97:ARG:HG2	1.55	0.88
1:B:150:TYR:CE2	1:B:166:ARG:HD3	2.08	0.88
1:D:221:LEU:HB3	1:D:354:THR:HB	1.54	0.88
1:A:361:ALA:HB3	1:A:362:PRO:HD3	1.55	0.88
1:B:120:ALA:HB1	1:B:121:PRO:HA	1.55	0.87
1:B:83:ASP:HB3	1:B:106:TRP:HD1	1.38	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ALA:HB1	1:B:64:VAL:HG22	1.56	0.86
1:B:94:THR:HG22	1:B:95:ALA:H	1.39	0.86
1:C:184:ILE:HG21	1:C:206:LEU:HD21	1.58	0.86
1:C:150:TYR:CE2	1:C:166:ARG:HD3	2.10	0.85
1:A:307:MSE:HE1	1:A:355:LEU:CB	2.06	0.85
1:C:49:GLN:NE2	1:C:204:ARG:HG3	1.92	0.84
1:B:259:GLN:HB2	1:B:262:GLU:CG	2.08	0.84
1:A:188:PHE:HD2	1:A:192:MSE:HG3	1.42	0.83
1:B:201:ILE:HG23	1:B:208:THR:CG2	2.06	0.83
1:C:33:SER:HB3	1:C:390:LEU:HD11	1.58	0.83
1:B:2:ALA:CB	1:D:334:ALA:HB1	2.08	0.83
1:A:287:ARG:HG2	1:A:306:LEU:HD23	1.58	0.83
1:D:21:ARG:HE	1:D:27:GLU:HG3	1.43	0.83
1:A:266:ALA:CB	1:A:269:LEU:HB2	2.07	0.82
1:D:218:LEU:HD12	1:D:219:ALA:H	1.42	0.82
1:D:266:ALA:HB1	1:D:269:LEU:HB2	1.60	0.82
1:B:224:ASN:HB3	1:B:377:THR:HB	1.61	0.82
1:B:366:ARG:HG3	1:B:366:ARG:HH11	1.44	0.81
1:C:237:PRO:HB2	1:C:241:ARG:HH21	1.46	0.81
1:B:188:PHE:CE1	1:B:206:LEU:HD11	2.15	0.81
1:C:213:LEU:HD13	1:C:295:LEU:HD21	1.62	0.81
1:B:14:ALA:HB1	1:B:18:ARG:HH12	1.41	0.81
1:B:150:TYR:CE2	1:B:166:ARG:HB3	2.16	0.81
1:D:291:ALA:HB1	1:D:303:PHE:CE1	2.15	0.80
1:D:266:ALA:CA	1:D:269:LEU:HD12	2.11	0.80
1:C:115:GLN:HG2	1:C:177:PHE:CZ	2.15	0.80
1:C:150:TYR:HE2	1:C:166:ARG:HD3	1.44	0.80
1:A:291:ALA:HB1	1:A:303:PHE:CE1	2.17	0.80
1:D:311:HIS:CD2	1:D:329:VAL:HG21	2.16	0.80
1:C:135:LEU:HD21	4:C:395:ANP:C5	2.13	0.79
1:A:304:GLY:HA2	1:A:307:MSE:CE	2.10	0.79
1:D:332:ALA:HB2	1:D:368:ILE:HD11	1.65	0.79
1:D:240:ARG:O	1:D:244:GLU:HG3	1.83	0.79
1:D:74:SER:HB2	1:D:89:GLN:HG3	1.64	0.79
1:B:116:TYR:O	1:B:117:TYR:C	2.22	0.78
1:B:188:PHE:HE1	1:B:206:LEU:HD21	1.47	0.78
1:D:37:ARG:HA	1:D:57:LEU:HG	1.65	0.78
1:D:304:GLY:HA2	1:D:307:MSE:HG3	1.64	0.78
1:C:63:LEU:CD1	1:C:129:VAL:HG22	2.13	0.78
1:D:236:TYR:HB3	1:D:237:PRO:HD3	1.66	0.78
1:B:338:VAL:HA	1:B:356:LEU:HB3	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLN:O	1:A:256:ARG:HD2	1.84	0.78
1:C:175:HIS:CE1	1:C:181:PRO:HA	2.19	0.77
1:B:4:LEU:HD23	1:B:379:TYR:CE2	2.20	0.77
1:C:90:PHE:HB2	1:C:91:PRO:HD2	1.66	0.77
1:C:92:LEU:HD11	1:C:123:PRO:O	1.83	0.77
1:D:49:GLN:O	1:D:256:ARG:HD3	1.84	0.77
1:D:68:ARG:HH12	1:D:72:LEU:HD12	1.50	0.77
1:B:198:ALA:HB2	1:B:213:LEU:HD11	1.67	0.76
1:B:361:ALA:O	1:B:365:MSE:HG3	1.86	0.76
1:D:219:ALA:HB3	1:D:356:LEU:HD13	1.66	0.76
1:B:142:SER:O	1:B:146:GLU:HG3	1.86	0.76
1:B:188:PHE:CE1	1:B:206:LEU:HD21	2.19	0.76
1:B:245:GLU:O	1:B:246:VAL:C	2.27	0.76
1:A:232:ALA:O	1:A:235:GLU:HB2	1.85	0.76
1:B:47:TYR:CD1	1:B:240:ARG:HG3	2.21	0.75
1:C:103:THR:HG23	1:C:104:PRO:HA	1.67	0.75
1:C:237:PRO:HB2	1:C:241:ARG:NH2	2.00	0.75
1:B:23:GLU:OE2	1:B:87:ARG:HD3	1.86	0.75
1:B:250:LEU:CD2	1:B:266:ALA:HB2	2.10	0.75
1:A:308:VAL:HG22	1:A:333:LEU:HD11	1.69	0.75
1:D:30:LEU:HD21	5:D:464:HOH:O	1.86	0.75
1:D:87:ARG:HG2	1:D:87:ARG:HH11	1.52	0.75
1:B:29:GLU:OE1	1:B:67:PRO:HD2	1.87	0.75
1:B:73:VAL:CG1	1:B:75:LEU:HD21	2.17	0.75
1:B:250:LEU:HD21	1:B:266:ALA:CB	2.09	0.74
1:D:260:LEU:HD12	1:D:260:LEU:O	1.87	0.74
1:A:246:VAL:CG2	1:A:270:VAL:HG11	2.15	0.74
1:C:292:ALA:O	1:C:296:ARG:HG3	1.87	0.74
1:D:70:ASP:OD1	5:D:465:HOH:O	2.05	0.74
1:C:264:GLU:OE2	1:C:267:ARG:HD3	1.87	0.74
1:A:236:TYR:HB3	1:A:237:PRO:HD3	1.68	0.74
1:B:164:ALA:O	1:B:168:GLN:HG3	1.88	0.74
1:A:8:GLN:O	1:A:11:GLU:HB2	1.87	0.73
1:A:120:ALA:HB1	1:A:121:PRO:HA	1.68	0.73
1:C:74:SER:HB2	1:C:89:GLN:CG	2.19	0.73
1:B:105:ARG:HG3	1:B:105:ARG:HH11	1.51	0.73
1:C:99:LEU:HD23	1:C:99:LEU:H	1.54	0.73
1:A:31:ALA:HB3	1:A:390:LEU:O	1.88	0.73
1:A:384:ALA:HB1	5:A:465:HOH:O	1.89	0.73
1:C:72:LEU:HD23	1:C:91:PRO:HA	1.69	0.73
1:A:94:THR:HG22	1:A:96:GLN:H	1.53	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:LEU:O	1:B:252:LYS:HG2	1.89	0.73
1:B:16:ALA:HB1	1:B:64:VAL:CG2	2.19	0.72
1:D:241:ARG:O	1:D:245:GLU:HG3	1.88	0.72
1:A:162:THR:HG23	1:A:165:ALA:H	1.53	0.72
1:C:120:ALA:HB1	1:C:121:PRO:HA	1.70	0.72
1:D:6:GLN:OE1	1:D:58:GLU:HB2	1.89	0.72
1:D:162:THR:O	1:D:165:ALA:HB3	1.89	0.72
1:C:72:LEU:CD2	1:C:91:PRO:HA	2.20	0.72
1:A:189:ILE:HD13	1:A:199:LEU:HG	1.72	0.72
1:B:92:LEU:O	1:B:97:ARG:HD3	1.89	0.72
1:B:198:ALA:HB2	1:B:213:LEU:CD1	2.19	0.72
1:A:187:GLN:O	1:A:191:LEU:HD12	1.90	0.71
1:A:366:ARG:O	1:A:367:HIS:C	2.30	0.71
1:B:286:ARG:O	1:B:290:GLN:HG3	1.89	0.71
1:A:49:GLN:HE21	1:A:204:ARG:HG3	1.55	0.71
1:C:113:VAL:HG11	1:C:149:THR:CG2	2.21	0.71
1:D:343:MSE:HE1	1:D:347:GLY:HA2	1.71	0.71
1:B:122:LEU:HD12	1:B:157:CYS:HB3	1.72	0.71
1:C:97:ARG:HH11	1:C:97:ARG:CB	2.00	0.71
1:A:8:GLN:HB2	1:A:11:GLU:OE1	1.89	0.71
1:A:322:CYS:HB2	1:A:323:PRO:HD2	1.72	0.71
1:D:185:MSE:O	1:D:189:ILE:HG22	1.91	0.71
1:D:302:ALA:O	1:D:306:LEU:HD12	1.89	0.71
1:C:267:ARG:HD2	1:C:275:PHE:CE1	2.25	0.71
1:C:21:ARG:HA	1:C:26:ALA:O	1.90	0.71
1:B:293:ALA:O	1:B:297:ARG:HB2	1.91	0.71
1:D:88:LEU:HD12	1:D:89:GLN:N	2.02	0.71
1:D:122:LEU:HD12	1:D:123:PRO:HD2	1.72	0.70
1:D:273:GLU:O	1:D:274:GLY:C	2.34	0.70
1:C:327:GLN:NE2	5:C:497:HOH:O	2.23	0.70
1:D:332:ALA:HB2	1:D:368:ILE:CD1	2.20	0.70
1:C:360:ALA:O	1:C:361:ALA:C	2.34	0.70
1:B:117:TYR:CD1	1:B:118:PRO:HD2	2.26	0.70
1:A:100:GLU:CG	1:A:101:PRO:HD2	2.20	0.70
1:A:198:ALA:HB2	1:A:213:LEU:HD13	1.74	0.70
1:B:192:MSE:HE3	1:B:192:MSE:HA	1.72	0.70
1:C:28:PRO:CB	1:C:64:VAL:HG13	2.22	0.70
1:C:241:ARG:O	1:C:245:GLU:HG3	1.91	0.70
1:B:7:PRO:HB2	1:B:12:LEU:HG	1.72	0.70
1:B:197:HIS:CD2	1:B:210:LEU:HB3	2.24	0.70
1:B:273:GLU:HA	1:B:276:ARG:CZ	2.22	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:HD23	1:C:99:LEU:N	2.06	0.70
1:B:258:VAL:HG11	1:B:263:LEU:HD12	1.74	0.69
1:C:323:PRO:O	1:C:327:GLN:HG3	1.91	0.69
1:B:235:GLU:O	1:B:238:VAL:HB	1.93	0.69
1:B:73:VAL:HG12	1:B:75:LEU:HD21	1.74	0.69
1:B:248:ARG:O	1:B:249:ALA:C	2.36	0.69
1:D:343:MSE:HE1	1:D:347:GLY:CA	2.22	0.69
1:C:311:HIS:HB2	1:C:342:ARG:CB	2.21	0.69
1:B:242:GLN:OE1	1:B:277:ARG:HG3	1.93	0.69
1:D:195:LYS:HB2	1:D:385:ASP:OD1	1.93	0.69
1:D:263:LEU:HG	1:D:275:PHE:CE1	2.27	0.69
1:A:68:ARG:HD2	1:A:125:PHE:C	2.17	0.69
1:C:184:ILE:HA	5:C:477:HOH:O	1.92	0.68
1:A:312:ARG:HE	1:A:315:ARG:NH1	1.91	0.68
1:D:197:HIS:HD2	1:D:210:LEU:HB3	1.58	0.68
1:A:150:TYR:HD2	1:A:154:GLN:HE21	1.38	0.68
1:B:188:PHE:HD2	1:B:192:MSE:HG3	1.59	0.68
1:C:91:PRO:HG2	1:C:97:ARG:NH2	2.08	0.68
1:B:88:LEU:HD12	1:B:107:ALA:CB	2.23	0.68
1:A:117:TYR:CD1	1:A:118:PRO:HD2	2.29	0.68
1:D:218:LEU:HD22	1:D:300:TYR:CE1	2.29	0.68
1:D:259:GLN:HB2	1:D:262:GLU:CD	2.18	0.68
1:D:339:TYR:CD1	1:D:356:LEU:HA	2.29	0.68
1:A:338:VAL:HA	1:A:356:LEU:HB3	1.75	0.68
1:C:74:SER:HB2	1:C:89:GLN:HG3	1.76	0.68
1:D:227:VAL:HG21	1:D:324:GLU:HG2	1.75	0.67
1:D:12:LEU:HD12	1:D:60:MSE:HE3	1.76	0.67
1:A:266:ALA:O	1:A:267:ARG:C	2.36	0.67
1:C:146:GLU:O	1:C:149:THR:HB	1.95	0.67
1:D:357:GLU:O	1:D:358:ALA:C	2.36	0.67
1:D:361:ALA:HB3	1:D:362:PRO:HD3	1.77	0.67
1:C:47:TYR:CD1	1:C:240:ARG:HG3	2.28	0.67
1:C:103:THR:CG2	1:C:104:PRO:HA	2.24	0.67
1:D:74:SER:CB	1:D:89:GLN:HG3	2.25	0.67
1:A:110:VAL:O	1:A:114:ILE:HG13	1.94	0.67
1:B:32:VAL:HA	1:B:390:LEU:HG	1.77	0.67
4:C:395:ANP:N7	5:C:439:HOH:O	2.28	0.67
1:D:147:VAL:HG21	1:D:190:SER:HB3	1.77	0.67
1:D:224:ASN:HB3	1:D:377:THR:HB	1.77	0.67
1:C:34:ALA:HB3	1:C:148:ALA:HB2	1.76	0.67
1:D:20:PHE:HD1	1:D:128:VAL:HG23	1.60	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:ALA:CB	1:D:368:ILE:HD11	2.24	0.67
1:A:164:ALA:O	1:A:168:GLN:HG3	1.94	0.67
1:C:154:GLN:C	1:C:155:GLN:HE21	2.03	0.67
1:A:117:TYR:CG	1:A:118:PRO:HD2	2.30	0.66
1:C:4:LEU:HG	1:C:377:THR:CG2	2.24	0.66
1:D:29:GLU:HB2	1:D:66:SER:OG	1.96	0.66
1:A:322:CYS:SG	1:A:325:LEU:HG	2.35	0.66
1:A:117:TYR:OH	1:A:154:GLN:HA	1.96	0.66
1:B:152:PHE:CE2	1:B:156:LEU:HD11	2.31	0.66
1:B:83:ASP:CB	1:B:106:TRP:HD1	2.09	0.66
1:D:218:LEU:HD12	1:D:219:ALA:N	2.10	0.66
1:D:266:ALA:CB	1:D:269:LEU:HB2	2.26	0.66
1:A:33:SER:HB3	1:A:390:LEU:HD11	1.76	0.66
1:A:45:THR:O	1:A:48:ASN:N	2.29	0.66
1:A:356:LEU:N	1:A:356:LEU:HD12	2.10	0.66
1:D:107:ALA:HB3	5:D:430:HOH:O	1.96	0.66
1:C:205:SER:HB2	1:C:207:GLU:HG3	1.77	0.65
1:D:68:ARG:HH12	1:D:72:LEU:CD1	2.08	0.65
1:D:95:ALA:O	1:D:96:GLN:C	2.38	0.65
1:D:236:TYR:HB3	1:D:237:PRO:CD	2.26	0.65
1:D:343:MSE:CE	1:D:347:GLY:HA2	2.26	0.65
1:B:153:LEU:N	1:B:153:LEU:HD23	2.11	0.65
1:B:273:GLU:HA	1:B:276:ARG:NH2	2.12	0.65
1:D:117:TYR:OH	1:D:154:GLN:HA	1.96	0.65
1:B:234:SER:O	1:B:238:VAL:HG23	1.96	0.65
1:B:366:ARG:HG3	1:B:366:ARG:NH1	2.10	0.65
1:C:6:GLN:HG2	1:C:59:LEU:HD21	1.78	0.65
1:D:273:GLU:O	1:D:276:ARG:N	2.30	0.65
1:A:68:ARG:N	1:A:124:GLY:O	2.30	0.65
1:B:29:GLU:HB2	1:B:66:SER:OG	1.97	0.65
1:B:94:THR:HG22	1:B:95:ALA:N	2.10	0.65
1:B:266:ALA:O	1:B:269:LEU:N	2.30	0.65
1:C:279:ARG:NH2	1:C:317:ASP:OD1	2.30	0.65
1:C:19:ALA:O	1:C:22:GLU:HB3	1.97	0.65
1:A:250:LEU:HD21	1:A:266:ALA:HB3	1.78	0.65
1:D:23:GLU:CD	1:D:87:ARG:HH12	2.04	0.65
1:D:85:PRO:HD2	1:D:104:PRO:CG	2.26	0.65
1:D:198:ALA:HB2	1:D:213:LEU:CD1	2.22	0.65
1:D:259:GLN:N	1:D:262:GLU:OE1	2.30	0.65
1:B:6:GLN:HG2	1:B:59:LEU:HD21	1.79	0.64
1:C:279:ARG:HH21	1:C:317:ASP:CG	2.04	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ASN:HD22	1:D:40:LEU:N	1.94	0.64
1:D:242:GLN:OE1	1:D:277:ARG:NE	2.29	0.64
1:A:92:LEU:HD11	1:A:123:PRO:O	1.97	0.64
1:D:250:LEU:N	1:D:250:LEU:HD23	2.11	0.64
1:D:266:ALA:O	1:D:269:LEU:N	2.30	0.64
1:C:110:VAL:O	1:C:114:ILE:HG13	1.98	0.64
1:C:135:LEU:HD22	4:C:395:ANP:C3'	2.26	0.64
1:B:8:GLN:O	1:B:9:VAL:C	2.39	0.64
1:C:356:LEU:HD12	1:C:356:LEU:N	2.13	0.64
1:A:243:CYS:O	1:A:246:VAL:N	2.30	0.64
1:A:272:LYS:O	1:A:275:PHE:N	2.29	0.64
1:C:242:GLN:OE1	1:C:277:ARG:NE	2.30	0.64
1:C:286:ARG:O	1:C:290:GLN:HG3	1.96	0.64
1:A:18:ARG:NH2	5:A:469:HOH:O	2.23	0.64
1:B:83:ASP:OD1	1:B:105:ARG:NH1	2.31	0.64
1:D:335:VAL:HG13	1:D:363:HIS:ND1	2.12	0.64
1:C:202:ASP:O	1:C:206:LEU:N	2.30	0.64
1:A:307:MSE:HE2	1:A:355:LEU:HD22	1.80	0.64
1:B:27:GLU:HA	1:B:27:GLU:OE1	1.97	0.64
1:B:149:THR:O	1:B:150:TYR:C	2.39	0.64
1:A:189:ILE:CD1	1:A:199:LEU:HG	2.28	0.63
1:A:227:VAL:HG21	1:A:324:GLU:HG2	1.81	0.63
1:B:88:LEU:HD12	1:B:107:ALA:HB2	1.81	0.63
1:B:117:TYR:CE2	1:B:119:ALA:HB3	2.33	0.63
1:C:63:LEU:HD11	1:C:129:VAL:HG22	1.79	0.63
1:C:68:ARG:NH1	1:C:70:ASP:HB2	2.14	0.63
1:D:283:GLY:O	1:D:287:ARG:HB2	1.97	0.63
1:A:302:ALA:O	1:A:306:LEU:HD12	1.96	0.63
1:B:4:LEU:HD23	1:B:379:TYR:HE2	1.63	0.63
1:D:226:ASN:ND2	1:D:375:THR:O	2.30	0.63
1:A:49:GLN:NE2	1:A:204:ARG:HG3	2.13	0.63
1:B:103:THR:HG23	1:B:104:PRO:HA	1.81	0.63
1:B:188:PHE:CD2	1:B:192:MSE:HG3	2.34	0.63
1:B:248:ARG:O	1:B:251:GLY:N	2.30	0.63
1:B:337:GLY:O	1:B:357:GLU:HG3	1.99	0.63
1:D:280:HIS:HA	5:D:412:HOH:O	1.98	0.63
1:D:7:PRO:HG2	1:D:12:LEU:HD21	1.79	0.63
1:D:20:PHE:CD1	1:D:128:VAL:HG23	2.33	0.63
1:A:98:SER:HB3	1:A:115:GLN:NE2	2.09	0.63
1:A:250:LEU:HD21	1:A:266:ALA:CB	2.28	0.63
1:D:103:THR:HA	1:D:104:PRO:C	2.24	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ASP:OD1	1:B:216:PRO:HD2	1.99	0.63
1:D:21:ARG:NE	1:D:27:GLU:HG3	2.11	0.63
1:D:304:GLY:HA2	1:D:307:MSE:HE2	1.79	0.63
1:B:248:ARG:O	1:B:250:LEU:N	2.32	0.62
1:B:259:GLN:CB	1:B:262:GLU:HG3	2.21	0.62
1:C:18:ARG:O	1:C:19:ALA:C	2.41	0.62
1:D:248:ARG:O	1:D:249:ALA:C	2.41	0.62
1:A:182:CYS:O	1:A:240:ARG:NH1	2.31	0.62
1:B:29:GLU:O	1:B:30:LEU:HD23	1.99	0.62
1:C:234:SER:O	1:C:238:VAL:HG23	1.98	0.62
1:C:356:LEU:HD12	1:C:356:LEU:H	1.63	0.62
1:A:296:ARG:HG2	5:A:461:HOH:O	1.98	0.62
1:C:97:ARG:HB2	1:C:97:ARG:NH1	2.04	0.62
1:C:250:LEU:N	1:C:250:LEU:HD12	2.13	0.62
1:B:145:LEU:O	1:B:146:GLU:C	2.41	0.62
1:C:335:VAL:HG13	1:C:363:HIS:ND1	2.14	0.62
1:B:42:GLY:O	1:B:52:VAL:HG12	1.98	0.62
1:D:4:LEU:HD13	5:D:457:HOH:O	1.99	0.62
1:B:97:ARG:HG3	1:B:97:ARG:HH11	1.64	0.62
1:D:271:SER:OG	1:D:274:GLY:N	2.33	0.62
1:A:194:GLN:OE1	1:B:192:MSE:HE1	2.00	0.62
1:D:237:PRO:O	1:D:241:ARG:HG3	2.00	0.62
1:A:28:PRO:CB	1:A:64:VAL:HG12	2.29	0.62
1:A:202:ASP:OD1	1:A:256:ARG:NH1	2.30	0.61
1:C:372:TYR:HA	5:C:497:HOH:O	1.99	0.61
1:B:105:ARG:HG3	1:B:105:ARG:NH1	2.13	0.61
1:B:322:CYS:HB2	1:B:323:PRO:HD2	1.81	0.61
1:C:194:GLN:HG2	1:D:163:ILE:CD1	2.30	0.61
1:C:312:ARG:HG2	1:C:312:ARG:HH11	1.65	0.61
1:C:92:LEU:O	1:C:97:ARG:HD3	2.00	0.61
1:D:361:ALA:O	1:D:364:ALA:HB3	1.99	0.61
1:A:291:ALA:HB1	1:A:303:PHE:CD1	2.35	0.61
1:A:266:ALA:O	1:A:269:LEU:N	2.30	0.61
1:C:219:ALA:HB3	1:C:356:LEU:HD13	1.81	0.61
1:C:283:GLY:HA3	5:C:414:HOH:O	2.00	0.61
1:D:89:GLN:HB2	5:D:469:HOH:O	2.01	0.61
1:D:238:VAL:O	1:D:239:ARG:C	2.38	0.61
1:B:339:TYR:CD1	1:B:356:LEU:HA	2.35	0.61
1:C:270:VAL:HG23	1:C:271:SER:O	2.01	0.61
1:D:277:ARG:HB3	1:D:318:TYR:CE1	2.36	0.61
1:A:252:LYS:HG2	1:A:257:GLU:HB3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:MSE:HE1	1:A:347:GLY:CA	2.30	0.61
1:C:149:THR:O	1:C:152:PHE:HB3	2.01	0.61
1:D:182:CYS:O	1:D:240:ARG:NH1	2.34	0.61
1:A:202:ASP:O	1:A:206:LEU:N	2.30	0.60
1:A:232:ALA:HB1	1:A:235:GLU:CG	2.31	0.60
1:D:77:THR:HG21	4:D:395:ANP:N1	2.16	0.60
1:A:138:GLY:HA2	4:A:395:ANP:O2G	2.00	0.60
1:C:49:GLN:HE21	1:C:204:ARG:CG	2.12	0.60
1:C:64:VAL:HG22	1:C:392:LEU:HD11	1.82	0.60
1:D:307:MSE:O	1:D:310:SER:HB3	2.00	0.60
1:B:254:SER:OG	1:B:256:ARG:HB3	2.00	0.60
1:C:188:PHE:CD2	1:C:192:MSE:HE3	2.35	0.60
1:C:232:ALA:HB1	1:C:235:GLU:HG2	1.84	0.60
1:D:261:GLU:N	1:D:261:GLU:OE1	2.34	0.60
1:D:311:HIS:HB2	1:D:342:ARG:HB3	1.83	0.60
1:A:236:TYR:HB3	1:A:237:PRO:CD	2.31	0.60
1:B:120:ALA:CB	1:B:121:PRO:HA	2.20	0.60
1:C:105:ARG:O	1:C:108:ASN:HB2	2.01	0.60
1:D:330:GLU:O	1:D:331:ALA:C	2.43	0.60
1:B:34:ALA:HB3	1:B:144:SER:O	2.01	0.60
1:B:103:THR:HA	1:B:104:PRO:C	2.27	0.60
1:B:23:GLU:HG3	1:B:23:GLU:O	2.02	0.60
1:C:335:VAL:HG13	1:C:363:HIS:CE1	2.37	0.60
1:D:43:GLU:OE1	1:D:43:GLU:HA	2.01	0.60
1:D:106:TRP:HB2	4:D:395:ANP:N3	2.16	0.60
1:B:169:VAL:HG12	1:B:170:CYS:N	2.15	0.60
1:B:188:PHE:CZ	1:B:206:LEU:HD11	2.36	0.60
1:B:23:GLU:CD	1:B:87:ARG:HH11	2.10	0.60
1:B:61:THR:HG23	1:B:130:VAL:O	2.02	0.60
1:B:224:ASN:O	1:B:376:ALA:HA	2.01	0.60
1:C:165:ALA:O	1:C:166:ARG:C	2.42	0.60
1:A:303:PHE:HD2	1:A:307:MSE:HE2	1.66	0.60
1:D:49:GLN:HG3	1:D:254:SER:CB	2.32	0.60
1:D:77:THR:HG22	1:D:78:THR:N	2.17	0.60
1:C:258:VAL:HG12	1:C:259:GLN:N	2.16	0.59
1:C:325:LEU:HD11	1:C:349:GLY:O	2.01	0.59
1:C:37:ARG:C	1:C:37:ARG:HD2	2.27	0.59
1:C:98:SER:O	1:C:99:LEU:C	2.46	0.59
1:C:167:ALA:HB2	1:C:191:LEU:HD12	1.83	0.59
1:D:23:GLU:OE2	1:D:87:ARG:NH1	2.34	0.59
1:A:304:GLY:HA3	1:A:339:TYR:C	2.27	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:PRO:HG3	1:B:99:LEU:HG	1.84	0.59
1:B:162:THR:O	1:B:165:ALA:HB3	2.01	0.59
1:B:152:PHE:HD2	1:B:153:LEU:CD2	2.14	0.59
1:B:231:LEU:C	1:B:233:SER:H	2.09	0.59
1:B:237:PRO:HB2	1:B:241:ARG:NH2	2.17	0.59
1:D:234:SER:O	1:D:238:VAL:HG23	2.02	0.59
1:D:264:GLU:O	1:D:266:ALA:N	2.35	0.59
1:A:254:SER:OG	1:A:256:ARG:N	2.30	0.59
1:B:188:PHE:O	1:B:192:MSE:N	2.30	0.59
1:C:103:THR:HA	1:C:104:PRO:C	2.26	0.59
1:C:338:VAL:HA	1:C:356:LEU:HB3	1.84	0.59
1:D:322:CYS:O	1:D:325:LEU:N	2.36	0.59
1:D:31:ALA:CB	1:D:64:VAL:HG12	2.32	0.59
1:B:41:ILE:HG22	1:B:53:LEU:HB3	1.85	0.59
1:C:224:ASN:HB3	1:C:377:THR:HB	1.85	0.59
1:D:277:ARG:O	1:D:280:HIS:HB3	2.02	0.59
1:B:138:GLY:H	4:B:395:ANP:HNB1	1.50	0.59
1:C:185:MSE:HG2	1:C:186:ASP:N	2.17	0.59
1:D:39:ASN:ND2	1:D:41:ILE:H	2.01	0.59
1:D:63:LEU:C	1:D:63:LEU:HD23	2.27	0.59
1:A:259:GLN:O	1:A:262:GLU:N	2.35	0.59
1:A:9:VAL:HG22	1:A:60:MSE:CE	2.33	0.59
1:A:77:THR:O	1:A:86:GLN:HG2	2.02	0.59
1:A:339:TYR:HB2	1:A:355:LEU:HB3	1.84	0.59
1:B:370:GLU:HB3	1:B:371:HIS:CD2	2.38	0.59
1:C:135:LEU:HD21	4:C:395:ANP:C4	2.33	0.59
1:A:0:HIS:O	1:A:1:HIS:C	2.44	0.58
1:A:23:GLU:O	1:A:23:GLU:HG3	2.02	0.58
1:A:335:VAL:HG13	1:A:363:HIS:ND1	2.18	0.58
1:B:21:ARG:HA	1:B:26:ALA:O	2.03	0.58
1:D:329:VAL:O	1:D:332:ALA:N	2.36	0.58
1:D:49:GLN:HB3	1:D:204:ARG:HB2	1.84	0.58
1:A:272:LYS:O	1:A:273:GLU:C	2.47	0.58
1:A:295:LEU:HD12	1:A:295:LEU:O	2.04	0.58
1:D:4:LEU:HD22	1:D:377:THR:CG2	2.34	0.58
1:B:147:VAL:HG21	1:B:190:SER:HB3	1.84	0.58
1:B:245:GLU:O	1:B:248:ARG:N	2.37	0.58
1:B:258:VAL:HG11	1:B:263:LEU:CD1	2.32	0.58
1:D:310:SER:OG	1:D:342:ARG:NH1	2.36	0.58
1:A:143:ALA:HB2	1:A:186:ASP:HB3	1.85	0.58
1:B:83:ASP:HB3	1:B:106:TRP:CD1	2.29	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:THR:N	1:C:97:ARG:O	2.35	0.58
1:D:242:GLN:OE1	1:D:277:ARG:HG3	2.03	0.58
1:D:266:ALA:HA	1:D:269:LEU:CD1	2.22	0.58
1:A:66:SER:HB3	1:A:67:PRO:HD2	1.86	0.58
1:A:368:ILE:O	1:A:369:GLN:C	2.45	0.58
1:C:184:ILE:CG2	1:C:206:LEU:HD21	2.33	0.58
1:D:362:PRO:HA	1:D:365:MSE:HE3	1.85	0.58
1:B:23:GLU:OE1	1:B:87:ARG:NH1	2.36	0.58
1:B:356:LEU:N	1:B:356:LEU:HD12	2.18	0.58
1:C:175:HIS:NE2	1:C:181:PRO:HA	2.18	0.58
1:B:105:ARG:O	1:B:108:ASN:HB2	2.04	0.58
1:C:49:GLN:O	1:C:256:ARG:HD3	2.04	0.58
1:C:117:TYR:OH	1:C:154:GLN:HA	2.04	0.58
1:A:45:THR:HB	1:A:50:GLY:HA3	1.85	0.58
1:C:311:HIS:HB2	1:C:342:ARG:HB3	1.86	0.58
1:B:58:GLU:HG2	1:B:384:ALA:HB2	1.85	0.57
1:C:4:LEU:HD23	1:C:4:LEU:N	2.18	0.57
1:D:249:ALA:C	1:D:250:LEU:HD23	2.29	0.57
1:D:304:GLY:HA3	1:D:339:TYR:O	2.04	0.57
1:A:188:PHE:CZ	1:A:206:LEU:HD23	2.39	0.57
1:A:335:VAL:HG13	1:A:363:HIS:CE1	2.39	0.57
1:B:150:TYR:HD2	1:B:154:GLN:HE21	1.51	0.57
1:B:338:VAL:HA	1:B:356:LEU:CB	2.34	0.57
1:A:331:ALA:O	1:A:334:ALA:HB3	2.04	0.57
1:B:73:VAL:HG23	1:B:92:LEU:HD12	1.86	0.57
1:B:97:ARG:HG3	1:B:97:ARG:NH1	2.20	0.57
1:D:242:GLN:O	1:D:243:CYS:C	2.47	0.57
1:C:189:ILE:HG23	1:C:190:SER:N	2.20	0.57
1:B:117:TYR:CG	1:B:118:PRO:HD2	2.40	0.57
1:C:37:ARG:HA	1:C:57:LEU:HG	1.87	0.57
1:D:135:LEU:N	1:D:135:LEU:HD23	2.19	0.57
1:B:142:SER:HB3	4:B:395:ANP:O2A	2.05	0.57
1:D:369:GLN:O	1:D:372:TYR:N	2.34	0.57
1:B:13:LEU:O	1:B:16:ALA:N	2.38	0.57
1:C:32:VAL:HG11	1:C:151:THR:HG22	1.86	0.57
1:C:88:LEU:HD22	1:C:104:PRO:HD2	1.87	0.57
1:D:197:HIS:CD2	1:D:210:LEU:HB3	2.38	0.57
1:D:242:GLN:O	1:D:245:GLU:N	2.36	0.57
1:A:94:THR:HG22	1:A:95:ALA:N	2.20	0.56
1:A:192:MSE:HE3	1:A:192:MSE:HA	1.87	0.56
1:A:320:VAL:O	1:A:348:PHE:N	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:O	1:C:21:ARG:N	2.38	0.56
1:C:76:LEU:HD13	1:C:87:ARG:CG	2.35	0.56
1:C:284:GLU:OE1	1:C:287:ARG:NH2	2.35	0.56
1:D:271:SER:HG	1:D:274:GLY:H	1.52	0.56
1:B:41:ILE:HG12	1:B:42:GLY:N	2.21	0.56
1:B:59:LEU:CB	1:B:133:VAL:HG22	2.35	0.56
1:B:68:ARG:HD2	1:B:126:SER:OG	2.06	0.56
1:B:73:VAL:HG23	1:B:92:LEU:CD1	2.35	0.56
1:B:153:LEU:HD22	1:B:156:LEU:CD1	2.35	0.56
1:C:76:LEU:HD13	1:C:87:ARG:HG3	1.88	0.56
1:C:91:PRO:HG2	1:C:97:ARG:CZ	2.35	0.56
1:C:343:MSE:HE1	1:C:347:GLY:CA	2.36	0.56
1:B:104:PRO:HB2	1:B:106:TRP:CD1	2.40	0.56
1:A:9:VAL:HG22	1:A:60:MSE:HE3	1.88	0.56
1:A:38:VAL:HG23	1:A:344:THR:HG21	1.86	0.56
1:B:77:THR:HG21	4:B:395:ANP:N1	2.21	0.56
1:A:94:THR:N	1:A:97:ARG:O	2.27	0.56
1:A:107:ALA:O	1:A:111:LYS:HG3	2.05	0.56
1:B:77:THR:HG22	1:B:78:THR:N	2.20	0.56
1:D:259:GLN:HB2	1:D:262:GLU:OE2	2.06	0.56
1:C:188:PHE:HZ	1:C:206:LEU:HD13	1.70	0.56
1:D:163:ILE:O	1:D:166:ARG:HB2	2.05	0.56
1:C:205:SER:CB	1:C:207:GLU:HG3	2.36	0.56
1:A:207:GLU:CD	1:B:296:ARG:HD3	2.31	0.56
1:B:250:LEU:O	1:B:251:GLY:C	2.49	0.56
1:C:382:GLN:O	1:C:383:ALA:C	2.49	0.56
1:D:218:LEU:HD22	1:D:300:TYR:CZ	2.41	0.56
1:A:143:ALA:HA	1:A:146:GLU:OE1	2.06	0.55
1:A:307:MSE:CE	1:A:355:LEU:HD22	2.35	0.55
1:C:236:TYR:HB3	1:C:237:PRO:HD3	1.86	0.55
1:D:157:CYS:O	1:D:158:PRO:C	2.49	0.55
1:A:59:LEU:HD23	1:A:59:LEU:N	2.20	0.55
1:B:226:ASN:ND2	1:B:375:THR:O	2.30	0.55
1:C:235:GLU:O	1:C:238:VAL:N	2.39	0.55
1:D:260:LEU:HD12	1:D:260:LEU:C	2.31	0.55
1:A:204:ARG:CZ	1:A:256:ARG:HD3	2.36	0.55
1:A:304:GLY:HA3	1:A:339:TYR:O	2.05	0.55
1:C:39:ASN:HD21	1:C:53:LEU:H	1.54	0.55
1:C:249:ALA:C	1:C:250:LEU:HD12	2.31	0.55
1:C:367:HIS:O	1:C:370:GLU:HB2	2.06	0.55
1:A:93:PRO:HB3	1:A:99:LEU:H	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLU:C	1:B:30:LEU:HD23	2.32	0.55
1:B:244:GLU:O	1:B:245:GLU:C	2.47	0.55
1:C:109:TYR:HB2	1:C:145:LEU:HD21	1.88	0.55
1:C:174:GLU:O	1:C:178:ALA:HB3	2.07	0.55
1:C:180:MSE:O	1:C:182:CYS:N	2.36	0.55
1:C:276:ARG:O	1:C:277:ARG:C	2.48	0.55
1:A:284:GLU:HB2	1:A:287:ARG:HH21	1.71	0.55
1:B:241:ARG:O	1:B:244:GLU:N	2.39	0.55
1:A:43:GLU:OE2	1:A:342:ARG:NH2	2.29	0.55
1:C:329:VAL:HG21	1:C:342:ARG:HA	1.89	0.55
1:A:27:GLU:HA	1:A:27:GLU:OE2	2.07	0.55
1:A:136:GLY:HA3	1:A:228:ARG:HD2	1.89	0.55
1:B:273:GLU:O	1:B:277:ARG:HG2	2.07	0.55
1:A:37:ARG:O	1:A:37:ARG:NH1	2.30	0.55
1:A:219:ALA:O	1:A:356:LEU:HD12	2.06	0.55
1:C:91:PRO:HG2	1:C:97:ARG:HH21	1.72	0.55
1:D:208:THR:HG22	1:D:209:SER:N	2.21	0.55
1:D:246:VAL:O	1:D:249:ALA:HB3	2.07	0.55
1:B:241:ARG:O	1:B:242:GLN:C	2.49	0.55
1:C:120:ALA:CB	1:C:121:PRO:HA	2.33	0.55
1:A:266:ALA:HA	1:A:269:LEU:HD12	1.89	0.54
1:B:247:ALA:HB2	1:B:255:LEU:HD23	1.88	0.54
1:A:75:LEU:CD2	1:A:127:ALA:HB3	2.38	0.54
1:A:308:VAL:CG2	1:A:333:LEU:HD11	2.38	0.54
1:B:2:ALA:HB3	1:D:334:ALA:O	2.06	0.54
1:A:112:GLY:HA3	1:A:173:ALA:HB1	1.89	0.54
1:B:30:LEU:O	1:B:64:VAL:HA	2.06	0.54
1:B:33:SER:HB3	1:B:390:LEU:HD11	1.88	0.54
1:C:77:THR:HG22	1:C:79:SER:H	1.70	0.54
1:D:248:ARG:O	1:D:251:GLY:N	2.30	0.54
1:D:293:ALA:O	1:D:294:ALA:C	2.49	0.54
1:D:325:LEU:HD11	1:D:349:GLY:H	1.71	0.54
1:D:339:TYR:HD1	1:D:356:LEU:HA	1.73	0.54
1:C:117:TYR:CE1	1:C:153:LEU:HB2	2.42	0.54
1:A:20:PHE:CE1	1:A:65:GLY:HA2	2.42	0.54
1:B:31:ALA:HA	1:B:63:LEU:O	2.08	0.54
1:C:243:CYS:O	1:C:244:GLU:C	2.49	0.54
1:D:302:ALA:O	1:D:305:ARG:HB2	2.07	0.54
1:D:327:GLN:OE1	1:D:372:TYR:HA	2.07	0.54
1:A:68:ARG:NH1	1:A:70:ASP:OD2	2.41	0.54
1:A:205:SER:OG	1:A:207:GLU:HB2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:CD1	1:B:157:CYS:HB3	2.37	0.54
1:D:215:ASP:OD1	1:D:216:PRO:HD2	2.07	0.54
1:D:304:GLY:HA2	1:D:307:MSE:CG	2.35	0.54
1:A:51:LEU:HD21	1:A:256:ARG:NH2	2.23	0.54
1:B:311:HIS:HB2	1:B:342:ARG:CB	2.38	0.54
1:C:167:ALA:HB2	1:C:191:LEU:CD1	2.38	0.54
1:D:38:VAL:HG12	1:D:57:LEU:HD21	1.89	0.54
1:B:6:GLN:O	1:B:7:PRO:C	2.50	0.54
1:B:266:ALA:HA	1:B:269:LEU:HB2	1.89	0.54
1:B:305:ARG:O	1:B:309:GLU:HG3	2.07	0.54
1:C:188:PHE:O	1:C:189:ILE:C	2.48	0.54
1:C:259:GLN:O	1:C:262:GLU:N	2.41	0.54
1:A:122:LEU:HD12	1:A:123:PRO:HD2	1.88	0.53
1:C:20:PHE:HD1	1:C:128:VAL:CG2	2.21	0.53
1:C:93:PRO:HG3	1:C:99:LEU:HG	1.90	0.53
1:C:256:ARG:O	1:C:256:ARG:HG3	2.06	0.53
1:A:205:SER:HG	1:A:207:GLU:HB2	1.71	0.53
1:A:287:ARG:O	1:A:306:LEU:HD22	2.07	0.53
1:B:45:THR:HG21	1:B:284:GLU:HB3	1.90	0.53
1:D:49:GLN:CB	1:D:204:ARG:HB2	2.38	0.53
1:D:133:VAL:CG1	1:D:134:PRO:HD2	2.39	0.53
1:D:218:LEU:CD1	1:D:219:ALA:H	2.17	0.53
1:A:188:PHE:CE1	1:A:206:LEU:HD23	2.43	0.53
1:C:135:LEU:CD2	4:C:395:ANP:H3'	2.32	0.53
1:C:236:TYR:O	1:C:237:PRO:C	2.50	0.53
1:D:259:GLN:HB2	1:D:262:GLU:OE1	2.08	0.53
1:A:87:ARG:HG3	5:A:444:HOH:O	2.07	0.53
1:B:175:HIS:CE1	1:B:181:PRO:HA	2.43	0.53
1:B:236:TYR:HB3	1:B:237:PRO:HD3	1.90	0.53
1:C:201:ILE:HG12	1:C:208:THR:HG22	1.90	0.53
1:C:281:VAL:O	1:C:285:ILE:HG13	2.08	0.53
1:B:49:GLN:OE1	1:B:254:SER:HB3	2.09	0.53
1:B:111:LYS:NZ	5:B:436:HOH:O	2.29	0.53
1:B:246:VAL:O	1:B:247:ALA:C	2.52	0.53
1:C:94:THR:HG22	1:C:95:ALA:N	2.23	0.53
1:D:8:GLN:O	1:D:9:VAL:C	2.49	0.53
1:D:43:GLU:HB3	1:D:314:LEU:HD21	1.91	0.53
1:D:89:GLN:NE2	5:D:469:HOH:O	2.41	0.53
1:A:150:TYR:CE2	1:A:166:ARG:HG2	2.44	0.53
1:B:149:THR:O	1:B:152:PHE:N	2.42	0.53
1:C:367:HIS:O	1:C:371:HIS:HD2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ASN:HA	1:D:54:PRO:HA	1.90	0.53
1:D:327:GLN:OE1	1:D:373:GLY:N	2.33	0.53
1:B:39:ASN:HD21	1:B:53:LEU:H	1.55	0.53
1:B:367:HIS:O	1:B:371:HIS:HD2	1.91	0.53
1:D:202:ASP:O	1:D:206:LEU:N	2.35	0.53
1:D:335:VAL:HG13	1:D:363:HIS:CE1	2.44	0.53
1:B:17:ARG:HG2	1:B:27:GLU:OE2	2.09	0.53
1:C:320:VAL:O	1:C:347:GLY:HA3	2.08	0.53
1:A:247:ALA:HB2	1:A:255:LEU:CD2	2.40	0.52
1:B:322:CYS:SG	1:B:325:LEU:HG	2.49	0.52
1:D:193:GLY:O	1:D:194:GLN:HG2	2.09	0.52
1:C:19:ALA:HB3	1:C:128:VAL:HG11	1.91	0.52
1:D:254:SER:OG	1:D:256:ARG:HB3	2.09	0.52
1:D:342:ARG:O	1:D:352:THR:HB	2.10	0.52
1:A:98:SER:CB	1:A:115:GLN:HE22	2.11	0.52
1:B:343:MSE:HE1	1:B:347:GLY:CA	2.39	0.52
1:C:259:GLN:H	1:C:262:GLU:HB2	1.74	0.52
1:A:45:THR:O	1:A:48:ASN:HB2	2.10	0.52
1:A:307:MSE:O	1:A:310:SER:HB3	2.09	0.52
1:B:101:PRO:HG3	1:B:177:PHE:CD2	2.45	0.52
1:D:18:ARG:HG3	1:D:22:GLU:OE2	2.10	0.52
1:D:162:THR:HB	5:D:449:HOH:O	2.09	0.52
1:A:192:MSE:HE1	1:B:194:GLN:HG2	1.92	0.52
1:B:259:GLN:O	1:B:260:LEU:C	2.53	0.52
1:D:78:THR:HB	1:D:129:VAL:O	2.10	0.52
1:B:143:ALA:HB2	1:B:186:ASP:HB3	1.92	0.52
1:C:90:PHE:HB2	1:C:91:PRO:CD	2.38	0.52
1:D:285:ILE:O	1:D:286:ARG:C	2.50	0.52
1:D:324:GLU:OE1	1:D:324:GLU:N	2.37	0.52
1:A:279:ARG:NH2	1:A:317:ASP:OD1	2.42	0.52
1:B:315:ARG:HG2	1:B:316:ASP:OD1	2.10	0.52
1:C:218:LEU:HD11	1:C:355:LEU:HG	1.91	0.52
1:A:5:ARG:C	1:A:7:PRO:HD3	2.35	0.52
1:B:116:TYR:CE1	1:B:177:PHE:HE1	2.27	0.52
1:B:239:ARG:HH11	1:B:239:ARG:HG2	1.74	0.52
1:C:20:PHE:HD1	1:C:128:VAL:HG23	1.75	0.52
1:D:83:ASP:OD2	1:D:105:ARG:N	2.30	0.52
1:D:285:ILE:O	1:D:288:THR:N	2.42	0.52
1:A:40:LEU:HB2	1:A:53:LEU:O	2.10	0.52
1:B:222:ILE:HB	1:B:379:TYR:HB2	1.92	0.52
1:B:239:ARG:HG2	1:B:239:ARG:NH1	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:PHE:HB2	1:C:128:VAL:HG21	1.91	0.52
1:A:72:LEU:HD23	1:A:91:PRO:HA	1.92	0.52
1:B:31:ALA:HB2	1:B:392:LEU:HD21	1.92	0.52
1:C:304:GLY:O	1:C:307:MSE:HB2	2.11	0.52
1:A:249:ALA:C	1:A:251:GLY:H	2.17	0.51
1:A:356:LEU:HD12	1:A:356:LEU:H	1.73	0.51
1:B:32:VAL:N	1:B:390:LEU:HD12	2.25	0.51
1:B:339:TYR:OH	1:B:357:GLU:HG2	2.09	0.51
1:C:91:PRO:HG2	1:C:97:ARG:NE	2.25	0.51
1:C:239:ARG:HG2	1:C:239:ARG:HH11	1.76	0.51
1:A:105:ARG:O	1:A:106:TRP:C	2.51	0.51
1:D:47:TYR:CD1	1:D:240:ARG:HG3	2.45	0.51
1:D:181:PRO:O	1:D:240:ARG:NH1	2.37	0.51
1:C:74:SER:HB2	1:C:89:GLN:HG2	1.91	0.51
1:D:221:LEU:HD13	1:D:380:LEU:HD21	1.92	0.51
1:D:329:VAL:O	1:D:330:GLU:C	2.52	0.51
1:A:335:VAL:HG13	1:A:336:PRO:HD2	1.92	0.51
1:D:88:LEU:HD22	1:D:104:PRO:HD2	1.93	0.51
1:D:202:ASP:OD1	1:D:204:ARG:HB3	2.10	0.51
1:A:29:GLU:O	1:A:30:LEU:HD23	2.11	0.51
1:A:245:GLU:HG3	1:A:248:ARG:HH21	1.74	0.51
1:A:259:GLN:O	1:A:260:LEU:C	2.53	0.51
1:B:206:LEU:O	5:B:397:HOH:O	2.19	0.51
1:C:68:ARG:N	1:C:124:GLY:O	2.44	0.51
1:C:143:ALA:O	1:C:144:SER:C	2.52	0.51
1:C:264:GLU:O	1:C:267:ARG:HB2	2.11	0.51
1:A:34:ALA:O	1:A:144:SER:OG	2.29	0.51
1:D:87:ARG:HG2	1:D:87:ARG:NH1	2.22	0.51
1:D:264:GLU:O	1:D:267:ARG:N	2.29	0.51
1:A:252:LYS:HG2	1:A:257:GLU:CB	2.40	0.51
1:B:97:ARG:HH11	1:B:97:ARG:CG	2.24	0.51
1:B:152:PHE:CD2	1:B:153:LEU:HD23	2.46	0.51
1:A:23:GLU:OE2	1:A:87:ARG:NE	2.31	0.51
1:A:294:ALA:HA	1:A:297:ARG:CZ	2.41	0.51
1:C:264:GLU:OE2	1:C:267:ARG:NH1	2.30	0.51
1:A:29:GLU:C	1:A:30:LEU:HD23	2.36	0.51
1:C:83:ASP:O	1:C:85:PRO:O	2.29	0.51
1:D:365:MSE:HG2	1:D:378:PHE:CD2	2.46	0.51
1:A:53:LEU:O	1:A:53:LEU:HG	2.11	0.50
1:A:175:HIS:CE1	1:A:181:PRO:HA	2.45	0.50
1:D:120:ALA:HB1	1:D:121:PRO:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLU:HB2	1:A:314:LEU:HD11	1.92	0.50
1:A:100:GLU:HG3	1:A:101:PRO:CD	2.31	0.50
1:A:246:VAL:O	1:A:247:ALA:C	2.53	0.50
1:C:94:THR:HG22	1:C:96:GLN:N	2.12	0.50
1:D:226:ASN:ND2	1:D:377:THR:OG1	2.33	0.50
1:D:358:ALA:O	1:D:359:SER:C	2.55	0.50
1:A:361:ALA:HB3	1:A:362:PRO:CD	2.36	0.50
1:A:215:ASP:OD1	1:A:216:PRO:HD2	2.11	0.50
1:A:367:HIS:O	1:A:371:HIS:HD2	1.94	0.50
1:B:16:ALA:O	1:B:17:ARG:C	2.53	0.50
1:D:7:PRO:CG	1:D:12:LEU:HD21	2.42	0.50
1:D:9:VAL:CG2	1:D:60:MSE:HE1	2.42	0.50
1:D:43:GLU:OE1	2:D:393:GLA:O6	2.29	0.50
1:D:133:VAL:HG12	1:D:134:PRO:HD2	1.93	0.50
1:D:302:ALA:C	1:D:306:LEU:HD12	2.35	0.50
1:D:308:VAL:O	1:D:312:ARG:HG3	2.11	0.50
1:A:75:LEU:HD23	1:A:127:ALA:HB3	1.94	0.50
1:B:31:ALA:CB	1:B:390:LEU:HB2	2.42	0.50
1:B:185:MSE:HG2	1:B:186:ASP:N	2.26	0.50
1:C:325:LEU:HD21	1:C:349:GLY:O	2.12	0.50
1:A:33:SER:HA	1:A:61:THR:O	2.12	0.50
1:A:169:VAL:HG12	1:A:170:CYS:N	2.26	0.50
1:A:180:MSE:O	1:A:182:CYS:N	2.44	0.50
1:B:184:ILE:N	1:B:184:ILE:HD12	2.26	0.50
1:C:77:THR:HG21	4:C:395:ANP:N1	2.27	0.50
1:C:187:GLN:O	1:C:191:LEU:HG	2.12	0.50
1:D:279:ARG:HG2	1:D:317:ASP:OD2	2.12	0.50
1:D:280:HIS:CD2	1:D:281:VAL:N	2.80	0.50
1:A:77:THR:HG22	1:A:79:SER:H	1.76	0.50
1:B:116:TYR:CZ	1:B:177:PHE:HE1	2.30	0.50
1:B:150:TYR:CE2	1:B:154:GLN:NE2	2.80	0.50
1:C:82:ALA:O	1:C:83:ASP:O	2.30	0.50
1:C:246:VAL:O	1:C:247:ALA:C	2.54	0.50
1:C:322:CYS:HB2	1:C:323:PRO:HD2	1.93	0.50
1:C:360:ALA:C	1:C:362:PRO:HD2	2.37	0.50
1:D:181:PRO:O	1:D:240:ARG:HD2	2.12	0.50
1:D:213:LEU:HD21	1:D:295:LEU:HD21	1.93	0.50
1:A:146:GLU:O	1:A:149:THR:HB	2.12	0.50
1:A:205:SER:OG	1:A:207:GLU:N	2.37	0.50
1:B:109:TYR:O	1:B:113:VAL:HG23	2.12	0.50
1:B:339:TYR:CZ	1:B:357:GLU:HG2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:TYR:CE1	1:B:177:PHE:CE1	3.00	0.49
1:B:135:LEU:HB3	4:B:395:ANP:H3'	1.93	0.49
1:C:37:ARG:HD2	1:C:37:ARG:O	2.12	0.49
1:C:194:GLN:O	1:C:195:LYS:C	2.55	0.49
1:B:35:PRO:O	1:B:144:SER:HB2	2.11	0.49
1:C:371:HIS:N	1:C:371:HIS:CD2	2.80	0.49
1:D:312:ARG:NH2	5:D:418:HOH:O	2.44	0.49
1:A:184:ILE:H	1:A:184:ILE:CD1	2.06	0.49
1:A:247:ALA:HB2	1:A:255:LEU:HD23	1.94	0.49
1:A:273:GLU:O	1:A:277:ARG:HG2	2.13	0.49
1:B:266:ALA:O	1:B:267:ARG:C	2.53	0.49
1:C:117:TYR:HE2	1:C:119:ALA:HB3	1.77	0.49
1:D:205:SER:O	1:D:206:LEU:HB2	2.11	0.49
1:B:361:ALA:HB3	1:B:362:PRO:HD3	1.94	0.49
1:B:371:HIS:CD2	1:B:371:HIS:N	2.80	0.49
1:C:177:PHE:N	1:C:177:PHE:CD1	2.80	0.49
1:A:34:ALA:HB3	1:A:148:ALA:HB2	1.94	0.49
1:C:245:GLU:O	1:C:246:VAL:C	2.52	0.49
1:C:261:GLU:OE2	1:C:286:ARG:NH1	2.43	0.49
1:C:320:VAL:O	1:C:348:PHE:N	2.45	0.49
1:D:142:SER:O	1:D:146:GLU:HG3	2.13	0.49
1:D:291:ALA:HB1	1:D:303:PHE:CD1	2.46	0.49
1:A:270:VAL:O	1:A:271:SER:O	2.30	0.49
1:B:13:LEU:O	1:B:16:ALA:HB3	2.13	0.49
1:C:98:SER:O	1:C:99:LEU:O	2.31	0.49
1:B:136:GLY:N	4:B:395:ANP:O2B	2.46	0.49
1:B:242:GLN:O	1:B:243:CYS:C	2.52	0.49
1:B:35:PRO:HA	1:B:60:MSE:CB	2.43	0.49
1:B:143:ALA:CB	1:B:186:ASP:HB3	2.43	0.49
1:B:205:SER:HB2	1:B:207:GLU:OE2	2.12	0.49
1:B:294:ALA:O	1:B:299:ASP:N	2.36	0.49
1:C:37:ARG:HG2	1:C:189:ILE:HG21	1.95	0.49
1:D:68:ARG:HD3	1:D:70:ASP:HB2	1.95	0.49
1:A:77:THR:HG21	4:A:395:ANP:C2	2.43	0.48
1:A:186:ASP:OD2	2:A:393:GLA:O2	2.30	0.48
1:B:280:HIS:CD2	1:B:318:TYR:CD1	3.00	0.48
1:D:51:LEU:HB3	1:D:200:LEU:HD11	1.94	0.48
1:B:53:LEU:N	1:B:54:PRO:HD3	2.28	0.48
1:B:59:LEU:HB2	1:B:133:VAL:HG22	1.94	0.48
1:B:181:PRO:O	1:B:236:TYR:HE2	1.97	0.48
1:B:239:ARG:HD2	1:B:318:TYR:CE2	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:THR:O	1:C:97:ARG:O	2.31	0.48
1:C:112:GLY:O	1:C:116:TYR:HD1	1.95	0.48
1:C:113:VAL:CG1	1:C:149:THR:HG22	2.33	0.48
1:C:192:MSE:HB2	1:C:199:LEU:CD2	2.43	0.48
1:C:220:VAL:HG22	1:C:355:LEU:HD12	1.95	0.48
1:A:35:PRO:HA	1:A:60:MSE:CB	2.43	0.48
1:C:21:ARG:O	1:C:25:GLY:N	2.44	0.48
1:C:194:GLN:O	1:C:195:LYS:O	2.31	0.48
1:C:314:LEU:O	1:C:319:GLU:N	2.47	0.48
1:D:85:PRO:HG2	1:D:87:ARG:O	2.12	0.48
1:D:95:ALA:O	1:D:96:GLN:O	2.30	0.48
1:D:105:ARG:O	1:D:106:TRP:C	2.53	0.48
1:D:163:ILE:O	1:D:166:ARG:N	2.42	0.48
1:D:366:ARG:O	1:D:370:GLU:HG3	2.13	0.48
1:A:235:GLU:O	1:A:238:VAL:HB	2.13	0.48
1:B:152:PHE:HD2	1:B:153:LEU:HD23	1.77	0.48
1:C:177:PHE:N	1:C:177:PHE:HD1	2.11	0.48
1:C:318:TYR:O	1:C:319:GLU:HB2	2.13	0.48
1:D:362:PRO:O	1:D:363:HIS:C	2.55	0.48
1:D:375:THR:O	1:D:375:THR:HG22	2.12	0.48
1:A:239:ARG:HD3	1:A:242:GLN:OE1	2.13	0.48
1:A:260:LEU:N	1:A:282:VAL:HG11	2.29	0.48
1:A:312:ARG:HE	1:A:315:ARG:HH12	1.59	0.48
1:B:9:VAL:HG23	5:B:479:HOH:O	2.13	0.48
1:B:24:PHE:CE1	1:B:126:SER:HB3	2.48	0.48
1:B:232:ALA:O	1:B:235:GLU:N	2.31	0.48
1:C:4:LEU:N	1:C:378:PHE:O	2.38	0.48
1:C:16:ALA:HB1	1:C:64:VAL:HB	1.95	0.48
1:C:37:ARG:NH2	1:C:186:ASP:OD1	2.42	0.48
1:C:242:GLN:OE1	1:C:277:ARG:HG2	2.14	0.48
1:D:43:GLU:OE2	1:D:345:GLY:N	2.44	0.48
1:D:73:VAL:HG11	1:D:90:PHE:CZ	2.48	0.48
1:D:281:VAL:O	1:D:284:GLU:N	2.47	0.48
1:A:1:HIS:HD2	1:A:3:ALA:HB3	1.78	0.48
1:A:207:GLU:OE2	1:B:296:ARG:HD3	2.14	0.48
1:B:7:PRO:HG2	1:B:132:SER:HB3	1.95	0.48
1:B:33:SER:HA	1:B:61:THR:O	2.13	0.48
1:D:94:THR:O	1:D:97:ARG:O	2.31	0.48
1:D:77:THR:HG22	1:D:79:SER:N	2.08	0.48
1:B:125:PHE:CG	1:B:152:PHE:HE2	2.31	0.48
1:B:141:SER:OG	4:B:395:ANP:O2B	2.30	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ASP:HB2	5:B:446:HOH:O	2.14	0.48
1:C:8:GLN:O	1:C:9:VAL:C	2.57	0.48
1:C:20:PHE:CD1	1:C:128:VAL:HG23	2.49	0.48
1:C:266:ALA:O	1:C:267:ARG:C	2.56	0.48
1:D:328:LEU:HD21	1:D:372:TYR:CG	2.48	0.48
1:A:49:GLN:HE21	1:A:204:ARG:CG	2.26	0.48
1:A:77:THR:HG21	4:A:395:ANP:H2	1.96	0.48
1:A:116:TYR:O	1:A:117:TYR:O	2.30	0.48
1:A:310:SER:O	1:A:311:HIS:C	2.57	0.48
1:B:54:PRO:HD2	1:B:199:LEU:O	2.14	0.48
1:A:43:GLU:CB	1:A:314:LEU:HD11	2.44	0.48
1:B:258:VAL:CG1	1:B:263:LEU:HD12	2.42	0.48
1:C:188:PHE:CZ	1:C:206:LEU:HD22	2.49	0.48
1:C:347:GLY:O	1:C:348:PHE:HB2	2.14	0.48
1:C:369:GLN:HA	1:C:369:GLN:NE2	2.29	0.48
1:D:279:ARG:O	1:D:280:HIS:C	2.57	0.48
1:D:304:GLY:CA	1:D:307:MSE:HE2	2.41	0.48
1:A:146:GLU:OE2	1:A:174:GLU:HB2	2.13	0.47
1:A:295:LEU:HD12	1:A:295:LEU:C	2.39	0.47
1:D:277:ARG:O	1:D:280:HIS:N	2.47	0.47
1:B:85:PRO:HA	5:B:453:HOH:O	2.13	0.47
1:C:211:VAL:O	1:C:212:PRO:C	2.55	0.47
1:D:202:ASP:C	1:D:204:ARG:H	2.22	0.47
1:D:358:ALA:O	1:D:360:ALA:N	2.48	0.47
1:A:391:CYS:HB3	5:A:489:HOH:O	2.13	0.47
1:B:9:VAL:O	1:B:10:ALA:C	2.56	0.47
1:B:171:GLN:HG2	1:B:175:HIS:HD2	1.78	0.47
1:B:204:ARG:HB2	1:B:256:ARG:NH1	2.30	0.47
1:C:84:GLU:HA	1:C:85:PRO:O	2.14	0.47
1:D:266:ALA:O	1:D:267:ARG:C	2.58	0.47
1:A:307:MSE:CE	1:A:355:LEU:HB2	2.21	0.47
1:B:138:GLY:HA2	4:B:395:ANP:O2G	2.13	0.47
1:B:299:ASP:OD1	1:B:302:ALA:HB2	2.14	0.47
1:C:63:LEU:HD12	1:C:129:VAL:HA	1.96	0.47
1:C:273:GLU:HB2	5:C:397:HOH:O	2.13	0.47
1:D:94:THR:OG1	1:D:97:ARG:HG2	2.15	0.47
1:D:163:ILE:O	1:D:164:ALA:C	2.56	0.47
1:C:32:VAL:CG1	1:C:151:THR:HG22	2.44	0.47
1:C:304:GLY:HA3	1:C:339:TYR:O	2.13	0.47
1:B:115:GLN:HG2	1:B:177:PHE:CZ	2.50	0.47
1:B:146:GLU:O	1:B:149:THR:HB	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:LEU:HD22	1:B:360:ALA:HB3	1.95	0.47
1:C:59:LEU:HD11	1:C:379:TYR:CD2	2.50	0.47
1:C:151:THR:O	1:C:154:GLN:HB2	2.14	0.47
1:C:227:VAL:HG21	1:C:324:GLU:HG2	1.96	0.47
1:C:370:GLU:HB3	1:C:371:HIS:CD2	2.49	0.47
1:D:1:HIS:CE1	1:D:366:ARG:HG2	2.49	0.47
1:D:246:VAL:O	1:D:247:ALA:C	2.57	0.47
1:D:292:ALA:O	1:D:296:ARG:N	2.45	0.47
1:A:18:ARG:O	1:A:19:ALA:C	2.57	0.47
1:B:124:GLY:O	1:B:125:PHE:HB3	2.15	0.47
1:D:152:PHE:O	1:D:153:LEU:C	2.55	0.47
1:D:274:GLY:O	1:D:275:PHE:C	2.57	0.47
1:B:211:VAL:HA	1:B:212:PRO:HD2	1.71	0.47
1:D:266:ALA:CB	1:D:269:LEU:HD12	2.44	0.47
1:B:12:LEU:HD23	1:B:12:LEU:HA	1.75	0.47
1:B:112:GLY:HA3	1:B:173:ALA:HB1	1.97	0.47
1:B:267:ARG:HG3	5:B:410:HOH:O	2.15	0.47
1:C:246:VAL:O	1:C:249:ALA:N	2.48	0.47
1:D:20:PHE:HD1	1:D:128:VAL:CG2	2.27	0.47
1:D:136:GLY:HA3	1:D:228:ARG:CZ	2.45	0.47
1:D:266:ALA:CA	1:D:269:LEU:HB2	2.44	0.47
1:A:171:GLN:HG2	1:A:175:HIS:CD2	2.49	0.46
1:A:252:LYS:NZ	1:A:257:GLU:O	2.45	0.46
1:C:213:LEU:HD12	1:C:213:LEU:HA	1.75	0.46
1:A:35:PRO:HA	1:A:60:MSE:HB2	1.97	0.46
1:A:339:TYR:CD1	1:A:356:LEU:HA	2.51	0.46
1:B:80:GLU:C	1:B:82:ALA:H	2.21	0.46
1:B:196:GLY:HA2	1:B:383:ALA:HB3	1.95	0.46
1:C:142:SER:OG	4:C:395:ANP:O1B	2.33	0.46
1:D:1:HIS:CG	1:D:366:ARG:HG2	2.50	0.46
1:D:39:ASN:HD22	1:D:39:ASN:C	2.22	0.46
1:A:33:SER:HB3	1:A:62:VAL:HG22	1.97	0.46
1:A:47:TYR:CD1	1:A:240:ARG:HG3	2.51	0.46
1:A:141:SER:OG	4:A:395:ANP:O2B	2.30	0.46
1:A:243:CYS:O	1:A:244:GLU:C	2.58	0.46
1:B:85:PRO:O	1:B:104:PRO:HG3	2.15	0.46
1:B:146:GLU:OE2	1:B:174:GLU:HB2	2.15	0.46
1:C:312:ARG:HG2	1:C:312:ARG:NH1	2.30	0.46
1:A:57:LEU:O	1:A:384:ALA:HB3	2.15	0.46
1:A:113:VAL:HB	1:A:149:THR:HG21	1.96	0.46
1:B:111:LYS:O	1:B:114:ILE:HB	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:LEU:HD21	1:D:208:THR:HG21	1.97	0.46
1:D:221:LEU:HD13	1:D:380:LEU:CD2	2.45	0.46
1:D:304:GLY:CA	1:D:307:MSE:HG3	2.39	0.46
1:A:188:PHE:HE1	1:A:206:LEU:CD2	2.28	0.46
1:A:284:GLU:OE1	1:A:287:ARG:NH2	2.46	0.46
1:B:92:LEU:HG	1:B:93:PRO:HD2	1.96	0.46
1:D:222:ILE:HB	1:D:379:TYR:HB2	1.96	0.46
1:A:188:PHE:CE1	1:A:206:LEU:CD2	2.99	0.46
1:A:281:VAL:O	1:A:285:ILE:HG13	2.15	0.46
1:B:148:ALA:O	1:B:149:THR:C	2.57	0.46
1:C:277:ARG:H	1:C:277:ARG:HD3	1.81	0.46
1:C:320:VAL:HG12	1:C:348:PHE:CE1	2.51	0.46
1:D:68:ARG:N	1:D:124:GLY:O	2.49	0.46
1:D:236:TYR:O	1:D:237:PRO:C	2.56	0.46
1:D:239:ARG:O	1:D:240:ARG:C	2.58	0.46
1:D:245:GLU:O	1:D:246:VAL:C	2.57	0.46
1:A:187:GLN:OE1	1:A:187:GLN:N	2.31	0.46
1:B:43:GLU:O	1:B:44:HIS:HB2	2.15	0.46
1:B:114:ILE:O	1:B:116:TYR:N	2.49	0.46
1:D:9:VAL:O	1:D:10:ALA:C	2.57	0.46
1:D:371:HIS:N	1:D:371:HIS:CD2	2.84	0.46
1:A:284:GLU:CB	1:A:287:ARG:HH21	2.28	0.46
1:C:83:ASP:OD2	1:C:105:ARG:N	2.40	0.46
1:C:303:PHE:O	1:C:307:MSE:HG3	2.15	0.46
1:D:59:LEU:HD22	1:D:132:SER:O	2.16	0.46
1:D:356:LEU:N	1:D:356:LEU:HD12	2.31	0.46
1:A:46:ASP:OD2	2:A:393:GLA:H4	2.16	0.46
1:A:221:LEU:HD13	1:A:380:LEU:HD21	1.96	0.46
1:A:308:VAL:O	1:A:309:GLU:C	2.59	0.46
1:A:58:GLU:HG3	1:A:384:ALA:HB2	1.97	0.46
1:B:292:ALA:O	1:B:296:ARG:HG3	2.16	0.46
1:B:325:LEU:HD13	1:B:343:MSE:CB	2.46	0.46
1:C:28:PRO:HB2	1:C:64:VAL:HG13	1.97	0.46
1:D:68:ARG:C	1:D:70:ASP:H	2.20	0.46
1:A:250:LEU:O	1:A:251:GLY:C	2.57	0.45
1:A:321:SER:OG	1:A:322:CYS:N	2.44	0.45
1:B:21:ARG:HB2	1:B:27:GLU:OE1	2.15	0.45
1:B:34:ALA:HB2	1:B:147:VAL:HG12	1.97	0.45
1:C:112:GLY:HA2	1:C:115:GLN:HB3	1.98	0.45
1:C:123:PRO:HG2	1:C:156:LEU:HB3	1.97	0.45
1:D:208:THR:CG2	1:D:209:SER:N	2.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLU:HA	1:A:287:ARG:NH2	2.31	0.45
1:B:188:PHE:CZ	1:B:206:LEU:HG	2.51	0.45
1:B:356:LEU:CD2	1:B:360:ALA:HB3	2.46	0.45
1:C:76:LEU:CD1	1:C:87:ARG:HG3	2.46	0.45
1:C:170:CYS:O	1:C:173:ALA:HB3	2.16	0.45
1:C:276:ARG:HG2	1:C:317:ASP:OD1	2.16	0.45
1:D:322:CYS:O	1:D:323:PRO:C	2.59	0.45
1:B:37:ARG:O	1:B:139:LEU:HA	2.17	0.45
1:B:311:HIS:HB2	1:B:342:ARG:HB2	1.97	0.45
1:B:356:LEU:HD12	1:B:356:LEU:H	1.81	0.45
1:C:239:ARG:O	1:C:240:ARG:C	2.57	0.45
1:A:44:HIS:ND1	1:A:318:TYR:HE2	2.14	0.45
1:A:192:MSE:HA	1:A:192:MSE:CE	2.46	0.45
1:A:284:GLU:CA	1:A:287:ARG:NH2	2.79	0.45
1:A:303:PHE:CD2	1:A:307:MSE:HE2	2.50	0.45
1:A:335:VAL:HG12	1:A:336:PRO:N	2.31	0.45
1:B:149:THR:O	1:B:152:PHE:HB3	2.16	0.45
1:B:192:MSE:HE3	1:B:192:MSE:CA	2.44	0.45
1:C:109:TYR:CB	1:C:145:LEU:HD21	2.47	0.45
1:C:184:ILE:HG21	1:C:206:LEU:CD2	2.38	0.45
1:C:361:ALA:N	1:C:362:PRO:CD	2.80	0.45
1:D:173:ALA:O	1:D:177:PHE:HB2	2.17	0.45
1:C:229:HIS:HE2	1:C:324:GLU:CD	2.24	0.45
1:D:239:ARG:NH2	1:D:319:GLU:O	2.48	0.45
1:D:297[A]:ARG:NH1	5:D:456:HOH:O	2.43	0.45
1:A:245:GLU:O	1:A:248:ARG:HB3	2.15	0.45
1:B:184:ILE:O	1:B:185:MSE:C	2.60	0.45
1:C:59:LEU:HD11	1:C:379:TYR:CE2	2.52	0.45
1:C:189:ILE:CG2	1:C:190:SER:N	2.80	0.45
1:D:53:LEU:N	1:D:54:PRO:CD	2.80	0.45
1:B:45:THR:CG2	1:B:284:GLU:HB3	2.46	0.45
1:B:185:MSE:O	1:B:189:ILE:HG22	2.16	0.45
1:C:307:MSE:O	1:C:310:SER:HB3	2.17	0.45
1:C:311:HIS:HB2	1:C:342:ARG:HB2	1.96	0.45
1:D:356:LEU:N	1:D:356:LEU:CD1	2.80	0.45
1:A:260:LEU:HG	1:A:282:VAL:HG12	1.99	0.45
1:B:40:LEU:O	1:B:41:ILE:HB	2.17	0.45
1:B:110:VAL:O	1:B:111:LYS:C	2.59	0.45
1:B:188:PHE:CZ	1:B:206:LEU:CG	3.00	0.45
1:B:202:ASP:OD1	1:B:204:ARG:HB3	2.17	0.45
1:D:235:GLU:O	1:D:236:TYR:C	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:MSE:HE3	1:D:343:MSE:HB2	1.52	0.45
1:D:357:GLU:O	1:D:360:ALA:N	2.48	0.45
1:A:13:LEU:HA	1:A:13:LEU:HD12	1.60	0.45
1:A:75:LEU:HD11	1:A:110:VAL:HG11	1.99	0.45
1:A:94:THR:CG2	1:A:95:ALA:N	2.80	0.45
1:A:122:LEU:HD21	1:A:153:LEU:HD22	1.98	0.45
1:A:218:LEU:HD11	1:A:355:LEU:HG	1.99	0.45
1:B:29:GLU:CD	1:B:67:PRO:HD2	2.42	0.45
1:B:117:TYR:OH	1:B:159:ASP:HB3	2.16	0.45
1:C:34:ALA:O	1:C:144:SER:OG	2.31	0.45
1:C:258:VAL:CG1	1:C:259:GLN:N	2.80	0.45
1:D:41:ILE:HD12	1:D:307:MSE:HA	1.98	0.45
1:D:287:ARG:HG3	1:D:287:ARG:HH11	1.82	0.45
1:B:51:LEU:HD23	1:B:202:ASP:HA	1.99	0.44
1:B:273:GLU:CA	1:B:276:ARG:NH2	2.80	0.44
1:C:117:TYR:CE2	1:C:119:ALA:HB3	2.52	0.44
1:C:227:VAL:CG1	1:C:228:ARG:N	2.80	0.44
1:C:238:VAL:HG12	1:C:242:GLN:HE21	1.81	0.44
1:D:335:VAL:CG1	1:D:363:HIS:ND1	2.80	0.44
1:B:20:PHE:O	1:B:21:ARG:C	2.59	0.44
1:C:73:VAL:CG1	1:C:125:PHE:CZ	3.00	0.44
1:A:20:PHE:HA	1:A:128:VAL:HG21	1.99	0.44
1:A:185:MSE:HG2	1:A:186:ASP:N	2.31	0.44
1:A:328:LEU:HA	1:A:328:LEU:HD23	1.67	0.44
1:B:20:PHE:CE2	1:B:28:PRO:HA	2.52	0.44
1:B:198:ALA:HB2	1:B:213:LEU:HD12	1.97	0.44
1:C:119:ALA:HB2	1:C:159:ASP:HA	1.98	0.44
1:C:215:ASP:HA	1:C:216:PRO:HD2	1.73	0.44
1:D:63:LEU:HD23	1:D:63:LEU:O	2.18	0.44
1:D:77:THR:O	1:D:86:GLN:HG2	2.18	0.44
1:D:131:SER:N	5:D:432:HOH:O	2.49	0.44
1:A:138:GLY:C	1:A:139:LEU:HD23	2.42	0.44
1:A:360:ALA:O	1:A:361:ALA:C	2.59	0.44
1:B:31:ALA:HB3	1:B:390:LEU:HB2	1.99	0.44
1:B:320:VAL:O	1:B:348:PHE:N	2.45	0.44
1:D:68:ARG:NH1	1:D:72:LEU:HD12	2.26	0.44
1:D:266:ALA:C	1:D:269:LEU:H	2.24	0.44
1:D:364:ALA:O	1:D:368:ILE:HG13	2.18	0.44
1:A:232:ALA:HB3	1:A:348:PHE:CD2	2.53	0.44
1:A:336:PRO:HD2	1:A:363:HIS:CE1	2.52	0.44
1:B:27:GLU:HA	1:B:28:PRO:HD3	1.75	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ILE:HG12	1:B:42:GLY:H	1.80	0.44
1:B:49:GLN:NE2	1:B:204:ARG:CG	2.80	0.44
1:B:109:TYR:CE2	1:B:178:ALA:CB	3.00	0.44
1:B:227:VAL:CG1	1:B:228:ARG:N	2.80	0.44
1:C:94:THR:CG2	1:C:95:ALA:N	2.81	0.44
1:C:227:VAL:HG13	1:C:229:HIS:CE1	2.53	0.44
1:D:97:ARG:NH2	1:D:99:LEU:HD23	2.33	0.44
1:D:272:LYS:O	1:D:276:ARG:HG3	2.17	0.44
1:A:219:ALA:HB3	1:A:356:LEU:HD13	2.00	0.44
1:A:229:HIS:HB2	1:A:348:PHE:O	2.17	0.44
1:A:243:CYS:O	1:A:245:GLU:N	2.51	0.44
1:B:41:ILE:CG1	1:B:42:GLY:N	2.80	0.44
1:B:356:LEU:N	1:B:356:LEU:CD1	2.81	0.44
1:C:13:LEU:O	1:C:14:ALA:C	2.61	0.44
1:C:356:LEU:N	1:C:356:LEU:CD1	2.80	0.44
1:D:47:TYR:CD1	1:D:240:ARG:CG	3.00	0.44
1:A:1:HIS:CD2	1:A:3:ALA:H	2.36	0.44
1:B:117:TYR:CD1	1:B:118:PRO:CD	3.00	0.44
1:C:113:VAL:O	1:C:117:TYR:N	2.50	0.44
1:C:250:LEU:N	1:C:250:LEU:CD1	2.81	0.44
1:C:261:GLU:HG3	5:C:480:HOH:O	2.17	0.44
1:D:34:ALA:HB3	1:D:148:ALA:HB2	1.99	0.44
1:D:136:GLY:HA3	1:D:228:ARG:NH1	2.33	0.44
1:A:9:VAL:CG2	1:A:60:MSE:HE1	2.47	0.44
1:A:336:PRO:HD2	1:A:363:HIS:HE1	1.83	0.44
1:B:34:ALA:O	1:B:144:SER:OG	2.29	0.44
1:B:260:LEU:HD12	1:B:260:LEU:HA	1.85	0.44
1:C:6:GLN:HG2	1:C:59:LEU:CD2	2.46	0.44
1:C:269:LEU:HD23	1:C:269:LEU:HA	1.69	0.44
1:D:53:LEU:N	1:D:54:PRO:HD3	2.33	0.44
1:A:34:ALA:HB3	1:A:144:SER:O	2.17	0.44
1:A:51:LEU:HD21	1:A:256:ARG:HH22	1.82	0.44
1:A:117:TYR:CD1	1:A:118:PRO:CD	3.00	0.44
1:A:188:PHE:HE1	1:A:206:LEU:HD21	1.82	0.44
1:A:224:ASN:N	1:A:377:THR:O	2.41	0.44
1:B:286:ARG:O	1:B:289:ALA:HB3	2.18	0.44
1:C:35:PRO:HG3	1:C:385:ASP:O	2.17	0.44
1:C:49:GLN:HB3	1:C:204:ARG:HB2	2.00	0.44
1:C:116:TYR:CE2	1:C:172:GLN:HG2	2.52	0.44
1:C:245:GLU:O	1:C:248:ARG:HB3	2.17	0.44
1:C:361:ALA:HB3	1:C:362:PRO:CD	2.37	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:ASP:O	1:D:327:GLN:C	2.59	0.44
1:A:28:PRO:HB3	1:A:64:VAL:HG12	2.00	0.43
1:A:56:ALA:O	1:A:383:ALA:HA	2.17	0.43
1:B:115:GLN:HG2	1:B:177:PHE:HZ	1.82	0.43
1:B:218:LEU:HD11	1:B:355:LEU:HG	2.00	0.43
1:B:232:ALA:O	1:B:235:GLU:HB2	2.17	0.43
1:B:311:HIS:ND1	1:B:343:MSE:HG2	2.33	0.43
1:B:356:LEU:HD13	1:B:356:LEU:C	2.42	0.43
1:C:24:PHE:HZ	1:C:74:SER:OG	2.01	0.43
1:C:261:GLU:OE2	1:C:286:ARG:NH2	2.49	0.43
1:D:259:GLN:O	1:D:262:GLU:N	2.50	0.43
1:B:150:TYR:HE1	1:B:169:VAL:HG21	1.83	0.43
1:C:14:ALA:O	1:C:15:GLU:C	2.60	0.43
1:C:72:LEU:HD22	1:C:91:PRO:HA	1.96	0.43
1:C:255:LEU:HA	1:C:255:LEU:HD23	1.55	0.43
1:D:9:VAL:HA	1:D:60:MSE:HE1	2.00	0.43
1:A:32:VAL:HG11	1:A:152:PHE:HA	1.99	0.43
1:C:235:GLU:O	1:C:236:TYR:C	2.61	0.43
1:D:159:ASP:HB2	5:D:472:HOH:O	2.18	0.43
1:A:150:TYR:OH	1:A:159:ASP:OD2	2.29	0.43
1:B:113:VAL:HB	1:B:149:THR:HG21	1.99	0.43
1:B:116:TYR:O	1:B:117:TYR:O	2.37	0.43
1:D:58:GLU:CD	1:D:382:GLN:HB2	2.42	0.43
1:A:113:VAL:HG11	1:A:150:TYR:N	2.34	0.43
1:A:149:THR:O	1:A:152:PHE:HB3	2.19	0.43
1:A:204:ARG:NH2	1:A:257:GLU:OE2	2.51	0.43
1:B:326:ASP:OD1	1:B:326:ASP:N	2.52	0.43
1:C:28:PRO:HB3	1:C:64:VAL:HG13	1.99	0.43
1:B:219:ALA:HB3	1:B:356:LEU:CD1	2.49	0.43
1:B:252:LYS:HB3	1:B:257:GLU:HB2	2.00	0.43
1:B:284:GLU:HA	1:B:284:GLU:OE1	2.18	0.43
1:C:236:TYR:HB3	1:C:237:PRO:CD	2.47	0.43
1:D:68:ARG:HB3	1:D:70:ASP:H	1.84	0.43
1:D:135:LEU:C	1:D:228:ARG:HH11	2.27	0.43
1:A:37:ARG:C	1:A:37:ARG:HD2	2.43	0.43
1:A:239:ARG:O	1:A:242:GLN:HB2	2.18	0.43
1:B:18:ARG:O	1:B:19:ALA:C	2.61	0.43
1:B:188:PHE:CZ	1:B:206:LEU:CD1	2.99	0.43
1:B:194:GLN:O	1:B:195:LYS:C	2.59	0.43
1:C:20:PHE:CE1	1:C:24:PHE:CD1	3.07	0.43
1:C:189:ILE:HD13	1:C:199:LEU:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:PRO:HG3	1:D:185:MSE:HG3	2.00	0.43
1:A:6:GLN:HE21	1:A:6:GLN:HB2	1.47	0.43
1:A:77:THR:CG2	4:A:395:ANP:N1	2.82	0.43
1:B:27:GLU:CD	1:B:28:PRO:HD2	2.44	0.43
1:B:222:ILE:HD12	1:B:222:ILE:HG21	1.77	0.43
1:B:364:ALA:O	1:B:365:MSE:C	2.62	0.43
1:C:192:MSE:HB2	1:C:199:LEU:HD21	2.00	0.43
1:D:164:ALA:O	1:D:168:GLN:HG3	2.18	0.43
1:D:309:GLU:O	1:D:310:SER:C	2.62	0.43
1:A:76:LEU:HD12	1:A:77:THR:H	1.83	0.43
1:A:372:TYR:C	1:A:374:GLY:H	2.27	0.43
1:C:9:VAL:O	1:C:13:LEU:N	2.51	0.43
1:C:68:ARG:NH1	1:C:70:ASP:CB	2.81	0.43
1:C:232:ALA:C	1:C:234:SER:H	2.27	0.43
1:C:304:GLY:HA3	1:C:339:TYR:C	2.44	0.43
1:D:77:THR:CG2	4:D:395:ANP:N1	2.80	0.43
1:D:192:MSE:O	1:D:193:GLY:C	2.61	0.43
1:A:68:ARG:NH1	1:A:72:LEU:CB	2.82	0.43
1:B:88:LEU:HG	1:B:104:PRO:HD2	2.00	0.43
1:C:44:HIS:H	2:C:393:GLA:HO6	1.66	0.43
1:C:93:PRO:HG3	1:C:99:LEU:CG	2.49	0.43
1:C:152:PHE:C	1:C:154:GLN:H	2.27	0.43
1:C:165:ALA:O	1:C:168:GLN:N	2.51	0.43
1:C:222:ILE:HB	1:C:379:TYR:HB2	2.00	0.43
1:D:38:VAL:O	1:D:38:VAL:HG13	2.19	0.43
1:D:287:ARG:HG2	1:D:306:LEU:HD23	1.99	0.43
1:A:28:PRO:HB2	1:A:64:VAL:HG12	2.00	0.42
1:A:68:ARG:HH12	1:A:72:LEU:CB	2.32	0.42
1:A:88:LEU:HD13	1:A:104:PRO:HD2	2.01	0.42
1:A:299:ASP:OD1	1:A:302:ALA:HB2	2.19	0.42
1:B:325:LEU:HD13	1:B:343:MSE:HB2	2.01	0.42
1:C:206:LEU:HD23	1:C:206:LEU:HA	1.69	0.42
1:D:133:VAL:HA	1:D:134:PRO:HD3	1.75	0.42
1:D:199:LEU:CD2	1:D:208:THR:HG21	2.49	0.42
1:A:204:ARG:NH2	1:A:256:ARG:HG2	2.34	0.42
1:B:266:ALA:CA	1:B:269:LEU:HB2	2.49	0.42
1:C:245:GLU:HA	1:C:248:ARG:CZ	2.49	0.42
1:C:275:PHE:O	1:C:278:ALA:HB3	2.19	0.42
1:D:218:LEU:HD12	1:D:356:LEU:O	2.18	0.42
1:D:333:LEU:HD21	1:D:340:GLY:C	2.44	0.42
1:A:49:GLN:HB3	1:A:204:ARG:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLU:HB2	1:A:287:ARG:NH2	2.33	0.42
1:A:329:VAL:O	1:A:330:GLU:C	2.61	0.42
1:B:240:ARG:O	1:B:244:GLU:HG3	2.19	0.42
1:B:291:ALA:O	1:B:294:ALA:HB3	2.19	0.42
1:C:158:PRO:HB3	5:C:444:HOH:O	2.18	0.42
1:D:264:GLU:O	1:D:265:ALA:C	2.62	0.42
1:A:361:ALA:HB3	5:A:454:HOH:O	2.19	0.42
1:B:83:ASP:OD2	1:B:105:ARG:N	2.47	0.42
1:B:171:GLN:HG3	1:B:182:CYS:SG	2.59	0.42
1:C:321:SER:OG	1:C:322:CYS:N	2.52	0.42
1:D:153:LEU:O	1:D:156:LEU:N	2.50	0.42
1:D:199:LEU:HD23	1:D:208:THR:HG23	2.01	0.42
1:D:221:LEU:O	1:D:354:THR:N	2.38	0.42
1:D:333:LEU:HA	1:D:333:LEU:HD23	1.74	0.42
1:A:68:ARG:HB3	1:A:70:ASP:HB3	2.02	0.42
1:B:76:LEU:HD12	1:B:86:GLN:O	2.20	0.42
1:B:188:PHE:HZ	1:B:206:LEU:HG	1.83	0.42
1:B:219:ALA:HB3	1:B:356:LEU:HD13	2.01	0.42
1:C:68:ARG:HD2	1:C:126:SER:OG	2.19	0.42
1:C:314:LEU:HD23	1:C:314:LEU:HA	1.82	0.42
1:D:37:ARG:HD2	1:D:37:ARG:C	2.43	0.42
1:D:223:THR:O	1:D:351:CYS:HA	2.19	0.42
1:A:57:LEU:C	1:A:384:ALA:HB3	2.45	0.42
1:A:213:LEU:HD11	1:A:295:LEU:HD21	2.02	0.42
1:A:227:VAL:CG1	1:A:228:ARG:N	2.80	0.42
1:B:366:ARG:NH1	5:B:452:HOH:O	2.51	0.42
1:C:74:SER:HA	1:C:89:GLN:HA	2.02	0.42
1:C:194:GLN:C	1:C:195:LYS:O	2.62	0.42
1:D:204:ARG:HB3	1:D:256:ARG:NH1	2.35	0.42
1:A:122:LEU:HD11	1:A:153:LEU:HD22	2.02	0.42
1:B:14:ALA:O	1:B:15:GLU:C	2.59	0.42
1:B:53:LEU:HD13	1:B:200:LEU:HD13	2.02	0.42
1:B:247:ALA:HB2	1:B:255:LEU:CD2	2.49	0.42
1:C:32:VAL:CA	1:C:390:LEU:HD12	2.50	0.42
1:C:240:ARG:O	1:C:244:GLU:HG3	2.20	0.42
1:D:235:GLU:O	1:D:238:VAL:N	2.53	0.42
1:D:303:PHE:O	1:D:307:MSE:HG3	2.20	0.42
1:B:109:TYR:CE2	1:B:178:ALA:HB2	2.54	0.42
1:B:171:GLN:HG2	1:B:175:HIS:CD2	2.54	0.42
1:B:173:ALA:O	1:B:177:PHE:HB2	2.20	0.42
1:B:370:GLU:CB	1:B:371:HIS:CD2	3.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:VAL:O	1:C:110:VAL:HG12	2.19	0.42
1:D:112:GLY:O	1:D:116:TYR:HD1	2.02	0.42
1:D:380:LEU:HD23	1:D:380:LEU:HA	1.70	0.42
1:B:246:VAL:HG12	1:B:250:LEU:HD12	2.00	0.42
1:C:31:ALA:CB	1:C:390:LEU:HB2	2.50	0.42
1:B:49:GLN:HE21	1:B:204:ARG:CG	2.32	0.42
1:C:117:TYR:CD1	1:C:153:LEU:HB2	2.55	0.42
1:C:172:GLN:O	1:C:173:ALA:C	2.61	0.42
1:C:256:ARG:HD3	1:C:256:ARG:HH11	1.53	0.42
1:D:47:TYR:CE1	1:D:240:ARG:HG3	2.55	0.42
1:D:84:GLU:HB2	5:D:446:HOH:O	2.19	0.42
1:D:88:LEU:CD1	1:D:89:GLN:N	2.80	0.42
1:D:252:LYS:CG	1:D:257:GLU:HB2	2.50	0.42
1:D:322:CYS:HA	1:D:323:PRO:HD2	1.77	0.42
1:D:329:VAL:HG12	1:D:330:GLU:N	2.34	0.42
1:A:152:PHE:O	1:A:155:GLN:HB2	2.20	0.41
1:A:293:ALA:O	1:A:297:ARG:HB3	2.20	0.41
1:B:99:LEU:N	1:B:115:GLN:OE1	2.53	0.41
1:C:4:LEU:HG	1:C:377:THR:HG23	2.02	0.41
1:C:341:SER:O	1:C:342:ARG:HB3	2.20	0.41
1:D:184:ILE:HG22	1:D:188:PHE:CD1	2.55	0.41
1:A:34:ALA:HA	1:A:35:PRO:HD3	1.92	0.41
1:A:113:VAL:CG1	1:A:149:THR:HG22	2.50	0.41
1:A:239:ARG:O	1:A:240:ARG:C	2.63	0.41
1:A:270:VAL:O	1:A:271:SER:C	2.63	0.41
1:A:361:ALA:N	1:A:362:PRO:CD	2.83	0.41
1:C:7:PRO:HB2	1:C:12:LEU:HG	2.02	0.41
1:C:10:ALA:O	1:C:13:LEU:N	2.52	0.41
1:C:122:LEU:HA	1:C:123:PRO:HD2	1.74	0.41
1:C:192:MSE:CB	1:C:199:LEU:HD21	2.50	0.41
1:C:261:GLU:CD	1:C:286:ARG:HH22	2.27	0.41
1:C:295:LEU:HD12	1:C:295:LEU:HA	1.63	0.41
1:D:12:LEU:HD23	1:D:12:LEU:HA	1.64	0.41
1:D:260:LEU:HB3	1:D:261:GLU:OE1	2.21	0.41
1:A:227:VAL:HG12	1:A:228:ARG:N	2.35	0.41
1:C:184:ILE:H	1:C:184:ILE:HG12	1.67	0.41
1:C:260:LEU:HD12	1:C:260:LEU:HA	1.86	0.41
1:D:238:VAL:HG12	1:D:242:GLN:HE21	1.85	0.41
1:D:286:ARG:O	1:D:287:ARG:C	2.61	0.41
1:D:314:LEU:O	1:D:319:GLU:N	2.44	0.41
1:A:361:ALA:O	1:A:364:ALA:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:MSE:HE1	5:B:479:HOH:O	2.21	0.41
1:B:117:TYR:OH	1:B:154:GLN:HA	2.21	0.41
1:B:199:LEU:HD11	1:B:210:LEU:CD2	2.51	0.41
1:B:205:SER:C	1:B:207:GLU:H	2.28	0.41
1:C:175:HIS:CD2	1:C:181:PRO:HA	2.55	0.41
1:C:193:GLY:O	1:C:386:GLY:N	2.53	0.41
1:A:140:SER:N	4:A:395:ANP:O3G	2.50	0.41
1:A:343:MSE:CE	1:A:347:GLY:HA2	2.50	0.41
1:B:12:LEU:O	1:B:13:LEU:C	2.64	0.41
1:B:295:LEU:HD22	1:B:303:PHE:CE1	2.56	0.41
1:B:321:SER:OG	1:B:326:ASP:OD1	2.30	0.41
1:B:77:THR:CG2	1:B:78:THR:N	2.83	0.41
1:D:320:VAL:O	1:D:348:PHE:N	2.52	0.41
1:D:332:ALA:O	1:D:333:LEU:C	2.63	0.41
1:A:262:GLU:O	1:A:265:ALA:HB3	2.20	0.41
1:B:98:SER:O	1:B:99:LEU:C	2.64	0.41
1:B:166:ARG:O	1:B:169:VAL:HB	2.20	0.41
1:B:184:ILE:HG22	1:B:188:PHE:CD1	2.55	0.41
1:C:8:GLN:N	1:C:11:GLU:HG3	2.36	0.41
1:C:20:PHE:CD2	1:C:28:PRO:HB3	2.56	0.41
1:C:189:ILE:HD12	1:C:189:ILE:HA	1.70	0.41
1:D:30:LEU:O	1:D:65:GLY:N	2.45	0.41
1:D:77:THR:CG2	1:D:78:THR:N	2.83	0.41
1:D:211:VAL:HA	1:D:212:PRO:HD2	1.57	0.41
1:A:12:LEU:HD12	1:A:12:LEU:HA	1.85	0.41
1:A:343:MSE:HE1	1:A:347:GLY:HA2	2.01	0.41
1:B:276:ARG:O	1:B:317:ASP:HB3	2.20	0.41
1:B:281:VAL:O	1:B:282:VAL:C	2.63	0.41
1:C:205:SER:O	1:C:206:LEU:HB2	2.20	0.41
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.89	0.41
1:A:53:LEU:N	1:A:54:PRO:CD	2.84	0.41
1:A:76:LEU:HD12	1:A:77:THR:N	2.36	0.41
1:A:113:VAL:HG11	1:A:149:THR:HG22	2.02	0.41
1:A:205:SER:O	1:A:206:LEU:HB2	2.20	0.41
1:B:63:LEU:HD12	1:B:129:VAL:HG22	2.02	0.41
1:B:184:ILE:HD12	1:B:184:ILE:H	1.85	0.41
1:B:239:ARG:HB3	1:B:318:TYR:CE2	2.54	0.41
1:B:325:LEU:HD23	1:B:325:LEU:HA	1.83	0.41
1:C:4:LEU:HD21	1:C:377:THR:HG23	2.03	0.41
1:C:61:THR:HA	1:C:130:VAL:O	2.20	0.41
1:C:78:THR:HG22	1:C:78:THR:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:SER:HA	1:D:61:THR:O	2.21	0.41
1:D:49:GLN:HB3	1:D:49:GLN:HE21	1.44	0.41
1:D:87:ARG:NH1	1:D:87:ARG:CG	2.79	0.41
1:D:99:LEU:HD23	1:D:99:LEU:HA	1.89	0.41
1:D:221:LEU:HD12	1:D:222:ILE:N	2.36	0.41
1:D:382:GLN:HE21	1:D:382:GLN:HB3	1.63	0.41
1:A:13:LEU:O	1:A:16:ALA:N	2.54	0.41
1:A:250:LEU:CD2	1:A:266:ALA:HB2	2.51	0.41
1:B:93:PRO:HA	1:B:97:ARG:CG	2.36	0.41
1:B:169:VAL:O	1:B:170:CYS:C	2.60	0.41
1:D:188:PHE:O	1:D:189:ILE:C	2.64	0.41
1:B:254:SER:O	1:B:257:GLU:HB2	2.21	0.40
1:B:307:MSE:HB3	1:B:342:ARG:HG2	2.03	0.40
1:C:20:PHE:CE2	1:C:28:PRO:HA	2.56	0.40
1:D:4:LEU:HD22	1:D:377:THR:HG22	2.02	0.40
1:D:20:PHE:CD1	1:D:128:VAL:CG2	3.03	0.40
1:D:59:LEU:HD11	1:D:379:TYR:CE2	2.56	0.40
1:D:261:GLU:N	1:D:261:GLU:CD	2.80	0.40
1:A:39:ASN:HD22	1:A:40:LEU:N	2.19	0.40
1:B:77:THR:HG22	1:B:79:SER:N	2.18	0.40
1:C:32:VAL:C	1:C:390:LEU:HD12	2.46	0.40
1:C:42:GLY:O	1:C:52:VAL:HG12	2.21	0.40
1:C:202:ASP:CG	1:C:256:ARG:HH12	2.27	0.40
1:C:372:TYR:HD1	5:C:497:HOH:O	2.03	0.40
1:D:70:ASP:OD2	1:D:70:ASP:N	2.54	0.40
1:D:315:ARG:NH1	5:D:418:HOH:O	2.51	0.40
1:D:328:LEU:HD21	1:D:372:TYR:CD1	2.56	0.40
1:A:135:LEU:N	1:A:135:LEU:HD23	2.36	0.40
1:A:250:LEU:CD2	1:A:266:ALA:CB	2.98	0.40
1:A:259:GLN:O	1:A:261:GLU:N	2.54	0.40
1:B:80:GLU:C	1:B:82:ALA:N	2.80	0.40
1:B:153:LEU:CD2	1:B:156:LEU:CD1	2.98	0.40
1:D:4:LEU:HA	1:D:4:LEU:HD12	1.59	0.40
1:D:73:VAL:O	1:D:89:GLN:HA	2.21	0.40
1:D:122:LEU:HD12	1:D:122:LEU:HA	1.93	0.40
1:A:52:VAL:HG23	1:A:54:PRO:CD	2.52	0.40
1:A:150:TYR:CD2	1:A:150:TYR:C	3.00	0.40
1:A:331:ALA:O	1:A:332:ALA:C	2.63	0.40
1:A:335:VAL:CG1	1:A:336:PRO:HD2	2.51	0.40
1:B:29:GLU:HB3	1:B:30:LEU:HG	2.03	0.40
1:B:232:ALA:C	1:B:234:SER:N	2.80	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:PHE:CD1	1:C:128:VAL:CG2	3.04	0.40
1:C:175:HIS:O	1:C:179:GLY:HA2	2.22	0.40
1:C:195:LYS:O	1:C:197:HIS:N	2.55	0.40
1:D:276:ARG:HB3	1:D:317:ASP:OD1	2.20	0.40
1:A:10:ALA:O	1:A:11:GLU:C	2.65	0.40
1:B:81:GLY:C	1:B:135:LEU:HD12	2.46	0.40
1:B:85:PRO:HD2	1:B:104:PRO:HG3	2.04	0.40
1:B:146:GLU:HB3	1:B:170:CYS:HB3	2.04	0.40
1:C:157:CYS:O	1:C:157:CYS:SG	2.80	0.40
1:C:232:ALA:C	1:C:234:SER:N	2.80	0.40
1:C:343:MSE:CE	1:C:347:GLY:HA2	2.51	0.40
1:D:59:LEU:HD23	1:D:59:LEU:HA	1.83	0.40
1:D:361:ALA:N	1:D:362:PRO:CD	2.85	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	387/399 (97%)	326 (84%)	52 (13%)	9 (2%)	5	8
1	B	386/399 (97%)	320 (83%)	50 (13%)	16 (4%)	2	3
1	C	386/399 (97%)	331 (86%)	42 (11%)	13 (3%)	3	4
1	D	387/399 (97%)	319 (82%)	52 (13%)	16 (4%)	2	3
All	All	1546/1596 (97%)	1296 (84%)	196 (13%)	54 (4%)	3	4

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	271	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	18	ARG
1	B	115	GLN
1	B	158	PRO
1	B	246	VAL
1	C	83	ASP
1	C	99	LEU
1	C	185	MSE
1	D	265	ALA
1	A	161	GLY
1	A	196	GLY
1	A	244	GLU
1	A	250	LEU
1	B	22	GLU
1	B	249	ALA
1	C	195	LYS
1	C	233	SER
1	D	9	VAL
1	D	285	ILE
1	A	46	ASP
1	A	260	LEU
1	B	123	PRO
1	B	248	ARG
1	C	10	ALA
1	C	186	ASP
1	D	158	PRO
1	D	281	VAL
1	D	359	SER
1	A	181	PRO
1	B	10	ALA
1	B	13	LEU
1	B	185	MSE
1	B	245	GLU
1	C	22	GLU
1	C	96	GLN
1	C	123	PRO
1	D	96	GLN
1	D	188	PHE
1	D	264	GLU
1	D	273	GLU
1	B	149	THR
1	D	323	PRO
1	D	358	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	369	GLN
1	B	233	SER
1	D	95	ALA
1	D	361	ALA
1	C	236	TYR
1	D	282	VAL
1	B	41	ILE
1	B	193	GLY
1	C	196	GLY
1	C	9	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	309/308 (100%)	258 (84%)	51 (16%)	2	4
1	B	307/308 (100%)	249 (81%)	58 (19%)	1	3
1	C	307/308 (100%)	266 (87%)	41 (13%)	4	8
1	D	309/308 (100%)	251 (81%)	58 (19%)	1	3
All	All	1232/1232 (100%)	1024 (83%)	208 (17%)	2	4

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	5	ARG
1	A	6	GLN
1	A	12	LEU
1	A	32	VAL
1	A	43	GLU
1	A	46	ASP
1	A	49	GLN
1	A	55	MSE
1	A	63	LEU
1	A	74	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	75	LEU
1	A	86	GLN
1	A	89	GLN
1	A	97	ARG
1	A	103	THR
1	A	105	ARG
1	A	132	SER
1	A	135	LEU
1	A	140	SER
1	A	163	ILE
1	A	176	SER
1	A	184	ILE
1	A	188	PHE
1	A	192	MSE
1	A	199	LEU
1	A	206	LEU
1	A	207	GLU
1	A	213	LEU
1	A	234	SER
1	A	248	ARG
1	A	250	LEU
1	A	252	LYS
1	A	257	GLU
1	A	270	VAL
1	A	271	SER
1	A	286	ARG
1	A	287	ARG
1	A	290	GLN
1	A	297	ARG
1	A	306	LEU
1	A	312	ARG
1	A	313	SER
1	A	326	ASP
1	A	342	ARG
1	A	355	LEU
1	A	356	LEU
1	A	366	ARG
1	A	370	GLU
1	A	390	LEU
1	A	391	CYS
1	B	6	GLN
1	B	13	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	17	ARG
1	B	27	GLU
1	B	37	ARG
1	B	49	GLN
1	B	55	MSE
1	B	63	LEU
1	B	68	ARG
1	B	69	LYS
1	B	75	LEU
1	B	76	LEU
1	B	79	SER
1	B	87	ARG
1	B	88	LEU
1	B	89	GLN
1	B	92	LEU
1	B	97	ARG
1	B	98	SER
1	B	100	GLU
1	B	105	ARG
1	B	122	LEU
1	B	128	VAL
1	B	140	SER
1	B	153	LEU
1	B	156	LEU
1	B	159	ASP
1	B	160	SER
1	B	163	ILE
1	B	166	ARG
1	B	188	PHE
1	B	191	LEU
1	B	194	GLN
1	B	195	LYS
1	B	199	LEU
1	B	201	ILE
1	B	204	ARG
1	B	206	LEU
1	B	217	LYS
1	B	218	LEU
1	B	222	ILE
1	B	234	SER
1	B	248	ARG
1	B	250	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	252	LYS
1	B	258	VAL
1	B	263	LEU
1	B	264	GLU
1	B	271	SER
1	B	315	ARG
1	B	326	ASP
1	B	342	ARG
1	B	355	LEU
1	B	356	LEU
1	B	359	SER
1	B	382	GLN
1	B	385	ASP
1	B	392	LEU
1	C	1	HIS
1	C	4	LEU
1	C	6	GLN
1	C	8	GLN
1	C	11	GLU
1	C	29	GLU
1	C	30	LEU
1	C	37	ARG
1	C	63	LEU
1	C	64	VAL
1	C	68	ARG
1	C	69	LYS
1	C	72	LEU
1	C	73	VAL
1	C	75	LEU
1	C	89	GLN
1	C	97	ARG
1	C	99	LEU
1	C	106	TRP
1	C	133	VAL
1	C	142	SER
1	C	145	LEU
1	C	154	GLN
1	C	157	CYS
1	C	163	ILE
1	C	187	GLN
1	C	194	GLN
1	C	209	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	214	SER
1	C	217	LYS
1	C	228	ARG
1	C	234	SER
1	C	248	ARG
1	C	250	LEU
1	C	252	LYS
1	C	261	GLU
1	C	271	SER
1	C	272	LYS
1	C	312	ARG
1	C	356	LEU
1	C	382	GLN
1	D	1	HIS
1	D	4	LEU
1	D	11	GLU
1	D	29	GLU
1	D	39	ASN
1	D	40	LEU
1	D	43	GLU
1	D	49	GLN
1	D	55	MSE
1	D	66	SER
1	D	70	ASP
1	D	72	LEU
1	D	78	THR
1	D	83	ASP
1	D	86	GLN
1	D	87	ARG
1	D	89	GLN
1	D	97	ARG
1	D	100	GLU
1	D	103	THR
1	D	169	VAL
1	D	180	MSE
1	D	184	ILE
1	D	187	GLN
1	D	192	MSE
1	D	194	GLN
1	D	195	LYS
1	D	199	LEU
1	D	200	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	204	ARG
1	D	217	LYS
1	D	218	LEU
1	D	233	SER
1	D	234	SER
1	D	240	ARG
1	D	246	VAL
1	D	248	ARG
1	D	250	LEU
1	D	255	LEU
1	D	260	LEU
1	D	262	GLU
1	D	264	GLU
1	D	272	LYS
1	D	277	ARG
1	D	279	ARG
1	D	290	GLN
1	D	306	LEU
1	D	312	ARG
1	D	313	SER
1	D	318	TYR
1	D	322	CYS
1	D	341	SER
1	D	342	ARG
1	D	343	MSE
1	D	356	LEU
1	D	375	THR
1	D	381	SER
1	D	382	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	39	ASN
1	A	48	ASN
1	A	49	GLN
1	A	115	GLN
1	A	175	HIS
1	A	327	GLN
1	A	369	GLN
1	A	371	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	382	GLN
1	B	8	GLN
1	B	39	ASN
1	B	49	GLN
1	B	89	GLN
1	B	154	GLN
1	B	171	GLN
1	B	327	GLN
1	B	367	HIS
1	B	371	HIS
1	B	382	GLN
1	C	39	ASN
1	C	49	GLN
1	C	86	GLN
1	C	89	GLN
1	C	154	GLN
1	C	155	GLN
1	C	187	GLN
1	C	194	GLN
1	C	259	GLN
1	C	369	GLN
1	C	371	HIS
1	C	382	GLN
1	D	39	ASN
1	D	49	GLN
1	D	187	GLN
1	D	194	GLN
1	D	197	HIS
1	D	226	ASN
1	D	259	GLN
1	D	371	HIS
1	D	382	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLA	B	393	-	12,12,12	0.55	0	17,17,17	1.44	4 (23%)
4	ANP	D	395	3	33,33,33	1.34	4 (12%)	45,52,52	1.31	4 (8%)
4	ANP	B	395	3	33,33,33	1.44	6 (18%)	45,52,52	1.44	8 (17%)
2	GLA	A	393	-	12,12,12	0.66	0	17,17,17	1.08	0
2	GLA	C	393	-	12,12,12	0.54	0	17,17,17	1.09	1 (5%)
2	GLA	D	393	-	12,12,12	0.52	0	17,17,17	1.04	0
4	ANP	C	395	3	33,33,33	1.42	6 (18%)	45,52,52	1.52	7 (15%)
4	ANP	A	395	3	33,33,33	1.38	6 (18%)	45,52,52	1.51	7 (15%)

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	GLA	B	393	-	-	1/2/22/22	0/1/1/1
4	ANP	D	395	3	-	8/18/38/38	0/3/3/3
4	ANP	B	395	3	-	6/18/38/38	0/3/3/3
2	GLA	A	393	-	-	1/2/22/22	0/1/1/1
2	GLA	C	393	-	-	1/2/22/22	0/1/1/1
2	GLA	D	393	-	-	1/2/22/22	0/1/1/1
4	ANP	C	395	3	-	8/18/38/38	0/3/3/3
4	ANP	A	395	3	-	10/18/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	395	ANP	C6-N6	-3.66	1.24	1.34
4	D	395	ANP	C6-N6	-3.60	1.25	1.34
4	B	395	ANP	C6-N6	-3.51	1.25	1.34
4	C	395	ANP	C6-N6	-3.36	1.25	1.34
4	C	395	ANP	PG-O2G	-3.26	1.48	1.56
4	C	395	ANP	PB-O2B	-3.23	1.48	1.56
4	B	395	ANP	PB-O1B	3.15	1.51	1.46
4	D	395	ANP	PG-O1G	3.04	1.50	1.46
4	D	395	ANP	PB-O1B	2.95	1.50	1.46
4	C	395	ANP	PG-O1G	2.82	1.50	1.46
4	B	395	ANP	PG-O1G	2.78	1.50	1.46
4	A	395	ANP	C2-N3	-2.65	1.29	1.33
4	B	395	ANP	O4'-C1'	-2.57	1.36	1.42
4	D	395	ANP	PG-O2G	-2.57	1.50	1.56
4	A	395	ANP	PB-O1B	2.52	1.50	1.46
4	A	395	ANP	PB-O2B	-2.42	1.50	1.56
4	B	395	ANP	C2-N3	-2.41	1.29	1.33
4	A	395	ANP	PG-O1G	2.25	1.49	1.46
4	C	395	ANP	PB-O1B	2.17	1.49	1.46
4	A	395	ANP	PG-O2G	-2.15	1.51	1.56
4	B	395	ANP	C2-N1	2.05	1.37	1.33
4	C	395	ANP	C2-N3	-2.02	1.30	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	395	ANP	C2-N1-C6	4.95	126.86	118.73
4	A	395	ANP	C2-N1-C6	4.67	126.40	118.73
4	B	395	ANP	C2-N1-C6	4.55	126.20	118.73
4	D	395	ANP	C2-N1-C6	4.48	126.10	118.73
4	A	395	ANP	O1B-PB-N3B	-4.43	105.25	111.77
4	C	395	ANP	O1B-PB-N3B	-4.11	105.72	111.77
4	D	395	ANP	N3-C2-N1	-3.66	123.03	128.58
4	B	395	ANP	N3-C2-N1	-3.50	123.28	128.58
4	D	395	ANP	O1B-PB-N3B	-3.18	107.08	111.77
4	C	395	ANP	N3-C2-N1	-3.13	123.84	128.58
4	B	395	ANP	O1G-PG-N3B	-3.04	107.30	111.77
4	A	395	ANP	N3-C2-N1	-3.00	124.05	128.58
2	C	393	GLA	O3-C3-C4	-2.93	103.47	110.38
4	A	395	ANP	C5-C6-N1	-2.93	110.08	117.51
4	C	395	ANP	C5-C6-N1	-2.89	110.17	117.51
2	B	393	GLA	O2-C2-C1	2.85	115.82	109.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	395	ANP	O3G-PG-O1G	-2.50	107.17	113.45
2	B	393	GLA	O3-C3-C2	-2.49	104.50	110.38
4	C	395	ANP	N6-C6-N1	2.45	123.83	118.38
4	C	395	ANP	C2'-C3'-C4'	-2.40	97.97	102.61
4	A	395	ANP	N6-C6-N1	2.35	123.60	118.38
4	A	395	ANP	O1G-PG-N3B	-2.33	108.34	111.77
2	B	393	GLA	O2-C2-C3	-2.28	105.01	110.38
4	B	395	ANP	C5-C6-N1	-2.27	111.75	117.51
4	D	395	ANP	C5-C6-N1	-2.27	111.75	117.51
4	A	395	ANP	O3G-PG-O1G	-2.23	107.86	113.45
4	B	395	ANP	O2B-PB-O3A	2.19	111.95	104.64
2	B	393	GLA	C3-C4-C5	-2.18	106.28	110.23
4	B	395	ANP	C2'-C3'-C4'	-2.17	98.41	102.61
4	C	395	ANP	O3G-PG-O1G	-2.09	108.21	113.45
4	B	395	ANP	O2G-PG-O3G	2.07	113.15	107.59

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	395	ANP	PB-N3B-PG-O1G
4	A	395	ANP	PA-O3A-PB-O2B
4	A	395	ANP	C5'-O5'-PA-O2A
4	A	395	ANP	O4'-C4'-C5'-O5'
4	B	395	ANP	C5'-O5'-PA-O2A
4	C	395	ANP	PB-N3B-PG-O1G
4	D	395	ANP	PB-N3B-PG-O1G
4	D	395	ANP	C5'-O5'-PA-O2A
4	D	395	ANP	O4'-C4'-C5'-O5'
4	D	395	ANP	C3'-C4'-C5'-O5'
4	A	395	ANP	C3'-C4'-C5'-O5'
2	A	393	GLA	O5-C5-C6-O6
2	D	393	GLA	O5-C5-C6-O6
4	B	395	ANP	O4'-C4'-C5'-O5'
2	B	393	GLA	O5-C5-C6-O6
2	C	393	GLA	O5-C5-C6-O6
4	B	395	ANP	C3'-C4'-C5'-O5'
4	B	395	ANP	PG-N3B-PB-O3A
4	A	395	ANP	C5'-O5'-PA-O1A
4	A	395	ANP	C5'-O5'-PA-O3A
4	B	395	ANP	C5'-O5'-PA-O1A
4	B	395	ANP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

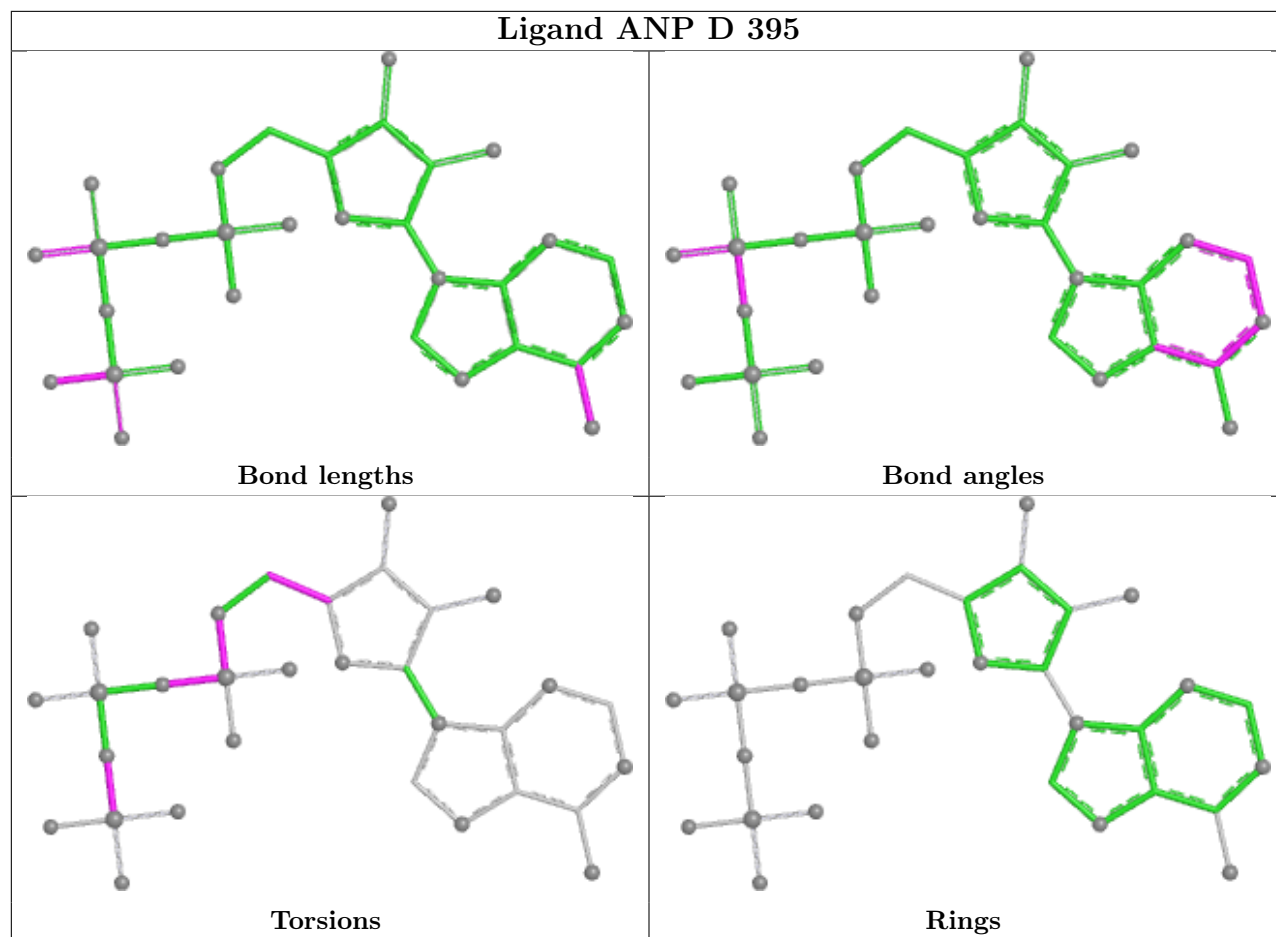
Mol	Chain	Res	Type	Atoms
4	C	395	ANP	C5'-O5'-PA-O1A
4	C	395	ANP	C5'-O5'-PA-O2A
4	C	395	ANP	C5'-O5'-PA-O3A
4	D	395	ANP	C5'-O5'-PA-O1A
4	D	395	ANP	C5'-O5'-PA-O3A
4	A	395	ANP	PB-O3A-PA-O2A
4	D	395	ANP	PB-O3A-PA-O2A
4	C	395	ANP	C3'-C4'-C5'-O5'
4	C	395	ANP	PA-O3A-PB-O2B
4	D	395	ANP	PB-O3A-PA-O1A
4	A	395	ANP	PA-O3A-PB-O1B
4	C	395	ANP	PA-O3A-PB-O1B
4	A	395	ANP	PB-O3A-PA-O1A
4	C	395	ANP	PB-O3A-PA-O1A

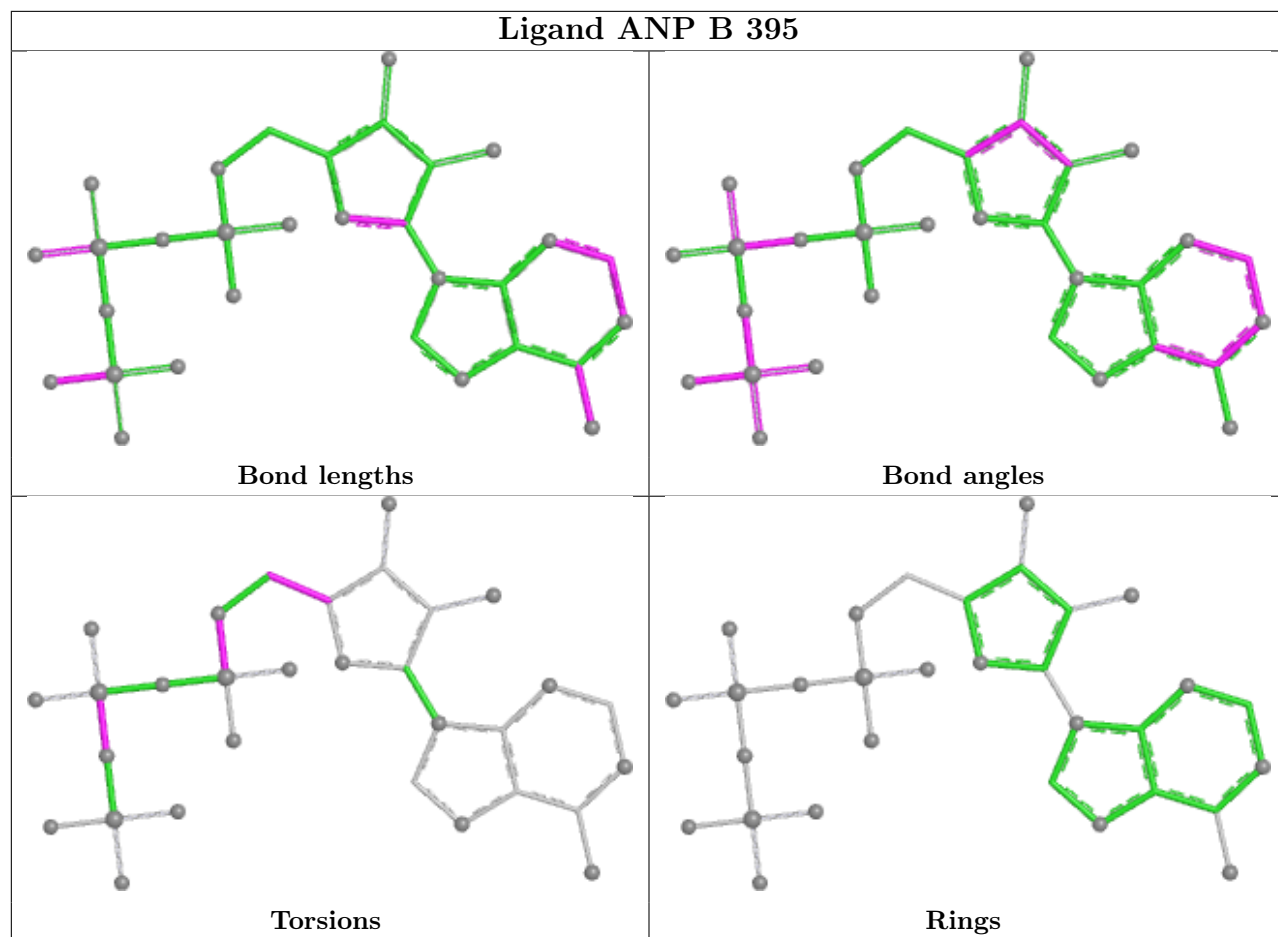
There are no ring outliers.

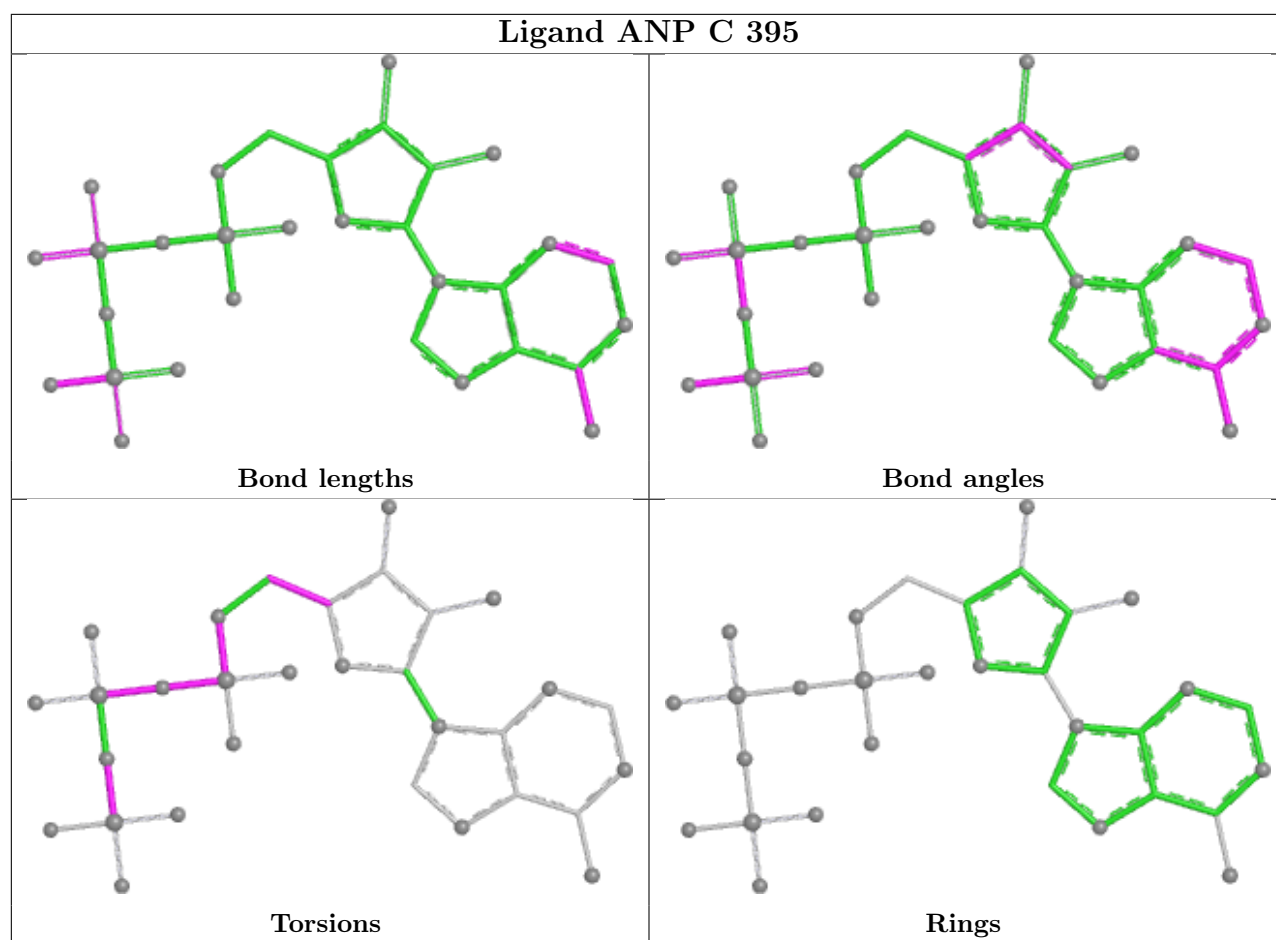
7 monomers are involved in 28 short contacts:

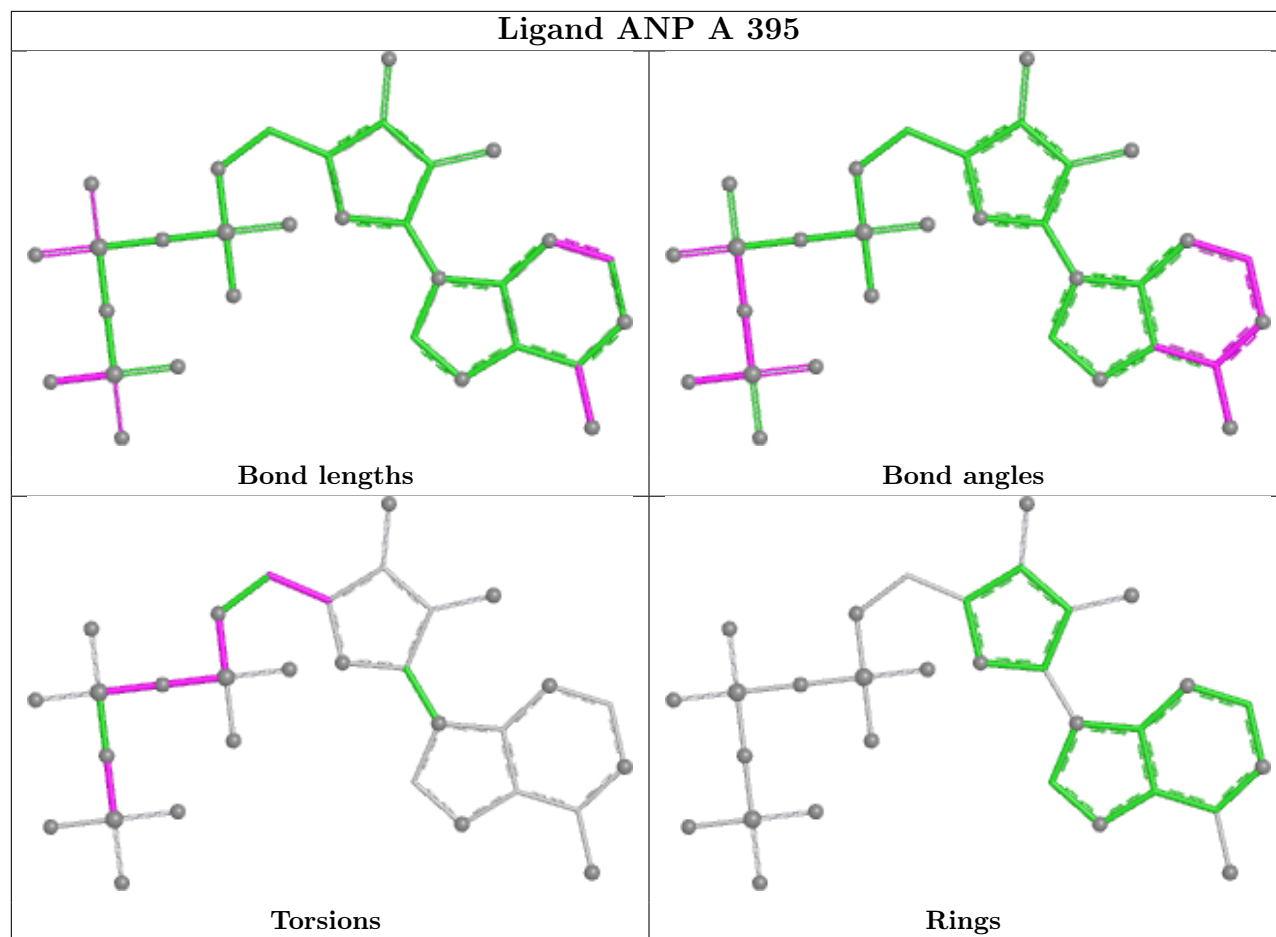
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	395	ANP	3	0
4	B	395	ANP	7	0
2	A	393	GLA	2	0
2	C	393	GLA	1	0
2	D	393	GLA	1	0
4	C	395	ANP	8	0
4	A	395	ANP	6	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	383/399 (95%)	-0.13	3 (0%) 82 80	22, 41, 69, 84	0
1	B	382/399 (95%)	0.06	4 (1%) 79 76	19, 48, 76, 93	0
1	C	382/399 (95%)	-0.15	3 (0%) 82 80	15, 40, 73, 90	0
1	D	382/399 (95%)	-0.13	3 (0%) 82 80	21, 41, 68, 88	1 (0%)
All	All	1529/1596 (95%)	-0.09	13 (0%) 81 78	15, 43, 73, 93	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	4.0
1	C	26	ALA	3.1
1	B	94	THR	3.1
1	C	86	GLN	2.8
1	D	245	GLU	2.5
1	B	99	LEU	2.4
1	B	264	GLU	2.4
1	A	219	ALA	2.2
1	A	232	ALA	2.2
1	A	157	CYS	2.1
1	D	70	ASP	2.1
1	C	327	GLN	2.1
1	D	233	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

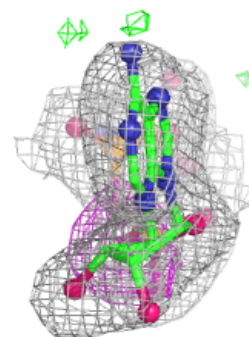
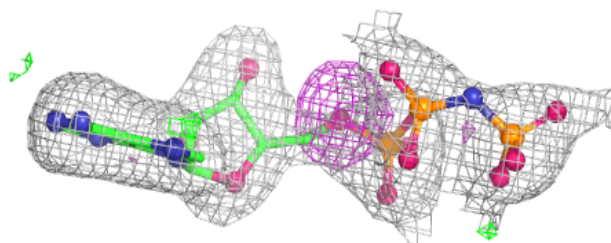
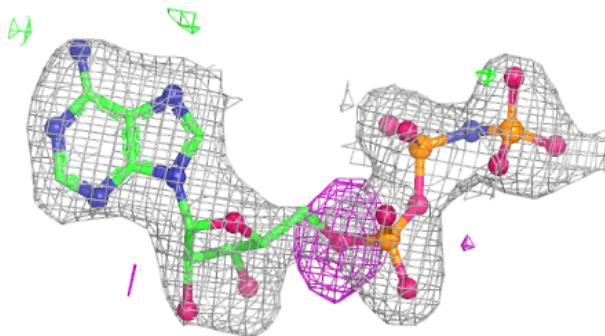
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ANP	B	395	31/31	0.89	0.10	0,44,81,94	0
3	MG	B	394	1/1	0.91	0.05	41,41,41,41	0
2	GLA	A	393	12/12	0.95	0.08	22,33,49,66	0
2	GLA	B	393	12/12	0.96	0.08	22,34,54,71	0
4	ANP	C	395	31/31	0.96	0.08	0,36,57,92	0
3	MG	D	394	1/1	0.97	0.06	27,27,27,27	0
4	ANP	A	395	31/31	0.97	0.06	19,34,50,66	0
3	MG	A	394	1/1	0.97	0.06	38,38,38,38	0
2	GLA	D	393	12/12	0.97	0.06	2,22,31,55	0
3	MG	C	394	1/1	0.98	0.04	26,26,26,26	0
4	ANP	D	395	31/31	0.98	0.06	12,26,51,80	0
2	GLA	C	393	12/12	0.99	0.06	6,19,58,80	0

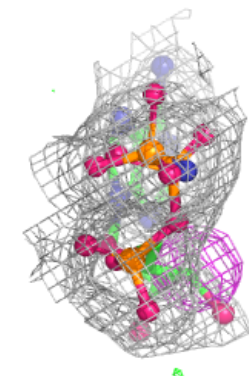
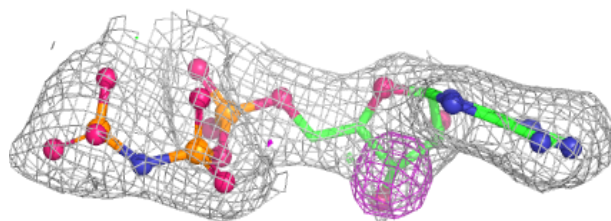
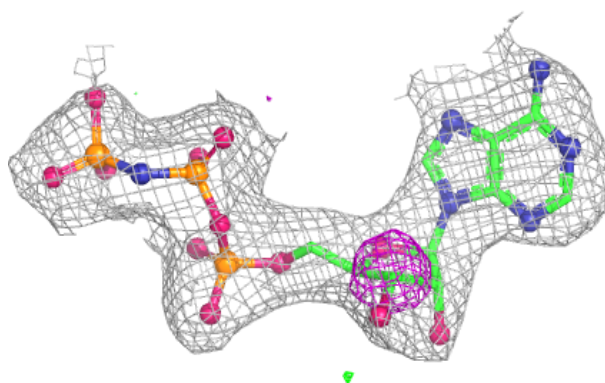
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 395:

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

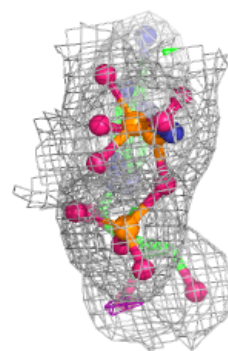
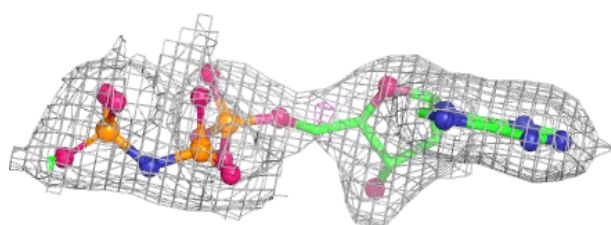
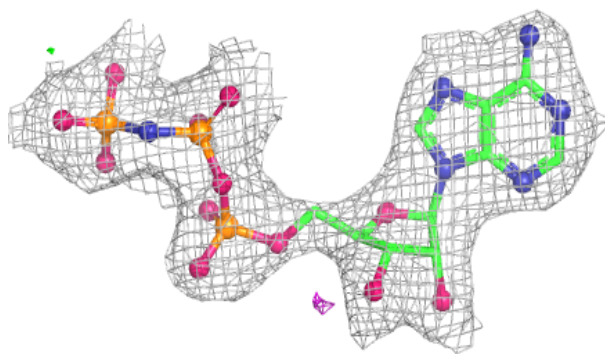
**Electron density around ANP C 395:**

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

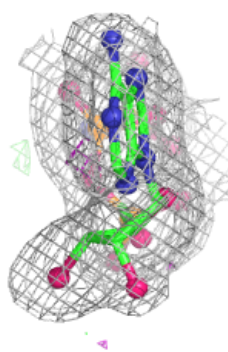
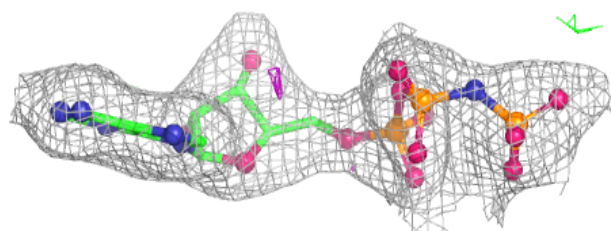
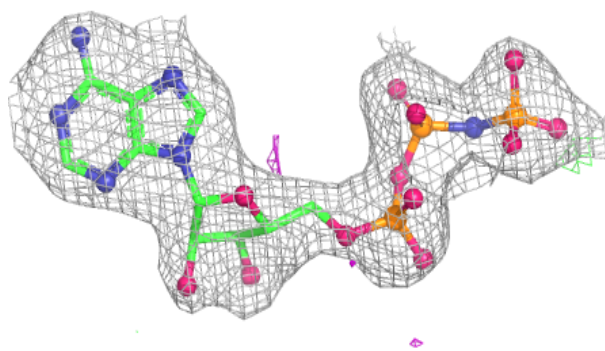


Electron density around ANP A 395:

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

**Electron density around ANP D 395:**

$2mF_o-DF_c$ (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.