Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:54 pm BST

PDB ID	:	4RB4
Title	:	Crystal structure of dodecameric iron-containing heptosyltransferase TibC in complex with ADP-D-beta-D-heptose at 3.9 angstrom resolution
Authors	:	Yao, Q.; Lu, Q.; Shao, F.
Deposited on	:	2014-09-12
Resolution	:	3.88 Å(reported)

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

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

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

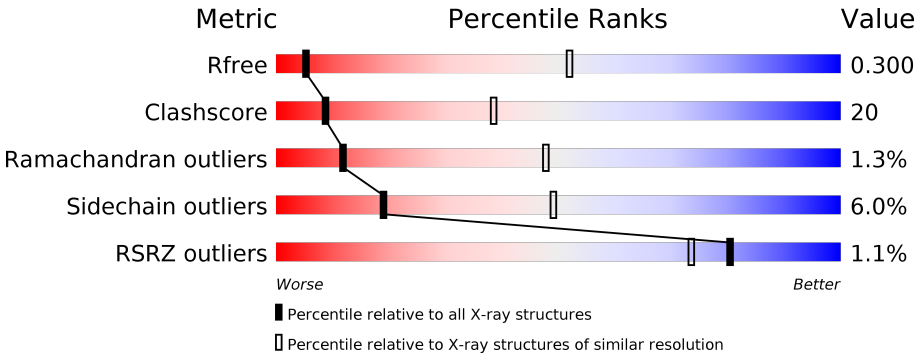
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.88 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (4.12-3.64)
Clashscore	141614	1045 (4.10-3.66)
Ramachandran outliers	138981	1008 (4.10-3.66)
Sidechain outliers	138945	1001 (4.10-3.66)
RSRZ outliers	127900	1213 (4.16-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	406	72% 17% • 6%
1	B	406	74% 16% 5% 6%
1	C	406	73% 19% • •
1	D	406	% 69% 21% • 6%
1	E	406	% 67% 24% 5% •
1	F	406	% 72% 19% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	406	2% 68% 21% 5%
1	H	406	2% 71% 19% 5%
1	I	406	% 72% 19%
1	J	406	% 72% 18% 5%
1	K	406	74% 18%
1	L	406	2% 62% 22% 8% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FE	A	501	-	-	X	-
2	FE	D	501	-	-	X	-
2	FE	G	501	-	-	-	X
2	FE	J	501	-	-	X	-
3	AQH	D	502	-	-	X	-
3	AQH	H	502	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 37611 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 Glycosyltransferase tibC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	390	Total	C	N	O	S	0	0	0
			3132	2016	546	557	13			
1	L	374	Total	C	N	O	S	0	0	0
			3008	1938	524	533	13			
1	C	389	Total	C	N	O	S	0	0	0
			3121	2007	545	556	13			
1	D	381	Total	C	N	O	S	0	0	0
			3061	1970	536	542	13			
1	E	390	Total	C	N	O	S	0	0	0
			3129	2013	546	557	13			
1	H	385	Total	C	N	O	S	0	0	0
			3093	1990	541	549	13			
1	B	383	Total	C	N	O	S	0	0	0
			3082	1987	538	544	13			
1	F	384	Total	C	N	O	S	0	0	0
			3084	1985	539	547	13			
1	G	389	Total	C	N	O	S	0	0	0
			3121	2007	545	556	13			
1	I	389	Total	C	N	O	S	0	0	0
			3121	2007	545	556	13			
1	J	385	Total	C	N	O	S	0	0	0
			3097	1996	541	547	13			
1	A	380	Total	C	N	O	S	0	0	0
			3058	1969	535	541	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	110	ALA	ASP	ENGINEERED MUTATION	UNP H5MH13
L	110	ALA	ASP	ENGINEERED MUTATION	UNP H5MH13
C	110	ALA	ASP	ENGINEERED MUTATION	UNP H5MH13
D	110	ALA	ASP	ENGINEERED MUTATION	UNP H5MH13
E	110	ALA	ASP	ENGINEERED MUTATION	UNP H5MH13

Continued on next page...

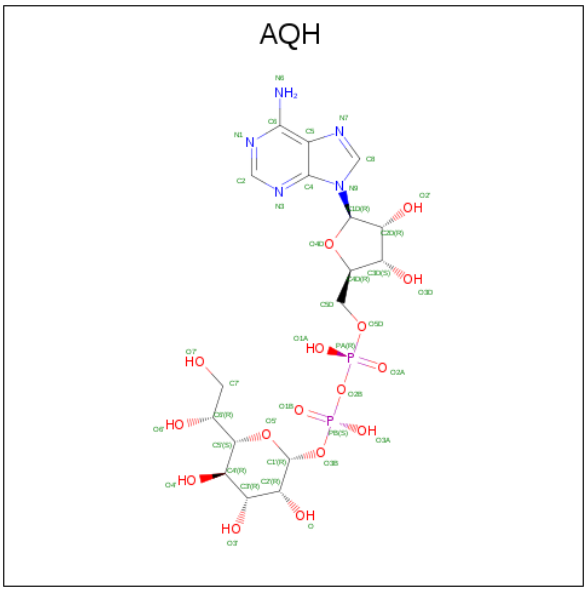
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	110	ALA	ASP	ENGINEERED MUTATION	UNP H5MH13
B	110	ALA	ASP	ENGINEERED MUTATION	UNP H5MH13
F	110	ALA	ASP	ENGINEERED MUTATION	UNP H5MH13
G	110	ALA	ASP	ENGINEERED MUTATION	UNP H5MH13
I	110	ALA	ASP	ENGINEERED MUTATION	UNP H5MH13
J	110	ALA	ASP	ENGINEERED MUTATION	UNP H5MH13
A	110	ALA	ASP	ENGINEERED MUTATION	UNP H5MH13

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

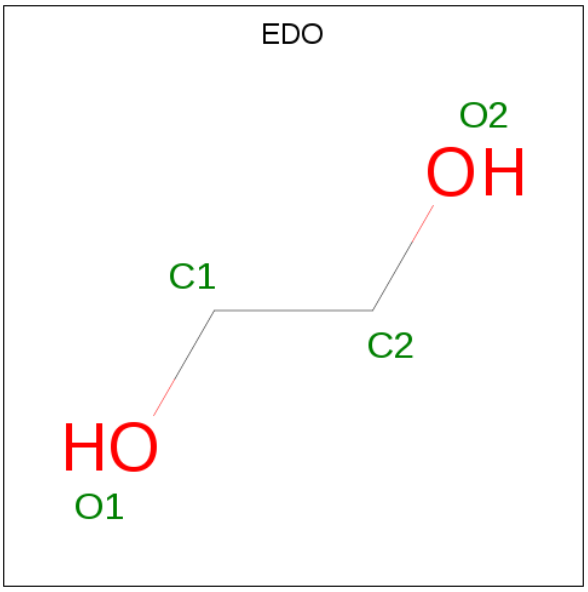
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Fe 1 1	0	0
2	J	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	K	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl] methyl (2R,3R,4R,5R,6S)-6-[(1R)-1,2-dihydroxyethyl]-3,4,5-trihydroxytetrahydro-2H-pyran-2-yl dihydrogen diphosphate (three-letter code: AQH) (formula: $C_{17}H_{27}N_5O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	K	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
3	L	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
3	C	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
3	D	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
3	E	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
3	H	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
3	B	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
3	F	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
3	G	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
3	I	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
3	J	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
3	A	1	Total	C	N	O	P	0	0
			40	17	5	16	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



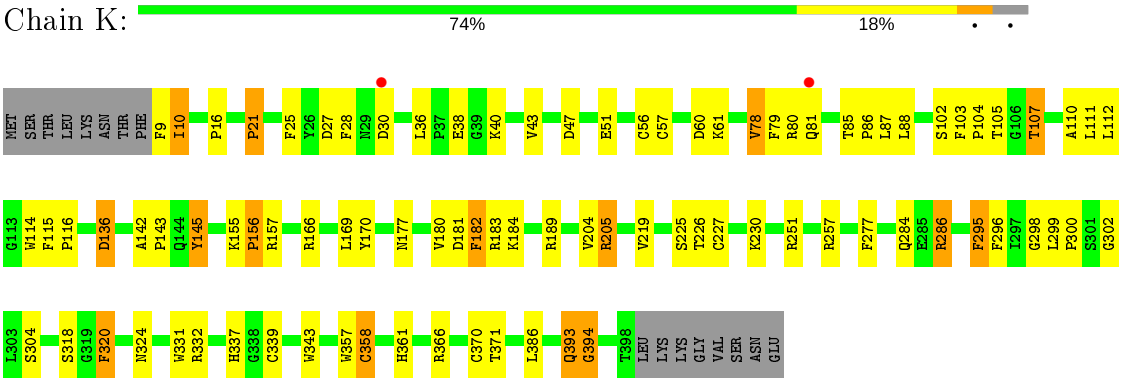
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		

3 Residue-property plots (i)

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

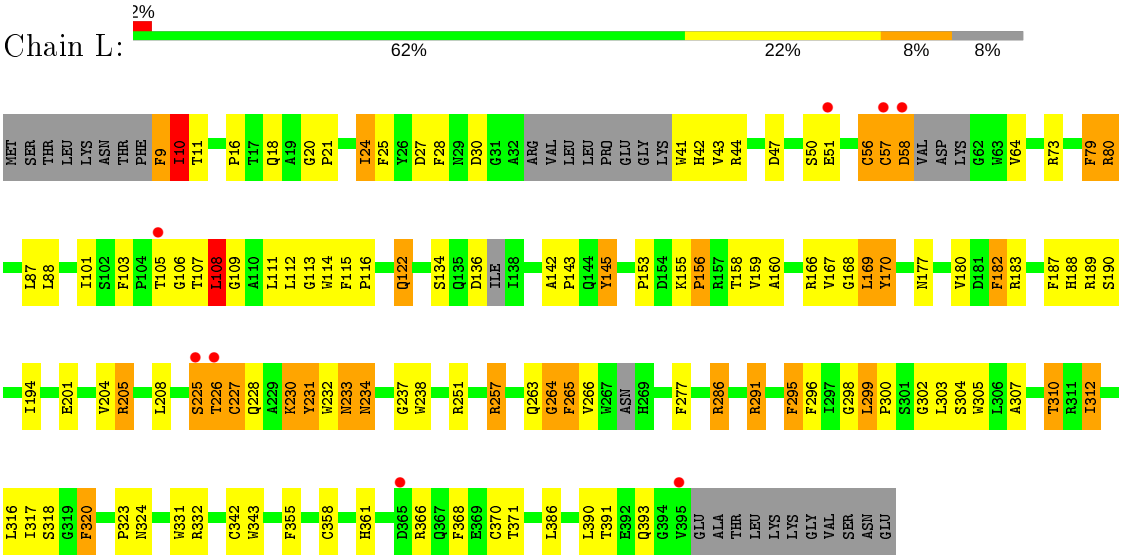
- Molecule 1: Glycosyltransferase tibC

Chain K:



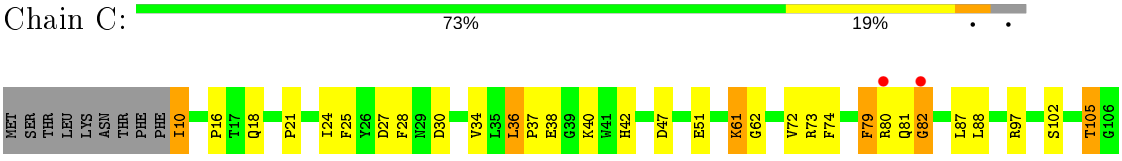
- Molecule 1: Glycosyltransferase tibC

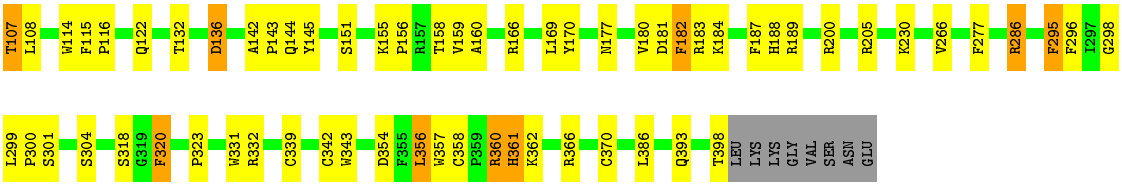
Chain L:



- Molecule 1: Glycosyltransferase tibC

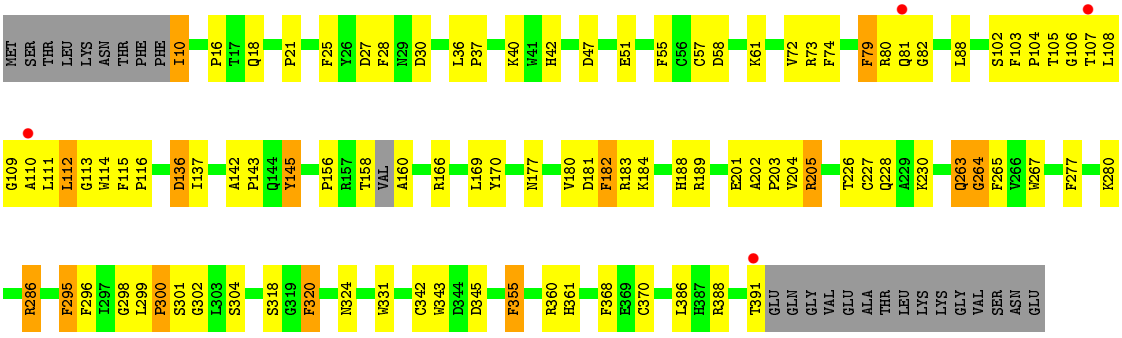
Chain C:





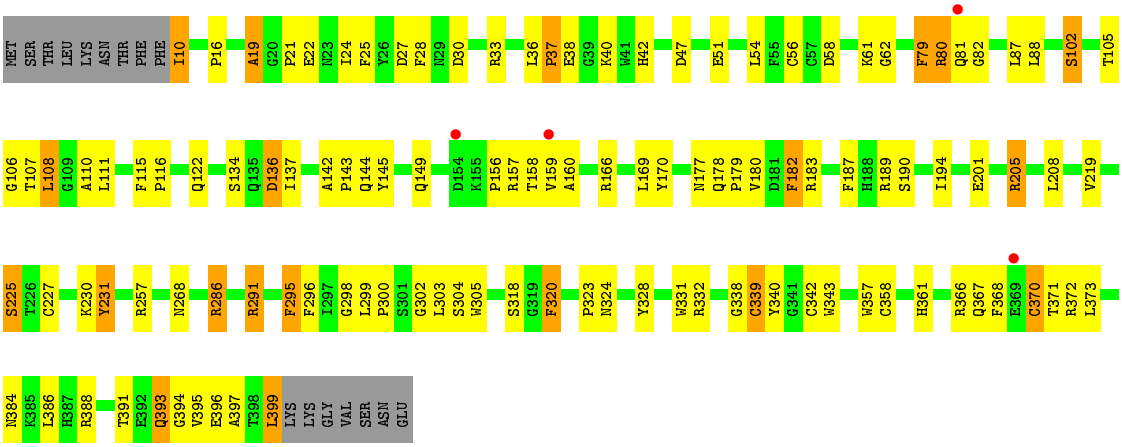
• Molecule 1: Glycosyltransferase tibC

Chain D:



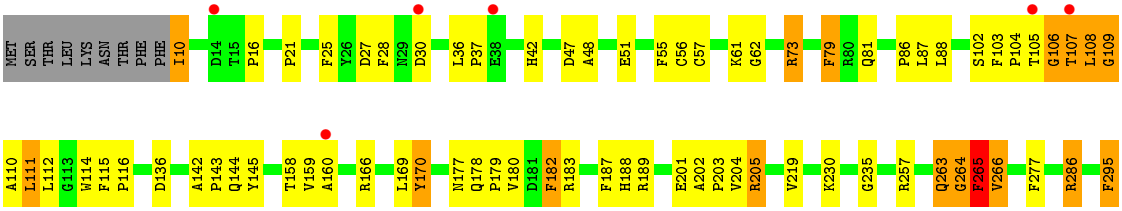
• Molecule 1: Glycosyltransferase tibC

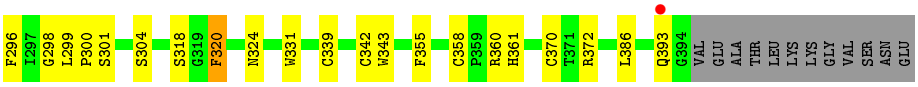
Chain E:



• Molecule 1: Glycosyltransferase tibC

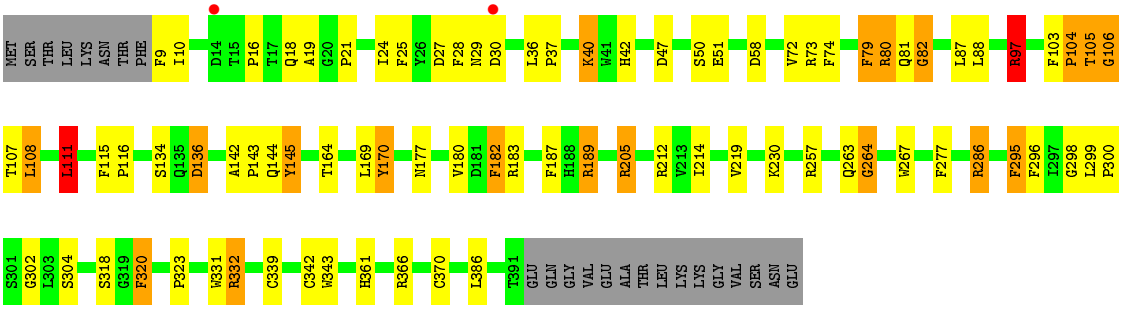
Chain H:





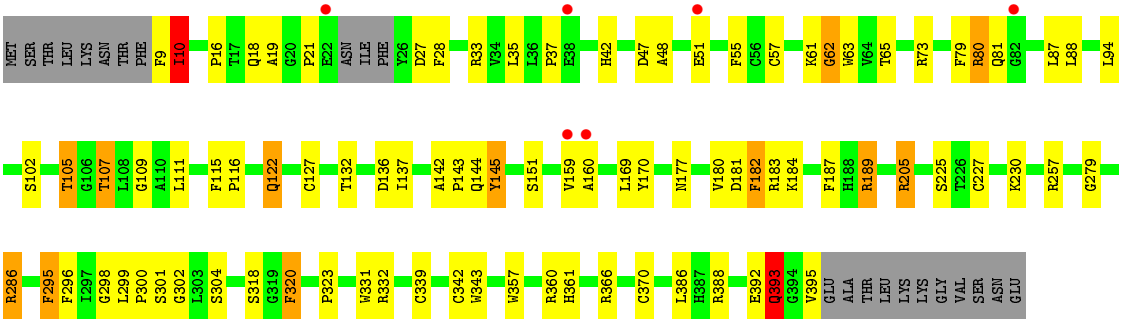
• Molecule 1: Glycosyltransferase tibC

Chain B:



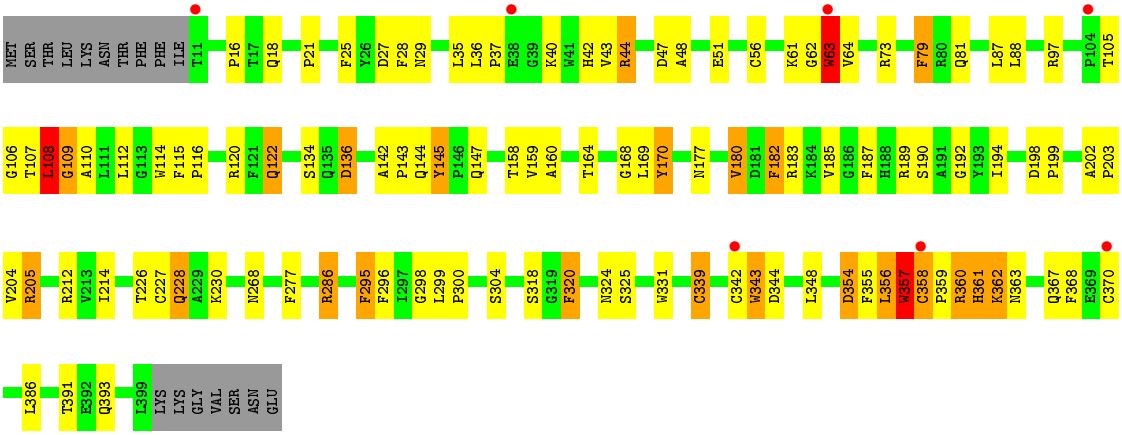
• Molecule 1: Glycosyltransferase tibC

Chain F:



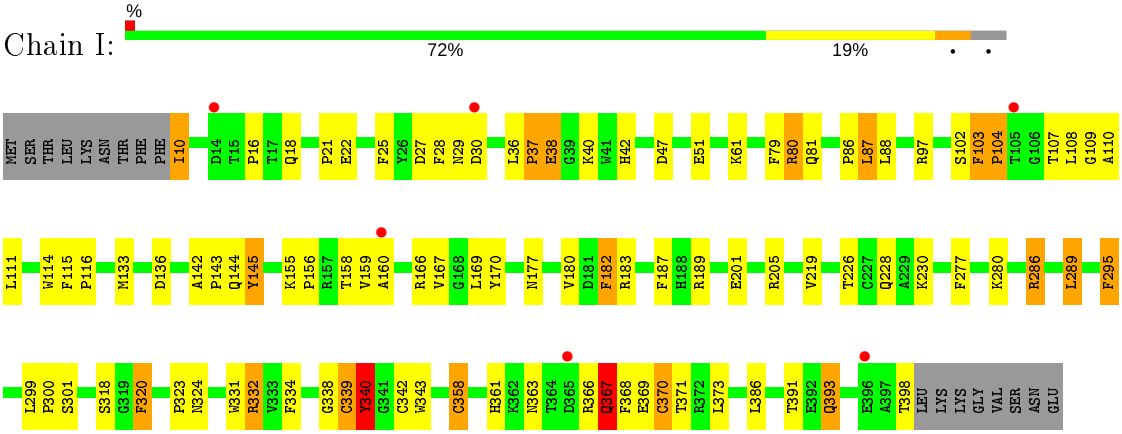
• Molecule 1: Glycosyltransferase tibC

Chain G:



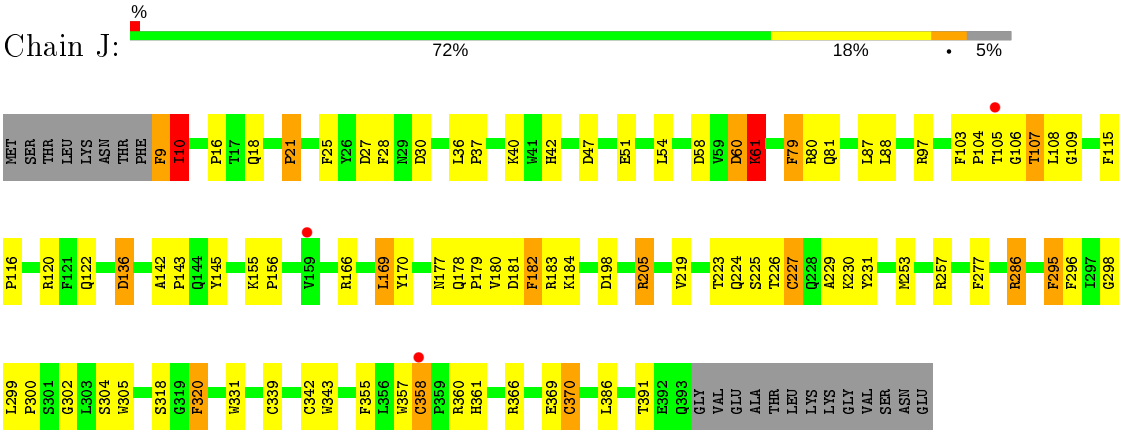
• Molecule 1: Glycosyltransferase tibC

Chain I:



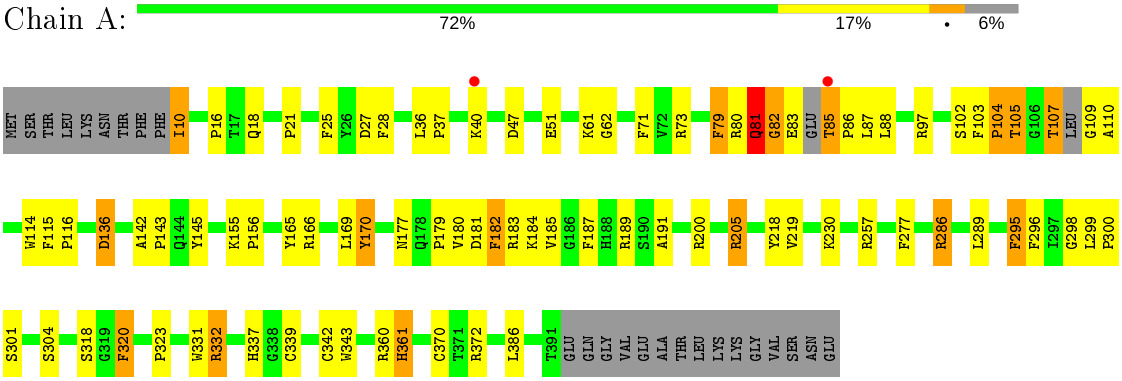
- Molecule 1: Glycosyltransferase tibC

Chain J:



- Molecule 1: Glycosyltransferase tibC

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.29Å 313.20Å 164.69Å 90.00° 101.26° 90.00°	Depositor
Resolution (Å)	20.04 – 3.88 20.03 – 3.88	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.04-3.88) 99.4 (20.03-3.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.74 (at 3.94Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.282 , 0.295 0.293 , 0.300	Depositor DCC
R_{free} test set	3995 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	98.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	37611	wwPDB-VP
Average B, all atoms (Å^2)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AQH, EDO, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.59	3/3154 (0.1%)	0.34	0/4298
1	B	0.65	4/3181 (0.1%)	0.34	0/4338
1	C	0.58	0/3219	0.35	0/4390
1	D	0.59	3/3158 (0.1%)	0.34	0/4305
1	E	0.58	3/3227 (0.1%)	0.35	0/4401
1	F	0.65	3/3181 (0.1%)	0.34	0/4336
1	G	0.64	4/3219 (0.1%)	0.36	0/4390
1	H	0.60	3/3191 (0.1%)	0.37	1/4351 (0.0%)
1	I	0.61	6/3219 (0.2%)	0.37	1/4390 (0.0%)
1	J	0.62	3/3196 (0.1%)	0.37	1/4358 (0.0%)
1	K	0.58	2/3231 (0.1%)	0.36	0/4406
1	L	0.62	2/3102 (0.1%)	0.37	0/4225
All	All	0.61	36/38278 (0.1%)	0.35	3/52188 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	3
1	D	0	1
1	E	0	3
1	F	0	4
1	G	0	2
1	H	0	2
1	I	0	1
1	J	0	2
1	K	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	26

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	ARG	CZ-NH1	-8.61	1.21	1.33
1	H	265	PHE	CG-CD1	-8.42	1.26	1.38
1	L	291	ARG	CZ-NH1	-8.40	1.22	1.33
1	E	291	ARG	CZ-NH1	-7.90	1.22	1.33
1	A	82	GLY	CA-C	7.82	1.64	1.51
1	G	63	TRP	CG-CD1	-7.69	1.25	1.36
1	D	355	PHE	CG-CD1	-7.52	1.27	1.38
1	L	265	PHE	CG-CD1	-7.32	1.27	1.38
1	I	340	TYR	CG-CD1	-6.56	1.30	1.39
1	F	10	ILE	CB-CG2	-6.54	1.32	1.52
1	G	63	TRP	CD2-CE2	-6.33	1.33	1.41
1	B	106	GLY	N-CA	-5.98	1.37	1.46
1	A	83	GLU	N-CA	5.97	1.58	1.46
1	K	358	CYS	CB-SG	5.94	1.92	1.82
1	I	340	TYR	CE2-CZ	-5.63	1.31	1.38
1	J	358	CYS	CB-SG	5.52	1.91	1.82
1	H	265	PHE	CE2-CZ	-5.51	1.26	1.37
1	D	355	PHE	CG-CD2	-5.50	1.30	1.38
1	J	10	ILE	CB-CG1	-5.48	1.38	1.54
1	H	358	CYS	CB-SG	5.44	1.91	1.82
1	D	355	PHE	CE2-CZ	-5.44	1.27	1.37
1	I	104	PRO	N-CD	5.39	1.55	1.47
1	B	111	LEU	CG-CD1	-5.38	1.31	1.51
1	I	358	CYS	CB-SG	5.38	1.91	1.82
1	G	228	GLN	CD-NE2	-5.24	1.19	1.32
1	E	231	TYR	CG-CD1	-5.17	1.32	1.39
1	I	367	GLN	CD-NE2	-5.16	1.20	1.32
1	A	82	GLY	N-CA	5.13	1.53	1.46
1	J	370	CYS	CB-SG	5.12	1.91	1.82
1	I	289	LEU	CG-CD2	-5.09	1.33	1.51
1	F	189	ARG	CZ-NH1	-5.07	1.26	1.33
1	K	157	ARG	CZ-NH2	-5.05	1.26	1.33
1	E	205	ARG	CZ-NH1	-5.05	1.26	1.33
1	B	189	ARG	CZ-NH1	-5.03	1.26	1.33
1	G	268	ASN	CG-ND2	-5.03	1.20	1.32
1	F	388	ARG	CD-NE	-5.01	1.38	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	109	GLY	N-CA-C	6.28	128.81	113.10
1	I	103	PHE	C-N-CD	5.59	140.14	128.40
1	J	105	THR	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	372	ARG	Sidechain
1	A	79	PHE	Peptide
1	B	30	ASP	Peptide
1	B	79	PHE	Peptide
1	C	105	THR	Peptide
1	C	114	TRP	Peptide
1	C	79	PHE	Peptide
1	D	79	PHE	Peptide
1	E	286	ARG	Sidechain
1	E	357	TRP	Peptide
1	E	79	PHE	Peptide
1	F	10	ILE	Peptide
1	F	105	THR	Peptide
1	F	357	TRP	Peptide
1	F	80	ARG	Sidechain
1	G	44	ARG	Sidechain
1	G	79	PHE	Peptide
1	H	205	ARG	Sidechain
1	H	79	PHE	Peptide
1	I	80	ARG	Sidechain
1	J	357	TRP	Peptide
1	J	79	PHE	Peptide
1	K	251	ARG	Sidechain
1	K	357	TRP	Peptide
1	L	79	PHE	Peptide
1	L	80	ARG	Sidechain

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3058	0	2956	95	0
1	B	3082	0	2979	87	0
1	C	3121	0	3016	98	0
1	D	3061	0	2952	137	0
1	E	3129	0	3027	134	0
1	F	3084	0	2979	96	0
1	G	3121	0	3016	128	0
1	H	3093	0	2988	116	0
1	I	3121	0	3015	120	0
1	J	3097	0	2993	100	0
1	K	3132	0	3024	118	0
1	L	3008	0	2882	268	0
2	A	1	0	0	2	0
2	B	1	0	0	1	0
2	C	1	0	0	1	0
2	D	1	0	0	3	0
2	E	1	0	0	1	0
2	F	1	0	0	1	0
2	G	1	0	0	1	0
2	H	1	0	0	1	0
2	I	1	0	0	1	0
2	J	1	0	0	3	0
2	K	1	0	0	1	0
2	L	1	0	0	1	0
3	A	40	0	25	13	0
3	B	40	0	25	8	0
3	C	40	0	25	12	0
3	D	40	0	25	23	0
3	E	40	0	25	10	0
3	F	40	0	25	19	0
3	G	40	0	25	12	0
3	H	40	0	25	24	0
3	I	40	0	25	11	0
3	J	40	0	25	8	0
3	K	40	0	25	16	0
3	L	40	0	25	17	0
4	C	4	0	6	1	0
4	I	4	0	6	1	0
4	J	4	0	6	0	0
All	All	37611	0	36145	1508	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 20.

All (1508) 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:L:296:PHE:CZ	1:L:298:GLY:HA3	1.21	1.68
1:L:107:THR:HG22	1:L:108:LEU:CD2	1.19	1.61
1:L:296:PHE:CE2	1:L:298:GLY:HA3	1.41	1.51
1:D:110:ALA:CB	1:D:137:ILE:HD12	1.07	1.50
1:D:110:ALA:HB1	1:D:137:ILE:CG2	1.43	1.49
1:L:107:THR:CG2	1:L:108:LEU:HD23	1.39	1.48
1:K:79:PHE:HE1	1:K:86:PRO:CA	1.20	1.48
1:L:107:THR:CG2	1:L:108:LEU:CD2	1.90	1.44
1:D:110:ALA:CB	1:D:137:ILE:HG23	1.45	1.42
1:K:79:PHE:CE1	1:K:86:PRO:CA	2.00	1.42
1:L:296:PHE:CE2	1:L:298:GLY:CA	2.03	1.42
1:D:110:ALA:CB	1:D:137:ILE:CD1	1.97	1.41
1:E:108:LEU:HD12	1:E:302:GLY:CA	1.49	1.41
1:L:230:LYS:HG3	1:L:320:PHE:CE1	1.56	1.39
1:L:57:CYS:SG	1:L:64:VAL:HG21	1.63	1.38
1:D:104:PRO:O	1:D:105:THR:CG2	1.71	1.38
1:L:296:PHE:CZ	1:L:298:GLY:CA	2.06	1.38
1:D:110:ALA:HB2	1:D:137:ILE:CD1	1.53	1.38
1:L:107:THR:HA	1:L:108:LEU:CB	1.24	1.38
1:K:79:PHE:CE1	1:K:86:PRO:HA	1.60	1.35
1:H:110:ALA:CB	3:H:502:AQH:O3'	1.73	1.34
1:L:107:THR:CB	1:L:108:LEU:HD23	1.59	1.33
1:C:169:LEU:HD23	1:C:182:PHE:CE2	1.62	1.33
1:L:107:THR:CA	1:L:108:LEU:HB3	1.60	1.32
1:E:339:CYS:O	1:E:370:CYS:HB3	1.28	1.32
1:L:107:THR:CA	1:L:108:LEU:HD23	1.57	1.31
1:K:78:VAL:CG2	1:K:88:LEU:HB3	1.60	1.31
1:K:79:PHE:HE1	1:K:86:PRO:N	1.28	1.31
1:L:101:ILE:CG2	1:L:103:PHE:CE2	2.16	1.28
1:L:307:ALA:O	1:L:312:ILE:CD1	1.78	1.28
1:A:107:THR:HG22	3:A:502:AQH:O1A	1.26	1.28
1:K:339:CYS:O	1:K:370:CYS:HB3	1.09	1.26
1:E:108:LEU:CD1	1:E:302:GLY:HA3	1.66	1.25
1:G:360:ARG:O	1:G:361:HIS:CG	1.89	1.24
1:L:107:THR:CA	1:L:108:LEU:CB	2.14	1.24
1:L:230:LYS:N	1:L:230:LYS:HE2	1.50	1.24
1:K:79:PHE:CD1	1:K:86:PRO:HA	1.75	1.22
1:D:226:THR:CG2	3:D:502:AQH:O3A	1.89	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:THR:HG23	3:D:502:AQH:O3A	1.40	1.19
1:L:230:LYS:HA	1:L:231:TYR:O	1.38	1.19
1:F:205:ARG:HH11	1:F:205:ARG:HG3	1.09	1.18
1:G:360:ARG:O	1:G:361:HIS:ND1	1.74	1.18
1:L:43:VAL:N	1:L:57:CYS:O	1.77	1.17
1:L:101:ILE:HG22	1:L:103:PHE:CE2	1.76	1.17
1:L:107:THR:HA	1:L:108:LEU:CG	1.73	1.16
1:A:107:THR:O	1:A:109:GLY:N	1.77	1.16
1:D:226:THR:CB	3:D:502:AQH:O3A	1.93	1.16
1:E:107:THR:HG21	1:E:110:ALA:HB3	1.25	1.14
1:L:107:THR:CA	1:L:108:LEU:CD2	2.24	1.14
1:K:79:PHE:CE1	1:K:86:PRO:N	2.13	1.13
1:L:233:ASN:O	1:L:234:ASN:O	1.66	1.13
1:E:108:LEU:O	1:E:108:LEU:HD13	1.44	1.13
1:L:312:ILE:HD13	1:L:312:ILE:O	1.47	1.13
1:D:104:PRO:O	1:D:105:THR:HG22	0.95	1.12
1:A:205:ARG:HG3	1:A:205:ARG:HH11	1.06	1.11
1:I:363:ASN:N	1:I:367:GLN:HE22	1.49	1.11
1:F:107:THR:OG1	3:F:502:AQH:O1A	1.69	1.10
1:L:299:LEU:CB	1:L:300:PRO:CD	2.30	1.10
1:H:360:ARG:O	1:H:361:HIS:ND1	1.83	1.10
1:L:107:THR:CG2	1:L:111:LEU:HG	1.80	1.09
1:D:110:ALA:HB3	1:D:137:ILE:HG23	1.27	1.09
1:K:10:ILE:HG12	1:K:102:SER:OG	1.50	1.09
1:L:101:ILE:HG21	1:L:103:PHE:CE2	1.88	1.09
1:E:108:LEU:CD1	1:E:302:GLY:CA	2.27	1.09
1:L:299:LEU:CB	1:L:300:PRO:HD2	1.82	1.09
1:L:44:ARG:HG2	1:L:56:CYS:HB2	1.27	1.08
1:C:36:LEU:H	1:C:36:LEU:CD2	1.61	1.08
1:K:339:CYS:O	1:K:370:CYS:CB	2.02	1.08
1:L:230:LYS:CA	1:L:230:LYS:HE2	1.83	1.07
1:C:36:LEU:N	1:C:36:LEU:HD22	1.55	1.07
1:I:107:THR:HG23	1:I:110:ALA:HB3	1.36	1.07
1:L:296:PHE:CE2	1:L:298:GLY:N	2.21	1.07
1:L:232:TRP:CH2	1:L:237:GLY:HA3	1.88	1.06
1:L:299:LEU:HB2	1:L:300:PRO:CD	1.84	1.06
1:L:230:LYS:CE	1:L:230:LYS:H	1.67	1.06
1:D:108:LEU:O	3:D:502:AQH:O2A	1.71	1.06
1:L:307:ALA:O	1:L:312:ILE:HD12	1.52	1.05
1:D:226:THR:OG1	3:D:502:AQH:O3A	1.73	1.05
1:D:110:ALA:HB1	1:D:137:ILE:CG1	1.85	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:228:GLN:O	1:L:231:TYR:HB3	1.57	1.05
1:E:339:CYS:O	1:E:370:CYS:CB	2.03	1.05
1:G:35:LEU:HD13	1:G:63:TRP:NE1	1.70	1.05
1:J:205:ARG:HG3	1:J:205:ARG:HH11	0.98	1.05
1:D:110:ALA:CA	1:D:137:ILE:HD12	1.86	1.05
1:C:169:LEU:HD23	1:C:182:PHE:HE2	0.90	1.05
1:L:43:VAL:HG12	1:L:57:CYS:O	1.56	1.05
1:L:299:LEU:HB2	1:L:300:PRO:HD2	1.09	1.05
1:D:110:ALA:CB	1:D:137:ILE:CG2	2.15	1.04
1:B:205:ARG:HH11	1:B:205:ARG:HG3	1.15	1.04
1:E:108:LEU:CD1	1:E:302:GLY:C	2.26	1.04
1:A:107:THR:CG2	3:A:502:AQH:O1A	2.06	1.04
1:D:110:ALA:HB1	1:D:137:ILE:CB	1.89	1.03
1:L:107:THR:N	1:L:108:LEU:HD23	1.73	1.03
1:G:35:LEU:HD13	1:G:63:TRP:HE1	1.22	1.02
1:L:107:THR:HG21	1:L:111:LEU:HG	1.04	1.02
1:L:230:LYS:HE2	1:L:230:LYS:H	1.00	1.02
1:L:307:ALA:O	1:L:312:ILE:HD11	1.55	1.02
1:L:41:TRP:O	1:L:58:ASP:C	1.98	1.02
1:K:10:ILE:CG1	1:K:102:SER:OG	2.08	1.02
1:D:300:PRO:O	3:D:502:AQH:O6'	1.79	1.00
1:E:106:GLY:HA3	1:E:134:SER:OG	1.61	1.00
1:H:110:ALA:HB2	3:H:502:AQH:O3'	1.58	1.00
1:C:36:LEU:H	1:C:36:LEU:HD22	0.84	1.00
1:I:228:GLN:HG3	1:I:368:PHE:HE2	1.26	0.99
1:I:27:ASP:OD1	1:I:28:PHE:N	1.95	0.99
1:C:169:LEU:CD2	1:C:182:PHE:HE2	1.76	0.99
1:D:104:PRO:C	1:D:105:THR:HG22	1.81	0.98
1:E:108:LEU:HD11	1:E:302:GLY:C	1.84	0.98
1:G:354:ASP:HB3	1:G:356:LEU:O	1.64	0.97
1:J:205:ARG:CG	1:J:205:ARG:HH11	1.78	0.97
1:K:78:VAL:HG23	1:K:88:LEU:HB3	1.43	0.97
1:L:230:LYS:HG3	1:L:320:PHE:CD1	1.99	0.97
1:I:228:GLN:CG	1:I:368:PHE:HE2	1.76	0.97
1:H:110:ALA:HB1	3:H:502:AQH:O3'	1.65	0.96
1:I:107:THR:CG2	1:I:110:ALA:HB3	1.95	0.96
1:K:226:THR:OG1	3:K:502:AQH:O1B	1.82	0.96
1:L:107:THR:CG2	1:L:108:LEU:HD21	1.75	0.96
1:J:107:THR:OG1	3:J:503:AQH:O2A	1.80	0.96
1:L:230:LYS:CG	1:L:320:PHE:CE1	2.48	0.96
1:L:107:THR:CB	1:L:108:LEU:CD2	2.27	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:43:VAL:O	1:L:57:CYS:N	1.98	0.96
1:L:300:PRO:O	3:L:502:AQH:O6'	1.84	0.96
1:E:394:GLY:O	1:E:396:GLU:N	1.99	0.95
1:E:107:THR:CG2	1:E:110:ALA:HB3	1.96	0.95
1:I:228:GLN:HG3	1:I:368:PHE:CE2	2.00	0.95
1:L:107:THR:HB	1:L:108:LEU:HG	1.48	0.95
1:L:43:VAL:HG12	1:L:57:CYS:C	1.73	0.95
1:D:107:THR:O	1:D:107:THR:HG23	1.65	0.94
1:I:363:ASN:H	1:I:367:GLN:HE22	1.06	0.94
1:L:57:CYS:SG	1:L:64:VAL:CG2	2.56	0.94
1:D:226:THR:CG2	3:D:502:AQH:PB	2.56	0.94
1:D:226:THR:OG1	3:D:502:AQH:PB	2.26	0.93
1:G:343:TRP:CZ3	3:G:502:AQH:O7'	2.22	0.93
1:H:108:LEU:HB3	3:H:502:AQH:O1A	1.67	0.93
1:H:110:ALA:HB2	3:H:502:AQH:H11	1.51	0.93
1:E:225:SER:N	1:E:231:TYR:HE1	1.65	0.93
1:G:108:LEU:HD23	1:G:109:GLY:H	1.34	0.93
1:E:300:PRO:HB2	3:E:502:AQH:O6'	1.68	0.93
1:L:101:ILE:CG2	1:L:103:PHE:HE2	1.83	0.92
1:E:108:LEU:HD12	1:E:302:GLY:HA3	0.92	0.92
1:L:107:THR:HA	1:L:108:LEU:CD2	1.91	0.92
1:I:226:THR:OG1	3:I:503:AQH:O3A	1.87	0.92
1:L:230:LYS:HE2	1:L:230:LYS:C	1.89	0.91
1:L:296:PHE:HZ	1:L:298:GLY:HA3	1.18	0.91
1:J:257:ARG:HD3	3:J:503:AQH:N7	1.86	0.91
1:B:299:LEU:HB3	1:B:300:PRO:HD2	1.51	0.91
1:G:108:LEU:O	1:G:110:ALA:N	2.04	0.91
1:L:227:CYS:O	1:L:230:LYS:NZ	2.03	0.91
1:L:257:ARG:HB3	3:L:502:AQH:C4	2.01	0.91
1:G:299:LEU:HB3	1:G:300:PRO:HD2	1.53	0.91
1:J:9:PHE:HD1	1:J:10:ILE:HG22	1.35	0.91
1:L:225:SER:O	1:L:226:THR:HG23	1.71	0.91
1:L:225:SER:O	3:L:502:AQH:O3D	1.87	0.91
1:L:107:THR:HG21	1:L:111:LEU:CG	1.97	0.91
1:K:299:LEU:HB3	1:K:300:PRO:HD2	1.51	0.90
1:D:391:THR:HG22	1:D:391:THR:O	1.69	0.90
1:J:299:LEU:HB3	1:J:300:PRO:HD2	1.53	0.90
1:K:79:PHE:CE1	1:K:86:PRO:CB	2.54	0.90
1:E:208:LEU:O	1:E:291:ARG:NH1	2.04	0.90
1:K:286:ARG:NH1	3:K:502:AQH:H17	1.88	0.89
1:D:299:LEU:HB3	1:D:300:PRO:HD2	1.54	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:GLY:HA3	3:F:502:AQH:H9	1.55	0.89
1:H:104:PRO:C	1:H:107:THR:HG21	1.91	0.89
1:A:79:PHE:HE1	1:A:86:PRO:HB3	1.38	0.88
1:L:107:THR:CA	1:L:108:LEU:CG	2.42	0.88
1:D:226:THR:HG21	3:D:502:AQH:O1B	1.71	0.88
1:L:107:THR:CB	1:L:108:LEU:CG	2.51	0.88
1:D:110:ALA:O	1:D:111:LEU:HG	1.73	0.88
1:J:205:ARG:NH1	1:J:205:ARG:HG3	1.81	0.88
3:K:502:AQH:H11	3:K:502:AQH:O2A	1.74	0.88
1:K:78:VAL:HG21	1:K:88:LEU:HB3	1.54	0.88
1:C:299:LEU:HB3	1:C:300:PRO:HD2	1.55	0.87
1:D:226:THR:HG23	3:D:502:AQH:PB	2.14	0.87
1:F:182:PHE:CE1	1:F:183:ARG:HG3	2.10	0.87
1:L:230:LYS:N	1:L:230:LYS:CE	2.30	0.87
1:E:299:LEU:HB3	1:E:300:PRO:HD2	1.55	0.87
1:L:158:THR:O	1:L:160:ALA:N	2.08	0.86
1:D:110:ALA:HB1	1:D:137:ILE:HD12	1.35	0.86
1:K:10:ILE:N	1:K:10:ILE:HD12	1.90	0.86
1:L:230:LYS:O	1:L:230:LYS:HE3	1.76	0.85
1:C:182:PHE:CE1	1:C:183:ARG:HG3	2.11	0.85
1:I:228:GLN:CG	1:I:368:PHE:CE2	2.57	0.85
1:H:299:LEU:HB3	1:H:300:PRO:HD2	1.58	0.85
1:L:43:VAL:HG13	1:L:57:CYS:H	1.39	0.85
1:E:340:TYR:OH	1:A:179:PRO:O	1.93	0.85
1:E:108:LEU:HD13	1:E:108:LEU:C	1.95	0.85
1:L:286:ARG:NH1	3:L:502:AQH:H17	1.92	0.85
1:A:299:LEU:HB3	1:A:300:PRO:HD2	1.59	0.84
1:D:106:GLY:O	1:D:107:THR:HG22	1.76	0.84
1:L:107:THR:OG1	1:L:111:LEU:HD12	1.76	0.84
1:L:299:LEU:HD22	1:L:317:ILE:HB	1.58	0.84
1:D:110:ALA:HB1	1:D:137:ILE:HG21	1.59	0.84
1:L:232:TRP:HD1	1:L:371:THR:HB	1.41	0.84
1:A:205:ARG:HH11	1:A:205:ARG:CG	1.89	0.84
1:G:158:THR:O	1:G:160:ALA:N	2.09	0.84
1:K:78:VAL:CG2	1:K:88:LEU:CB	2.53	0.84
1:A:79:PHE:CE1	1:A:86:PRO:HB3	2.12	0.83
1:K:182:PHE:CE1	1:K:183:ARG:HG3	2.11	0.83
1:L:228:GLN:O	1:L:231:TYR:CB	2.26	0.83
1:G:35:LEU:HD13	1:G:63:TRP:CD1	2.14	0.83
1:F:299:LEU:HB3	1:F:300:PRO:HD2	1.59	0.82
1:L:103:PHE:CE1	1:L:167:VAL:HB	2.14	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:PHE:CE1	1:A:183:ARG:HG3	2.13	0.82
1:H:106:GLY:N	1:H:107:THR:HG22	1.94	0.82
1:C:107:THR:OG1	3:C:503:AQH:O2A	1.97	0.82
1:E:108:LEU:C	1:E:108:LEU:CD1	2.48	0.82
1:L:299:LEU:HB3	1:L:300:PRO:CD	2.08	0.82
1:K:10:ILE:HG12	1:K:102:SER:CB	2.09	0.82
1:I:230:LYS:CE	3:I:503:AQH:O6'	2.28	0.82
1:I:103:PHE:CD2	1:I:111:LEU:CD2	2.63	0.81
1:D:182:PHE:CE1	1:D:183:ARG:HG3	2.15	0.81
1:E:108:LEU:HD12	1:E:302:GLY:C	1.96	0.81
1:B:182:PHE:CE1	1:B:183:ARG:HG3	2.16	0.81
1:L:342:CYS:SG	2:L:501:FE:FE	1.71	0.81
1:H:360:ARG:C	1:H:361:HIS:HD1	1.83	0.81
1:L:227:CYS:C	1:L:230:LYS:NZ	2.34	0.81
1:E:342:CYS:SG	2:E:501:FE:FE	1.73	0.80
1:F:169:LEU:HD23	1:F:182:PHE:CD2	2.15	0.80
1:L:101:ILE:HG21	1:L:103:PHE:CZ	2.16	0.80
1:I:27:ASP:CG	1:I:28:PHE:H	1.85	0.80
1:A:205:ARG:NH1	1:A:205:ARG:HG3	1.88	0.80
1:E:158:THR:O	1:E:160:ALA:N	2.13	0.80
1:J:300:PRO:HB2	3:J:503:AQH:O6'	1.80	0.80
1:A:370:CYS:SG	2:A:501:FE:FE	1.71	0.80
1:E:108:LEU:CG	1:E:302:GLY:HA3	2.11	0.80
1:J:226:THR:OG1	3:J:503:AQH:O1B	1.99	0.80
1:H:110:ALA:HB2	3:H:502:AQH:C3'	2.11	0.80
1:K:286:ARG:HH11	3:K:502:AQH:H17	1.47	0.80
1:L:230:LYS:CE	1:L:230:LYS:C	2.50	0.80
1:I:103:PHE:CE2	1:I:115:PHE:HD1	2.00	0.80
1:J:182:PHE:CE1	1:J:183:ARG:HG3	2.17	0.80
1:L:230:LYS:O	1:L:230:LYS:CE	2.30	0.80
1:C:158:THR:O	1:C:160:ALA:N	2.15	0.80
1:B:19:ALA:O	1:B:24:ILE:O	2.00	0.80
1:L:208:LEU:O	1:L:291:ARG:NH1	2.15	0.79
1:L:42:HIS:NE2	1:L:56:CYS:SG	2.55	0.79
1:I:299:LEU:HB3	1:I:300:PRO:HD2	1.62	0.79
1:K:79:PHE:CE1	1:K:85:THR:C	2.54	0.79
1:J:300:PRO:O	3:J:503:AQH:H6	1.82	0.79
1:G:370:CYS:SG	2:G:501:FE:FE	1.74	0.79
1:L:225:SER:O	1:L:226:THR:CG2	2.30	0.79
1:L:232:TRP:O	1:L:233:ASN:CB	2.30	0.79
1:L:302:GLY:O	1:L:305:TRP:N	2.16	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:SER:H	1:E:231:TYR:HE1	1.28	0.79
1:A:187:PHE:CZ	3:A:502:AQH:O4'	2.35	0.78
1:F:370:CYS:SG	2:F:501:FE:FE	1.74	0.78
1:L:107:THR:HG22	1:L:108:LEU:HD21	0.79	0.78
1:B:318:SER:HB3	1:B:332:ARG:HH12	1.48	0.78
1:F:205:ARG:NH1	1:F:205:ARG:HG3	1.90	0.78
1:L:107:THR:CG2	1:L:111:LEU:CG	2.59	0.78
1:D:226:THR:N	3:D:502:AQH:O3A	2.17	0.78
1:F:205:ARG:CG	1:F:205:ARG:HH11	1.93	0.78
1:L:101:ILE:CG2	1:L:103:PHE:CZ	2.66	0.78
1:H:182:PHE:CE1	1:H:183:ARG:HG3	2.18	0.77
1:H:110:ALA:HB3	3:H:502:AQH:O3'	1.81	0.77
1:D:158:THR:O	1:D:160:ALA:N	2.17	0.77
1:H:110:ALA:HB2	3:H:502:AQH:C2'	2.14	0.77
1:K:226:THR:CG2	3:K:502:AQH:O1B	2.33	0.77
1:L:107:THR:HA	1:L:108:LEU:HB3	0.78	0.77
1:B:205:ARG:NH1	1:B:205:ARG:HG3	1.94	0.77
1:C:169:LEU:HD23	1:C:182:PHE:CD2	2.20	0.76
1:E:205:ARG:HH11	1:E:205:ARG:HG3	1.47	0.76
1:G:122:GLN:O	1:G:122:GLN:OE1	2.02	0.76
1:K:9:PHE:HB2	1:K:10:ILE:HD12	1.67	0.76
3:K:502:AQH:H11	3:K:502:AQH:PA	2.26	0.76
1:D:300:PRO:O	3:D:502:AQH:C6'	2.34	0.76
1:L:232:TRP:CH2	1:L:237:GLY:CA	2.67	0.76
1:L:299:LEU:HB3	1:L:300:PRO:HD3	1.67	0.76
1:B:182:PHE:HD1	1:B:183:ARG:N	1.82	0.76
1:L:182:PHE:CE1	1:L:183:ARG:HG3	2.21	0.76
1:L:187:PHE:CZ	3:L:502:AQH:O7'	2.39	0.76
1:K:107:THR:OG1	3:K:502:AQH:O2A	2.04	0.76
1:A:110:ALA:N	3:A:502:AQH:O3'	2.18	0.76
1:H:104:PRO:O	1:H:107:THR:HG21	1.86	0.75
1:B:370:CYS:SG	2:B:501:FE:FE	1.77	0.75
1:J:169:LEU:HB3	1:J:182:PHE:CE2	2.21	0.75
1:L:230:LYS:CA	1:L:230:LYS:CE	2.62	0.75
1:C:370:CYS:SG	2:C:501:FE:FE	1.78	0.75
1:L:312:ILE:O	1:L:312:ILE:CD1	2.30	0.75
1:E:170:TYR:CE2	1:E:177:ASN:HB3	2.22	0.75
1:H:108:LEU:O	3:H:502:AQH:O1A	2.05	0.75
1:L:43:VAL:CG1	1:L:57:CYS:O	2.35	0.75
1:D:226:THR:HG1	3:D:502:AQH:PB	2.06	0.74
1:H:263:GLN:HG3	1:H:355:PHE:HB3	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:9:PHE:CD1	1:J:10:ILE:HG22	2.21	0.74
1:K:286:ARG:HH11	3:K:502:AQH:C2	1.99	0.74
1:E:108:LEU:O	1:E:108:LEU:CD1	2.30	0.74
1:H:370:CYS:SG	2:H:501:FE:FE	1.78	0.74
1:L:107:THR:N	1:L:108:LEU:CD2	2.46	0.74
1:E:338:GLY:HA3	1:E:373:LEU:HD12	1.68	0.74
1:A:257:ARG:HD3	3:A:502:AQH:N7	2.02	0.74
1:D:110:ALA:HB2	1:D:137:ILE:HD12	0.75	0.74
1:D:169:LEU:HD22	1:D:182:PHE:CE2	2.23	0.74
1:H:182:PHE:HD1	1:H:183:ARG:N	1.86	0.74
1:D:110:ALA:HB1	1:D:137:ILE:CD1	1.84	0.74
3:E:502:AQH:O4'	3:E:502:AQH:H2	1.86	0.74
1:D:110:ALA:C	1:D:111:LEU:HG	2.08	0.74
1:I:342:CYS:SG	2:I:501:FE:FE	1.77	0.74
1:L:296:PHE:HE2	1:L:298:GLY:CA	1.97	0.74
1:L:298:GLY:O	1:L:304:SER:OG	2.04	0.74
1:F:107:THR:HB	3:F:502:AQH:O2A	1.88	0.73
1:K:78:VAL:HG23	1:K:88:LEU:CB	2.17	0.73
1:L:114:TRP:NE1	1:L:188:HIS:HA	2.03	0.73
1:E:339:CYS:O	1:E:370:CYS:SG	2.46	0.73
1:G:325:SER:HG	1:G:343:TRP:HZ2	1.36	0.73
1:D:110:ALA:O	1:D:111:LEU:CG	2.36	0.73
1:I:295:PHE:HD2	1:I:386:LEU:CD2	2.01	0.73
1:E:338:GLY:HA3	1:E:373:LEU:CD1	2.19	0.73
1:H:158:THR:O	1:H:160:ALA:N	2.21	0.73
1:L:232:TRP:O	1:L:371:THR:OG1	2.03	0.73
1:G:35:LEU:CD1	1:G:63:TRP:CD1	2.72	0.73
1:H:170:TYR:CD2	1:H:177:ASN:HB2	2.23	0.73
1:H:265:PHE:CD2	1:H:266:VAL:HG23	2.23	0.73
1:J:16:PRO:HB3	1:J:27:ASP:HB2	1.71	0.73
1:K:286:ARG:NH1	3:K:502:AQH:C2	2.51	0.73
1:L:187:PHE:CE1	3:L:502:AQH:O7'	2.40	0.73
1:L:233:ASN:O	1:L:234:ASN:C	2.26	0.73
1:D:226:THR:CG2	3:D:502:AQH:O1B	2.36	0.73
1:F:169:LEU:HD23	1:F:182:PHE:CE2	2.23	0.73
1:L:233:ASN:ND2	1:L:368:PHE:HB3	2.04	0.73
1:A:170:TYR:CE2	1:A:177:ASN:CB	2.72	0.72
1:D:370:CYS:SG	2:D:501:FE:FE	1.79	0.72
1:G:356:LEU:N	1:G:356:LEU:HD23	2.04	0.72
1:A:360:ARG:C	1:A:361:HIS:HD1	1.92	0.72
1:G:27:ASP:OD1	1:G:28:PHE:N	2.21	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:43:VAL:CG1	1:L:57:CYS:H	2.03	0.72
1:K:226:THR:HG23	3:K:502:AQH:O1B	1.89	0.72
1:K:302:GLY:N	3:K:502:AQH:O1A	2.23	0.72
3:G:502:AQH:O2B	3:G:502:AQH:O	2.07	0.72
1:I:338:GLY:HA3	1:I:373:LEU:HD12	1.72	0.72
1:D:110:ALA:O	1:D:137:ILE:HG21	1.90	0.72
1:E:384:ASN:O	1:E:388:ARG:HG3	1.90	0.72
1:H:105:THR:O	1:H:107:THR:HB	1.89	0.72
1:J:61:LYS:HG3	1:J:61:LYS:O	1.89	0.72
1:K:169:LEU:HD22	1:K:182:PHE:CE2	2.25	0.72
1:I:27:ASP:OD2	1:I:29:ASN:ND2	2.22	0.72
1:L:265:PHE:HD1	1:E:368:PHE:HD2	1.35	0.72
1:L:230:LYS:CG	1:L:320:PHE:CD1	2.72	0.72
1:L:43:VAL:CG1	1:L:57:CYS:N	2.52	0.72
1:H:170:TYR:CE2	1:H:177:ASN:CB	2.73	0.71
1:L:286:ARG:NH1	3:L:502:AQH:C2	2.52	0.71
1:L:114:TRP:HE1	1:L:188:HIS:HA	1.55	0.71
1:E:225:SER:N	1:E:231:TYR:CE1	2.55	0.71
1:F:170:TYR:CE2	1:F:177:ASN:HB3	2.24	0.71
1:I:363:ASN:N	1:I:367:GLN:NE2	2.34	0.71
1:D:170:TYR:CE2	1:D:177:ASN:HB3	2.25	0.71
1:G:343:TRP:CE3	3:G:502:AQH:O7'	2.44	0.71
1:A:104:PRO:O	1:A:105:THR:HG23	1.90	0.71
1:L:107:THR:OG1	1:L:111:LEU:HB2	1.91	0.71
1:A:170:TYR:CD2	1:A:177:ASN:HB2	2.25	0.71
1:B:182:PHE:HE1	1:B:183:ARG:HG3	1.54	0.71
1:J:10:ILE:HG23	1:J:10:ILE:O	1.88	0.71
1:B:21:PRO:HD2	1:B:88:LEU:HD12	1.72	0.71
1:E:10:ILE:O	1:E:10:ILE:HG23	1.91	0.71
1:I:170:TYR:CE2	1:I:177:ASN:HB3	2.26	0.71
1:I:230:LYS:HE2	3:I:503:AQH:O6'	1.89	0.71
1:L:103:PHE:CD1	1:L:167:VAL:HB	2.25	0.71
1:D:112:LEU:HD12	1:D:113:GLY:H	1.55	0.70
1:L:232:TRP:O	1:L:233:ASN:CG	2.30	0.70
1:A:71:PHE:HD1	1:A:165:TYR:HH	1.39	0.70
1:E:21:PRO:HD2	1:E:88:LEU:HD12	1.72	0.70
1:A:318:SER:HB3	1:A:332:ARG:HH12	1.56	0.70
1:L:232:TRP:O	1:L:233:ASN:HB2	1.91	0.70
1:L:43:VAL:HG13	1:L:57:CYS:N	1.99	0.70
1:C:170:TYR:CE2	1:C:177:ASN:HB3	2.26	0.70
1:I:230:LYS:NZ	3:I:503:AQH:O6'	2.23	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:277:PHE:O	1:G:286:ARG:NH2	2.26	0.69
1:L:302:GLY:N	3:L:502:AQH:O3A	2.18	0.69
1:F:302:GLY:N	3:F:502:AQH:H11	2.07	0.69
1:D:10:ILE:HD11	1:D:102:SER:OG	1.91	0.69
1:I:107:THR:HG23	1:I:110:ALA:CB	2.19	0.69
1:E:300:PRO:O	3:E:502:AQH:H6	1.91	0.69
1:A:257:ARG:HD3	3:A:502:AQH:C8	2.23	0.69
1:C:115:PHE:HE2	1:C:145:TYR:HD2	1.40	0.69
1:E:22:GLU:OE2	1:E:80:ARG:NH1	2.24	0.69
1:G:356:LEU:O	1:G:357:TRP:HB3	1.91	0.69
1:G:286:ARG:NH1	3:G:502:AQH:H17	2.08	0.69
1:G:360:ARG:O	1:G:361:HIS:CB	2.41	0.69
1:I:228:GLN:HG2	1:I:368:PHE:HE2	1.58	0.68
1:L:101:ILE:HG21	1:L:103:PHE:HE2	1.45	0.68
1:A:18:GLN:OE1	1:A:97:ARG:NH2	2.27	0.68
1:J:358:CYS:SG	2:J:501:FE:FE	1.85	0.68
1:F:299:LEU:O	1:F:304:SER:OG	2.09	0.68
1:G:357:TRP:O	1:G:357:TRP:CD2	2.46	0.68
1:H:105:THR:C	1:H:107:THR:HB	2.14	0.68
1:L:107:THR:HG23	1:L:108:LEU:HD23	1.67	0.68
1:B:27:ASP:OD1	1:B:28:PHE:N	2.26	0.68
1:C:360:ARG:O	1:C:361:HIS:ND1	2.27	0.68
1:F:360:ARG:O	1:F:361:HIS:ND1	2.26	0.68
1:B:16:PRO:HB3	1:B:27:ASP:HB2	1.76	0.68
1:K:79:PHE:HD1	1:K:86:PRO:HA	1.53	0.68
1:D:115:PHE:N	1:D:116:PRO:CD	2.57	0.68
1:G:182:PHE:CE1	1:G:183:ARG:HG3	2.29	0.68
1:K:43:VAL:HG12	1:K:57:CYS:SG	2.34	0.67
1:C:16:PRO:HB3	1:C:27:ASP:HB2	1.76	0.67
1:I:363:ASN:H	1:I:367:GLN:NE2	1.87	0.67
1:D:107:THR:O	1:D:107:THR:CG2	2.39	0.67
1:E:300:PRO:HB2	3:E:502:AQH:H5	1.60	0.67
1:K:79:PHE:CE1	1:K:86:PRO:HB3	2.28	0.67
1:L:101:ILE:HG22	1:L:103:PHE:CD2	2.28	0.67
1:B:277:PHE:O	1:B:286:ARG:NH2	2.27	0.67
1:D:103:PHE:CB	1:D:111:LEU:HD13	2.24	0.67
1:A:103:PHE:HB3	1:A:104:PRO:HD2	1.77	0.67
1:D:16:PRO:HB3	1:D:27:ASP:HB2	1.75	0.67
1:G:348:LEU:HD13	1:G:359:PRO:CG	2.24	0.67
1:H:30:ASP:HB2	1:H:166:ARG:HH21	1.60	0.67
1:G:356:LEU:O	1:G:357:TRP:CB	2.41	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:PHE:O	1:D:286:ARG:NH2	2.28	0.67
1:D:368:PHE:HD2	1:H:265:PHE:CE1	2.12	0.67
1:F:302:GLY:N	3:F:502:AQH:C2'	2.58	0.67
1:A:342:CYS:SG	2:A:501:FE:FE	1.87	0.67
1:D:170:TYR:HE2	1:D:177:ASN:HB3	1.59	0.67
1:K:358:CYS:SG	2:K:501:FE:FE	1.87	0.67
1:I:107:THR:CG2	1:I:110:ALA:CB	2.72	0.66
1:L:43:VAL:O	1:L:56:CYS:HA	1.93	0.66
1:D:342:CYS:SG	2:D:501:FE:FE	1.86	0.66
1:L:299:LEU:CD2	1:L:317:ILE:HB	2.26	0.66
1:F:170:TYR:HE2	1:F:177:ASN:HB3	1.60	0.66
1:H:182:PHE:HE1	1:H:183:ARG:HG3	1.59	0.66
1:I:182:PHE:CE1	1:I:183:ARG:HG3	2.31	0.66
1:K:43:VAL:CG1	1:K:57:CYS:SG	2.83	0.66
1:L:103:PHE:CE1	1:L:167:VAL:CB	2.78	0.66
1:L:107:THR:HB	1:L:108:LEU:CG	2.15	0.66
1:L:228:GLN:NE2	1:L:231:TYR:CE2	2.63	0.66
1:L:44:ARG:HA	1:L:56:CYS:HA	1.77	0.66
1:B:286:ARG:NH1	3:B:502:AQH:H17	2.09	0.66
1:E:27:ASP:OD1	1:E:28:PHE:N	2.28	0.66
1:L:265:PHE:CD1	1:E:368:PHE:HD2	2.13	0.66
1:G:360:ARG:C	1:G:361:HIS:ND1	2.47	0.66
1:J:223:THR:O	1:J:299:LEU:HD11	1.95	0.66
1:J:342:CYS:SG	2:J:501:FE:FE	1.88	0.66
1:F:302:GLY:CA	3:F:502:AQH:H11	2.25	0.66
1:L:296:PHE:CD2	1:L:298:GLY:N	2.57	0.66
1:L:114:TRP:CD1	1:L:188:HIS:HA	2.31	0.66
1:J:370:CYS:SG	2:J:501:FE:FE	1.88	0.66
1:A:16:PRO:HB3	1:A:27:ASP:HB2	1.77	0.66
1:H:189:ARG:NH2	1:H:324:ASN:O	2.29	0.66
3:I:503:AQH:O1B	3:I:503:AQH:O	2.12	0.66
1:K:27:ASP:OD1	1:K:28:PHE:N	2.28	0.66
1:D:103:PHE:HB3	1:D:111:LEU:HD13	1.78	0.65
1:F:301:SER:HA	3:F:502:AQH:H13	1.76	0.65
3:E:502:AQH:H23	3:E:502:AQH:O1B	1.95	0.65
1:J:170:TYR:CD2	1:J:177:ASN:HB2	2.30	0.65
1:L:226:THR:O	1:L:355:PHE:HE1	1.79	0.65
1:G:108:LEU:HD23	1:G:109:GLY:N	2.10	0.65
1:K:16:PRO:HB3	1:K:27:ASP:HB2	1.78	0.65
1:L:16:PRO:HB2	1:L:25:PHE:HB3	1.78	0.65
1:L:226:THR:O	1:L:355:PHE:CE1	2.48	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:41:TRP:O	1:L:58:ASP:CA	2.44	0.65
1:C:115:PHE:HE2	1:C:145:TYR:CD2	2.14	0.65
1:J:104:PRO:O	1:J:106:GLY:N	2.30	0.65
1:C:230:LYS:HE2	3:C:503:AQH:O6'	1.97	0.65
1:H:104:PRO:HB2	1:H:107:THR:OG1	1.95	0.65
1:L:43:VAL:O	1:L:56:CYS:CA	2.45	0.65
1:D:170:TYR:CD2	1:D:177:ASN:HB2	2.32	0.65
1:H:27:ASP:OD1	1:H:28:PHE:N	2.29	0.65
1:H:299:LEU:O	1:H:304:SER:OG	2.11	0.65
1:L:265:PHE:CE1	1:E:368:PHE:HE2	2.15	0.65
1:B:106:GLY:HA3	1:B:134:SER:OG	1.96	0.65
1:C:145:TYR:CE1	1:C:205:ARG:NH1	2.65	0.65
1:D:112:LEU:HD12	1:D:113:GLY:N	2.12	0.65
1:D:286:ARG:NH1	3:D:502:AQH:H17	2.11	0.65
1:E:170:TYR:CE2	1:E:177:ASN:CB	2.80	0.65
1:D:170:TYR:CE2	1:D:177:ASN:CB	2.80	0.64
1:I:158:THR:O	1:I:160:ALA:N	2.28	0.64
1:L:42:HIS:HA	1:L:58:ASP:HA	1.78	0.64
1:D:114:TRP:HE1	1:D:188:HIS:HA	1.61	0.64
1:H:277:PHE:O	1:H:286:ARG:NH2	2.29	0.64
1:F:187:PHE:CZ	3:F:502:AQH:O4'	2.50	0.64
1:H:170:TYR:CE2	1:H:177:ASN:HB3	2.31	0.64
1:I:103:PHE:HE2	1:I:115:PHE:HD1	1.45	0.64
1:C:115:PHE:N	1:C:116:PRO:CD	2.60	0.64
1:E:16:PRO:HB3	1:E:27:ASP:HB2	1.80	0.64
1:I:339:CYS:O	1:I:370:CYS:HB3	1.98	0.64
1:A:85:THR:HG22	1:A:86:PRO:HD2	1.80	0.64
1:I:170:TYR:CE2	1:I:177:ASN:CB	2.81	0.64
1:I:295:PHE:CD2	1:I:386:LEU:CD2	2.80	0.64
1:L:264:GLY:O	1:L:266:VAL:N	2.25	0.64
1:L:107:THR:HG23	1:L:111:LEU:CD1	2.28	0.64
1:E:107:THR:H	1:E:111:LEU:HD12	1.62	0.64
1:G:228:GLN:HG3	1:G:368:PHE:HE2	1.63	0.64
1:G:357:TRP:CE3	1:G:357:TRP:O	2.51	0.64
1:L:9:PHE:O	1:L:10:ILE:HB	1.97	0.64
1:G:299:LEU:O	1:G:304:SER:OG	2.08	0.64
1:K:103:PHE:HB3	1:K:104:PRO:HD2	1.79	0.64
1:J:227:CYS:SG	1:J:229:ALA:HB3	2.39	0.63
1:K:169:LEU:HD22	1:K:182:PHE:CD2	2.32	0.63
1:G:348:LEU:HD13	1:G:359:PRO:HG2	1.80	0.63
1:F:109:GLY:HA3	3:F:502:AQH:C3'	2.27	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:PRO:HB2	1:H:25:PHE:HB3	1.81	0.63
1:L:361:HIS:HD2	1:L:366:ARG:HB2	1.62	0.63
1:C:21:PRO:HD2	1:C:88:LEU:HD12	1.80	0.63
1:J:182:PHE:HE1	1:J:183:ARG:HG3	1.64	0.63
1:K:182:PHE:HE1	1:K:183:ARG:HG3	1.62	0.63
1:K:226:THR:CB	3:K:502:AQH:O1B	2.46	0.63
1:L:257:ARG:HB2	3:L:502:AQH:C6	2.27	0.63
1:D:226:THR:CA	3:D:502:AQH:O3A	2.45	0.63
1:F:302:GLY:HA2	3:F:502:AQH:H11	1.80	0.63
1:I:366:ARG:O	1:I:369:GLU:HB2	1.99	0.63
1:D:110:ALA:O	1:D:111:LEU:CB	2.47	0.63
1:E:19:ALA:O	1:E:24:ILE:O	2.16	0.63
1:G:325:SER:OG	1:G:343:TRP:HZ2	1.80	0.63
1:K:361:HIS:HD2	1:K:366:ARG:HB2	1.63	0.63
1:J:115:PHE:N	1:J:116:PRO:CD	2.61	0.63
1:J:169:LEU:C	1:J:170:TYR:HD1	2.02	0.63
1:L:257:ARG:HB3	3:L:502:AQH:C5	2.29	0.63
1:D:10:ILE:HG23	1:D:10:ILE:O	1.99	0.63
1:E:208:LEU:HB3	1:E:291:ARG:HH11	1.64	0.63
1:F:169:LEU:HD23	1:F:182:PHE:HD2	1.64	0.63
1:H:16:PRO:HB3	1:H:27:ASP:HB2	1.80	0.63
1:L:230:LYS:O	1:L:230:LYS:HG2	1.99	0.63
1:G:359:PRO:HB2	1:G:360:ARG:HG3	1.81	0.63
1:I:338:GLY:HA3	1:I:373:LEU:CD1	2.29	0.63
1:K:79:PHE:CE1	1:K:86:PRO:CD	2.81	0.63
1:A:80:ARG:O	1:A:82:GLY:N	2.29	0.62
1:L:312:ILE:H	1:L:312:ILE:CD1	2.12	0.62
1:E:189:ARG:NH2	1:E:324:ASN:O	2.32	0.62
1:A:16:PRO:HB2	1:A:25:PHE:HB3	1.81	0.62
1:B:10:ILE:O	1:B:10:ILE:HG23	1.99	0.62
1:K:170:TYR:CE2	1:K:177:ASN:HB3	2.35	0.62
1:G:40:LYS:HB3	1:G:81:GLN:OE1	1.99	0.62
1:J:60:ASP:O	1:J:61:LYS:O	2.16	0.62
1:D:320:PHE:CE2	1:D:343:TRP:HB2	2.34	0.62
1:F:27:ASP:OD1	1:F:28:PHE:N	2.33	0.62
1:B:264:GLY:O	1:B:267:TRP:NE1	2.33	0.62
1:F:170:TYR:CD2	1:F:177:ASN:HB2	2.34	0.62
1:J:10:ILE:CG2	1:J:10:ILE:O	2.47	0.62
1:L:182:PHE:HD1	1:L:183:ARG:N	1.98	0.62
1:B:169:LEU:HB3	1:B:182:PHE:HE2	1.65	0.62
1:I:103:PHE:HE2	1:I:115:PHE:CD1	2.17	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:189:ARG:NH2	1:I:324:ASN:O	2.33	0.62
1:L:277:PHE:O	1:L:286:ARG:NH2	2.33	0.62
1:I:103:PHE:CE2	1:I:115:PHE:CD1	2.85	0.62
1:I:334:PHE:CZ	1:I:340:TYR:HD2	2.18	0.62
1:J:21:PRO:HD2	1:J:88:LEU:HD12	1.82	0.62
1:L:114:TRP:CH2	1:L:168:GLY:HA2	2.35	0.61
1:A:21:PRO:HD2	1:A:88:LEU:HD12	1.80	0.61
1:H:182:PHE:C	1:H:182:PHE:HD1	2.03	0.61
1:K:115:PHE:N	1:K:116:PRO:CD	2.63	0.61
1:L:230:LYS:HB2	1:L:300:PRO:HG3	1.81	0.61
1:E:182:PHE:CE1	1:E:183:ARG:HG3	2.35	0.61
1:F:61:LYS:O	1:F:62:GLY:O	2.18	0.61
1:G:228:GLN:CG	1:G:368:PHE:HE2	2.13	0.61
1:I:228:GLN:HG2	1:I:368:PHE:CE2	2.34	0.61
1:I:286:ARG:NH1	3:I:503:AQH:H17	2.16	0.61
1:L:265:PHE:CE1	1:E:368:PHE:CE2	2.88	0.61
1:C:170:TYR:CE2	1:C:177:ASN:CB	2.84	0.61
1:E:115:PHE:N	1:E:116:PRO:CD	2.63	0.61
1:E:170:TYR:CD2	1:E:177:ASN:HB2	2.36	0.61
1:E:170:TYR:HE2	1:E:177:ASN:HB3	1.65	0.61
1:G:182:PHE:C	1:G:182:PHE:HD1	2.04	0.61
1:G:286:ARG:HH11	3:G:502:AQH:H17	1.66	0.61
1:I:10:ILE:O	1:I:10:ILE:HG23	2.00	0.61
1:J:170:TYR:CE2	1:J:177:ASN:CB	2.83	0.61
1:L:107:THR:CG2	1:L:111:LEU:CD1	2.79	0.61
1:I:339:CYS:O	1:I:370:CYS:CB	2.49	0.61
1:I:189:ARG:HD3	4:I:502:EDO:H12	1.82	0.61
1:L:16:PRO:HB3	1:L:27:ASP:HB2	1.81	0.61
1:B:263:GLN:O	1:B:264:GLY:C	2.37	0.61
3:B:502:AQH:O1A	3:B:502:AQH:H13	2.01	0.61
1:D:16:PRO:HB2	1:D:25:PHE:HB3	1.81	0.61
1:D:21:PRO:HD2	1:D:88:LEU:HD12	1.83	0.61
1:L:225:SER:C	1:L:226:THR:HG23	2.21	0.61
1:G:360:ARG:O	1:G:361:HIS:CE1	2.53	0.61
1:H:21:PRO:HD2	1:H:88:LEU:HD12	1.83	0.61
1:I:219:VAL:HG21	1:I:295:PHE:HE1	1.65	0.61
1:C:107:THR:HG1	3:C:503:AQH:PA	2.22	0.60
1:D:114:TRP:NE1	1:D:188:HIS:HA	2.15	0.60
1:D:228:GLN:HB2	1:D:355:PHE:CE1	2.36	0.60
1:F:35:LEU:HD13	1:F:63:TRP:CE2	2.36	0.60
1:K:277:PHE:O	1:K:286:ARG:NH2	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:265:PHE:CD1	1:E:368:PHE:CD2	2.88	0.60
1:A:115:PHE:N	1:A:116:PRO:CD	2.62	0.60
1:G:115:PHE:N	1:G:116:PRO:CD	2.64	0.60
1:I:170:TYR:CD2	1:I:177:ASN:HB2	2.36	0.60
1:D:104:PRO:O	1:D:105:THR:HG23	1.89	0.60
1:F:170:TYR:CE2	1:F:177:ASN:CB	2.83	0.60
1:I:115:PHE:N	1:I:116:PRO:CD	2.64	0.60
1:B:29:ASN:O	1:B:164:THR:HB	2.01	0.60
1:I:219:VAL:CG2	1:I:295:PHE:HE1	2.15	0.60
1:K:9:PHE:CD1	1:K:105:THR:OG1	2.54	0.60
1:B:182:PHE:HD1	1:B:182:PHE:C	2.04	0.60
1:C:170:TYR:CD2	1:C:177:ASN:HB2	2.36	0.60
1:H:169:LEU:HB3	1:H:182:PHE:HE2	1.66	0.60
1:E:106:GLY:HA2	1:E:111:LEU:HD11	1.81	0.60
1:F:361:HIS:HD2	1:F:366:ARG:HB2	1.67	0.60
1:L:238:TRP:HZ2	1:L:299:LEU:HD11	1.66	0.60
1:A:277:PHE:O	1:A:286:ARG:NH2	2.35	0.60
1:F:115:PHE:N	1:F:116:PRO:CD	2.65	0.60
1:L:208:LEU:HB3	1:L:291:ARG:HH11	1.67	0.60
1:B:103:PHE:O	1:B:104:PRO:O	2.19	0.60
1:C:10:ILE:HG23	1:C:10:ILE:O	2.01	0.60
1:D:169:LEU:HD22	1:D:182:PHE:CD2	2.35	0.60
1:G:16:PRO:HB3	1:G:27:ASP:HB2	1.84	0.60
1:I:170:TYR:HE2	1:I:177:ASN:HB3	1.65	0.60
1:A:170:TYR:CE2	1:A:177:ASN:HB3	2.36	0.60
1:A:169:LEU:HD22	1:A:182:PHE:CD2	2.37	0.60
1:I:103:PHE:CD2	1:I:111:LEU:HD21	2.37	0.60
1:A:27:ASP:OD1	1:A:28:PHE:N	2.35	0.60
1:B:16:PRO:HB2	1:B:25:PHE:HB3	1.84	0.60
1:F:301:SER:HA	3:F:502:AQH:C1'	2.31	0.59
1:K:16:PRO:HB2	1:K:25:PHE:HB3	1.82	0.59
1:L:42:HIS:CD2	1:L:56:CYS:SG	2.95	0.59
1:D:27:ASP:OD1	1:D:28:PHE:N	2.35	0.59
1:I:16:PRO:HB2	1:I:25:PHE:HB3	1.83	0.59
1:K:9:PHE:HB2	1:K:10:ILE:CD1	2.31	0.59
1:E:320:PHE:CE2	1:E:343:TRP:HB2	2.37	0.59
1:L:41:TRP:C	1:L:58:ASP:C	2.60	0.59
1:E:10:ILE:HD11	1:E:102:SER:OG	2.02	0.59
1:E:231:TYR:HE2	1:E:268:ASN:ND2	2.00	0.59
1:F:109:GLY:CA	3:F:502:AQH:H9	2.30	0.59
1:H:263:GLN:O	1:H:264:GLY:C	2.40	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:115:PHE:N	1:L:116:PRO:CD	2.65	0.59
1:B:205:ARG:HH11	1:B:205:ARG:CG	1.99	0.59
1:E:361:HIS:HD2	1:E:366:ARG:HB2	1.67	0.59
1:H:103:PHE:HB3	1:H:111:LEU:HD21	1.82	0.59
1:H:182:PHE:C	1:H:182:PHE:CD1	2.76	0.59
1:J:361:HIS:HD2	1:J:366:ARG:HB2	1.67	0.59
1:C:266:VAL:HG21	1:C:356:LEU:CD2	2.32	0.59
1:H:169:LEU:C	1:H:170:TYR:HD1	2.05	0.59
1:C:136:ASP:OD1	1:C:136:ASP:N	2.36	0.59
1:C:301:SER:HB2	3:C:503:AQH:H21	1.85	0.59
1:F:10:ILE:HD11	1:F:102:SER:OG	2.03	0.59
1:C:142:ALA:HB3	1:C:143:PRO:HD3	1.85	0.59
1:G:182:PHE:HD1	1:G:183:ARG:N	2.01	0.58
1:D:368:PHE:CD2	1:H:265:PHE:CE1	2.91	0.58
1:I:277:PHE:O	1:I:286:ARG:NH2	2.36	0.58
1:L:182:PHE:C	1:L:182:PHE:HD1	2.07	0.58
1:L:30:ASP:HB2	1:L:166:ARG:HH21	1.67	0.58
1:L:257:ARG:CB	3:L:502:AQH:C5	2.81	0.58
1:B:320:PHE:CE2	1:B:343:TRP:HB2	2.38	0.58
1:G:170:TYR:CD2	1:G:177:ASN:HB2	2.37	0.58
1:I:10:ILE:HD11	1:I:102:SER:OG	2.03	0.58
1:L:265:PHE:HD2	1:L:266:VAL:HG23	1.67	0.58
1:G:21:PRO:HD2	1:G:88:LEU:HD12	1.85	0.58
1:A:169:LEU:HD22	1:A:182:PHE:CE2	2.38	0.58
1:B:115:PHE:N	1:B:116:PRO:CD	2.66	0.58
1:C:16:PRO:HB2	1:C:25:PHE:HB3	1.85	0.58
1:G:227:CYS:SG	1:G:230:LYS:HE3	2.44	0.58
1:I:182:PHE:HD1	1:I:182:PHE:C	2.07	0.58
1:C:24:ILE:HG12	1:C:37:PRO:HD2	1.84	0.58
1:D:169:LEU:HD22	1:D:182:PHE:HE2	1.68	0.58
1:F:21:PRO:HD2	1:F:88:LEU:HD12	1.85	0.58
1:I:182:PHE:HD1	1:I:183:ARG:N	2.02	0.58
1:L:320:PHE:CE2	1:L:343:TRP:HB2	2.39	0.58
1:L:21:PRO:HD2	1:L:88:LEU:HD12	1.83	0.58
1:B:170:TYR:CE2	1:B:177:ASN:CB	2.87	0.58
1:D:112:LEU:O	1:D:116:PRO:HD3	2.03	0.58
1:G:182:PHE:CD1	1:G:182:PHE:C	2.76	0.58
1:H:320:PHE:CE2	1:H:343:TRP:HB2	2.39	0.58
1:A:182:PHE:HE1	1:A:183:ARG:HG3	1.67	0.58
1:D:345:ASP:OD2	1:D:360:ARG:NH1	2.36	0.58
1:L:307:ALA:C	1:L:312:ILE:HD11	2.22	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ASP:OD1	1:C:28:PHE:N	2.37	0.58
1:G:16:PRO:HB2	1:G:25:PHE:HB3	1.86	0.58
1:J:169:LEU:HB3	1:J:182:PHE:HE2	1.64	0.58
1:J:18:GLN:OE1	1:J:97:ARG:NH2	2.36	0.58
1:K:10:ILE:CG2	1:K:166:ARG:NH1	2.67	0.58
1:E:40:LYS:HB3	1:E:81:GLN:OE1	2.04	0.57
1:G:170:TYR:CE2	1:G:177:ASN:CB	2.87	0.57
1:I:295:PHE:CD2	1:I:386:LEU:HD23	2.39	0.57
1:I:318:SER:HB3	1:I:332:ARG:HH12	1.69	0.57
1:E:136:ASP:N	1:E:136:ASP:OD1	2.35	0.57
1:H:115:PHE:N	1:H:116:PRO:CD	2.68	0.57
1:I:334:PHE:HZ	1:I:340:TYR:HD2	1.49	0.57
1:L:189:ARG:NH2	1:L:324:ASN:O	2.37	0.57
1:L:230:LYS:O	1:L:230:LYS:CG	2.52	0.57
1:B:115:PHE:HE2	1:B:145:TYR:CD2	2.22	0.57
1:I:136:ASP:OD1	1:I:136:ASP:N	2.38	0.57
1:K:21:PRO:HD2	1:K:88:LEU:HD12	1.87	0.57
1:B:182:PHE:CD1	1:B:182:PHE:C	2.78	0.57
1:D:189:ARG:NH2	1:D:324:ASN:O	2.37	0.57
1:I:219:VAL:CG2	1:I:295:PHE:CE1	2.88	0.57
1:K:79:PHE:CZ	1:K:86:PRO:HD3	2.40	0.57
1:H:108:LEU:C	3:H:502:AQH:O1A	2.42	0.57
1:A:300:PRO:HD3	1:A:318:SER:HB2	1.87	0.57
1:B:170:TYR:CD2	1:B:177:ASN:HB2	2.39	0.57
1:F:182:PHE:HE1	1:F:183:ARG:HG3	1.69	0.57
1:I:182:PHE:CD1	1:I:182:PHE:C	2.78	0.57
1:A:323:PRO:HA	1:A:332:ARG:HE	1.69	0.57
1:D:108:LEU:N	1:D:109:GLY:CA	2.68	0.57
1:I:103:PHE:CZ	1:I:115:PHE:HD1	2.22	0.57
1:L:291:ARG:HA	1:L:310:THR:CG2	2.34	0.57
3:D:502:AQH:H13	3:D:502:AQH:PA	2.45	0.57
1:J:27:ASP:OD1	1:J:28:PHE:N	2.38	0.57
1:F:159:VAL:O	1:F:160:ALA:HB3	2.05	0.57
1:F:169:LEU:CD2	1:F:182:PHE:CE2	2.88	0.57
1:F:392:GLU:O	1:F:393:GLN:C	2.43	0.57
1:K:103:PHE:CE2	1:K:115:PHE:HD1	2.23	0.57
3:C:503:AQH:O3A	3:C:503:AQH:O	2.22	0.57
1:E:205:ARG:NH1	1:E:205:ARG:HG3	2.16	0.57
1:G:343:TRP:CD1	1:G:344:ASP:N	2.73	0.56
3:G:502:AQH:H26	3:G:502:AQH:H22	1.87	0.56
1:L:182:PHE:C	1:L:182:PHE:CD1	2.79	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:TYR:HE2	1:C:177:ASN:HB3	1.67	0.56
1:E:169:LEU:HD21	1:E:187:PHE:HB2	1.87	0.56
1:K:10:ILE:CD1	1:K:10:ILE:N	2.62	0.56
1:C:277:PHE:O	1:C:286:ARG:NH2	2.39	0.56
1:G:107:THR:O	1:G:108:LEU:O	2.23	0.56
1:L:232:TRP:HH2	1:L:237:GLY:CA	2.15	0.56
1:I:104:PRO:HD2	1:I:114:TRP:HZ3	1.69	0.56
1:J:60:ASP:N	1:J:60:ASP:OD1	2.39	0.56
1:K:136:ASP:OD1	1:K:136:ASP:N	2.34	0.56
1:K:110:ALA:N	3:K:502:AQH:O3'	2.38	0.56
1:J:16:PRO:HB2	1:J:25:PHE:HB3	1.87	0.56
1:H:265:PHE:CE2	1:H:266:VAL:HG23	2.41	0.56
1:B:40:LYS:HB3	1:B:81:GLN:OE1	2.06	0.56
1:I:331:TRP:CE2	1:I:386:LEU:HD13	2.41	0.56
1:J:225:SER:N	1:J:231:TYR:CE1	2.73	0.56
1:L:169:LEU:HD21	1:L:187:PHE:HB2	1.88	0.56
1:A:187:PHE:CE1	3:A:502:AQH:O4'	2.59	0.56
1:C:122:GLN:C	1:C:122:GLN:OE1	2.45	0.56
1:C:361:HIS:HD2	1:C:366:ARG:HB2	1.71	0.56
1:D:55:PHE:HE2	1:D:57:CYS:HG	1.51	0.56
1:L:265:PHE:CD2	1:L:266:VAL:HG23	2.40	0.56
1:B:136:ASP:OD1	1:B:136:ASP:N	2.37	0.55
1:G:187:PHE:CE1	3:G:502:AQH:O4'	2.58	0.55
1:I:103:PHE:CD2	1:I:111:LEU:HD22	2.41	0.55
1:I:361:HIS:HD2	1:I:366:ARG:HB2	1.71	0.55
1:G:18:GLN:OE1	1:G:97:ARG:NH2	2.40	0.55
1:H:265:PHE:O	1:H:266:VAL:HB	2.05	0.55
1:I:142:ALA:HB3	1:I:143:PRO:HD3	1.88	0.55
1:I:40:LYS:HB3	1:I:81:GLN:OE1	2.05	0.55
1:J:225:SER:N	1:J:231:TYR:CZ	2.57	0.55
1:L:265:PHE:HE1	1:E:368:PHE:HE2	1.52	0.55
1:K:142:ALA:HB3	1:K:143:PRO:HD3	1.89	0.55
1:K:9:PHE:CE1	1:K:105:THR:OG1	2.55	0.55
1:J:142:ALA:HB3	1:J:143:PRO:HD3	1.86	0.55
1:J:257:ARG:HD3	3:J:503:AQH:C5	2.35	0.55
1:K:182:PHE:CD1	1:K:183:ARG:N	2.74	0.55
1:L:238:TRP:CZ2	1:L:299:LEU:HD21	2.41	0.55
1:E:182:PHE:C	1:E:182:PHE:CD1	2.80	0.55
1:E:399:LEU:C	1:E:399:LEU:HD23	2.27	0.55
1:E:61:LYS:HG2	1:E:62:GLY:N	2.22	0.55
1:G:142:ALA:HB3	1:G:143:PRO:HD3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:339:CYS:C	1:K:370:CYS:HB3	2.13	0.55
1:K:79:PHE:HZ	1:K:86:PRO:HD3	1.70	0.55
1:A:301:SER:HA	3:A:502:AQH:O3B	2.07	0.55
1:C:36:LEU:CD2	1:C:36:LEU:N	2.30	0.55
1:E:106:GLY:CA	1:E:134:SER:OG	2.47	0.55
1:F:300:PRO:O	3:F:502:AQH:H6	2.07	0.55
1:L:169:LEU:HD23	1:L:182:PHE:CD2	2.41	0.55
1:B:361:HIS:HD2	1:B:366:ARG:HB2	1.72	0.55
1:D:286:ARG:NH1	3:D:502:AQH:C2	2.69	0.55
1:F:257:ARG:HD3	3:F:502:AQH:N7	2.22	0.55
1:G:108:LEU:CD2	1:G:109:GLY:H	2.15	0.55
1:C:230:LYS:CE	3:C:503:AQH:O6'	2.54	0.55
1:E:16:PRO:HB2	1:E:25:PHE:HB3	1.87	0.55
1:E:231:TYR:CE2	1:E:268:ASN:CG	2.80	0.55
3:C:503:AQH:O4'	3:C:503:AQH:H2	2.06	0.55
1:A:10:ILE:HG23	1:A:10:ILE:O	2.07	0.55
1:H:136:ASP:N	1:H:136:ASP:OD1	2.40	0.55
1:J:103:PHE:HB3	1:J:104:PRO:HD2	1.89	0.55
1:J:108:LEU:O	1:J:108:LEU:HD23	2.07	0.55
1:J:299:LEU:O	1:J:304:SER:OG	2.16	0.55
3:L:502:AQH:O	3:L:502:AQH:O2B	2.25	0.55
1:K:10:ILE:CD1	1:K:102:SER:OG	2.56	0.54
1:F:169:LEU:CD2	1:F:182:PHE:HE2	2.20	0.54
1:H:10:ILE:O	1:H:10:ILE:HG23	2.06	0.54
1:K:78:VAL:HG22	1:K:88:LEU:HB3	1.76	0.54
1:G:35:LEU:CD1	1:G:63:TRP:NE1	2.59	0.54
1:K:182:PHE:HD1	1:K:183:ARG:N	2.06	0.54
1:B:182:PHE:CD1	1:B:183:ARG:N	2.72	0.54
1:D:169:LEU:CD2	1:D:182:PHE:CD2	2.90	0.54
1:J:182:PHE:HD1	1:J:183:ARG:N	2.06	0.54
1:F:107:THR:HG1	3:F:502:AQH:PA	2.24	0.54
1:K:78:VAL:HG21	1:K:88:LEU:CB	2.30	0.54
1:L:263:GLN:O	1:L:264:GLY:O	2.26	0.54
1:L:298:GLY:C	1:L:304:SER:OG	2.46	0.54
1:C:300:PRO:HD3	1:C:318:SER:HB2	1.90	0.54
1:L:302:GLY:O	1:L:304:SER:N	2.40	0.54
1:G:363:ASN:H	1:G:367:GLN:NE2	2.05	0.54
1:H:142:ALA:N	1:H:143:PRO:CD	2.71	0.54
1:K:189:ARG:NH2	1:K:324:ASN:O	2.41	0.54
1:L:263:GLN:O	1:L:264:GLY:C	2.44	0.54
1:L:265:PHE:HE1	1:E:368:PHE:CE2	2.24	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:TYR:CE2	1:E:268:ASN:ND2	2.76	0.54
1:F:320:PHE:CE2	1:F:343:TRP:HB2	2.43	0.54
1:G:189:ARG:NH1	1:G:324:ASN:O	2.41	0.54
1:K:205:ARG:HH11	1:K:205:ARG:HB2	1.73	0.54
1:K:299:LEU:O	1:K:304:SER:OG	2.16	0.54
1:C:40:LYS:HB3	1:C:81:GLN:OE1	2.07	0.54
1:D:110:ALA:CA	1:D:137:ILE:CD1	2.67	0.54
1:D:110:ALA:HA	1:D:137:ILE:CD1	2.38	0.54
1:H:286:ARG:HH11	3:H:502:AQH:H17	1.73	0.54
1:L:299:LEU:O	1:L:304:SER:OG	2.23	0.54
1:D:331:TRP:CE2	1:D:386:LEU:HD13	2.43	0.54
3:D:502:AQH:H13	3:D:502:AQH:O1A	2.08	0.54
1:F:295:PHE:CD2	1:F:386:LEU:CD2	2.91	0.54
1:G:29:ASN:O	1:G:164:THR:HB	2.08	0.54
1:H:107:THR:O	1:H:107:THR:HG23	2.08	0.54
1:J:30:ASP:HB2	1:J:166:ARG:HH21	1.73	0.54
1:L:230:LYS:HG3	1:L:320:PHE:HE1	1.51	0.54
1:B:331:TRP:CE2	1:B:386:LEU:HD13	2.43	0.53
1:J:182:PHE:CD1	1:J:183:ARG:N	2.76	0.53
1:K:337:HIS:CD2	1:J:54:LEU:HD21	2.42	0.53
1:L:106:GLY:O	1:L:108:LEU:HB3	2.09	0.53
1:L:232:TRP:O	1:L:371:THR:CB	2.56	0.53
1:B:205:ARG:NH1	1:B:205:ARG:CG	2.65	0.53
1:G:185:VAL:O	1:G:189:ARG:NE	2.41	0.53
1:I:18:GLN:OE1	1:I:97:ARG:NH2	2.41	0.53
1:D:300:PRO:HD3	1:D:318:SER:HB2	1.90	0.53
1:I:21:PRO:HD2	1:I:88:LEU:HD12	1.90	0.53
1:C:342:CYS:SG	1:C:370:CYS:SG	3.07	0.53
1:F:144:GLN:C	1:F:145:TYR:HD1	2.11	0.53
1:H:170:TYR:HD1	1:H:170:TYR:N	2.07	0.53
1:L:80:ARG:HG2	1:L:80:ARG:HH11	1.72	0.53
1:C:182:PHE:CD1	1:C:183:ARG:N	2.77	0.53
1:E:142:ALA:HB3	1:E:143:PRO:HD3	1.90	0.53
1:F:33:ARG:HG2	1:F:65:THR:HG22	1.89	0.53
1:I:366:ARG:HE	1:I:369:GLU:CD	2.11	0.53
1:J:224:GLN:HA	1:J:231:TYR:CE2	2.43	0.53
1:L:291:ARG:HA	1:L:310:THR:HG21	1.91	0.53
1:B:142:ALA:HB3	1:B:143:PRO:HD3	1.91	0.53
1:D:189:ARG:NH1	1:D:201:GLU:OE1	2.41	0.53
1:J:115:PHE:N	1:J:116:PRO:HD2	2.24	0.53
1:K:331:TRP:CE2	1:K:386:LEU:HD13	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:233:ASN:HD22	1:L:368:PHE:HB3	1.73	0.53
1:B:300:PRO:HD3	1:B:318:SER:HB2	1.91	0.53
1:I:295:PHE:HD2	1:I:386:LEU:HD21	1.73	0.53
1:L:142:ALA:N	1:L:143:PRO:CD	2.72	0.53
1:L:182:PHE:CD1	1:L:183:ARG:N	2.76	0.53
1:B:230:LYS:NZ	3:B:502:AQH:O1B	2.41	0.53
1:C:10:ILE:HD11	1:C:102:SER:OG	2.09	0.53
1:D:169:LEU:CD2	1:D:182:PHE:HD2	2.22	0.53
1:E:189:ARG:NH1	1:E:201:GLU:OE1	2.41	0.53
1:K:30:ASP:HB2	1:K:166:ARG:HH21	1.74	0.53
1:L:205:ARG:HH11	1:L:205:ARG:HB2	1.74	0.53
1:A:170:TYR:CE2	1:A:177:ASN:HB2	2.40	0.52
1:C:320:PHE:CE2	1:C:343:TRP:HB2	2.44	0.52
1:F:10:ILE:HD11	1:F:102:SER:CB	2.38	0.52
1:I:144:GLN:C	1:I:145:TYR:HD1	2.12	0.52
1:K:169:LEU:CD2	1:K:182:PHE:CD2	2.92	0.52
1:F:142:ALA:HB3	1:F:143:PRO:HD3	1.90	0.52
1:G:339:CYS:SG	1:G:342:CYS:SG	3.07	0.52
1:J:142:ALA:N	1:J:143:PRO:CD	2.72	0.52
1:K:300:PRO:HD3	1:K:318:SER:HB2	1.91	0.52
1:K:320:PHE:CE2	1:K:343:TRP:HB2	2.44	0.52
1:C:182:PHE:HE1	1:C:183:ARG:HG3	1.69	0.52
1:E:106:GLY:HA3	1:E:134:SER:HG	1.73	0.52
1:A:142:ALA:N	1:A:143:PRO:CD	2.73	0.52
1:C:18:GLN:OE1	1:C:97:ARG:NH2	2.40	0.52
1:D:110:ALA:HB2	1:D:137:ILE:HD13	1.75	0.52
1:D:136:ASP:OD1	1:D:136:ASP:N	2.40	0.52
1:E:149:GLN:OE1	1:E:157:ARG:HD3	2.09	0.52
1:G:368:PHE:N	1:G:368:PHE:CD1	2.77	0.52
1:H:182:PHE:CD1	1:H:183:ARG:HG3	2.44	0.52
1:H:300:PRO:HD3	1:H:318:SER:HB2	1.91	0.52
1:L:136:ASP:OD1	1:L:136:ASP:N	2.37	0.52
1:L:169:LEU:HD23	1:L:182:PHE:CE2	2.44	0.52
1:A:320:PHE:CE2	1:A:343:TRP:HB2	2.45	0.52
1:C:339:CYS:SG	1:C:370:CYS:SG	3.04	0.52
1:F:115:PHE:N	1:F:116:PRO:HD2	2.25	0.52
1:H:142:ALA:HB3	1:H:143:PRO:HD3	1.92	0.52
1:J:342:CYS:SG	1:J:370:CYS:SG	3.06	0.52
1:E:106:GLY:HA2	1:E:111:LEU:CD1	2.40	0.52
1:F:16:PRO:HB3	1:F:27:ASP:HB2	1.91	0.52
1:J:320:PHE:CE2	1:J:343:TRP:HB2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:299:LEU:CB	1:K:300:PRO:HD2	2.33	0.52
1:D:302:GLY:N	3:D:502:AQH:O1A	2.43	0.52
1:E:108:LEU:N	3:E:502:AQH:O1A	2.42	0.52
1:F:142:ALA:N	1:F:143:PRO:CD	2.73	0.52
1:H:169:LEU:HD21	1:H:187:PHE:HB2	1.92	0.52
1:C:200:ARG:HA	4:C:502:EDO:H11	1.92	0.52
1:F:136:ASP:OD1	1:F:136:ASP:N	2.40	0.52
1:F:182:PHE:CD1	1:F:183:ARG:N	2.77	0.52
1:A:360:ARG:O	1:A:361:HIS:ND1	2.33	0.52
1:E:142:ALA:N	1:E:143:PRO:CD	2.73	0.52
1:H:144:GLN:C	1:H:145:TYR:HD1	2.13	0.52
1:E:368:PHE:O	1:E:372:ARG:HG3	2.09	0.52
1:F:107:THR:CB	3:F:502:AQH:O2A	2.58	0.52
1:I:145:TYR:HD1	1:I:145:TYR:N	2.08	0.52
1:K:299:LEU:HB3	1:K:300:PRO:CD	2.33	0.52
1:L:115:PHE:HE2	1:L:145:TYR:CD2	2.28	0.52
1:C:115:PHE:N	1:C:116:PRO:HD2	2.24	0.51
1:C:144:GLN:C	1:C:145:TYR:HD1	2.13	0.51
1:D:142:ALA:HB3	1:D:143:PRO:HD3	1.93	0.51
1:E:257:ARG:HB2	3:E:502:AQH:C4	2.39	0.51
1:G:115:PHE:HE2	1:G:145:TYR:CD2	2.28	0.51
1:H:170:TYR:CD1	1:H:170:TYR:N	2.78	0.51
3:L:502:AQH:H23	3:L:502:AQH:O1B	2.11	0.51
1:E:108:LEU:HD11	1:E:303:LEU:N	2.25	0.51
1:E:144:GLN:C	1:E:145:TYR:HD1	2.14	0.51
1:G:142:ALA:N	1:G:143:PRO:CD	2.73	0.51
1:G:182:PHE:CD1	1:G:183:ARG:N	2.78	0.51
1:J:300:PRO:CB	3:J:503:AQH:O6'	2.55	0.51
1:K:142:ALA:N	1:K:143:PRO:CD	2.73	0.51
1:K:170:TYR:CE2	1:K:177:ASN:CB	2.93	0.51
1:L:331:TRP:CE2	1:L:386:LEU:HD13	2.45	0.51
1:D:142:ALA:N	1:D:143:PRO:CD	2.73	0.51
1:E:115:PHE:N	1:E:116:PRO:HD2	2.25	0.51
1:E:80:ARG:O	1:E:82:GLY:N	2.44	0.51
1:J:104:PRO:C	1:J:106:GLY:N	2.62	0.51
1:K:115:PHE:N	1:K:116:PRO:HD2	2.25	0.51
1:B:107:THR:O	1:B:111:LEU:HB2	2.11	0.51
1:C:142:ALA:N	1:C:143:PRO:CD	2.74	0.51
1:G:299:LEU:CB	1:G:300:PRO:HD2	2.34	0.51
1:L:43:VAL:CA	1:L:57:CYS:O	2.56	0.51
1:A:40:LYS:HB3	1:A:81:GLN:OE1	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:356:LEU:N	1:G:356:LEU:CD2	2.74	0.51
1:G:228:GLN:HG3	1:G:368:PHE:CE2	2.43	0.51
1:H:115:PHE:HE2	1:H:145:TYR:CD2	2.28	0.51
1:I:145:TYR:N	1:I:145:TYR:CD1	2.79	0.51
1:J:115:PHE:HE2	1:J:145:TYR:CD2	2.29	0.51
1:J:342:CYS:SG	1:J:358:CYS:SG	3.07	0.51
1:L:227:CYS:O	1:L:230:LYS:CE	2.59	0.51
1:D:114:TRP:CD1	1:D:188:HIS:HA	2.46	0.51
1:H:103:PHE:HB3	1:H:104:PRO:HD2	1.92	0.51
1:I:115:PHE:N	1:I:116:PRO:HD2	2.26	0.51
1:L:296:PHE:CE2	1:L:298:GLY:C	2.81	0.51
1:A:182:PHE:CD1	1:A:183:ARG:N	2.79	0.51
1:B:115:PHE:N	1:B:116:PRO:HD2	2.26	0.51
1:B:182:PHE:CD1	1:B:183:ARG:HG3	2.46	0.51
1:B:97:ARG:HH11	1:B:97:ARG:CG	2.24	0.51
1:C:354:ASP:HB3	1:C:357:TRP:HB2	1.92	0.51
1:L:182:PHE:HE1	1:L:183:ARG:HG3	1.72	0.51
1:C:357:TRP:O	1:C:357:TRP:CE3	2.63	0.50
1:D:30:ASP:HB2	1:D:166:ARG:HH21	1.76	0.50
1:F:145:TYR:HD1	1:F:145:TYR:N	2.09	0.50
1:H:339:CYS:SG	1:H:370:CYS:SG	3.06	0.50
1:I:142:ALA:N	1:I:143:PRO:CD	2.73	0.50
1:L:115:PHE:N	1:L:116:PRO:HD2	2.27	0.50
1:L:312:ILE:H	1:L:312:ILE:HD12	1.76	0.50
1:L:342:CYS:SG	1:L:370:CYS:SG	3.10	0.50
1:C:318:SER:HB3	1:C:332:ARG:NH1	2.26	0.50
1:C:34:VAL:HG22	1:C:36:LEU:HD13	1.92	0.50
1:E:182:PHE:HD1	1:E:182:PHE:C	2.14	0.50
1:G:357:TRP:CG	1:G:357:TRP:O	2.63	0.50
1:K:169:LEU:CD2	1:K:182:PHE:HD2	2.24	0.50
1:B:286:ARG:NH1	3:B:502:AQH:C2	2.73	0.50
1:E:145:TYR:HE1	1:E:205:ARG:HB2	1.76	0.50
1:E:300:PRO:HD3	1:E:318:SER:HB2	1.93	0.50
1:E:331:TRP:CE2	1:E:386:LEU:HD13	2.47	0.50
1:L:230:LYS:HB3	1:L:320:PHE:CD1	2.46	0.50
1:L:80:ARG:HH11	1:L:80:ARG:CG	2.24	0.50
1:D:227:CYS:SG	1:D:230:LYS:HE3	2.52	0.50
1:I:169:LEU:HB3	1:I:182:PHE:HE2	1.77	0.50
1:J:136:ASP:N	1:J:136:ASP:OD1	2.39	0.50
1:K:181:ASP:HB3	1:K:184:LYS:HG3	1.93	0.50
1:L:228:GLN:NE2	1:L:231:TYR:CD2	2.80	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ALA:N	1:B:143:PRO:CD	2.75	0.50
1:L:103:PHE:CE1	1:L:167:VAL:HG21	2.46	0.50
1:I:27:ASP:CG	1:I:28:PHE:N	2.52	0.50
1:I:38:GLU:O	1:I:38:GLU:HG3	2.11	0.50
1:K:115:PHE:HE2	1:K:145:TYR:CD2	2.29	0.50
1:A:295:PHE:CD2	1:A:386:LEU:HD23	2.47	0.50
1:C:169:LEU:CD2	1:C:182:PHE:CE2	2.58	0.50
1:E:296:PHE:CE2	1:E:298:GLY:HA3	2.46	0.50
1:F:189:ARG:HG3	1:F:189:ARG:HH11	1.76	0.50
1:F:339:CYS:SG	1:F:370:CYS:SG	3.08	0.50
1:K:10:ILE:HG21	1:K:166:ARG:NH1	2.27	0.50
1:K:170:TYR:CD2	1:K:177:ASN:HB2	2.46	0.50
1:A:296:PHE:CE2	1:A:298:GLY:HA3	2.47	0.50
1:H:295:PHE:CD2	1:H:386:LEU:HD23	2.47	0.50
1:K:230:LYS:HG2	1:K:320:PHE:CE1	2.47	0.50
1:E:115:PHE:HE2	1:E:145:TYR:CD2	2.30	0.50
1:F:10:ILE:HD11	1:F:102:SER:HB2	1.94	0.50
1:F:279:GLY:O	1:F:286:ARG:NH1	2.44	0.50
1:F:296:PHE:CE2	1:F:298:GLY:HA3	2.47	0.50
1:F:94:LEU:O	1:F:127:CYS:HB3	2.12	0.50
1:H:112:LEU:HD22	1:H:204:VAL:HG21	1.93	0.50
1:I:22:GLU:OE2	1:I:87:LEU:HD11	2.12	0.50
1:J:300:PRO:HD3	1:J:318:SER:HB2	1.93	0.50
1:A:71:PHE:HD1	1:A:165:TYR:OH	1.94	0.49
1:D:205:ARG:HH11	1:D:205:ARG:HB2	1.76	0.49
1:D:391:THR:CG2	1:D:391:THR:O	2.43	0.49
1:L:107:THR:OG1	1:L:111:LEU:CD1	2.55	0.49
1:B:295:PHE:CD2	1:B:386:LEU:CD2	2.95	0.49
1:F:205:ARG:NH1	1:F:205:ARG:CG	2.63	0.49
1:F:342:CYS:SG	1:F:370:CYS:SG	3.10	0.49
1:A:115:PHE:HE2	1:A:145:TYR:CD2	2.30	0.49
1:G:331:TRP:CE2	1:G:386:LEU:HD13	2.47	0.49
1:H:145:TYR:HD1	1:H:145:TYR:N	2.09	0.49
1:H:182:PHE:CD1	1:H:183:ARG:N	2.74	0.49
1:I:170:TYR:CE2	1:I:177:ASN:HB2	2.48	0.49
1:L:142:ALA:HB3	1:L:143:PRO:HD3	1.94	0.49
1:D:169:LEU:HD23	1:D:182:PHE:HD2	1.78	0.49
1:E:299:LEU:O	1:E:304:SER:OG	2.15	0.49
1:F:331:TRP:CE2	1:F:386:LEU:HD13	2.46	0.49
1:J:230:LYS:HG2	1:J:320:PHE:CE1	2.47	0.49
1:K:318:SER:HB3	1:K:332:ARG:NH1	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:300:PRO:O	3:K:502:AQH:H6	2.11	0.49
1:A:331:TRP:CE2	1:A:386:LEU:HD13	2.47	0.49
1:C:331:TRP:CE2	1:C:386:LEU:HD13	2.48	0.49
1:G:189:ARG:O	1:G:192:GLY:N	2.45	0.49
1:J:170:TYR:CE2	1:J:177:ASN:HB3	2.47	0.49
1:J:295:PHE:CD2	1:J:386:LEU:CD2	2.95	0.49
1:A:205:ARG:NH1	1:A:205:ARG:CG	2.59	0.49
1:C:132:THR:HA	1:C:151:SER:O	2.13	0.49
1:D:170:TYR:CE2	1:D:177:ASN:HB2	2.47	0.49
1:H:145:TYR:CD1	1:H:145:TYR:N	2.80	0.49
1:I:340:TYR:N	1:I:340:TYR:HD1	2.09	0.49
1:C:354:ASP:OD2	1:C:357:TRP:HA	2.13	0.49
3:F:502:AQH:H26	3:F:502:AQH:H22	1.94	0.49
1:B:145:TYR:CD1	1:B:145:TYR:N	2.81	0.49
1:C:189:ARG:HH11	1:C:189:ARG:HG3	1.77	0.49
1:G:320:PHE:CE2	1:G:343:TRP:HB3	2.48	0.49
1:I:104:PRO:CD	1:I:114:TRP:HZ3	2.25	0.49
1:L:103:PHE:CE1	1:L:167:VAL:CG2	2.96	0.49
1:L:230:LYS:CD	1:L:230:LYS:N	2.75	0.49
1:L:302:GLY:C	1:L:304:SER:N	2.66	0.49
1:A:115:PHE:N	1:A:116:PRO:HD2	2.26	0.49
1:A:299:LEU:CB	1:A:300:PRO:HD2	2.39	0.49
1:C:145:TYR:CD1	1:C:145:TYR:N	2.81	0.49
1:D:370:CYS:HG	2:D:501:FE:FE	1.29	0.49
1:F:145:TYR:CD1	1:F:145:TYR:N	2.81	0.49
1:F:300:PRO:HD3	1:F:318:SER:HB2	1.95	0.49
1:H:342:CYS:SG	1:H:370:CYS:SG	3.10	0.49
1:L:318:SER:HB3	1:L:332:ARG:NH1	2.28	0.49
1:B:169:LEU:HB3	1:B:182:PHE:CE2	2.47	0.49
1:D:115:PHE:HE2	1:D:145:TYR:CD2	2.30	0.49
1:E:318:SER:HB3	1:E:332:ARG:NH1	2.28	0.49
1:E:367:GLN:O	1:E:372:ARG:NH1	2.46	0.49
1:G:35:LEU:CD1	1:G:63:TRP:HE1	2.10	0.49
1:I:342:CYS:SG	1:I:358:CYS:SG	3.07	0.49
1:I:80:ARG:HH11	1:I:80:ARG:HG2	1.78	0.49
1:E:54:LEU:HD21	1:A:337:HIS:CD2	2.48	0.48
1:D:230:LYS:HG2	1:D:320:PHE:CE1	2.48	0.48
1:E:399:LEU:CD2	1:E:399:LEU:N	2.74	0.48
1:G:106:GLY:HA3	1:G:134:SER:OG	2.13	0.48
1:I:182:PHE:CD1	1:I:183:ARG:N	2.81	0.48
1:A:169:LEU:CD2	1:A:182:PHE:HD2	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:SER:HA	3:A:502:AQH:C1'	2.43	0.48
1:B:299:LEU:HB3	1:B:300:PRO:CD	2.33	0.48
1:D:115:PHE:N	1:D:116:PRO:HD2	2.28	0.48
1:L:170:TYR:CD2	1:L:177:ASN:HB2	2.49	0.48
1:L:233:ASN:ND2	1:L:368:PHE:CB	2.74	0.48
1:L:312:ILE:N	1:L:312:ILE:CD1	2.74	0.48
1:A:295:PHE:N	1:A:295:PHE:CD1	2.81	0.48
1:B:257:ARG:HB3	3:B:502:AQH:O2'	2.14	0.48
1:D:300:PRO:O	3:D:502:AQH:H6	2.13	0.48
1:G:358:CYS:H	1:G:362:LYS:HB2	1.77	0.48
1:G:368:PHE:HD1	1:G:368:PHE:N	2.09	0.48
1:G:47:ASP:O	1:G:51:GLU:N	2.45	0.48
1:K:295:PHE:CD2	1:K:386:LEU:HD23	2.48	0.48
1:K:79:PHE:CZ	1:K:86:PRO:CD	2.97	0.48
1:L:286:ARG:HH12	3:L:502:AQH:C2	2.23	0.48
1:C:299:LEU:CB	1:C:300:PRO:HD2	2.35	0.48
3:K:502:AQH:C2'	3:K:502:AQH:PA	3.00	0.48
1:F:302:GLY:CA	3:F:502:AQH:C2'	2.90	0.48
1:H:301:SER:HA	3:H:502:AQH:H13	1.96	0.48
1:I:219:VAL:HG22	1:I:295:PHE:CE1	2.48	0.48
1:J:182:PHE:C	1:J:182:PHE:CD1	2.87	0.48
1:L:228:GLN:HB3	1:L:368:PHE:CZ	2.48	0.48
3:G:502:AQH:PB	3:G:502:AQH:H27	2.37	0.48
3:A:502:AQH:O3A	3:A:502:AQH:O	2.32	0.48
1:G:122:GLN:C	1:G:122:GLN:OE1	2.52	0.48
1:L:286:ARG:HH12	3:L:502:AQH:H17	1.76	0.48
1:B:145:TYR:HD1	1:B:145:TYR:N	2.11	0.48
1:C:295:PHE:CD2	1:C:386:LEU:HD23	2.48	0.48
1:F:182:PHE:CD1	1:F:183:ARG:HG3	2.48	0.48
1:H:265:PHE:O	1:H:266:VAL:CB	2.62	0.48
1:D:296:PHE:CE2	1:D:298:GLY:HA3	2.48	0.48
1:I:334:PHE:HZ	1:I:340:TYR:CD2	2.30	0.48
1:L:265:PHE:HD1	1:E:368:PHE:CD2	2.20	0.48
1:C:360:ARG:O	1:C:361:HIS:CG	2.67	0.48
1:E:42:HIS:C	1:E:42:HIS:CD2	2.88	0.48
3:E:502:AQH:H27	3:E:502:AQH:PB	2.36	0.48
1:G:354:ASP:CB	1:G:356:LEU:O	2.50	0.48
1:J:299:LEU:HB3	1:J:300:PRO:CD	2.36	0.48
1:A:142:ALA:HB3	1:A:143:PRO:HD3	1.94	0.47
1:H:108:LEU:O	3:H:502:AQH:PA	2.72	0.47
1:B:342:CYS:SG	1:B:370:CYS:SG	3.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LEU:CD2	1:C:62:GLY:O	2.62	0.47
1:G:205:ARG:HH11	1:G:205:ARG:HB2	1.80	0.47
1:J:296:PHE:CE2	1:J:298:GLY:HA3	2.49	0.47
1:L:112:LEU:O	1:L:204:VAL:HG13	2.14	0.47
1:L:232:TRP:CD1	1:L:371:THR:HB	2.33	0.47
1:L:42:HIS:HB3	1:L:79:PHE:HB2	1.94	0.47
1:B:107:THR:OG1	1:B:108:LEU:N	2.47	0.47
1:J:226:THR:O	1:J:355:PHE:CE1	2.67	0.47
1:J:40:LYS:HB3	1:J:81:GLN:OE1	2.14	0.47
1:K:9:PHE:C	1:K:10:ILE:HD12	2.32	0.47
1:L:145:TYR:CD1	1:L:145:TYR:N	2.82	0.47
1:C:299:LEU:HB3	1:C:300:PRO:CD	2.38	0.47
1:D:106:GLY:O	1:D:107:THR:CG2	2.57	0.47
1:D:47:ASP:O	1:D:51:GLU:N	2.46	0.47
1:I:300:PRO:HD3	1:I:318:SER:HB2	1.96	0.47
1:L:302:GLY:HA2	1:L:305:TRP:HD1	1.79	0.47
1:C:145:TYR:HE1	1:C:205:ARG:HB2	1.80	0.47
1:L:145:TYR:HD1	1:L:145:TYR:N	2.13	0.47
1:A:170:TYR:N	1:A:170:TYR:HD1	2.12	0.47
1:B:299:LEU:CB	1:B:300:PRO:HD2	2.33	0.47
1:G:35:LEU:HD12	1:G:63:TRP:CD1	2.47	0.47
1:K:182:PHE:C	1:K:182:PHE:CD1	2.85	0.47
1:A:169:LEU:C	1:A:170:TYR:HD1	2.17	0.47
1:B:170:TYR:CE2	1:B:177:ASN:HB3	2.50	0.47
1:B:318:SER:HB3	1:B:332:ARG:NH1	2.25	0.47
1:B:323:PRO:HA	1:B:332:ARG:HE	1.79	0.47
1:C:72:VAL:O	1:C:74:PHE:N	2.47	0.47
1:E:42:HIS:O	1:E:79:PHE:HB2	2.14	0.47
1:H:47:ASP:O	1:H:51:GLU:N	2.44	0.47
1:L:20:GLY:N	1:L:24:ILE:O	2.45	0.47
1:L:43:VAL:O	1:L:56:CYS:C	2.52	0.47
1:A:182:PHE:HD1	1:A:183:ARG:N	2.12	0.47
1:G:299:LEU:HB3	1:G:300:PRO:CD	2.36	0.47
1:H:106:GLY:N	1:H:107:THR:CG2	2.73	0.47
1:H:115:PHE:N	1:H:116:PRO:HD2	2.30	0.47
1:H:331:TRP:CE2	1:H:386:LEU:HD13	2.49	0.47
1:L:190:SER:O	1:L:194:ILE:HG13	2.14	0.47
1:A:170:TYR:N	1:A:170:TYR:CD1	2.83	0.47
1:C:61:LYS:HE2	1:C:61:LYS:HB3	1.48	0.47
1:D:182:PHE:CD1	1:D:183:ARG:N	2.82	0.47
1:D:265:PHE:HB3	1:H:372:ARG:HD2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:THR:OG1	3:E:502:AQH:O1A	2.31	0.47
1:H:169:LEU:HB3	1:H:182:PHE:CE2	2.48	0.47
1:H:187:PHE:CZ	3:H:502:AQH:O3'	2.64	0.47
1:H:296:PHE:CE2	1:H:298:GLY:HA3	2.50	0.47
1:I:115:PHE:CE1	1:I:133:MET:HE1	2.50	0.47
1:C:299:LEU:O	1:C:304:SER:OG	2.21	0.47
1:D:300:PRO:O	3:D:502:AQH:C5'	2.63	0.47
1:E:122:GLN:OE1	1:E:122:GLN:C	2.54	0.47
1:I:340:TYR:N	1:I:340:TYR:CD1	2.82	0.47
1:J:108:LEU:HD23	1:J:108:LEU:C	2.35	0.47
1:L:233:ASN:C	1:L:234:ASN:O	2.48	0.47
1:G:358:CYS:HB3	1:G:362:LYS:N	2.30	0.47
1:L:230:LYS:CB	1:L:320:PHE:CD1	2.98	0.47
1:L:286:ARG:NH1	3:L:502:AQH:N1	2.62	0.47
1:L:27:ASP:OD1	1:L:28:PHE:N	2.48	0.47
1:A:136:ASP:OD1	1:A:136:ASP:N	2.38	0.46
1:C:354:ASP:CG	1:C:357:TRP:HB2	2.35	0.46
1:F:122:GLN:O	1:F:122:GLN:OE1	2.33	0.46
1:F:295:PHE:HD2	1:F:386:LEU:CD2	2.27	0.46
1:G:115:PHE:N	1:G:116:PRO:HD2	2.29	0.46
1:G:120:ARG:NH1	1:G:198:ASP:O	2.48	0.46
1:K:182:PHE:CD1	1:K:183:ARG:HG3	2.48	0.46
1:L:228:GLN:HE22	1:L:231:TYR:HE2	1.59	0.46
1:C:266:VAL:HG21	1:C:356:LEU:HD22	1.97	0.46
1:F:230:LYS:HG2	1:F:320:PHE:CE1	2.49	0.46
1:I:47:ASP:O	1:I:51:GLU:N	2.46	0.46
1:B:144:GLN:C	1:B:145:TYR:HD1	2.19	0.46
1:I:42:HIS:O	1:I:79:PHE:HB2	2.16	0.46
1:D:299:LEU:C	1:D:301:SER:H	2.19	0.46
1:E:47:ASP:O	1:E:51:GLU:N	2.47	0.46
1:G:169:LEU:HD21	1:G:187:PHE:HB2	1.97	0.46
1:L:105:THR:HB	1:L:134:SER:HB3	1.98	0.46
1:I:169:LEU:HB3	1:I:182:PHE:CE2	2.51	0.46
1:L:296:PHE:CZ	1:L:298:GLY:N	2.66	0.46
1:D:299:LEU:O	1:D:304:SER:OG	2.18	0.46
1:E:393:GLN:O	1:E:397:ALA:HB2	2.15	0.46
1:G:348:LEU:HD22	1:G:359:PRO:HB3	1.97	0.46
1:H:301:SER:HA	3:H:502:AQH:C1'	2.45	0.46
1:H:61:LYS:HG2	1:H:62:GLY:N	2.28	0.46
1:L:43:VAL:CB	1:L:57:CYS:O	2.63	0.46
1:A:182:PHE:CD1	1:A:183:ARG:HG3	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:PHE:CE2	1:C:298:GLY:HA3	2.51	0.46
1:D:40:LYS:HB3	1:D:81:GLN:OE1	2.16	0.46
1:E:145:TYR:CD1	1:E:145:TYR:N	2.83	0.46
1:E:54:LEU:CD2	1:A:337:HIS:CD2	2.99	0.46
1:H:109:GLY:HA3	3:H:502:AQH:O2A	2.16	0.46
1:J:122:GLN:C	1:J:122:GLN:OE1	2.54	0.46
1:K:145:TYR:N	1:K:145:TYR:CD1	2.84	0.46
1:B:219:VAL:CG2	1:B:295:PHE:CE1	2.99	0.46
1:E:227:CYS:SG	1:E:230:LYS:HG3	2.56	0.46
1:G:35:LEU:HD12	1:G:63:TRP:HD1	1.81	0.46
1:H:42:HIS:NE2	1:H:56:CYS:SG	2.88	0.46
1:A:299:LEU:O	1:A:304:SER:OG	2.19	0.46
1:B:296:PHE:CE2	1:B:298:GLY:HA3	2.50	0.46
1:C:187:PHE:CE1	3:C:503:AQH:O4'	2.67	0.46
1:K:295:PHE:N	1:K:295:PHE:CD1	2.84	0.46
1:C:145:TYR:HE1	1:C:205:ARG:NH1	2.10	0.46
1:E:145:TYR:HD1	1:E:145:TYR:N	2.14	0.46
1:F:318:SER:HB3	1:F:332:ARG:NH1	2.30	0.46
1:I:169:LEU:HD21	1:I:187:PHE:HB2	1.97	0.46
1:K:10:ILE:CG2	1:K:166:ARG:HH12	2.29	0.46
1:L:170:TYR:CE2	1:L:177:ASN:CB	2.99	0.46
1:G:360:ARG:C	1:G:361:HIS:HD1	2.19	0.45
1:A:169:LEU:CD2	1:A:182:PHE:CD2	2.99	0.45
1:B:9:PHE:CD1	1:B:9:PHE:N	2.84	0.45
1:C:295:PHE:CD1	1:C:295:PHE:N	2.84	0.45
1:D:181:ASP:HB3	1:D:184:LYS:HG3	1.99	0.45
1:D:42:HIS:O	1:D:79:PHE:HB2	2.15	0.45
1:E:108:LEU:HD11	1:E:302:GLY:O	2.14	0.45
1:G:136:ASP:N	1:G:136:ASP:OD1	2.36	0.45
1:C:181:ASP:HB3	1:C:184:LYS:HG3	1.97	0.45
1:C:42:HIS:C	1:C:42:HIS:CD2	2.90	0.45
1:D:103:PHE:CG	1:D:111:LEU:HD13	2.52	0.45
1:G:187:PHE:HB3	1:G:343:TRP:HH2	1.81	0.45
1:H:286:ARG:NH1	3:H:502:AQH:H17	2.32	0.45
1:L:257:ARG:HB2	3:L:502:AQH:C5	2.47	0.45
1:B:257:ARG:HB2	3:B:502:AQH:C4	2.47	0.45
1:H:230:LYS:HG2	1:H:320:PHE:CE1	2.52	0.45
1:E:295:PHE:CD1	1:E:295:PHE:N	2.85	0.45
1:E:399:LEU:HD22	1:E:399:LEU:N	2.31	0.45
1:H:295:PHE:CD1	1:H:295:PHE:N	2.85	0.45
1:A:61:LYS:HG2	1:A:62:GLY:N	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:PHE:HE1	1:B:183:ARG:CG	2.26	0.45
3:D:502:AQH:H26	3:D:502:AQH:H22	1.99	0.45
1:E:182:PHE:HB2	1:E:187:PHE:HA	1.98	0.45
1:H:10:ILE:HD11	1:H:102:SER:OG	2.17	0.45
1:D:105:THR:HA	1:D:106:GLY:HA2	1.75	0.45
1:G:114:TRP:CH2	1:G:168:GLY:HA2	2.52	0.45
1:G:230:LYS:HG2	1:G:320:PHE:CE1	2.52	0.45
1:G:44:ARG:HD3	1:G:56:CYS:SG	2.56	0.45
1:H:10:ILE:O	1:H:10:ILE:CG2	2.63	0.45
1:I:30:ASP:HB2	1:I:166:ARG:HH21	1.82	0.45
1:J:109:GLY:HA3	3:J:503:AQH:O3'	2.17	0.45
1:J:331:TRP:CE2	1:J:386:LEU:HD13	2.51	0.45
1:L:361:HIS:HD2	1:L:366:ARG:CB	2.29	0.45
1:A:299:LEU:HB3	1:A:300:PRO:CD	2.41	0.45
1:C:354:ASP:CB	1:C:357:TRP:HB2	2.47	0.45
1:D:182:PHE:CD1	1:D:183:ARG:HG3	2.52	0.45
1:G:170:TYR:CE2	1:G:177:ASN:HB3	2.51	0.45
1:J:295:PHE:C	1:J:295:PHE:HD1	2.20	0.45
1:A:10:ILE:HD11	1:A:102:SER:OG	2.17	0.45
1:D:295:PHE:CD1	1:D:295:PHE:N	2.85	0.45
1:D:295:PHE:CD2	1:D:386:LEU:HD23	2.52	0.45
1:B:170:TYR:N	1:B:170:TYR:CD1	2.83	0.45
1:I:42:HIS:CD2	1:I:42:HIS:C	2.90	0.45
1:J:277:PHE:O	1:J:286:ARG:NH1	2.49	0.45
1:L:189:ARG:NH1	1:L:201:GLU:OE1	2.50	0.45
1:L:47:ASP:O	1:L:51:GLU:N	2.47	0.45
1:G:145:TYR:CD1	1:G:145:TYR:N	2.85	0.44
1:G:170:TYR:CD1	1:G:170:TYR:N	2.85	0.44
1:D:182:PHE:HE1	1:D:183:ARG:HG3	1.74	0.44
1:G:358:CYS:O	1:G:362:LYS:HB3	2.17	0.44
1:H:170:TYR:HE2	1:H:177:ASN:CB	2.27	0.44
1:K:169:LEU:HD23	1:K:182:PHE:HD2	1.83	0.44
1:L:182:PHE:CD1	1:L:183:ARG:HG3	2.51	0.44
1:D:110:ALA:HA	1:D:137:ILE:HD12	1.87	0.44
1:F:227:CYS:SG	1:F:230:LYS:HE3	2.57	0.44
1:G:42:HIS:CD2	1:G:42:HIS:C	2.90	0.44
1:H:105:THR:C	1:H:107:THR:CG2	2.85	0.44
1:H:170:TYR:CE2	1:H:177:ASN:HB2	2.45	0.44
1:I:393:GLN:H	1:I:393:GLN:HG2	1.60	0.44
3:I:503:AQH:PB	3:I:503:AQH:H27	2.38	0.44
1:J:170:TYR:N	1:J:170:TYR:CD1	2.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:PHE:CD1	1:C:183:ARG:HG3	2.49	0.44
1:D:105:THR:OG1	1:D:106:GLY:CA	2.65	0.44
1:G:145:TYR:HD1	1:G:145:TYR:N	2.16	0.44
1:J:205:ARG:NH1	1:J:205:ARG:CG	2.51	0.44
1:L:323:PRO:HA	1:L:332:ARG:NH2	2.32	0.44
1:A:182:PHE:CD1	1:A:182:PHE:C	2.90	0.44
1:A:339:CYS:SG	1:A:370:CYS:SG	3.09	0.44
1:F:182:PHE:HD1	1:F:183:ARG:N	2.15	0.44
1:I:301:SER:HA	3:I:503:AQH:H13	2.00	0.44
1:B:230:LYS:HG2	1:B:320:PHE:CE1	2.52	0.44
1:B:339:CYS:SG	1:B:370:CYS:SG	3.10	0.44
1:G:189:ARG:HG2	1:G:199:PRO:O	2.18	0.44
1:B:170:TYR:N	1:B:170:TYR:HD1	2.16	0.44
1:C:107:THR:HG1	1:C:108:LEU:N	2.16	0.44
1:E:302:GLY:O	1:E:305:TRP:N	2.50	0.44
3:G:502:AQH:H27	3:G:502:AQH:PA	2.37	0.44
1:H:230:LYS:HE2	3:H:502:AQH:O6'	2.18	0.44
1:L:107:THR:CB	1:L:108:LEU:HG	2.16	0.44
1:A:218:TYR:OH	1:A:289:LEU:O	2.27	0.44
1:B:169:LEU:HD21	1:B:187:PHE:HB2	1.99	0.44
1:H:55:PHE:HE2	1:H:57:CYS:HG	1.65	0.44
1:I:219:VAL:HG21	1:I:295:PHE:CE1	2.47	0.44
1:L:291:ARG:HA	1:L:310:THR:HG22	1.99	0.44
1:B:212:ARG:NE	1:B:214:ILE:O	2.51	0.44
1:B:295:PHE:HD2	1:B:386:LEU:CD2	2.31	0.44
1:C:30:ASP:HB2	1:C:166:ARG:HH21	1.83	0.44
1:C:358:CYS:O	1:C:362:LYS:HB2	2.18	0.44
1:D:18:GLN:NE2	1:D:18:GLN:HA	2.32	0.44
1:G:61:LYS:O	1:G:62:GLY:O	2.36	0.44
1:C:80:ARG:O	1:C:82:GLY:N	2.48	0.43
1:E:299:LEU:HB3	1:E:300:PRO:CD	2.37	0.43
1:E:230:LYS:HG2	1:E:320:PHE:CE1	2.52	0.43
1:F:181:ASP:HB3	1:F:184:LYS:HG3	2.00	0.43
1:F:42:HIS:O	1:F:79:PHE:HB2	2.17	0.43
1:G:42:HIS:HE2	1:G:56:CYS:HG	1.64	0.43
1:J:170:TYR:N	1:J:170:TYR:HD1	2.16	0.43
1:K:169:LEU:HD22	1:K:182:PHE:HE2	1.76	0.43
1:F:331:TRP:CZ2	1:F:386:LEU:HD13	2.53	0.43
1:I:182:PHE:CD1	1:I:183:ARG:HG3	2.53	0.43
1:I:323:PRO:HA	1:I:332:ARG:HE	1.83	0.43
1:K:227:CYS:SG	1:K:230:LYS:HE3	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:THR:CG2	1:L:153:PRO:HG2	2.48	0.43
1:E:30:ASP:HB2	1:E:166:ARG:HH21	1.83	0.43
1:E:342:CYS:SG	1:E:358:CYS:SG	3.06	0.43
1:G:145:TYR:CE1	1:G:205:ARG:NH1	2.87	0.43
1:H:189:ARG:NH1	1:H:201:GLU:OE1	2.51	0.43
1:B:189:ARG:HH11	1:B:189:ARG:HG3	1.83	0.43
1:E:182:PHE:CD1	1:E:183:ARG:N	2.87	0.43
1:F:299:LEU:CB	1:F:300:PRO:HD2	2.39	0.43
1:G:144:GLN:C	1:G:145:TYR:HD1	2.22	0.43
1:G:296:PHE:CE2	1:G:298:GLY:HA3	2.52	0.43
1:H:300:PRO:O	3:H:502:AQH:H6	2.19	0.43
1:L:228:GLN:OE1	1:L:228:GLN:HA	2.18	0.43
1:A:18:GLN:HE21	1:A:18:GLN:HA	1.84	0.43
1:J:339:CYS:SG	1:J:370:CYS:SG	3.16	0.43
1:K:145:TYR:HD1	1:K:145:TYR:N	2.17	0.43
1:K:393:GLN:O	1:K:394:GLY:O	2.37	0.43
1:D:331:TRP:CZ2	1:D:386:LEU:HD13	2.54	0.43
1:I:80:ARG:CG	1:I:80:ARG:HH11	2.31	0.43
1:K:60:ASP:N	1:K:60:ASP:OD1	2.49	0.43
1:L:170:TYR:N	1:L:170:TYR:CD1	2.85	0.43
1:B:72:VAL:O	1:B:74:PHE:N	2.52	0.43
1:C:37:PRO:O	1:C:38:GLU:C	2.56	0.43
1:E:338:GLY:O	1:E:340:TYR:HD2	2.02	0.43
1:E:399:LEU:HD22	1:E:399:LEU:H	1.84	0.43
1:F:42:HIS:HB3	1:F:79:PHE:HB2	2.00	0.43
1:H:178:GLN:HA	1:H:179:PRO:HD3	1.94	0.43
1:I:115:PHE:HE2	1:I:145:TYR:CD2	2.37	0.43
1:I:189:ARG:NH1	1:I:201:GLU:OE1	2.51	0.43
1:J:145:TYR:N	1:J:145:TYR:CD1	2.87	0.43
1:J:295:PHE:C	1:J:295:PHE:CD1	2.92	0.43
1:J:42:HIS:O	1:J:79:PHE:HB2	2.18	0.43
1:K:103:PHE:CD2	1:K:111:LEU:CD2	3.02	0.43
1:A:110:ALA:HA	1:A:187:PHE:HE2	1.84	0.43
1:A:295:PHE:N	1:A:295:PHE:HD1	2.16	0.43
1:E:170:TYR:CE2	1:E:177:ASN:HB2	2.52	0.43
1:D:267:TRP:CG	1:H:235:GLY:HA2	2.54	0.43
1:H:257:ARG:HB2	3:H:502:AQH:C4	2.49	0.43
1:I:104:PRO:HD3	1:I:167:VAL:O	2.18	0.43
1:J:302:GLY:O	1:J:305:TRP:N	2.50	0.43
1:E:190:SER:O	1:E:194:ILE:HG13	2.18	0.43
1:F:111:LEU:HD13	1:F:137:ILE:HG13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:TYR:HE1	1:F:205:ARG:HB2	1.82	0.43
1:G:295:PHE:CD2	1:G:386:LEU:CD2	3.02	0.43
1:I:145:TYR:CE1	1:I:205:ARG:NH1	2.87	0.43
1:D:145:TYR:N	1:D:145:TYR:CD1	2.87	0.42
1:G:300:PRO:HD3	1:G:318:SER:HB2	2.01	0.42
1:G:358:CYS:H	1:G:362:LYS:CB	2.32	0.42
1:G:367:GLN:HG2	1:G:368:PHE:CD1	2.54	0.42
1:I:182:PHE:HB2	1:I:187:PHE:HA	2.01	0.42
1:I:299:LEU:HB3	1:I:300:PRO:CD	2.41	0.42
1:J:299:LEU:CB	1:J:300:PRO:HD2	2.34	0.42
1:K:104:PRO:CG	1:K:114:TRP:HZ3	2.32	0.42
1:A:181:ASP:HB3	1:A:184:LYS:HG3	2.00	0.42
1:A:219:VAL:HG22	1:A:295:PHE:CE1	2.53	0.42
1:B:50:SER:O	1:B:51:GLU:HB2	2.19	0.42
1:E:295:PHE:CD2	1:E:386:LEU:HD23	2.54	0.42
1:F:295:PHE:CD2	1:F:386:LEU:HD23	2.54	0.42
1:F:47:ASP:O	1:F:51:GLU:N	2.46	0.42
1:I:107:THR:O	1:I:107:THR:HG23	2.20	0.42
1:L:18:GLN:HE21	1:L:18:GLN:HA	1.83	0.42
1:A:47:ASP:O	1:A:51:GLU:N	2.46	0.42
1:B:42:HIS:O	1:B:79:PHE:HB2	2.19	0.42
1:E:323:PRO:HA	1:E:332:ARG:NH2	2.33	0.42
1:E:42:HIS:HE2	1:E:56:CYS:HG	1.66	0.42
1:F:18:GLN:HA	1:F:18:GLN:NE2	2.35	0.42
1:H:105:THR:C	1:H:107:THR:CB	2.85	0.42
1:I:103:PHE:CZ	1:I:115:PHE:CD1	3.03	0.42
1:I:320:PHE:HZ	3:I:503:AQH:H3	1.66	0.42
1:L:50:SER:O	1:L:51:GLU:HB2	2.20	0.42
1:F:42:HIS:CD2	1:F:42:HIS:C	2.93	0.42
1:G:182:PHE:HE1	1:G:183:ARG:HG3	1.80	0.42
1:G:190:SER:O	1:G:194:ILE:HG13	2.19	0.42
1:H:114:TRP:CD1	1:H:188:HIS:HA	2.54	0.42
1:K:219:VAL:HG22	1:K:295:PHE:CE1	2.54	0.42
1:A:103:PHE:HB3	1:A:104:PRO:CD	2.46	0.42
1:A:145:TYR:CD1	1:A:145:TYR:N	2.88	0.42
1:A:342:CYS:SG	1:A:370:CYS:SG	3.17	0.42
1:D:18:GLN:HE21	1:D:18:GLN:HA	1.85	0.42
1:G:107:THR:HG23	1:G:107:THR:O	2.20	0.42
1:L:169:LEU:C	1:L:170:TYR:HD1	2.23	0.42
1:B:111:LEU:HD13	1:B:111:LEU:HA	1.80	0.42
1:H:145:TYR:HE1	1:H:205:ARG:HB2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:331:TRP:CZ2	1:I:386:LEU:HD13	2.55	0.42
1:K:296:PHE:CE2	1:K:298:GLY:HA3	2.55	0.42
1:A:300:PRO:O	3:A:502:AQH:H6	2.20	0.42
1:C:42:HIS:O	1:C:79:PHE:HB2	2.20	0.42
1:C:47:ASP:O	1:C:51:GLU:N	2.46	0.42
1:G:170:TYR:N	1:G:170:TYR:HD1	2.17	0.42
1:K:103:PHE:CE2	1:K:115:PHE:CD1	3.04	0.42
1:K:257:ARG:HB2	3:K:502:AQH:C4	2.49	0.42
1:A:230:LYS:HG2	1:A:320:PHE:CE1	2.55	0.42
1:H:42:HIS:O	1:H:79:PHE:HB2	2.20	0.42
1:L:114:TRP:CE3	1:L:167:VAL:HG12	2.55	0.42
1:A:155:LYS:N	1:A:156:PRO:HD3	2.34	0.42
1:D:111:LEU:O	1:D:114:TRP:N	2.51	0.42
1:E:299:LEU:CB	1:E:300:PRO:HD2	2.35	0.42
1:F:9:PHE:C	1:F:10:ILE:HG23	2.40	0.42
1:G:226:THR:OG1	3:G:502:AQH:O1B	2.26	0.42
1:J:9:PHE:HB3	1:J:10:ILE:H	1.63	0.42
1:J:295:PHE:HD2	1:J:386:LEU:CD2	2.33	0.42
1:K:78:VAL:HG23	1:K:88:LEU:H	1.85	0.42
1:L:390:LEU:HA	1:L:390:LEU:HD23	1.92	0.42
1:D:72:VAL:O	1:D:74:PHE:N	2.53	0.42
1:G:42:HIS:O	1:G:79:PHE:HB2	2.19	0.42
1:J:178:GLN:HA	1:J:179:PRO:HD3	1.92	0.42
1:J:42:HIS:ND1	1:J:58:ASP:OD1	2.53	0.42
1:L:296:PHE:HE2	1:L:298:GLY:C	2.21	0.42
1:G:18:GLN:NE2	1:G:18:GLN:HA	2.35	0.41
1:I:286:ARG:HH11	3:I:503:AQH:H17	1.85	0.41
1:K:103:PHE:CZ	1:K:115:PHE:HD1	2.38	0.41
1:L:18:GLN:NE2	1:L:18:GLN:HA	2.35	0.41
1:L:295:PHE:CD1	1:L:295:PHE:C	2.94	0.41
1:A:185:VAL:O	1:A:189:ARG:HD2	2.20	0.41
1:B:299:LEU:O	1:B:304:SER:OG	2.17	0.41
1:C:145:TYR:HD1	1:C:145:TYR:N	2.17	0.41
1:D:112:LEU:O	1:D:116:PRO:CD	2.68	0.41
1:E:328:TYR:HE2	1:E:399:LEU:HD11	1.85	0.41
1:J:181:ASP:HB3	1:J:184:LYS:HG3	2.01	0.41
1:K:155:LYS:N	1:K:156:PRO:HD3	2.34	0.41
1:B:97:ARG:HD2	1:B:97:ARG:HA	1.87	0.41
1:G:169:LEU:HB3	1:G:182:PHE:CE2	2.56	0.41
1:I:37:PRO:HB2	1:I:38:GLU:H	1.74	0.41
1:K:104:PRO:CD	1:K:114:TRP:HZ3	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:ASP:O	1:K:51:GLU:N	2.47	0.41
1:L:232:TRP:CZ2	1:L:234:ASN:HB3	2.55	0.41
1:A:18:GLN:NE2	1:A:18:GLN:HA	2.36	0.41
3:A:502:AQH:PB	3:A:502:AQH:O	2.79	0.41
1:A:85:THR:CG2	1:A:86:PRO:HD2	2.47	0.41
1:B:302:GLY:N	3:B:502:AQH:O1A	2.54	0.41
1:C:323:PRO:HA	1:C:332:ARG:NH2	2.36	0.41
1:E:111:LEU:HD13	1:E:137:ILE:HG13	2.01	0.41
1:F:132:THR:HA	1:F:151:SER:O	2.20	0.41
1:F:55:PHE:HE2	1:F:57:CYS:HG	1.67	0.41
1:G:112:LEU:HD22	1:G:204:VAL:HG21	2.03	0.41
1:L:312:ILE:HD13	1:L:312:ILE:H	1.85	0.41
1:C:182:PHE:HD1	1:C:183:ARG:N	2.16	0.41
1:C:230:LYS:HG2	1:C:320:PHE:CE1	2.56	0.41
1:C:301:SER:HB2	3:C:503:AQH:H23	2.03	0.41
1:I:108:LEU:HD23	1:I:109:GLY:N	2.35	0.41
1:J:219:VAL:CG2	1:J:295:PHE:CE1	3.04	0.41
1:J:360:ARG:C	1:J:361:HIS:ND1	2.74	0.41
1:K:170:TYR:HE2	1:K:177:ASN:HB3	1.83	0.41
1:L:170:TYR:N	1:L:170:TYR:HD1	2.18	0.41
1:L:295:PHE:HD1	1:L:295:PHE:C	2.23	0.41
1:A:114:TRP:CD1	1:A:191:ALA:HB2	2.56	0.41
1:E:178:GLN:HA	1:E:179:PRO:HD3	1.94	0.41
3:E:502:AQH:O	3:E:502:AQH:PB	2.79	0.41
1:F:169:LEU:HD22	1:F:182:PHE:HE2	1.85	0.41
1:F:189:ARG:HG3	1:F:189:ARG:NH1	2.35	0.41
3:F:502:AQH:H2	3:F:502:AQH:O4'	2.20	0.41
1:J:253:MET:SD	1:J:277:PHE:CE1	3.14	0.41
1:L:122:GLN:OE1	1:L:122:GLN:O	2.38	0.41
1:C:155:LYS:N	1:C:156:PRO:HD3	2.35	0.41
1:C:80:ARG:C	1:C:82:GLY:H	2.23	0.41
1:E:27:ASP:OD2	1:E:33:ARG:NH2	2.54	0.41
1:F:295:PHE:C	1:F:295:PHE:HD1	2.24	0.41
1:F:360:ARG:C	1:F:361:HIS:ND1	2.73	0.41
1:G:169:LEU:C	1:G:170:TYR:HD1	2.24	0.41
1:G:43:VAL:HG11	1:G:64:VAL:HG21	2.02	0.41
1:I:79:PHE:CD1	1:I:86:PRO:HA	2.56	0.41
1:K:337:HIS:CD2	1:J:54:LEU:CD2	3.04	0.41
1:L:291:ARG:CA	1:L:310:THR:HG21	2.50	0.41
1:L:299:LEU:O	1:L:316:LEU:HG	2.21	0.41
1:L:331:TRP:CZ2	1:L:386:LEU:HD13	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ARG:O	1:B:82:GLY:N	2.47	0.41
1:C:301:SER:HA	3:C:503:AQH:H13	2.03	0.41
1:D:202:ALA:HA	1:D:203:PRO:HD3	1.88	0.41
1:J:169:LEU:C	1:J:170:TYR:CD1	2.89	0.41
1:B:219:VAL:HG21	1:B:295:PHE:HE1	1.85	0.41
1:C:360:ARG:HE	1:C:360:ARG:HB2	1.67	0.41
1:D:263:GLN:O	1:D:264:GLY:O	2.38	0.41
1:H:286:ARG:HH11	3:H:502:AQH:C2	2.34	0.41
1:H:42:HIS:CD2	1:H:42:HIS:C	2.93	0.41
3:H:502:AQH:H19	3:H:502:AQH:H26	2.03	0.41
1:J:366:ARG:O	1:J:369:GLU:HB2	2.21	0.41
1:L:10:ILE:HG12	1:L:11:THR:N	2.36	0.41
1:B:219:VAL:HG21	1:B:295:PHE:CE1	2.56	0.41
3:C:503:AQH:O	3:C:503:AQH:PB	2.79	0.41
1:D:299:LEU:CB	1:D:300:PRO:HD2	2.33	0.41
1:E:338:GLY:HA3	1:E:373:LEU:HD11	2.00	0.41
1:G:48:ALA:HB1	1:G:73:ARG:HH21	1.85	0.41
1:G:107:THR:OG1	3:G:502:AQH:O1A	2.36	0.41
1:H:182:PHE:HE1	1:H:183:ARG:CG	2.30	0.41
3:H:502:AQH:PB	3:H:502:AQH:O	2.79	0.41
1:J:155:LYS:N	1:J:156:PRO:HD3	2.36	0.41
1:J:360:ARG:O	1:J:361:HIS:ND1	2.54	0.41
1:L:109:GLY:O	1:L:112:LEU:N	2.52	0.41
1:L:342:CYS:SG	1:L:358:CYS:SG	3.13	0.41
1:B:9:PHE:HA	1:B:10:ILE:HA	1.63	0.41
1:B:169:LEU:C	1:B:170:TYR:HD1	2.24	0.41
3:B:502:AQH:H13	3:B:502:AQH:PA	2.60	0.41
1:D:267:TRP:CE2	1:H:235:GLY:HA3	2.56	0.41
1:F:323:PRO:HA	1:F:332:ARG:NH2	2.35	0.41
1:H:169:LEU:HD22	1:H:182:PHE:CE2	2.56	0.41
1:H:79:PHE:HE1	1:H:86:PRO:HB3	1.86	0.41
1:J:10:ILE:HA	1:J:10:ILE:HD12	1.79	0.41
1:J:120:ARG:NH1	1:J:198:ASP:O	2.54	0.41
1:A:230:LYS:NZ	3:A:502:AQH:O3A	2.53	0.40
1:B:18:GLN:NE2	1:B:18:GLN:HA	2.36	0.40
1:D:112:LEU:HA	1:D:204:VAL:HG11	2.03	0.40
1:G:227:CYS:SG	1:G:230:LYS:HG3	2.60	0.40
1:J:182:PHE:CD1	1:J:183:ARG:HG3	2.53	0.40
1:J:295:PHE:CD2	1:J:386:LEU:HD23	2.56	0.40
1:E:399:LEU:HD12	1:A:200:ARG:HH22	1.87	0.40
1:C:188:HIS:CE1	1:C:189:ARG:NH1	2.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:VAL:HG22	1:E:295:PHE:CE1	2.56	0.40
1:E:58:ASP:HB3	1:E:81:GLN:NE2	2.36	0.40
1:F:295:PHE:C	1:F:295:PHE:CD1	2.94	0.40
1:F:48:ALA:HB1	1:F:73:ARG:HH21	1.86	0.40
1:H:187:PHE:CE1	3:H:502:AQH:O4'	2.74	0.40
1:H:202:ALA:HA	1:H:203:PRO:HD3	1.87	0.40
1:K:112:LEU:HD22	1:K:204:VAL:HG21	2.03	0.40
1:B:104:PRO:HB2	1:B:105:THR:H	1.59	0.40
1:B:47:ASP:O	1:B:51:GLU:N	2.49	0.40
1:F:18:GLN:HE21	1:F:18:GLN:HA	1.86	0.40
1:G:169:LEU:HB3	1:G:182:PHE:HE2	1.86	0.40
1:G:202:ALA:HA	1:G:203:PRO:HD3	1.87	0.40
1:G:212:ARG:NE	1:G:214:ILE:O	2.54	0.40
1:H:107:THR:CG2	1:H:107:THR:O	2.70	0.40
1:H:299:LEU:HB3	1:H:300:PRO:CD	2.41	0.40
1:H:48:ALA:HB1	1:H:73:ARG:HH21	1.86	0.40
1:I:155:LYS:N	1:I:156:PRO:HD3	2.37	0.40
1:K:284:GLN:NE2	1:K:284:GLN:HA	2.36	0.40
1:L:155:LYS:N	1:L:156:PRO:HD3	2.37	0.40
1:A:85:THR:CB	1:A:86:PRO:HD2	2.51	0.40
1:E:37:PRO:HB2	1:E:38:GLU:H	1.65	0.40
3:G:502:AQH:PA	3:G:502:AQH:O	2.79	0.40
1:G:42:HIS:NE2	1:G:56:CYS:SG	2.88	0.40
3:I:503:AQH:PB	3:I:503:AQH:O	2.79	0.40
1:J:47:ASP:O	1:J:51:GLU:N	2.50	0.40
1:L:113:GLY:O	1:L:116:PRO:HD2	2.21	0.40
1:B:58:ASP:HB3	1:B:81:GLN:NE2	2.37	0.40
1:C:300:PRO:O	3:C:503:AQH:H6	2.21	0.40
1:D:182:PHE:HD1	1:D:183:ARG:N	2.20	0.40
1:D:58:ASP:HB3	1:D:81:GLN:NE2	2.36	0.40
1:G:180:VAL:HG13	1:I:340:TYR:HE2	1.87	0.40
1:H:219:VAL:HG22	1:H:295:PHE:CE1	2.57	0.40
1:J:18:GLN:HA	1:J:18:GLN:NE2	2.35	0.40
1:L:182:PHE:HB2	1:L:187:PHE:HA	2.03	0.40
1:L:230:LYS:HA	1:L:231:TYR:C	2.13	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	374/406 (92%)	360 (96%)	10 (3%)	4 (1%)	14	51
1	B	381/406 (94%)	364 (96%)	12 (3%)	5 (1%)	12	48
1	C	387/406 (95%)	367 (95%)	15 (4%)	5 (1%)	12	48
1	D	377/406 (93%)	356 (94%)	15 (4%)	6 (2%)	9	44
1	E	388/406 (96%)	366 (94%)	18 (5%)	4 (1%)	15	52
1	F	380/406 (94%)	355 (93%)	20 (5%)	5 (1%)	12	48
1	G	387/406 (95%)	365 (94%)	16 (4%)	6 (2%)	9	44
1	H	383/406 (94%)	370 (97%)	7 (2%)	6 (2%)	9	44
1	I	387/406 (95%)	364 (94%)	21 (5%)	2 (0%)	29	67
1	J	383/406 (94%)	368 (96%)	11 (3%)	4 (1%)	15	52
1	K	388/406 (96%)	377 (97%)	9 (2%)	2 (0%)	29	67
1	L	364/406 (90%)	338 (93%)	14 (4%)	12 (3%)	4	31
All	All	4579/4872 (94%)	4350 (95%)	168 (4%)	61 (1%)	12	48

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	10	ILE
1	L	231	TYR
1	L	233	ASN
1	L	234	ASN
1	L	299	LEU
1	E	37	PRO
1	B	37	PRO
1	B	104	PRO
1	F	393	GLN
1	G	108	LEU
1	G	357	TRP
1	G	361	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	10	ILE
1	J	61	LYS
1	L	108	LEU
1	L	159	VAL
1	L	264	GLY
1	L	303	LEU
1	D	264	GLY
1	E	395	VAL
1	H	106	GLY
1	H	264	GLY
1	B	264	GLY
1	F	37	PRO
1	G	37	PRO
1	G	109	GLY
1	G	159	VAL
1	I	37	PRO
1	K	21	PRO
1	L	226	THR
1	C	73	ARG
1	C	105	THR
1	D	37	PRO
1	E	19	ALA
1	E	159	VAL
1	H	266	VAL
1	B	73	ARG
1	F	19	ALA
1	J	21	PRO
1	A	37	PRO
1	A	81	GLN
1	A	104	PRO
1	L	225	SER
1	D	73	ARG
1	D	263	GLN
1	H	37	PRO
1	B	82	GLY
1	F	105	THR
1	A	73	ARG
1	C	361	HIS
1	D	82	GLY
1	H	73	ARG
1	K	394	GLY
1	L	73	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	82	GLY
1	C	159	VAL
1	H	159	VAL
1	F	62	GLY
1	J	37	PRO
1	I	159	VAL
1	D	300	PRO

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	329/355 (93%)	311 (94%)	18 (6%)	21	52
1	B	331/355 (93%)	313 (95%)	18 (5%)	22	52
1	C	335/355 (94%)	320 (96%)	15 (4%)	27	56
1	D	328/355 (92%)	311 (95%)	17 (5%)	23	53
1	E	336/355 (95%)	315 (94%)	21 (6%)	18	47
1	F	331/355 (93%)	316 (96%)	15 (4%)	27	56
1	G	335/355 (94%)	308 (92%)	27 (8%)	11	40
1	H	332/355 (94%)	316 (95%)	16 (5%)	25	54
1	I	335/355 (94%)	312 (93%)	23 (7%)	15	45
1	J	332/355 (94%)	315 (95%)	17 (5%)	24	53
1	K	336/355 (95%)	313 (93%)	23 (7%)	16	46
1	L	322/355 (91%)	295 (92%)	27 (8%)	11	39
All	All	3982/4260 (94%)	3745 (94%)	237 (6%)	19	49

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	10	ILE
1	K	36	LEU
1	K	38	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	40	LYS
1	K	56	CYS
1	K	61	LYS
1	K	78	VAL
1	K	80	ARG
1	K	81	GLN
1	K	87	LEU
1	K	107	THR
1	K	136	ASP
1	K	145	TYR
1	K	156	PRO
1	K	180	VAL
1	K	182	PHE
1	K	205	ARG
1	K	225	SER
1	K	286	ARG
1	K	295	PHE
1	K	320	PHE
1	K	371	THR
1	K	393	GLN
1	L	9	PHE
1	L	10	ILE
1	L	24	ILE
1	L	56	CYS
1	L	57	CYS
1	L	58	ASP
1	L	87	LEU
1	L	108	LEU
1	L	122	GLN
1	L	145	TYR
1	L	156	PRO
1	L	169	LEU
1	L	170	TYR
1	L	180	VAL
1	L	182	PHE
1	L	205	ARG
1	L	227	CYS
1	L	230	LYS
1	L	251	ARG
1	L	257	ARG
1	L	286	ARG
1	L	295	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	310	THR
1	L	312	ILE
1	L	320	PHE
1	L	391	THR
1	L	393	GLN
1	C	10	ILE
1	C	36	LEU
1	C	61	LYS
1	C	87	LEU
1	C	107	THR
1	C	136	ASP
1	C	180	VAL
1	C	182	PHE
1	C	286	ARG
1	C	295	PHE
1	C	320	PHE
1	C	356	LEU
1	C	360	ARG
1	C	393	GLN
1	C	398	THR
1	D	10	ILE
1	D	36	LEU
1	D	61	LYS
1	D	80	ARG
1	D	112	LEU
1	D	136	ASP
1	D	145	TYR
1	D	156	PRO
1	D	180	VAL
1	D	182	PHE
1	D	205	ARG
1	D	280	LYS
1	D	286	ARG
1	D	295	PHE
1	D	320	PHE
1	D	361	HIS
1	D	388	ARG
1	E	10	ILE
1	E	36	LEU
1	E	80	ARG
1	E	87	LEU
1	E	102	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	105	THR
1	E	108	LEU
1	E	136	ASP
1	E	156	PRO
1	E	180	VAL
1	E	182	PHE
1	E	225	SER
1	E	286	ARG
1	E	295	PHE
1	E	320	PHE
1	E	339	CYS
1	E	370	CYS
1	E	371	THR
1	E	391	THR
1	E	393	GLN
1	E	399	LEU
1	H	10	ILE
1	H	36	LEU
1	H	81	GLN
1	H	87	LEU
1	H	107	THR
1	H	108	LEU
1	H	111	LEU
1	H	170	TYR
1	H	180	VAL
1	H	182	PHE
1	H	263	GLN
1	H	265	PHE
1	H	286	ARG
1	H	295	PHE
1	H	320	PHE
1	H	393	GLN
1	B	36	LEU
1	B	40	LYS
1	B	80	ARG
1	B	87	LEU
1	B	97	ARG
1	B	105	THR
1	B	108	LEU
1	B	111	LEU
1	B	136	ASP
1	B	145	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	170	TYR
1	B	180	VAL
1	B	182	PHE
1	B	205	ARG
1	B	286	ARG
1	B	295	PHE
1	B	320	PHE
1	B	332	ARG
1	F	80	ARG
1	F	81	GLN
1	F	87	LEU
1	F	107	THR
1	F	122	GLN
1	F	145	TYR
1	F	180	VAL
1	F	182	PHE
1	F	205	ARG
1	F	225	SER
1	F	286	ARG
1	F	295	PHE
1	F	320	PHE
1	F	393	GLN
1	F	395	VAL
1	G	36	LEU
1	G	63	TRP
1	G	87	LEU
1	G	105	THR
1	G	108	LEU
1	G	122	GLN
1	G	136	ASP
1	G	145	TYR
1	G	147	GLN
1	G	170	TYR
1	G	180	VAL
1	G	182	PHE
1	G	205	ARG
1	G	286	ARG
1	G	295	PHE
1	G	320	PHE
1	G	339	CYS
1	G	343	TRP
1	G	354	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	355	PHE
1	G	356	LEU
1	G	357	TRP
1	G	358	CYS
1	G	360	ARG
1	G	362	LYS
1	G	391	THR
1	G	393	GLN
1	I	10	ILE
1	I	36	LEU
1	I	38	GLU
1	I	61	LYS
1	I	87	LEU
1	I	145	TYR
1	I	180	VAL
1	I	182	PHE
1	I	280	LYS
1	I	286	ARG
1	I	289	LEU
1	I	295	PHE
1	I	320	PHE
1	I	332	ARG
1	I	339	CYS
1	I	340	TYR
1	I	343	TRP
1	I	367	GLN
1	I	370	CYS
1	I	371	THR
1	I	391	THR
1	I	393	GLN
1	I	398	THR
1	J	9	PHE
1	J	36	LEU
1	J	60	ASP
1	J	61	LYS
1	J	80	ARG
1	J	87	LEU
1	J	107	THR
1	J	136	ASP
1	J	169	LEU
1	J	180	VAL
1	J	182	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	205	ARG
1	J	227	CYS
1	J	286	ARG
1	J	295	PHE
1	J	320	PHE
1	J	391	THR
1	A	10	ILE
1	A	36	LEU
1	A	81	GLN
1	A	85	THR
1	A	87	LEU
1	A	105	THR
1	A	107	THR
1	A	136	ASP
1	A	166	ARG
1	A	170	TYR
1	A	180	VAL
1	A	182	PHE
1	A	205	ARG
1	A	286	ARG
1	A	295	PHE
1	A	320	PHE
1	A	332	ARG
1	A	361	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	284	GLN
1	G	367	GLN
1	I	367	GLN
1	A	337	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AQH	C	503	-	37,43,43	1.83	9 (24%)	47,66,66	2.19	10 (21%)
3	AQH	L	502	-	37,43,43	1.89	11 (29%)	47,66,66	2.33	14 (29%)
4	EDO	C	502	-	3,3,3	0.31	0	2,2,2	0.31	0
4	EDO	J	502	-	3,3,3	0.27	0	2,2,2	0.31	0
4	EDO	I	502	-	3,3,3	0.22	0	2,2,2	0.31	0
3	AQH	J	503	-	37,43,43	1.80	10 (27%)	47,66,66	2.31	9 (19%)
3	AQH	I	503	-	37,43,43	1.83	9 (24%)	47,66,66	2.19	10 (21%)
3	AQH	G	502	-	37,43,43	1.87	10 (27%)	47,66,66	2.35	14 (29%)
3	AQH	B	502	-	37,43,43	1.84	10 (27%)	47,66,66	2.29	12 (25%)
3	AQH	A	502	-	37,43,43	1.83	10 (27%)	47,66,66	2.18	10 (21%)
3	AQH	D	502	-	37,43,43	1.82	11 (29%)	47,66,66	2.26	11 (23%)
3	AQH	K	502	-	37,43,43	1.81	11 (29%)	47,66,66	2.29	10 (21%)
3	AQH	F	502	-	37,43,43	1.89	10 (27%)	47,66,66	2.33	14 (29%)
3	AQH	E	502	-	37,43,43	1.82	10 (27%)	47,66,66	2.19	10 (21%)
3	AQH	H	502	-	37,43,43	1.83	10 (27%)	47,66,66	2.19	10 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AQH	C	503	-	-	14/23/63/63	0/4/4/4
3	AQH	L	502	-	-	16/23/63/63	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	502	-	-	1/1/1/1	-
4	EDO	J	502	-	-	0/1/1/1	-
4	EDO	I	502	-	-	0/1/1/1	-
3	AQH	J	503	-	-	8/23/63/63	0/4/4/4
3	AQH	I	503	-	-	12/23/63/63	0/4/4/4
3	AQH	G	502	-	-	12/23/63/63	0/4/4/4
3	AQH	B	502	-	-	7/23/63/63	0/4/4/4
3	AQH	A	502	-	-	9/23/63/63	0/4/4/4
3	AQH	D	502	-	-	11/23/63/63	0/4/4/4
3	AQH	K	502	-	-	15/23/63/63	0/4/4/4
3	AQH	F	502	-	-	9/23/63/63	0/4/4/4
3	AQH	E	502	-	-	16/23/63/63	0/4/4/4
3	AQH	H	502	-	-	10/23/63/63	0/4/4/4

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	502	AQH	O-C2'	4.89	1.54	1.43
3	D	502	AQH	O-C2'	4.88	1.54	1.43
3	F	502	AQH	O-C2'	4.87	1.54	1.43
3	K	502	AQH	O-C2'	4.86	1.54	1.43
3	B	502	AQH	O-C2'	4.86	1.54	1.43
3	I	503	AQH	O-C2'	4.84	1.54	1.43
3	H	502	AQH	O-C2'	4.84	1.54	1.43
3	E	502	AQH	O-C2'	4.82	1.54	1.43
3	C	503	AQH	O-C2'	4.82	1.54	1.43
3	G	502	AQH	O-C2'	4.82	1.54	1.43
3	A	502	AQH	O-C2'	4.80	1.54	1.43
3	J	503	AQH	O-C2'	4.79	1.54	1.43
3	J	503	AQH	C2-N3	4.45	1.39	1.32
3	E	502	AQH	C2-N3	4.44	1.39	1.32
3	A	502	AQH	C2-N3	4.43	1.39	1.32
3	H	502	AQH	C2-N3	4.43	1.39	1.32
3	F	502	AQH	C2-N3	4.43	1.39	1.32
3	C	503	AQH	C2-N3	4.43	1.39	1.32
3	G	502	AQH	C2-N3	4.42	1.39	1.32
3	I	503	AQH	C2-N3	4.42	1.39	1.32
3	L	502	AQH	C2-N3	4.42	1.39	1.32
3	K	502	AQH	C2-N3	4.41	1.39	1.32
3	B	502	AQH	C2-N3	4.41	1.39	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	AQH	C2-N3	4.39	1.39	1.32
3	F	502	AQH	O5'-C5'	4.12	1.50	1.44
3	L	502	AQH	O5'-C5'	4.07	1.50	1.44
3	G	502	AQH	O5'-C5'	4.01	1.50	1.44
3	B	502	AQH	O5'-C5'	3.73	1.49	1.44
3	C	503	AQH	O5'-C5'	3.67	1.49	1.44
3	A	502	AQH	O5'-C5'	3.63	1.49	1.44
3	E	502	AQH	O5'-C5'	3.62	1.49	1.44
3	I	503	AQH	O5'-C5'	3.61	1.49	1.44
3	A	502	AQH	C4-N3	3.60	1.40	1.35
3	H	502	AQH	O5'-C5'	3.60	1.49	1.44
3	I	503	AQH	C4-N3	3.59	1.40	1.35
3	B	502	AQH	C4-N3	3.58	1.40	1.35
3	D	502	AQH	C4-N3	3.58	1.40	1.35
3	L	502	AQH	C4-N3	3.55	1.40	1.35
3	H	502	AQH	C4-N3	3.54	1.40	1.35
3	F	502	AQH	C4-N3	3.54	1.40	1.35
3	D	502	AQH	O5'-C5'	3.53	1.49	1.44
3	K	502	AQH	O5'-C5'	3.53	1.49	1.44
3	E	502	AQH	C4-N3	3.52	1.40	1.35
3	G	502	AQH	C4-N3	3.49	1.40	1.35
3	C	503	AQH	C4-N3	3.48	1.40	1.35
3	J	503	AQH	C4-N3	3.46	1.40	1.35
3	K	502	AQH	C4-N3	3.46	1.40	1.35
3	J	503	AQH	O5'-C5'	3.41	1.49	1.44
3	J	503	AQH	PA-O1A	-2.95	1.41	1.55
3	G	502	AQH	PA-O1A	-2.93	1.41	1.55
3	C	503	AQH	PA-O1A	-2.92	1.41	1.55
3	K	502	AQH	PA-O1A	-2.92	1.41	1.55
3	E	502	AQH	PA-O1A	-2.92	1.41	1.55
3	A	502	AQH	PA-O1A	-2.91	1.41	1.55
3	F	502	AQH	PA-O1A	-2.91	1.41	1.55
3	B	502	AQH	PA-O1A	-2.91	1.41	1.55
3	D	502	AQH	PA-O1A	-2.91	1.41	1.55
3	H	502	AQH	PA-O1A	-2.91	1.41	1.55
3	I	503	AQH	PA-O1A	-2.91	1.41	1.55
3	L	502	AQH	PA-O1A	-2.90	1.41	1.55
3	C	503	AQH	C2-N1	2.59	1.38	1.33
3	F	502	AQH	C2-N1	2.59	1.38	1.33
3	E	502	AQH	C2-N1	2.57	1.38	1.33
3	B	502	AQH	C2-N1	2.56	1.38	1.33
3	H	502	AQH	C2-N1	2.56	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	503	AQH	C2-N1	2.55	1.38	1.33
3	K	502	AQH	C2-N1	2.53	1.38	1.33
3	A	502	AQH	C2-N1	2.53	1.38	1.33
3	J	503	AQH	C2-N1	2.52	1.38	1.33
3	D	502	AQH	C2-N1	2.51	1.38	1.33
3	G	502	AQH	C2-N1	2.51	1.38	1.33
3	L	502	AQH	C2-N1	2.50	1.38	1.33
3	G	502	AQH	O5'-C1'	2.37	1.47	1.41
3	F	502	AQH	O5'-C1'	2.35	1.47	1.41
3	L	502	AQH	O5'-C1'	2.35	1.47	1.41
3	I	503	AQH	O5'-C1'	2.16	1.47	1.41
3	B	502	AQH	O5'-C1'	2.14	1.47	1.41
3	H	502	AQH	O5'-C1'	2.14	1.47	1.41
3	A	502	AQH	O5'-C1'	2.14	1.47	1.41
3	C	503	AQH	O5'-C1'	2.14	1.47	1.41
3	C	503	AQH	C5-N7	-2.10	1.32	1.39
3	I	503	AQH	C5-N7	-2.10	1.32	1.39
3	J	503	AQH	C5-N7	-2.10	1.32	1.39
3	K	502	AQH	C5-N7	-2.10	1.32	1.39
3	E	502	AQH	O5'-C1'	2.09	1.47	1.41
3	F	502	AQH	C5-N7	-2.09	1.32	1.39
3	B	502	AQH	C5-N7	-2.09	1.32	1.39
3	H	502	AQH	C5-N7	-2.09	1.32	1.39
3	E	502	AQH	C5-N7	-2.09	1.32	1.39
3	G	502	AQH	C6'-C5'	2.09	1.57	1.52
3	A	502	AQH	C5-N7	-2.09	1.32	1.39
3	D	502	AQH	C6'-C5'	2.08	1.57	1.52
3	L	502	AQH	C5-N7	-2.08	1.32	1.39
3	G	502	AQH	C5-N7	-2.08	1.32	1.39
3	D	502	AQH	C5-N7	-2.08	1.32	1.39
3	C	503	AQH	C6'-C5'	2.08	1.57	1.52
3	I	503	AQH	C6'-C5'	2.07	1.57	1.52
3	B	502	AQH	C6'-C5'	2.07	1.57	1.52
3	A	502	AQH	C6'-C5'	2.05	1.57	1.52
3	F	502	AQH	C6'-C5'	2.05	1.57	1.52
3	K	502	AQH	C3D-C4D	-2.04	1.47	1.53
3	H	502	AQH	C6'-C5'	2.04	1.57	1.52
3	J	503	AQH	C3D-C4D	-2.04	1.47	1.53
3	L	502	AQH	C6'-C5'	2.04	1.57	1.52
3	E	502	AQH	C6'-C5'	2.03	1.57	1.52
3	F	502	AQH	C3D-C4D	-2.03	1.47	1.53
3	D	502	AQH	O5'-C1'	2.03	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	AQH	C3D-C4D	-2.03	1.47	1.53
3	K	502	AQH	C6'-C5'	2.03	1.57	1.52
3	J	503	AQH	O5'-C1'	2.03	1.47	1.41
3	K	502	AQH	O5'-C1'	2.03	1.47	1.41
3	G	502	AQH	C3D-C4D	-2.03	1.47	1.53
3	A	502	AQH	C3D-C4D	-2.03	1.47	1.53
3	L	502	AQH	C3D-C4D	-2.02	1.47	1.53
3	K	502	AQH	PB-O1B	-2.02	1.43	1.50
3	L	502	AQH	PB-O1B	-2.02	1.43	1.50
3	E	502	AQH	C3D-C4D	-2.01	1.47	1.53
3	J	503	AQH	C6'-C5'	2.01	1.57	1.52
3	D	502	AQH	C3D-C4D	-2.00	1.47	1.53
3	D	502	AQH	PB-O1B	-2.00	1.43	1.50
3	H	502	AQH	C3D-C4D	-2.00	1.47	1.53

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	503	AQH	O-C2'-C1'	-9.75	86.37	110.05
3	K	502	AQH	O-C2'-C1'	-9.71	86.45	110.05
3	L	502	AQH	O-C2'-C1'	-9.59	86.74	110.05
3	F	502	AQH	O-C2'-C1'	-9.58	86.76	110.05
3	B	502	AQH	O-C2'-C1'	-9.58	86.77	110.05
3	D	502	AQH	O-C2'-C1'	-9.57	86.80	110.05
3	G	502	AQH	O-C2'-C1'	-9.50	86.97	110.05
3	C	503	AQH	O-C2'-C1'	-9.14	87.85	110.05
3	I	503	AQH	O-C2'-C1'	-9.14	87.85	110.05
3	H	502	AQH	O-C2'-C1'	-9.14	87.85	110.05
3	E	502	AQH	O-C2'-C1'	-9.13	87.87	110.05
3	A	502	AQH	O-C2'-C1'	-9.12	87.90	110.05
3	C	503	AQH	N3-C2-N1	-7.04	117.68	128.68
3	F	502	AQH	N3-C2-N1	-7.03	117.69	128.68
3	K	502	AQH	N3-C2-N1	-7.02	117.71	128.68
3	G	502	AQH	N3-C2-N1	-7.01	117.72	128.68
3	E	502	AQH	N3-C2-N1	-7.01	117.72	128.68
3	H	502	AQH	N3-C2-N1	-7.00	117.73	128.68
3	B	502	AQH	N3-C2-N1	-7.00	117.74	128.68
3	J	503	AQH	N3-C2-N1	-7.00	117.75	128.68
3	L	502	AQH	N3-C2-N1	-6.99	117.76	128.68
3	I	503	AQH	N3-C2-N1	-6.98	117.76	128.68
3	D	502	AQH	N3-C2-N1	-6.98	117.77	128.68
3	A	502	AQH	N3-C2-N1	-6.97	117.79	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	503	AQH	O5'-C1'-O3B	-5.48	104.20	111.36
3	G	502	AQH	O5'-C1'-O3B	-4.71	105.21	111.36
3	K	502	AQH	O5'-C1'-O3B	-4.67	105.27	111.36
3	F	502	AQH	O5'-C1'-O3B	-4.49	105.49	111.36
3	B	502	AQH	O5'-C1'-O3B	-4.48	105.50	111.36
3	L	502	AQH	O5'-C1'-O3B	-4.47	105.53	111.36
3	D	502	AQH	O5'-C1'-O3B	-4.33	105.70	111.36
3	H	502	AQH	O3B-C1'-C2'	3.51	114.81	108.38
3	C	503	AQH	O3B-C1'-C2'	3.51	114.80	108.38
3	I	503	AQH	O3B-C1'-C2'	3.51	114.80	108.38
3	E	502	AQH	O3B-C1'-C2'	3.49	114.78	108.38
3	A	502	AQH	O3B-C1'-C2'	3.46	114.72	108.38
3	K	502	AQH	O3B-C1'-C2'	2.87	113.64	108.38
3	G	502	AQH	O-C2'-C3'	2.80	116.83	110.35
3	B	502	AQH	O-C2'-C3'	2.73	116.66	110.35
3	D	502	AQH	O-C2'-C3'	2.72	116.64	110.35
3	F	502	AQH	O-C2'-C3'	2.72	116.64	110.35
3	L	502	AQH	O-C2'-C3'	2.71	116.62	110.35
3	J	503	AQH	O3B-C1'-C2'	2.68	113.29	108.38
3	D	502	AQH	O3B-C1'-C2'	2.67	113.28	108.38
3	K	502	AQH	O-C2'-C3'	2.65	116.48	110.35
3	G	502	AQH	O7'-C7'-C6'	2.60	116.75	111.07
3	G	502	AQH	C1'-O5'-C5'	2.60	117.25	113.06
3	G	502	AQH	C3'-C4'-C5'	2.60	115.62	109.68
3	K	502	AQH	C2'-C3'-C4'	-2.59	106.29	110.82
3	L	502	AQH	C1'-O5'-C5'	2.59	117.24	113.06
3	B	502	AQH	O3B-C1'-C2'	2.59	113.13	108.38
3	L	502	AQH	O3B-C1'-C2'	2.58	113.12	108.38
3	F	502	AQH	C1'-O5'-C5'	2.58	117.21	113.06
3	F	502	AQH	O7'-C7'-C6'	2.56	116.66	111.07
3	J	503	AQH	O-C2'-C3'	2.56	116.27	110.35
3	C	503	AQH	C2'-C3'-C4'	-2.56	106.36	110.82
3	F	502	AQH	O3B-C1'-C2'	2.55	113.06	108.38
3	J	503	AQH	C5D-C4D-C3D	-2.55	105.62	115.18
3	A	502	AQH	O7'-C7'-C6'	2.55	116.63	111.07
3	B	502	AQH	O7'-C7'-C6'	2.55	116.62	111.07
3	L	502	AQH	O7'-C7'-C6'	2.55	116.62	111.07
3	C	503	AQH	O7'-C7'-C6'	2.54	116.61	111.07
3	E	502	AQH	C2'-C3'-C4'	-2.54	106.39	110.82
3	D	502	AQH	O7'-C7'-C6'	2.54	116.60	111.07
3	H	502	AQH	O7'-C7'-C6'	2.54	116.60	111.07
3	E	502	AQH	O7'-C7'-C6'	2.54	116.60	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	AQH	C2'-C3'-C4'	-2.54	106.40	110.82
3	H	502	AQH	C2'-C3'-C4'	-2.53	106.40	110.82
3	I	503	AQH	C2'-C3'-C4'	-2.53	106.41	110.82
3	I	503	AQH	O7'-C7'-C6'	2.53	116.58	111.07
3	C	503	AQH	O-C2'-C3'	2.49	116.10	110.35
3	A	502	AQH	O-C2'-C3'	2.47	116.07	110.35
3	K	502	AQH	O7'-C7'-C6'	2.47	116.46	111.07
3	C	503	AQH	O3A-PB-O3B	2.47	116.53	106.78
3	E	502	AQH	O-C2'-C3'	2.47	116.05	110.35
3	I	503	AQH	O3A-PB-O3B	2.46	116.50	106.78
3	E	502	AQH	O3A-PB-O3B	2.46	116.48	106.78
3	H	502	AQH	O-C2'-C3'	2.46	116.03	110.35
3	I	503	AQH	O-C2'-C3'	2.46	116.03	110.35
3	H	502	AQH	O3A-PB-O3B	2.46	116.47	106.78
3	D	502	AQH	O3A-PB-O3B	2.45	116.47	106.78
3	B	502	AQH	O3A-PB-O3B	2.45	116.45	106.78
3	F	502	AQH	O3A-PB-O3B	2.45	116.45	106.78
3	A	502	AQH	O3A-PB-O3B	2.45	116.45	106.78
3	L	502	AQH	O3A-PB-O3B	2.45	116.44	106.78
3	K	502	AQH	C5D-C4D-C3D	-2.45	106.02	115.18
3	K	502	AQH	O3A-PB-O3B	2.44	116.39	106.78
3	G	502	AQH	O3A-PB-O3B	2.43	116.35	106.78
3	I	503	AQH	C5D-C4D-C3D	-2.40	106.20	115.18
3	G	502	AQH	C5D-C4D-C3D	-2.40	106.20	115.18
3	D	502	AQH	C5D-C4D-C3D	-2.39	106.22	115.18
3	C	503	AQH	C5D-C4D-C3D	-2.39	106.22	115.18
3	B	502	AQH	C5D-C4D-C3D	-2.39	106.23	115.18
3	A	502	AQH	C5D-C4D-C3D	-2.39	106.24	115.18
3	F	502	AQH	C5D-C4D-C3D	-2.38	106.25	115.18
3	E	502	AQH	C5D-C4D-C3D	-2.38	106.25	115.18
3	L	502	AQH	C5D-C4D-C3D	-2.38	106.25	115.18
3	H	502	AQH	C5D-C4D-C3D	-2.38	106.27	115.18
3	F	502	AQH	O5'-C5'-C4'	2.34	111.16	107.87
3	G	502	AQH	O3B-C1'-C2'	2.34	112.67	108.38
3	L	502	AQH	O5'-C5'-C4'	2.34	111.15	107.87
3	B	502	AQH	O5'-C5'-C4'	2.34	111.15	107.87
3	J	503	AQH	C2'-C3'-C4'	-2.33	106.75	110.82
3	D	502	AQH	C2'-C3'-C4'	-2.32	106.78	110.82
3	J	503	AQH	O7'-C7'-C6'	2.22	115.91	111.07
3	G	502	AQH	O5'-C1'-C2'	2.20	115.00	110.35
3	C	503	AQH	O4D-C4D-C3D	2.17	109.41	105.11
3	B	502	AQH	O4D-C4D-C3D	2.16	109.39	105.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	AQH	C2'-C3'-C4'	-2.16	107.06	110.82
3	I	503	AQH	O4D-C4D-C3D	2.15	109.36	105.11
3	D	502	AQH	O4D-C4D-C3D	2.15	109.36	105.11
3	G	502	AQH	O5'-C5'-C4'	2.15	110.88	107.87
3	H	502	AQH	O4D-C4D-C3D	2.14	109.35	105.11
3	F	502	AQH	O4D-C4D-C3D	2.14	109.35	105.11
3	E	502	AQH	O4D-C4D-C3D	2.14	109.34	105.11
3	L	502	AQH	O4D-C4D-C3D	2.13	109.33	105.11
3	A	502	AQH	O4D-C4D-C3D	2.11	109.29	105.11
3	J	503	AQH	O3A-PB-O3B	2.11	115.09	106.78
3	A	502	AQH	C4-C5-N7	-2.09	107.22	109.40
3	B	502	AQH	C4-C5-N7	-2.08	107.23	109.40
3	L	502	AQH	C4-C5-N7	-2.08	107.23	109.40
3	F	502	AQH	C3'-C4'-C5'	2.08	114.42	109.68
3	L	502	AQH	C3'-C4'-C5'	2.07	114.42	109.68
3	K	502	AQH	C4-C5-N7	-2.07	107.24	109.40
3	I	503	AQH	C4-C5-N7	-2.07	107.24	109.40
3	F	502	AQH	C4-C5-N7	-2.07	107.25	109.40
3	F	502	AQH	O5'-C1'-C2'	2.05	114.68	110.35
3	C	503	AQH	C4-C5-N7	-2.03	107.28	109.40
3	E	502	AQH	C4-C5-N7	-2.03	107.28	109.40
3	L	502	AQH	O5'-C1'-C2'	2.03	114.64	110.35
3	G	502	AQH	C4-C5-N7	-2.03	107.28	109.40
3	D	502	AQH	C4-C5-N7	-2.01	107.30	109.40
3	H	502	AQH	C4-C5-N7	-2.01	107.31	109.40
3	G	502	AQH	O4D-C1D-C2D	-2.00	104.00	106.93

There are no chirality outliers.

All (140) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	503	AQH	C5D-O5D-PA-O2A
3	I	503	AQH	O6'-C6'-C7'-O7'
3	I	503	AQH	C5'-C6'-C7'-O7'
3	I	503	AQH	O5'-C1'-O3B-PB
3	L	502	AQH	C5D-O5D-PA-O2B
3	L	502	AQH	C1'-O3B-PB-O2B
3	L	502	AQH	O6'-C6'-C7'-O7'
3	L	502	AQH	C5'-C6'-C7'-O7'
3	L	502	AQH	O5'-C5'-C6'-C7'
3	L	502	AQH	C4'-C5'-C6'-C7'
3	L	502	AQH	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	L	502	AQH	C4'-C5'-C6'-O6'
3	L	502	AQH	C3D-C4D-C5D-O5D
3	L	502	AQH	O4D-C4D-C5D-O5D
3	C	503	AQH	C5D-O5D-PA-O1A
3	C	503	AQH	C5D-O5D-PA-O2A
3	C	503	AQH	C5D-O5D-PA-O2B
3	C	503	AQH	O5'-C1'-O3B-PB
3	C	503	AQH	C3D-C4D-C5D-O5D
3	C	503	AQH	O4D-C4D-C5D-O5D
3	G	502	AQH	C5D-O5D-PA-O1A
3	G	502	AQH	O5'-C5'-C6'-C7'
3	G	502	AQH	C4'-C5'-C6'-C7'
3	G	502	AQH	O5'-C5'-C6'-O6'
3	G	502	AQH	C4'-C5'-C6'-O6'
3	A	502	AQH	C1'-O3B-PB-O3A
3	A	502	AQH	O6'-C6'-C7'-O7'
3	A	502	AQH	O5'-C1'-O3B-PB
3	F	502	AQH	O6'-C6'-C7'-O7'
3	F	502	AQH	C5'-C6'-C7'-O7'
3	J	503	AQH	C1'-O3B-PB-O2B
3	J	503	AQH	O5'-C1'-O3B-PB
3	B	502	AQH	C1'-O3B-PB-O2B
3	B	502	AQH	O6'-C6'-C7'-O7'
3	B	502	AQH	C5'-C6'-C7'-O7'
3	B	502	AQH	C4'-C5'-C6'-C7'
3	B	502	AQH	C3D-C4D-C5D-O5D
3	E	502	AQH	C5D-O5D-PA-O2A
3	E	502	AQH	C1'-O3B-PB-O3A
3	E	502	AQH	O6'-C6'-C7'-O7'
3	E	502	AQH	C5'-C6'-C7'-O7'
3	E	502	AQH	O5'-C5'-C6'-C7'
3	E	502	AQH	C4'-C5'-C6'-C7'
3	E	502	AQH	O5'-C5'-C6'-O6'
3	E	502	AQH	C4'-C5'-C6'-O6'
3	E	502	AQH	O5'-C1'-O3B-PB
3	H	502	AQH	C5D-O5D-PA-O1A
3	H	502	AQH	C5D-O5D-PA-O2A
3	H	502	AQH	C5D-O5D-PA-O2B
3	H	502	AQH	PA-O2B-PB-O3B
3	H	502	AQH	C1'-O3B-PB-O3A
3	H	502	AQH	O5'-C1'-O3B-PB
3	D	502	AQH	C5D-O5D-PA-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	502	AQH	C1'-O3B-PB-O2B
3	D	502	AQH	O5'-C5'-C6'-C7'
3	D	502	AQH	C4'-C5'-C6'-C7'
3	D	502	AQH	O5'-C5'-C6'-O6'
3	D	502	AQH	C4'-C5'-C6'-O6'
3	D	502	AQH	O5'-C1'-O3B-PB
3	K	502	AQH	C5D-O5D-PA-O2B
3	K	502	AQH	C1'-O3B-PB-O2B
3	K	502	AQH	O6'-C6'-C7'-O7'
3	K	502	AQH	C5'-C6'-C7'-O7'
3	K	502	AQH	O5'-C5'-C6'-C7'
3	K	502	AQH	C4'-C5'-C6'-C7'
3	K	502	AQH	O5'-C5'-C6'-O6'
3	K	502	AQH	C4'-C5'-C6'-O6'
3	K	502	AQH	O5'-C1'-O3B-PB
3	K	502	AQH	C2'-C1'-O3B-PB
3	A	502	AQH	C5'-C6'-C7'-O7'
3	J	503	AQH	C3D-C4D-C5D-O5D
3	J	503	AQH	O4D-C4D-C5D-O5D
3	E	502	AQH	O4D-C4D-C5D-O5D
3	E	502	AQH	C1'-O3B-PB-O2B
3	H	502	AQH	C1'-O3B-PB-O2B
3	I	503	AQH	O4D-C4D-C5D-O5D
3	E	502	AQH	C3D-C4D-C5D-O5D
3	I	503	AQH	C1'-O3B-PB-O2B
3	A	502	AQH	C1'-O3B-PB-O2B
3	I	503	AQH	C3D-C4D-C5D-O5D
3	C	503	AQH	O6'-C6'-C7'-O7'
3	D	502	AQH	C2'-C1'-O3B-PB
3	C	503	AQH	PA-O2B-PB-O1B
3	J	503	AQH	PA-O2B-PB-O1B
3	K	502	AQH	PA-O2B-PB-O1B
3	B	502	AQH	O4D-C4D-C5D-O5D
3	I	503	AQH	C1'-O3B-PB-O3A
3	F	502	AQH	C1'-O3B-PB-O3A
3	C	503	AQH	C5'-C6'-C7'-O7'
3	J	503	AQH	C4D-C5D-O5D-PA
3	D	502	AQH	C4D-C5D-O5D-PA
3	K	502	AQH	C4D-C5D-O5D-PA
3	I	503	AQH	PA-O2B-PB-O3B
3	L	502	AQH	PB-O2B-PA-O5D
3	A	502	AQH	PA-O2B-PB-O3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	502	AQH	PA-O2B-PB-O3B
3	G	502	AQH	C1'-O3B-PB-O2B
3	F	502	AQH	C1'-O3B-PB-O2B
3	G	502	AQH	C5D-O5D-PA-O2B
3	E	502	AQH	C5D-O5D-PA-O2B
3	G	502	AQH	C3D-C4D-C5D-O5D
3	L	502	AQH	C1'-O3B-PB-O1B
3	A	502	AQH	PA-O2B-PB-O1B
3	A	502	AQH	C1'-O3B-PB-O1B
3	F	502	AQH	C1'-O3B-PB-O1B
3	J	503	AQH	C1'-O3B-PB-O1B
3	E	502	AQH	C1'-O3B-PB-O1B
3	H	502	AQH	C1'-O3B-PB-O1B
3	L	502	AQH	C5D-O5D-PA-O1A
3	L	502	AQH	C5D-O5D-PA-O2A
3	G	502	AQH	C5D-O5D-PA-O2A
3	D	502	AQH	C5D-O5D-PA-O1A
3	D	502	AQH	C5D-O5D-PA-O2A
3	K	502	AQH	C5D-O5D-PA-O1A
3	J	503	AQH	C4'-C5'-C6'-C7'
3	I	503	AQH	O5'-C5'-C6'-O6'
3	L	502	AQH	O5'-C1'-O3B-PB
3	G	502	AQH	O5'-C1'-O3B-PB
3	I	503	AQH	PB-O2B-PA-O2A
3	G	502	AQH	PA-O2B-PB-O3A
4	C	502	EDO	O1-C1-C2-O2
3	L	502	AQH	PA-O2B-PB-O3A
3	C	503	AQH	PA-O2B-PB-O3B
3	F	502	AQH	PA-O2B-PB-O3B
3	C	503	AQH	C1'-O3B-PB-O2B
3	I	503	AQH	C4'-C5'-C6'-O6'
3	C	503	AQH	C4'-C5'-C6'-O6'
3	F	502	AQH	C4'-C5'-C6'-O6'
3	B	502	AQH	C4'-C5'-C6'-O6'
3	H	502	AQH	C4'-C5'-C6'-O6'
3	C	503	AQH	C1'-O3B-PB-O1B
3	G	502	AQH	PA-O2B-PB-O1B
3	F	502	AQH	PB-O2B-PA-O1A
3	K	502	AQH	PB-O2B-PA-O1A
3	F	502	AQH	C5D-O5D-PA-O2A
3	E	502	AQH	C5D-O5D-PA-O1A
3	K	502	AQH	C5D-O5D-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	502	AQH	O4D-C4D-C5D-O5D
3	H	502	AQH	O4D-C4D-C5D-O5D
3	C	503	AQH	C1'-O3B-PB-O3A

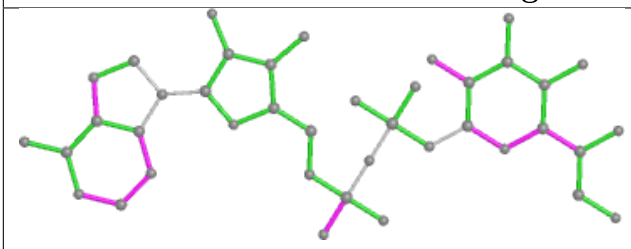
There are no ring outliers.

14 monomers are involved in 175 short contacts:

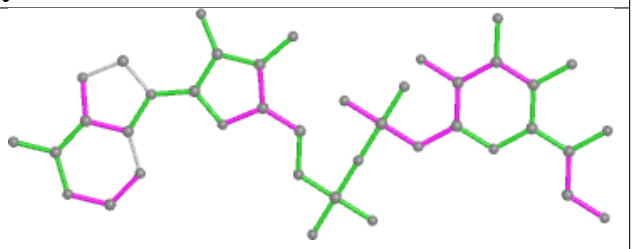
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	AQH	12	0
3	L	502	AQH	17	0
4	C	502	EDO	1	0
4	I	502	EDO	1	0
3	J	503	AQH	8	0
3	I	503	AQH	11	0
3	G	502	AQH	12	0
3	B	502	AQH	8	0
3	A	502	AQH	13	0
3	D	502	AQH	23	0
3	K	502	AQH	16	0
3	F	502	AQH	19	0
3	E	502	AQH	10	0
3	H	502	AQH	24	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

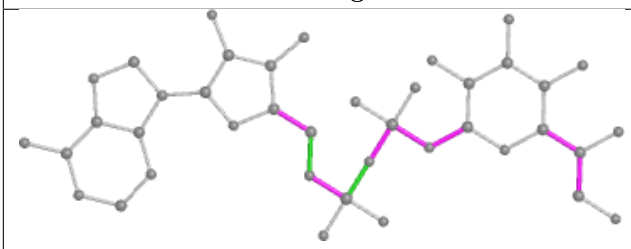
Ligand AQH C 503



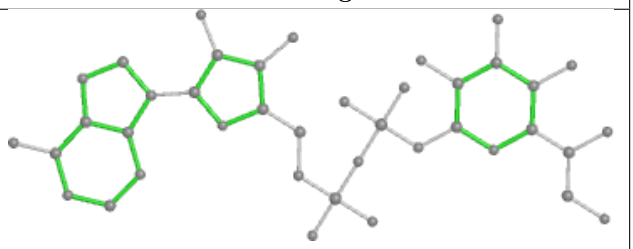
Bond lengths



Bond angles

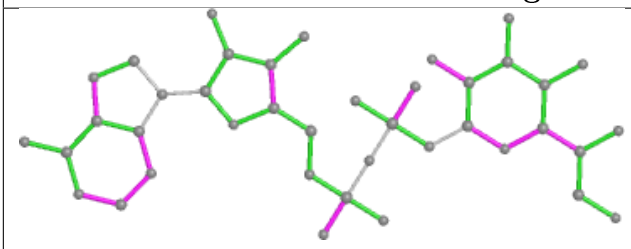


Torsions

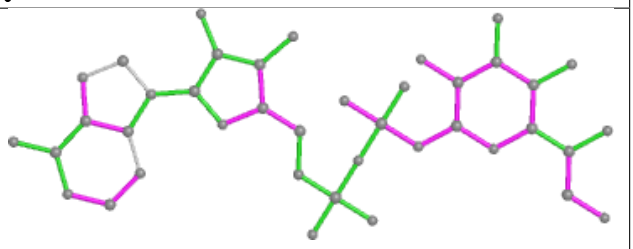


Rings

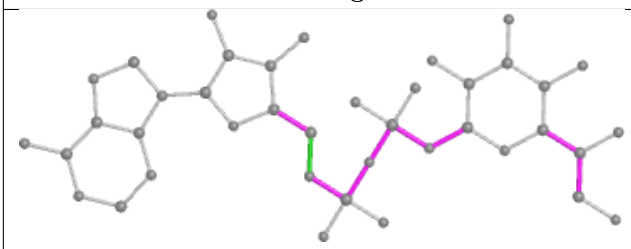
Ligand AQH L 502



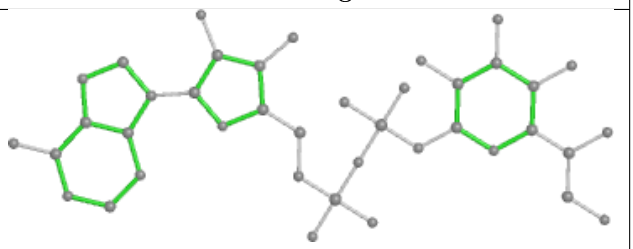
Bond lengths



Bond angles

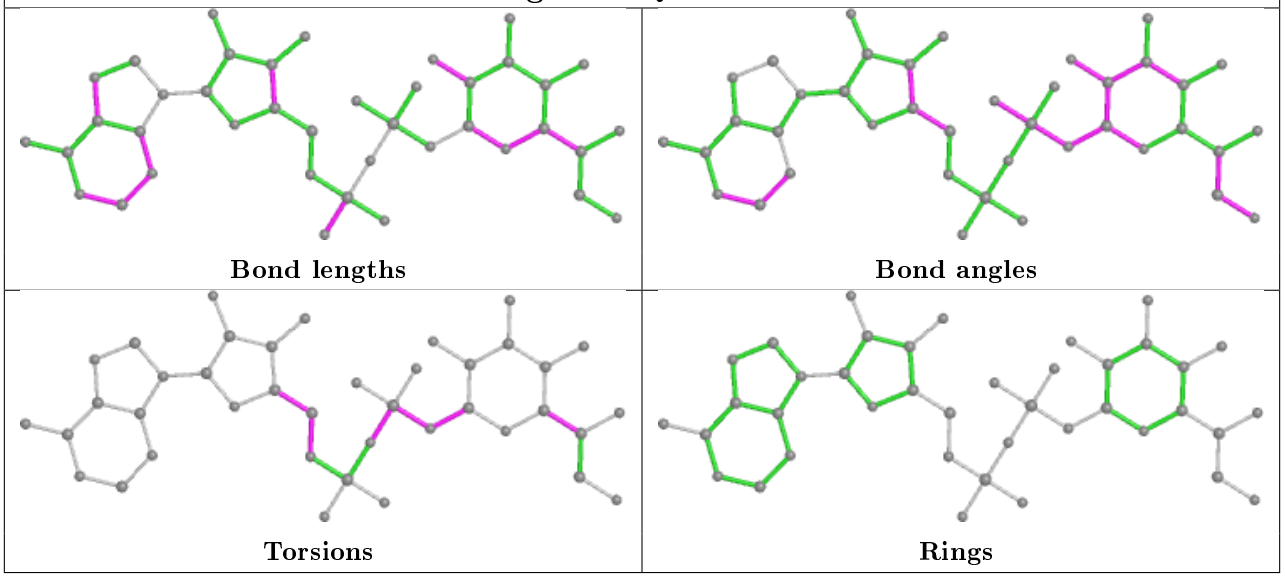


Torsions

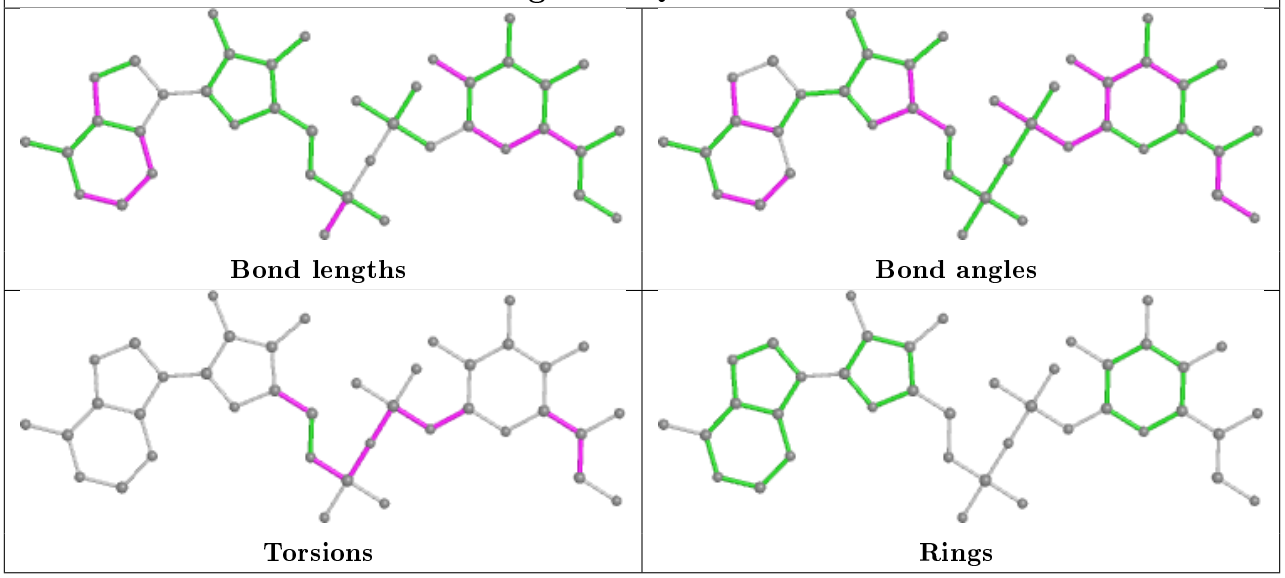


Rings

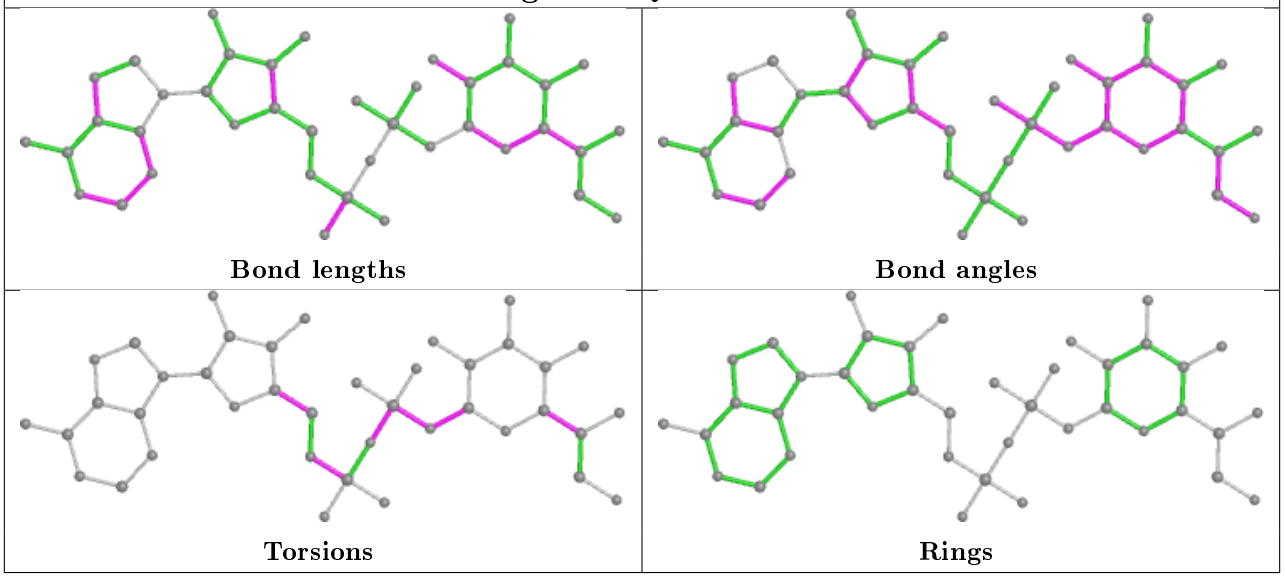
Ligand AQH J 503



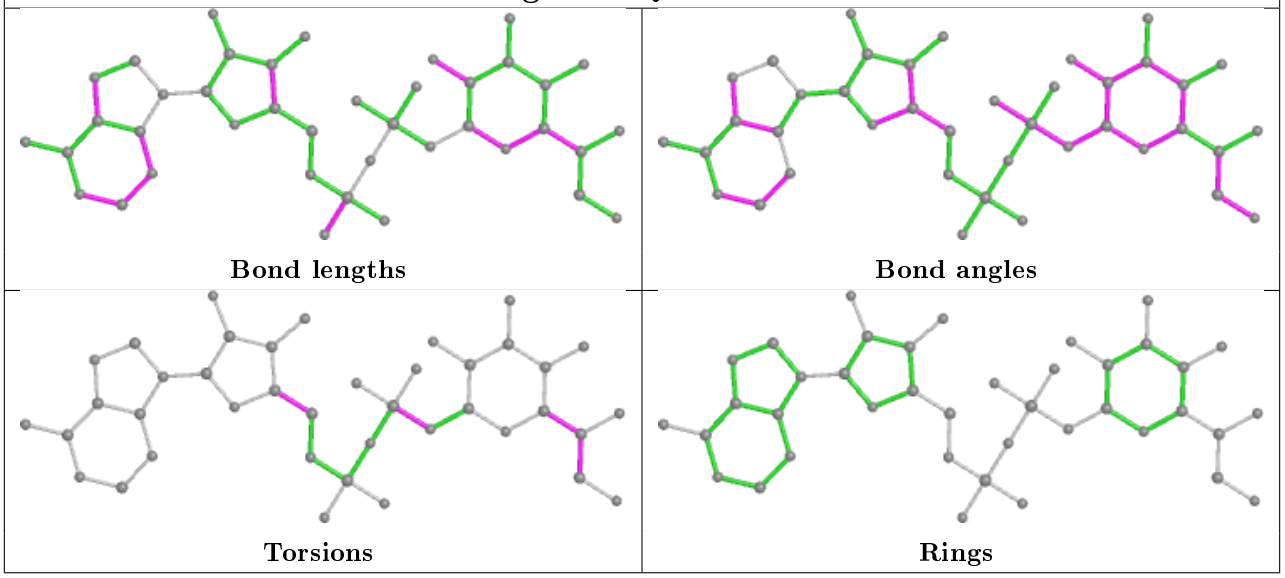
Ligand AQH I 503



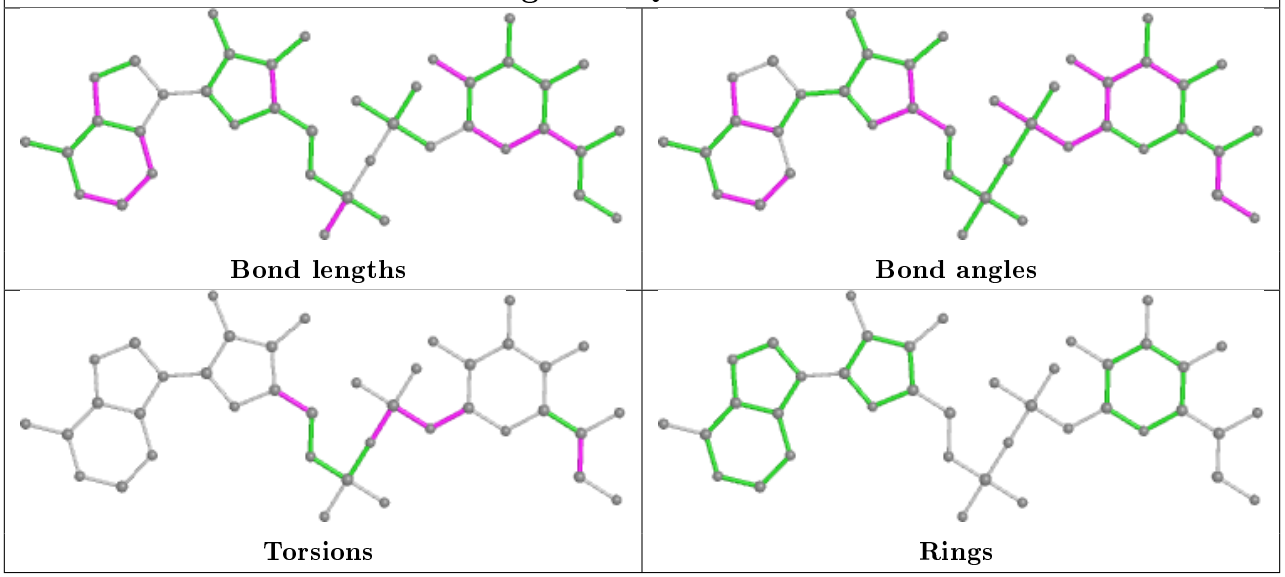
Ligand AQH G 502



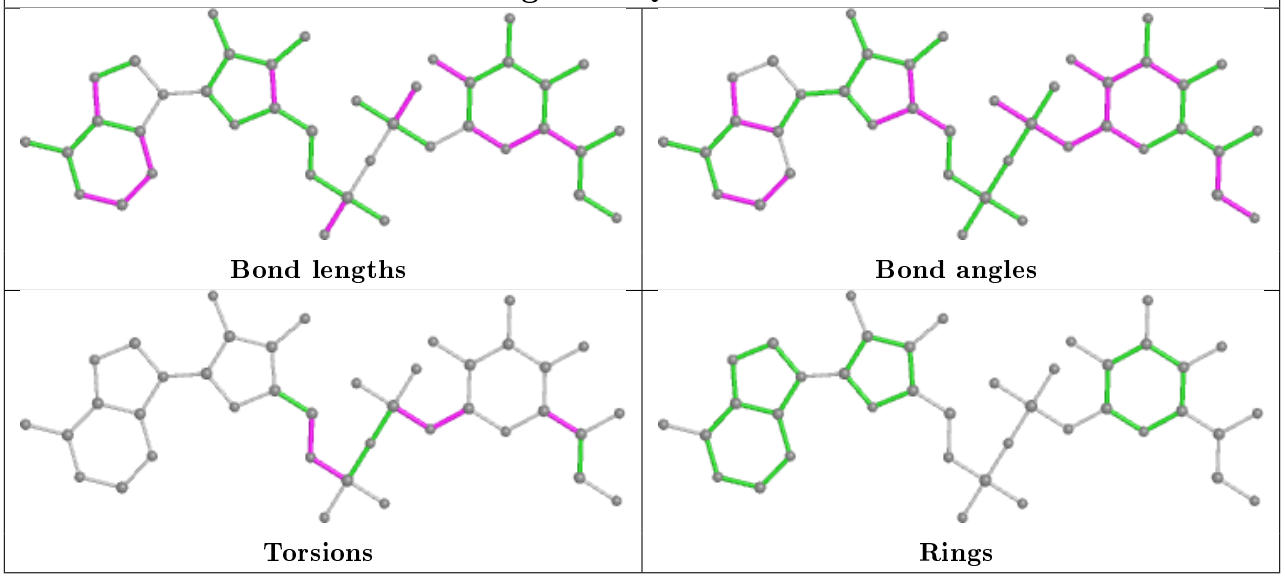
Ligand AQH B 502



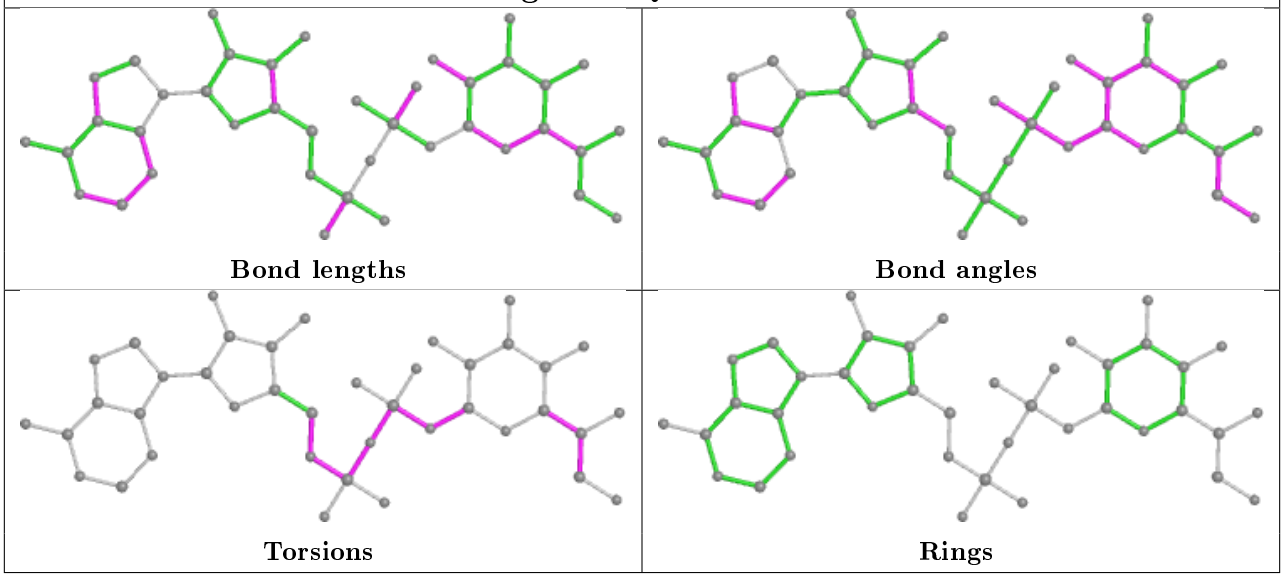
Ligand AQH A 502



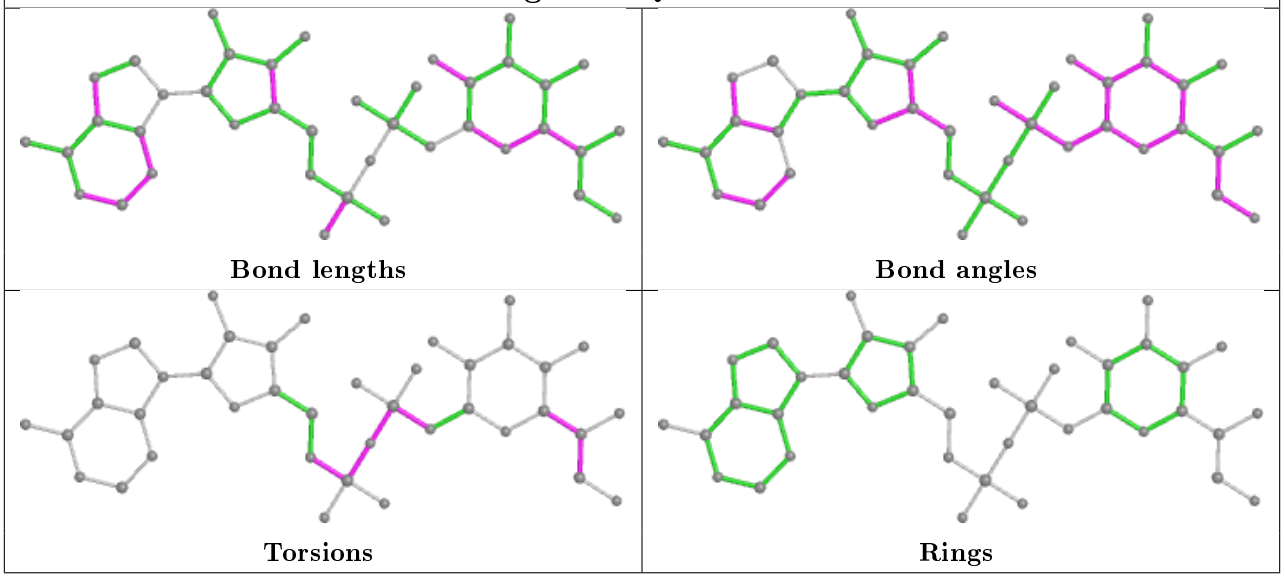
Ligand AQH D 502

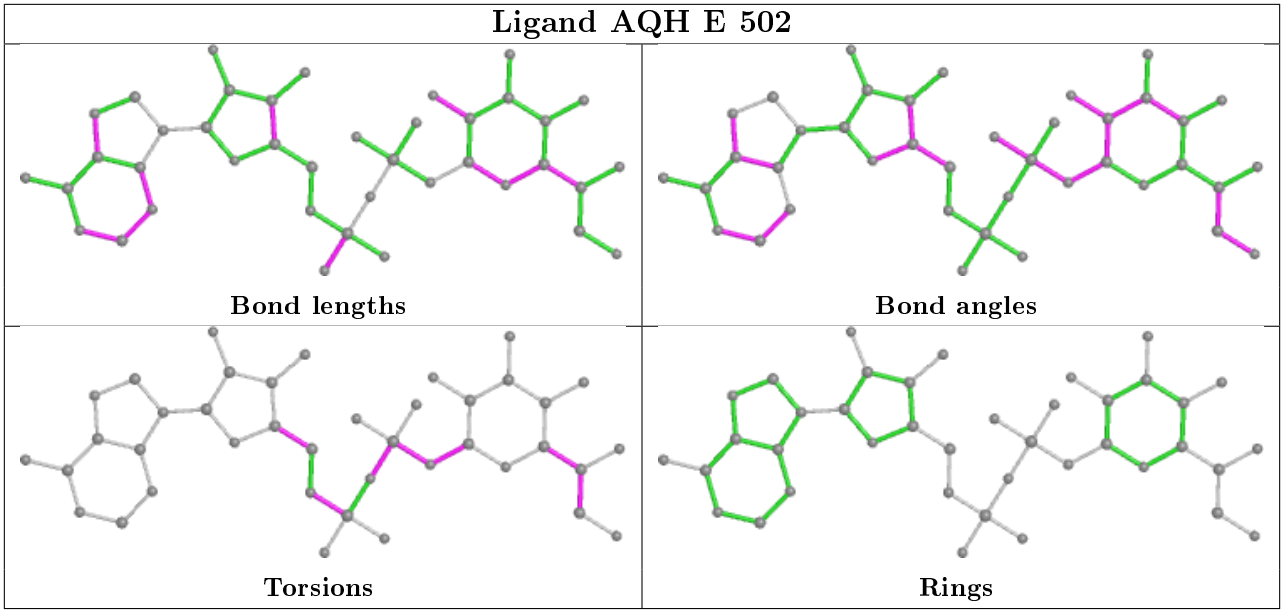


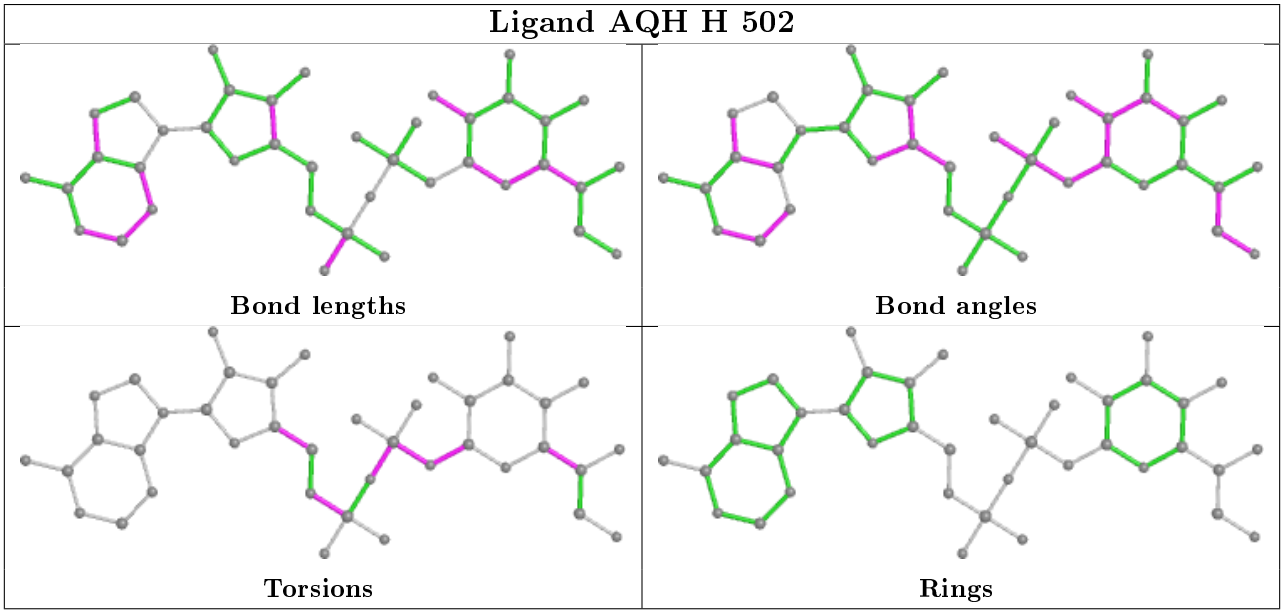
Ligand AQH K 502



Ligand AQH F 502







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	380/406 (93%)	-0.10	2 (0%)	91	86	150, 150, 150, 150	0
1	B	383/406 (94%)	-0.18	2 (0%)	91	86	150, 150, 150, 150	0
1	C	389/406 (95%)	-0.14	2 (0%)	91	86	150, 150, 150, 150	0
1	D	381/406 (93%)	-0.12	4 (1%)	82	76	30, 150, 150, 150	0
1	E	390/406 (96%)	-0.10	4 (1%)	82	76	124, 150, 150, 150	0
1	F	384/406 (94%)	-0.07	6 (1%)	72	63	150, 150, 150, 150	0
1	G	389/406 (95%)	-0.08	7 (1%)	68	60	150, 150, 150, 150	0
1	H	385/406 (94%)	-0.10	7 (1%)	68	60	25, 150, 150, 150	0
1	I	389/406 (95%)	-0.10	6 (1%)	73	65	85, 150, 150, 150	0
1	J	385/406 (94%)	-0.20	3 (0%)	86	80	150, 150, 150, 150	0
1	K	390/406 (96%)	-0.14	2 (0%)	91	86	150, 150, 150, 150	0
1	L	374/406 (92%)	-0.02	8 (2%)	63	54	23, 150, 150, 150	0
All	All	4619/4872 (94%)	-0.11	53 (1%)	80	73	23, 150, 150, 150	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	57	CYS	6.1
1	D	110	ALA	5.6
1	A	85	THR	3.9
1	L	225	SER	3.6
1	F	160	ALA	3.0
1	D	81	GLN	3.0
1	F	159	VAL	3.0
1	H	38	GLU	2.9
1	H	105	THR	2.9
1	L	395	VAL	2.8
1	E	159	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	391	THR	2.8
1	H	14	ASP	2.7
1	G	38	GLU	2.6
1	E	81	GLN	2.6
1	F	51	GLU	2.6
1	H	160	ALA	2.6
1	L	105	THR	2.5
1	I	105	THR	2.5
1	F	38	GLU	2.5
1	H	107	THR	2.5
1	G	63	TRP	2.5
1	C	82	GLY	2.5
1	B	30	ASP	2.4
1	J	159	VAL	2.4
1	I	30	ASP	2.4
1	L	365	ASP	2.4
1	L	58	ASP	2.4
1	J	105	THR	2.3
1	I	365	ASP	2.3
1	C	80	ARG	2.3
1	H	30	ASP	2.3
1	K	30	ASP	2.3
1	A	40	LYS	2.2
1	D	107	THR	2.2
1	G	104	PRO	2.2
1	L	51	GLU	2.2
1	G	370	CYS	2.2
1	K	81	GLN	2.2
1	F	22	GLU	2.1
1	H	393	GLN	2.1
1	F	82	GLY	2.1
1	G	342	CYS	2.1
1	I	396	GLU	2.1
1	B	14	ASP	2.1
1	G	11	THR	2.1
1	E	369	GLU	2.1
1	E	154	ASP	2.1
1	I	14	ASP	2.1
1	L	226	THR	2.1
1	I	160	ALA	2.0
1	G	358	CYS	2.0
1	J	358	CYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

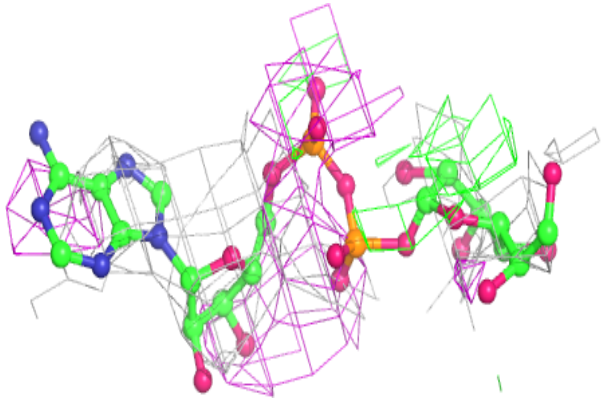
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

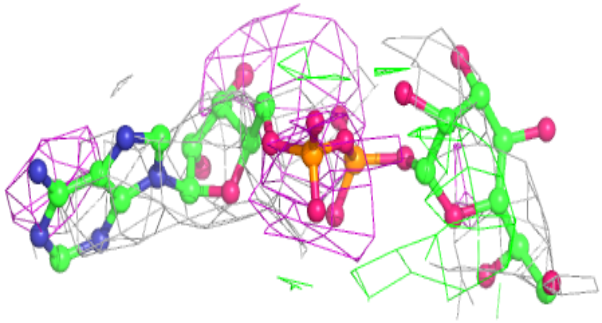
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	G	501	1/1	0.71	0.58	150,150,150,150	0
3	AQH	L	502	40/40	0.76	0.40	150,150,150,150	0
3	AQH	A	502	40/40	0.76	0.35	150,150,150,150	40
4	EDO	C	502	4/4	0.78	0.33	150,150,150,150	0
3	AQH	H	502	40/40	0.80	0.33	150,150,150,150	0
3	AQH	I	503	40/40	0.81	0.33	150,150,150,150	0
4	EDO	I	502	4/4	0.82	0.33	150,150,150,150	0
3	AQH	D	502	40/40	0.82	0.28	150,150,150,150	40
3	AQH	E	502	40/40	0.85	0.24	150,150,150,150	0
4	EDO	J	502	4/4	0.85	0.37	150,150,150,150	0
3	AQH	F	502	40/40	0.85	0.27	150,150,150,150	0
3	AQH	C	503	40/40	0.87	0.25	150,150,150,150	0
3	AQH	G	502	40/40	0.87	0.27	150,150,150,150	40
3	AQH	B	502	40/40	0.87	0.27	150,150,150,150	0
3	AQH	J	503	40/40	0.88	0.25	150,150,150,150	0
3	AQH	K	502	40/40	0.89	0.23	150,150,150,150	0
2	FE	E	501	1/1	0.91	0.52	150,150,150,150	0
2	FE	K	501	1/1	0.91	0.66	150,150,150,150	0
2	FE	I	501	1/1	0.94	0.52	150,150,150,150	0
2	FE	C	501	1/1	0.94	0.53	150,150,150,150	0
2	FE	B	501	1/1	0.98	0.43	150,150,150,150	0
2	FE	J	501	1/1	0.98	0.48	150,150,150,150	0
2	FE	D	501	1/1	0.98	0.47	150,150,150,150	0
2	FE	H	501	1/1	0.98	0.45	150,150,150,150	0
2	FE	A	501	1/1	0.99	0.46	150,150,150,150	0
2	FE	L	501	1/1	0.99	0.46	150,150,150,150	0
2	FE	F	501	1/1	0.99	0.46	150,150,150,150	0

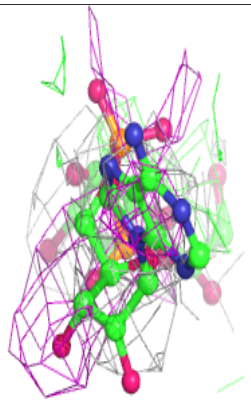
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AQH L 502:

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

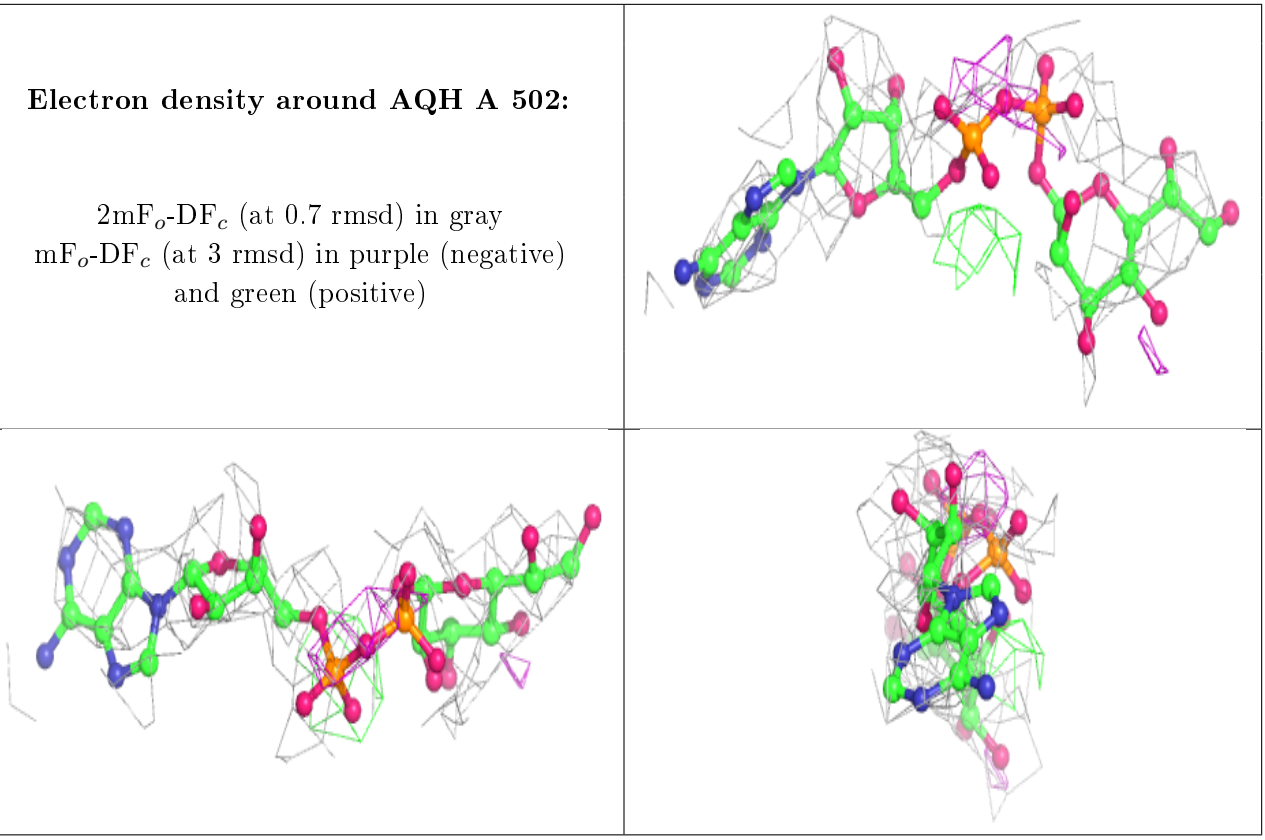






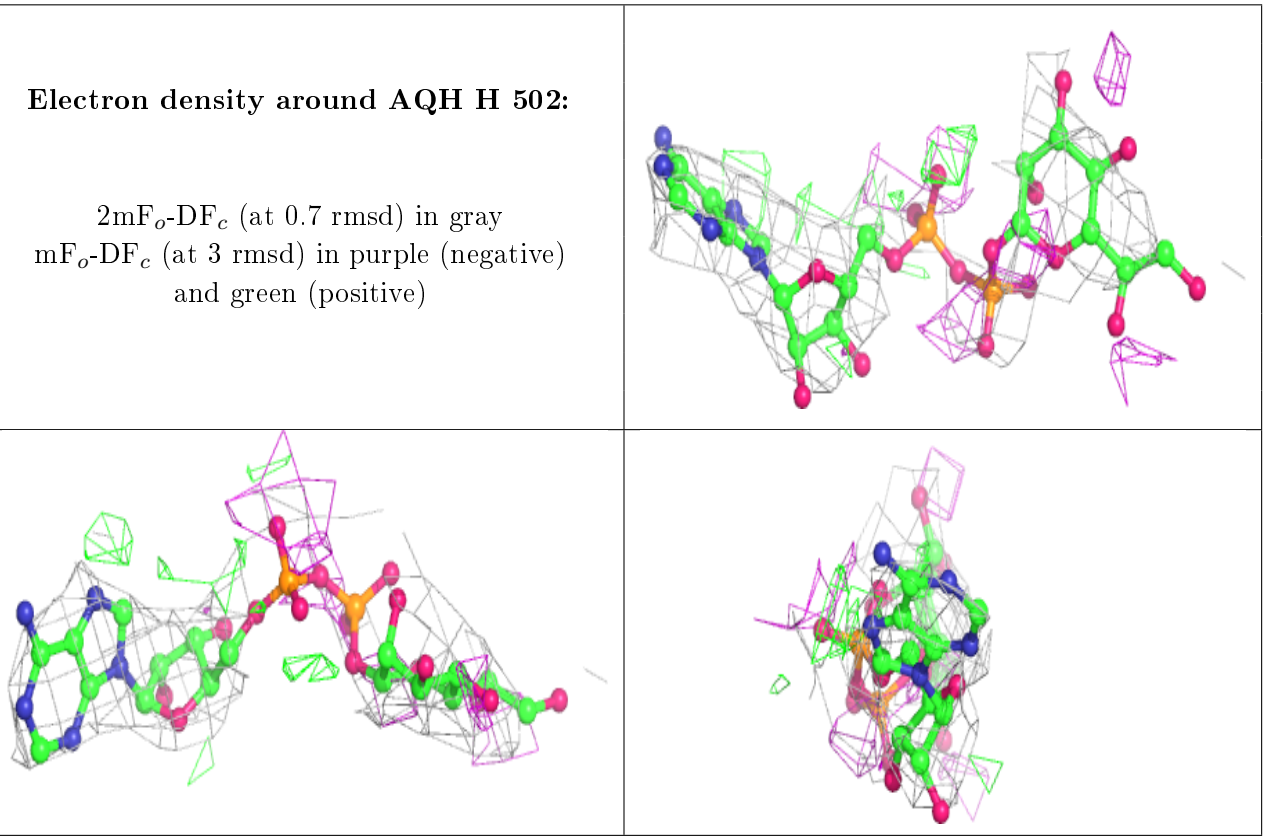
Electron density around AQH A 502:

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



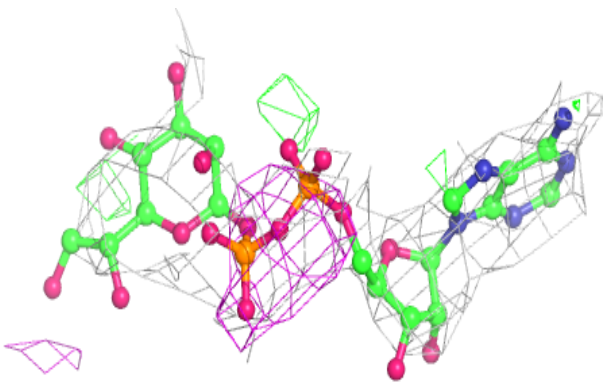
Electron density around AQH H 502:

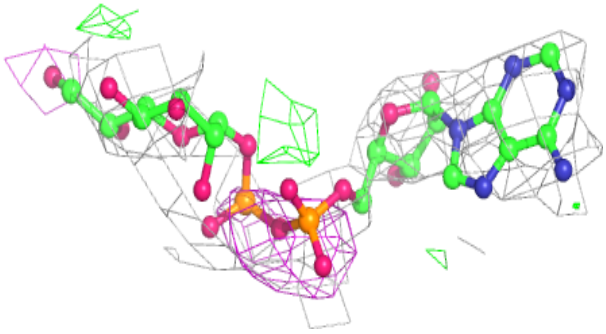
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around AQH I 503:

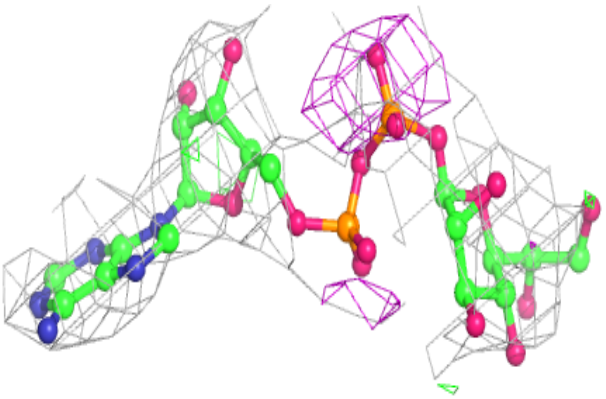
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

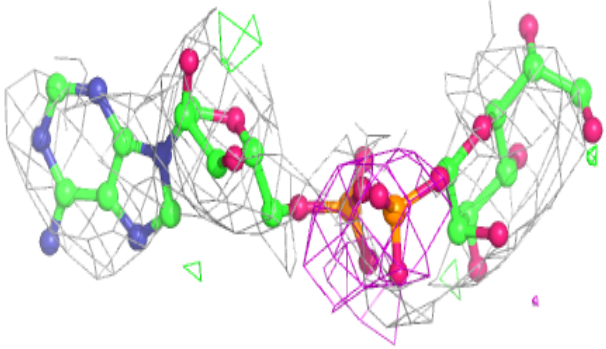


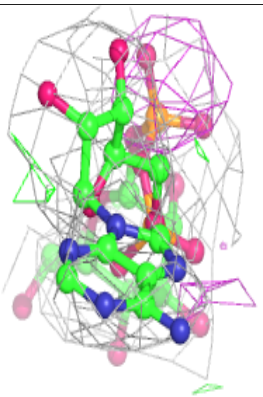


Electron density around AQH D 502:

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

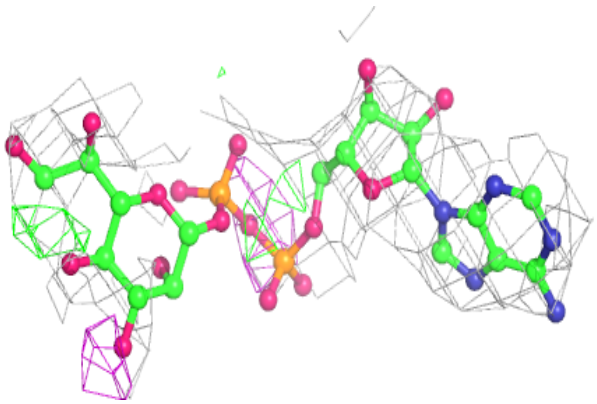


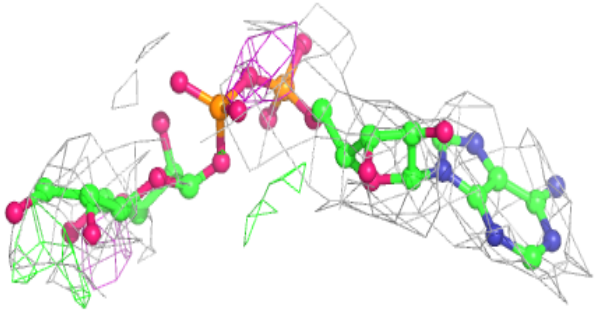


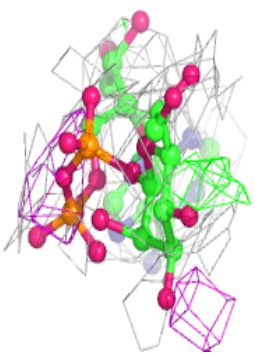


Electron density around AQH E 502:

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

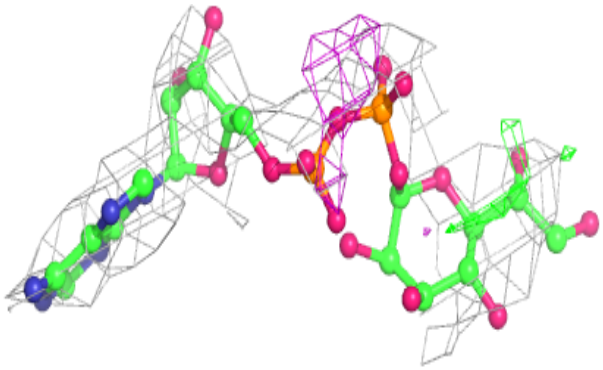


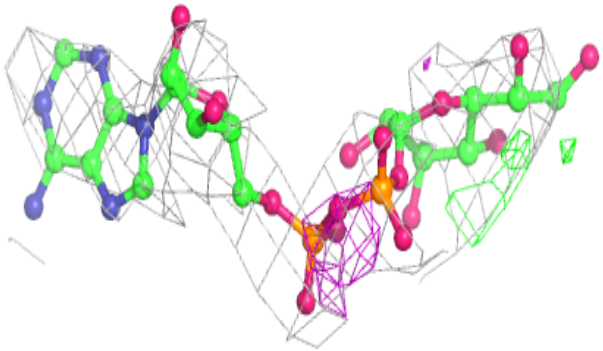


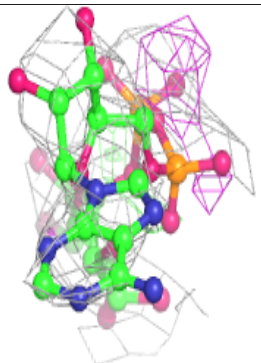


Electron density around AQH F 502:

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

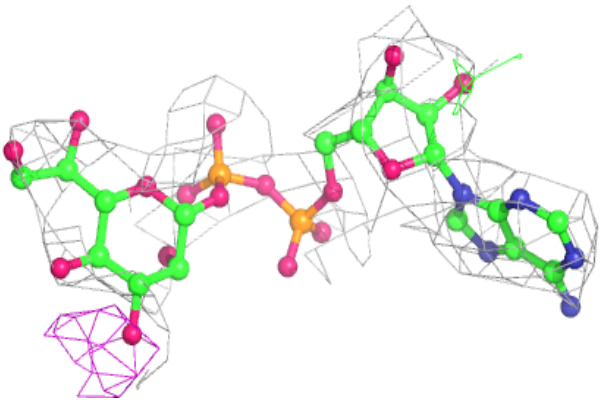


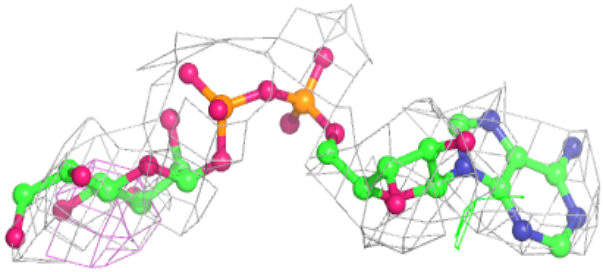


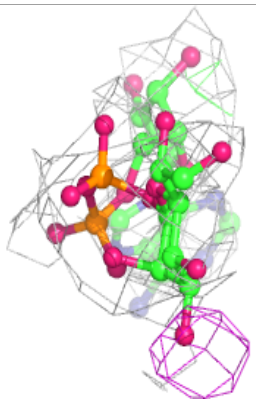


Electron density around AQH C 503:

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

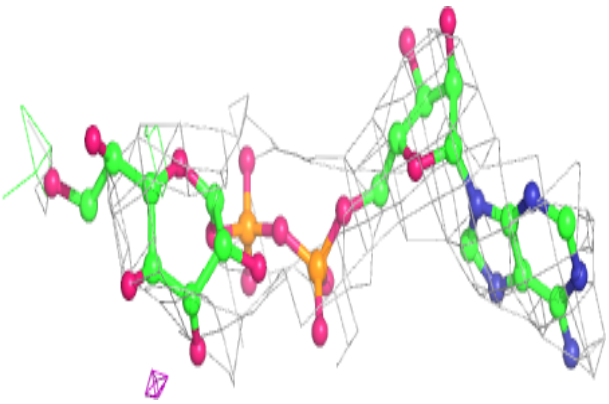


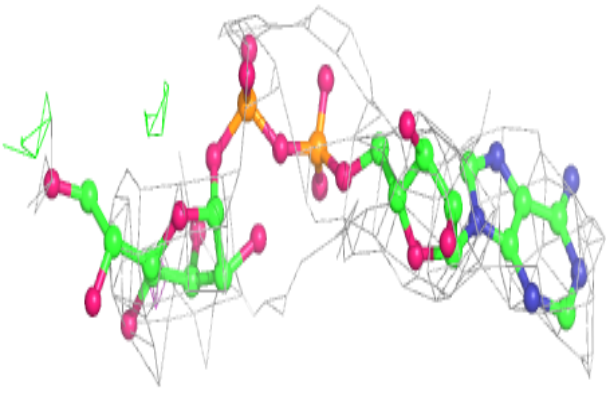


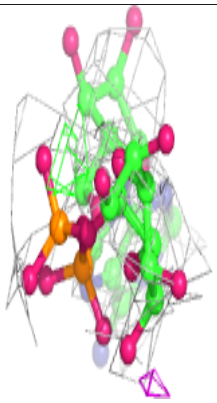


Electron density around AQH G 502:

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

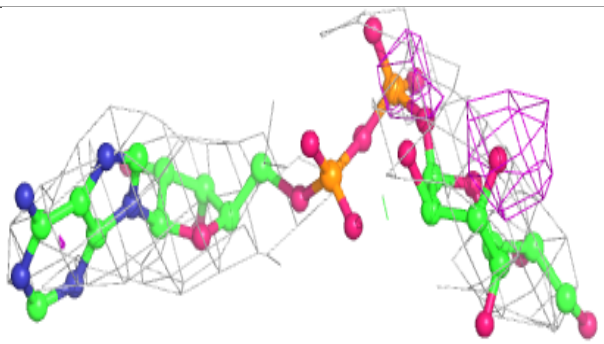


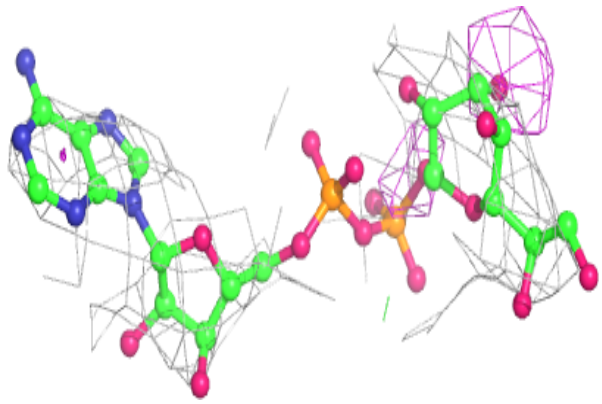


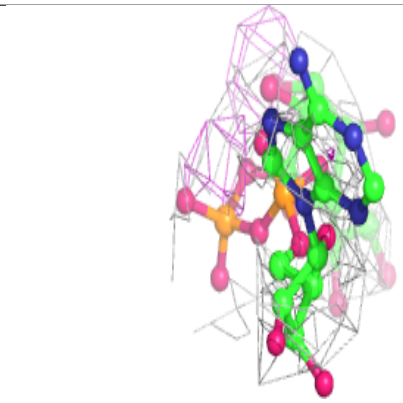


Electron density around AQH B 502:

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

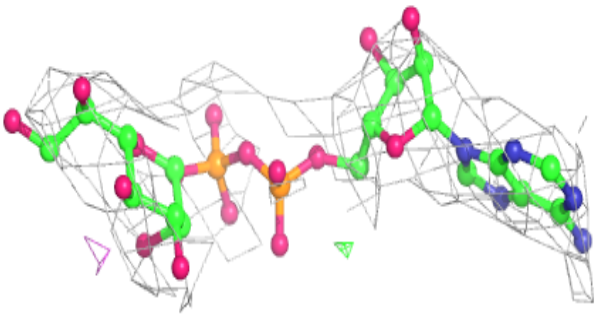


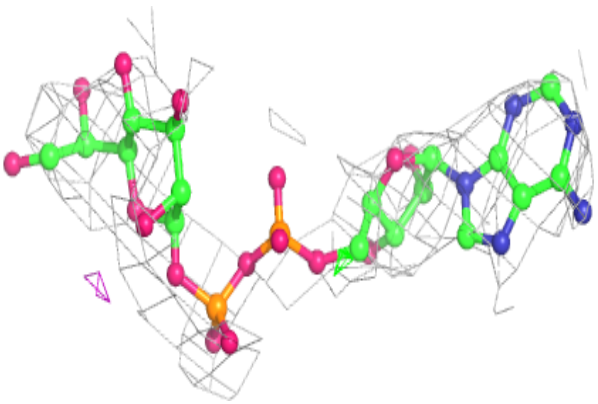


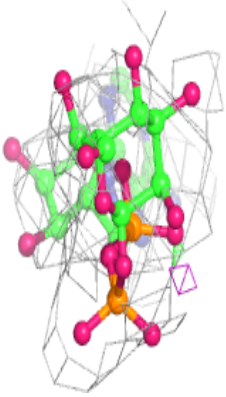


Electron density around AQH J 503:

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

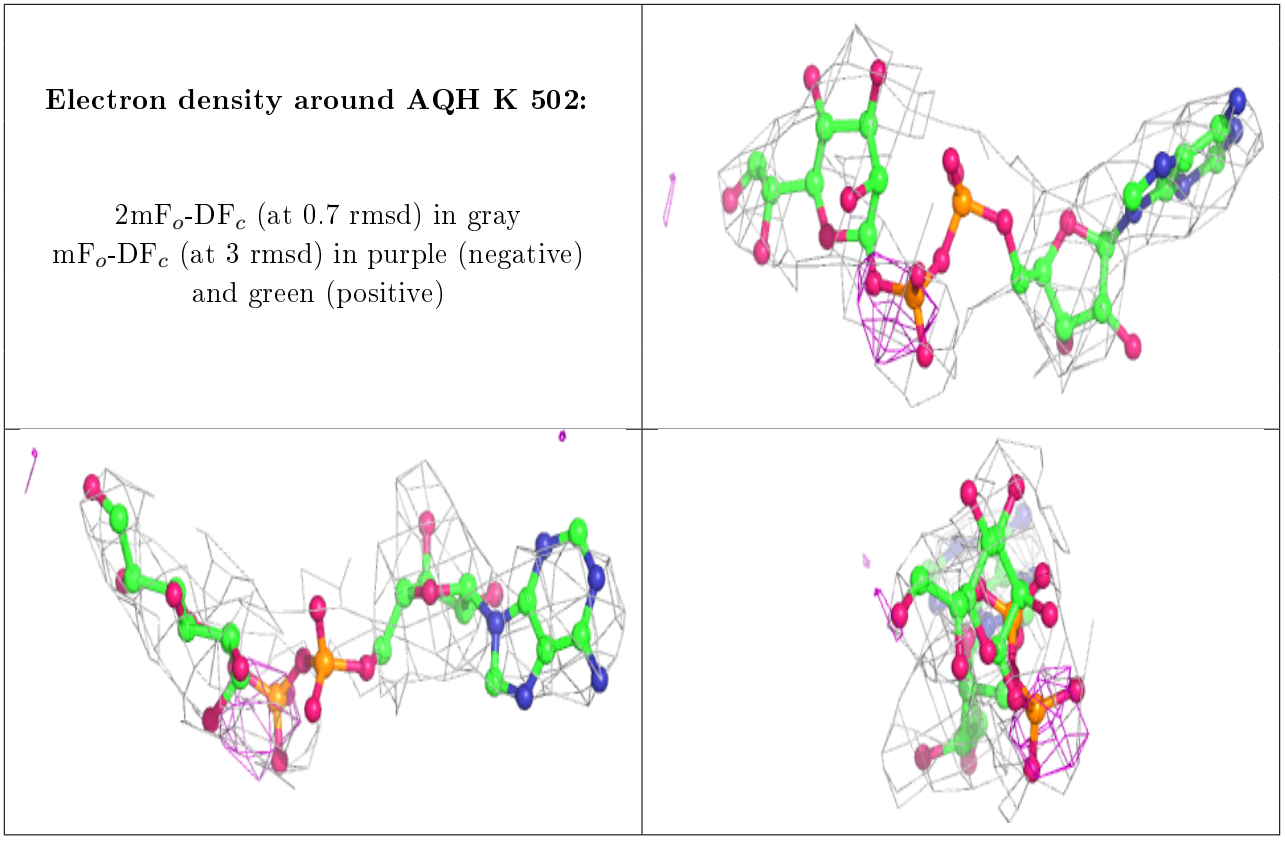






Electron density around AQH K 502:

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



6.5 Other polymers

There are no such residues in this entry.