Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2024 – 07:23 AM EST

PDB ID	:	3KOZ
Title	:	Crystal Structure of ornithine 4,5 aminomutase in complex with ornithine (Anaerobic)
Authors	:	Wolthers, K.R.; Levy, C.W.; Scrutton, N.S.; Leys, D.
Deposited on	:	2009-11-14
Resolution	:	2.80 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

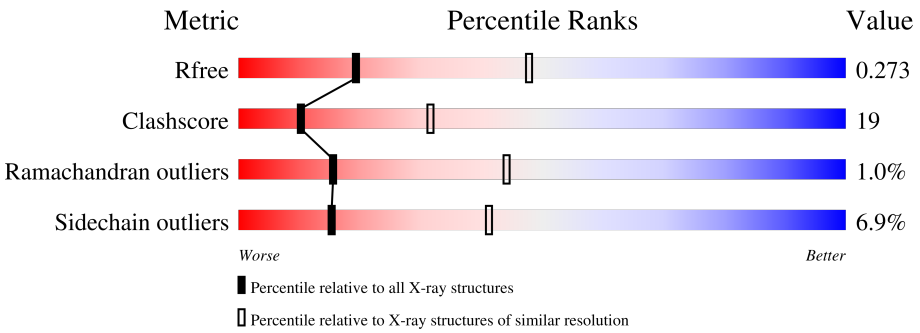
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	763	61% 31% • 5%
1	B	763	59% 33% • 5%
1	C	763	63% 30% • 5%
1	D	763	64% 29% • 5%
2	E	121	49% 36% 6% 9%
2	F	121	60% 24% 7% 9%
2	G	121	59% 30% • 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	121	61% 26% • 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	B12	A	1801	X	-	-	-
3	B12	B	1801	X	-	X	-
3	B12	C	1801	X	-	X	-
3	B12	D	1801	X	-	X	-
4	5AD	A	1500	X	-	-	-
4	5AD	B	1500	X	-	-	-
4	5AD	C	1500	X	-	-	-
4	5AD	D	1500	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26616 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 D-ornithine aminomutase E component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	5651	3561	981	1075	34	0	0	0
1	B	728	5672	3579	984	1075	34	0	0	0
1	C	728	5654	3570	981	1069	34	0	0	0
1	D	728	5664	3575	984	1071	34	0	0	0

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
A	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
A	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
A	744	SER	-	expression tag	UNP Q8VPJ5
A	745	GLU	-	expression tag	UNP Q8VPJ5
A	746	ASP	-	expression tag	UNP Q8VPJ5
A	747	PRO	-	expression tag	UNP Q8VPJ5
A	748	ASN	-	expression tag	UNP Q8VPJ5
A	749	SER	-	expression tag	UNP Q8VPJ5
A	750	SER	-	expression tag	UNP Q8VPJ5
A	751	SER	-	expression tag	UNP Q8VPJ5
A	752	VAL	-	expression tag	UNP Q8VPJ5
A	753	ASP	-	expression tag	UNP Q8VPJ5
A	754	LYS	-	expression tag	UNP Q8VPJ5
A	755	LEU	-	expression tag	UNP Q8VPJ5
A	756	ALA	-	expression tag	UNP Q8VPJ5
A	757	ALA	-	expression tag	UNP Q8VPJ5
A	758	ALA	-	expression tag	UNP Q8VPJ5
A	759	LEU	-	expression tag	UNP Q8VPJ5
A	760	GLU	-	expression tag	UNP Q8VPJ5
A	761	HIS	-	expression tag	UNP Q8VPJ5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	762	HIS	-	expression tag	UNP Q8VPJ5
A	763	HIS	-	expression tag	UNP Q8VPJ5
A	764	HIS	-	expression tag	UNP Q8VPJ5
A	765	HIS	-	expression tag	UNP Q8VPJ5
A	766	HIS	-	expression tag	UNP Q8VPJ5
B	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
B	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
B	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
B	744	SER	-	expression tag	UNP Q8VPJ5
B	745	GLU	-	expression tag	UNP Q8VPJ5
B	746	ASP	-	expression tag	UNP Q8VPJ5
B	747	PRO	-	expression tag	UNP Q8VPJ5
B	748	ASN	-	expression tag	UNP Q8VPJ5
B	749	SER	-	expression tag	UNP Q8VPJ5
B	750	SER	-	expression tag	UNP Q8VPJ5
B	751	SER	-	expression tag	UNP Q8VPJ5
B	752	VAL	-	expression tag	UNP Q8VPJ5
B	753	ASP	-	expression tag	UNP Q8VPJ5
B	754	LYS	-	expression tag	UNP Q8VPJ5
B	755	LEU	-	expression tag	UNP Q8VPJ5
B	756	ALA	-	expression tag	UNP Q8VPJ5
B	757	ALA	-	expression tag	UNP Q8VPJ5
B	758	ALA	-	expression tag	UNP Q8VPJ5
B	759	LEU	-	expression tag	UNP Q8VPJ5
B	760	GLU	-	expression tag	UNP Q8VPJ5
B	761	HIS	-	expression tag	UNP Q8VPJ5
B	762	HIS	-	expression tag	UNP Q8VPJ5
B	763	HIS	-	expression tag	UNP Q8VPJ5
B	764	HIS	-	expression tag	UNP Q8VPJ5
B	765	HIS	-	expression tag	UNP Q8VPJ5
B	766	HIS	-	expression tag	UNP Q8VPJ5
C	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
C	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
C	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
C	744	SER	-	expression tag	UNP Q8VPJ5
C	745	GLU	-	expression tag	UNP Q8VPJ5
C	746	ASP	-	expression tag	UNP Q8VPJ5
C	747	PRO	-	expression tag	UNP Q8VPJ5
C	748	ASN	-	expression tag	UNP Q8VPJ5
C	749	SER	-	expression tag	UNP Q8VPJ5
C	750	SER	-	expression tag	UNP Q8VPJ5
C	751	SER	-	expression tag	UNP Q8VPJ5

Continued on next page...

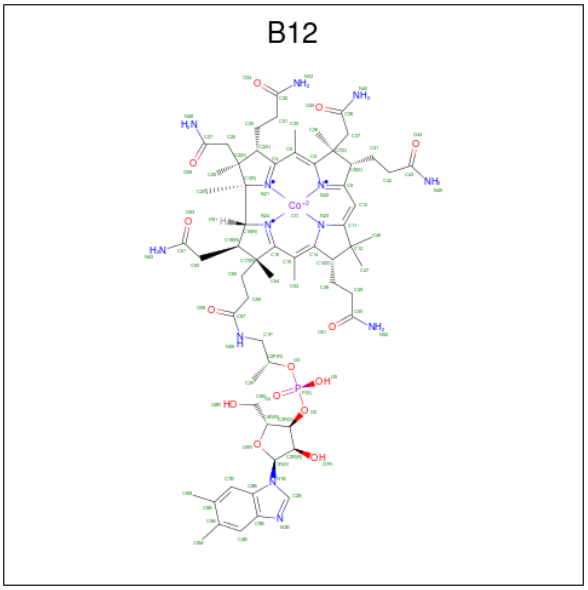
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	752	VAL	-	expression tag	UNP Q8VPJ5
C	753	ASP	-	expression tag	UNP Q8VPJ5
C	754	LYS	-	expression tag	UNP Q8VPJ5
C	755	LEU	-	expression tag	UNP Q8VPJ5
C	756	ALA	-	expression tag	UNP Q8VPJ5
C	757	ALA	-	expression tag	UNP Q8VPJ5
C	758	ALA	-	expression tag	UNP Q8VPJ5
C	759	LEU	-	expression tag	UNP Q8VPJ5
C	760	GLU	-	expression tag	UNP Q8VPJ5
C	761	HIS	-	expression tag	UNP Q8VPJ5
C	762	HIS	-	expression tag	UNP Q8VPJ5
C	763	HIS	-	expression tag	UNP Q8VPJ5
C	764	HIS	-	expression tag	UNP Q8VPJ5
C	765	HIS	-	expression tag	UNP Q8VPJ5
C	766	HIS	-	expression tag	UNP Q8VPJ5
D	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
D	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
D	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
D	744	SER	-	expression tag	UNP Q8VPJ5
D	745	GLU	-	expression tag	UNP Q8VPJ5
D	746	ASP	-	expression tag	UNP Q8VPJ5
D	747	PRO	-	expression tag	UNP Q8VPJ5
D	748	ASN	-	expression tag	UNP Q8VPJ5
D	749	SER	-	expression tag	UNP Q8VPJ5
D	750	SER	-	expression tag	UNP Q8VPJ5
D	751	SER	-	expression tag	UNP Q8VPJ5
D	752	VAL	-	expression tag	UNP Q8VPJ5
D	753	ASP	-	expression tag	UNP Q8VPJ5
D	754	LYS	-	expression tag	UNP Q8VPJ5
D	755	LEU	-	expression tag	UNP Q8VPJ5
D	756	ALA	-	expression tag	UNP Q8VPJ5
D	757	ALA	-	expression tag	UNP Q8VPJ5
D	758	ALA	-	expression tag	UNP Q8VPJ5
D	759	LEU	-	expression tag	UNP Q8VPJ5
D	760	GLU	-	expression tag	UNP Q8VPJ5
D	761	HIS	-	expression tag	UNP Q8VPJ5
D	762	HIS	-	expression tag	UNP Q8VPJ5
D	763	HIS	-	expression tag	UNP Q8VPJ5
D	764	HIS	-	expression tag	UNP Q8VPJ5
D	765	HIS	-	expression tag	UNP Q8VPJ5
D	766	HIS	-	expression tag	UNP Q8VPJ5

- Molecule 2 is a protein called D-ornithine aminomutase S component.

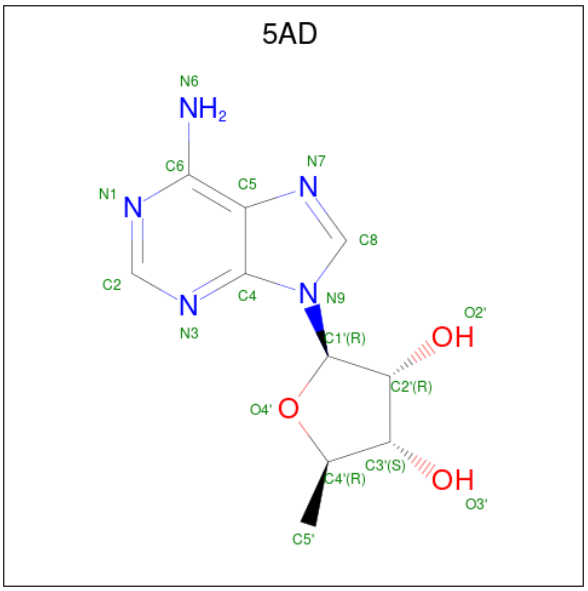
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	110	860	541	153	162	4	0	0	0
			Total	C	N	O	S			
2	F	110	863	542	153	164	4	0	0	0
			Total	C	N	O	S			
2	G	110	860	541	153	162	4	0	0	0
			Total	C	N	O	S			
2	H	110	860	541	153	162	4	0	0	0

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



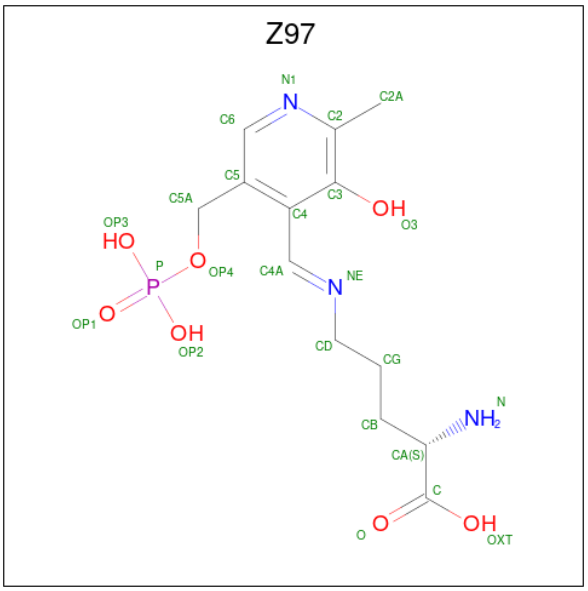
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Co	N	O	P		
3	A	1	91	62	1	13	14	1	0	0
			Total	C	Co	N	O	P		
3	B	1	91	62	1	13	14	1	0	0
			Total	C	Co	N	O	P		
3	C	1	91	62	1	13	14	1	0	0
			Total	C	Co	N	O	P		
3	D	1	91	62	1	13	14	1	0	0

- Molecule 4 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	18	10	5	3	0	0
4	B	1	18	10	5	3	0	0
4	C	1	18	10	5	3	0	0
4	D	1	18	10	5	3	0	0

- Molecule 5 is (E)-N 5 -({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyl idene)-L-ornithine (three-letter code: Z97) (formula: $C_{13}H_{20}N_3O_7P$).



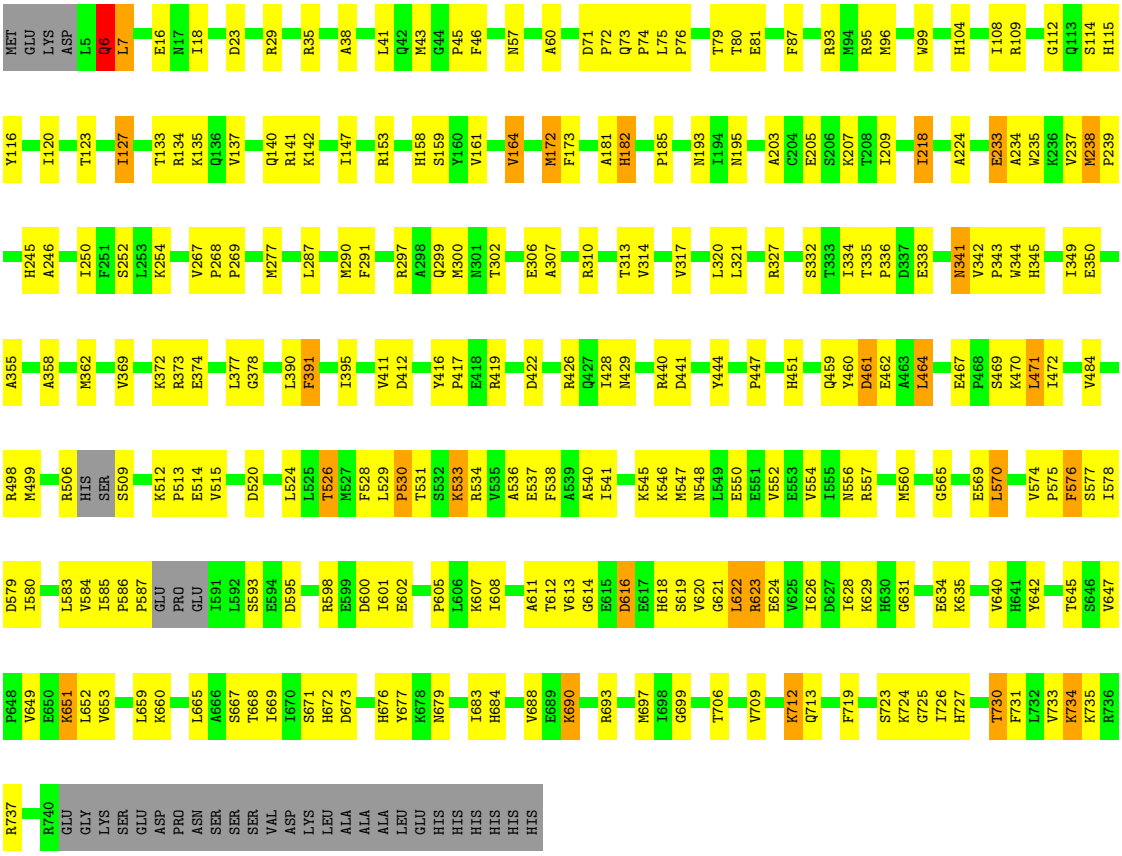
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	24	13	3	7	1	0	0
			Total	C	N	O	P		
5	B	1	24	13	3	7	1	0	0
			Total	C	N	O	P		
5	C	1	24	13	3	7	1	0	0
			Total	C	N	O	P		
5	D	1	24	13	3	7	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

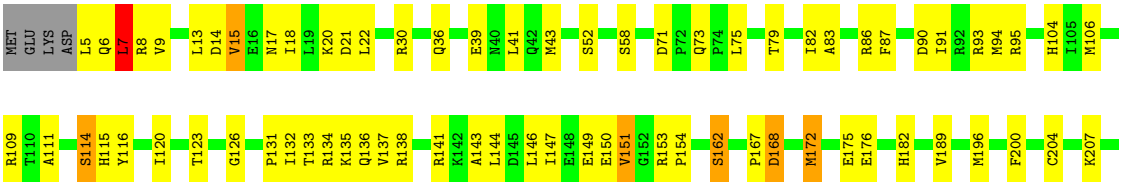
• Molecule 1: D-ornithine aminomutase E component

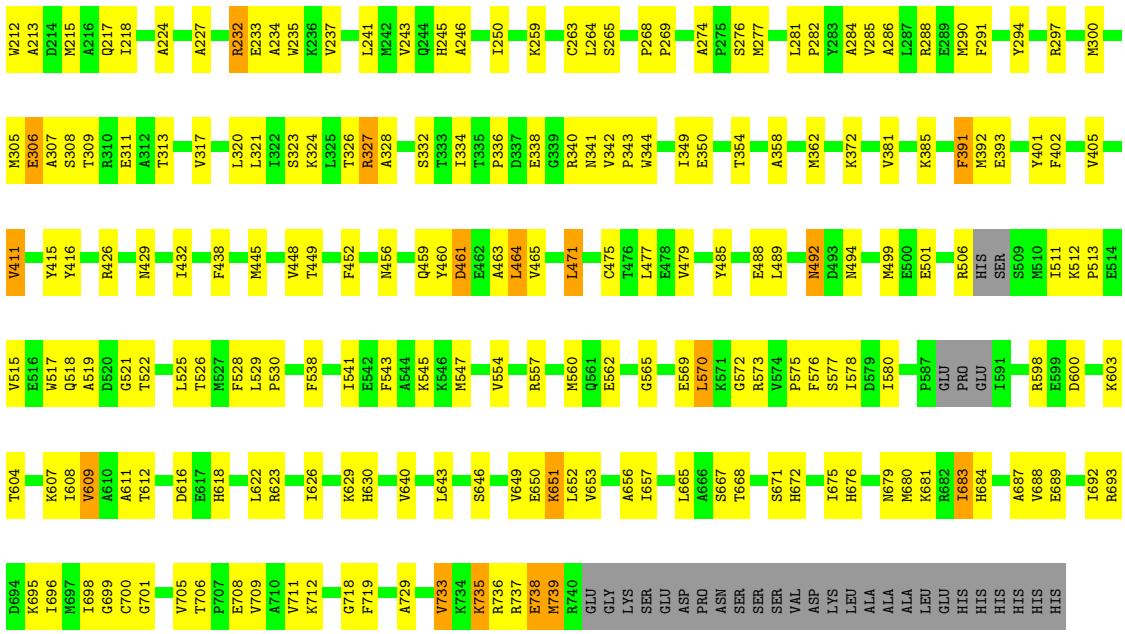
Chain A: 61% 31% • 5%



• Molecule 1: D-ornithine aminomutase E component

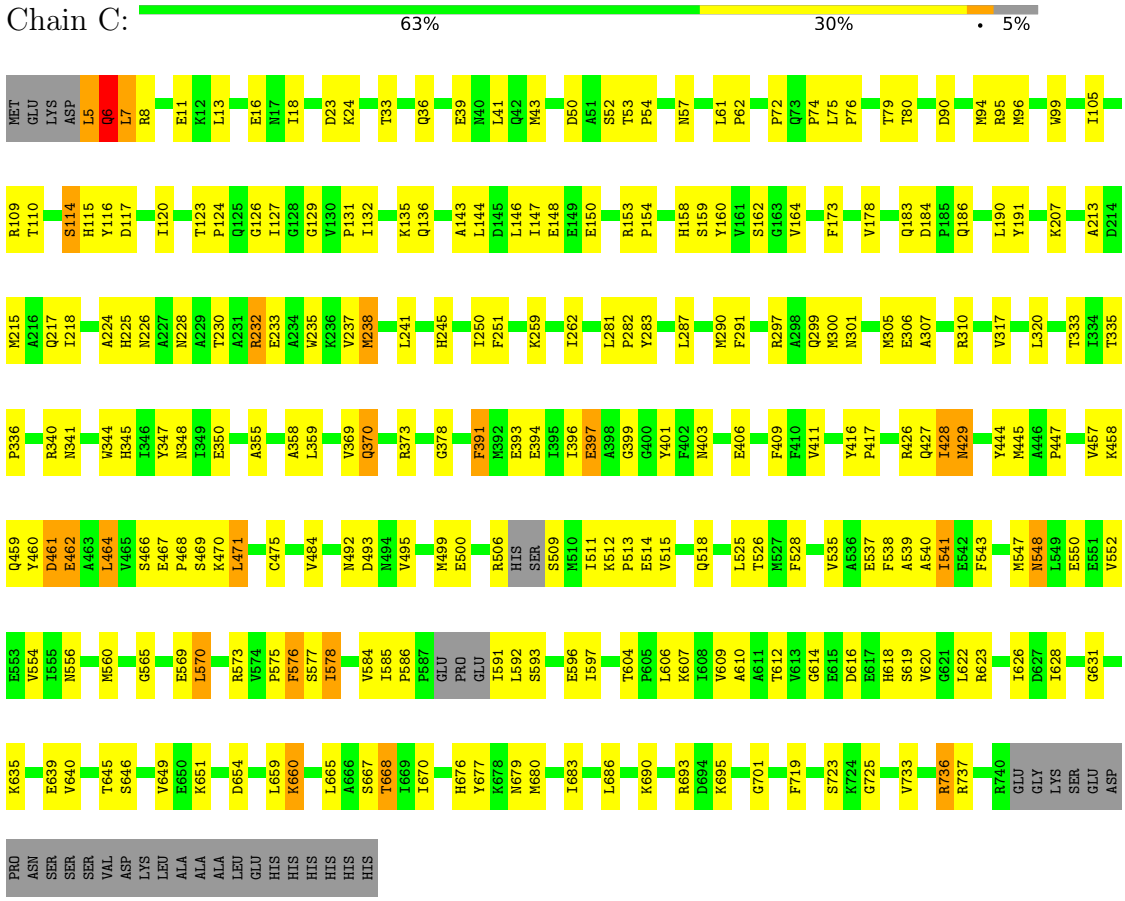
Chain B: 59% 33% • 5%





• Molecule 1: D-ornithine aminomutase E component

Chain C:



• Molecule 1: D-ornithine aminomutase E component

Chain D:

MET GLU LYS ASP L5 Q6 L7 R8 V9 N10 E11 I18 D23 K24 Y25 T26 P27 K28 R29 R30 G31 E39 N40 L41 Q42 M43 D50 T53 N57 S63 A64 K65 P72 T79 G85 R86 F87 E88 D89 D90 M94 W99 H104 I108 R109 T110

A111 S114 H115 Y116 I120 T123 P124 I127 G128 G129 V130 P131 I132 T133 R134 K135 Q136 V137 R138 E150 H158 V161 S162 M172 F173 E176 N179 Q186 Y187 N188 V189 R192 M196 C204 E205 W212 I218 D219 G223 A224 R232 E233 A234

W235 K236 V237 M238 H245 N248 S249 I250 F251 V255 L264 V267 P268 P269 P275 L279 D280 L281 P282 A286 M290 F291 M305 E306 A307 R310 H316 N319 L320 D337 E338 G339 R340 N341 V342 P343 W344 A355 A358 Q370 R373 E374

V381 R382 V389 L390 F391 E394 I395 I396 E397 A398 G399 G400 Y401 F402 N403 E406 F409 F410 V411 Y415 Y416 P417 E418 I424 I428 F438 D443 Y444 M445 A446 P447 V448 T449 A450 H451 F452 N456 Q459 Y460 D461 E462 A463 L464 E467 P468 L471

L477 E478 V479 P480 Y485 E491 N492 D493 N494 V497 R498 M499 E500 E501 T502 R506 HIS SER S509 M510 I511 K512 P513 E514 V515 Q518 T522 V523 L524 L525 T526 M527 F528 L529 P530 V535 A536 E537 I541 E542 F543 M547 V554 M560 Q561 E562 A563 E564

E569 V574 P575 F576 S577 I578 I585 P586 P587 GLU PRO GLU I591 R598 K607 I608 V609 A610 A611 H618 S619 V620 G621 L622 R623 I626 D627 I628 G632 I633 E634 Y642 L643 V647 P648 V649 E650 K651 L652 V653 K660 A663 I664 L665 A666 S667 T668

S671 D674 I675 H676 I683 H684 A687 V688 E689 K690 R693 D694 K695 I696 M697 C700 E708 V711 G718 R721 G725 F731 K734 K735 R736 M739 R740 GLU GLY LYS SER GLU ASP PRO ASN SER SER SER VAL ASP LYS LEU ALA ALA ALA LEU GLU

HIS HIS HIS HIS HIS

- Molecule 2: D-ornithine aminomutase S component

Chain E:

MET LYS ARG ALA D5 D6 F7 R10 L14 E20 E21 L22 Q23 F26 E31 D35 P36 K42 P47 S48 I49 E50 R51 S52 V53 L54 L55 R56 M57 S60 E63 A64 I67 V68 D69 K70 T71 M72 D73 R74 G75 L76 M77 G78 K79 G80 A81 G82 H83

I84 V85 I88 A89 K90 E91 K92 N93 E98 A99 A102 K107 Y108 W109 D110 D111 A112 I113 Q114 ILE PHE LYS GLY GLY VAL LYS

- Molecule 2: D-ornithine aminomutase S component

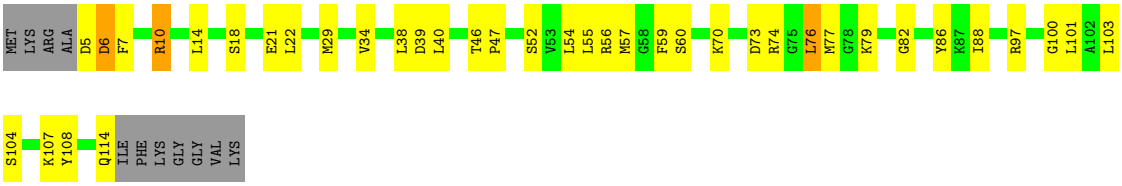
Chain F:

MET LYS ARG ALA D5 D6 F7 R10 R11 E20 Q23 T24 R25 E28 M29 K32 P36 L37 S52 V53 L54 L55 R56 M57 G58 F59 E63 A64 K65 A66 I67 K70 L76 M77 I84 I88 I94 R97 G100 L101 A102 L103 S104 E105

W109 A112 I113 Q114 ILE PHE LYS GLY GLY VAL LYS

- Molecule 2: D-ornithine aminomutase S component

Chain G:



• Molecule 2: D-ornithine aminomutase S component

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.52Å 233.22Å 124.14Å 90.00° 103.43° 90.00°	Depositor
Resolution (Å)	60.37 – 2.80 65.36 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.8 (60.37-2.80) 97.9 (65.36-2.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.5_2, REFMAC 5.5.0102	Depositor
R, R_{free}	0.185 , 0.254 0.264 , 0.273	Depositor DCC
R_{free} test set	5217 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	26616	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.40% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: Z97, B12, 5AD

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	0.45	0/5756	0.63	1/7794 (0.0%)
1	B	0.45	0/5777	0.63	1/7818 (0.0%)
1	C	0.44	0/5759	0.62	0/7796
1	D	0.45	0/5769	0.62	0/7808
2	E	0.45	0/872	0.61	0/1170
2	F	0.45	0/875	0.65	0/1174
2	G	0.43	0/872	0.58	0/1170
2	H	0.46	0/872	0.61	0/1170
All	All	0.45	0/26552	0.62	2/35900 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	164	VAL	CB-CA-C	-5.23	101.47	111.40
1	B	7	LEU	CA-CB-CG	-5.14	103.47	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5651	0	5584	210	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5672	0	5644	236	0
1	C	5654	0	5621	207	0
1	D	5664	0	5636	206	0
2	E	860	0	865	41	0
2	F	863	0	867	35	0
2	G	860	0	865	30	0
2	H	860	0	865	36	0
3	A	91	0	87	19	0
3	B	91	0	87	24	0
3	C	91	0	87	24	0
3	D	91	0	87	31	0
4	A	18	0	7	3	0
4	B	18	0	7	3	0
4	C	18	0	7	3	0
4	D	18	0	7	3	0
5	A	24	0	18	3	0
5	B	24	0	18	3	0
5	C	24	0	18	3	0
5	D	24	0	18	7	0
All	All	26616	0	26395	996	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 19.

All (996) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:ASP:HA	2:E:7:PHE:N	1.61	1.16
2:F:5:ASP:HA	2:F:7:PHE:N	1.66	1.08
2:G:5:ASP:HA	2:G:7:PHE:N	1.70	1.07
1:D:537:GLU:HG3	1:D:554:VAL:HG21	1.39	1.04
2:F:5:ASP:HA	2:F:7:PHE:H	1.21	0.99
3:A:1801:B12:H262	3:A:1801:B12:H601	1.45	0.98
2:G:5:ASP:HA	2:G:7:PHE:H	1.26	0.97
1:C:649:VAL:HG13	1:C:683:ILE:HG12	1.47	0.97
1:B:525:LEU:HD23	1:B:570:LEU:HD11	1.45	0.96
1:B:526:THR:HG23	1:B:569:GLU:HG2	1.48	0.94
2:E:5:ASP:HA	2:E:7:PHE:H	1.24	0.93
3:C:1801:B12:H401	3:C:1801:B12:H8	1.33	0.92
1:B:109:ARG:HG2	1:B:132:ILE:HG13	1.54	0.89
1:C:668:THR:HG23	1:C:676:HIS:HB2	1.51	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:HD11	3:C:1801:B12:H1P1	1.54	0.89
1:B:14:ASP:OD2	1:B:17:ASN:HB2	1.72	0.89
2:H:25:ARG:HA	2:H:28:GLU:HG3	1.54	0.89
3:C:1801:B12:H362	3:C:1801:B12:H351	1.54	0.88
1:B:577:SER:O	1:B:578:ILE:HD12	1.75	0.86
2:H:5:ASP:HA	2:H:7:PHE:N	1.90	0.86
1:D:611:ALA:HB2	1:D:643:LEU:HB2	1.56	0.85
1:B:598:ARG:NH2	1:D:232:ARG:HH21	1.76	0.84
1:C:612:THR:HB	1:C:645:THR:HG22	1.59	0.84
1:B:393:GLU:HG3	2:F:29:MET:CE	2.09	0.82
1:C:525:LEU:HB3	1:C:570:LEU:HD12	1.61	0.82
1:D:109:ARG:NH2	5:D:767:Z97:OP2	2.14	0.81
1:C:668:THR:CG2	1:C:676:HIS:HB2	2.10	0.80
1:C:41:LEU:HD21	1:C:43:MET:HE2	1.64	0.80
1:D:88:GLU:OE2	1:D:498:ARG:HD2	1.82	0.80
1:C:213:ALA:HB3	1:C:215:MET:HG3	1.63	0.79
2:F:88:ILE:HG13	2:F:103:LEU:HD11	1.65	0.79
1:A:577:SER:O	1:A:578:ILE:HD12	1.83	0.79
1:B:207:LYS:HZ2	1:B:217:GLN:NE2	1.80	0.79
1:B:649:VAL:HG13	1:B:683:ILE:HG12	1.65	0.79
3:D:1801:B12:H362	3:D:1801:B12:H351	1.65	0.78
1:B:456:ASN:OD1	1:B:459:GLN:HB3	1.83	0.78
1:C:460:TYR:O	1:C:461:ASP:HB2	1.82	0.78
1:D:394:GLU:HG2	1:D:409:PHE:CE2	2.19	0.78
1:A:267:VAL:HG22	1:A:299:GLN:HB3	1.66	0.77
1:D:394:GLU:HG2	1:D:409:PHE:HE2	1.47	0.77
1:B:207:LYS:HZ2	1:B:217:GLN:HE22	1.33	0.77
1:D:5:LEU:HD23	1:D:6:GLN:HB2	1.66	0.77
1:D:652:LEU:HD23	1:D:683:ILE:HD11	1.67	0.76
3:B:1801:B12:H291	3:B:1801:B12:H251	1.50	0.76
1:A:724:LYS:HB2	1:A:726:ILE:HG22	1.67	0.76
1:C:250:ILE:HG23	2:G:34:VAL:HG21	1.68	0.76
1:D:512:LYS:HB2	1:D:513:PRO:HD2	1.68	0.76
1:C:123:THR:HG23	1:C:135:LYS:HD3	1.67	0.75
1:A:528:PHE:CE1	1:A:565:GLY:HA3	2.20	0.75
1:B:506:ARG:HH11	1:B:518:GLN:HE22	1.32	0.75
3:B:1801:B12:N40	3:B:1801:B12:H8	2.00	0.74
1:B:41:LEU:HD23	1:B:43:MET:HE2	1.69	0.74
1:B:233:GLU:HG2	1:B:235:TRP:CH2	2.21	0.74
1:B:651:LYS:HE3	1:B:651:LYS:HA	1.68	0.74
1:C:514:GLU:OE2	1:C:518:GLN:HA	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1801:B12:H362	3:A:1801:B12:H351	1.69	0.74
1:C:512:LYS:HB2	1:C:513:PRO:HD2	1.69	0.74
2:F:109:TRP:O	2:F:113:ILE:HG13	1.88	0.73
1:A:18:ILE:HG23	1:A:142:LYS:HD3	1.69	0.73
1:A:560:MET:HB3	1:C:96:MET:HE3	1.69	0.73
3:B:1801:B12:H8	3:B:1801:B12:H401	1.53	0.73
1:D:541:ILE:HD11	1:D:554:VAL:HG23	1.71	0.73
3:A:1801:B12:H2B	3:A:1801:B12:O7R	1.89	0.72
1:B:109:ARG:HG2	1:B:132:ILE:CG1	2.19	0.72
3:D:1801:B12:H601	3:D:1801:B12:H262	1.72	0.72
2:F:6:ASP:O	2:F:10:ARG:HG2	1.90	0.72
1:C:540:ALA:HB1	1:C:570:LEU:HD21	1.71	0.72
3:B:1801:B12:H362	3:B:1801:B12:H351	1.69	0.71
1:B:653:VAL:O	1:B:657:ILE:HG13	1.89	0.71
4:B:1500:5AD:H5'3	3:D:1801:B12:C16	2.18	0.71
1:C:577:SER:O	1:C:578:ILE:HD12	1.90	0.71
2:H:57:MET:HE1	2:H:82:GLY:HA2	1.70	0.71
1:D:467:GLU:HA	1:D:467:GLU:OE1	1.90	0.71
1:B:393:GLU:HG3	2:F:29:MET:HE1	1.72	0.71
2:H:95:SER:OG	2:H:98:GLU:HG2	1.89	0.71
1:A:254:LYS:HE2	2:E:31:GLU:HG3	1.72	0.70
1:B:600:ASP:OD2	1:B:733:VAL:HG23	1.90	0.70
1:A:712:LYS:HD2	1:A:713:GLN:NE2	2.05	0.70
1:C:467:GLU:HB3	1:C:470:LYS:HG3	1.73	0.70
1:A:79:THR:HB	1:A:332:SER:HA	1.72	0.69
1:A:684:HIS:O	1:A:688:VAL:HG23	1.92	0.69
3:A:1801:B12:H401	3:A:1801:B12:H8	1.57	0.69
2:H:59:PHE:CE1	2:H:100:GLY:HA3	2.27	0.69
3:A:1801:B12:H8	3:A:1801:B12:N40	2.07	0.69
1:C:373:ARG:NH1	1:C:378:GLY:HA2	2.08	0.69
2:G:57:MET:HE1	2:G:82:GLY:HA2	1.75	0.69
3:B:1801:B12:C16	4:D:1500:5AD:H5'3	2.21	0.68
3:C:1801:B12:H8	3:C:1801:B12:N40	2.05	0.68
1:B:393:GLU:HG3	2:F:29:MET:HE2	1.75	0.68
1:B:688:VAL:HG22	1:B:693:ARG:HG2	1.75	0.68
1:A:74:PRO:HB2	1:A:76:PRO:HD2	1.74	0.68
1:B:8:ARG:HH11	1:B:8:ARG:HB2	1.59	0.67
2:F:63:GLU:O	2:F:67:ILE:HG13	1.93	0.67
1:C:396:ILE:CD1	2:G:29:MET:HG2	2.25	0.67
1:B:82:ILE:HG12	1:B:93:ARG:HD2	1.75	0.67
1:A:626:ILE:O	1:A:634:GLU:HB2	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:VAL:HG22	1:A:693:ARG:HG2	1.77	0.67
3:A:1801:B12:H601	3:A:1801:B12:C26	2.23	0.67
1:C:399:GLY:HA3	1:C:403:ASN:HD22	1.59	0.67
1:A:540:ALA:HB1	1:A:570:LEU:HD11	1.77	0.67
1:B:111:ALA:O	1:D:620:VAL:HG11	1.96	0.66
1:C:543:PHE:O	1:C:547:MET:HG3	1.95	0.66
2:G:6:ASP:O	2:G:10:ARG:HG3	1.95	0.66
1:D:79:THR:HG23	1:D:104:HIS:CG	2.30	0.66
1:A:537:GLU:HG3	1:A:554:VAL:HG21	1.77	0.66
2:H:54:LEU:HD23	2:H:57:MET:CE	2.25	0.66
1:A:158:HIS:HE1	1:A:218:ILE:HG13	1.61	0.66
1:A:440:ARG:NH1	1:A:444:TYR:CE2	2.64	0.66
1:B:729:ALA:O	1:B:733:VAL:HG12	1.95	0.66
1:B:320:LEU:HD13	1:B:358:ALA:HB3	1.78	0.66
1:A:120:ILE:HG13	1:A:133:THR:HG22	1.78	0.65
3:A:1801:B12:C16	4:C:1500:5AD:H5'3	2.25	0.65
2:F:54:LEU:HD23	2:F:57:MET:CE	2.26	0.65
1:C:259:LYS:HA	1:C:262:ILE:HD12	1.78	0.65
1:B:735:LYS:O	1:B:735:LYS:HG3	1.95	0.65
1:B:196:MET:SD	1:B:402:PHE:CD1	2.90	0.65
1:B:393:GLU:OE2	2:F:25:ARG:NH1	2.29	0.65
1:D:671:SER:HB2	1:D:676:HIS:ND1	2.12	0.65
3:D:1801:B12:O2	3:D:1801:B12:H2B	1.97	0.65
2:H:108:TYR:HA	2:H:111:ASP:OD2	1.97	0.65
1:A:112:GLY:HA3	1:C:620:VAL:HG13	1.78	0.65
1:C:550:GLU:HG3	1:C:573:ARG:NH2	2.12	0.65
3:D:1801:B12:N40	3:D:1801:B12:H8	2.11	0.65
1:B:393:GLU:HA	2:F:29:MET:HE1	1.79	0.65
1:D:234:ALA:O	1:D:237:VAL:HG12	1.97	0.65
1:D:464:LEU:HD23	1:D:471:LEU:HD13	1.79	0.65
3:C:1801:B12:H301	3:C:1801:B12:H203	1.78	0.64
1:C:394:GLU:HG2	1:C:409:PHE:CE2	2.31	0.64
1:D:652:LEU:HD23	1:D:683:ILE:CD1	2.27	0.64
1:C:16:GLU:HG3	1:C:499:MET:CE	2.27	0.64
1:B:464:LEU:HD23	1:B:471:LEU:HD13	1.80	0.64
1:D:224:ALA:HB3	1:D:245:HIS:CE1	2.33	0.64
1:B:598:ARG:HH22	1:D:232:ARG:HH21	1.42	0.63
1:C:606:LEU:HB2	1:C:736:ARG:NH2	2.13	0.63
1:A:618:HIS:CD2	3:A:1801:B12:H482	2.33	0.63
1:B:391:PHE:HA	1:B:416:TYR:CZ	2.33	0.63
1:C:593:SER:O	1:C:597:ILE:HG12	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:59:PHE:CZ	2:G:100:GLY:HA3	2.33	0.63
1:B:687:ALA:HB3	1:B:693:ARG:HD3	1.80	0.63
1:C:43:MET:HE1	1:C:72:PRO:HA	1.81	0.63
1:B:115:HIS:CE1	1:D:623:ARG:HD3	2.34	0.63
1:D:123:THR:HG23	1:D:135:LYS:HD3	1.79	0.63
2:G:54:LEU:HA	2:G:57:MET:HE2	1.80	0.63
1:B:73:GLN:HE21	1:B:153:ARG:HH22	1.47	0.62
1:B:120:ILE:HG13	1:B:133:THR:HG22	1.80	0.62
1:B:300:MET:HB2	1:B:334:ILE:HG12	1.81	0.62
1:B:393:GLU:CG	2:F:29:MET:HE1	2.28	0.62
1:A:158:HIS:CE1	1:A:218:ILE:HG13	2.35	0.62
3:A:1801:B12:O7R	3:A:1801:B12:C2B	2.47	0.62
2:E:109:TRP:O	2:E:113:ILE:HG13	1.99	0.62
2:E:107:LYS:O	2:E:108:TYR:HB2	1.99	0.62
1:C:537:GLU:HG3	1:C:554:VAL:HG21	1.82	0.62
1:C:607:LYS:HE2	1:C:639:GLU:OE2	2.00	0.62
1:B:623:ARG:HD3	1:D:115:HIS:CE1	2.35	0.62
1:D:721:ARG:HG3	1:D:721:ARG:HH11	1.63	0.62
2:H:47:PRO:O	2:H:51:ARG:HG3	1.98	0.62
1:B:313:THR:O	1:B:317:VAL:HG23	2.00	0.62
1:C:126:GLY:O	1:C:127:ILE:HD13	1.98	0.62
1:D:397:GLU:O	1:D:397:GLU:HG2	1.98	0.62
1:A:620:VAL:HG21	1:C:116:TYR:HE1	1.64	0.62
1:B:680:MET:HE1	1:B:705:VAL:HG22	1.82	0.61
1:B:232:ARG:NH2	1:D:598:ARG:NH2	2.48	0.61
1:B:671:SER:HB2	1:B:676:HIS:CE1	2.34	0.61
1:B:675:ILE:HD11	1:B:679:ASN:HD21	1.65	0.61
1:C:445:MET:HE1	1:C:447:PRO:HB3	1.81	0.61
1:D:459:GLN:HG3	1:D:460:TYR:CD2	2.36	0.61
1:C:307:ALA:O	1:C:340:ARG:HD3	2.00	0.61
1:B:79:THR:HA	1:B:104:HIS:HB3	1.82	0.61
1:B:143:ALA:O	1:B:147:ILE:HG13	2.00	0.61
1:C:41:LEU:CD2	1:C:43:MET:HE2	2.30	0.61
1:A:137:VAL:HB	1:A:172:MET:HE1	1.83	0.61
1:B:153:ARG:HG2	1:B:154:PRO:HD2	1.83	0.61
1:B:232:ARG:CZ	1:D:598:ARG:CZ	2.79	0.60
2:E:81:ALA:O	2:E:85:VAL:HG23	2.02	0.60
1:B:207:LYS:NZ	1:B:217:GLN:NE2	2.48	0.60
1:C:158:HIS:CD2	1:C:159:SER:N	2.68	0.60
3:C:1801:B12:H362	3:C:1801:B12:C35	2.27	0.60
1:D:90:ASP:O	1:D:94:MET:HG3	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:MET:HE3	1:D:447:PRO:N	2.15	0.60
1:C:506:ARG:HH11	1:C:518:GLN:HE22	1.50	0.60
2:G:97:ARG:O	2:G:101:LEU:HB2	2.01	0.60
2:H:5:ASP:HA	2:H:6:ASP:C	2.19	0.60
3:B:1801:B12:H261	4:D:1500:5AD:H5'2	1.83	0.60
1:A:671:SER:HB2	1:A:676:HIS:CE1	2.37	0.60
1:A:43:MET:HE3	1:A:72:PRO:HB3	1.82	0.60
1:B:344:TRP:CG	1:B:515:VAL:HB	2.37	0.60
1:C:626:ILE:HG23	1:C:640:VAL:HG21	1.84	0.60
1:B:372:LYS:HE2	1:D:370:GLN:NE2	2.17	0.60
1:C:475:CYS:HB2	2:G:56:ARG:O	2.02	0.60
1:C:610:ALA:HB1	1:C:622:LEU:HD21	1.84	0.60
1:A:185:PRO:HG3	1:A:203:ALA:CB	2.32	0.60
1:C:397:GLU:HG3	1:C:397:GLU:O	2.02	0.60
1:B:290:MET:SD	2:F:23:GLN:HG3	2.41	0.59
2:H:5:ASP:HA	2:H:7:PHE:H	1.62	0.59
1:C:109:ARG:HH21	5:C:767:Z97:P	2.24	0.59
1:D:537:GLU:CG	1:D:554:VAL:HG21	2.26	0.59
1:C:459:GLN:HG3	1:C:460:TYR:CD2	2.36	0.59
1:B:73:GLN:NE2	1:B:153:ARG:HH22	2.00	0.59
1:A:224:ALA:HB3	1:A:245:HIS:CE1	2.37	0.59
1:A:459:GLN:HG3	1:A:460:TYR:CD2	2.37	0.59
2:H:107:LYS:NZ	2:H:107:LYS:HB3	2.18	0.59
1:D:161:VAL:HG12	1:D:161:VAL:O	2.03	0.59
1:A:619:SER:HB3	1:A:645:THR:CG2	2.33	0.59
1:B:607:LYS:C	1:B:608:ILE:HD12	2.23	0.59
1:C:471:LEU:HD12	2:G:86:TYR:OH	2.02	0.59
1:A:607:LYS:O	1:A:608:ILE:HD12	2.03	0.59
1:C:373:ARG:HH11	1:C:378:GLY:HA2	1.67	0.59
1:A:541:ILE:O	1:A:545:LYS:HG2	2.03	0.58
1:C:396:ILE:HD11	2:G:29:MET:HG2	1.84	0.58
3:B:1801:B12:H203	3:B:1801:B12:H301	1.85	0.58
1:B:259:LYS:HE3	1:B:294:TYR:CZ	2.39	0.58
1:C:132:ILE:HA	1:C:136:GLN:OE1	2.03	0.58
1:A:161:VAL:HG23	1:A:181:ALA:HB1	1.86	0.58
1:A:621:GLY:O	1:A:624:GLU:HB2	2.04	0.58
1:B:738:GLU:O	1:B:738:GLU:HG2	2.03	0.58
1:B:264:LEU:HD21	1:B:291:PHE:CD1	2.38	0.58
1:B:277:MET:HE2	1:B:321:LEU:HD23	1.84	0.58
1:B:475:CYS:HB2	2:F:56:ARG:O	2.03	0.58
1:C:528:PHE:CE1	1:C:565:GLY:HA3	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:619:SER:HB3	1:C:645:THR:HG21	1.84	0.58
1:C:649:VAL:HG12	1:C:686:LEU:CD1	2.33	0.58
1:C:679:ASN:O	1:C:683:ILE:HG13	2.03	0.58
1:A:668:THR:HG23	1:A:668:THR:O	2.03	0.58
1:B:506:ARG:HH11	1:B:518:GLN:NE2	1.99	0.58
1:D:236:LYS:HG2	1:D:415:TYR:HB2	1.86	0.58
2:H:57:MET:CE	2:H:82:GLY:HA2	2.34	0.58
1:A:134:ARG:HA	1:A:172:MET:HE3	1.85	0.58
1:B:217:GLN:O	1:B:263:CYS:HB2	2.03	0.58
3:B:1801:B12:H251	3:B:1801:B12:N29	2.17	0.58
3:B:1801:B12:N23	4:D:1500:5AD:C4'	2.67	0.58
1:C:618:HIS:CE1	3:C:1801:B12:N22	2.72	0.58
1:A:43:MET:CE	1:A:72:PRO:HA	2.34	0.58
1:A:60:ALA:HB2	1:A:71:ASP:HB2	1.86	0.58
1:B:120:ILE:HG13	1:B:133:THR:CG2	2.35	0.57
3:D:1801:B12:H203	3:D:1801:B12:H301	1.86	0.57
1:B:115:HIS:HB3	1:D:623:ARG:HH11	1.69	0.57
1:C:428:ILE:HG12	1:C:428:ILE:O	2.04	0.57
3:C:1801:B12:H262	3:C:1801:B12:H601	1.86	0.57
1:B:259:LYS:HE3	1:B:294:TYR:CE2	2.40	0.57
1:C:43:MET:CE	1:C:72:PRO:HA	2.35	0.57
2:E:5:ASP:HA	2:E:6:ASP:C	2.20	0.57
1:B:123:THR:HG23	1:B:135:LYS:HD3	1.87	0.57
1:A:612:THR:HG22	1:A:616:ASP:HB3	1.87	0.57
1:D:690:LYS:O	1:D:690:LYS:HD3	2.04	0.57
1:A:601:ILE:HG22	1:A:601:ILE:O	2.04	0.57
1:B:511:ILE:CG1	1:D:530:PRO:HD2	2.34	0.57
1:B:668:THR:O	1:B:668:THR:HG23	2.05	0.57
2:F:112:ALA:C	2:F:114:GLN:H	2.08	0.57
1:D:468:PRO:O	1:D:471:LEU:HB2	2.05	0.57
1:A:556:ASN:HB3	1:A:569:GLU:HB2	1.87	0.57
1:B:281:LEU:O	1:B:285:VAL:HG23	2.04	0.57
1:C:320:LEU:HD13	1:C:358:ALA:HB3	1.87	0.57
1:D:232:ARG:HA	1:D:232:ARG:HH11	1.70	0.57
3:D:1801:B12:H601	3:D:1801:B12:H252	1.86	0.57
2:G:59:PHE:CE1	2:G:100:GLY:HA3	2.40	0.56
1:D:41:LEU:HD23	1:D:43:MET:HE2	1.86	0.56
1:A:290:MET:SD	2:E:23:GLN:HG3	2.46	0.56
1:C:668:THR:CG2	1:C:668:THR:O	2.53	0.56
1:A:43:MET:HE3	1:A:72:PRO:CB	2.36	0.56
1:B:286:ALA:HB2	1:B:381:VAL:HG13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1500:5AD:H5'2	3:D:1801:B12:H261	1.87	0.56
1:A:622:LEU:HD21	1:A:642:TYR:HE1	1.70	0.56
1:C:457:VAL:HG13	1:C:471:LEU:HD21	1.87	0.56
1:A:75:LEU:N	1:A:76:PRO:CD	2.68	0.56
1:A:440:ARG:HD2	2:E:42:LYS:O	2.06	0.56
1:B:709:VAL:O	1:B:712:LYS:HB2	2.06	0.56
1:C:394:GLU:HG2	1:C:409:PHE:HE2	1.71	0.56
1:A:579:ASP:O	1:A:583:LEU:HG	2.06	0.56
1:D:86:ARG:HD3	1:D:498:ARG:HD3	1.87	0.56
1:A:550:GLU:HG3	1:A:575:PRO:HG3	1.88	0.56
3:A:1801:B12:C15	4:C:1500:5AD:H5'3	2.37	0.56
1:B:116:TYR:CE1	3:D:1801:B12:H491	2.41	0.56
1:C:5:LEU:HD22	1:C:6:GLN:HB2	1.87	0.56
1:D:688:VAL:HG22	1:D:693:ARG:HG2	1.88	0.56
1:A:277:MET:CE	1:A:321:LEU:HD23	2.35	0.55
1:B:604:THR:HG22	1:B:736:ARG:NH2	2.21	0.55
2:H:24:THR:O	2:H:28:GLU:HG2	2.06	0.55
2:H:5:ASP:CB	2:H:8:GLN:H	2.19	0.55
1:B:95:ARG:HD3	1:D:564:GLU:HG2	1.86	0.55
1:B:126:GLY:CA	1:B:131:PRO:HD3	2.36	0.55
1:B:488:GLU:O	1:B:489:LEU:HD23	2.07	0.55
2:F:5:ASP:CA	2:F:7:PHE:H	2.06	0.55
1:C:5:LEU:O	1:C:6:GLN:HB3	2.07	0.55
1:C:191:TYR:CE1	1:C:230:THR:HG21	2.42	0.55
1:D:320:LEU:HD13	1:D:358:ALA:HB3	1.88	0.55
1:A:726:ILE:HG23	1:A:727:HIS:N	2.21	0.55
1:C:226:ASN:O	1:C:230:THR:HG23	2.05	0.55
1:B:460:TYR:O	1:B:461:ASP:HB2	2.06	0.55
1:B:554:VAL:HA	1:B:570:LEU:HB3	1.88	0.55
1:C:74:PRO:HB2	1:C:76:PRO:HD2	1.88	0.55
1:D:250:ILE:HG23	2:H:34:VAL:HG21	1.87	0.55
1:D:264:LEU:HD21	1:D:291:PHE:CD1	2.41	0.55
1:A:668:THR:OG1	1:A:676:HIS:HB2	2.07	0.55
1:B:464:LEU:N	1:B:464:LEU:HD13	2.21	0.55
1:B:651:LYS:HE3	1:B:651:LYS:CA	2.37	0.55
1:D:79:THR:HG23	1:D:104:HIS:ND1	2.21	0.55
1:D:667:SER:HA	3:D:1801:B12:H4B	1.89	0.55
1:A:233:GLU:HG2	1:A:235:TRP:CH2	2.41	0.55
1:C:213:ALA:CB	1:C:215:MET:HG3	2.35	0.55
1:D:537:GLU:O	1:D:541:ILE:HG12	2.06	0.55
1:A:631:GLY:O	1:A:725:GLY:HA3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:VAL:HG13	2:H:29:MET:HE1	1.87	0.55
2:F:97:ARG:O	2:F:101:LEU:HB2	2.07	0.54
3:C:1801:B12:H531	3:C:1801:B12:H543	1.89	0.54
1:A:116:TYR:CE2	1:A:120:ILE:HD13	2.42	0.54
1:D:668:THR:HG23	1:D:668:THR:O	2.07	0.54
1:B:326:THR:OG1	1:B:327:ARG:N	2.39	0.54
1:A:484:VAL:HG11	2:E:60:SER:HB3	1.89	0.54
1:A:622:LEU:HB2	1:A:667:SER:HB2	1.88	0.54
2:E:49:ILE:O	2:E:53:VAL:HG23	2.07	0.54
1:B:612:THR:HG22	1:B:616:ASP:HB3	1.90	0.54
1:A:668:THR:OG1	1:A:676:HIS:CB	2.56	0.54
1:A:712:LYS:HD2	1:A:713:GLN:HE22	1.70	0.54
1:B:277:MET:CE	1:B:321:LEU:HD23	2.38	0.54
1:D:632:GLY:HA2	1:D:725:GLY:HA3	1.88	0.54
1:A:237:VAL:HG22	1:A:237:VAL:O	2.08	0.54
1:A:416:TYR:CG	1:A:417:PRO:HA	2.43	0.54
1:B:86:ARG:HG3	1:B:517:TRP:NE1	2.23	0.54
2:F:7:PHE:O	2:F:11:ARG:HG2	2.08	0.54
1:C:467:GLU:N	1:C:468:PRO:HD3	2.23	0.54
1:A:623:ARG:HD3	1:C:115:HIS:CE1	2.43	0.53
1:B:676:HIS:O	1:B:680:MET:HE3	2.08	0.53
1:B:132:ILE:HA	1:B:136:GLN:OE1	2.08	0.53
1:C:628:ILE:HD12	1:C:635:LYS:HA	1.89	0.53
1:A:531:THR:CG2	1:A:536:ALA:HB2	2.38	0.53
1:A:628:ILE:HG13	1:A:635:LYS:HB2	1.90	0.53
1:B:86:ARG:HG3	1:B:517:TRP:CE2	2.42	0.53
1:B:207:LYS:NZ	1:B:217:GLN:HE22	2.04	0.53
1:B:464:LEU:N	1:B:464:LEU:CD1	2.72	0.53
1:D:43:MET:HE3	1:D:72:PRO:HB3	1.90	0.53
1:A:57:ASN:HB3	1:A:99:TRP:CH2	2.44	0.53
1:A:580:ILE:HA	1:A:583:LEU:HD12	1.91	0.53
1:B:7:LEU:HG	1:B:146:LEU:HB3	1.91	0.53
1:A:205:GLU:O	1:A:209:ILE:HD12	2.08	0.53
1:D:416:TYR:CG	1:D:417:PRO:HA	2.43	0.53
1:A:585:ILE:HG12	1:C:538:PHE:CD2	2.43	0.53
1:C:649:VAL:CG1	1:C:683:ILE:HG12	2.29	0.53
2:H:107:LYS:HB3	2:H:107:LYS:HZ3	1.74	0.53
1:B:541:ILE:HD11	1:B:554:VAL:HG23	1.90	0.53
3:B:1801:B12:H531	3:B:1801:B12:C55	2.39	0.53
1:B:41:LEU:HD23	1:B:43:MET:CE	2.37	0.53
1:B:147:ILE:O	1:B:151:VAL:HG13	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:VAL:HG13	1:C:241:LEU:HG	1.90	0.53
1:C:614:GLY:O	1:C:646:SER:HA	2.09	0.53
3:D:1801:B12:H262	3:D:1801:B12:C60	2.38	0.53
1:B:114:SER:HB2	5:B:767:Z97:OP2	2.09	0.52
1:B:306:GLU:CG	1:D:65:LYS:HE2	2.39	0.52
3:D:1801:B12:O7R	3:D:1801:B12:C2B	2.57	0.52
1:A:123:THR:O	1:A:498:ARG:NH2	2.42	0.52
1:C:541:ILE:HG23	1:C:552:VAL:CG1	2.40	0.52
1:A:416:TYR:CD1	1:A:417:PRO:HA	2.44	0.52
1:A:6:GLN:CG	1:A:7:LEU:H	2.22	0.52
1:B:578:ILE:HD13	1:D:543:PHE:CZ	2.45	0.52
1:C:556:ASN:HB3	1:C:569:GLU:HB2	1.90	0.52
2:H:59:PHE:CZ	2:H:100:GLY:HA3	2.44	0.52
1:A:514:GLU:HA	1:A:520:ASP:OD1	2.08	0.52
1:D:618:HIS:CE1	3:D:1801:B12:N22	2.77	0.52
1:A:671:SER:HA	1:A:676:HIS:ND1	2.25	0.52
1:C:677:TYR:HA	1:C:680:MET:HE3	1.92	0.52
1:C:701:GLY:HA2	1:C:719:PHE:O	2.10	0.52
1:A:428:ILE:HG23	1:A:429:ASN:N	2.25	0.52
1:C:541:ILE:HG23	1:C:552:VAL:HG11	1.92	0.52
1:D:120:ILE:HG13	1:D:133:THR:HG22	1.90	0.52
1:A:373:ARG:HH11	1:A:378:GLY:HA2	1.74	0.52
1:D:373:ARG:HD2	1:D:373:ARG:O	2.10	0.52
1:A:313:THR:O	1:A:317:VAL:HG23	2.09	0.52
4:A:1500:5AD:C4'	3:C:1801:B12:N23	2.72	0.52
1:A:613:VAL:HG13	1:A:614:GLY:N	2.25	0.51
1:B:15:VAL:HG22	1:B:499:MET:CE	2.40	0.51
1:B:153:ARG:HG2	1:B:154:PRO:CD	2.40	0.51
1:C:391:PHE:HA	1:C:416:TYR:CZ	2.45	0.51
1:C:612:THR:CB	1:C:645:THR:HG22	2.37	0.51
1:D:57:ASN:HB3	1:D:99:TRP:CH2	2.45	0.51
1:D:189:VAL:CG2	1:D:196:MET:HA	2.40	0.51
2:E:74:ARG:NH2	2:E:109:TRP:HB2	2.25	0.51
1:B:189:VAL:CG2	1:B:196:MET:HA	2.40	0.51
1:C:6:GLN:CG	1:C:7:LEU:N	2.73	0.51
1:C:75:LEU:N	1:C:76:PRO:CD	2.73	0.51
1:C:183:GLN:OE1	1:C:207:LYS:HE2	2.10	0.51
2:G:57:MET:HE1	2:G:82:GLY:CA	2.39	0.51
1:B:675:ILE:HD11	1:B:679:ASN:ND2	2.25	0.51
1:B:737:ARG:O	1:B:739:MET:N	2.40	0.51
1:D:307:ALA:HB1	1:D:340:ARG:HG3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:574:VAL:HG13	1:D:576:PHE:CE1	2.46	0.51
1:A:109:ARG:HH21	5:A:767:Z97:P	2.33	0.51
1:A:123:THR:HG23	1:A:135:LYS:HD3	1.91	0.51
1:C:719:PHE:HB3	1:C:723:SER:OG	2.11	0.51
3:C:1801:B12:H531	3:C:1801:B12:C55	2.40	0.51
2:H:35:ASP:HB2	2:H:36:PRO:HD3	1.93	0.51
1:A:611:ALA:HB3	1:A:652:LEU:HD13	1.91	0.51
1:C:5:LEU:HD22	1:C:5:LEU:C	2.31	0.51
2:E:72:MET:HG2	2:E:77:MET:HG3	1.93	0.51
1:B:232:ARG:NH2	1:D:598:ARG:CZ	2.74	0.51
1:B:274:ALA:O	1:B:276:SER:N	2.44	0.51
1:B:700:CYS:O	1:B:718:GLY:HA2	2.10	0.51
1:C:36:GLN:O	1:C:52:SER:HB2	2.09	0.51
3:C:1801:B12:H251	3:C:1801:B12:N29	2.25	0.51
1:A:526:THR:HG23	1:A:569:GLU:HG3	1.93	0.51
1:B:618:HIS:HD2	3:B:1801:B12:H482	1.76	0.51
1:B:665:LEU:HA	1:B:699:GLY:O	2.10	0.51
1:C:416:TYR:CD1	1:C:417:PRO:HA	2.46	0.51
1:A:310:ARG:O	1:A:314:VAL:HG23	2.10	0.51
1:A:358:ALA:O	1:A:362:MET:HG3	2.10	0.51
1:A:528:PHE:CZ	1:A:565:GLY:HA3	2.46	0.51
1:C:547:MET:O	1:C:548:ASN:HB2	2.11	0.51
1:C:668:THR:HG23	1:C:676:HIS:CB	2.33	0.51
3:A:1801:B12:H362	3:A:1801:B12:C35	2.39	0.50
3:B:1801:B12:H362	3:B:1801:B12:C35	2.37	0.50
1:C:525:LEU:HD23	1:C:570:LEU:CD1	2.41	0.50
1:B:204:CYS:HB3	1:B:452:PHE:CD2	2.47	0.50
1:C:124:PRO:HA	1:C:493:ASP:O	2.11	0.50
1:D:109:ARG:HG2	1:D:132:ILE:CG1	2.41	0.50
1:D:607:LYS:O	1:D:608:ILE:HD12	2.11	0.50
3:D:1801:B12:H362	3:D:1801:B12:C35	2.37	0.50
3:A:1801:B12:H351	3:A:1801:B12:H372	1.93	0.50
2:E:57:MET:HE1	2:E:82:GLY:HA2	1.92	0.50
1:B:224:ALA:HB3	1:B:245:HIS:CE1	2.47	0.50
1:B:342:VAL:HG12	1:B:343:PRO:HD2	1.94	0.50
1:C:218:ILE:HD13	1:C:297:ARG:HD2	1.93	0.50
2:G:70:LYS:O	2:G:74:ARG:HG2	2.11	0.50
2:E:51:ARG:HG2	2:E:68:VAL:HG21	1.94	0.50
1:B:13:LEU:HD22	1:B:18:ILE:HD11	1.93	0.50
1:A:688:VAL:HG22	1:A:693:ARG:CG	2.40	0.50
1:D:541:ILE:CD1	1:D:554:VAL:HG23	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:LEU:HB3	1:C:526:THR:HB	1.93	0.50
1:A:719:PHE:HB3	1:A:723:SER:OG	2.11	0.50
1:C:16:GLU:HG3	1:C:499:MET:HE3	1.93	0.50
1:C:144:LEU:O	1:C:148:GLU:HG2	2.12	0.50
1:C:444:TYR:C	1:C:444:TYR:CD2	2.85	0.50
2:H:6:ASP:O	2:H:10:ARG:HG3	2.11	0.50
4:A:1500:5AD:H5'3	3:C:1801:B12:C16	2.41	0.50
1:B:189:VAL:HG22	1:B:196:MET:HA	1.93	0.50
1:C:649:VAL:HG12	1:C:686:LEU:HD13	1.93	0.50
1:C:733:VAL:O	1:C:737:ARG:HG3	2.11	0.50
1:D:290:MET:SD	2:H:23:GLN:HB2	2.51	0.50
1:A:612:THR:CG2	1:A:616:ASP:HB3	2.42	0.50
1:B:671:SER:HA	1:B:676:HIS:ND1	2.26	0.50
3:C:1801:B12:H471	3:C:1801:B12:H492	1.94	0.50
1:D:233:GLU:HG2	1:D:235:TRP:CH2	2.47	0.50
1:D:735:LYS:O	1:D:739:MET:HG3	2.12	0.50
1:A:116:TYR:HE2	1:A:120:ILE:HD13	1.76	0.49
2:E:70:LYS:O	2:E:74:ARG:HG2	2.12	0.49
1:B:8:ARG:HH11	1:B:8:ARG:CB	2.24	0.49
1:B:611:ALA:HB2	1:B:643:LEU:HB2	1.94	0.49
1:D:23:ASP:OD2	1:D:24:LYS:HE3	2.11	0.49
1:A:470:LYS:O	1:A:472:ILE:N	2.45	0.49
1:C:622:LEU:HB2	1:C:667:SER:HB2	1.94	0.49
3:C:1801:B12:H492	3:C:1801:B12:C47	2.43	0.49
1:D:671:SER:HB2	1:D:676:HIS:CE1	2.47	0.49
1:A:159:SER:HB3	1:A:173:PHE:CZ	2.48	0.49
1:A:679:ASN:O	1:A:683:ILE:HG13	2.12	0.49
2:E:64:ALA:O	2:E:68:VAL:HG23	2.12	0.49
1:B:372:LYS:HE2	1:D:370:GLN:HE21	1.76	0.49
1:B:607:LYS:O	1:B:608:ILE:HD12	2.12	0.49
2:G:54:LEU:HD23	2:G:57:MET:CE	2.43	0.49
3:D:1801:B12:H492	3:D:1801:B12:H471	1.95	0.49
1:B:234:ALA:O	1:B:237:VAL:HG12	2.11	0.49
1:B:464:LEU:HD23	1:B:471:LEU:CD1	2.43	0.49
1:C:539:ALA:O	1:C:543:PHE:HD2	1.96	0.49
1:B:512:LYS:HB2	1:B:513:PRO:CD	2.42	0.49
1:B:708:GLU:O	1:B:711:VAL:HG12	2.13	0.49
1:C:116:TYR:CE2	1:C:120:ILE:HD13	2.48	0.49
1:A:45:PRO:HD2	1:A:46:PHE:CD2	2.48	0.49
1:A:580:ILE:HD12	1:C:535:VAL:CG1	2.42	0.49
3:A:1801:B12:N29	3:A:1801:B12:H251	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:TYR:HE2	1:C:120:ILE:HD13	1.77	0.49
1:D:135:LYS:HG3	1:D:485:TYR:OH	2.12	0.49
1:A:618:HIS:CD2	3:A:1801:B12:N24	2.80	0.49
1:A:619:SER:HB3	1:A:645:THR:HG23	1.94	0.49
1:A:733:VAL:O	1:A:737:ARG:HG3	2.13	0.49
2:E:54:LEU:HD23	2:E:57:MET:CE	2.42	0.49
1:D:114:SER:OG	5:D:767:Z97:OP2	2.22	0.48
1:D:204:CYS:HB3	1:D:452:PHE:CD2	2.47	0.48
1:A:690:LYS:HE3	1:A:690:LYS:HA	1.94	0.48
3:A:1801:B12:H251	3:A:1801:B12:H291	1.78	0.48
1:B:432:ILE:N	1:B:432:ILE:HD13	2.27	0.48
1:C:610:ALA:HA	1:C:665:LEU:O	2.12	0.48
1:D:478:GLU:O	1:D:480:PRO:HD3	2.13	0.48
1:B:511:ILE:HG12	1:D:530:PRO:HD2	1.95	0.48
1:C:8:ARG:HD3	1:C:11:GLU:OE1	2.13	0.48
1:C:406:GLU:HG2	1:C:426:ARG:O	2.13	0.48
1:C:668:THR:HG21	1:C:680:MET:HE2	1.94	0.48
1:D:316:HIS:O	1:D:319:ASN:HB2	2.13	0.48
1:D:449:THR:HB	1:D:477:LEU:HD12	1.95	0.48
1:A:218:ILE:HD13	1:A:297:ARG:HG3	1.94	0.48
2:E:80:GLY:O	2:E:84:ILE:HG12	2.14	0.48
2:E:20:GLU:H	2:E:20:GLU:CD	2.17	0.48
1:A:79:THR:HG22	1:A:80:THR:N	2.29	0.48
1:A:344:TRP:CG	1:A:515:VAL:HB	2.49	0.48
1:A:552:VAL:HG13	1:A:570:LEU:HD23	1.96	0.48
1:B:448:VAL:HB	2:F:56:ARG:HD2	1.96	0.48
1:B:706:THR:HB	1:B:709:VAL:HG23	1.95	0.48
1:C:416:TYR:CG	1:C:417:PRO:HA	2.49	0.48
1:D:684:HIS:O	1:D:687:ALA:HB3	2.12	0.48
1:A:531:THR:HG22	1:A:536:ALA:HB2	1.95	0.48
1:A:134:ARG:HA	1:A:172:MET:CE	2.43	0.48
1:A:730:THR:O	1:A:734:LYS:HB2	2.14	0.48
4:A:1500:5AD:H5'2	3:C:1801:B12:H261	1.96	0.48
2:E:63:GLU:O	2:E:67:ILE:HG13	2.14	0.48
1:B:137:VAL:HB	1:B:172:MET:HE3	1.96	0.48
1:B:212:TRP:CZ2	1:B:477:LEU:HB3	2.49	0.48
1:C:75:LEU:N	1:C:76:PRO:HD3	2.28	0.48
1:C:355:ALA:O	1:C:359:LEU:HD12	2.14	0.48
1:D:7:LEU:HD23	1:D:7:LEU:HA	1.73	0.48
1:D:438:PHE:CD2	2:H:77:MET:HG3	2.49	0.48
3:D:1801:B12:H421	3:D:1801:B12:C10	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1801:B12:H552	3:D:1801:B12:H531	1.96	0.48
1:A:287:LEU:HD12	1:A:291:PHE:CD2	2.49	0.48
1:A:526:THR:HG23	1:A:569:GLU:CG	2.44	0.48
1:B:560:MET:HB2	1:B:565:GLY:O	2.14	0.48
1:B:683:ILE:CG2	1:B:698:ILE:HD13	2.44	0.48
2:F:59:PHE:CE1	2:F:100:GLY:HA3	2.49	0.48
1:C:225:HIS:O	1:C:228:ASN:HB2	2.13	0.48
2:G:18:SER:OG	2:G:21:GLU:HG3	2.14	0.48
1:D:281:LEU:HB3	1:D:282:PRO:HD3	1.94	0.48
2:F:113:ILE:HG22	2:F:113:ILE:O	2.13	0.48
1:C:335:THR:HG22	1:C:348:ASN:HA	1.96	0.48
1:D:251:PHE:O	1:D:255:VAL:HG23	2.14	0.48
2:E:107:LYS:O	2:E:108:TYR:CB	2.62	0.47
1:B:311:GLU:OE2	1:D:63:SER:HB2	2.14	0.47
1:C:143:ALA:O	1:C:146:LEU:HB2	2.14	0.47
1:D:189:VAL:HG22	1:D:196:MET:HA	1.96	0.47
1:A:390:LEU:HD13	2:E:10:ARG:HB3	1.96	0.47
2:E:99:ALA:O	2:E:102:ALA:HB3	2.14	0.47
1:B:123:THR:O	1:B:494:ASN:HA	2.14	0.47
1:B:246:ALA:O	1:B:250:ILE:HG22	2.13	0.47
4:B:1500:5AD:H5'3	3:D:1801:B12:C15	2.39	0.47
1:D:124:PRO:O	1:D:131:PRO:HG2	2.14	0.47
1:D:219:ASP:HB3	1:D:248:ASN:ND2	2.29	0.47
2:H:103:LEU:HD22	2:H:109:TRP:CZ2	2.49	0.47
1:A:547:MET:O	1:A:548:ASN:HB2	2.15	0.47
1:D:86:ARG:CD	1:D:498:ARG:HD3	2.44	0.47
1:D:511:ILE:HG22	1:D:578:ILE:O	2.14	0.47
1:A:137:VAL:HB	1:A:172:MET:CE	2.44	0.47
1:A:537:GLU:O	1:A:541:ILE:HG13	2.14	0.47
1:C:238:MET:HE3	1:C:283:TYR:HB2	1.97	0.47
1:C:458:LYS:HE2	1:C:462:GLU:HG2	1.96	0.47
1:C:466:SER:O	1:C:467:GLU:HG2	2.14	0.47
1:A:238:MET:O	1:A:239:PRO:C	2.53	0.47
1:B:90:ASP:O	1:B:94:MET:HG3	2.14	0.47
1:B:309:THR:HG22	1:B:336:PRO:O	2.13	0.47
1:C:427:GLN:C	1:C:429:ASN:H	2.17	0.47
2:E:47:PRO:O	2:E:51:ARG:HG3	2.14	0.47
2:E:54:LEU:HD23	2:E:57:MET:HE2	1.96	0.47
1:B:609:VAL:HG23	1:B:652:LEU:HD11	1.97	0.47
1:C:233:GLU:HG2	1:C:235:TRP:CH2	2.50	0.47
1:C:612:THR:HG22	1:C:616:ASP:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:LYS:HB2	1:C:695:LYS:HE3	1.61	0.47
2:G:107:LYS:HG2	2:G:108:TYR:CD1	2.50	0.47
1:D:25:TYR:HD2	1:D:138:ARG:HG2	1.80	0.47
3:D:1801:B12:H351	3:D:1801:B12:H372	1.97	0.47
3:D:1801:B12:H531	3:D:1801:B12:H543	1.97	0.47
1:A:538:PHE:CD2	1:C:585:ILE:HG12	2.50	0.47
1:C:467:GLU:O	1:C:469:SER:N	2.48	0.47
1:D:374:GLU:HA	1:D:374:GLU:OE1	2.14	0.47
1:D:561:GLN:HB3	1:D:564:GLU:HB2	1.96	0.47
1:A:159:SER:O	1:A:181:ALA:HA	2.15	0.47
1:A:268:PRO:HA	1:A:269:PRO:HD3	1.81	0.47
1:A:341:ASN:ND2	1:A:342:VAL:O	2.45	0.47
1:A:649:VAL:O	1:A:653:VAL:HG23	2.15	0.47
3:A:1801:B12:H531	3:A:1801:B12:H543	1.97	0.47
2:E:23:GLN:O	2:E:26:PHE:HB3	2.15	0.47
1:B:8:ARG:CB	1:B:8:ARG:NH1	2.77	0.47
1:B:305:MET:HE3	1:B:305:MET:HB2	1.88	0.47
1:B:324:LYS:HE2	1:B:362:MET:O	2.15	0.47
1:D:411:VAL:HG12	1:D:411:VAL:O	2.15	0.47
1:A:6:GLN:CG	1:A:7:LEU:N	2.77	0.47
1:C:238:MET:CE	1:C:283:TYR:HB2	2.44	0.47
3:C:1801:B12:C2B	3:C:1801:B12:O7R	2.63	0.47
1:D:416:TYR:CD2	1:D:417:PRO:HA	2.50	0.47
3:D:1801:B12:C49	3:D:1801:B12:C47	2.87	0.47
1:A:43:MET:HE3	1:A:72:PRO:CA	2.44	0.46
1:A:622:LEU:HD11	1:A:626:ILE:HD11	1.97	0.46
1:B:541:ILE:HG22	1:B:545:LYS:HZ2	1.80	0.46
1:C:117:ASP:HA	1:C:164:VAL:HG23	1.97	0.46
1:C:495:VAL:O	1:C:499:MET:HG2	2.14	0.46
1:C:299:GLN:HG3	1:C:300:MET:N	2.30	0.46
1:C:444:TYR:HA	2:G:79:LYS:O	2.15	0.46
1:C:550:GLU:HB2	1:C:573:ARG:HB3	1.96	0.46
1:D:219:ASP:HB3	1:D:248:ASN:HD22	1.80	0.46
1:A:534:ARG:NH2	1:C:586:PRO:O	2.35	0.46
2:F:5:ASP:N	2:F:6:ASP:HB3	2.30	0.46
1:C:7:LEU:HA	1:C:7:LEU:HD23	1.63	0.46
1:C:158:HIS:HD2	1:C:159:SER:N	2.09	0.46
2:H:24:THR:O	2:H:28:GLU:CG	2.64	0.46
1:B:622:LEU:HB2	1:B:667:SER:HB2	1.96	0.46
1:B:684:HIS:O	1:B:688:VAL:HG23	2.15	0.46
1:C:184:ASP:OD1	1:C:186:GLN:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:46:THR:HB	2:G:47:PRO:HD2	1.97	0.46
1:D:187:TYR:CG	5:D:767:Z97:H2AB	2.50	0.46
1:D:196:MET:SD	1:D:402:PHE:CD1	3.08	0.46
1:D:736:ARG:HG2	1:D:736:ARG:O	2.15	0.46
1:B:13:LEU:HD13	1:B:91:ILE:HG22	1.96	0.46
1:B:120:ILE:C	1:B:133:THR:HG22	2.35	0.46
2:F:5:ASP:HA	2:F:6:ASP:C	2.28	0.46
1:D:344:TRP:CD1	1:D:515:VAL:HB	2.51	0.46
1:A:612:THR:HB	1:A:645:THR:HA	1.98	0.46
1:D:510:MET:CE	1:D:577:SER:HB2	2.46	0.46
1:D:721:ARG:HG3	1:D:721:ARG:NH1	2.27	0.46
1:B:290:MET:HE3	1:B:385:LYS:HG2	1.97	0.46
3:B:1801:B12:H351	3:B:1801:B12:H372	1.98	0.46
3:D:1801:B12:H552	3:D:1801:B12:C53	2.46	0.46
1:A:350:GLU:CG	1:C:310:ARG:HD3	2.46	0.46
1:B:79:THR:HB	1:B:332:SER:HA	1.98	0.46
1:B:115:HIS:HB3	1:D:623:ARG:NH1	2.30	0.46
1:B:506:ARG:HD3	1:B:518:GLN:HE22	1.80	0.46
3:B:1801:B12:H531	3:B:1801:B12:H543	1.98	0.46
1:C:50:ASP:O	1:C:75:LEU:HG	2.15	0.46
1:C:173:PHE:CD1	1:C:178:VAL:HG21	2.51	0.46
1:C:281:LEU:HB3	1:C:282:PRO:HD3	1.98	0.46
1:D:459:GLN:CG	1:D:460:TYR:CD2	2.98	0.46
1:D:578:ILE:HD13	1:D:578:ILE:HA	1.76	0.46
1:A:182:HIS:HB3	5:A:767:Z97:H2AA	1.98	0.46
1:A:349:ILE:HD12	1:A:349:ILE:N	2.30	0.46
1:A:462:GLU:CD	1:A:462:GLU:H	2.19	0.46
1:A:618:HIS:CG	1:A:669:ILE:HG21	2.51	0.46
1:C:336:PRO:HD2	1:C:347:TYR:HB3	1.97	0.46
1:C:659:LEU:C	1:C:660:LYS:HG2	2.36	0.46
1:D:192:ARG:HD3	1:D:192:ARG:HA	1.81	0.46
1:B:36:GLN:O	1:B:52:SER:HB2	2.16	0.46
1:B:580:ILE:HD12	1:D:535:VAL:HG11	1.96	0.46
1:D:8:ARG:HG3	1:D:11:GLU:OE1	2.16	0.46
1:A:307:ALA:HB1	1:A:556:ASN:HB2	1.98	0.45
1:A:344:TRP:CD1	1:A:515:VAL:HB	2.51	0.45
1:C:186:GLN:HG2	1:C:401:TYR:OH	2.16	0.45
1:C:396:ILE:HD12	2:G:29:MET:HG2	1.98	0.45
1:D:43:MET:CE	1:D:72:PRO:HB3	2.46	0.45
1:D:399:GLY:HA3	1:D:403:ASN:HD22	1.81	0.45
1:B:7:LEU:HD13	1:B:150:GLU:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ILE:HG22	1:B:90:ASP:HB3	1.99	0.45
1:B:538:PHE:CD2	1:D:585:ILE:HG23	2.51	0.45
1:B:543:PHE:O	1:B:547:MET:HG3	2.17	0.45
1:D:286:ALA:HB2	1:D:381:VAL:HG13	1.98	0.45
1:A:460:TYR:O	1:A:461:ASP:HB2	2.16	0.45
3:B:1801:B12:H252	3:B:1801:B12:H601	1.99	0.45
1:D:7:LEU:HD13	1:D:150:GLU:CD	2.37	0.45
1:D:305:MET:HE1	1:D:316:HIS:NE2	2.31	0.45
1:D:622:LEU:HD23	1:D:642:TYR:HE1	1.81	0.45
1:A:373:ARG:NH1	1:A:378:GLY:HA2	2.31	0.45
1:A:412:ASP:OD1	1:A:419:ARG:HG3	2.17	0.45
1:A:541:ILE:HG23	1:A:552:VAL:CG1	2.47	0.45
1:A:576:PHE:CD2	1:A:576:PHE:N	2.84	0.45
2:E:57:MET:CE	2:E:82:GLY:HA2	2.46	0.45
1:B:15:VAL:CG2	1:B:499:MET:HE2	2.47	0.45
1:B:676:HIS:O	1:B:680:MET:HG3	2.16	0.45
2:F:6:ASP:OD1	2:F:10:ARG:HD2	2.17	0.45
1:C:345:HIS:CD2	1:C:515:VAL:O	2.70	0.45
1:D:622:LEU:HB2	1:D:667:SER:HB2	1.98	0.45
1:D:675:ILE:O	1:D:675:ILE:HG13	2.14	0.45
1:B:557:ARG:HG3	1:B:557:ARG:HH11	1.80	0.45
1:C:61:LEU:O	1:C:62:PRO:C	2.53	0.45
1:C:233:GLU:HB3	1:C:235:TRP:CZ3	2.51	0.45
1:C:654:ASP:OD1	1:C:690:LYS:HE2	2.16	0.45
1:D:622:LEU:HG	1:D:626:ILE:HD12	1.98	0.45
1:A:607:LYS:NZ	1:A:659:LEU:O	2.45	0.45
1:B:237:VAL:O	1:B:237:VAL:HG22	2.17	0.45
1:A:246:ALA:O	1:A:250:ILE:HG22	2.16	0.45
1:A:300:MET:HB2	1:A:334:ILE:HG12	1.98	0.45
1:A:350:GLU:HG2	1:C:310:ARG:HD3	1.98	0.45
1:A:647:VAL:HG13	1:A:651:LYS:HD2	1.99	0.45
2:E:60:SER:H	2:E:63:GLU:HG3	1.80	0.45
1:B:323:SER:HB3	1:B:328:ALA:HB2	1.98	0.45
1:D:109:ARG:HG2	1:D:132:ILE:HG12	1.99	0.45
1:D:187:TYR:CB	5:D:767:Z97:H2AB	2.46	0.45
3:D:1801:B12:H291	3:D:1801:B12:H251	1.81	0.45
1:B:626:ILE:HD13	1:B:640:VAL:HG11	1.99	0.45
1:C:547:MET:O	1:C:548:ASN:CB	2.65	0.45
3:D:1801:B12:H601	3:D:1801:B12:C26	2.45	0.45
2:E:60:SER:OG	2:E:63:GLU:HG2	2.17	0.45
1:B:401:TYR:O	1:B:405:VAL:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:PHE:CE2	1:D:585:ILE:HG23	2.52	0.45
1:C:287:LEU:O	1:C:291:PHE:HD2	2.00	0.45
2:G:38:LEU:HD23	2:G:38:LEU:HA	1.74	0.45
1:D:116:TYR:CD1	1:D:116:TYR:N	2.85	0.45
1:D:158:HIS:HE1	1:D:218:ILE:HG13	1.82	0.45
1:D:510:MET:HE3	1:D:577:SER:HB2	1.99	0.45
1:B:176:GLU:OE1	1:B:176:GLU:HA	2.17	0.44
1:D:123:THR:O	1:D:494:ASN:HA	2.16	0.44
1:D:250:ILE:HD12	1:D:250:ILE:HA	1.68	0.44
1:B:426:ARG:NH1	1:D:634:GLU:OE2	2.32	0.44
1:C:6:GLN:CG	1:C:7:LEU:H	2.30	0.44
1:D:26:THR:HG22	1:D:27:PRO:HD2	2.00	0.44
1:D:162:SER:HB2	5:D:767:Z97:H6	1.98	0.44
1:D:461:ASP:OD1	1:D:463:ALA:HB3	2.17	0.44
1:C:290:MET:HE3	1:C:290:MET:HB2	1.83	0.44
1:D:734:LYS:HB3	1:D:734:LYS:HE2	1.78	0.44
1:A:38:ALA:HB1	1:A:41:LEU:HB2	1.99	0.44
1:A:574:VAL:HA	1:A:575:PRO:HD3	1.69	0.44
3:A:1801:B12:H18	3:A:1801:B12:H561	1.64	0.44
1:B:213:ALA:HB3	1:B:215:MET:HG3	1.98	0.44
2:F:20:GLU:CD	2:F:20:GLU:H	2.21	0.44
1:D:116:TYR:N	1:D:116:TYR:HD1	2.15	0.44
1:D:424:ILE:HD13	1:D:424:ILE:HA	1.71	0.44
1:D:610:ALA:HA	1:D:665:LEU:O	2.17	0.44
1:C:23:ASP:OD2	1:C:24:LYS:HE3	2.18	0.44
1:D:445:MET:HE3	1:D:447:PRO:CD	2.48	0.44
1:A:441:ASP:HB2	2:E:78:GLY:O	2.18	0.44
1:D:406:GLU:OE2	1:D:428:ILE:HG23	2.18	0.44
1:A:234:ALA:O	1:A:237:VAL:HG12	2.18	0.44
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.76	0.44
2:E:74:ARG:HB2	2:E:76:LEU:HD22	2.00	0.44
1:B:538:PHE:CZ	1:D:586:PRO:HD2	2.52	0.44
1:B:687:ALA:O	1:B:692:ILE:HG13	2.17	0.44
1:D:31:GLY:O	1:D:179:ASN:HB3	2.17	0.44
1:A:369:VAL:CG1	1:C:369:VAL:HG13	2.47	0.44
1:B:650:GLU:HB3	1:B:651:LYS:HZ2	1.82	0.44
1:C:90:ASP:O	1:C:94:MET:HG3	2.17	0.44
2:G:40:LEU:HD23	2:G:40:LEU:HA	1.74	0.44
1:B:126:GLY:HA3	1:B:131:PRO:HD3	1.99	0.44
3:B:1801:B12:H301	3:B:1801:B12:H253	1.75	0.44
1:D:116:TYR:CE2	1:D:120:ILE:HD13	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:VAL:HG22	1:A:693:ARG:CB	2.48	0.43
1:A:735:LYS:O	1:A:735:LYS:HG3	2.18	0.43
1:C:160:TYR:OH	5:C:767:Z97:HBA	2.18	0.43
1:C:300:MET:HE3	1:C:333:THR:HG22	2.00	0.43
1:A:195:ASN:ND2	1:A:428:ILE:O	2.50	0.43
1:A:372:LYS:HG2	1:C:370:GLN:NE2	2.33	0.43
1:B:232:ARG:CZ	1:D:598:ARG:NH2	2.80	0.43
1:B:712:LYS:HA	1:B:712:LYS:HD3	1.71	0.43
2:F:54:LEU:HD23	2:F:57:MET:HE3	1.99	0.43
1:C:344:TRP:CG	1:C:515:VAL:HB	2.54	0.43
1:D:233:GLU:HG2	1:D:235:TRP:CZ2	2.53	0.43
2:H:10:ARG:HE	2:H:10:ARG:HB3	1.57	0.43
1:A:598:ARG:NH1	1:C:232:ARG:HD2	2.34	0.43
1:C:144:LEU:HD23	1:C:147:ILE:HD12	2.00	0.43
1:C:190:LEU:O	1:C:426:ARG:NH2	2.50	0.43
1:D:445:MET:HG2	1:D:446:ALA:N	2.32	0.43
1:A:87:PHE:HB2	1:A:140:GLN:NE2	2.34	0.43
1:A:586:PRO:HA	1:A:587:PRO:HD3	1.85	0.43
2:E:6:ASP:OD1	2:E:10:ARG:HG2	2.19	0.43
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.81	0.43
1:B:522:THR:HA	1:B:572:GLY:O	2.18	0.43
1:B:526:THR:HB	1:D:524:LEU:HB3	2.00	0.43
1:B:608:ILE:HG21	1:B:665:LEU:HD12	2.00	0.43
1:B:672:HIS:O	1:B:675:ILE:HG22	2.19	0.43
1:C:94:MET:SD	1:C:105:ILE:HG21	2.58	0.43
3:C:1801:B12:O7R	3:C:1801:B12:H2B	2.17	0.43
1:D:591:ILE:HD12	1:D:591:ILE:N	2.32	0.43
1:A:310:ARG:HD3	1:C:350:GLU:HG2	1.99	0.43
1:A:320:LEU:HD11	1:A:355:ALA:HA	2.01	0.43
1:A:528:PHE:HE1	1:A:565:GLY:HA3	1.79	0.43
1:B:297:ARG:O	1:B:297:ARG:HD3	2.18	0.43
1:B:576:PHE:HE1	1:D:543:PHE:HD1	1.67	0.43
1:B:689:GLU:O	1:B:689:GLU:HG2	2.19	0.43
1:A:726:ILE:CG2	1:A:727:HIS:N	2.82	0.43
1:B:109:ARG:HH21	5:B:767:Z97:P	2.42	0.43
1:D:108:ILE:H	1:D:108:ILE:HG12	1.55	0.43
1:D:397:GLU:O	1:D:397:GLU:CG	2.64	0.43
2:H:103:LEU:HD22	2:H:109:TRP:CE2	2.53	0.43
1:B:265:SER:OG	1:B:297:ARG:NH1	2.49	0.43
3:B:1801:B12:H412	3:B:1801:B12:H363	1.48	0.43
1:C:317:VAL:HA	1:C:320:LEU:HD12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:723:SER:O	3:C:1801:B12:C5R	2.67	0.43
2:G:14:LEU:HD22	2:G:22:LEU:CD1	2.49	0.43
2:G:76:LEU:O	2:G:77:MET:C	2.56	0.43
2:H:74:ARG:HE	2:H:109:TRP:HB3	1.84	0.43
2:H:101:LEU:HD12	2:H:101:LEU:HA	1.88	0.43
1:A:43:MET:HE3	1:A:72:PRO:HA	1.98	0.43
1:A:43:MET:HE1	1:A:72:PRO:HA	2.00	0.43
1:A:618:HIS:CE1	3:A:1801:B12:N22	2.86	0.43
1:A:628:ILE:O	1:A:629:LYS:C	2.56	0.43
1:B:578:ILE:HD13	1:D:543:PHE:CE1	2.53	0.43
3:B:1801:B12:H2B	3:B:1801:B12:O7R	2.19	0.43
1:C:53:THR:HA	1:C:54:PRO:HD3	1.85	0.43
1:C:670:ILE:HG23	3:C:1801:B12:O34	2.18	0.43
1:D:337:ASP:O	1:D:338:GLU:C	2.57	0.43
3:D:1801:B12:H421	3:D:1801:B12:H10	2.00	0.43
2:H:51:ARG:HG2	2:H:68:VAL:HG21	2.01	0.43
1:A:310:ARG:HD3	1:C:350:GLU:CG	2.49	0.43
1:B:58:SER:HB2	1:B:71:ASP:OD2	2.18	0.43
1:B:126:GLY:HA2	1:B:131:PRO:HD3	2.01	0.43
1:D:663:ALA:HB2	1:D:697:MET:HE3	2.01	0.43
3:D:1801:B12:H531	3:D:1801:B12:C55	2.49	0.43
1:A:349:ILE:HG21	1:C:560:MET:HE2	2.01	0.43
1:A:373:ARG:HA	1:A:377:LEU:HD23	2.01	0.43
1:A:391:PHE:O	1:A:395:ILE:HG13	2.19	0.43
1:A:464:LEU:HA	1:A:464:LEU:HD12	1.67	0.43
1:A:584:VAL:C	1:A:585:ILE:HG13	2.40	0.43
1:C:391:PHE:HD2	1:C:391:PHE:O	2.02	0.43
1:D:5:LEU:HD23	1:D:5:LEU:C	2.39	0.43
1:D:123:THR:O	1:D:498:ARG:NH2	2.48	0.43
2:H:5:ASP:HA	2:H:6:ASP:CB	2.49	0.43
1:A:533:LYS:HG3	1:A:534:ARG:N	2.33	0.42
1:A:600:ASP:OD1	1:A:733:VAL:HB	2.18	0.42
1:A:611:ALA:CB	1:A:652:LEU:HD13	2.49	0.42
1:A:697:MET:HG2	1:A:735:LYS:HG3	2.01	0.42
1:B:7:LEU:HA	1:B:7:LEU:HD23	1.28	0.42
1:C:250:ILE:CG2	1:C:251:PHE:N	2.82	0.42
1:C:492:ASN:N	1:C:492:ASN:HD22	2.17	0.42
1:C:575:PRO:HD2	1:C:576:PHE:CE2	2.53	0.42
1:C:626:ILE:HG21	1:C:640:VAL:HG11	2.01	0.42
3:C:1801:B12:H301	3:C:1801:B12:H253	1.83	0.42
2:G:76:LEU:HD12	2:G:76:LEU:HA	1.80	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:650:GLU:O	1:D:653:VAL:HG23	2.19	0.42
3:D:1801:B12:H562	3:D:1801:B12:H18	1.73	0.42
1:B:8:ARG:HB2	1:B:8:ARG:NH1	2.32	0.42
1:B:116:TYR:CE2	1:B:120:ILE:HD13	2.54	0.42
1:B:529:LEU:HA	1:B:530:PRO:HD3	1.64	0.42
1:D:608:ILE:HG13	1:D:663:ALA:HB3	2.01	0.42
1:D:618:HIS:CD2	3:D:1801:B12:N24	2.87	0.42
1:D:700:CYS:O	1:D:718:GLY:HA2	2.19	0.42
1:A:73:GLN:OE1	1:A:153:ARG:NH2	2.49	0.42
1:A:75:LEU:N	1:A:76:PRO:HD3	2.34	0.42
1:B:22:LEU:HD23	1:B:22:LEU:HA	1.79	0.42
1:B:138:ARG:NH1	1:B:485:TYR:CD1	2.87	0.42
1:B:268:PRO:HA	1:B:269:PRO:HD3	1.73	0.42
1:B:609:VAL:HG11	1:B:656:ALA:HA	2.00	0.42
1:C:224:ALA:HB3	1:C:245:HIS:CE1	2.54	0.42
1:B:547:MET:HB3	1:D:547:MET:HB3	2.00	0.42
1:B:706:THR:HB	1:B:709:VAL:CG2	2.49	0.42
3:B:1801:B12:H601	3:B:1801:B12:H262	2.01	0.42
1:C:399:GLY:HA3	1:C:403:ASN:ND2	2.30	0.42
1:C:592:LEU:HD22	1:C:596:GLU:CB	2.49	0.42
1:A:467:GLU:O	1:A:469:SER:N	2.52	0.42
1:C:109:ARG:NH2	5:C:767:Z97:P	2.91	0.42
1:D:186:GLN:HG2	1:D:401:TYR:OH	2.19	0.42
1:D:307:ALA:O	1:D:340:ARG:HD3	2.20	0.42
1:A:233:GLU:HB3	1:A:235:TRP:CZ3	2.55	0.42
1:B:737:ARG:C	1:B:739:MET:N	2.73	0.42
1:D:342:VAL:O	1:D:343:PRO:C	2.57	0.42
1:D:684:HIS:O	1:D:688:VAL:HG23	2.19	0.42
1:A:444:TYR:CE1	2:E:80:GLY:HA2	2.55	0.42
1:B:350:GLU:HB3	1:D:310:ARG:HD3	2.02	0.42
1:B:354:THR:OG1	1:D:310:ARG:HD2	2.20	0.42
1:B:521:GLY:O	1:B:573:ARG:HA	2.20	0.42
3:B:1801:B12:C53	3:B:1801:B12:H552	2.49	0.42
3:C:1801:B12:N40	3:C:1801:B12:C8	2.81	0.42
1:D:396:ILE:C	1:D:398:ALA:H	2.23	0.42
1:D:443:ASP:OD1	2:H:79:LYS:HE3	2.20	0.42
1:D:506:ARG:HD3	1:D:518:GLN:HE22	1.85	0.42
1:D:574:VAL:HG13	1:D:576:PHE:CD1	2.55	0.42
1:A:207:LYS:HD3	1:A:252:SER:OG	2.19	0.42
1:A:616:ASP:OD2	1:A:669:ILE:HB	2.20	0.42
1:A:712:LYS:HG2	1:A:712:LYS:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:55:LEU:HD23	2:E:55:LEU:HA	1.92	0.42
1:C:95:ARG:HH21	1:C:150:GLU:CD	2.22	0.42
1:C:126:GLY:HA3	1:C:129:GLY:O	2.20	0.42
1:D:528:PHE:CE1	1:D:560:MET:HG3	2.54	0.42
1:A:16:GLU:OE1	1:A:506:ARG:NH2	2.45	0.42
1:A:512:LYS:HB2	1:A:513:PRO:CD	2.50	0.42
1:C:191:TYR:HE1	1:C:230:THR:HG21	1.85	0.42
1:D:212:TRP:CZ2	1:D:477:LEU:HB3	2.55	0.42
1:D:522:THR:HG22	1:D:523:VAL:N	2.35	0.42
1:A:349:ILE:N	1:A:349:ILE:CD1	2.82	0.42
1:A:546:LYS:O	1:C:548:ASN:ND2	2.52	0.42
1:A:593:SER:OG	1:A:595:ASP:HB2	2.19	0.42
1:B:492:ASN:HD22	1:B:492:ASN:HA	1.53	0.42
1:D:85:GLY:HA2	1:D:129:GLY:O	2.20	0.42
1:D:399:GLY:HA3	1:D:403:ASN:ND2	2.35	0.42
1:A:585:ILE:HA	1:A:586:PRO:HD3	1.81	0.41
1:B:134:ARG:NH2	1:B:175:GLU:OE2	2.44	0.41
1:B:512:LYS:HD3	1:B:519:ALA:HB1	2.02	0.41
1:B:665:LEU:HB3	3:B:1801:B12:C5M	2.50	0.41
1:C:6:GLN:HG2	1:C:7:LEU:N	2.35	0.41
2:G:88:ILE:HG13	2:G:103:LEU:HD11	2.02	0.41
1:D:320:LEU:HD11	1:D:355:ALA:HA	2.02	0.41
1:A:96:MET:HG2	1:C:560:MET:HB3	2.02	0.41
1:A:115:HIS:CE1	1:C:623:ARG:HD3	2.55	0.41
1:A:302:THR:HG22	1:A:334:ILE:HG21	2.02	0.41
1:A:341:ASN:C	1:A:341:ASN:HD22	2.23	0.41
3:A:1801:B12:N23	4:C:1500:5AD:C4'	2.74	0.41
1:B:182:HIS:HA	1:B:218:ILE:O	2.20	0.41
1:B:200:PHE:CD2	2:F:37:LEU:HD13	2.55	0.41
1:B:668:THR:HG21	1:B:680:MET:HE2	2.01	0.41
1:B:701:GLY:HA2	1:B:719:PHE:O	2.20	0.41
1:C:53:THR:HG22	1:C:54:PRO:O	2.20	0.41
1:C:305:MET:HE3	1:C:305:MET:HB2	1.85	0.41
1:C:393:GLU:O	1:C:397:GLU:HB3	2.20	0.41
1:D:205:GLU:OE2	1:D:451:HIS:HA	2.20	0.41
1:A:335:THR:HA	1:A:336:PRO:HD3	1.85	0.41
1:B:511:ILE:HD11	1:D:530:PRO:HD2	2.01	0.41
1:C:18:ILE:HD13	1:C:143:ALA:HB2	2.02	0.41
1:C:110:THR:HG22	1:C:131:PRO:HA	2.01	0.41
1:C:250:ILE:HG23	1:C:251:PHE:N	2.34	0.41
1:C:554:VAL:HG22	1:C:570:LEU:HD23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:TRP:CH2	1:D:477:LEU:HB3	2.55	0.41
1:D:344:TRP:CG	1:D:515:VAL:HB	2.55	0.41
1:D:444:TYR:CD2	1:D:444:TYR:C	2.93	0.41
1:D:529:LEU:HA	1:D:530:PRO:HD3	1.85	0.41
1:A:95:ARG:HA	1:A:147:ILE:HD13	2.03	0.41
1:B:162:SER:CB	5:B:767:Z97:H6	2.50	0.41
1:B:411:VAL:HG12	1:B:411:VAL:O	2.21	0.41
1:C:57:ASN:HB3	1:C:99:TRP:CH2	2.56	0.41
1:C:153:ARG:HA	1:C:154:PRO:HD3	1.85	0.41
1:C:406:GLU:OE2	1:C:428:ILE:HG22	2.20	0.41
1:C:619:SER:HB3	1:C:645:THR:CG2	2.49	0.41
1:C:620:VAL:HG23	3:C:1801:B12:O51	2.20	0.41
1:C:719:PHE:CD2	3:C:1801:B12:HM63	2.55	0.41
1:A:79:THR:HA	1:A:104:HIS:HB3	2.02	0.41
1:A:193:ASN:HB2	1:A:426:ARG:CZ	2.50	0.41
1:A:447:PRO:HG2	2:E:57:MET:SD	2.61	0.41
1:B:629:LYS:NZ	5:D:767:Z97:HDA	2.35	0.41
1:C:207:LYS:HZ2	1:C:217:GLN:HE22	1.69	0.41
1:C:484:VAL:HG11	2:G:60:SER:HB3	2.01	0.41
1:D:275:PRO:HD2	1:D:279:LEU:HD11	2.02	0.41
1:D:344:TRP:CE2	1:D:515:VAL:HG11	2.55	0.41
1:D:561:GLN:O	1:D:562:GLU:C	2.58	0.41
3:D:1801:B12:H2B	3:D:1801:B12:O7R	2.20	0.41
2:H:6:ASP:HB3	2:H:7:PHE:H	1.74	0.41
1:A:224:ALA:CB	1:A:245:HIS:CE1	3.03	0.41
1:B:20:LYS:O	1:B:21:ASP:HB2	2.21	0.41
1:B:438:PHE:CD2	2:F:77:MET:HG3	2.55	0.41
1:B:680:MET:CE	1:B:705:VAL:HG22	2.50	0.41
2:F:112:ALA:C	2:F:114:GLN:N	2.72	0.41
1:C:464:LEU:HD12	1:C:464:LEU:HA	1.80	0.41
1:D:269:PRO:HD2	1:D:280:ASP:CG	2.41	0.41
1:D:416:TYR:HA	1:D:418:GLU:N	2.35	0.41
1:D:628:ILE:HG12	1:D:628:ILE:O	2.20	0.41
1:D:711:VAL:HG12	1:D:711:VAL:O	2.19	0.41
1:A:342:VAL:CG1	1:A:343:PRO:HD2	2.50	0.41
2:E:35:ASP:HB2	2:E:36:PRO:HD3	2.03	0.41
1:B:243:VAL:HG22	1:B:392:MET:HG3	2.03	0.41
1:B:629:LYS:HZ1	5:D:767:Z97:HDA	1.86	0.41
1:C:649:VAL:HG12	1:C:686:LEU:HD12	2.01	0.41
2:G:52:SER:HA	2:G:55:LEU:HD12	2.03	0.41
1:D:109:ARG:HG2	1:D:132:ILE:HG13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:ILE:O	1:D:428:ILE:HG13	2.21	0.41
1:D:492:ASN:O	1:D:497:VAL:HG21	2.20	0.41
1:D:526:THR:HG23	1:D:569:GLU:HG2	2.02	0.41
1:D:574:VAL:HA	1:D:575:PRO:HD3	1.97	0.41
1:D:607:LYS:C	1:D:608:ILE:HD12	2.41	0.41
1:A:93:ARG:HG3	1:A:345:HIS:ND1	2.36	0.41
1:A:512:LYS:HB2	1:A:513:PRO:HD2	2.03	0.41
1:B:15:VAL:HG22	1:B:499:MET:HE2	2.02	0.41
1:B:172:MET:HE2	1:B:176:GLU:CG	2.51	0.41
1:B:281:LEU:O	1:B:281:LEU:HD12	2.20	0.41
1:B:307:ALA:O	1:B:340:ARG:HD3	2.21	0.41
3:B:1801:B12:N40	3:B:1801:B12:C8	2.80	0.41
1:D:443:ASP:HA	1:D:456:ASN:HD22	1.85	0.41
2:H:35:ASP:CB	2:H:36:PRO:HD3	2.51	0.41
1:A:578:ILE:CG2	1:A:579:ASP:N	2.84	0.41
1:A:665:LEU:HA	1:A:699:GLY:O	2.20	0.41
2:E:90:LYS:HE2	2:E:90:LYS:HB3	1.83	0.41
1:B:79:THR:HG23	1:B:104:HIS:ND1	2.35	0.41
1:B:86:ARG:O	1:B:87:PHE:C	2.59	0.41
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.89	0.41
1:B:344:TRP:CD1	1:B:515:VAL:HB	2.56	0.41
1:B:415:TYR:O	1:B:416:TYR:C	2.59	0.41
1:B:461:ASP:OD1	1:B:463:ALA:HB3	2.21	0.41
1:B:528:PHE:CZ	1:B:565:GLY:HA3	2.56	0.41
1:B:530:PRO:HD2	1:D:511:ILE:HD11	2.03	0.41
3:B:1801:B12:O7R	3:B:1801:B12:C2B	2.68	0.41
2:F:66:ALA:O	2:F:70:LYS:HG3	2.21	0.41
2:F:76:LEU:HG	2:F:84:ILE:HD11	2.03	0.41
1:D:138:ARG:HE	1:D:176:GLU:CD	2.24	0.41
1:D:382:ARG:CZ	2:H:22:LEU:HD22	2.50	0.41
1:D:585:ILE:HA	1:D:586:PRO:HD3	1.76	0.41
3:D:1801:B12:H492	3:D:1801:B12:C47	2.51	0.41
1:A:709:VAL:HG12	1:A:709:VAL:O	2.21	0.41
1:A:116:TYR:HE1	1:C:620:VAL:HG21	1.86	0.40
1:A:422:ASP:OD1	1:A:422:ASP:N	2.50	0.40
1:A:440:ARG:HH22	1:A:451:HIS:CE1	2.38	0.40
1:A:677:TYR:CE1	1:A:709:VAL:HB	2.56	0.40
1:B:41:LEU:CD2	1:B:43:MET:HE2	2.46	0.40
1:B:281:LEU:HB3	1:B:282:PRO:HD3	2.03	0.40
1:B:284:ALA:O	1:B:288:ARG:HD3	2.20	0.40
2:F:32:LYS:O	2:F:36:PRO:HD3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ARG:NH2	1:C:114:SER:OG	2.51	0.40
1:C:537:GLU:O	1:C:540:ALA:HB3	2.20	0.40
1:C:631:GLY:O	1:C:725:GLY:HA3	2.21	0.40
3:D:1801:B12:H412	3:D:1801:B12:H363	1.86	0.40
2:H:106:GLY:HA2	2:H:109:TRP:HD1	1.87	0.40
1:B:14:ASP:O	1:B:18:ILE:HG13	2.21	0.40
1:B:479:VAL:HG12	1:B:479:VAL:O	2.20	0.40
2:F:25:ARG:O	2:F:29:MET:HG3	2.21	0.40
1:C:7:LEU:HD12	1:C:146:LEU:HB3	2.04	0.40
2:G:10:ARG:HE	2:G:10:ARG:HB3	1.19	0.40
1:D:172:MET:HE1	1:D:173:PHE:HD1	1.86	0.40
1:A:35:ARG:HH12	1:A:74:PRO:HD2	1.86	0.40
1:A:81:GLU:OE2	5:A:767:Z97:N	2.52	0.40
1:A:684:HIS:CE1	1:A:693:ARG:HE	2.39	0.40
2:E:112:ALA:C	2:E:114:GLN:N	2.74	0.40
1:B:137:VAL:CB	1:B:172:MET:HE3	2.51	0.40
1:C:6:GLN:HB3	1:C:6:GLN:HE21	1.59	0.40
1:C:668:THR:HG23	1:C:668:THR:O	2.21	0.40
1:D:172:MET:O	1:D:172:MET:HE2	2.21	0.40
1:D:267:VAL:HG12	1:D:268:PRO:O	2.21	0.40
2:H:5:ASP:CA	2:H:6:ASP:CB	3.00	0.40
1:B:167:PRO:O	1:B:168:ASP:C	2.60	0.40
1:B:167:PRO:HB2	2:F:52:SER:HB3	2.02	0.40
1:C:79:THR:HG22	1:C:80:THR:N	2.37	0.40
1:D:575:PRO:HG2	1:D:576:PHE:CD2	2.57	0.40
1:A:390:LEU:HD23	2:E:14:LEU:HD11	2.03	0.40
1:A:541:ILE:HG23	1:A:552:VAL:HG12	2.04	0.40
1:A:671:SER:O	1:A:672:HIS:C	2.59	0.40
1:A:688:VAL:HG22	1:A:693:ARG:HB2	2.04	0.40
2:E:88:ILE:HD13	2:E:88:ILE:HA	1.85	0.40
1:B:227:ALA:HB3	1:B:241:LEU:CD2	2.51	0.40
1:B:471:LEU:HD12	1:B:471:LEU:HA	1.86	0.40
1:B:629:LYS:HE3	1:B:630:HIS:NE2	2.37	0.40
3:B:1801:B12:C61	3:B:1801:B12:H562	2.51	0.40
1:C:693:ARG:HD2	1:C:693:ARG:HA	1.72	0.40
1:D:132:ILE:HA	1:D:136:GLN:OE1	2.21	0.40
1:D:238:MET:H	1:D:238:MET:HG3	1.55	0.40
1:D:305:MET:HB2	1:D:305:MET:HE3	1.78	0.40
1:D:647:VAL:HA	1:D:648:PRO:HD3	1.95	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	722/763 (95%)	664 (92%)	51 (7%)	7 (1%)	15	44
1	B	722/763 (95%)	660 (91%)	54 (8%)	8 (1%)	14	41
1	C	722/763 (95%)	673 (93%)	43 (6%)	6 (1%)	19	49
1	D	722/763 (95%)	663 (92%)	54 (8%)	5 (1%)	22	53
2	E	108/121 (89%)	95 (88%)	11 (10%)	2 (2%)	8	26
2	F	108/121 (89%)	99 (92%)	6 (6%)	3 (3%)	5	17
2	G	108/121 (89%)	98 (91%)	9 (8%)	1 (1%)	17	46
2	H	108/121 (89%)	97 (90%)	11 (10%)	0	100	100
All	All	3320/3536 (94%)	3049 (92%)	239 (7%)	32 (1%)	15	44

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
2	E	6	ASP
2	E	93	ASN
1	B	461	ASP
1	C	6	GLN
1	C	461	ASP
2	G	6	ASP
1	A	461	ASP
1	A	471	LEU
1	B	738	GLU
1	B	739	MET
2	F	6	ASP
1	D	7	LEU
1	D	338	GLU
1	A	660	LYS
1	B	168	ASP
1	D	6	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	111	ALA
1	C	341	ASN
1	B	83	ALA
1	B	735	LYS
2	F	84	ILE
1	C	548	ASN
1	B	575	PRO
2	F	113	ILE
1	C	7	LEU
1	A	411	VAL
1	A	530	PRO
1	B	411	VAL
1	A	605	PRO
1	C	411	VAL
1	D	411	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	598/644 (93%)	556 (93%)	42 (7%)	15	40
1	B	604/644 (94%)	563 (93%)	41 (7%)	16	42
1	C	600/644 (93%)	566 (94%)	34 (6%)	20	50
1	D	602/644 (94%)	561 (93%)	41 (7%)	16	42
2	E	89/100 (89%)	78 (88%)	11 (12%)	4	14
2	F	90/100 (90%)	81 (90%)	9 (10%)	7	22
2	G	89/100 (89%)	83 (93%)	6 (7%)	16	43
2	H	89/100 (89%)	83 (93%)	6 (7%)	16	43
All	All	2761/2976 (93%)	2571 (93%)	190 (7%)	15	41

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	LEU
1	A	23	ASP
1	A	29	ARG
1	A	108	ILE
1	A	114	SER
1	A	127	ILE
1	A	141	ARG
1	A	164	VAL
1	A	172	MET
1	A	182	HIS
1	A	218	ILE
1	A	233	GLU
1	A	238	MET
1	A	306	GLU
1	A	327	ARG
1	A	338	GLU
1	A	341	ASN
1	A	374	GLU
1	A	391	PHE
1	A	464	LEU
1	A	471	LEU
1	A	499	MET
1	A	509	SER
1	A	526	THR
1	A	533	LYS
1	A	557	ARG
1	A	570	LEU
1	A	576	PHE
1	A	602	GLU
1	A	616	ASP
1	A	622	LEU
1	A	623	ARG
1	A	640	VAL
1	A	651	LYS
1	A	673	ASP
1	A	690	LYS
1	A	706	THR
1	A	712	LYS
1	A	730	THR
1	A	731	PHE
1	A	734	LYS
2	E	21	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	23	GLN
2	E	63	GLU
2	E	73	ASP
2	E	76	LEU
2	E	91	GLU
2	E	93	ASN
2	E	98	GLU
2	E	107	LYS
2	E	111	ASP
2	E	114	GLN
1	B	5	LEU
1	B	6	GLN
1	B	7	LEU
1	B	9	VAL
1	B	15	VAL
1	B	30	ARG
1	B	39	GLU
1	B	106	MET
1	B	114	SER
1	B	141	ARG
1	B	149	GLU
1	B	151	VAL
1	B	162	SER
1	B	172	MET
1	B	232	ARG
1	B	306	GLU
1	B	308	SER
1	B	327	ARG
1	B	338	GLU
1	B	341	ASN
1	B	349	ILE
1	B	391	PHE
1	B	429	ASN
1	B	445	MET
1	B	449	THR
1	B	464	LEU
1	B	465	VAL
1	B	471	LEU
1	B	492	ASN
1	B	501	GLU
1	B	562	GLU
1	B	570	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	603	LYS
1	B	609	VAL
1	B	646	SER
1	B	651	LYS
1	B	681	LYS
1	B	683	ILE
1	B	695	LYS
1	B	696	ILE
1	B	733	VAL
2	F	10	ARG
2	F	23	GLN
2	F	28	GLU
2	F	29	MET
2	F	65	LYS
2	F	76	LEU
2	F	94	ILE
2	F	101	LEU
2	F	105	GLU
1	C	5	LEU
1	C	6	GLN
1	C	13	LEU
1	C	33	THR
1	C	39	GLU
1	C	114	SER
1	C	162	SER
1	C	232	ARG
1	C	238	MET
1	C	301	ASN
1	C	306	GLU
1	C	370	GLN
1	C	391	PHE
1	C	397	GLU
1	C	428	ILE
1	C	429	ASN
1	C	462	GLU
1	C	464	LEU
1	C	471	LEU
1	C	500	GLU
1	C	509	SER
1	C	511	ILE
1	C	541	ILE
1	C	570	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	576	PHE
1	C	578	ILE
1	C	584	VAL
1	C	591	ILE
1	C	604	THR
1	C	609	VAL
1	C	651	LYS
1	C	660	LYS
1	C	668	THR
1	C	736	ARG
2	G	10	ARG
2	G	39	ASP
2	G	73	ASP
2	G	76	LEU
2	G	104	SER
2	G	114	GLN
1	D	6	GLN
1	D	7	LEU
1	D	8	ARG
1	D	9	VAL
1	D	18	ILE
1	D	26	THR
1	D	29	ARG
1	D	39	GLU
1	D	50	ASP
1	D	53	THR
1	D	63	SER
1	D	79	THR
1	D	108	ILE
1	D	127	ILE
1	D	172	MET
1	D	179	ASN
1	D	232	ARG
1	D	250	ILE
1	D	306	GLU
1	D	341	ASN
1	D	370	GLN
1	D	391	PHE
1	D	428	ILE
1	D	471	LEU
1	D	491	GLU
1	D	500	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	501	GLU
1	D	502	THR
1	D	576	PHE
1	D	577	SER
1	D	608	ILE
1	D	653	VAL
1	D	660	LYS
1	D	674	ASP
1	D	675	ILE
1	D	690	LYS
1	D	695	LYS
1	D	696	ILE
1	D	708	GLU
1	D	731	PHE
1	D	736	ARG
2	H	23	GLN
2	H	25	ARG
2	H	28	GLU
2	H	39	ASP
2	H	76	LEU
2	H	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	HIS
1	A	331	GLN
1	A	341	ASN
1	A	370	GLN
1	A	492	ASN
1	A	679	ASN
1	A	713	GLN
1	B	73	GLN
1	B	217	GLN
1	B	331	GLN
1	B	370	GLN
1	B	429	ASN
1	B	492	ASN
1	B	518	GLN
1	B	679	ASN
1	B	713	GLN
1	C	217	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	245	HIS
1	C	370	GLN
1	C	403	ASN
1	C	407	GLN
1	C	429	ASN
1	C	492	ASN
1	C	518	GLN
2	G	8	GLN
2	G	16	ASN
1	D	331	GLN
1	D	370	GLN
1	D	492	ASN
1	D	518	GLN
2	H	16	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	Z97	D	767	-	23,24,24	2.31	8 (34%)	29,33,33	1.81	5 (17%)
4	5AD	A	1500	3	17,20,20	2.43	8 (47%)	15,30,30	4.29	10 (66%)
3	B12	A	1801	1,4	90,101,101	1.32	10 (11%)	137,166,166	2.38	32 (23%)
5	Z97	C	767	-	23,24,24	2.21	7 (30%)	29,33,33	1.74	8 (27%)
3	B12	C	1801	1,4	90,101,101	1.40	8 (8%)	137,166,166	2.37	31 (22%)
4	5AD	C	1500	3	17,20,20	2.44	7 (41%)	15,30,30	4.26	7 (46%)
4	5AD	B	1500	3	17,20,20	2.40	7 (41%)	15,30,30	4.42	8 (53%)
4	5AD	D	1500	3	17,20,20	2.33	7 (41%)	15,30,30	4.25	9 (60%)
5	Z97	A	767	-	23,24,24	2.25	6 (26%)	29,33,33	1.83	7 (24%)
3	B12	B	1801	1,4	90,101,101	1.36	9 (10%)	137,166,166	2.26	28 (20%)
5	Z97	B	767	-	23,24,24	2.16	6 (26%)	29,33,33	1.85	5 (17%)
3	B12	D	1801	1,4	90,101,101	1.36	10 (11%)	137,166,166	2.32	31 (22%)

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
5	Z97	D	767	-	-	9/18/18/18	0/1/1/1
4	5AD	A	1500	3	3/3/4/4	0/0/20/20	0/3/3/3
3	B12	A	1801	1,4	1/1/36/38	21/52/223/223	0/3/11/11
5	Z97	C	767	-	-	8/18/18/18	0/1/1/1
3	B12	C	1801	1,4	1/1/36/38	8/52/223/223	0/3/11/11
4	5AD	C	1500	3	2/2/4/4	0/0/20/20	0/3/3/3
4	5AD	B	1500	3	2/2/4/4	0/0/20/20	0/3/3/3
4	5AD	D	1500	3	3/3/4/4	0/0/20/20	0/3/3/3
5	Z97	A	767	-	-	6/18/18/18	0/1/1/1
3	B12	B	1801	1,4	1/1/36/38	11/52/223/223	0/3/11/11
5	Z97	B	767	-	-	7/18/18/18	0/1/1/1
3	B12	D	1801	1,4	1/1/36/38	20/52/223/223	0/3/11/11

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	767	Z97	C4-C5	5.83	1.49	1.42
4	C	1500	5AD	C2-N3	5.52	1.41	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1500	5AD	C2-N3	5.50	1.41	1.32
4	B	1500	5AD	C2-N3	5.47	1.40	1.32
5	C	767	Z97	C4-C5	5.45	1.48	1.42
5	A	767	Z97	C4-C5	5.44	1.48	1.42
5	D	767	Z97	C4A-NE	5.28	1.45	1.27
3	B	1801	B12	C14-N23	5.24	1.41	1.35
3	C	1801	B12	C19-N24	-5.19	1.39	1.48
5	B	767	Z97	C4-C5	5.17	1.48	1.42
4	D	1500	5AD	C2-N3	5.09	1.40	1.32
3	C	1801	B12	C14-N23	5.03	1.41	1.35
5	B	767	Z97	C4A-NE	4.97	1.43	1.27
5	A	767	Z97	C4A-NE	4.77	1.43	1.27
5	C	767	Z97	C4A-NE	4.75	1.43	1.27
4	C	1500	5AD	O4'-C4'	-4.60	1.30	1.44
3	B	1801	B12	C9-N22	4.41	1.42	1.30
4	B	1500	5AD	O4'-C4'	-4.36	1.31	1.44
3	B	1801	B12	C19-N24	-4.31	1.40	1.48
3	A	1801	B12	C14-N23	4.30	1.40	1.35
5	D	767	Z97	C4-C4A	4.27	1.54	1.46
3	D	1801	B12	C14-N23	4.25	1.40	1.35
3	C	1801	B12	C9-N22	4.23	1.41	1.30
5	A	767	Z97	C4-C4A	4.21	1.54	1.46
3	A	1801	B12	C9-N22	4.16	1.41	1.30
5	B	767	Z97	C4-C4A	4.16	1.54	1.46
3	D	1801	B12	C8B-C9B	4.13	1.48	1.40
3	C	1801	B12	C8B-C9B	4.11	1.48	1.40
3	A	1801	B12	C8B-C9B	4.06	1.48	1.40
4	A	1500	5AD	C8-N7	4.05	1.41	1.34
3	B	1801	B12	C8B-C9B	4.01	1.48	1.40
3	D	1801	B12	C9-N22	4.00	1.41	1.30
5	C	767	Z97	C4-C4A	3.96	1.54	1.46
4	D	1500	5AD	C8-N7	3.96	1.41	1.34
3	C	1801	B12	C16-C15	-3.83	1.34	1.44
3	D	1801	B12	C16-C15	-3.79	1.34	1.44
3	B	1801	B12	C16-C15	-3.72	1.34	1.44
3	A	1801	B12	C11-N23	3.72	1.44	1.37
3	D	1801	B12	C19-N24	-3.71	1.41	1.48
3	D	1801	B12	C11-N23	3.70	1.44	1.37
3	B	1801	B12	C11-N23	3.53	1.43	1.37
3	A	1801	B12	C16-C15	-3.49	1.34	1.44
3	A	1801	B12	C19-N24	-3.46	1.42	1.48
5	C	767	Z97	C2-N1	3.44	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1500	5AD	O4'-C4'	-3.44	1.34	1.44
4	C	1500	5AD	C8-N7	3.40	1.40	1.34
3	D	1801	B12	C6B-C5B	3.35	1.49	1.40
3	A	1801	B12	C6B-C5B	3.33	1.49	1.40
5	A	767	Z97	C3-C2	3.30	1.44	1.40
3	C	1801	B12	C6B-C5B	3.28	1.49	1.40
3	C	1801	B12	C11-N23	3.27	1.43	1.37
3	B	1801	B12	C6B-C5B	3.19	1.48	1.40
4	B	1500	5AD	C6-N6	3.01	1.45	1.34
3	A	1801	B12	C10-C9	2.97	1.47	1.39
3	D	1801	B12	C10-C9	2.97	1.47	1.39
4	D	1500	5AD	O4'-C4'	-2.94	1.35	1.44
5	B	767	Z97	C4-C3	-2.92	1.36	1.40
5	A	767	Z97	C2-N1	2.90	1.39	1.33
5	B	767	Z97	C2-N1	2.90	1.39	1.33
4	C	1500	5AD	C6-N6	2.87	1.44	1.34
4	A	1500	5AD	O3'-C3'	-2.85	1.36	1.43
4	D	1500	5AD	O3'-C3'	-2.78	1.36	1.43
5	D	767	Z97	C2-N1	2.78	1.39	1.33
5	D	767	Z97	OXT-C	2.74	1.39	1.30
5	A	767	Z97	OXT-C	2.71	1.39	1.30
4	A	1500	5AD	C6-N6	2.71	1.43	1.34
4	C	1500	5AD	O3'-C3'	-2.68	1.36	1.43
4	D	1500	5AD	C6-N6	2.66	1.43	1.34
4	B	1500	5AD	O3'-C3'	-2.66	1.36	1.43
5	D	767	Z97	C3-C2	2.60	1.43	1.40
4	C	1500	5AD	C2-N1	2.44	1.38	1.33
5	C	767	Z97	OXT-C	2.43	1.38	1.30
4	D	1500	5AD	C6-C5	-2.41	1.34	1.43
3	B	1801	B12	C10-C9	2.39	1.46	1.39
4	B	1500	5AD	C6-C5	-2.39	1.34	1.43
4	D	1500	5AD	O4'-C1'	2.35	1.44	1.41
5	C	767	Z97	C4-C3	-2.32	1.37	1.40
3	D	1801	B12	C14-C15	2.31	1.48	1.38
5	D	767	Z97	C6-N1	2.29	1.39	1.34
3	C	1801	B12	C10-C9	2.28	1.45	1.39
5	B	767	Z97	OXT-C	2.27	1.38	1.30
5	C	767	Z97	C6-N1	2.26	1.39	1.34
4	A	1500	5AD	C6-C5	-2.26	1.34	1.43
4	B	1500	5AD	C8-N7	2.25	1.38	1.34
3	B	1801	B12	C14-C15	2.23	1.47	1.38
4	C	1500	5AD	C6-C5	-2.20	1.35	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1801	B12	C14-C15	2.16	1.47	1.38
4	A	1500	5AD	O4'-C1'	2.15	1.44	1.41
3	D	1801	B12	C1-C2	-2.15	1.53	1.58
5	D	767	Z97	C4-C3	-2.11	1.37	1.40
4	A	1500	5AD	C2-N1	2.03	1.37	1.33
4	B	1500	5AD	C5-N7	-2.01	1.32	1.39
3	A	1801	B12	C20-C1	-2.01	1.49	1.53

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1500	5AD	C5'-C4'-C3'	11.37	127.64	115.70
4	C	1500	5AD	C5'-C4'-C3'	11.25	127.51	115.70
4	D	1500	5AD	C5'-C4'-C3'	10.68	126.91	115.70
3	A	1801	B12	C1-C19-N24	9.84	117.31	106.24
4	A	1500	5AD	C5'-C4'-C3'	9.73	125.92	115.70
3	D	1801	B12	C1-C19-N24	9.72	117.17	106.24
3	B	1801	B12	C13-C12-C11	-8.75	91.07	100.97
3	C	1801	B12	C20-C1-C19	-8.67	101.00	109.36
3	B	1801	B12	C1-C19-N24	8.61	115.92	106.24
3	A	1801	B12	C13-C12-C11	-8.11	91.79	100.97
3	C	1801	B12	C13-C12-C11	-7.95	91.97	100.97
3	D	1801	B12	C13-C12-C11	-7.90	92.03	100.97
3	D	1801	B12	C46-C12-C13	-7.81	80.93	112.72
3	C	1801	B12	C46-C12-C13	-7.75	81.18	112.72
3	D	1801	B12	C47-C12-C46	7.68	122.32	109.35
3	C	1801	B12	C1-C19-N24	7.62	114.81	106.24
3	A	1801	B12	C12-C11-N23	7.47	122.25	111.83
3	A	1801	B12	C47-C12-C46	7.34	121.75	109.35
3	B	1801	B12	C1-C19-C18	7.17	133.65	121.88
3	C	1801	B12	C47-C12-C46	7.13	121.39	109.35
3	A	1801	B12	C46-C12-C13	-7.10	83.80	112.72
3	C	1801	B12	C1-C19-C18	7.05	133.46	121.88
5	D	767	Z97	OP4-C5A-C5	6.86	122.42	109.35
3	A	1801	B12	C12-C11-C10	-6.66	114.70	123.37
3	D	1801	B12	C12-C11-N23	6.62	121.05	111.83
3	C	1801	B12	C55-C17-C16	-6.50	103.82	116.65
3	B	1801	B12	C46-C12-C13	-6.36	86.81	112.72
3	D	1801	B12	C12-C11-C10	-6.33	115.13	123.37
4	A	1500	5AD	N3-C2-N1	-6.31	118.81	128.68
3	B	1801	B12	C47-C12-C46	6.26	119.94	109.35
4	C	1500	5AD	N3-C2-N1	-6.07	119.19	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1500	5AD	O3'-C3'-C4'	6.04	125.27	110.47
3	A	1801	B12	C47-C12-C13	-6.00	88.27	112.72
3	D	1801	B12	C1-C19-C18	5.92	131.60	121.88
4	B	1500	5AD	O3'-C3'-C4'	5.91	124.94	110.47
4	B	1500	5AD	O2'-C2'-C3'	5.89	130.86	111.82
3	A	1801	B12	C1-C19-C18	5.83	131.46	121.88
4	A	1500	5AD	O2'-C2'-C3'	5.83	130.67	111.82
5	A	767	Z97	OP4-C5A-C5	5.78	120.37	109.35
4	B	1500	5AD	N3-C2-N1	-5.76	119.68	128.68
4	D	1500	5AD	N3-C2-N1	-5.72	119.74	128.68
3	A	1801	B12	C18-C19-N24	5.69	110.97	102.31
4	A	1500	5AD	O3'-C3'-C4'	5.66	124.33	110.47
3	D	1801	B12	C18-C19-N24	5.63	110.88	102.31
3	B	1801	B12	C12-C11-N23	5.63	119.68	111.83
5	B	767	Z97	OP4-C5A-C5	5.63	120.07	109.35
3	B	1801	B12	C12-C11-C10	-5.59	116.09	123.37
4	A	1500	5AD	O3'-C3'-C2'	5.58	129.88	111.82
3	B	1801	B12	C47-C12-C13	-5.56	90.09	112.72
3	C	1801	B12	C18-C19-N24	5.45	110.61	102.31
3	C	1801	B12	C12-C11-C10	-5.41	116.32	123.37
5	C	767	Z97	OP4-C5A-C5	5.34	119.53	109.35
4	C	1500	5AD	O3'-C3'-C4'	5.13	123.04	110.47
3	D	1801	B12	C47-C12-C13	-5.10	91.97	112.72
3	B	1801	B12	C20-C1-C19	-5.00	104.54	109.36
4	C	1500	5AD	O2'-C2'-C1'	5.00	129.31	110.85
3	C	1801	B12	C12-C11-N23	4.98	118.78	111.83
3	B	1801	B12	C18-C19-N24	4.96	109.86	102.31
3	C	1801	B12	C47-C12-C13	-4.84	93.03	112.72
3	A	1801	B12	C20-C1-C19	-4.79	104.74	109.36
3	C	1801	B12	C26-C2-C1	4.68	117.30	110.01
3	B	1801	B12	C2P-C1P-N59	-4.61	106.14	112.93
3	A	1801	B12	C15-C14-N23	-4.59	120.66	126.26
4	D	1500	5AD	O2'-C2'-C3'	4.58	126.65	111.82
3	B	1801	B12	C55-C17-C16	-4.58	107.61	116.65
4	C	1500	5AD	O2'-C2'-C3'	4.57	126.61	111.82
3	A	1801	B12	C13-C14-N23	4.55	115.29	109.10
4	C	1500	5AD	O3'-C3'-C2'	4.48	126.31	111.82
4	D	1500	5AD	O3'-C3'-C2'	4.40	126.05	111.82
3	C	1801	B12	C2-C1-C19	4.37	125.49	118.60
3	A	1801	B12	C26-C2-C1	4.34	116.78	110.01
4	B	1500	5AD	O2'-C2'-C1'	4.28	126.65	110.85
3	D	1801	B12	C55-C17-C16	-4.26	108.23	116.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1801	B12	C20-C1-C19	-4.25	105.26	109.36
3	B	1801	B12	C19-C1-N21	4.21	106.47	102.16
3	C	1801	B12	C19-C1-N21	4.13	106.40	102.16
4	D	1500	5AD	O2'-C2'-C1'	4.13	126.11	110.85
3	D	1801	B12	C30-C3-C2	-4.08	110.45	119.09
4	B	1500	5AD	O3'-C3'-C2'	4.04	124.89	111.82
3	C	1801	B12	C15-C14-N23	-3.99	121.39	126.26
3	D	1801	B12	C15-C14-N23	-3.95	121.43	126.26
3	B	1801	B12	C47-C12-C11	3.88	124.03	110.08
3	B	1801	B12	C15-C14-N23	-3.88	121.53	126.26
3	C	1801	B12	C2-C1-N21	3.75	107.00	101.77
4	A	1500	5AD	O2'-C2'-C1'	3.75	124.71	110.85
3	D	1801	B12	C13-C14-N23	3.73	114.18	109.10
3	A	1801	B12	C55-C17-C16	-3.70	109.33	116.65
3	C	1801	B12	C13-C14-N23	3.69	114.13	109.10
3	D	1801	B12	C2-C1-N21	3.53	106.69	101.77
5	B	767	Z97	C5-C6-N1	-3.53	117.94	123.82
3	C	1801	B12	C25-C2-C1	-3.50	108.51	113.78
3	D	1801	B12	C19-C1-N21	3.48	105.73	102.16
5	B	767	Z97	OXT-C-O	-3.46	116.23	124.09
3	A	1801	B12	C9-C10-C11	-3.44	121.00	125.97
4	B	1500	5AD	O4'-C4'-C5'	3.42	127.08	110.29
4	C	1500	5AD	O4'-C4'-C5'	3.41	127.01	110.29
3	D	1801	B12	C26-C2-C1	3.37	115.26	110.01
4	A	1500	5AD	O4'-C4'-C5'	3.33	126.61	110.29
3	B	1801	B12	C2-C1-N21	3.29	106.36	101.77
3	A	1801	B12	C30-C3-C2	-3.29	112.13	119.09
3	D	1801	B12	C25-C2-C1	-3.27	108.85	113.78
3	C	1801	B12	C18-C60-C61	-3.26	105.83	113.97
3	B	1801	B12	C26-C2-C1	3.21	115.02	110.01
3	A	1801	B12	C2-C1-N21	3.21	106.24	101.77
4	D	1500	5AD	O4'-C4'-C5'	3.20	126.00	110.29
3	D	1801	B12	C12-C13-C14	3.11	107.46	102.26
3	B	1801	B12	C2-C26-C27	-3.09	106.54	115.22
3	A	1801	B12	C2-C1-C19	3.08	123.45	118.60
3	A	1801	B12	C19-C1-N21	3.05	105.29	102.16
3	B	1801	B12	C30-C3-C2	-3.02	112.69	119.09
3	B	1801	B12	C13-C14-N23	3.01	113.19	109.10
3	A	1801	B12	C12-C13-C14	2.99	107.25	102.26
3	B	1801	B12	C20-C1-C2	-2.93	108.39	113.28
3	B	1801	B12	C1-C2-C3	2.89	105.28	101.60
5	B	767	Z97	CD-NE-C4A	-2.83	110.21	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1801	B12	C47-C12-C11	2.78	120.09	110.08
3	B	1801	B12	C2-C1-C19	2.77	122.98	118.60
3	B	1801	B12	C1P-N59-C57	-2.77	116.65	122.69
4	D	1500	5AD	C3'-C2'-C1'	2.77	105.14	100.98
3	C	1801	B12	O6R-C4R-C5R	-2.76	103.24	109.21
3	B	1801	B12	C25-C2-C1	-2.76	109.62	113.78
3	B	1801	B12	C12-C13-C14	2.76	106.87	102.26
5	A	767	Z97	CD-NE-C4A	-2.75	110.45	118.90
3	A	1801	B12	C18-C60-C61	-2.74	107.12	113.97
3	A	1801	B12	C1-C2-C3	2.74	105.10	101.60
5	C	767	Z97	CD-NE-C4A	-2.71	110.59	118.90
3	D	1801	B12	C54-C17-C55	2.67	113.66	109.25
3	D	1801	B12	C46-C12-C11	2.63	119.55	110.08
3	A	1801	B12	C47-C12-C11	2.62	119.50	110.08
5	D	767	Z97	CD-NE-C4A	-2.62	110.86	118.90
5	D	767	Z97	CG-CD-NE	2.57	117.23	110.93
3	D	1801	B12	C7-C6-N22	2.54	112.57	107.94
3	A	1801	B12	C20-C1-C2	-2.53	109.07	113.28
5	A	767	Z97	OP4-P-OP1	2.52	113.55	106.47
3	C	1801	B12	C30-C3-C2	-2.51	113.78	119.09
3	A	1801	B12	C3R-C2R-C1R	2.51	105.45	99.89
5	A	767	Z97	C5-C6-N1	-2.49	119.67	123.82
5	C	767	Z97	C5-C6-N1	-2.45	119.73	123.82
5	C	767	Z97	C2A-C2-N1	2.45	122.45	117.67
3	C	1801	B12	C20-C1-N21	-2.44	106.27	110.27
3	A	1801	B12	C7-C6-N22	2.41	112.35	107.94
3	A	1801	B12	C54-C17-C18	-2.40	109.44	112.98
3	D	1801	B12	C30-C31-C32	-2.40	104.47	112.59
3	C	1801	B12	C20-C1-C2	-2.39	109.29	113.28
3	D	1801	B12	C18-C60-C61	-2.39	108.00	113.97
5	B	767	Z97	C6-N1-C2	2.38	123.57	119.17
5	A	767	Z97	CG-CD-NE	2.36	116.71	110.93
3	B	1801	B12	C3R-C2R-C1R	2.35	105.09	99.89
3	D	1801	B12	C20-C1-C2	-2.34	109.38	113.28
5	A	767	Z97	C5-C4-C4A	-2.33	117.72	121.56
4	A	1500	5AD	C1'-N9-C4	-2.33	122.55	126.64
3	C	1801	B12	C12-C13-C14	2.33	106.16	102.26
5	D	767	Z97	CB-CA-N	2.32	116.26	110.17
3	A	1801	B12	C18-C17-C16	2.32	103.49	100.67
3	D	1801	B12	C9-C10-C11	-2.31	122.63	125.97
3	C	1801	B12	C46-C12-C11	2.31	118.38	110.08
3	A	1801	B12	C46-C12-C11	2.30	118.36	110.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1500	5AD	C4-C5-N7	-2.30	107.00	109.40
3	D	1801	B12	C18-C17-C16	2.29	103.45	100.67
3	D	1801	B12	C56-C55-C17	-2.25	111.17	115.52
4	A	1500	5AD	O4'-C1'-C2'	-2.25	103.64	106.93
5	C	767	Z97	OXT-C-O	-2.24	119.01	124.09
3	C	1801	B12	C48-C13-C14	2.22	114.03	108.49
5	C	767	Z97	C2A-C2-C3	-2.22	118.14	120.89
5	A	767	Z97	OXT-C-CA	2.20	120.88	113.38
3	C	1801	B12	C2-C26-C27	-2.20	109.04	115.22
3	C	1801	B12	C54-C17-C55	2.18	112.84	109.25
4	B	1500	5AD	O4'-C1'-C2'	-2.17	103.75	106.93
3	D	1801	B12	C1-C2-C3	2.17	104.37	101.60
3	D	1801	B12	C47-C12-C11	2.16	117.84	110.08
3	A	1801	B12	C60-C18-C17	-2.16	110.52	115.74
4	A	1500	5AD	C4-C5-N7	-2.15	107.16	109.40
5	C	767	Z97	CG-CD-NE	2.14	116.19	110.93
5	D	767	Z97	C5-C6-N1	-2.14	120.25	123.82
3	C	1801	B12	C7-C6-N22	2.14	111.84	107.94
5	C	767	Z97	CB-CA-N	2.08	115.61	110.17
3	D	1801	B12	C7-C6-C5	-2.07	124.82	128.07
3	B	1801	B12	C18-C17-C16	2.05	103.16	100.67
3	A	1801	B12	C25-C2-C1	-2.04	110.70	113.78
3	A	1801	B12	C7-C6-C5	-2.04	124.86	128.07
3	C	1801	B12	C2P-C1P-N59	-2.01	109.97	112.93

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1801	B12	C19
3	B	1801	B12	C19
3	C	1801	B12	C19
3	D	1801	B12	C19
4	A	1500	5AD	C4'
4	A	1500	5AD	C3'
4	A	1500	5AD	C2'
4	B	1500	5AD	C4'
4	B	1500	5AD	C2'
4	C	1500	5AD	C4'
4	C	1500	5AD	C3'
4	D	1500	5AD	C4'
4	D	1500	5AD	C3'
4	D	1500	5AD	C2'

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C2-C3-C30-C31
3	A	1801	B12	C14-C13-C48-C49
3	A	1801	B12	C16-C17-C55-C56
3	A	1801	B12	C54-C17-C55-C56
3	A	1801	B12	C18-C17-C55-C56
3	A	1801	B12	C56-C57-N59-C1P
3	A	1801	B12	C1P-C2P-O3-P
3	B	1801	B12	C42-C41-C8-C9
3	B	1801	B12	C16-C17-C55-C56
3	B	1801	B12	C54-C17-C55-C56
3	B	1801	B12	C18-C17-C55-C56
3	C	1801	B12	C16-C17-C55-C56
3	C	1801	B12	C54-C17-C55-C56
3	C	1801	B12	C18-C17-C55-C56
3	D	1801	B12	C16-C17-C55-C56
3	D	1801	B12	C54-C17-C55-C56
3	D	1801	B12	C18-C17-C55-C56
3	D	1801	B12	C3P-C2P-O3-P
5	B	767	Z97	C5A-OP4-P-OP2
5	B	767	Z97	C5A-OP4-P-OP3
5	B	767	Z97	N-CA-CB-CG
5	C	767	Z97	C5A-OP4-P-OP1
3	A	1801	B12	O58-C57-N59-C1P
3	D	1801	B12	O6R-C4R-C5R-O8R
3	D	1801	B12	C3R-C4R-C5R-O8R
3	A	1801	B12	C12-C13-C48-C49
3	B	1801	B12	C42-C41-C8-C7
3	A	1801	B12	C4-C3-C30-C31
5	A	767	Z97	OXT-C-CA-N
3	C	1801	B12	C7-C37-C38-N40
5	A	767	Z97	NE-CD-CG-CB
5	B	767	Z97	NE-CD-CG-CB
5	C	767	Z97	NE-CD-CG-CB
3	D	1801	B12	C2-C3-C30-C31
5	D	767	Z97	OXT-C-CA-CB
5	D	767	Z97	CG-CD-NE-C4A
3	A	1801	B12	C8-C41-C42-C43
3	B	1801	B12	C2-C26-C27-N29
3	C	1801	B12	C7-C37-C38-O39
5	D	767	Z97	O-C-CA-CB
5	D	767	Z97	CA-CB-CG-CD
5	D	767	Z97	NE-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C3P-C2P-O3-P
3	D	1801	B12	C1P-C2P-O3-P
3	C	1801	B12	O6R-C4R-C5R-O8R
3	B	1801	B12	C2-C26-C27-O28
3	B	1801	B12	C7-C37-C38-O39
3	B	1801	B12	C7-C37-C38-N40
3	D	1801	B12	C2-C26-C27-N29
5	C	767	Z97	CA-CB-CG-CD
3	D	1801	B12	O58-C57-N59-C1P
3	D	1801	B12	C18-C60-C61-O63
3	D	1801	B12	C18-C60-C61-N62
3	A	1801	B12	C42-C41-C8-C9
3	A	1801	B12	C13-C48-C49-C50
5	C	767	Z97	OXT-C-CA-N
3	D	1801	B12	C56-C57-N59-C1P
3	D	1801	B12	C38-C37-C7-C6
3	D	1801	B12	C2-C26-C27-O28
3	D	1801	B12	C4-C3-C30-C31
5	D	767	Z97	OXT-C-CA-N
5	A	767	Z97	O-C-CA-N
5	B	767	Z97	CA-CB-CG-CD
3	D	1801	B12	C2P-O3-P-O2
3	B	1801	B12	C14-C13-C48-C49
5	C	767	Z97	C5A-OP4-P-OP2
3	A	1801	B12	C41-C42-C43-N45
3	D	1801	B12	C38-C37-C7-C8
5	A	767	Z97	O-C-CA-CB
3	A	1801	B12	C41-C42-C43-O44
3	B	1801	B12	C3-C2-C26-C27
3	D	1801	B12	C3-C2-C26-C27
5	A	767	Z97	OXT-C-CA-CB
5	D	767	Z97	C5A-OP4-P-OP1
5	B	767	Z97	OXT-C-CA-CB
5	C	767	Z97	O-C-CA-CB
5	D	767	Z97	O-C-CA-N
5	C	767	Z97	OXT-C-CA-CB
5	D	767	Z97	C5A-OP4-P-OP2
3	D	1801	B12	C25-C2-C26-C27
3	A	1801	B12	C7-C37-C38-O39
3	A	1801	B12	C19-C18-C60-C61
3	C	1801	B12	C19-C18-C60-C61
5	C	767	Z97	C3-C4-C4A-NE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1801	B12	C2P-O3-P-O2
3	A	1801	B12	C2P-C1P-N59-C57
3	A	1801	B12	C7-C37-C38-N40
5	B	767	Z97	OXT-C-CA-N
5	A	767	Z97	C4-C4A-NE-CD
3	A	1801	B12	C17-C18-C60-C61

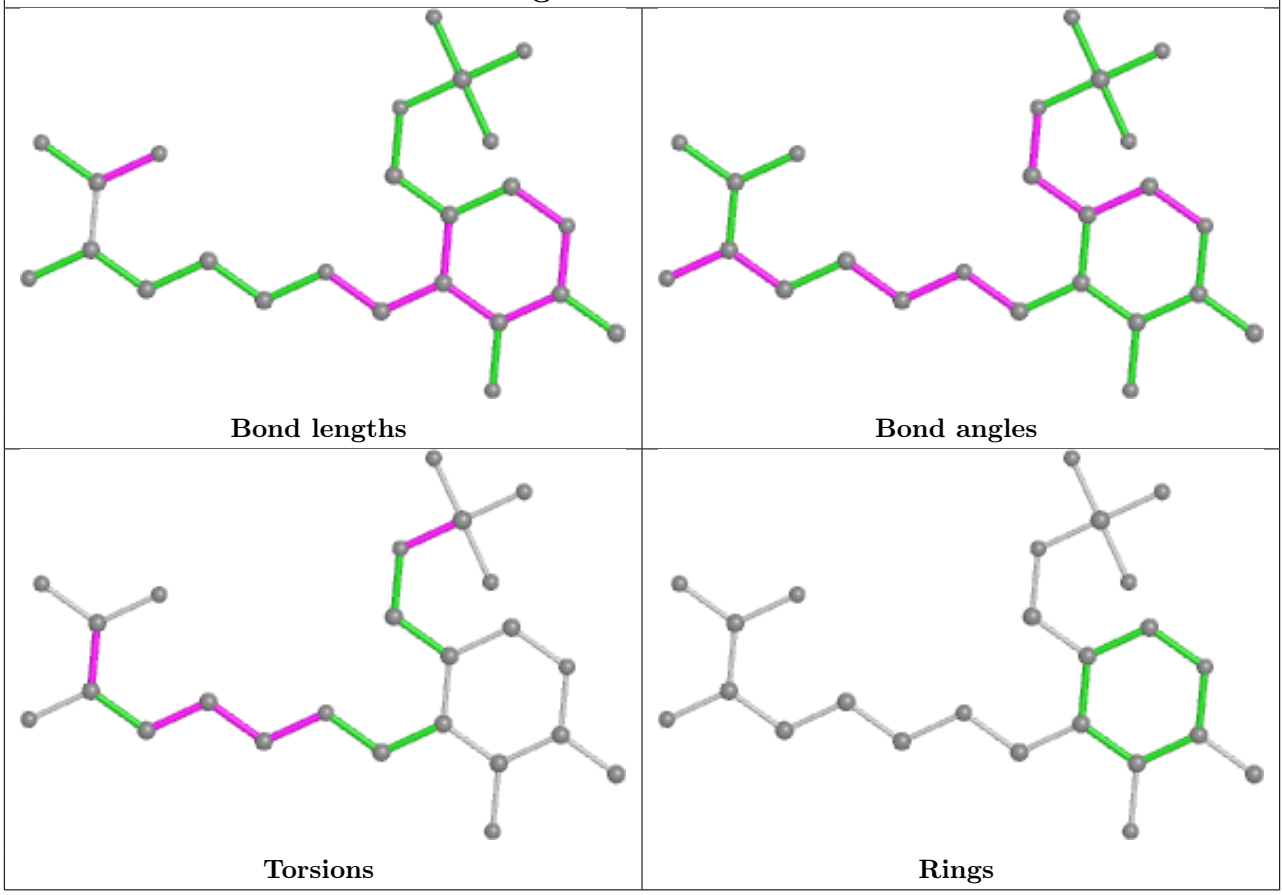
There are no ring outliers.

12 monomers are involved in 114 short contacts:

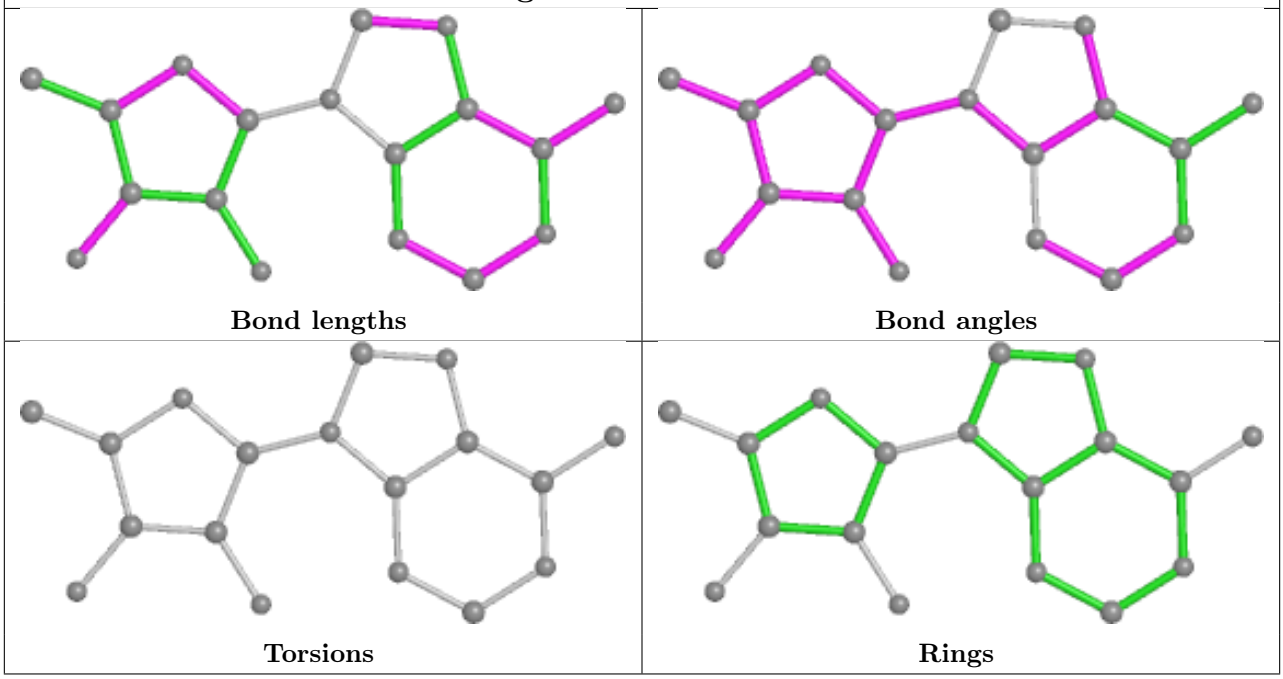
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	767	Z97	7	0
4	A	1500	5AD	3	0
3	A	1801	B12	19	0
5	C	767	Z97	3	0
3	C	1801	B12	24	0
4	C	1500	5AD	3	0
4	B	1500	5AD	3	0
4	D	1500	5AD	3	0
5	A	767	Z97	3	0
3	B	1801	B12	24	0
5	B	767	Z97	3	0
3	D	1801	B12	31	0

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.

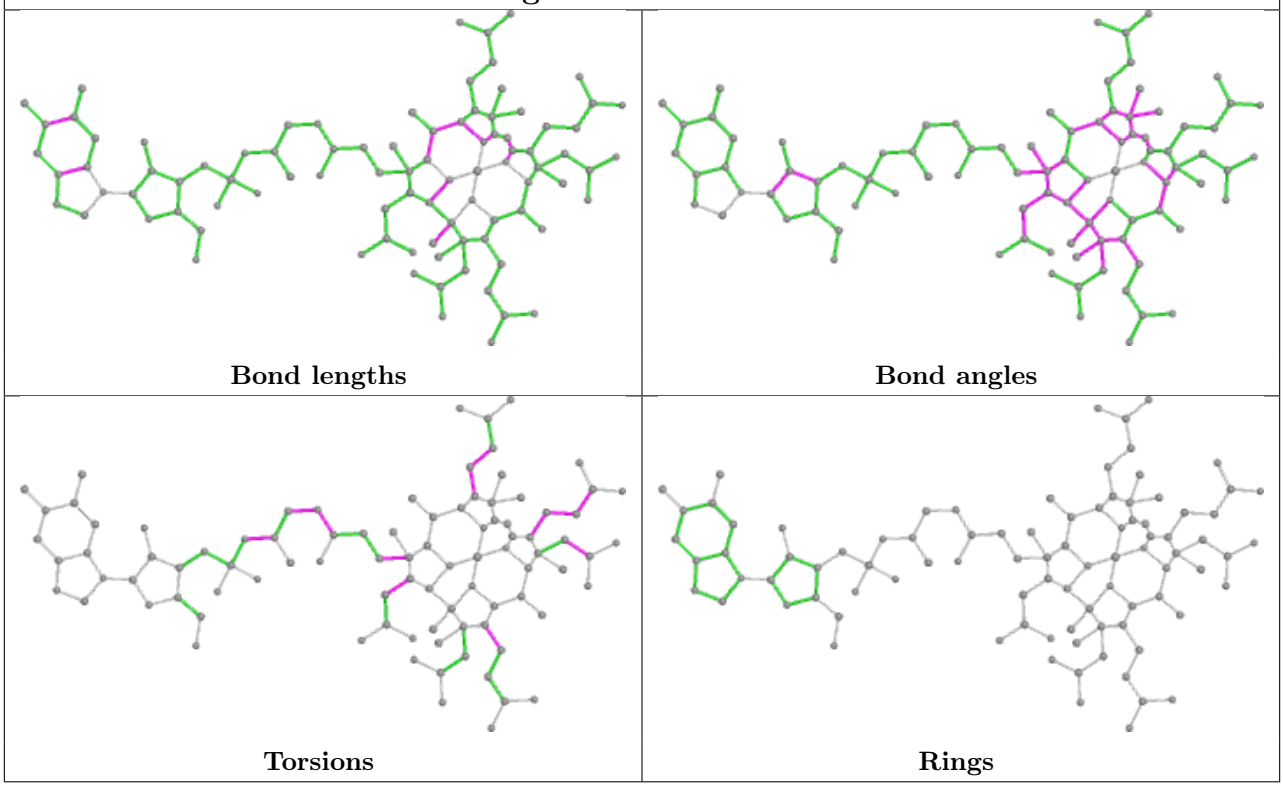
Ligand Z97 D 767



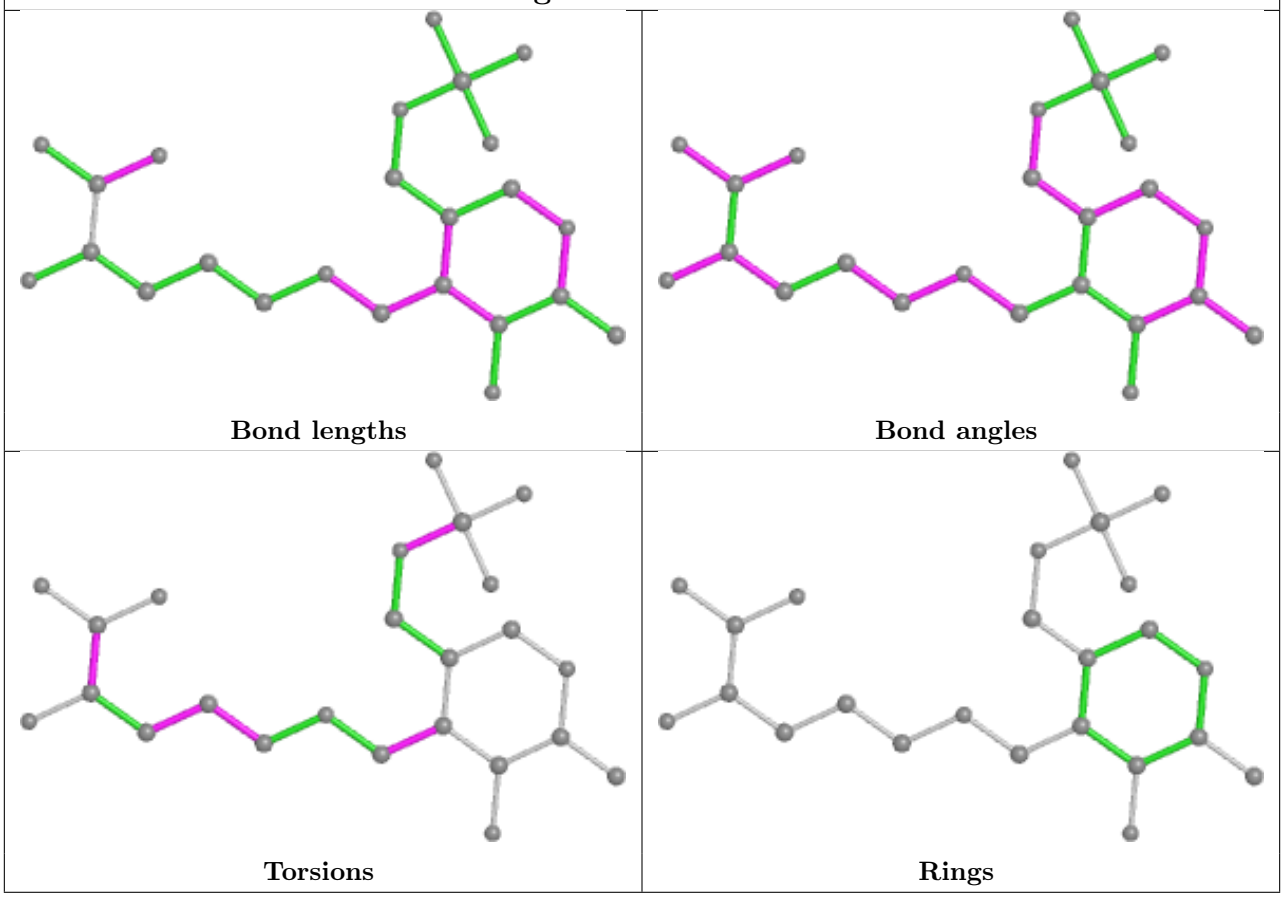
Ligand 5AD A 1500



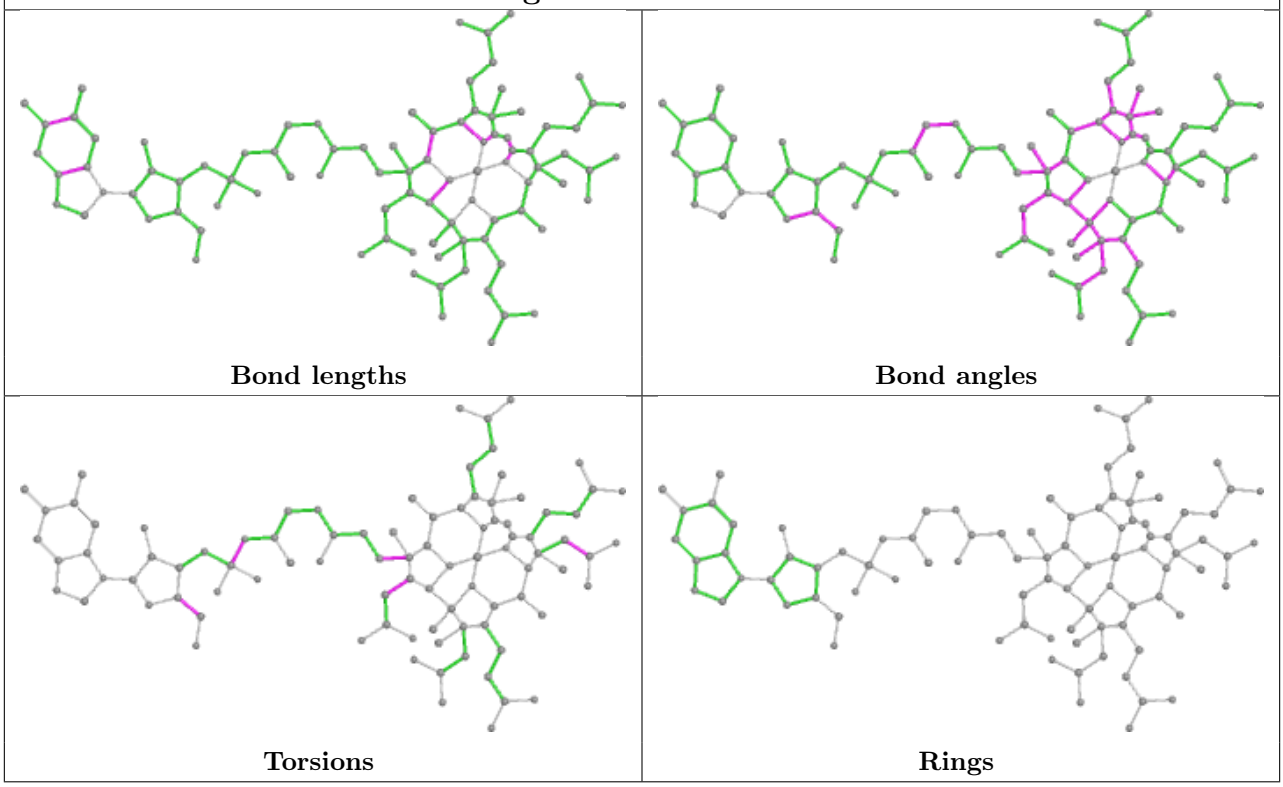
Ligand B12 A 1801



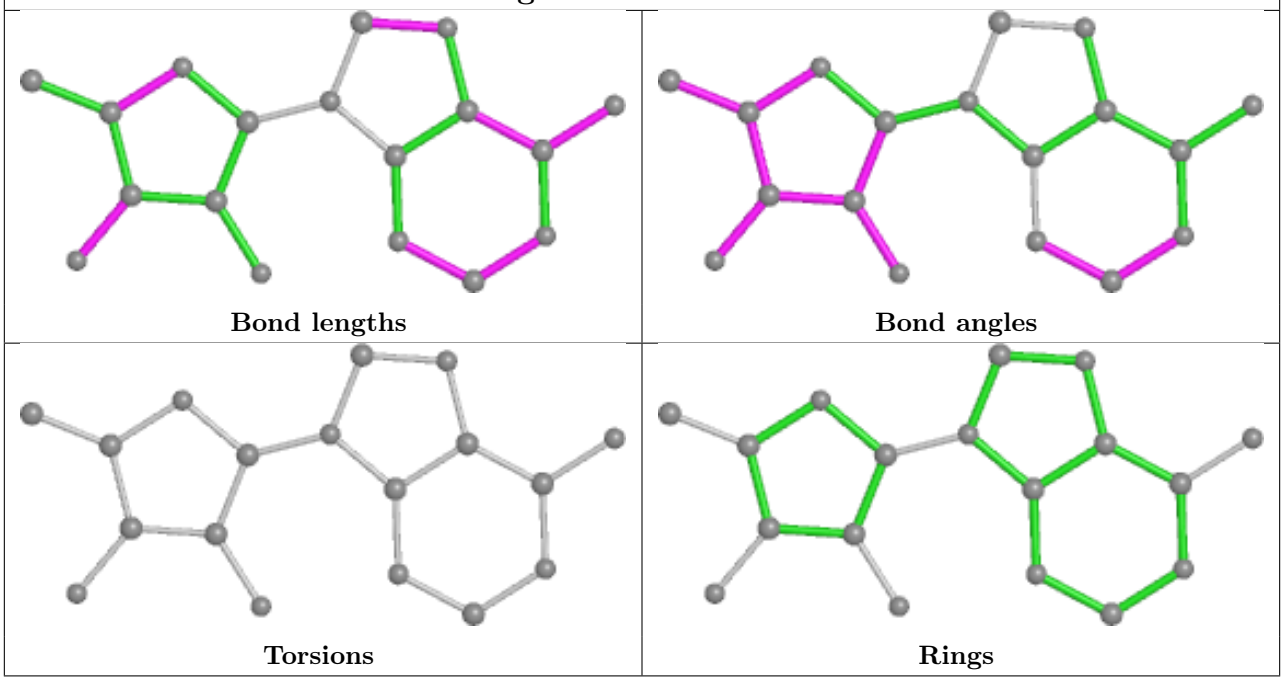
Ligand Z97 C 767



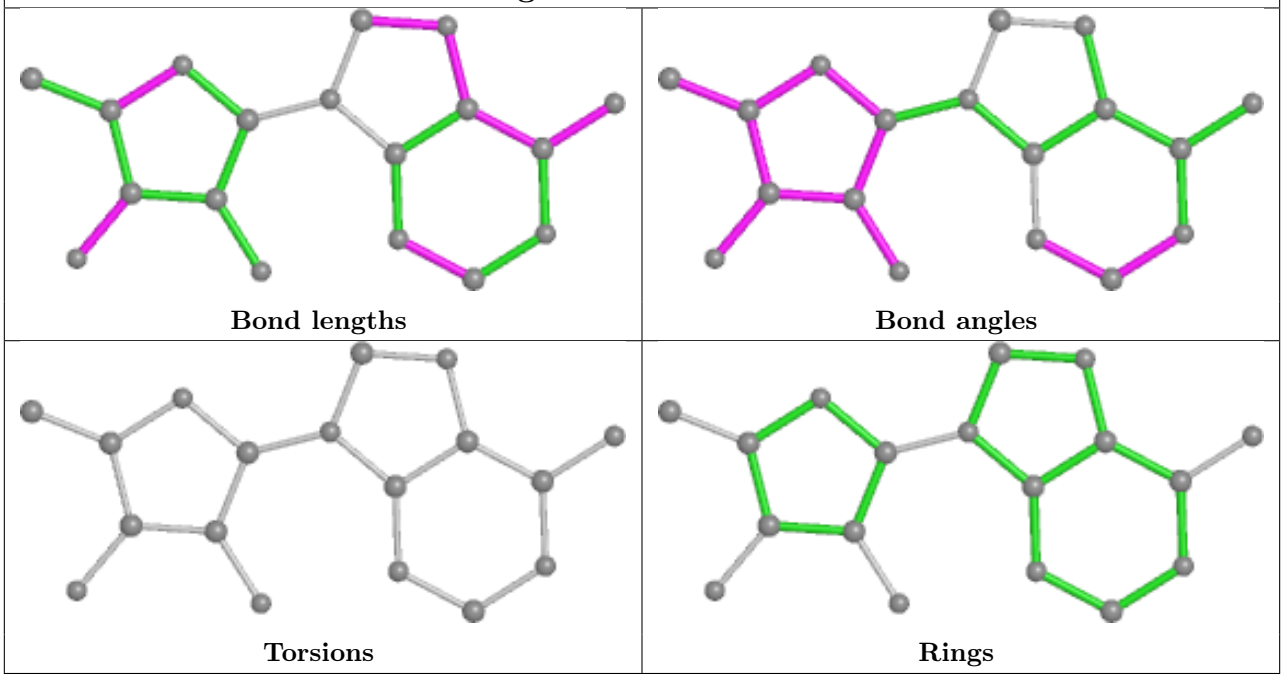
Ligand B12 C 1801



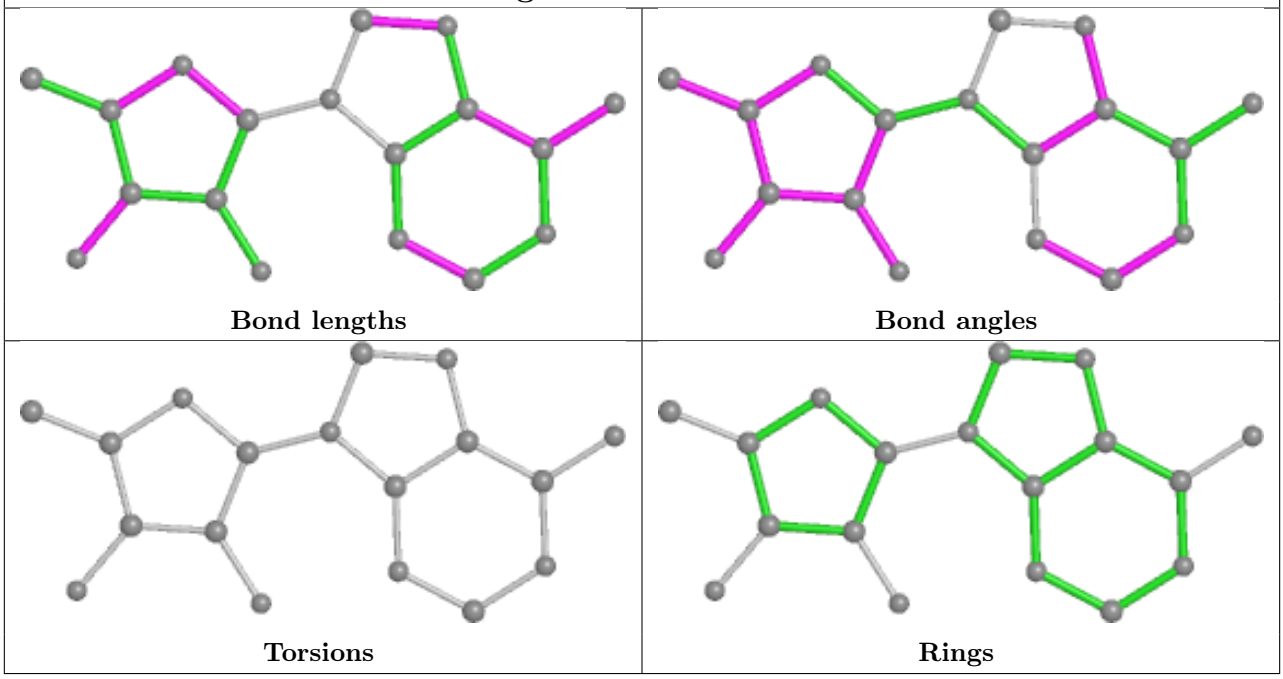
Ligand 5AD C 1500



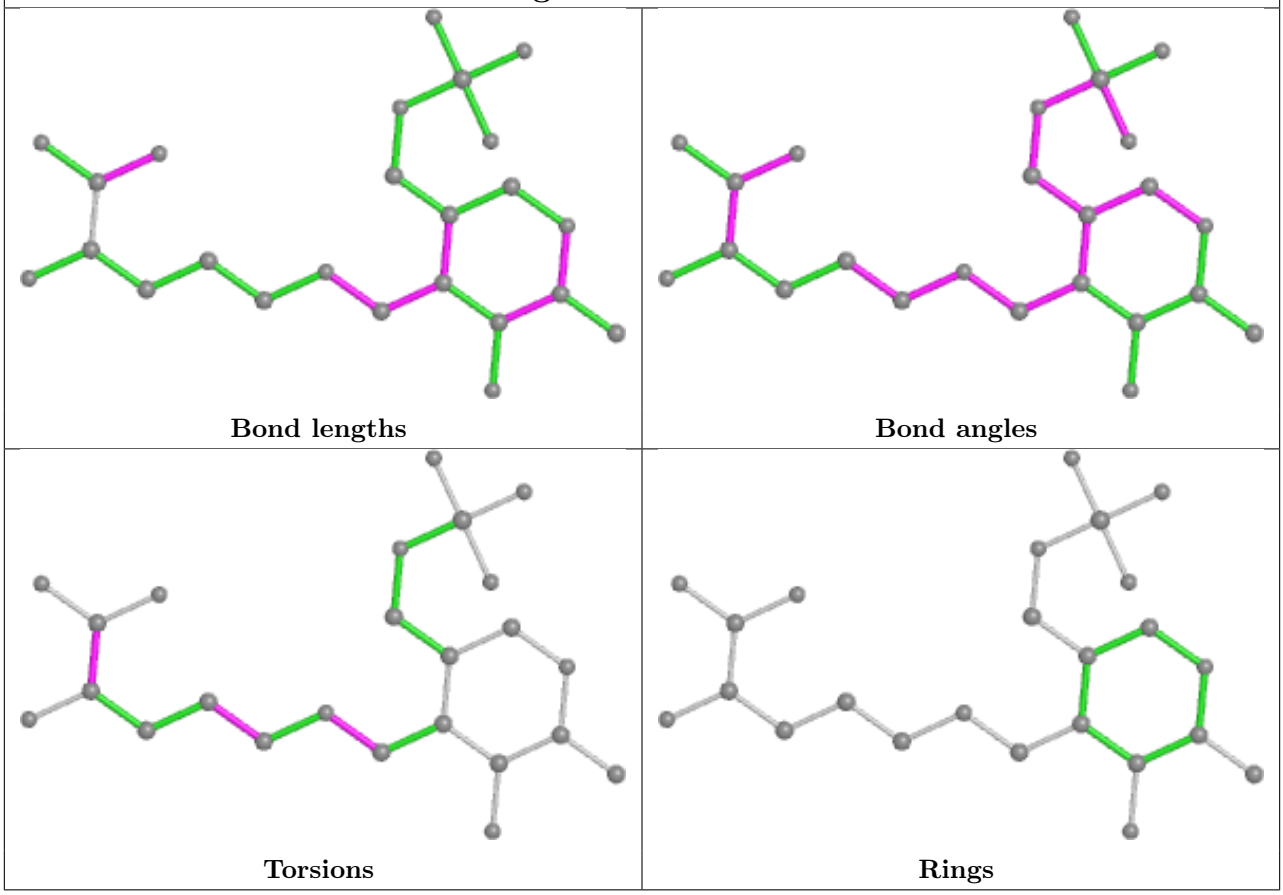
Ligand 5AD B 1500



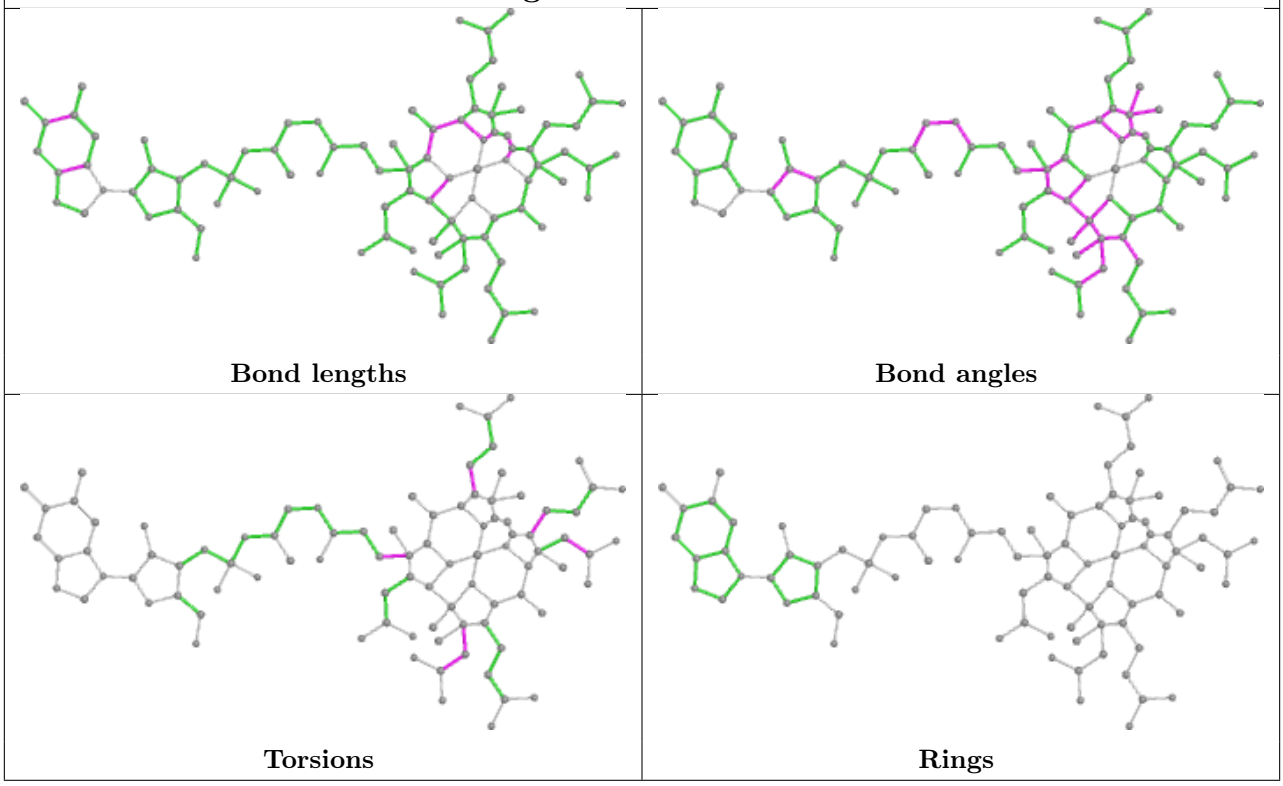
Ligand 5AD D 1500



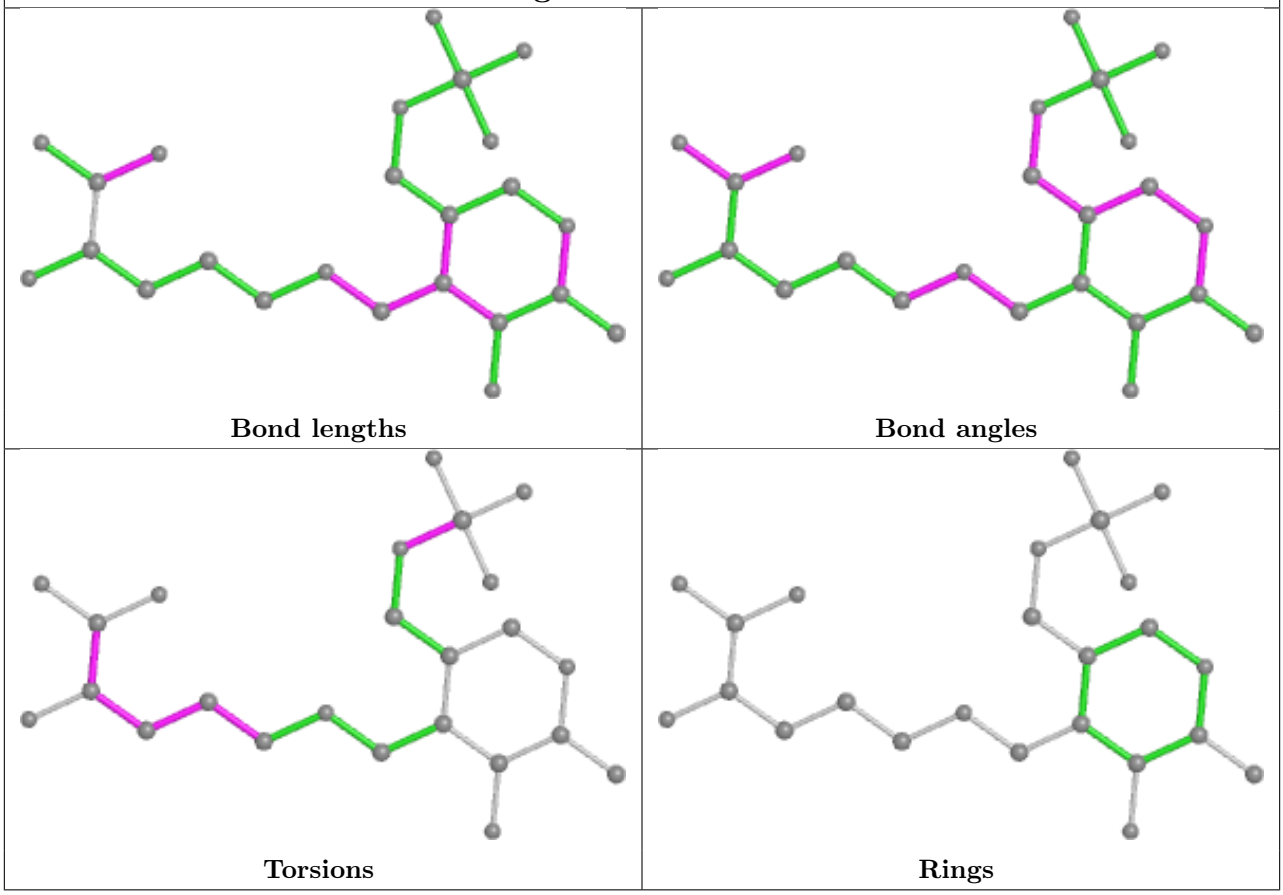
Ligand Z97 A 767



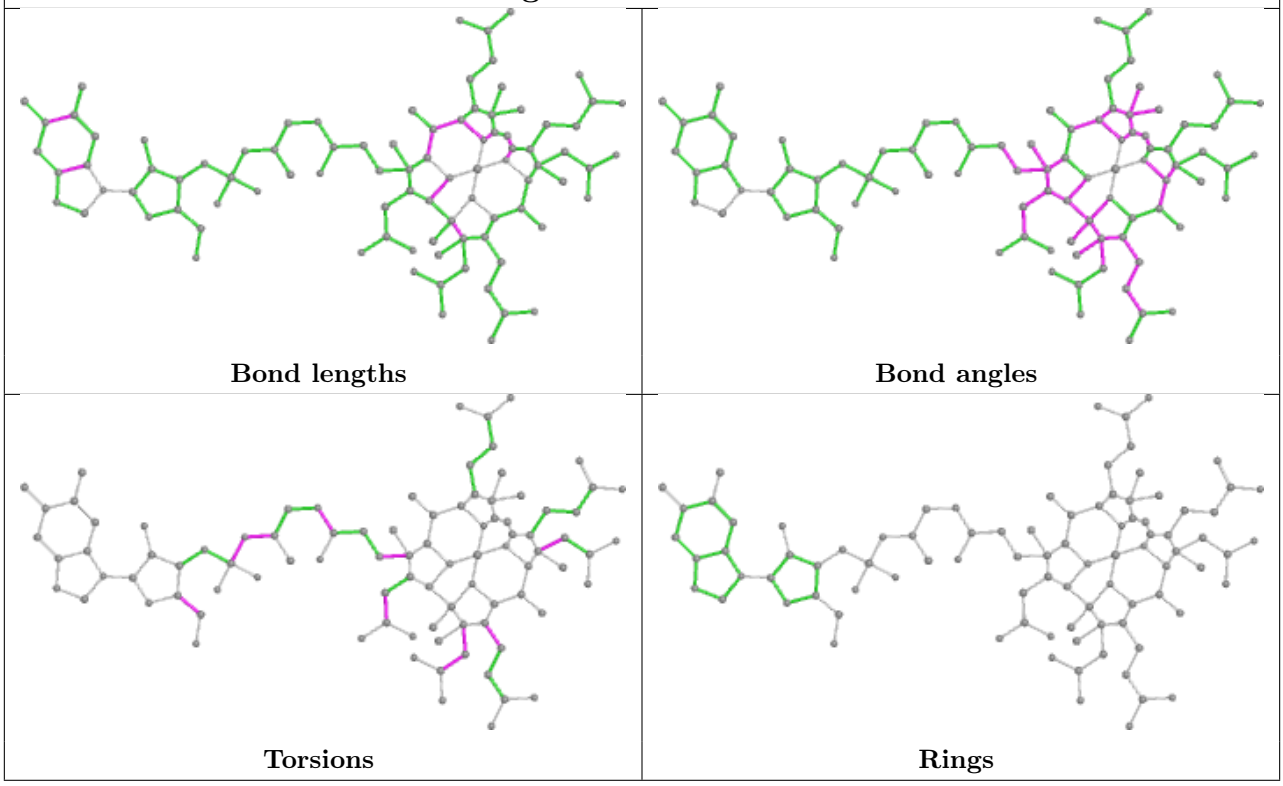
Ligand B12 B 1801



Ligand Z97 B 767



Ligand B12 D 1801



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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

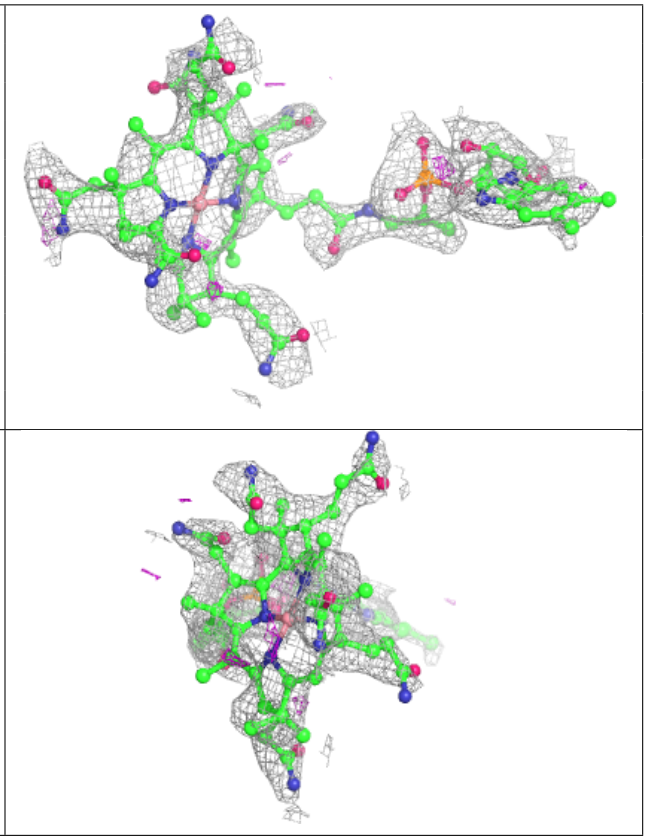
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

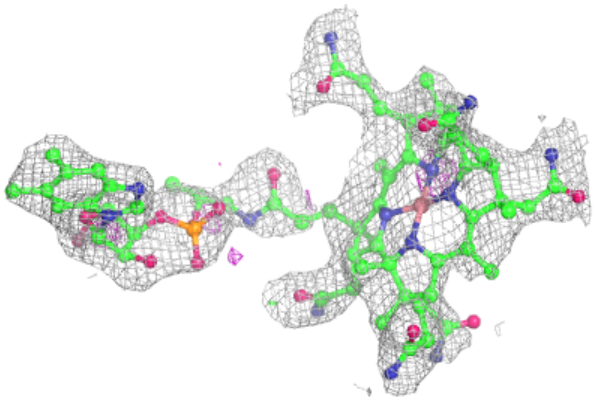
Electron density around B12 A 1801:

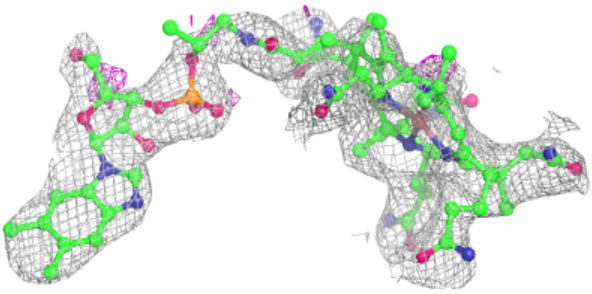
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

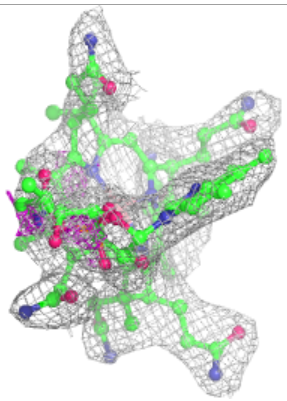


Electron density around B12 B 1801:

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

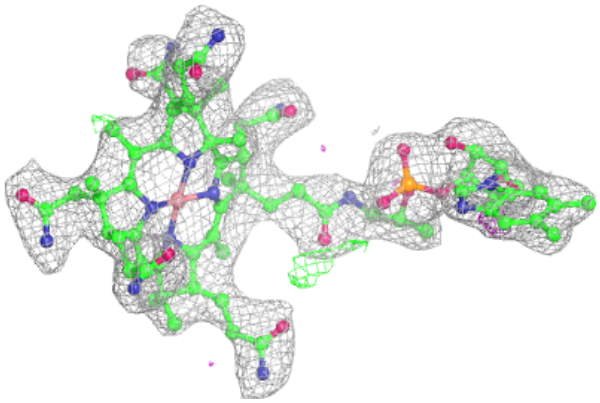


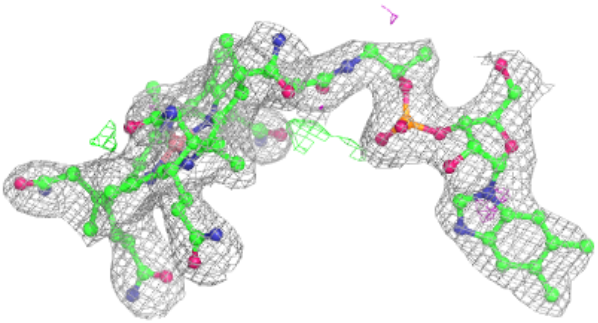


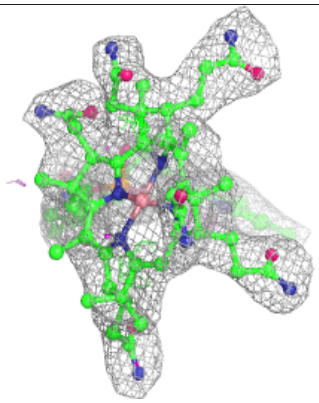


Electron density around B12 C 1801:

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

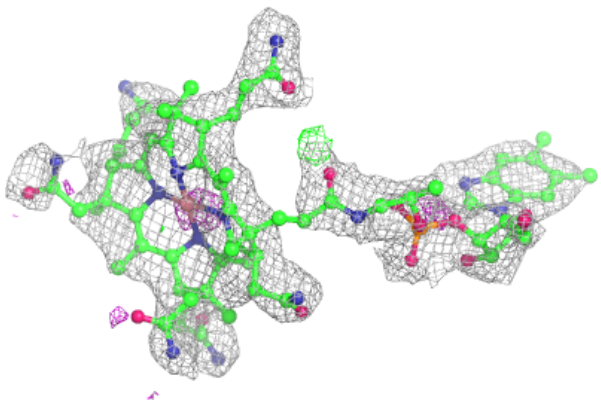


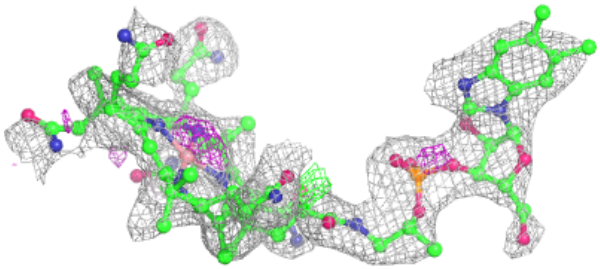


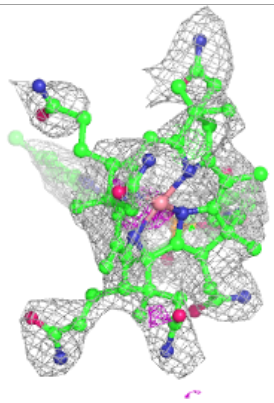


Electron density around B12 D 1801:

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

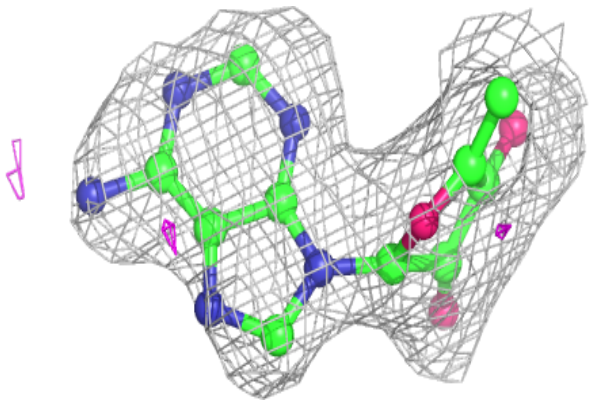


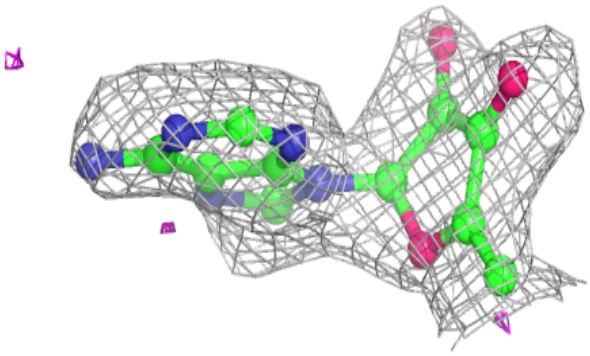


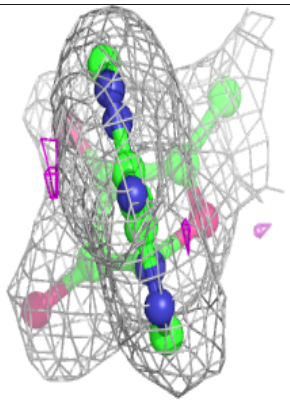


Electron density around 5AD A 1500:

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

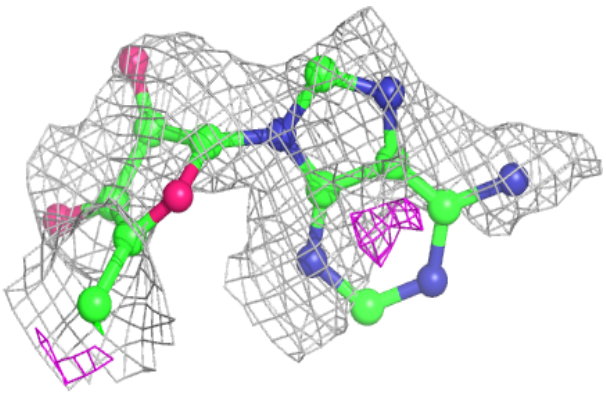


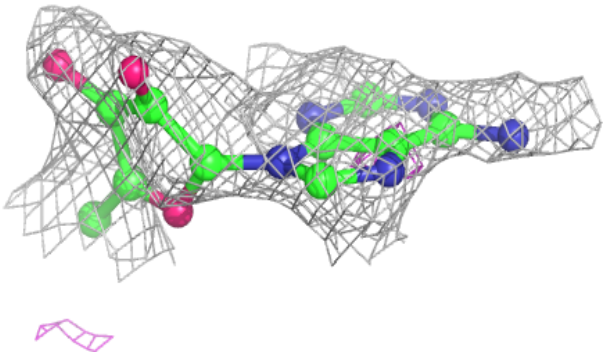


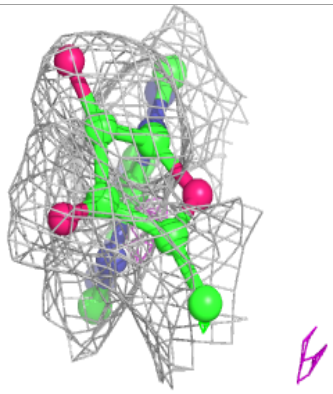


Electron density around 5AD B 1500:

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

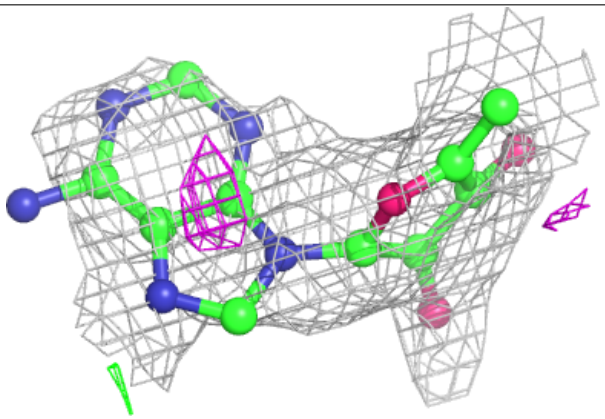


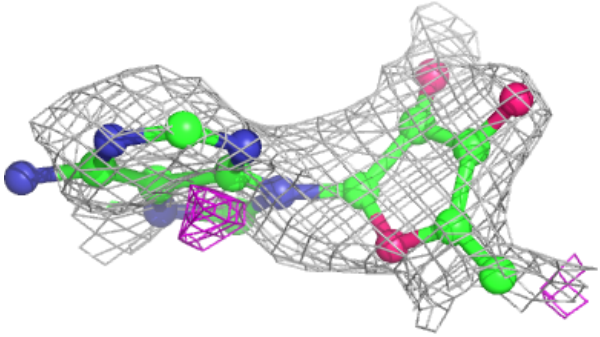


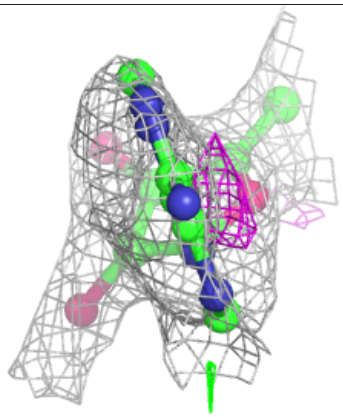


Electron density around 5AD C 1500:

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

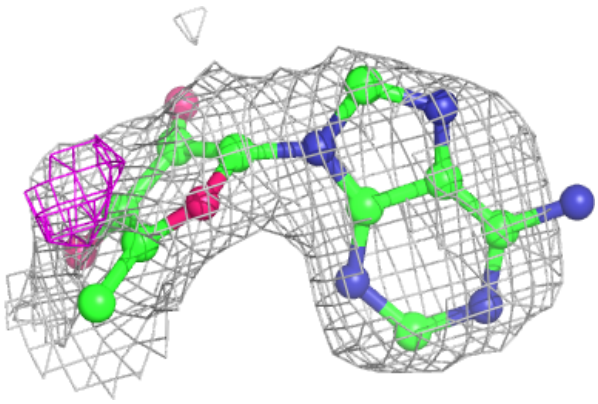


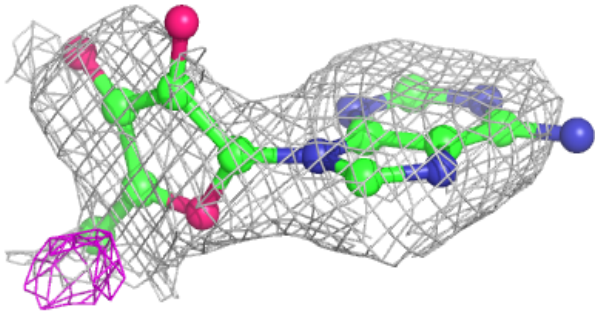


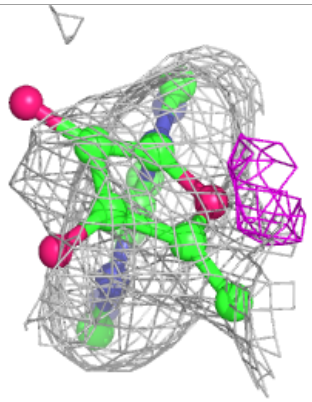


Electron density around 5AD D 1500:

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

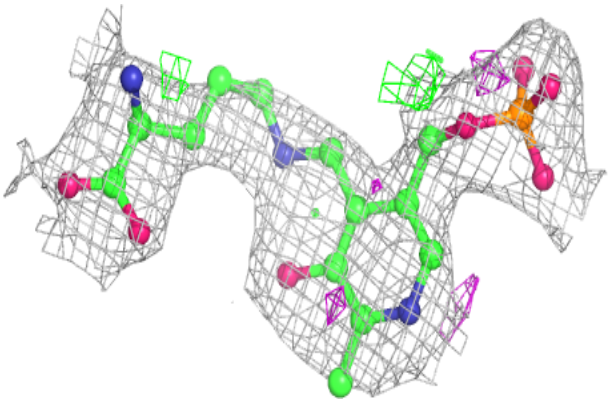


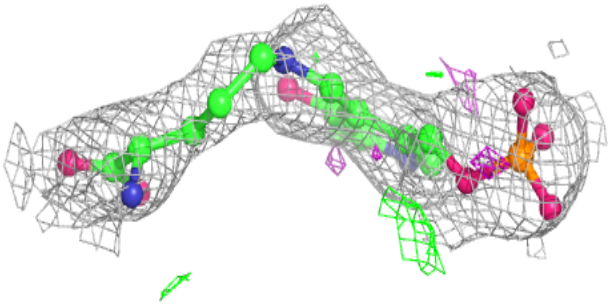


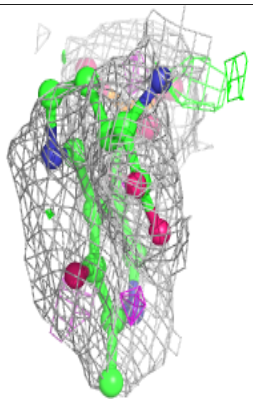


Electron density around Z97 A 767:

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

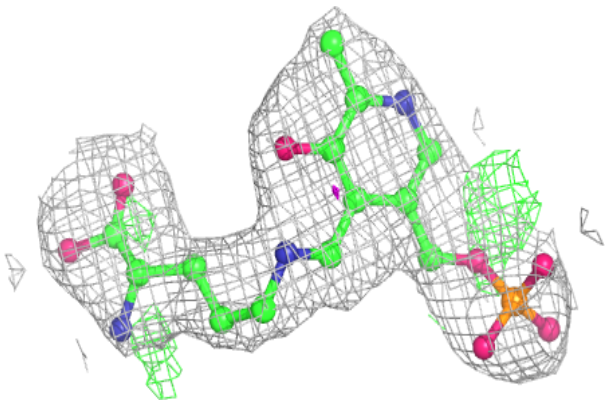


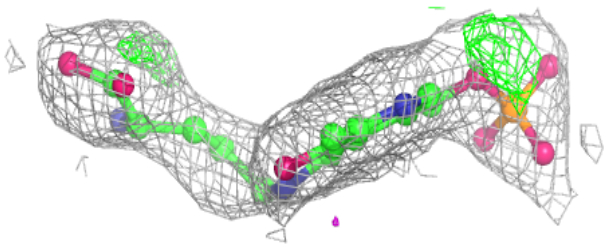


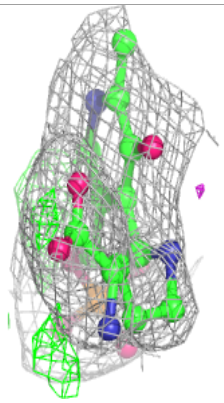


Electron density around Z97 B 767:

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

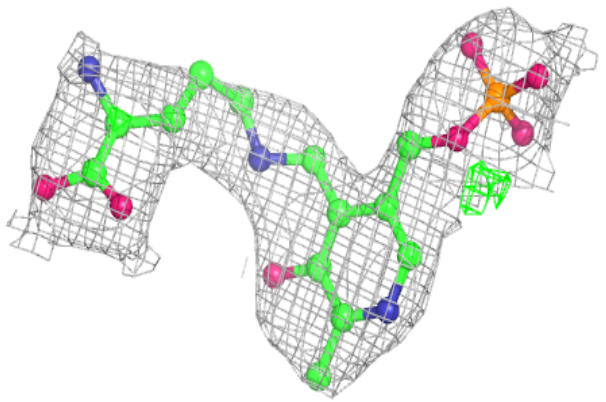


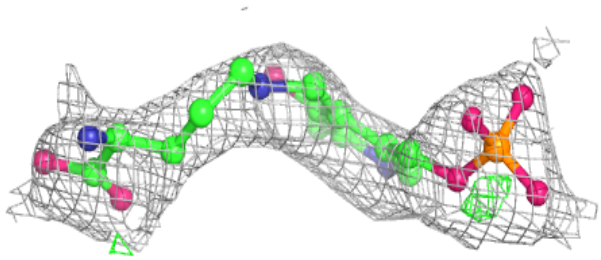


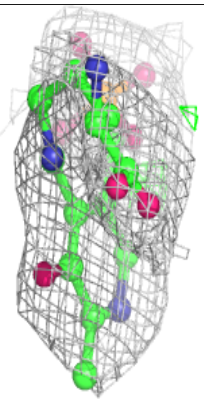


Electron density around Z97 C 767:

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

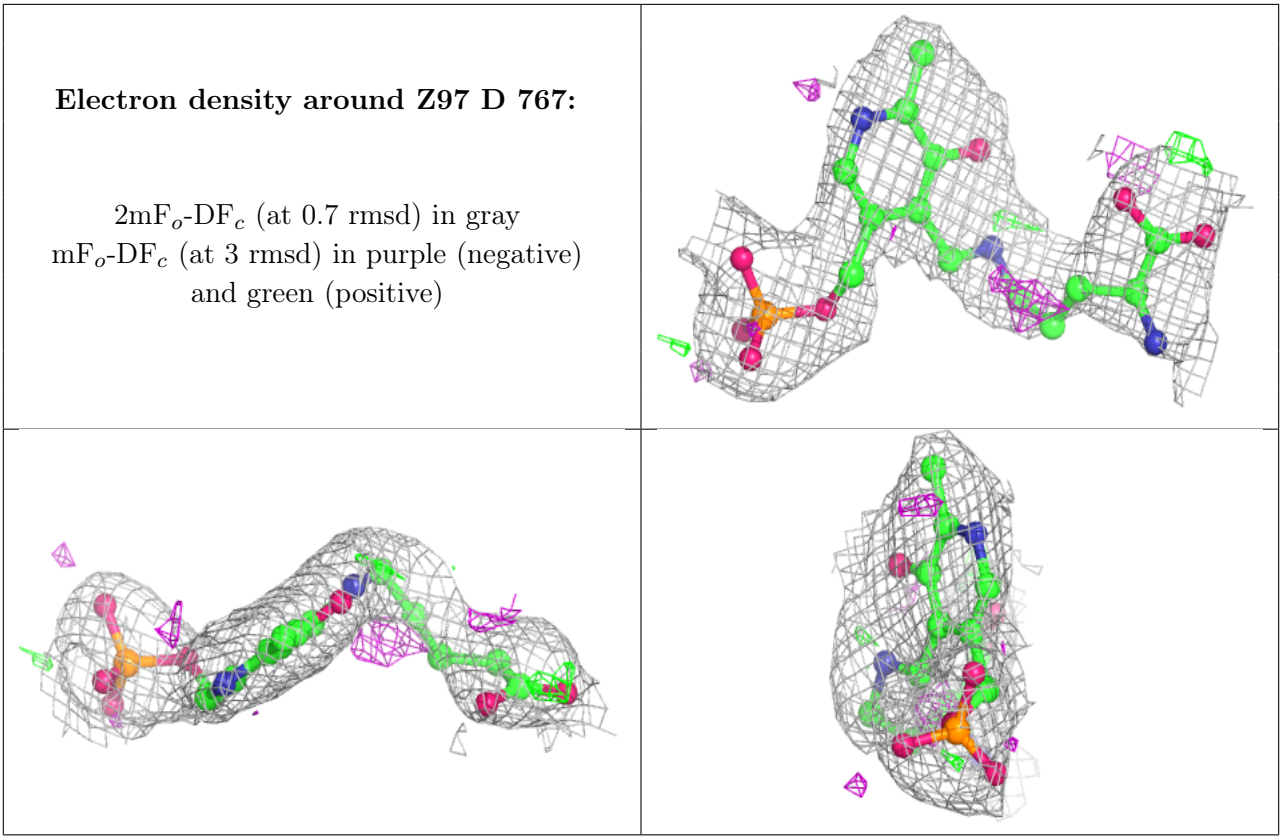






Electron density around Z97 D 767:

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



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.