



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 04:31 AM EST

PDB ID : 3KOY
Title : Crystal Structure of ornithine 4,5 aminomutase in complex with ornithine (Aerobic)
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-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

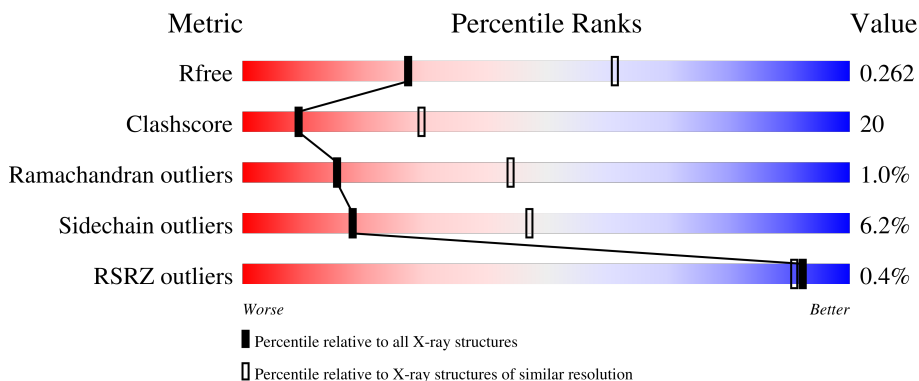
1 Overall quality at a glance

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)
RSRZ outliers	127900	3078 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	763	
1	B	763	
1	C	763	
1	D	763	
2	E	121	

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Mol	Chain	Length	Quality of chain
2	F	121	
2	G	121	
2	H	121	

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	-	X	-
3	B12	B	1801	X	-	X	-
3	B12	C	1801	X	-	X	-
3	B12	D	1801	X	-	X	-
5	5AD	A	1500	X	-	-	-
5	5AD	B	1500	X	-	-	-
5	5AD	C	1500	X	-	-	-
5	5AD	D	1500	X	-	-	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 26592 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	5634	3550	976	1075	33	0	0	0
1	B	728	5665	3574	983	1074	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

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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

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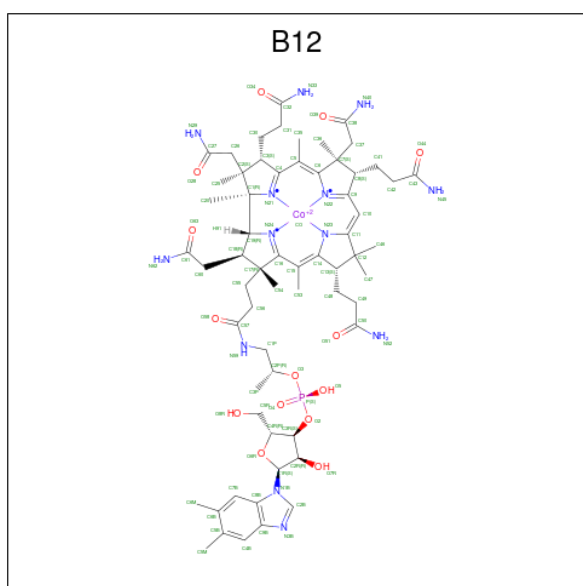
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Chain	Residue	Modelled	Actual	Comment	Reference
C	752	VAL	-	expression tag	UNP Q8VPJ5
C	753	ASP	-	expression tag	UNP Q8VPJ5
C	754	LYS	-	expression tag	UNP Q8VPJ5
C	755	LEU	-	expression tag	UNP Q8VPJ5
C	756	ALA	-	expression tag	UNP Q8VPJ5
C	757	ALA	-	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.

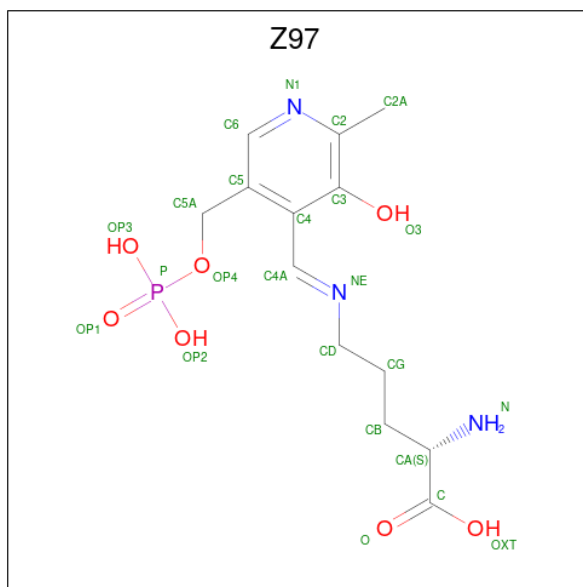
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	110	Total 860	C 541	N 153	O 162	S 4	0	0	0
2	F	110	Total 863	C 542	N 153	O 164	S 4	0	0	0
2	G	110	Total 860	C 541	N 153	O 162	S 4	0	0	0
2	H	110	Total 860	C 541	N 153	O 162	S 4	0	0	0

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



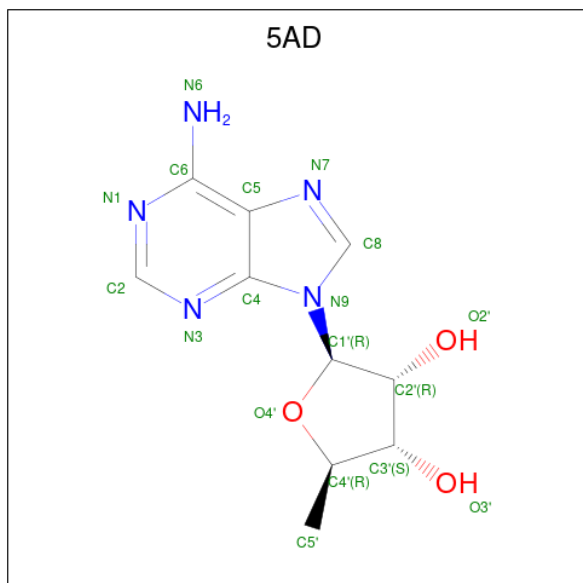
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
3	A	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	C	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	D	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

- Molecule 4 is (E)-N 5 -({3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methylidene)-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		
4	A	1	Total	C	N	O	P	0	0
			24	13	3	7	1		
4	B	1	Total	C	N	O	P	0	0
			24	13	3	7	1		
4	C	1	Total	C	N	O	P	0	0
			24	13	3	7	1		
4	D	1	Total	C	N	O	P	0	0
			24	13	3	7	1		

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

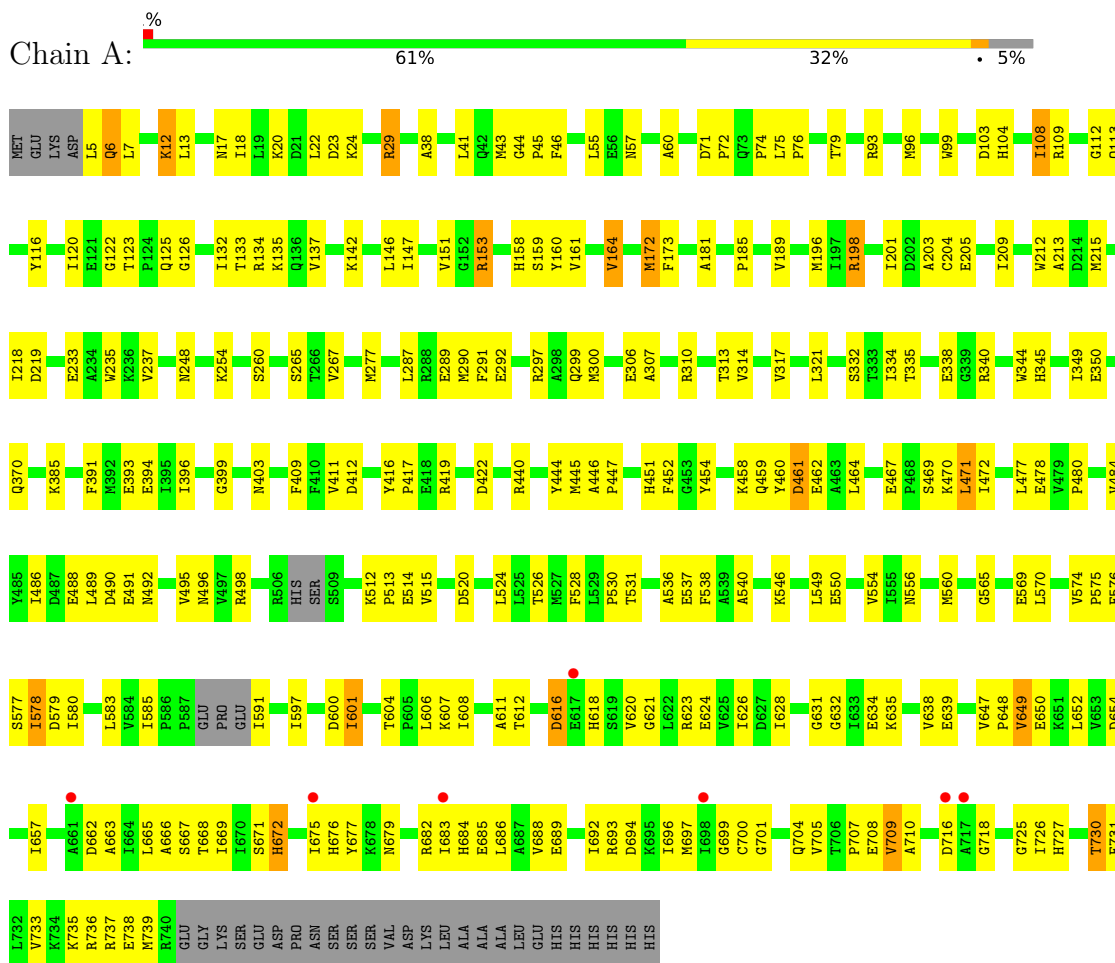


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	10	5	3		
5	B	1	Total	C	N	O	0	0
			18	10	5	3		
5	C	1	Total	C	N	O	0	0
			18	10	5	3		
5	D	1	Total	C	N	O	0	0
			18	10	5	3		

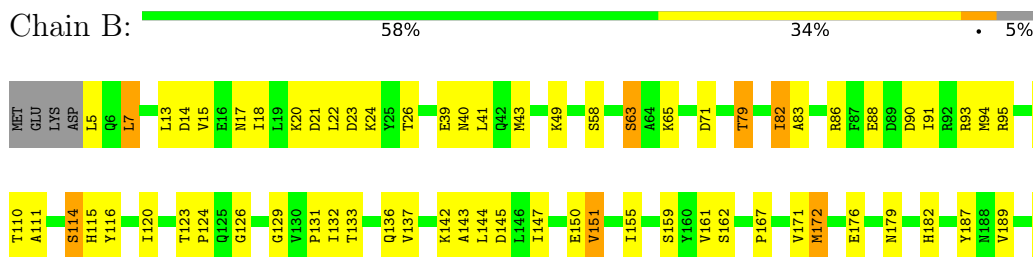
3 Residue-property plots i

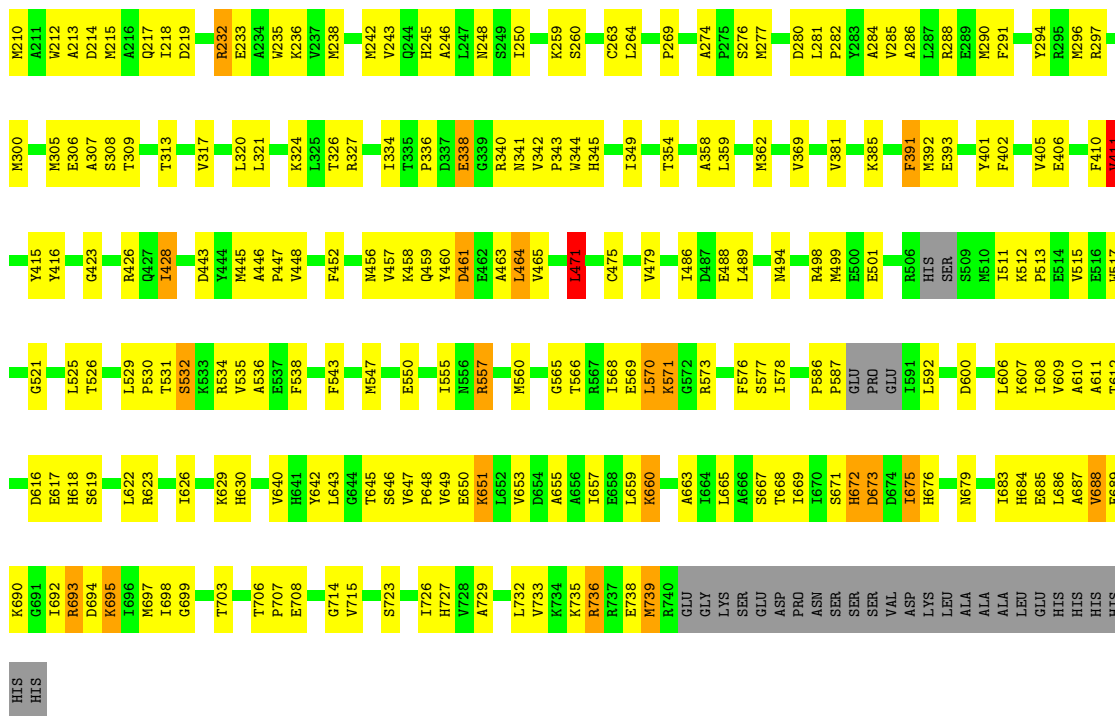
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: D-ornithine aminomutase E component



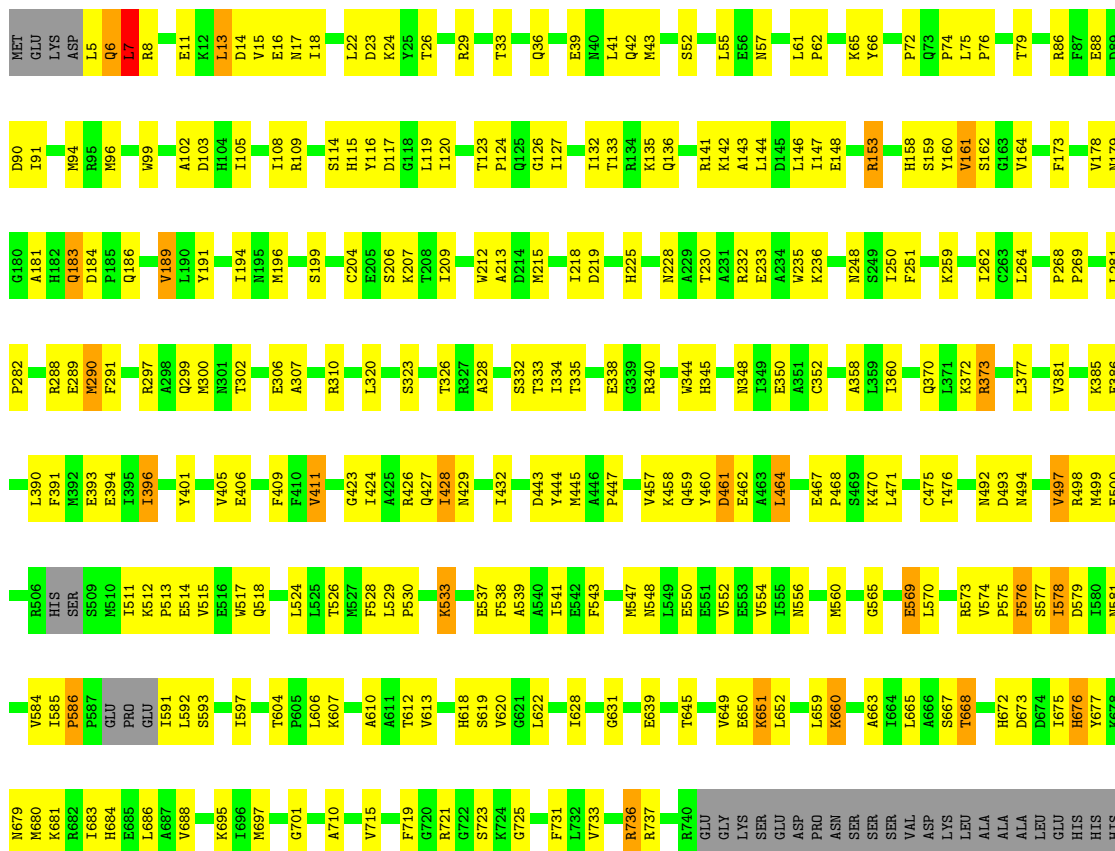
• Molecule 1: D-ornithine aminomutase E component





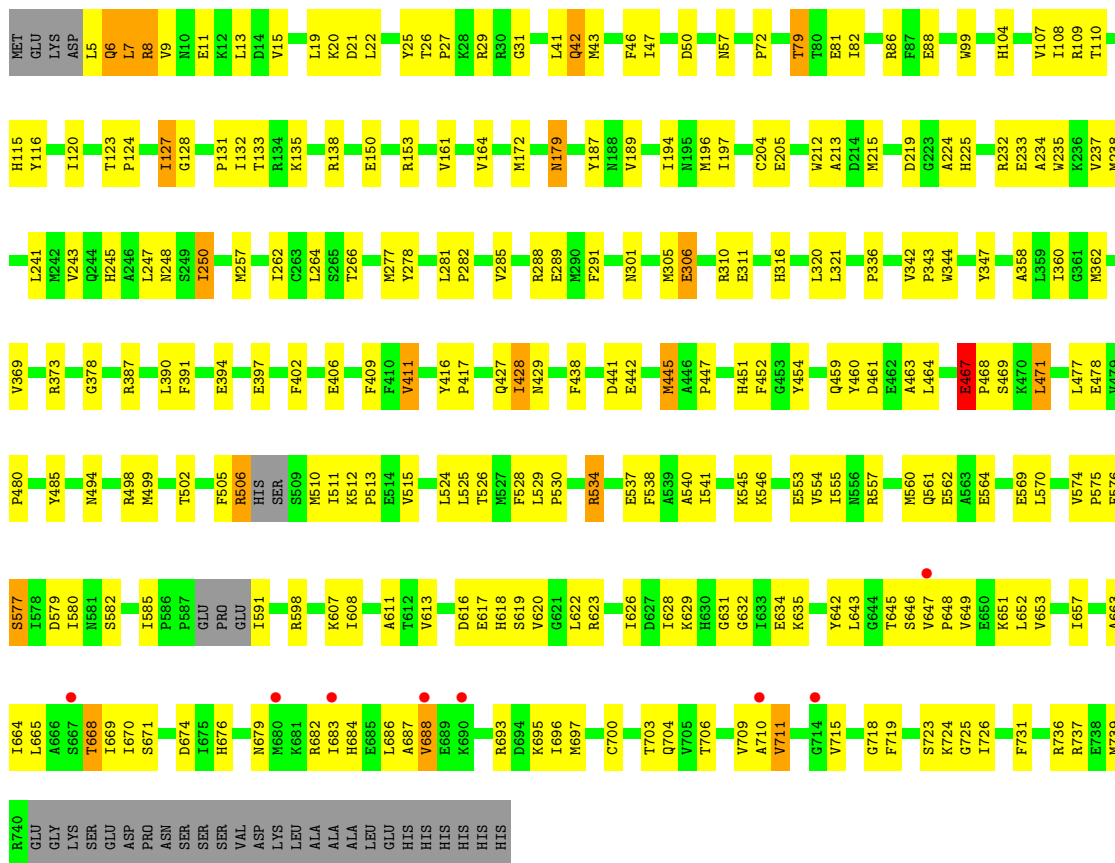
• Molecule 1: D-ornithine aminomutase E component

Chain C:



HIS
HIS
HIS

• Molecule 1: D-ornithine aminomutase E component

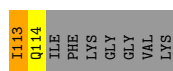


• Molecule 2: D-ornithine aminomutase S component



• Molecule 2: D-ornithine aminomutase S component





- Molecule 2: D-ornithine aminomutase S component

Chain G: 55% 32% 9%



- Molecule 2: D-ornithine aminomutase S component

Chain H: 60% 31% 9%



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 64.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (60.37-2.80) 93.8 (64.70-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.5_2, REFMAC 5.5.0066	Depositor
R, R_{free}	0.183 , 0.263 0.183 , 0.262	Depositor DCC
R_{free} test set	4265 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtrriage
Anisotropy	0.571	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26592	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.43	0/5739	0.61	0/7776
1	B	0.44	0/5770	0.61	0/7809
1	C	0.43	0/5759	0.60	0/7796
1	D	0.44	0/5769	0.61	0/7808
2	E	0.44	0/872	0.59	0/1170
2	F	0.44	0/875	0.63	0/1174
2	G	0.42	0/872	0.58	0/1170
2	H	0.46	0/872	0.57	0/1170
All	All	0.43	0/26528	0.61	0/35873

There are no bond length outliers.

There are no bond angle outliers.

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	5634	0	5544	217	0
1	B	5665	0	5629	238	0
1	C	5654	0	5621	223	0
1	D	5664	0	5636	231	0
2	E	860	0	865	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	863	0	867	30	0
2	G	860	0	865	42	0
2	H	860	0	865	34	0
3	A	91	0	87	24	0
3	B	91	0	87	22	0
3	C	91	0	87	26	0
3	D	91	0	87	33	0
4	A	24	0	18	0	0
4	B	24	0	18	4	0
4	C	24	0	18	2	0
4	D	24	0	18	3	0
5	A	18	0	8	3	0
5	B	18	0	8	4	0
5	C	18	0	9	2	0
5	D	18	0	8	2	0
All	All	26592	0	26345	1054	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1054) 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	1.53	1.22
2:F:5:ASP:HA	2:F:7:PHE:N	1.61	1.13
1:A:43:MET:HE1	1:A:72:PRO:HA	1.30	1.09
1:D:537:GLU:HG3	1:D:554:VAL:HG21	1.36	1.07
1:A:306:GLU:HG3	1:A:307:ALA:H	0.87	1.03
1:C:458:LYS:HG3	1:C:462:GLU:HG3	1.41	1.01
1:A:526:THR:HG22	1:A:569:GLU:HG2	1.39	1.01
3:B:1801:B12:H261	5:D:1500:5AD:H5'2	1.42	1.00
2:G:5:ASP:HA	2:G:7:PHE:N	1.76	0.99
2:F:5:ASP:HA	2:F:7:PHE:H	0.84	0.98
5:B:1500:5AD:H5'3	3:D:1801:B12:C16	1.93	0.98
3:B:1801:B12:C16	5:D:1500:5AD:H5'3	1.90	0.98
1:A:306:GLU:HG3	1:A:307:ALA:N	1.67	0.98
3:C:1801:B12:H401	3:C:1801:B12:H8	1.30	0.95
1:D:459:GLN:HG3	1:D:460:TYR:CD2	2.03	0.94
1:C:458:LYS:HE3	1:C:462:GLU:HG2	1.52	0.92
1:C:668:THR:HG23	1:C:676:HIS:HB2	1.49	0.92
1:A:306:GLU:CG	1:A:307:ALA:H	1.80	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:ASP:HA	2:E:7:PHE:H	1.22	0.90
1:C:373:ARG:HH11	1:C:373:ARG:HG3	1.37	0.88
2:F:5:ASP:CA	2:F:7:PHE:H	1.81	0.88
3:D:1801:B12:H601	3:D:1801:B12:H262	1.55	0.88
2:H:5:ASP:HA	2:H:7:PHE:N	1.89	0.88
1:A:396:ILE:HD12	2:E:29:MET:HE3	1.56	0.87
1:D:394:GLU:HG2	1:D:409:PHE:CE2	2.11	0.86
1:B:526:THR:HG23	1:B:569:GLU:HG2	1.56	0.86
1:A:96:MET:HG2	1:C:560:MET:HB3	1.59	0.84
1:D:394:GLU:HG2	1:D:409:PHE:HE2	1.38	0.84
1:B:23:ASP:OD2	1:B:24:LYS:HE3	1.78	0.83
3:B:1801:B12:H8	3:B:1801:B12:H401	1.43	0.83
2:G:87:LYS:O	2:G:91:GLU:HB2	1.79	0.83
2:H:5:ASP:HA	2:H:7:PHE:H	1.44	0.82
3:A:1801:B12:H262	3:A:1801:B12:H601	1.62	0.81
1:A:577:SER:O	1:A:578:ILE:HD12	1.79	0.81
1:B:232:ARG:HH21	1:D:598:ARG:HH22	1.28	0.81
1:A:682:ARG:HG2	1:A:686:LEU:HD13	1.63	0.81
1:B:577:SER:O	1:B:578:ILE:HD12	1.82	0.80
1:C:218:ILE:HD13	1:C:297:ARG:HD2	1.62	0.80
1:C:668:THR:CG2	1:C:676:HIS:HB2	2.11	0.80
1:A:233:GLU:HG2	1:A:235:TRP:CH2	2.16	0.79
1:B:393:GLU:HG3	2:F:29:MET:CE	2.12	0.79
3:C:1801:B12:H362	3:C:1801:B12:H351	1.63	0.79
5:B:1500:5AD:H5'2	3:D:1801:B12:H261	1.64	0.79
1:D:459:GLN:HG3	1:D:460:TYR:HD2	1.46	0.79
1:A:618:HIS:HB2	1:A:669:ILE:HG13	1.64	0.78
1:D:233:GLU:HG2	1:D:235:TRP:CZ2	2.19	0.78
1:D:406:GLU:OE2	1:D:428:ILE:HG23	1.83	0.78
1:A:606:LEU:HD12	1:A:607:LYS:H	1.48	0.78
3:D:1801:B12:N40	3:D:1801:B12:H8	1.99	0.78
1:D:649:VAL:HG11	1:D:682:ARG:HB3	1.64	0.77
2:F:6:ASP:O	2:F:10:ARG:HG3	1.84	0.77
1:A:464:LEU:HD23	1:A:471:LEU:HD23	1.67	0.77
1:B:525:LEU:HD23	1:B:570:LEU:HD13	1.65	0.77
1:B:14:ASP:OD2	1:B:17:ASN:HB2	1.85	0.76
1:A:445:MET:HE1	1:A:471:LEU:HD12	1.68	0.76
1:A:738:GLU:HG3	1:A:739:MET:N	1.99	0.76
1:D:611:ALA:HB2	1:D:643:LEU:HB2	1.67	0.76
1:D:88:GLU:OE2	1:D:498:ARG:HD2	1.86	0.76
1:A:459:GLN:HG3	1:A:460:TYR:HD2	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:THR:HG23	1:D:135:LYS:HD3	1.67	0.75
1:C:577:SER:O	1:C:578:ILE:HD12	1.87	0.75
1:A:123:THR:HG23	1:A:135:LYS:HD3	1.69	0.75
3:B:1801:B12:H8	3:B:1801:B12:N40	1.98	0.75
1:B:82:ILE:HD13	1:B:93:ARG:HD2	1.69	0.74
1:C:459:GLN:HG3	1:C:460:TYR:CD2	2.22	0.74
1:B:534:ARG:HG3	1:B:534:ARG:HH11	1.52	0.74
1:B:488:GLU:O	1:B:489:LEU:HD23	1.88	0.73
1:B:623:ARG:HD3	1:D:115:HIS:CE1	2.24	0.73
1:C:259:LYS:HA	1:C:262:ILE:HD12	1.70	0.73
1:C:225:HIS:O	1:C:228:ASN:HB2	1.89	0.73
1:A:18:ILE:HG23	1:A:142:LYS:HD3	1.70	0.72
1:A:459:GLN:HG3	1:A:460:TYR:CD2	2.24	0.72
1:B:196:MET:SD	1:B:402:PHE:CD1	2.83	0.72
1:A:668:THR:HG21	1:A:676:HIS:HA	1.71	0.72
1:B:109:ARG:HG2	1:B:132:ILE:HG13	1.72	0.72
1:C:189:VAL:HG11	1:C:196:MET:HB3	1.68	0.72
1:C:512:LYS:HB2	1:C:513:PRO:HD2	1.70	0.72
2:F:109:TRP:O	2:F:113:ILE:HG13	1.90	0.71
1:B:88:GLU:OE2	1:B:498:ARG:HD2	1.90	0.71
1:C:233:GLU:HB3	1:C:235:TRP:CZ3	2.24	0.71
1:C:575:PRO:HD2	1:C:576:PHE:CE2	2.26	0.71
3:A:1801:B12:H5R1	3:A:1801:B12:H3P1	1.71	0.71
1:D:219:ASP:HB3	1:D:248:ASN:ND2	2.06	0.71
3:D:1801:B12:H262	3:D:1801:B12:C60	2.21	0.71
1:A:528:PHE:CE1	1:A:565:GLY:HA3	2.25	0.70
1:C:213:ALA:HB3	1:C:215:MET:HG3	1.73	0.70
1:B:232:ARG:HE	1:D:598:ARG:CZ	2.04	0.70
1:B:120:ILE:HG13	1:B:133:THR:HG22	1.73	0.70
1:A:396:ILE:HD12	2:E:29:MET:CE	2.21	0.70
3:A:1801:B12:H2B	3:A:1801:B12:O7R	1.91	0.70
1:D:510:MET:CE	1:D:577:SER:HB2	2.21	0.70
1:A:120:ILE:HG13	1:A:133:THR:HG22	1.73	0.70
1:C:610:ALA:HB1	1:C:622:LEU:HD21	1.74	0.70
2:G:54:LEU:HA	2:G:57:MET:HE2	1.74	0.69
1:C:460:TYR:O	1:C:461:ASP:HB2	1.92	0.69
3:D:1801:B12:H362	3:D:1801:B12:H351	1.75	0.69
1:A:612:THR:HG22	1:A:616:ASP:HB3	1.75	0.69
2:E:54:LEU:HD23	2:E:57:MET:HE2	1.75	0.69
1:A:550:GLU:HG3	1:A:575:PRO:HG3	1.76	0.68
1:A:671:SER:HB2	1:A:676:HIS:CE1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:74:ARG:O	2:F:76:LEU:HD13	1.94	0.68
1:A:277:MET:CE	1:A:321:LEU:HD23	2.24	0.68
3:A:1801:B12:H401	3:A:1801:B12:H8	1.57	0.67
1:B:606:LEU:HD21	1:B:732:LEU:HB3	1.76	0.67
1:A:677:TYR:CE1	1:A:709:VAL:HB	2.29	0.67
3:A:1801:B12:H362	3:A:1801:B12:H351	1.74	0.67
3:A:1801:B12:H8	3:A:1801:B12:N40	2.08	0.67
2:H:5:ASP:HA	2:H:6:ASP:HB3	1.76	0.67
1:A:103:ASP:HB3	1:A:153:ARG:NH1	2.09	0.67
1:C:250:ILE:HG23	2:G:34:VAL:HG21	1.75	0.67
1:A:43:MET:HE1	1:A:72:PRO:CA	2.17	0.67
1:B:243:VAL:HG22	1:B:392:MET:HG3	1.76	0.67
2:H:59:PHE:CE1	2:H:100:GLY:HA3	2.30	0.67
1:C:43:MET:HE1	1:C:72:PRO:HA	1.76	0.66
2:G:5:ASP:HA	2:G:6:ASP:C	2.14	0.66
1:A:41:LEU:HD21	1:A:43:MET:HE2	1.78	0.66
1:D:526:THR:HG23	1:D:569:GLU:HG2	1.77	0.66
1:A:137:VAL:HB	1:A:172:MET:HE1	1.77	0.66
1:A:445:MET:CE	1:A:471:LEU:HD12	2.25	0.66
2:F:63:GLU:O	2:F:67:ILE:HG13	1.95	0.66
1:D:649:VAL:HG13	1:D:683:ILE:HG13	1.78	0.66
1:D:120:ILE:HG13	1:D:133:THR:HG22	1.76	0.66
1:A:385:LYS:HE2	2:E:23:GLN:HE21	1.60	0.66
1:C:74:PRO:HB2	1:C:76:PRO:HD2	1.78	0.66
1:C:579:ASP:OD1	1:C:581:ASN:HB2	1.95	0.66
1:C:593:SER:O	1:C:597:ILE:HG12	1.96	0.66
1:D:649:VAL:CG1	1:D:683:ILE:HG13	2.25	0.66
1:A:738:GLU:HG3	1:A:739:MET:H	1.60	0.66
2:E:5:ASP:CA	2:E:7:PHE:H	2.01	0.66
3:B:1801:B12:H362	3:B:1801:B12:H351	1.76	0.65
2:G:97:ARG:O	2:G:101:LEU:HB2	1.95	0.65
1:D:632:GLY:HA2	1:D:725:GLY:HA3	1.78	0.65
1:A:440:ARG:NH1	1:A:444:TYR:CE2	2.65	0.65
1:A:484:VAL:HG11	2:E:60:SER:HB3	1.77	0.65
1:B:115:HIS:CE1	1:D:623:ARG:HD3	2.31	0.65
2:F:88:ILE:HG13	2:F:103:LEU:HD11	1.79	0.65
1:A:486:ILE:N	1:A:486:ILE:HD12	2.11	0.65
1:D:512:LYS:HB2	1:D:513:PRO:HD2	1.79	0.65
3:D:1801:B12:H421	3:D:1801:B12:H10	1.79	0.65
1:B:79:THR:HG23	1:B:104:HIS:CG	2.32	0.65
1:C:458:LYS:HE3	1:C:462:GLU:CG	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:TYR:CE1	2:H:86:TYR:HE2	2.15	0.64
1:B:277:MET:HE2	1:B:321:LEU:HD23	1.77	0.64
1:C:649:VAL:HG12	1:C:686:LEU:HD12	1.78	0.64
2:G:95:SER:OG	2:G:98:GLU:HG2	1.98	0.64
1:B:86:ARG:HG3	1:B:517:TRP:CE2	2.33	0.64
1:C:543:PHE:O	1:C:547:MET:HG3	1.97	0.64
1:D:109:ARG:HG2	1:D:132:ILE:HG12	1.80	0.64
1:C:124:PRO:HA	1:C:493:ASP:OD1	1.98	0.64
1:C:475:CYS:HB2	2:G:56:ARG:O	1.98	0.64
3:D:1801:B12:H311	3:D:1801:B12:H353	1.80	0.64
1:A:580:ILE:HA	1:A:583:LEU:HD12	1.80	0.64
1:B:671:SER:HA	1:B:676:HIS:ND1	2.13	0.64
1:B:689:GLU:O	1:B:689:GLU:HG2	1.97	0.64
1:C:612:THR:HB	1:C:645:THR:HG22	1.80	0.64
1:B:162:SER:HB2	4:B:767:Z97:H6	1.80	0.63
2:F:54:LEU:HD23	2:F:57:MET:CE	2.27	0.63
3:C:1801:B12:H262	3:C:1801:B12:H601	1.79	0.63
1:C:550:GLU:HG3	1:C:573:ARG:NH2	2.13	0.63
1:A:335:THR:O	1:A:338:GLU:HB2	1.98	0.63
3:A:1801:B12:O7R	3:A:1801:B12:C2B	2.46	0.63
1:A:254:LYS:HE2	2:E:31:GLU:HG3	1.81	0.63
1:A:526:THR:OG1	1:C:524:LEU:HB3	1.98	0.63
1:A:606:LEU:HD12	1:A:607:LYS:N	2.14	0.63
1:C:394:GLU:HG2	1:C:409:PHE:CE2	2.34	0.63
1:B:608:ILE:HG21	1:B:665:LEU:HD12	1.81	0.63
1:A:537:GLU:HG3	1:A:554:VAL:HG21	1.81	0.63
1:A:560:MET:HB3	1:C:96:MET:HE2	1.80	0.63
3:B:1801:B12:H203	3:B:1801:B12:H301	1.81	0.63
1:B:277:MET:CE	1:B:321:LEU:HD23	2.29	0.62
1:D:619:SER:HB2	1:D:623:ARG:CZ	2.29	0.62
1:C:550:GLU:HB2	1:C:573:ARG:HB3	1.81	0.62
1:D:724:LYS:HB2	1:D:726:ILE:HG22	1.81	0.62
1:C:677:TYR:HA	1:C:680:MET:HE3	1.81	0.62
2:G:52:SER:HA	2:G:55:LEU:HD12	1.80	0.62
2:E:47:PRO:O	2:E:51:ARG:HG3	2.00	0.62
1:A:218:ILE:HD13	1:A:297:ARG:HD2	1.80	0.62
1:A:205:GLU:O	1:A:209:ILE:HD12	1.99	0.62
1:B:79:THR:HA	1:B:104:HIS:HB3	1.81	0.62
1:A:628:ILE:HG13	1:A:635:LYS:HB2	1.82	0.62
2:H:47:PRO:O	2:H:51:ARG:HG3	2.00	0.62
1:B:426:ARG:NH1	1:D:634:GLU:OE2	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:MET:SD	1:D:402:PHE:CD1	2.93	0.61
1:D:219:ASP:HB3	1:D:248:ASN:HD22	1.63	0.61
2:F:97:ARG:O	2:F:101:LEU:HB2	2.00	0.61
2:G:18:SER:OG	2:G:21:GLU:HG3	1.99	0.61
1:B:668:THR:O	1:B:668:THR:HG23	2.00	0.61
1:A:514:GLU:HA	1:A:520:ASP:OD1	2.01	0.61
2:E:74:ARG:HB2	2:E:76:LEU:HD12	1.82	0.61
1:C:649:VAL:HG12	1:C:686:LEU:CD1	2.31	0.61
3:D:1801:B12:H421	3:D:1801:B12:C10	2.31	0.61
1:D:277:MET:HE1	1:D:321:LEU:HG	1.83	0.61
1:B:391:PHE:HA	1:B:416:TYR:CZ	2.36	0.61
2:E:49:ILE:O	2:E:53:VAL:HG23	2.00	0.61
2:F:54:LEU:HD23	2:F:57:MET:HE2	1.83	0.61
1:B:653:VAL:O	1:B:657:ILE:HG13	2.01	0.60
1:C:514:GLU:OE2	1:C:518:GLN:HA	2.01	0.60
3:C:1801:B12:H8	3:C:1801:B12:N40	2.05	0.60
1:C:233:GLU:HB3	1:C:235:TRP:CH2	2.36	0.60
1:B:393:GLU:HG3	2:F:29:MET:HE1	1.81	0.60
1:D:224:ALA:HB3	1:D:245:HIS:CE1	2.36	0.60
1:A:667:SER:HB2	3:A:1801:B12:H4B	1.83	0.60
1:C:126:GLY:O	1:C:127:ILE:HD13	2.02	0.60
1:B:459:GLN:HG3	1:B:460:TYR:CD2	2.36	0.60
1:B:204:CYS:HB3	1:B:452:PHE:CD2	2.37	0.60
1:C:29:ARG:NH2	1:C:148:GLU:OE2	2.32	0.60
2:G:88:ILE:HG13	2:G:103:LEU:HD11	1.84	0.60
1:D:79:THR:HG23	1:D:104:HIS:CG	2.36	0.60
3:D:1801:B12:H601	3:D:1801:B12:C26	2.32	0.60
1:C:43:MET:CE	1:C:72:PRO:HA	2.32	0.60
1:A:685:GLU:O	1:A:689:GLU:HB2	2.01	0.60
2:E:107:LYS:O	2:E:108:TYR:HB2	2.00	0.60
1:B:532:SER:OG	1:B:535:VAL:HG23	2.02	0.60
1:A:604:THR:HB	1:A:736:ARG:HH12	1.66	0.59
1:A:684:HIS:O	1:A:688:VAL:HG23	2.02	0.59
3:A:1801:B12:H351	3:A:1801:B12:H372	1.84	0.59
2:E:81:ALA:O	2:E:85:VAL:HG23	2.01	0.59
1:B:324:LYS:HE2	1:B:362:MET:O	2.02	0.59
1:C:428:ILE:HG12	1:C:428:ILE:O	2.01	0.59
1:D:358:ALA:O	1:D:362:MET:HG3	2.03	0.59
1:D:668:THR:HG23	1:D:668:THR:O	2.02	0.59
1:A:546:LYS:NZ	1:C:578:ILE:HD11	2.17	0.59
2:E:5:ASP:HA	2:E:6:ASP:C	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ARG:HG2	1:D:132:ILE:CG1	2.32	0.59
1:D:464:LEU:HD23	1:D:471:LEU:HD13	1.84	0.59
1:A:267:VAL:HG22	1:A:299:GLN:HB3	1.83	0.59
1:C:659:LEU:O	1:C:660:LYS:HG2	2.02	0.59
1:D:250:ILE:HG23	2:H:34:VAL:HG21	1.84	0.59
1:D:416:TYR:CG	1:D:417:PRO:HA	2.37	0.59
1:A:606:LEU:HB2	1:A:736:ARG:NH2	2.18	0.59
1:B:109:ARG:HG2	1:B:132:ILE:CG1	2.33	0.58
1:B:111:ALA:O	1:D:620:VAL:HG11	2.03	0.58
1:B:281:LEU:O	1:B:285:VAL:HG23	2.03	0.58
1:B:300:MET:HB2	1:B:334:ILE:HG12	1.85	0.58
2:F:5:ASP:N	2:F:6:ASP:HB3	2.18	0.58
1:A:585:ILE:HG12	1:C:538:PHE:CD2	2.38	0.58
1:C:158:HIS:CD2	1:C:159:SER:N	2.71	0.58
1:C:109:ARG:HH21	4:C:767:Z97:P	2.27	0.58
1:B:217:GLN:O	1:B:263:CYS:HB2	2.03	0.58
1:C:41:LEU:HD21	1:C:43:MET:HE2	1.86	0.58
3:C:1801:B12:H203	3:C:1801:B12:H302	1.84	0.58
1:C:307:ALA:O	1:C:340:ARG:HD3	2.03	0.58
1:C:373:ARG:HH11	1:C:373:ARG:CG	2.15	0.58
1:D:669:ILE:HG22	3:D:1801:B12:H202	1.85	0.58
2:G:54:LEU:HD23	2:G:57:MET:CE	2.33	0.58
1:C:109:ARG:HG2	1:C:132:ILE:HG12	1.84	0.58
1:B:264:LEU:HD21	1:B:291:PHE:CD1	2.39	0.57
1:D:6:GLN:HG2	1:D:7:LEU:N	2.19	0.57
1:D:653:VAL:O	1:D:657:ILE:HG12	2.04	0.57
2:E:109:TRP:O	2:E:113:ILE:HG13	2.04	0.57
1:B:120:ILE:HG13	1:B:133:THR:CG2	2.33	0.57
1:B:461:ASP:OD1	1:B:463:ALA:HB3	2.04	0.57
1:A:370:GLN:HG2	1:C:372:LYS:HG3	1.86	0.57
1:B:660:LYS:HG3	1:B:660:LYS:O	2.02	0.57
1:B:464:LEU:HD23	1:B:471:LEU:CD1	2.34	0.57
1:C:218:ILE:HD13	1:C:297:ARG:CD	2.32	0.57
1:D:124:PRO:O	1:D:131:PRO:HG2	2.03	0.57
1:C:335:THR:HG22	1:C:348:ASN:HA	1.86	0.57
1:A:60:ALA:HB2	1:A:71:ASP:HB2	1.86	0.57
1:A:79:THR:HB	1:A:332:SER:HA	1.86	0.57
1:B:286:ALA:HB2	1:B:381:VAL:HG13	1.87	0.57
1:C:443:ASP:OD1	2:G:79:LYS:HE2	2.05	0.57
1:B:464:LEU:HD23	1:B:471:LEU:HD13	1.87	0.57
3:C:1801:B12:O7R	3:C:1801:B12:H2B	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ILE:HD11	1:D:428:ILE:CD1	2.34	0.57
1:C:109:ARG:HG2	1:C:132:ILE:CG1	2.35	0.57
1:D:526:THR:HG23	1:D:569:GLU:CG	2.35	0.57
1:A:631:GLY:O	1:A:725:GLY:HA3	2.05	0.56
1:B:232:ARG:HH21	1:D:598:ARG:NH2	1.99	0.56
3:C:1801:B12:H531	3:C:1801:B12:H543	1.87	0.56
2:F:49:ILE:O	2:F:53:VAL:HG23	2.04	0.56
5:A:1500:5AD:C4'	3:C:1801:B12:N23	2.67	0.56
1:B:649:VAL:HG12	1:B:686:LEU:CD1	2.36	0.56
1:D:6:GLN:HG2	1:D:7:LEU:H	1.69	0.56
2:H:5:ASP:HA	2:H:6:ASP:CB	2.32	0.56
1:B:63:SER:HB2	1:D:311:GLU:OE2	2.06	0.56
2:F:112:ALA:C	2:F:114:GLN:H	2.09	0.56
3:C:1801:B12:O7R	3:C:1801:B12:C2B	2.53	0.56
1:D:467:GLU:HA	1:D:467:GLU:OE1	2.04	0.56
1:B:313:THR:O	1:B:317:VAL:HG23	2.06	0.56
1:D:25:TYR:HD2	1:D:138:ARG:HG2	1.71	0.56
1:B:557:ARG:HG3	1:B:557:ARG:HH11	1.69	0.56
3:B:1801:B12:H291	3:B:1801:B12:H251	1.70	0.56
1:B:534:ARG:HG3	1:B:534:ARG:NH1	2.18	0.56
1:B:86:ARG:HG3	1:B:517:TRP:NE1	2.20	0.56
1:B:672:HIS:O	1:B:673:ASP:HB2	2.06	0.56
1:A:57:ASN:HB3	1:A:99:TRP:CH2	2.41	0.55
1:B:246:ALA:O	1:B:250:ILE:HG22	2.05	0.55
1:C:36:GLN:O	1:C:52:SER:HB2	2.04	0.55
1:D:41:LEU:HD23	1:D:43:MET:HE2	1.89	0.55
3:D:1801:B12:H531	3:D:1801:B12:H543	1.87	0.55
1:D:618:HIS:HB2	1:D:669:ILE:HG13	1.87	0.55
1:A:540:ALA:HB1	1:A:570:LEU:HD11	1.88	0.55
1:B:619:SER:HB2	1:B:623:ARG:CZ	2.36	0.55
2:F:92:LYS:HG3	2:F:108:TYR:CE1	2.40	0.55
1:D:608:ILE:HG13	1:D:663:ALA:HB3	1.88	0.55
1:D:626:ILE:O	1:D:634:GLU:HB2	2.06	0.55
1:B:612:THR:HG22	1:B:616:ASP:HB3	1.88	0.55
1:D:468:PRO:O	1:D:471:LEU:HB2	2.06	0.55
1:B:445:MET:HE1	1:B:447:PRO:HB3	1.88	0.55
1:D:541:ILE:HD11	1:D:554:VAL:HG23	1.89	0.55
1:A:7:LEU:HD12	1:A:146:LEU:HB3	1.88	0.55
1:A:707:PRO:HA	1:A:718:GLY:HA3	1.89	0.55
1:D:561:GLN:HB3	1:D:564:GLU:HB2	1.88	0.55
1:A:290:MET:SD	2:E:23:GLN:HG2	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LYS:HG3	1:A:462:GLU:HA	1.88	0.55
1:D:79:THR:HG23	1:D:104:HIS:ND1	2.22	0.55
3:A:1801:B12:H601	3:A:1801:B12:C26	2.36	0.55
1:B:7:LEU:HD13	1:B:150:GLU:HB2	1.88	0.55
1:B:147:ILE:O	1:B:151:VAL:HG13	2.07	0.55
1:C:123:THR:HG23	1:C:135:LYS:HD3	1.89	0.55
1:D:26:THR:HG22	1:D:27:PRO:HD2	1.89	0.55
1:D:109:ARG:HH21	4:D:767:Z97:P	2.30	0.55
2:E:5:ASP:CA	2:E:7:PHE:N	2.47	0.55
1:C:411:VAL:O	1:C:423:GLY:HA2	2.06	0.55
1:B:649:VAL:HG12	1:B:686:LEU:HD12	1.89	0.54
3:C:1801:B12:H362	3:C:1801:B12:C35	2.34	0.54
1:D:441:ASP:OD2	2:H:79:LYS:NZ	2.39	0.54
1:D:706:THR:HB	1:D:709:VAL:HG23	1.88	0.54
1:D:719:PHE:HB3	1:D:723:SER:OG	2.07	0.54
1:C:467:GLU:HB3	1:C:470:LYS:HG2	1.88	0.54
1:A:277:MET:HE2	1:A:321:LEU:HD23	1.90	0.54
1:B:344:TRP:CG	1:B:515:VAL:HB	2.42	0.54
1:D:510:MET:HE2	1:D:577:SER:HB2	1.87	0.54
1:D:205:GLU:OE2	1:D:451:HIS:HA	2.07	0.54
1:C:411:VAL:HB	1:C:424:ILE:H	1.73	0.54
3:A:1801:B12:C15	5:C:1500:5AD:H5'3	2.32	0.54
1:C:445:MET:HE1	1:C:447:PRO:HB3	1.88	0.54
2:E:54:LEU:HD23	2:E:57:MET:CE	2.38	0.54
1:C:103:ASP:HB3	1:C:153:ARG:NH1	2.23	0.54
1:C:219:ASP:O	1:C:225:HIS:HE1	1.90	0.54
1:A:185:PRO:HG3	1:A:203:ALA:CB	2.38	0.54
2:F:113:ILE:HG22	2:F:113:ILE:O	2.06	0.54
1:D:116:TYR:CE2	1:D:120:ILE:HD13	2.43	0.54
1:D:622:LEU:HG	1:D:626:ILE:HD12	1.90	0.54
1:A:307:ALA:HB1	1:A:556:ASN:HB2	1.89	0.54
1:A:447:PRO:HG2	2:E:57:MET:SD	2.48	0.54
1:B:167:PRO:HD2	2:F:48:SER:OG	2.08	0.54
1:C:132:ILE:HA	1:C:136:GLN:OE1	2.08	0.54
1:C:649:VAL:CG1	1:C:686:LEU:HD12	2.38	0.54
1:C:719:PHE:HB3	1:C:723:SER:OG	2.08	0.54
1:A:464:LEU:HD23	1:A:471:LEU:CD2	2.36	0.54
1:D:373:ARG:NH1	1:D:378:GLY:HA2	2.23	0.54
1:A:123:THR:O	1:A:498:ARG:NH2	2.42	0.53
1:B:393:GLU:OE2	2:F:25:ARG:NH1	2.39	0.53
1:D:19:LEU:HD23	1:D:22:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:591:ILE:HD12	1:D:591:ILE:N	2.23	0.53
1:A:607:LYS:HG3	1:A:639:GLU:HB3	1.89	0.53
1:C:6:GLN:HG2	1:C:8:ARG:HG3	1.89	0.53
1:C:41:LEU:CD2	1:C:43:MET:HE2	2.39	0.53
1:C:631:GLY:O	1:C:725:GLY:HA3	2.08	0.53
3:C:1801:B12:H251	3:C:1801:B12:N29	2.22	0.53
2:G:59:PHE:CZ	2:G:100:GLY:HA3	2.43	0.53
1:A:416:TYR:CD1	1:A:417:PRO:HA	2.43	0.53
1:C:461:ASP:HB3	1:C:464:LEU:HD22	1.89	0.53
1:D:123:THR:O	1:D:498:ARG:NH2	2.42	0.53
1:A:585:ILE:HG23	1:C:538:PHE:CE2	2.43	0.53
1:B:162:SER:OG	4:B:767:Z97:N1	2.40	0.53
1:B:687:ALA:C	1:B:693:ARG:HB2	2.28	0.53
1:A:604:THR:HB	1:A:736:ARG:NH1	2.24	0.53
1:B:137:VAL:HG21	1:B:172:MET:HE3	1.90	0.53
1:C:75:LEU:N	1:C:76:PRO:CD	2.71	0.53
1:D:6:GLN:CG	1:D:7:LEU:H	2.20	0.53
3:B:1801:B12:H351	3:B:1801:B12:H372	1.91	0.53
1:D:204:CYS:HB3	1:D:452:PHE:CD2	2.44	0.53
1:D:438:PHE:CD2	2:H:77:MET:HG3	2.43	0.53
3:D:1801:B12:H302	3:D:1801:B12:H203	1.91	0.53
1:A:708:GLU:C	1:A:710:ALA:H	2.13	0.53
1:B:13:LEU:HD13	1:B:91:ILE:HG22	1.91	0.53
1:B:79:THR:HG23	1:B:104:HIS:ND1	2.24	0.53
1:D:671:SER:OG	1:D:704:GLN:HG3	2.09	0.53
1:C:427:GLN:C	1:C:429:ASN:H	2.13	0.53
1:D:233:GLU:HG2	1:D:235:TRP:CH2	2.44	0.53
1:D:411:VAL:HG12	1:D:411:VAL:O	2.10	0.53
2:H:5:ASP:CB	2:H:8:GLN:HG2	2.39	0.53
1:A:13:LEU:HD22	1:A:18:ILE:HD11	1.90	0.52
1:B:683:ILE:HG22	1:B:698:ILE:HD13	1.91	0.52
3:A:1801:B12:H353	3:A:1801:B12:H311	1.92	0.52
1:B:512:LYS:HB2	1:B:513:PRO:CD	2.39	0.52
1:B:557:ARG:HH11	1:B:557:ARG:CG	2.22	0.52
1:C:86:ARG:HG3	1:C:517:TRP:NE1	2.23	0.52
1:C:471:LEU:HD12	2:G:86:TYR:OH	2.09	0.52
1:D:161:VAL:HG12	1:D:161:VAL:O	2.10	0.52
1:A:716:ASP:OD2	1:A:735:LYS:HE2	2.10	0.52
1:B:475:CYS:HB2	2:F:56:ARG:O	2.09	0.52
2:E:25:ARG:O	2:E:29:MET:HG3	2.08	0.52
1:B:172:MET:HE2	1:B:176:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1801:B12:H251	3:C:1801:B12:H291	1.75	0.52
1:B:606:LEU:HD21	1:B:732:LEU:HD22	1.91	0.52
1:B:671:SER:HB2	1:B:676:HIS:CE1	2.44	0.52
1:C:123:THR:O	1:C:494:ASN:HA	2.09	0.52
1:D:671:SER:HB2	1:D:676:HIS:ND1	2.24	0.52
3:D:1801:B12:H601	3:D:1801:B12:H252	1.92	0.52
1:A:549:LEU:HD21	1:A:574:VAL:HG23	1.92	0.52
1:B:550:GLU:HG3	1:B:573:ARG:NH2	2.24	0.52
1:D:688:VAL:HG22	1:D:693:ARG:HG2	1.91	0.52
2:H:65:LYS:HG2	2:H:69:ASP:OD2	2.09	0.52
1:B:445:MET:HE3	1:B:457:VAL:HG22	1.91	0.52
1:B:695:LYS:HB2	1:B:695:LYS:NZ	2.25	0.52
1:C:189:VAL:HG11	1:C:196:MET:CB	2.38	0.52
1:C:18:ILE:HG23	1:C:142:LYS:HD3	1.91	0.52
1:C:373:ARG:HD2	1:C:373:ARG:O	2.09	0.52
1:A:147:ILE:O	1:A:151:VAL:HG22	2.10	0.52
1:A:440:ARG:HH22	1:A:451:HIS:CE1	2.28	0.52
1:B:320:LEU:HD13	1:B:358:ALA:HB3	1.91	0.52
1:D:537:GLU:O	1:D:541:ILE:HG12	2.10	0.52
1:A:666:ALA:O	1:A:700:CYS:HA	2.10	0.52
1:B:651:LYS:HA	1:B:651:LYS:NZ	2.24	0.52
1:C:610:ALA:HA	1:C:665:LEU:O	2.10	0.52
1:D:454:TYR:C	1:D:454:TYR:CD2	2.84	0.52
1:A:688:VAL:HG22	1:A:693:ARG:CB	2.40	0.51
1:C:406:GLU:HG2	1:C:426:ARG:O	2.10	0.51
1:D:189:VAL:CG2	1:D:196:MET:HA	2.40	0.51
1:A:738:GLU:CG	1:A:739:MET:N	2.70	0.51
1:C:320:LEU:HD13	1:C:358:ALA:HB3	1.91	0.51
1:C:541:ILE:HG23	1:C:552:VAL:HG11	1.92	0.51
1:C:668:THR:CG2	1:C:668:THR:O	2.58	0.51
1:A:116:TYR:CE2	1:A:120:ILE:HD13	2.46	0.51
1:D:684:HIS:O	1:D:687:ALA:HB3	2.09	0.51
1:A:75:LEU:N	1:A:76:PRO:CD	2.73	0.51
1:A:618:HIS:ND1	1:A:669:ILE:HB	2.26	0.51
1:C:55:LEU:CD2	1:C:153:ARG:HB2	2.40	0.51
1:C:460:TYR:CE1	2:G:86:TYR:HE2	2.29	0.51
2:G:88:ILE:HG22	2:G:99:ALA:HB1	1.91	0.51
1:A:96:MET:HG2	1:C:560:MET:CB	2.37	0.51
1:B:126:GLY:HA3	1:B:129:GLY:O	2.11	0.51
1:B:460:TYR:O	1:B:461:ASP:HB2	2.09	0.51
1:B:219:ASP:HB3	1:B:248:ASN:HD22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:735:LYS:O	1:B:735:LYS:HG3	2.09	0.51
2:H:57:MET:HE1	2:H:82:GLY:HA2	1.91	0.51
2:G:70:LYS:O	2:G:74:ARG:HG2	2.10	0.51
1:D:461:ASP:OD1	1:D:463:ALA:HB3	2.11	0.51
1:A:601:ILE:HG22	1:A:601:ILE:O	2.10	0.51
1:A:738:GLU:CG	1:A:739:MET:H	2.22	0.51
1:B:274:ALA:O	1:B:276:SER:N	2.44	0.51
3:B:1801:B12:H362	3:B:1801:B12:C35	2.41	0.51
1:C:90:ASP:O	1:C:94:MET:HG3	2.11	0.51
1:D:541:ILE:HG22	1:D:545:LYS:HE3	1.93	0.51
1:A:74:PRO:HB2	1:A:76:PRO:HD2	1.91	0.51
3:B:1801:B12:H252	3:B:1801:B12:H601	1.93	0.51
1:A:164:VAL:O	1:A:198:ARG:NH2	2.43	0.51
1:A:579:ASP:O	1:A:583:LEU:HG	2.11	0.51
1:B:684:HIS:CG	1:B:714:GLY:HA3	2.45	0.51
1:C:556:ASN:HB3	1:C:569:GLU:HB2	1.93	0.51
1:A:693:ARG:HH22	1:A:716:ASP:CG	2.14	0.50
1:B:686:LEU:O	1:B:690:LYS:HG2	2.10	0.50
1:C:476:THR:OG1	2:G:56:ARG:HA	2.11	0.50
1:D:285:VAL:O	1:D:289:GLU:HG3	2.11	0.50
1:C:547:MET:O	1:C:548:ASN:HB2	2.12	0.50
1:D:616:ASP:HA	1:D:670:ILE:HD12	1.92	0.50
1:A:688:VAL:HG22	1:A:693:ARG:HG2	1.92	0.50
2:F:66:ALA:O	2:F:70:LYS:HG3	2.10	0.50
1:D:510:MET:HE3	1:D:577:SER:HB2	1.94	0.50
1:D:575:PRO:HD2	1:D:576:PHE:CE2	2.46	0.50
1:A:287:LEU:HD12	1:A:291:PHE:CD2	2.47	0.50
1:A:528:PHE:CZ	1:A:565:GLY:HA3	2.46	0.50
1:A:575:PRO:HD2	1:A:576:PHE:CE2	2.46	0.50
1:A:626:ILE:O	1:A:634:GLU:HB2	2.12	0.50
1:A:682:ARG:HG2	1:A:686:LEU:CD1	2.39	0.50
1:B:143:ALA:O	1:B:147:ILE:HG13	2.10	0.50
1:B:406:GLU:HG3	1:B:428:ILE:HG22	1.93	0.50
1:B:512:LYS:HB2	1:B:513:PRO:HD2	1.93	0.50
1:B:115:HIS:HB3	1:D:623:ARG:HH11	1.76	0.50
3:B:1801:B12:H531	3:B:1801:B12:C55	2.42	0.50
3:C:1801:B12:H203	3:C:1801:B12:C30	2.41	0.50
1:D:31:GLY:O	1:D:179:ASN:HB3	2.11	0.50
1:D:416:TYR:CD1	1:D:417:PRO:HA	2.46	0.50
1:C:194:ILE:HG12	1:C:432:ILE:HB	1.94	0.50
1:D:737:ARG:C	1:D:739:MET:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:HG3	1:A:29:ARG:HH11	1.77	0.50
1:A:300:MET:HB2	1:A:334:ILE:HG12	1.92	0.50
1:B:232:ARG:HE	1:D:598:ARG:NH1	2.10	0.50
1:D:305:MET:HE1	1:D:316:HIS:NE2	2.27	0.50
1:C:158:HIS:HD2	1:C:159:SER:N	2.09	0.50
1:D:653:VAL:O	1:D:653:VAL:HG12	2.10	0.50
1:B:655:ALA:O	1:B:659:LEU:HG	2.12	0.50
2:F:59:PHE:CE1	2:F:100:GLY:HA3	2.47	0.50
1:D:135:LYS:HG3	1:D:485:TYR:OH	2.12	0.50
1:B:167:PRO:O	1:B:171:VAL:HG23	2.11	0.49
1:C:467:GLU:N	1:C:468:PRO:HD3	2.27	0.49
1:C:528:PHE:CE1	1:C:565:GLY:HA3	2.47	0.49
1:C:710:ALA:O	1:C:715:VAL:HG22	2.12	0.49
1:D:164:VAL:HG12	1:D:194:ILE:HG23	1.94	0.49
1:D:668:THR:O	1:D:668:THR:CG2	2.60	0.49
1:D:671:SER:HB2	1:D:676:HIS:CE1	2.46	0.49
1:D:688:VAL:HG22	1:D:693:ARG:CG	2.42	0.49
1:A:313:THR:O	1:A:317:VAL:HG23	2.12	0.49
1:A:495:VAL:HG13	1:A:496:ASN:N	2.27	0.49
1:B:284:ALA:O	1:B:288:ARG:HD3	2.12	0.49
1:C:373:ARG:HG3	1:C:373:ARG:NH1	2.16	0.49
1:D:336:PRO:HD2	1:D:347:TYR:HB3	1.93	0.49
1:A:399:GLY:HA3	1:A:403:ASN:HD22	1.76	0.49
1:A:416:TYR:CG	1:A:417:PRO:HA	2.47	0.49
1:D:668:THR:HG23	1:D:676:HIS:HB2	1.94	0.49
1:A:113:GLN:HG3	1:A:116:TYR:CD2	2.47	0.49
1:B:570:LEU:HD12	1:B:570:LEU:H	1.78	0.49
1:C:290:MET:HB3	1:C:291:PHE:CD2	2.46	0.49
1:A:123:THR:CG2	1:A:135:LYS:HD3	2.41	0.49
2:E:70:LYS:O	2:E:74:ARG:HG2	2.13	0.49
1:B:290:MET:HE3	1:B:385:LYS:HG2	1.95	0.49
1:C:5:LEU:O	1:C:6:GLN:CB	2.61	0.49
1:D:234:ALA:O	1:D:237:VAL:HG12	2.13	0.49
1:A:45:PRO:HD2	1:A:46:PHE:CD2	2.47	0.49
1:A:618:HIS:CB	1:A:669:ILE:HG13	2.37	0.49
1:B:693:ARG:HG3	1:B:693:ARG:O	2.12	0.49
2:G:6:ASP:O	2:G:10:ARG:HG3	2.12	0.49
1:D:631:GLY:HA2	1:D:635:LYS:HD2	1.95	0.49
1:A:5:LEU:O	1:A:6:GLN:HB2	2.13	0.49
1:A:159:SER:HB3	1:A:173:PHE:CZ	2.47	0.49
3:B:1801:B12:H251	3:B:1801:B12:N29	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LEU:HD23	1:C:147:ILE:HD12	1.94	0.49
2:G:86:TYR:O	2:G:87:LYS:C	2.51	0.49
1:D:579:ASP:HB3	1:D:582:SER:OG	2.13	0.49
1:A:531:THR:CG2	1:A:536:ALA:HB2	2.43	0.49
1:B:116:TYR:CE1	3:D:1801:B12:H491	2.48	0.49
1:B:410:PHE:C	1:B:411:VAL:HG23	2.33	0.49
3:B:1801:B12:H601	3:B:1801:B12:H262	1.94	0.49
1:A:237:VAL:HG22	1:A:237:VAL:O	2.13	0.49
2:F:74:ARG:HG3	2:F:74:ARG:HH11	1.78	0.49
1:D:42:GLN:HG3	1:D:47:ILE:HG13	1.95	0.49
1:A:538:PHE:CD2	1:C:585:ILE:HG12	2.48	0.48
1:B:543:PHE:O	1:B:547:MET:HG3	2.14	0.48
1:C:618:HIS:CE1	3:C:1801:B12:N22	2.81	0.48
1:A:38:ALA:HB1	1:A:41:LEU:HB2	1.94	0.48
2:F:20:GLU:H	2:F:20:GLU:CD	2.17	0.48
1:C:541:ILE:HG23	1:C:552:VAL:CG1	2.43	0.48
3:D:1801:B12:H362	3:D:1801:B12:C35	2.43	0.48
2:H:5:ASP:HA	2:H:6:ASP:C	2.29	0.48
1:B:232:ARG:HH11	1:B:232:ARG:HA	1.78	0.48
1:B:411:VAL:O	1:B:423:GLY:HA2	2.13	0.48
1:C:161:VAL:HG23	1:C:181:ALA:HB1	1.94	0.48
1:C:386:GLU:O	1:C:390:LEU:HG	2.13	0.48
3:D:1801:B12:H492	3:D:1801:B12:H471	1.95	0.48
1:A:679:ASN:O	1:A:683:ILE:HG13	2.14	0.48
1:B:570:LEU:HD12	1:B:570:LEU:N	2.27	0.48
1:C:405:VAL:CG1	1:C:426:ARG:HB2	2.43	0.48
1:C:668:THR:HG23	1:C:676:HIS:CB	2.34	0.48
1:D:700:CYS:O	1:D:718:GLY:HA2	2.13	0.48
3:D:1801:B12:O7R	3:D:1801:B12:C2B	2.61	0.48
1:C:444:TYR:C	1:C:444:TYR:CD2	2.87	0.48
1:D:607:LYS:C	1:D:608:ILE:HD12	2.33	0.48
1:D:723:SER:H	3:D:1801:B12:H5R2	1.77	0.48
1:A:344:TRP:CG	1:A:515:VAL:HB	2.49	0.48
1:A:478:GLU:O	1:A:480:PRO:HD3	2.14	0.48
2:H:5:ASP:CA	2:H:6:ASP:CB	2.91	0.48
1:A:422:ASP:OD1	1:A:422:ASP:N	2.46	0.48
1:B:629:LYS:O	1:B:630:HIS:HD2	1.97	0.48
3:D:1801:B12:H253	3:D:1801:B12:H301	1.52	0.48
1:A:5:LEU:O	1:A:6:GLN:CB	2.62	0.48
1:A:735:LYS:O	1:A:735:LYS:HG3	2.14	0.48
1:B:58:SER:HB2	1:B:71:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:VAL:HG12	1:B:161:VAL:O	2.14	0.48
1:C:651:LYS:O	1:C:652:LEU:C	2.52	0.48
2:G:76:LEU:HB3	2:G:84:ILE:HD11	1.95	0.48
1:D:622:LEU:HD23	1:D:642:TYR:HE1	1.79	0.48
1:A:6:GLN:O	1:A:7:LEU:HB2	2.13	0.48
3:A:1801:B12:H362	3:A:1801:B12:C35	2.41	0.48
1:B:618:HIS:CE1	3:B:1801:B12:N21	2.81	0.48
1:C:13:LEU:HD13	1:C:91:ILE:HG22	1.96	0.48
1:C:164:VAL:HG13	1:C:194:ILE:HD13	1.95	0.48
1:D:288:ARG:HG3	1:D:288:ARG:HH11	1.79	0.48
1:A:394:GLU:HG2	1:A:409:PHE:CE2	2.48	0.47
1:A:470:LYS:O	1:A:472:ILE:N	2.47	0.47
1:A:606:LEU:HB2	1:A:736:ARG:HH21	1.78	0.47
2:E:59:PHE:CE1	2:E:100:GLY:HA3	2.48	0.47
1:C:79:THR:HB	1:C:332:SER:HA	1.96	0.47
1:C:492:ASN:O	1:C:497:VAL:HG11	2.13	0.47
1:C:607:LYS:HE2	1:C:639:GLU:OE2	2.14	0.47
1:D:25:TYR:CD2	1:D:138:ARG:HG2	2.48	0.47
1:A:267:VAL:CG2	1:A:299:GLN:HB3	2.44	0.47
1:B:132:ILE:HA	1:B:136:GLN:OE1	2.14	0.47
1:B:189:VAL:HG22	1:B:196:MET:HA	1.96	0.47
1:C:14:ASP:CG	1:C:17:ASN:HB2	2.34	0.47
1:D:5:LEU:O	1:D:6:GLN:HB2	2.13	0.47
3:D:1801:B12:O28	3:D:1801:B12:H3	2.15	0.47
2:E:23:GLN:O	2:E:26:PHE:HB3	2.15	0.47
1:B:95:ARG:HD3	1:D:564:GLU:HG2	1.96	0.47
1:C:344:TRP:CG	1:C:515:VAL:HB	2.49	0.47
2:G:59:PHE:CE1	2:G:100:GLY:HA3	2.49	0.47
2:H:6:ASP:O	2:H:10:ARG:HG3	2.13	0.47
1:A:122:GLY:O	1:A:133:THR:HG21	2.14	0.47
1:B:5:LEU:HD23	1:B:5:LEU:O	2.14	0.47
1:B:123:THR:O	1:B:498:ARG:NH2	2.44	0.47
1:B:137:VAL:CG2	1:B:172:MET:HE3	2.45	0.47
1:C:672:HIS:O	1:C:673:ASP:CB	2.62	0.47
2:G:76:LEU:O	2:G:77:MET:C	2.52	0.47
1:C:96:MET:CE	1:C:345:HIS:HB3	2.44	0.47
1:C:299:GLN:HG3	1:C:300:MET:N	2.29	0.47
1:D:7:LEU:HD13	1:D:150:GLU:CD	2.35	0.47
1:A:96:MET:CE	1:A:345:HIS:HB3	2.44	0.47
1:A:467:GLU:O	1:A:469:SER:N	2.47	0.47
3:A:1801:B12:C16	5:C:1500:5AD:H5'3	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:MET:HB3	1:B:210:MET:HE2	1.84	0.47
1:B:326:THR:OG1	1:B:327:ARG:N	2.46	0.47
1:B:622:LEU:HB2	1:B:667:SER:HB2	1.96	0.47
1:B:651:LYS:HA	1:B:651:LYS:CE	2.45	0.47
1:C:373:ARG:HA	1:C:377:LEU:HD23	1.97	0.47
3:D:1801:B12:H351	3:D:1801:B12:H372	1.95	0.47
2:H:25:ARG:HA	2:H:28:GLU:HB2	1.97	0.47
1:B:607:LYS:C	1:B:608:ILE:HD12	2.35	0.47
1:C:377:LEU:O	1:C:381:VAL:HG23	2.14	0.47
1:D:387:ARG:NH1	1:D:416:TYR:O	2.48	0.47
1:D:688:VAL:HG22	1:D:693:ARG:CB	2.44	0.47
1:B:297:ARG:O	1:B:297:ARG:HD3	2.15	0.47
1:B:359:LEU:HD23	1:B:359:LEU:HA	1.73	0.47
3:D:1801:B12:O2	3:D:1801:B12:H2B	2.15	0.47
2:H:35:ASP:HB2	2:H:36:PRO:HD3	1.97	0.47
1:A:75:LEU:N	1:A:76:PRO:HD3	2.30	0.47
1:A:112:GLY:HA3	1:C:620:VAL:HG13	1.96	0.47
1:C:612:THR:CB	1:C:645:THR:HG22	2.44	0.47
2:G:53:VAL:HG12	2:G:57:MET:HE1	1.97	0.47
1:B:39:GLU:O	1:B:40:ASN:C	2.53	0.46
1:B:511:ILE:CG1	1:D:530:PRO:HD2	2.45	0.46
1:B:606:LEU:CD2	1:B:732:LEU:HB3	2.44	0.46
1:C:219:ASP:HB3	1:C:248:ASN:ND2	2.31	0.46
1:C:444:TYR:HA	2:G:79:LYS:O	2.15	0.46
1:C:612:THR:HG21	1:C:618:HIS:O	2.14	0.46
1:A:672:HIS:O	1:A:675:ILE:HG22	2.15	0.46
1:A:621:GLY:O	1:A:624:GLU:HB2	2.15	0.46
1:B:600:ASP:OD2	1:B:733:VAL:HG23	2.16	0.46
1:C:209:ILE:O	1:C:212:TRP:HB3	2.14	0.46
1:A:125:GLN:HG3	1:A:126:GLY:N	2.30	0.46
1:A:344:TRP:CD1	1:A:515:VAL:HB	2.50	0.46
1:C:233:GLU:OE1	1:C:236:LYS:HD2	2.16	0.46
1:B:120:ILE:C	1:B:133:THR:HG22	2.35	0.46
1:C:394:GLU:HG2	1:C:409:PHE:HE2	1.80	0.46
1:C:396:ILE:CD1	2:G:29:MET:HG3	2.45	0.46
1:D:197:ILE:HD11	1:D:428:ILE:HD11	1.97	0.46
1:A:79:THR:HA	1:A:104:HIS:HB3	1.97	0.46
1:A:109:ARG:HG2	1:A:132:ILE:HG12	1.98	0.46
1:A:310:ARG:O	1:A:314:VAL:HG23	2.15	0.46
1:A:692:ILE:O	1:A:696:ILE:HG22	2.15	0.46
1:B:20:LYS:O	1:B:21:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ALA:O	1:C:146:LEU:HB2	2.15	0.46
1:C:393:GLU:OE2	2:G:25:ARG:NH1	2.49	0.46
1:D:611:ALA:HB1	1:D:647:VAL:HG21	1.97	0.46
1:D:652:LEU:HD23	1:D:683:ILE:HD13	1.96	0.46
3:B:1801:B12:H492	3:B:1801:B12:C47	2.46	0.46
1:C:539:ALA:O	1:C:543:PHE:HD2	1.99	0.46
1:D:43:MET:HE3	1:D:72:PRO:HB3	1.96	0.46
1:D:711:VAL:O	1:D:711:VAL:CG1	2.63	0.46
1:B:124:PRO:O	1:B:131:PRO:HG2	2.16	0.46
1:B:560:MET:HB2	1:B:565:GLY:O	2.16	0.46
1:B:576:PHE:CZ	1:D:546:LYS:HB3	2.50	0.46
1:B:647:VAL:HG12	1:B:648:PRO:O	2.16	0.46
3:B:1801:B12:H531	3:B:1801:B12:H543	1.98	0.46
1:C:701:GLY:HA2	1:C:719:PHE:O	2.16	0.46
1:D:8:ARG:HG3	1:D:11:GLU:OE1	2.14	0.46
1:D:390:LEU:HD21	2:H:10:ARG:O	2.14	0.46
1:D:478:GLU:O	1:D:480:PRO:HD3	2.16	0.46
1:A:709:VAL:HG12	1:A:709:VAL:O	2.16	0.46
1:B:106:MET:CE	1:B:218:ILE:HD12	2.46	0.46
1:B:144:LEU:HD22	1:B:155:ILE:HG21	1.97	0.46
1:B:245:HIS:CG	1:B:264:LEU:HD23	2.51	0.46
1:B:611:ALA:HB2	1:B:643:LEU:HB2	1.98	0.46
1:C:281:LEU:HB3	1:C:282:PRO:HD3	1.97	0.46
1:C:684:HIS:O	1:C:688:VAL:HG23	2.16	0.46
1:B:182:HIS:HA	1:B:218:ILE:O	2.16	0.46
1:B:649:VAL:CG1	1:B:686:LEU:HD12	2.45	0.46
1:A:218:ILE:HD13	1:A:297:ARG:CD	2.45	0.45
1:B:126:GLY:HA3	1:B:131:PRO:HD3	1.98	0.45
3:B:1801:B12:H2B	3:B:1801:B12:O2	2.15	0.45
1:D:42:GLN:HG2	1:D:46:PHE:O	2.16	0.45
1:A:612:THR:CG2	1:A:616:ASP:HB3	2.43	0.45
3:A:1801:B12:H18	3:A:1801:B12:H561	1.55	0.45
1:B:7:LEU:HD23	1:B:7:LEU:HA	1.44	0.45
1:B:530:PRO:HD2	1:D:511:ILE:HD11	1.98	0.45
1:B:612:THR:HB	1:B:645:THR:HA	1.99	0.45
1:B:729:ALA:O	1:B:733:VAL:HG12	2.15	0.45
1:B:735:LYS:HD2	1:B:738:GLU:OE1	2.16	0.45
2:F:7:PHE:O	2:F:11:ARG:HG2	2.16	0.45
1:D:688:VAL:HG22	1:D:693:ARG:HB2	1.97	0.45
1:D:737:ARG:C	1:D:739:MET:N	2.68	0.45
3:D:1801:B12:H8	3:D:1801:B12:H401	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ILE:HG23	1:A:727:HIS:N	2.31	0.45
1:B:354:THR:OG1	1:D:310:ARG:HD2	2.16	0.45
1:B:529:LEU:HA	1:B:530:PRO:HD3	1.64	0.45
1:B:608:ILE:HG23	1:B:609:VAL:O	2.15	0.45
1:C:373:ARG:CG	1:C:373:ARG:NH1	2.78	0.45
1:C:668:THR:HG21	1:C:680:MET:HE2	1.98	0.45
1:C:695:LYS:HB2	1:C:695:LYS:HE3	1.71	0.45
1:D:373:ARG:HD2	1:D:373:ARG:O	2.16	0.45
1:D:674:ASP:HA	1:D:676:HIS:CE1	2.51	0.45
2:H:53:VAL:O	2:H:57:MET:HG3	2.16	0.45
1:A:109:ARG:HG2	1:A:132:ILE:CG1	2.46	0.45
1:A:349:ILE:HD12	1:A:349:ILE:N	2.31	0.45
1:C:61:LEU:O	1:C:62:PRO:C	2.54	0.45
1:C:184:ASP:OD1	1:C:186:GLN:HB2	2.16	0.45
1:D:7:LEU:HD23	1:D:7:LEU:HA	1.60	0.45
1:D:648:PRO:HD2	1:D:651:LYS:HE3	1.98	0.45
1:D:663:ALA:HB2	1:D:697:MET:HE3	1.98	0.45
3:A:1801:B12:H301	3:A:1801:B12:H253	1.51	0.45
2:E:72:MET:HG2	2:E:77:MET:HG3	1.99	0.45
1:B:137:VAL:HB	1:B:172:MET:HE3	1.99	0.45
2:F:112:ALA:O	2:F:114:GLN:N	2.50	0.45
1:C:6:GLN:HG2	1:C:7:LEU:N	2.31	0.45
1:C:41:LEU:HG	1:C:42:GLN:N	2.31	0.45
1:D:445:MET:HE3	1:D:447:PRO:N	2.32	0.45
1:D:723:SER:O	3:D:1801:B12:H5R1	2.16	0.45
1:A:607:LYS:O	1:A:608:ILE:HD12	2.17	0.45
1:D:264:LEU:HD21	1:D:291:PHE:CD1	2.52	0.45
1:A:213:ALA:HB3	1:A:215:MET:HG3	1.98	0.45
1:A:289:GLU:O	1:A:292:GLU:HG3	2.17	0.45
1:A:733:VAL:O	1:A:737:ARG:HD2	2.17	0.45
2:E:64:ALA:O	2:E:68:VAL:HG23	2.16	0.45
1:B:65:LYS:HE2	1:D:306:GLU:CG	2.47	0.45
1:B:626:ILE:HD13	1:B:640:VAL:HG11	1.98	0.45
1:B:672:HIS:O	1:B:673:ASP:CB	2.64	0.45
1:B:692:ILE:O	1:B:694:ASP:N	2.50	0.45
1:C:191:TYR:CE1	1:C:230:THR:HG21	2.51	0.45
1:C:592:LEU:HD23	1:C:592:LEU:HA	1.86	0.45
1:D:197:ILE:HD11	1:D:428:ILE:HD12	1.99	0.45
1:D:710:ALA:O	1:D:715:VAL:HG22	2.16	0.45
2:H:7:PHE:O	2:H:11:ARG:HG2	2.17	0.45
1:A:460:TYR:O	1:A:461:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:VAL:HG12	1:B:499:MET:CE	2.47	0.45
1:B:309:THR:HG22	1:B:336:PRO:O	2.16	0.45
1:C:302:THR:HG22	1:C:334:ILE:HG13	1.99	0.45
1:D:86:ARG:HD3	1:D:498:ARG:HD3	1.99	0.45
2:H:17:LEU:HD22	2:H:21:GLU:HB3	1.98	0.45
1:B:232:ARG:NH2	1:D:635:LYS:HE2	2.31	0.45
1:B:550:GLU:HA	1:B:550:GLU:OE1	2.17	0.45
1:B:609:VAL:HG12	1:B:659:LEU:HD12	1.99	0.45
1:B:687:ALA:HB3	1:B:693:ARG:HD3	1.97	0.45
1:D:123:THR:O	1:D:494:ASN:HA	2.15	0.45
1:D:257:MET:HB3	1:D:262:ILE:HD11	1.99	0.45
1:C:186:GLN:HG2	1:C:401:TYR:OH	2.17	0.45
1:C:606:LEU:HB2	1:C:736:ARG:NH2	2.32	0.45
3:C:1801:B12:H471	3:C:1801:B12:H492	1.98	0.45
1:D:618:HIS:NE2	3:D:1801:B12:N22	2.64	0.45
2:E:5:ASP:CB	2:E:8:GLN:HG2	2.47	0.44
1:B:49:LYS:HE2	1:D:278:TYR:OH	2.17	0.44
1:B:90:ASP:O	1:B:94:MET:HG3	2.17	0.44
1:B:162:SER:CB	4:B:767:Z97:H6	2.47	0.44
1:B:629:LYS:HE3	1:B:630:HIS:NE2	2.32	0.44
3:B:1801:B12:H412	3:B:1801:B12:H363	1.52	0.44
1:C:607:LYS:NZ	1:C:660:LYS:HD3	2.32	0.44
1:D:127:ILE:HD12	1:D:128:GLY:N	2.32	0.44
1:D:212:TRP:CH2	1:D:477:LEU:HB3	2.52	0.44
1:D:406:GLU:CD	1:D:428:ILE:HG23	2.36	0.44
1:D:416:TYR:CD2	1:D:417:PRO:HA	2.52	0.44
1:A:17:ASN:HA	1:A:20:LYS:HE2	1.99	0.44
1:A:55:LEU:HD21	1:A:153:ARG:CZ	2.47	0.44
1:B:187:TYR:OH	1:D:629:LYS:HD3	2.18	0.44
1:B:657:ILE:HG12	1:B:692:ILE:HD13	1.99	0.44
1:C:18:ILE:HD13	1:C:143:ALA:HB2	1.98	0.44
1:D:445:MET:O	2:H:83:HIS:HB2	2.16	0.44
1:D:525:LEU:O	1:D:569:GLU:HA	2.17	0.44
1:D:553:GLU:O	1:D:555:ILE:HG23	2.16	0.44
1:D:622:LEU:HD23	1:D:642:TYR:CE1	2.52	0.44
1:D:628:ILE:HG12	1:D:628:ILE:O	2.17	0.44
1:C:75:LEU:N	1:C:76:PRO:HD3	2.31	0.44
1:C:345:HIS:ND1	1:C:515:VAL:O	2.43	0.44
3:C:1801:B12:H531	3:C:1801:B12:C55	2.47	0.44
1:D:164:VAL:HG12	1:D:194:ILE:CG2	2.47	0.44
1:D:459:GLN:CG	1:D:460:TYR:HD2	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ARG:HD3	1:C:350:GLU:CG	2.48	0.44
1:A:647:VAL:HA	1:A:648:PRO:HD3	1.81	0.44
1:B:232:ARG:HA	1:B:232:ARG:NH1	2.32	0.44
1:C:360:ILE:HD13	1:C:360:ILE:HA	1.77	0.44
1:C:411:VAL:O	1:C:411:VAL:HG12	2.17	0.44
1:C:679:ASN:O	1:C:683:ILE:HG13	2.18	0.44
1:C:733:VAL:O	1:C:737:ARG:HG3	2.16	0.44
1:D:288:ARG:HG3	1:D:288:ARG:NH1	2.32	0.44
1:A:620:VAL:HG21	1:C:116:TYR:HE1	1.82	0.44
1:B:212:TRP:C	1:B:214:ASP:H	2.21	0.44
1:B:538:PHE:CD2	1:D:585:ILE:HG23	2.53	0.44
1:C:88:GLU:OE1	1:C:498:ARG:NH1	2.50	0.44
1:C:663:ALA:HB2	1:C:697:MET:HB2	2.00	0.44
1:C:94:MET:SD	1:C:105:ILE:HG21	2.57	0.44
1:C:109:ARG:NH2	1:C:114:SER:OG	2.48	0.44
1:C:396:ILE:HD11	2:G:29:MET:HG3	1.99	0.44
3:C:1801:B12:C53	3:C:1801:B12:H552	2.47	0.44
1:A:669:ILE:HG22	3:A:1801:B12:H202	1.99	0.44
1:B:446:ALA:HA	1:B:447:PRO:HD3	1.67	0.44
1:C:584:VAL:O	1:C:586:PRO:HD3	2.17	0.44
1:D:250:ILE:HD12	1:D:250:ILE:HA	1.65	0.44
1:C:622:LEU:HB2	1:C:667:SER:HB2	1.98	0.44
2:G:46:THR:HB	2:G:47:PRO:HD2	1.99	0.44
1:D:696:ILE:HG12	1:D:697:MET:H	1.81	0.44
1:A:350:GLU:CG	1:C:310:ARG:HD3	2.48	0.44
1:A:618:HIS:HD2	3:A:1801:B12:C48	2.31	0.44
1:B:110:THR:HG22	1:B:131:PRO:HA	2.00	0.44
1:B:116:TYR:HE1	1:D:620:VAL:HG21	1.83	0.44
1:C:335:THR:O	1:C:338:GLU:HB2	2.17	0.44
2:H:25:ARG:O	2:H:29:MET:HG3	2.18	0.44
3:A:1801:B12:H451	3:A:1801:B12:H411	1.54	0.43
3:A:1801:B12:H531	3:A:1801:B12:H543	2.00	0.43
1:B:18:ILE:HG23	1:B:142:LYS:HD3	2.00	0.43
1:B:607:LYS:O	1:B:608:ILE:HD12	2.18	0.43
1:B:617:GLU:HA	1:B:645:THR:HB	2.00	0.43
1:B:618:HIS:HD2	3:B:1801:B12:H482	1.83	0.43
1:B:663:ALA:HB2	1:B:697:MET:HE3	2.00	0.43
1:B:675:ILE:HD11	1:B:679:ASN:HD21	1.81	0.43
1:C:204:CYS:HG	1:C:251:PHE:HZ	1.66	0.43
1:C:457:VAL:HG13	1:C:471:LEU:HD21	1.99	0.43
1:D:445:MET:HE1	1:D:447:PRO:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:ILE:O	1:D:665:LEU:HD23	2.18	0.43
1:A:12:LYS:CE	1:C:530:PRO:O	2.66	0.43
1:B:142:LYS:O	1:B:145:ASP:HB2	2.17	0.43
2:F:57:MET:CE	2:F:82:GLY:HA2	2.49	0.43
3:C:1801:B12:H363	3:C:1801:B12:H412	1.48	0.43
1:D:291:PHE:CE1	2:H:27:TRP:CH2	3.06	0.43
1:D:471:LEU:HD12	1:D:471:LEU:HA	1.60	0.43
1:A:310:ARG:HD3	1:C:350:GLU:HG2	1.99	0.43
1:B:93:ARG:HD3	1:B:345:HIS:HA	2.00	0.43
1:A:349:ILE:N	1:A:349:ILE:CD1	2.81	0.43
1:A:665:LEU:HA	1:A:699:GLY:O	2.18	0.43
1:B:443:ASP:HA	1:B:456:ASN:HD22	1.84	0.43
3:C:1801:B12:H351	3:C:1801:B12:H372	1.99	0.43
3:C:1801:B12:H301	3:C:1801:B12:H253	1.54	0.43
1:D:668:THR:CG2	1:D:676:HIS:HB2	2.48	0.43
2:H:5:ASP:CA	2:H:6:ASP:HB3	2.46	0.43
1:A:7:LEU:HA	1:A:7:LEU:HD23	1.72	0.43
1:A:212:TRP:CZ2	1:A:477:LEU:HB3	2.54	0.43
1:A:307:ALA:O	1:A:340:ARG:HD3	2.18	0.43
1:C:189:VAL:CG1	1:C:196:MET:HB3	2.44	0.43
1:D:574:VAL:HA	1:D:575:PRO:HD3	1.77	0.43
1:C:23:ASP:OD2	1:C:24:LYS:HG2	2.18	0.43
1:B:236:LYS:HB3	1:B:415:TYR:HB2	2.01	0.43
1:D:243:VAL:O	1:D:247:LEU:HG	2.19	0.43
1:D:266:THR:O	1:D:266:THR:HG23	2.17	0.43
1:D:617:GLU:HB2	3:D:1801:B12:C43	2.49	0.43
1:B:126:GLY:CA	1:B:131:PRO:HD3	2.48	0.43
1:B:233:GLU:HB3	1:B:235:TRP:CH2	2.54	0.43
1:B:521:GLY:O	1:B:573:ARG:HA	2.18	0.43
1:B:612:THR:CG2	1:B:616:ASP:HB3	2.48	0.43
1:C:65:LYS:HE2	1:C:66:TYR:CZ	2.54	0.43
1:C:268:PRO:HA	1:C:269:PRO:HD3	1.71	0.43
1:D:57:ASN:HB3	1:D:99:TRP:CH2	2.53	0.43
1:D:116:TYR:CD1	1:D:116:TYR:N	2.86	0.43
1:D:204:CYS:SG	2:H:41:GLY:HA3	2.59	0.43
1:A:189:VAL:CG2	1:A:196:MET:HA	2.49	0.43
1:A:412:ASP:OD1	1:A:419:ARG:HG3	2.19	0.43
1:A:601:ILE:HD13	1:A:638:VAL:HG22	2.01	0.43
1:B:665:LEU:HA	1:B:699:GLY:O	2.19	0.43
1:C:7:LEU:HD23	1:C:7:LEU:HA	1.49	0.43
1:C:537:GLU:HG3	1:C:554:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:MET:HE3	1:D:305:MET:HB2	1.84	0.43
1:A:462:GLU:CD	1:A:462:GLU:H	2.22	0.43
3:A:1801:B12:H541	3:A:1801:B12:H602	1.76	0.43
1:B:650:GLU:O	1:B:651:LYS:C	2.55	0.43
2:F:74:ARG:HG3	2:F:74:ARG:NH1	2.33	0.43
1:C:6:GLN:CG	1:C:7:LEU:N	2.82	0.43
2:G:95:SER:O	2:G:96:VAL:C	2.56	0.43
1:D:561:GLN:O	1:D:562:GLU:C	2.56	0.43
1:A:649:VAL:HG12	1:A:686:LEU:HD22	2.00	0.42
3:A:1801:B12:H601	3:A:1801:B12:H252	2.00	0.42
1:C:116:TYR:HE2	1:C:120:ILE:HD13	1.83	0.42
1:C:464:LEU:HG	1:C:470:LYS:HB2	2.00	0.42
1:D:20:LYS:O	1:D:21:ASP:HB2	2.18	0.42
1:A:93:ARG:HG3	1:A:345:HIS:ND1	2.33	0.42
1:D:82:ILE:O	1:D:107:VAL:HG22	2.20	0.42
1:D:360:ILE:HD13	1:D:360:ILE:HA	1.87	0.42
1:A:524:LEU:HB3	1:C:526:THR:HB	2.01	0.42
1:A:574:VAL:HA	1:A:575:PRO:HD3	1.79	0.42
1:B:342:VAL:HG12	1:B:343:PRO:HD2	2.01	0.42
1:B:586:PRO:HA	1:B:587:PRO:HD3	1.87	0.42
1:B:706:THR:HA	1:B:707:PRO:HD3	1.92	0.42
3:C:1801:B12:H562	3:C:1801:B12:H18	1.85	0.42
2:E:36:PRO:O	2:E:40:LEU:HG	2.19	0.42
1:B:448:VAL:HB	2:F:56:ARG:HD2	2.01	0.42
1:B:693:ARG:O	1:B:693:ARG:CG	2.67	0.42
2:G:14:LEU:HD23	2:G:14:LEU:HA	1.86	0.42
1:D:613:VAL:HG11	1:D:679:ASN:HB3	2.02	0.42
1:A:446:ALA:HA	1:A:447:PRO:HD3	1.82	0.42
3:A:1801:B12:H203	3:A:1801:B12:H302	2.02	0.42
1:B:115:HIS:ND1	1:D:623:ARG:HD3	2.34	0.42
1:B:526:THR:HB	1:D:524:LEU:HB3	2.01	0.42
1:C:57:ASN:HB3	1:C:99:TRP:CH2	2.54	0.42
1:D:5:LEU:O	1:D:5:LEU:HD23	2.20	0.42
1:D:116:TYR:N	1:D:116:TYR:HD1	2.17	0.42
1:D:529:LEU:HA	1:D:530:PRO:HD3	1.84	0.42
3:D:1801:B12:C49	3:D:1801:B12:C47	2.88	0.42
1:A:623:ARG:HD3	1:C:115:HIS:CE1	2.54	0.42
1:B:114:SER:HB2	4:B:767:Z97:OP2	2.19	0.42
1:B:479:VAL:HG12	1:B:479:VAL:O	2.18	0.42
1:D:81:GLU:CD	4:D:767:Z97:HN	2.21	0.42
1:D:120:ILE:HG13	1:D:133:THR:CG2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:ARG:HH11	1:D:378:GLY:HA2	1.85	0.42
1:A:12:LYS:HE2	1:C:530:PRO:O	2.20	0.42
1:A:22:LEU:HD23	1:A:22:LEU:HA	1.88	0.42
1:B:171:VAL:HG22	1:B:209:ILE:HD13	2.02	0.42
1:B:471:LEU:HD12	1:B:471:LEU:HA	1.83	0.42
1:B:706:THR:HG22	1:B:708:GLU:H	1.85	0.42
5:B:1500:5AD:H5'3	3:D:1801:B12:C15	2.29	0.42
1:C:117:ASP:HA	1:C:164:VAL:HG23	2.01	0.42
1:C:120:ILE:HG13	1:C:133:THR:HG22	2.02	0.42
1:C:675:ILE:O	1:C:675:ILE:HD12	2.20	0.42
3:C:1801:B12:H492	3:C:1801:B12:C47	2.49	0.42
2:G:20:GLU:H	2:G:20:GLU:CD	2.22	0.42
2:G:40:LEU:HA	2:G:40:LEU:HD23	1.76	0.42
1:D:5:LEU:HD23	1:D:6:GLN:HB2	2.00	0.42
1:D:212:TRP:CZ2	1:D:477:LEU:HB3	2.55	0.42
1:D:540:ALA:HB1	1:D:570:LEU:HD11	2.01	0.42
2:H:5:ASP:CB	2:H:8:GLN:H	2.33	0.42
2:H:59:PHE:CZ	2:H:100:GLY:HA3	2.53	0.42
1:A:546:LYS:HZ2	1:C:578:ILE:HD11	1.82	0.42
1:A:662:ASP:O	1:A:663:ALA:HB2	2.20	0.42
1:B:123:THR:O	1:B:494:ASN:HA	2.19	0.42
1:B:137:VAL:CB	1:B:172:MET:HE3	2.49	0.42
1:C:160:TYR:HD1	4:C:767:Z97:C6	2.33	0.42
1:C:406:GLU:OE1	1:C:428:ILE:HB	2.19	0.42
1:C:411:VAL:HB	1:C:424:ILE:HG12	2.00	0.42
2:G:38:LEU:HA	2:G:38:LEU:HD23	1.82	0.42
2:G:57:MET:CE	2:G:82:GLY:HA2	2.50	0.42
1:D:26:THR:CG2	1:D:27:PRO:HD2	2.49	0.42
1:D:512:LYS:HE3	1:D:576:PHE:O	2.19	0.42
1:D:711:VAL:O	1:D:711:VAL:HG13	2.20	0.42
1:A:204:CYS:HB3	1:A:452:PHE:CD2	2.55	0.42
1:A:445:MET:HE2	1:A:446:ALA:C	2.39	0.42
1:A:597:ILE:HD11	1:A:730:THR:OG1	2.20	0.42
1:A:618:HIS:HD2	3:A:1801:B12:H482	1.84	0.42
1:B:14:ASP:O	1:B:18:ILE:HG13	2.20	0.42
1:B:176:GLU:OE1	1:B:176:GLU:HA	2.19	0.42
1:B:445:MET:CE	1:B:471:LEU:HD23	2.49	0.42
1:B:555:ILE:HG21	1:B:571:LYS:HG2	2.02	0.42
1:B:739:MET:HE2	1:B:739:MET:HB2	1.78	0.42
1:C:183:GLN:OE1	1:C:207:LYS:HE2	2.19	0.42
1:C:592:LEU:HD13	1:C:597:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:GLU:HG3	1:D:428:ILE:HG22	2.01	0.42
1:D:628:ILE:HG13	1:D:635:LYS:HB2	2.01	0.42
1:A:108:ILE:HA	1:A:160:TYR:CE2	2.55	0.42
1:B:618:HIS:HD2	3:B:1801:B12:C48	2.33	0.42
1:A:546:LYS:NZ	1:C:578:ILE:CD1	2.83	0.41
1:A:704:GLN:O	1:A:705:VAL:HG23	2.20	0.41
1:B:281:LEU:HB3	1:B:282:PRO:HD3	2.02	0.41
1:B:688:VAL:N	1:B:693:ARG:HB2	2.35	0.41
1:B:689:GLU:O	1:B:689:GLU:CG	2.67	0.41
1:C:116:TYR:CE2	1:C:120:ILE:HD13	2.55	0.41
1:C:250:ILE:HD12	1:C:250:ILE:HA	1.96	0.41
2:G:5:ASP:CA	2:G:7:PHE:N	2.66	0.41
1:D:187:TYR:CG	4:D:767:Z97:H2AB	2.55	0.41
1:D:696:ILE:HG23	1:D:697:MET:N	2.35	0.41
1:A:7:LEU:CD1	1:A:146:LEU:HB3	2.50	0.41
1:A:688:VAL:HG22	1:A:693:ARG:CG	2.49	0.41
1:A:697:MET:CE	1:A:736:ARG:HB2	2.50	0.41
2:E:62:LEU:HA	2:E:62:LEU:HD23	1.73	0.41
1:B:13:LEU:CD1	1:B:91:ILE:HG22	2.50	0.41
1:C:554:VAL:HA	1:C:570:LEU:HB3	2.01	0.41
1:C:668:THR:HG23	1:C:668:THR:O	2.20	0.41
1:D:467:GLU:N	1:D:468:PRO:HD3	2.35	0.41
1:D:618:HIS:HD2	3:D:1801:B12:H481	1.84	0.41
3:D:1801:B12:H351	3:D:1801:B12:C37	2.50	0.41
1:A:488:GLU:O	1:A:489:LEU:HD23	2.20	0.41
1:A:512:LYS:HB2	1:A:513:PRO:CD	2.50	0.41
1:B:41:LEU:HD23	1:B:43:MET:CE	2.51	0.41
1:B:320:LEU:HD22	1:B:359:LEU:HG	2.03	0.41
1:B:606:LEU:HD13	1:B:736:ARG:CZ	2.50	0.41
1:B:610:ALA:O	1:B:611:ALA:HB2	2.20	0.41
1:C:250:ILE:HG23	1:C:251:PHE:N	2.35	0.41
1:C:533:LYS:HB2	1:C:533:LYS:NZ	2.36	0.41
2:G:29:MET:HB2	2:G:29:MET:HE2	1.59	0.41
1:D:342:VAL:O	1:D:343:PRO:C	2.58	0.41
1:D:505:PHE:C	1:D:506:ARG:HG2	2.40	0.41
1:D:645:THR:O	1:D:646:SER:HB2	2.20	0.41
1:A:134:ARG:HA	1:A:172:MET:CE	2.50	0.41
5:A:1500:5AD:H5'3	3:C:1801:B12:C16	2.50	0.41
1:C:119:LEU:HD23	1:C:119:LEU:HA	1.84	0.41
1:D:189:VAL:HG21	1:D:196:MET:HA	2.02	0.41
1:A:393:GLU:OE2	2:E:25:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:ASP:OD2	1:A:736:ARG:NH1	2.53	0.41
1:C:22:LEU:C	1:C:24:LYS:H	2.22	0.41
1:C:300:MET:CE	1:C:333:THR:HG22	2.50	0.41
1:D:460:TYR:CE1	2:H:86:TYR:CE2	3.04	0.41
1:A:575:PRO:HD2	1:A:576:PHE:CD2	2.55	0.41
1:A:611:ALA:HB3	1:A:652:LEU:HD13	2.01	0.41
2:E:22:LEU:HD12	2:E:22:LEU:HA	1.89	0.41
2:E:39:ASP:HA	2:E:42:LYS:HD2	2.02	0.41
1:B:238:MET:O	1:B:242:MET:HG3	2.19	0.41
1:B:264:LEU:HD13	1:B:296:MET:CE	2.49	0.41
5:B:1500:5AD:C4'	3:D:1801:B12:N23	2.79	0.41
1:A:650:GLU:HG2	1:A:654:ASP:OD2	2.21	0.41
1:B:264:LEU:HD13	1:B:296:MET:HE2	2.03	0.41
1:B:334:ILE:HG23	1:B:338:GLU:HG3	2.02	0.41
1:B:531:THR:HG23	1:B:532:SER:O	2.21	0.41
1:C:173:PHE:CD1	1:C:178:VAL:HG21	2.55	0.41
1:D:447:PRO:HG2	2:H:57:MET:SD	2.60	0.41
1:D:534:ARG:O	1:D:538:PHE:HD2	2.03	0.41
1:D:574:VAL:HG13	1:D:576:PHE:CE1	2.55	0.41
1:D:723:SER:N	3:D:1801:B12:H5R2	2.35	0.41
5:A:1500:5AD:H5'2	3:C:1801:B12:H261	2.02	0.41
1:B:305:MET:HE3	1:B:305:MET:HB2	1.96	0.41
1:B:369:VAL:HG13	1:D:369:VAL:HG13	2.03	0.41
1:C:102:ALA:HB2	1:C:352:CYS:SG	2.61	0.41
3:C:1801:B12:H601	3:C:1801:B12:H252	2.02	0.41
2:H:103:LEU:HD22	2:H:109:TRP:CZ2	2.56	0.41
1:A:440:ARG:NH1	1:A:454:TYR:O	2.53	0.41
1:A:688:VAL:HG22	1:A:693:ARG:HB3	2.03	0.41
1:B:232:ARG:NE	1:D:598:ARG:NH1	2.69	0.41
1:B:307:ALA:O	1:B:340:ARG:HD3	2.20	0.41
1:B:623:ARG:HH21	1:B:642:TYR:HE2	1.69	0.41
1:C:141:ARG:NH1	1:C:179:ASN:OD1	2.54	0.41
1:C:264:LEU:HD12	1:C:264:LEU:N	2.35	0.41
1:C:289:GLU:OE2	1:C:385:LYS:NZ	2.44	0.41
3:C:1801:B12:H531	3:C:1801:B12:H552	2.03	0.41
1:D:5:LEU:HD23	1:D:5:LEU:C	2.40	0.41
1:D:8:ARG:HG3	1:D:11:GLU:CD	2.41	0.41
1:D:116:TYR:HE2	1:D:120:ILE:HD13	1.84	0.41
1:D:189:VAL:HG22	1:D:196:MET:HA	2.03	0.41
1:D:320:LEU:HD13	1:D:358:ALA:HB3	2.02	0.41
1:D:580:ILE:HD13	1:D:580:ILE:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ILE:HG21	1:C:560:MET:HE2	2.03	0.41
1:A:735:LYS:HD2	1:A:738:GLU:OE2	2.21	0.41
2:E:88:ILE:HD13	2:E:88:ILE:HA	1.80	0.41
1:B:566:THR:HG22	1:B:568:ILE:HG12	2.03	0.41
1:C:529:LEU:HA	1:C:530:PRO:HD3	1.73	0.41
1:C:619:SER:HB3	1:C:645:THR:HG21	2.02	0.41
1:A:201:ILE:HG23	2:E:41:GLY:HA2	2.02	0.40
1:A:297:ARG:HH21	1:A:332:SER:CB	2.34	0.40
1:B:259:LYS:HE2	1:B:294:TYR:CZ	2.55	0.40
1:B:269:PRO:HD2	1:B:280:ASP:OD1	2.21	0.40
1:B:401:TYR:O	1:B:405:VAL:HG23	2.20	0.40
1:B:531:THR:CG2	1:B:536:ALA:HB2	2.51	0.40
1:C:6:GLN:HG3	1:C:8:ARG:HD2	2.03	0.40
1:C:16:GLU:HG3	1:C:499:MET:HE1	2.02	0.40
2:G:57:MET:HE2	2:G:57:MET:HB2	1.95	0.40
1:D:344:TRP:CD1	1:D:515:VAL:HB	2.56	0.40
1:A:44:GLY:HA3	1:A:45:PRO:HD3	1.84	0.40
1:A:632:GLY:O	1:A:634:GLU:N	2.54	0.40
1:B:213:ALA:HB3	1:B:215:MET:HG3	2.02	0.40
1:B:669:ILE:HG22	3:B:1801:B12:H202	2.03	0.40
1:B:726:ILE:HG23	1:B:727:HIS:N	2.36	0.40
1:C:161:VAL:HG12	1:C:161:VAL:O	2.21	0.40
1:C:460:TYR:CD1	2:G:86:TYR:HE2	2.38	0.40
1:C:574:VAL:O	1:C:574:VAL:HG12	2.20	0.40
2:G:76:LEU:HD12	2:G:76:LEU:HA	1.86	0.40
1:D:281:LEU:HB3	1:D:282:PRO:HD3	2.01	0.40
1:D:445:MET:HE3	1:D:447:PRO:CD	2.50	0.40
1:A:635:LYS:HG3	1:C:232:ARG:HH22	1.86	0.40
1:A:701:GLY:HA2	1:A:705:VAL:HG11	2.01	0.40
1:B:685:GLU:O	1:B:688:VAL:HG12	2.20	0.40
3:B:1801:B12:H301	3:B:1801:B12:H253	1.82	0.40
1:C:144:LEU:O	1:C:148:GLU:HG2	2.21	0.40
1:D:116:TYR:CD2	1:D:120:ILE:HD13	2.55	0.40
1:D:528:PHE:CE1	1:D:560:MET:HG3	2.56	0.40
1:A:158:HIS:NE2	1:A:181:ALA:HA	2.36	0.40
1:C:323:SER:HB3	1:C:328:ALA:HB2	2.03	0.40
1:C:411:VAL:CB	1:C:424:ILE:HG12	2.51	0.40
2:G:54:LEU:HD23	2:G:57:MET:HE3	2.02	0.40
1:D:213:ALA:HB3	1:D:215:MET:HG3	2.02	0.40
1:D:238:MET:O	1:D:241:LEU:HB2	2.20	0.40
2:H:10:ARG:HE	2:H:10:ARG:HB3	1.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:98:GLU:H	2:H:98:GLU:HG2	1.72	0.40
1:A:161:VAL:HG12	1:A:161:VAL:O	2.22	0.40
1:A:189:VAL:HG22	1:A:196:MET:HA	2.04	0.40
1:A:219:ASP:HB3	1:A:248:ASN:ND2	2.35	0.40
1:A:467:GLU:C	1:A:469:SER:H	2.25	0.40
1:A:531:THR:HG22	1:A:536:ALA:HB2	2.03	0.40
1:A:654:ASP:O	1:A:657:ILE:HB	2.22	0.40
1:B:22:LEU:HA	1:B:22:LEU:HD23	1.87	0.40
1:B:415:TYR:O	1:B:416:TYR:C	2.60	0.40
1:C:96:MET:HE1	1:C:345:HIS:HB3	2.04	0.40
1:C:288:ARG:HD2	1:C:326:THR:HB	2.02	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%)	651 (90%)	61 (8%)	10 (1%)	11 34
1	B	722/763 (95%)	659 (91%)	56 (8%)	7 (1%)	15 44
1	C	722/763 (95%)	658 (91%)	58 (8%)	6 (1%)	19 49
1	D	722/763 (95%)	670 (93%)	49 (7%)	3 (0%)	34 66
2	E	108/121 (89%)	102 (94%)	5 (5%)	1 (1%)	17 46
2	F	108/121 (89%)	100 (93%)	6 (6%)	2 (2%)	8 26
2	G	108/121 (89%)	98 (91%)	8 (7%)	2 (2%)	8 26
2	H	108/121 (89%)	95 (88%)	12 (11%)	1 (1%)	17 46
All	All	3320/3536 (94%)	3033 (91%)	255 (8%)	32 (1%)	15 44

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
2	E	6	ASP
1	C	6	GLN
1	C	461	ASP
2	G	6	ASP
1	A	471	LEU
1	B	461	ASP
1	B	693	ARG
1	D	6	GLN
2	H	108	TYR
1	A	12	LYS
1	A	461	ASP
1	A	601	ILE
1	A	649	VAL
1	B	458	LYS
2	F	6	ASP
2	F	113	ILE
1	C	7	LEU
2	G	86	TYR
1	A	694	ASP
1	B	471	LEU
1	A	411	VAL
1	B	83	ALA
1	B	7	LEU
1	D	411	VAL
1	A	530	PRO
1	A	709	VAL
1	C	586	PRO
1	D	467	GLU
1	B	411	VAL
1	C	161	VAL
1	C	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	594/644 (92%)	574 (97%)	20 (3%)	37	71
1	B	602/644 (94%)	560 (93%)	42 (7%)	15	40
1	C	600/644 (93%)	558 (93%)	42 (7%)	15	40
1	D	602/644 (94%)	558 (93%)	44 (7%)	14	38
2	E	89/100 (89%)	83 (93%)	6 (7%)	16	43
2	F	90/100 (90%)	84 (93%)	6 (7%)	16	43
2	G	89/100 (89%)	83 (93%)	6 (7%)	16	43
2	H	89/100 (89%)	83 (93%)	6 (7%)	16	43
All	All	2755/2976 (93%)	2583 (94%)	172 (6%)	18	47

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	24	LYS
1	A	29	ARG
1	A	108	ILE
1	A	153	ARG
1	A	164	VAL
1	A	172	MET
1	A	198	ARG
1	A	260	SER
1	A	265	SER
1	A	391	PHE
1	A	490	ASP
1	A	491	GLU
1	A	492	ASN
1	A	578	ILE
1	A	591	ILE
1	A	616	ASP
1	A	672	HIS
1	A	730	THR
1	A	731	PHE
2	E	9	GLN
2	E	21	GLU
2	E	73	ASP
2	E	93	ASN
2	E	101	LEU
2	E	111	ASP
1	B	26	THR

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Mol	Chain	Res	Type
1	B	63	SER
1	B	79	THR
1	B	82	ILE
1	B	114	SER
1	B	151	VAL
1	B	159	SER
1	B	172	MET
1	B	179	ASN
1	B	232	ARG
1	B	260	SER
1	B	306	GLU
1	B	308	SER
1	B	338	GLU
1	B	341	ASN
1	B	349	ILE
1	B	391	PHE
1	B	411	VAL
1	B	428	ILE
1	B	464	LEU
1	B	465	VAL
1	B	471	LEU
1	B	486	ILE
1	B	501	GLU
1	B	532	SER
1	B	557	ARG
1	B	570	LEU
1	B	571	LYS
1	B	592	LEU
1	B	646	SER
1	B	651	LYS
1	B	660	LYS
1	B	672	HIS
1	B	673	ASP
1	B	675	ILE
1	B	688	VAL
1	B	695	LYS
1	B	703	THR
1	B	715	VAL
1	B	723	SER
1	B	736	ARG
1	B	739	MET
2	F	23	GLN

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Mol	Chain	Res	Type
2	F	48	SER
2	F	65	LYS
2	F	76	LEU
2	F	93	ASN
2	F	101	LEU
1	C	7	LEU
1	C	11	GLU
1	C	13	LEU
1	C	15	VAL
1	C	26	THR
1	C	33	THR
1	C	39	GLU
1	C	108	ILE
1	C	153	ARG
1	C	162	SER
1	C	183	GLN
1	C	189	VAL
1	C	199	SER
1	C	206	SER
1	C	290	MET
1	C	306	GLU
1	C	370	GLN
1	C	373	ARG
1	C	391	PHE
1	C	396	ILE
1	C	428	ILE
1	C	464	LEU
1	C	497	VAL
1	C	500	GLU
1	C	511	ILE
1	C	533	LYS
1	C	569	GLU
1	C	576	PHE
1	C	578	ILE
1	C	591	ILE
1	C	604	THR
1	C	613	VAL
1	C	628	ILE
1	C	650	GLU
1	C	651	LYS
1	C	660	LYS
1	C	668	THR

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Mol	Chain	Res	Type
1	C	676	HIS
1	C	681	LYS
1	C	721	ARG
1	C	731	PHE
1	C	736	ARG
2	G	9	GLN
2	G	29	MET
2	G	39	ASP
2	G	65	LYS
2	G	76	LEU
2	G	91	GLU
1	D	7	LEU
1	D	8	ARG
1	D	9	VAL
1	D	13	LEU
1	D	15	VAL
1	D	29	ARG
1	D	42	GLN
1	D	50	ASP
1	D	79	THR
1	D	108	ILE
1	D	110	THR
1	D	127	ILE
1	D	153	ARG
1	D	172	MET
1	D	179	ASN
1	D	225	HIS
1	D	232	ARG
1	D	250	ILE
1	D	301	ASN
1	D	306	GLU
1	D	391	PHE
1	D	397	GLU
1	D	427	GLN
1	D	428	ILE
1	D	429	ASN
1	D	442	GLU
1	D	445	MET
1	D	467	GLU
1	D	469	SER
1	D	471	LEU
1	D	499	MET

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Mol	Chain	Res	Type
1	D	502	THR
1	D	506	ARG
1	D	534	ARG
1	D	557	ARG
1	D	577	SER
1	D	668	THR
1	D	686	LEU
1	D	688	VAL
1	D	695	LYS
1	D	703	THR
1	D	711	VAL
1	D	731	PHE
1	D	736	ARG
2	H	25	ARG
2	H	39	ASP
2	H	76	LEU
2	H	101	LEU
2	H	107	LYS
2	H	111	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	23	GLN
1	B	630	HIS
1	C	245	HIS
1	D	115	HIS
1	D	245	HIS
1	D	248	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
4	Z97	A	767	-	23,24,24	2.59	9 (39%)	29,33,33	1.74	8 (27%)
4	Z97	D	767	-	23,24,24	2.56	8 (34%)	29,33,33	1.87	6 (20%)
5	5AD	C	1500	3	17,20,20	2.25	5 (29%)	15,30,30	4.14	8 (53%)
5	5AD	D	1500	3	17,20,20	2.28	6 (35%)	15,30,30	4.13	8 (53%)
4	Z97	B	767	-	23,24,24	2.40	7 (30%)	29,33,33	1.58	4 (13%)
3	B12	A	1801	1,5	90,101,101	1.34	8 (8%)	137,166,166	2.31	35 (25%)
3	B12	B	1801	1,5	90,101,101	1.36	9 (10%)	137,166,166	2.25	30 (21%)
5	5AD	A	1500	3	17,20,20	2.09	4 (23%)	15,30,30	4.04	7 (46%)
3	B12	D	1801	1,5	90,101,101	1.39	10 (11%)	137,166,166	2.28	26 (18%)
5	5AD	B	1500	3	17,20,20	2.31	5 (29%)	15,30,30	4.57	7 (46%)
3	B12	C	1801	1,5	90,101,101	1.41	9 (10%)	137,166,166	2.40	29 (21%)
4	Z97	C	767	-	23,24,24	2.57	7 (30%)	29,33,33	1.65	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Z97	A	767	-	-	6/18/18/18	0/1/1/1
4	Z97	D	767	-	-	9/18/18/18	0/1/1/1
5	5AD	C	1500	3	3/3/4/4	0/0/20/20	0/3/3/3
5	5AD	D	1500	3	3/3/4/4	0/0/20/20	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Z97	B	767	-	-	10/18/18/18	0/1/1/1
3	B12	A	1801	1,5	1/1/36/38	23/52/223/223	0/3/11/11
3	B12	B	1801	1,5	1/1/36/38	16/52/223/223	0/3/11/11
5	5AD	A	1500	3	2/2/4/4	0/0/20/20	0/3/3/3
3	B12	D	1801	1,5	1/1/36/38	16/52/223/223	0/3/11/11
5	5AD	B	1500	3	2/2/4/4	0/0/20/20	0/3/3/3
3	B12	C	1801	1,5	1/1/36/38	9/52/223/223	0/3/11/11
4	Z97	C	767	-	-	10/18/18/18	0/1/1/1

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	767	Z97	C4-C5	6.96	1.50	1.42
4	D	767	Z97	C4-C5	6.81	1.50	1.42
4	A	767	Z97	C4-C5	6.66	1.50	1.42
4	B	767	Z97	C4-C5	6.42	1.50	1.42
3	D	1801	B12	C14-N23	5.84	1.42	1.35
3	B	1801	B12	C14-N23	5.76	1.42	1.35
3	C	1801	B12	C14-N23	5.50	1.42	1.35
3	A	1801	B12	C14-N23	5.44	1.42	1.35
4	C	767	Z97	C4A-NE	5.38	1.45	1.27
5	C	1500	5AD	C2-N3	5.37	1.40	1.32
4	B	767	Z97	C4A-NE	5.35	1.45	1.27
5	B	1500	5AD	C2-N3	5.29	1.40	1.32
4	D	767	Z97	C4A-NE	5.25	1.44	1.27
5	D	1500	5AD	C2-N3	5.16	1.40	1.32
4	A	767	Z97	C4A-NE	5.13	1.44	1.27
5	A	1500	5AD	C2-N3	5.06	1.40	1.32
4	C	767	Z97	C2-N1	4.90	1.43	1.33
4	A	767	Z97	C2-N1	4.76	1.42	1.33
4	D	767	Z97	C2-N1	4.54	1.42	1.33
3	C	1801	B12	C19-N24	-4.47	1.40	1.48
3	D	1801	B12	C9-N22	4.45	1.42	1.30
3	C	1801	B12	C8B-C9B	4.43	1.49	1.40
3	A	1801	B12	C9-N22	4.41	1.42	1.30
3	B	1801	B12	C9-N22	4.40	1.42	1.30
5	B	1500	5AD	O4'-C1'	4.39	1.47	1.41
5	D	1500	5AD	O4'-C1'	4.32	1.47	1.41
4	C	767	Z97	C6-N1	4.24	1.43	1.34
3	C	1801	B12	C9-N22	4.24	1.41	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1500	5AD	O4'-C1'	4.09	1.46	1.41
3	B	1801	B12	C8B-C9B	4.06	1.48	1.40
3	C	1801	B12	C16-C15	-4.05	1.33	1.44
4	D	767	Z97	C6-N1	4.05	1.43	1.34
4	B	767	Z97	C2-N1	4.04	1.41	1.33
3	A	1801	B12	C8B-C9B	4.02	1.48	1.40
3	D	1801	B12	C8B-C9B	3.98	1.48	1.40
3	D	1801	B12	C16-C15	-3.91	1.33	1.44
3	D	1801	B12	C19-N24	-3.82	1.41	1.48
3	B	1801	B12	C19-N24	-3.79	1.41	1.48
3	B	1801	B12	C16-C15	-3.78	1.34	1.44
4	A	767	Z97	C6-N1	3.76	1.42	1.34
3	A	1801	B12	C19-N24	-3.75	1.41	1.48
3	A	1801	B12	C16-C15	-3.72	1.34	1.44
5	A	1500	5AD	O4'-C1'	3.53	1.46	1.41
3	B	1801	B12	C11-N23	3.42	1.43	1.37
4	A	767	Z97	C3-C2	3.40	1.44	1.40
3	C	1801	B12	C6B-C5B	3.36	1.49	1.40
3	D	1801	B12	C11-N23	3.35	1.43	1.37
4	B	767	Z97	C6-N1	3.34	1.41	1.34
3	D	1801	B12	C6B-C5B	3.34	1.49	1.40
3	A	1801	B12	C11-N23	3.30	1.43	1.37
3	A	1801	B12	C6B-C5B	3.25	1.49	1.40
4	A	767	Z97	C4-C4A	3.12	1.52	1.46
4	D	767	Z97	C4-C3	-3.06	1.36	1.40
3	B	1801	B12	C6B-C5B	3.05	1.48	1.40
5	A	1500	5AD	C8-N7	3.01	1.40	1.34
5	B	1500	5AD	C8-N7	3.00	1.40	1.34
3	D	1801	B12	C10-C9	2.93	1.47	1.39
3	C	1801	B12	C11-N23	2.92	1.42	1.37
3	A	1801	B12	C10-C9	2.88	1.47	1.39
5	D	1500	5AD	C8-N7	2.88	1.39	1.34
4	B	767	Z97	C4-C4A	2.84	1.52	1.46
5	C	1500	5AD	C8-N7	2.79	1.39	1.34
4	B	767	Z97	C4-C3	-2.71	1.36	1.40
4	C	767	Z97	C4-C4A	2.70	1.51	1.46
4	D	767	Z97	C4-C4A	2.65	1.51	1.46
3	C	1801	B12	C10-C9	2.57	1.46	1.39
4	D	767	Z97	OXT-C	2.53	1.38	1.30
4	C	767	Z97	C4-C3	-2.50	1.37	1.40
5	D	1500	5AD	C6-N6	2.49	1.43	1.34
4	C	767	Z97	OXT-C	2.48	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	767	Z97	OXT-C	2.47	1.38	1.30
5	A	1500	5AD	C6-N6	2.43	1.42	1.34
3	B	1801	B12	C10-C9	2.41	1.46	1.39
5	C	1500	5AD	C6-N6	2.37	1.42	1.34
5	B	1500	5AD	C6-N6	2.34	1.42	1.34
5	D	1500	5AD	O2'-C2'	-2.22	1.37	1.43
4	B	767	Z97	OXT-C	2.20	1.37	1.30
4	D	767	Z97	C3-C2	2.19	1.43	1.40
5	D	1500	5AD	C6-C5	-2.19	1.35	1.43
3	D	1801	B12	O6R-C1R	2.14	1.44	1.41
3	D	1801	B12	C14-C15	2.12	1.47	1.38
5	B	1500	5AD	C6-C5	-2.10	1.35	1.43
3	C	1801	B12	C1-C19	-2.09	1.50	1.55
5	C	1500	5AD	C6-C5	-2.04	1.35	1.43
4	A	767	Z97	C2A-C2	2.02	1.53	1.50
3	B	1801	B12	C14-C15	2.02	1.47	1.38
4	A	767	Z97	C4-C3	-2.00	1.37	1.40

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1500	5AD	C5'-C4'-C3'	12.46	128.78	115.70
5	C	1500	5AD	C5'-C4'-C3'	10.53	126.75	115.70
5	D	1500	5AD	C5'-C4'-C3'	10.12	126.33	115.70
5	A	1500	5AD	C5'-C4'-C3'	9.85	126.04	115.70
3	A	1801	B12	C1-C19-N24	9.39	116.81	106.24
3	C	1801	B12	C20-C1-C19	-9.34	100.35	109.36
3	D	1801	B12	C1-C19-N24	8.84	116.18	106.24
3	B	1801	B12	C1-C19-N24	8.56	115.87	106.24
3	B	1801	B12	C13-C12-C11	-8.42	91.44	100.97
3	C	1801	B12	C1-C19-N24	8.03	115.27	106.24
3	C	1801	B12	C46-C12-C13	-7.82	80.89	112.72
3	D	1801	B12	C46-C12-C13	-7.81	80.92	112.72
3	A	1801	B12	C13-C12-C11	-7.56	92.42	100.97
3	C	1801	B12	C47-C12-C46	7.49	122.01	109.35
3	A	1801	B12	C46-C12-C13	-7.47	82.29	112.72
3	C	1801	B12	C13-C12-C11	-7.43	92.56	100.97
3	D	1801	B12	C47-C12-C46	7.41	121.88	109.35
3	B	1801	B12	C1-C19-C18	7.26	133.80	121.88
3	A	1801	B12	C47-C12-C46	7.25	121.60	109.35
3	D	1801	B12	C13-C12-C11	-7.15	92.87	100.97
3	B	1801	B12	C47-C12-C46	6.73	120.72	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1801	B12	C12-C11-N23	6.71	121.18	111.83
5	B	1500	5AD	O3'-C3'-C4'	6.63	126.72	110.47
3	B	1801	B12	C46-C12-C13	-6.61	85.80	112.72
3	A	1801	B12	C12-C11-N23	6.60	121.03	111.83
3	C	1801	B12	C1-C19-C18	6.54	132.62	121.88
5	D	1500	5AD	O3'-C3'-C4'	6.16	125.56	110.47
3	D	1801	B12	C18-C19-N24	6.16	111.68	102.31
3	D	1801	B12	C1-C19-C18	6.09	131.87	121.88
5	C	1500	5AD	O3'-C3'-C4'	6.08	125.37	110.47
5	A	1500	5AD	O3'-C3'-C4'	6.01	125.20	110.47
3	A	1801	B12	C1-C19-C18	5.97	131.68	121.88
3	B	1801	B12	C12-C11-N23	5.96	120.14	111.83
3	C	1801	B12	C26-C2-C1	5.94	119.27	110.01
3	C	1801	B12	C18-C19-N24	5.87	111.24	102.31
3	A	1801	B12	C18-C19-N24	5.86	111.22	102.31
5	D	1500	5AD	N3-C2-N1	-5.82	119.58	128.68
3	A	1801	B12	C47-C12-C13	-5.81	89.06	112.72
3	D	1801	B12	C12-C11-C10	-5.74	115.89	123.37
3	B	1801	B12	C12-C11-C10	-5.67	115.98	123.37
3	B	1801	B12	C47-C12-C13	-5.64	89.74	112.72
5	B	1500	5AD	N3-C2-N1	-5.60	119.92	128.68
5	C	1500	5AD	N3-C2-N1	-5.56	119.99	128.68
3	A	1801	B12	C12-C11-C10	-5.36	116.39	123.37
4	D	767	Z97	OP4-C5A-C5	5.29	119.43	109.35
5	A	1500	5AD	N3-C2-N1	-5.28	120.43	128.68
3	A	1801	B12	C20-C1-C19	-5.22	104.33	109.36
3	C	1801	B12	C30-C3-C2	-5.20	108.09	119.09
3	C	1801	B12	C12-C11-N23	5.19	119.06	111.83
3	C	1801	B12	C12-C11-C10	-5.15	116.66	123.37
3	C	1801	B12	C55-C17-C16	-5.14	106.49	116.65
3	D	1801	B12	C47-C12-C13	-5.09	91.99	112.72
3	D	1801	B12	C30-C3-C2	-5.03	108.43	119.09
5	A	1500	5AD	O3'-C3'-C2'	5.03	128.09	111.82
3	C	1801	B12	C47-C12-C13	-4.99	92.40	112.72
3	B	1801	B12	C18-C19-N24	4.99	109.90	102.31
5	B	1500	5AD	O2'-C2'-C3'	4.95	127.84	111.82
3	B	1801	B12	C55-C17-C16	-4.95	106.88	116.65
4	C	767	Z97	OP4-C5A-C5	4.94	118.76	109.35
5	A	1500	5AD	O2'-C2'-C3'	4.90	127.68	111.82
3	D	1801	B12	C19-C1-N21	4.82	107.10	102.16
5	B	1500	5AD	O3'-C3'-C2'	4.78	127.28	111.82
3	D	1801	B12	C55-C17-C16	-4.65	107.47	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1500	5AD	O2'-C2'-C3'	4.54	126.49	111.82
4	D	767	Z97	CD-NE-C4A	-4.49	105.11	118.90
5	D	1500	5AD	O2'-C2'-C3'	4.40	126.06	111.82
5	A	1500	5AD	O2'-C2'-C1'	4.39	127.07	110.85
3	D	1801	B12	C20-C1-C19	-4.39	105.13	109.36
5	B	1500	5AD	O2'-C2'-C1'	4.39	127.05	110.85
5	C	1500	5AD	O2'-C2'-C1'	4.33	126.86	110.85
3	B	1801	B12	C19-C1-N21	4.32	106.59	102.16
3	B	1801	B12	C2P-C1P-N59	-4.27	106.64	112.93
3	A	1801	B12	C30-C3-C2	-4.21	110.18	119.09
5	D	1500	5AD	O3'-C3'-C2'	4.20	125.40	111.82
3	A	1801	B12	C19-C1-N21	4.17	106.43	102.16
5	D	1500	5AD	O2'-C2'-C1'	4.15	126.18	110.85
4	A	767	Z97	CG-CD-NE	4.13	121.05	110.93
3	C	1801	B12	C19-C1-N21	4.07	106.33	102.16
3	C	1801	B12	C2-C1-N21	4.04	107.40	101.77
5	C	1500	5AD	O3'-C3'-C2'	4.03	124.85	111.82
3	C	1801	B12	C2-C1-C19	4.01	124.93	118.60
5	D	1500	5AD	C3'-C2'-C1'	3.90	106.85	100.98
4	A	767	Z97	OP4-C5A-C5	3.90	116.78	109.35
4	B	767	Z97	OP4-C5A-C5	3.87	116.72	109.35
3	B	1801	B12	C20-C1-C19	-3.83	105.67	109.36
3	D	1801	B12	C2-C1-N21	3.81	107.08	101.77
3	C	1801	B12	C13-C14-N23	3.80	114.27	109.10
3	B	1801	B12	C2-C1-N21	3.71	106.94	101.77
3	A	1801	B12	C55-C17-C16	-3.70	109.34	116.65
3	C	1801	B12	C15-C14-N23	-3.67	121.78	126.26
3	A	1801	B12	C26-C2-C1	3.63	115.67	110.01
3	D	1801	B12	C12-C13-C14	3.63	108.33	102.26
3	B	1801	B12	C47-C12-C11	3.54	122.82	110.08
3	A	1801	B12	C2-C1-N21	3.50	106.64	101.77
3	A	1801	B12	C13-C14-N23	3.49	113.85	109.10
3	C	1801	B12	C18-C60-C61	-3.35	105.61	113.97
3	A	1801	B12	C12-C13-C14	3.30	107.78	102.26
4	D	767	Z97	CG-CD-NE	3.28	118.97	110.93
3	B	1801	B12	C15-C14-N23	-3.27	122.27	126.26
3	D	1801	B12	C13-C14-N23	3.22	113.48	109.10
3	D	1801	B12	C25-C2-C1	-3.17	109.01	113.78
4	D	767	Z97	C3-C4-C5	3.15	120.67	118.26
3	C	1801	B12	C25-C2-C1	-3.11	109.09	113.78
3	A	1801	B12	C15-C14-N23	-3.09	122.49	126.26
5	C	1500	5AD	C3'-C2'-C1'	3.08	105.62	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	767	Z97	CD-NE-C4A	-3.05	109.52	118.90
3	A	1801	B12	C7-C6-N22	3.01	113.44	107.94
3	D	1801	B12	C26-C2-C1	2.98	114.66	110.01
4	A	767	Z97	CD-NE-C4A	-2.98	109.75	118.90
3	D	1801	B12	C46-C12-C11	2.96	120.74	110.08
3	D	1801	B12	C18-C17-C16	2.94	104.24	100.67
3	B	1801	B12	C13-C14-N23	2.92	113.08	109.10
3	D	1801	B12	C7-C6-N22	2.92	113.27	107.94
5	B	1500	5AD	O4'-C4'-C5'	2.91	124.58	110.29
3	B	1801	B12	C26-C2-C1	2.90	114.52	110.01
3	B	1801	B12	C12-C13-C14	2.90	107.11	102.26
5	A	1500	5AD	O4'-C4'-C5'	2.88	124.42	110.29
3	B	1801	B12	C30-C3-C2	-2.87	113.01	119.09
3	B	1801	B12	C20-C1-C2	-2.85	108.52	113.28
5	C	1500	5AD	O4'-C4'-C5'	2.85	124.25	110.29
4	C	767	Z97	CD-NE-C4A	-2.83	110.20	118.90
5	D	1500	5AD	O4'-C4'-C5'	2.81	124.08	110.29
4	B	767	Z97	OXT-C-O	-2.78	117.79	124.09
3	D	1801	B12	C15-C14-N23	-2.73	122.92	126.26
4	A	767	Z97	C5-C4-C4A	-2.71	117.11	121.56
3	A	1801	B12	C46-C12-C11	2.69	119.76	110.08
4	B	767	Z97	C5-C6-N1	-2.67	119.37	123.82
3	C	1801	B12	C47-C12-C11	2.66	119.66	110.08
3	A	1801	B12	C16-C15-C14	-2.60	117.31	121.25
3	A	1801	B12	C3R-C2R-C1R	2.59	105.62	99.89
3	D	1801	B12	C20-C1-C2	-2.57	108.99	113.28
4	A	767	Z97	OXT-C-O	-2.55	118.31	124.09
3	C	1801	B12	C7-C6-N22	2.54	112.58	107.94
3	C	1801	B12	C30-C31-C32	-2.53	104.02	112.59
3	B	1801	B12	C2-C26-C27	-2.50	108.19	115.22
3	A	1801	B12	C20-C1-C2	-2.50	109.11	113.28
3	A	1801	B12	C9-C10-C11	-2.48	122.38	125.97
3	C	1801	B12	C20-C1-C2	-2.42	109.24	113.28
3	B	1801	B12	C9-C10-C11	-2.41	122.48	125.97
3	A	1801	B12	C18-C17-C16	2.40	103.59	100.67
3	D	1801	B12	C30-C31-C32	-2.39	104.48	112.59
3	B	1801	B12	C7-C6-N22	2.38	112.29	107.94
4	C	767	Z97	CG-CD-NE	2.38	116.76	110.93
3	B	1801	B12	C18-C17-C16	2.38	103.56	100.67
3	A	1801	B12	C7-C6-C5	-2.36	124.35	128.07
3	B	1801	B12	C3R-C2R-C1R	2.35	105.09	99.89
4	D	767	Z97	O3-C3-C2	2.33	122.58	117.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1801	B12	O6R-C1R-C2R	-2.32	103.53	106.93
3	B	1801	B12	C25-C2-C1	-2.31	110.30	113.78
3	B	1801	B12	C1-C2-C3	2.29	104.53	101.60
3	A	1801	B12	C18-C60-C61	-2.29	108.25	113.97
4	C	767	Z97	C3-C4-C5	2.29	120.02	118.26
4	C	767	Z97	OXT-C-O	-2.29	118.90	124.09
3	C	1801	B12	C48-C13-C14	2.27	114.15	108.49
3	A	1801	B12	C47-C12-C11	2.26	118.23	110.08
3	C	1801	B12	C46-C12-C11	2.24	118.16	110.08
4	D	767	Z97	C5-C6-N1	-2.24	120.09	123.82
3	A	1801	B12	C25-C2-C1	-2.22	110.43	113.78
4	C	767	Z97	OXT-C-CA	2.22	120.96	113.38
3	A	1801	B12	C30-C31-C32	-2.21	105.10	112.59
4	A	767	Z97	CB-CA-N	2.20	115.95	110.17
3	D	1801	B12	C7-C6-C5	-2.19	124.63	128.07
3	A	1801	B12	C1-C2-C3	2.18	104.38	101.60
3	A	1801	B12	C2P-C1P-N59	-2.17	109.73	112.93
3	C	1801	B12	C18-C17-C16	2.16	103.30	100.67
4	A	767	Z97	C3-C4-C4A	2.15	124.42	120.41
4	A	767	Z97	OP2-P-OP4	2.13	112.40	106.73
3	D	1801	B12	C2P-C1P-N59	-2.12	109.80	112.93
3	A	1801	B12	C54-C17-C18	-2.12	109.86	112.98
3	A	1801	B12	C2-C1-C19	2.11	121.94	118.60
3	C	1801	B12	C12-C13-C14	2.09	105.75	102.26
3	C	1801	B12	C7-C6-C5	-2.05	124.85	128.07
3	A	1801	B12	C53-C15-C16	2.04	123.89	120.38
3	B	1801	B12	C18-C60-C61	-2.04	108.89	113.97

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
5	A	1500	5AD	C2'
5	A	1500	5AD	C3'
5	B	1500	5AD	C2'
5	B	1500	5AD	C3'
5	C	1500	5AD	C2'
5	C	1500	5AD	C4'
5	C	1500	5AD	C3'

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Mol	Chain	Res	Type	Atom
5	D	1500	5AD	C2'
5	D	1500	5AD	C3'
5	D	1500	5AD	C4'

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	A	1801	B12	C3P-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	C42-C41-C8-C9
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	C38-C37-C7-C6
3	D	1801	B12	C38-C37-C7-C8
3	D	1801	B12	C16-C17-C55-C56
3	D	1801	B12	C54-C17-C55-C56
3	D	1801	B12	C18-C17-C55-C56
4	A	767	Z97	C-CA-CB-CG
4	A	767	Z97	N-CA-CB-CG
4	A	767	Z97	CA-CB-CG-CD
4	A	767	Z97	C4-C4A-NE-CD
4	B	767	Z97	C5A-OP4-P-OP1
4	B	767	Z97	C5A-OP4-P-OP2
4	B	767	Z97	C5A-OP4-P-OP3
4	C	767	Z97	C5A-OP4-P-OP2
4	D	767	Z97	C-CA-CB-CG
3	A	1801	B12	O58-C57-N59-C1P
3	A	1801	B12	C12-C13-C48-C49
3	B	1801	B12	C42-C41-C8-C7
3	C	1801	B12	C42-C41-C8-C7
3	A	1801	B12	C4-C3-C30-C31
3	C	1801	B12	C7-C37-C38-N40

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Mol	Chain	Res	Type	Atoms
4	B	767	Z97	NE-CD-CG-CB
4	C	767	Z97	NE-CD-CG-CB
3	A	1801	B12	C42-C41-C8-C9
4	D	767	Z97	OXT-C-CA-N
3	C	1801	B12	C4-C3-C30-C31
3	B	1801	B12	C7-C37-C38-N40
3	C	1801	B12	C7-C37-C38-O39
4	D	767	Z97	NE-CD-CG-CB
4	A	767	Z97	O-C-CA-CB
3	A	1801	B12	C7-C37-C38-N40
3	B	1801	B12	C7-C37-C38-O39
4	A	767	Z97	CG-CD-NE-C4A
3	A	1801	B12	C8-C41-C42-C43
4	B	767	Z97	OXT-C-CA-N
3	D	1801	B12	C18-C60-C61-N62
3	D	1801	B12	C4-C3-C30-C31
3	A	1801	B12	C13-C48-C49-C50
3	D	1801	B12	C7-C37-C38-N40
4	C	767	Z97	C5A-OP4-P-OP1
4	D	767	Z97	C5A-OP4-P-OP1
3	D	1801	B12	O58-C57-N59-C1P
3	B	1801	B12	C41-C42-C43-O44
3	B	1801	B12	C41-C42-C43-N45
4	C	767	Z97	OXT-C-CA-N
3	A	1801	B12	C7-C37-C38-O39
3	D	1801	B12	C7-C37-C38-O39
4	C	767	Z97	CA-CB-CG-CD
4	D	767	Z97	O-C-CA-N
3	B	1801	B12	O6R-C4R-C5R-O8R
3	D	1801	B12	C18-C60-C61-O63
3	D	1801	B12	C56-C57-N59-C1P
3	C	1801	B12	C2P-O3-P-O2
4	C	767	Z97	C5A-OP4-P-OP3
3	B	1801	B12	O58-C57-N59-C1P
4	B	767	Z97	N-CA-CB-CG
4	B	767	Z97	CG-CD-NE-C4A
4	D	767	Z97	O-C-CA-CB
3	A	1801	B12	C30-C31-C32-N33
3	B	1801	B12	C2-C26-C27-N29
3	A	1801	B12	C2-C3-C30-C31
3	A	1801	B12	C17-C18-C60-C61
3	D	1801	B12	C1P-C2P-O3-P

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Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C30-C31-C32-O34
4	C	767	Z97	OXT-C-CA-CB
4	C	767	Z97	C3-C4-C4A-NE
3	B	1801	B12	C56-C57-N59-C1P
4	C	767	Z97	O-C-CA-CB
3	B	1801	B12	C2-C26-C27-O28
4	B	767	Z97	O-C-CA-CB
3	A	1801	B12	C19-C18-C60-C61
4	C	767	Z97	O-C-CA-N
4	B	767	Z97	OXT-C-CA-CB
4	D	767	Z97	C5A-OP4-P-OP2
3	A	1801	B12	C3-C2-C26-C27
3	A	1801	B12	C41-C42-C43-N45
3	B	1801	B12	C3-C2-C26-C27
4	B	767	Z97	CA-CB-CG-CD
4	D	767	Z97	OXT-C-CA-CB
3	D	1801	B12	C17-C18-C60-C61
4	D	767	Z97	CA-CB-CG-CD
3	D	1801	B12	N59-C1P-C2P-O3
3	A	1801	B12	C41-C42-C43-O44
3	B	1801	B12	C19-C18-C60-C61
3	D	1801	B12	C19-C18-C60-C61

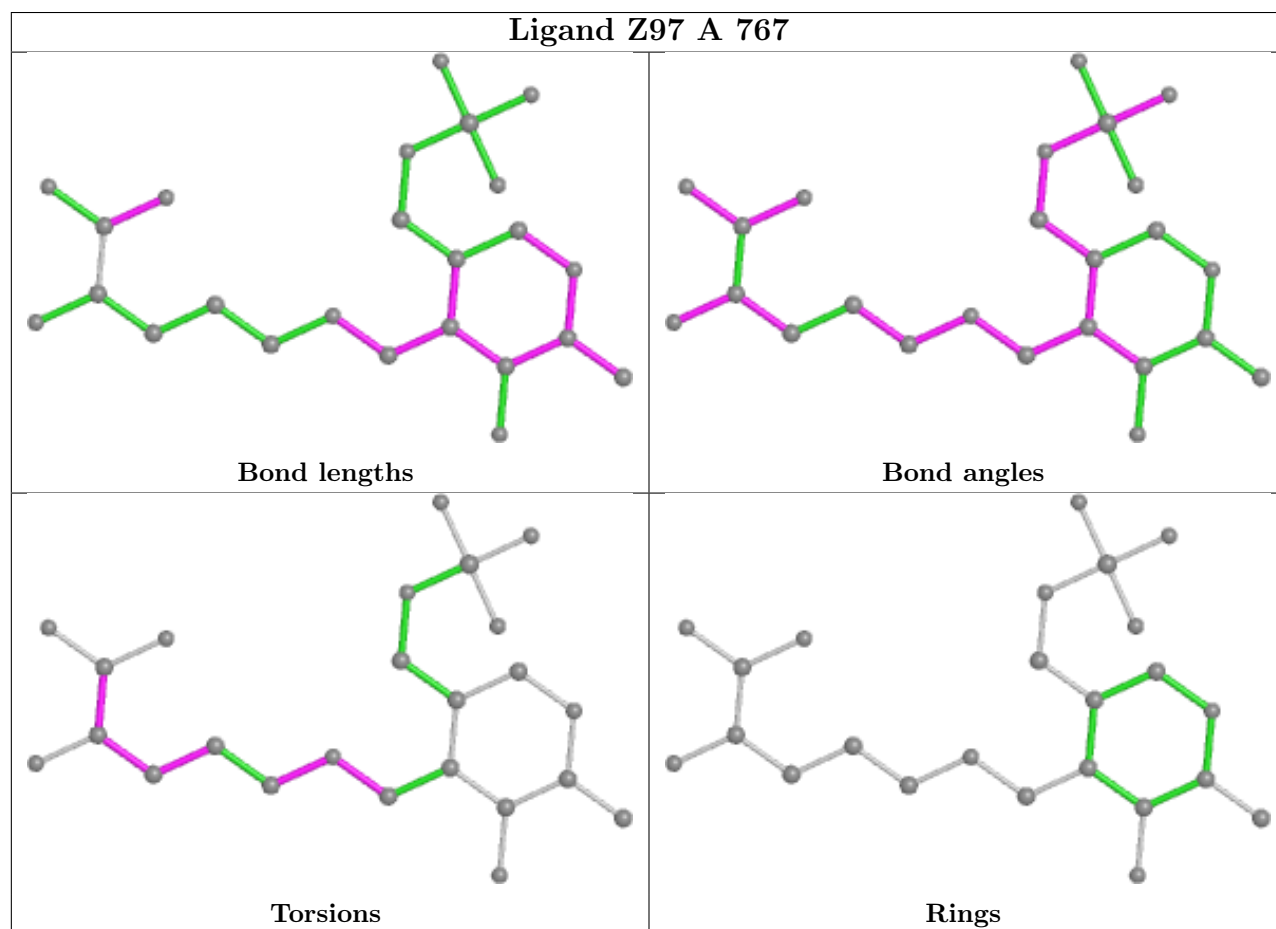
There are no ring outliers.

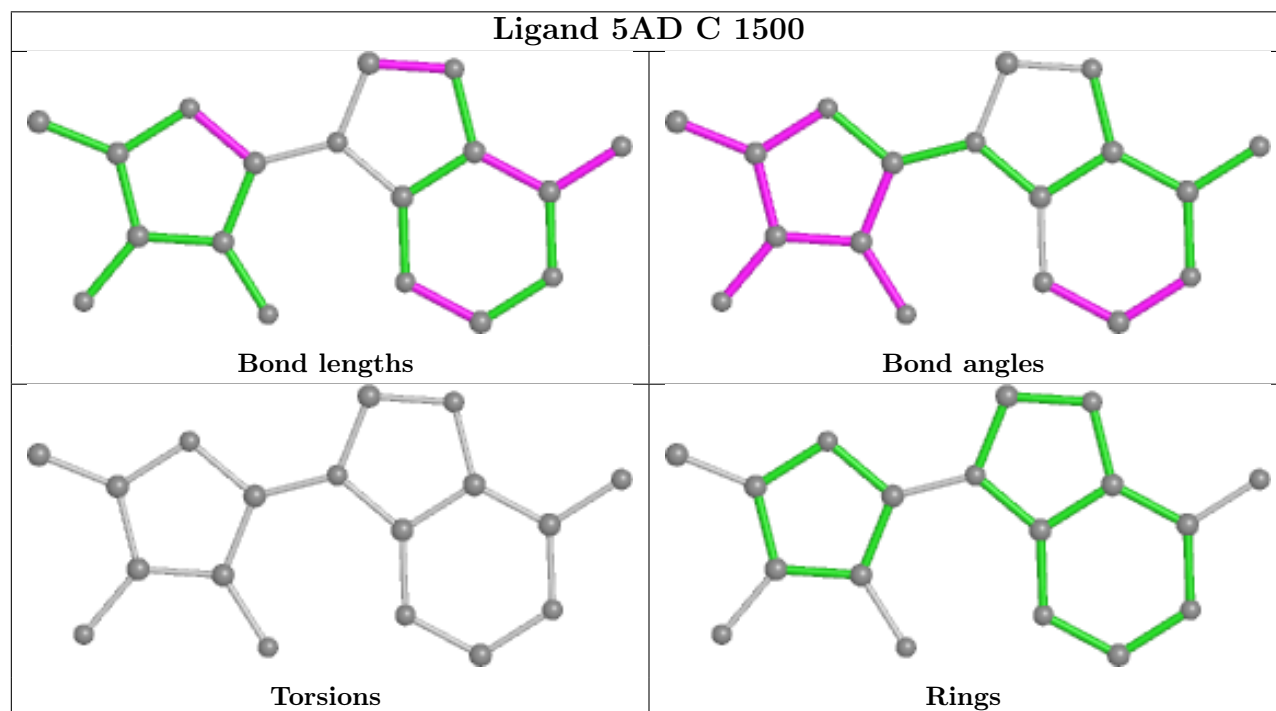
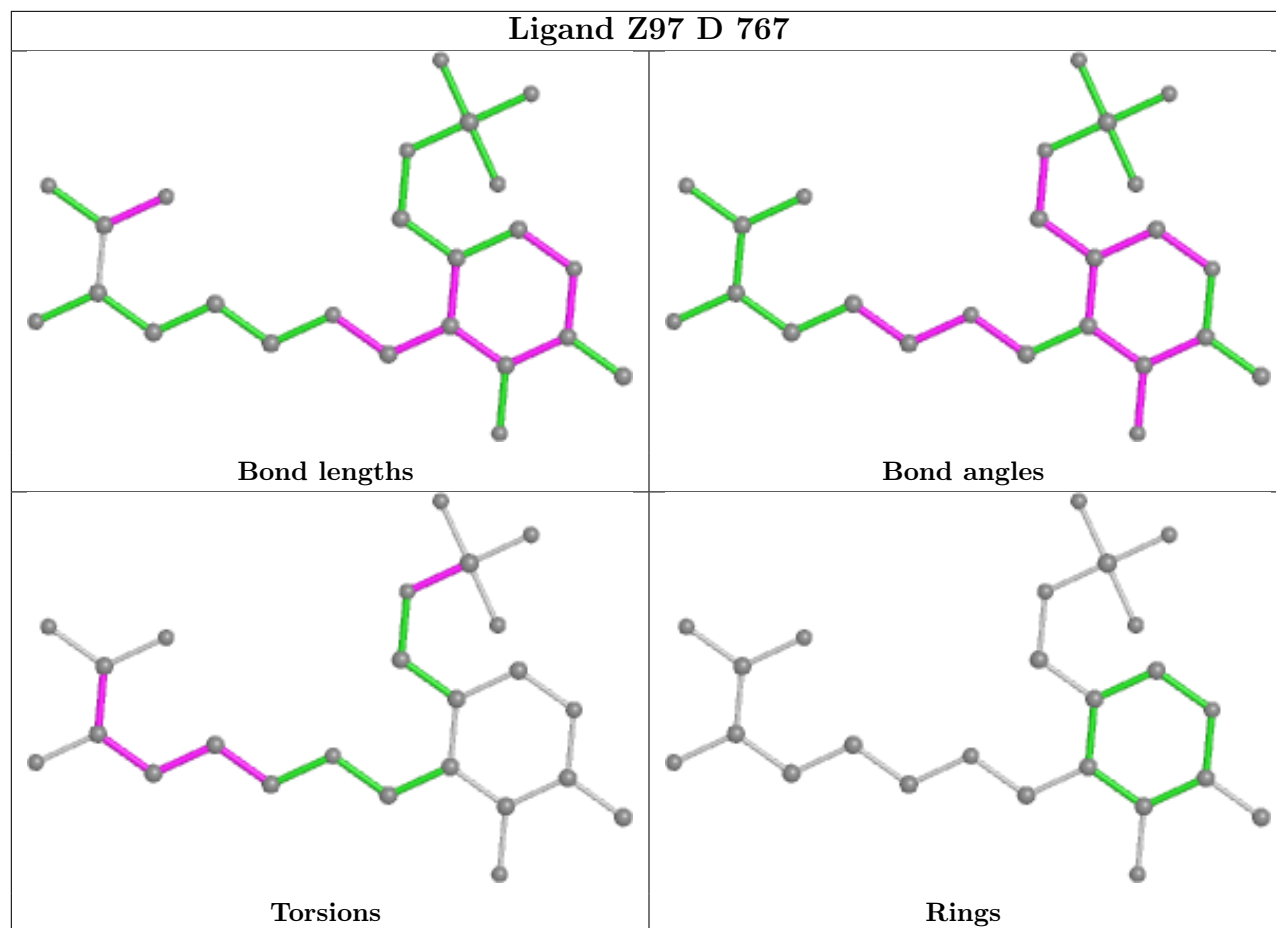
11 monomers are involved in 114 short contacts:

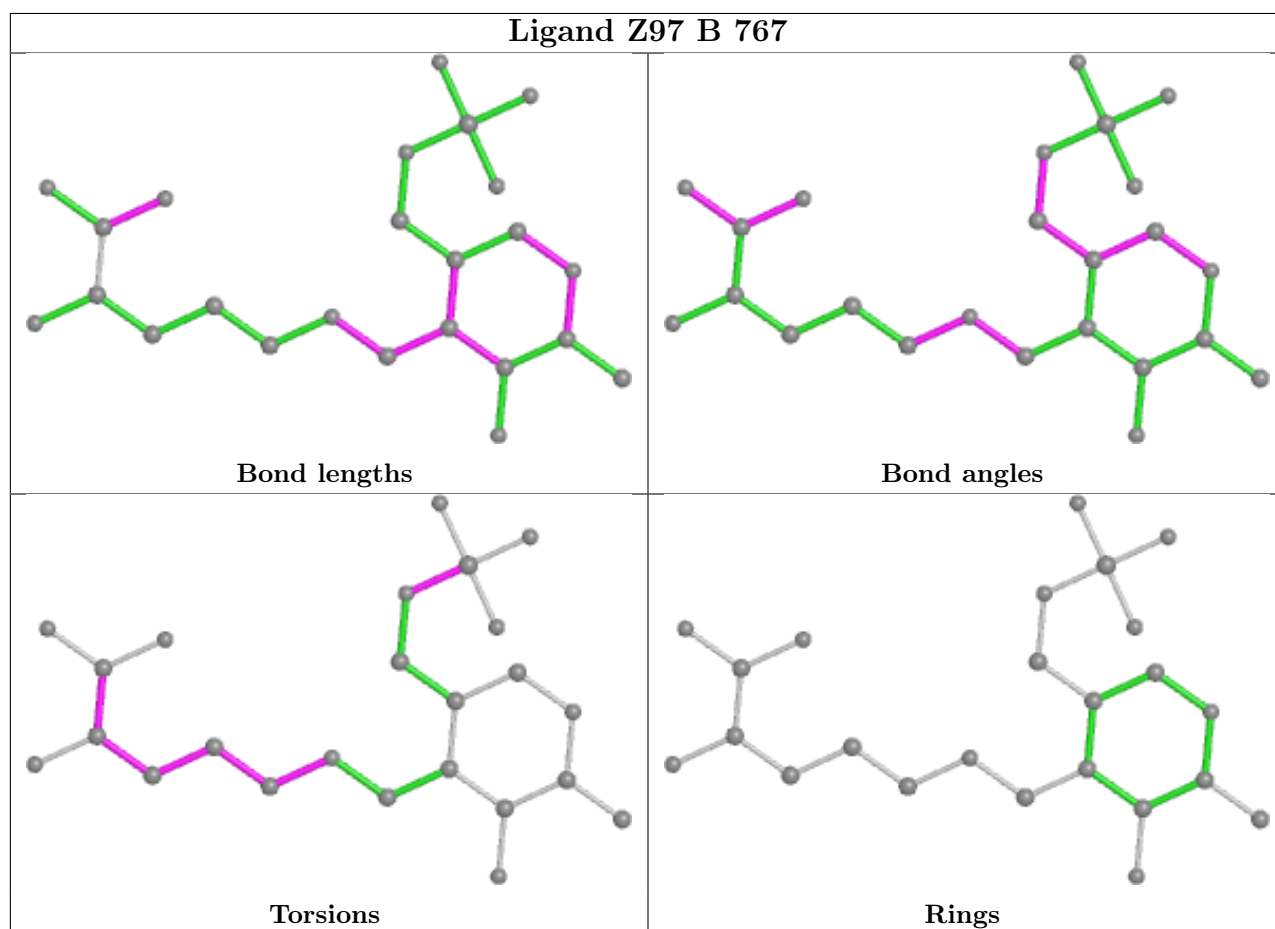
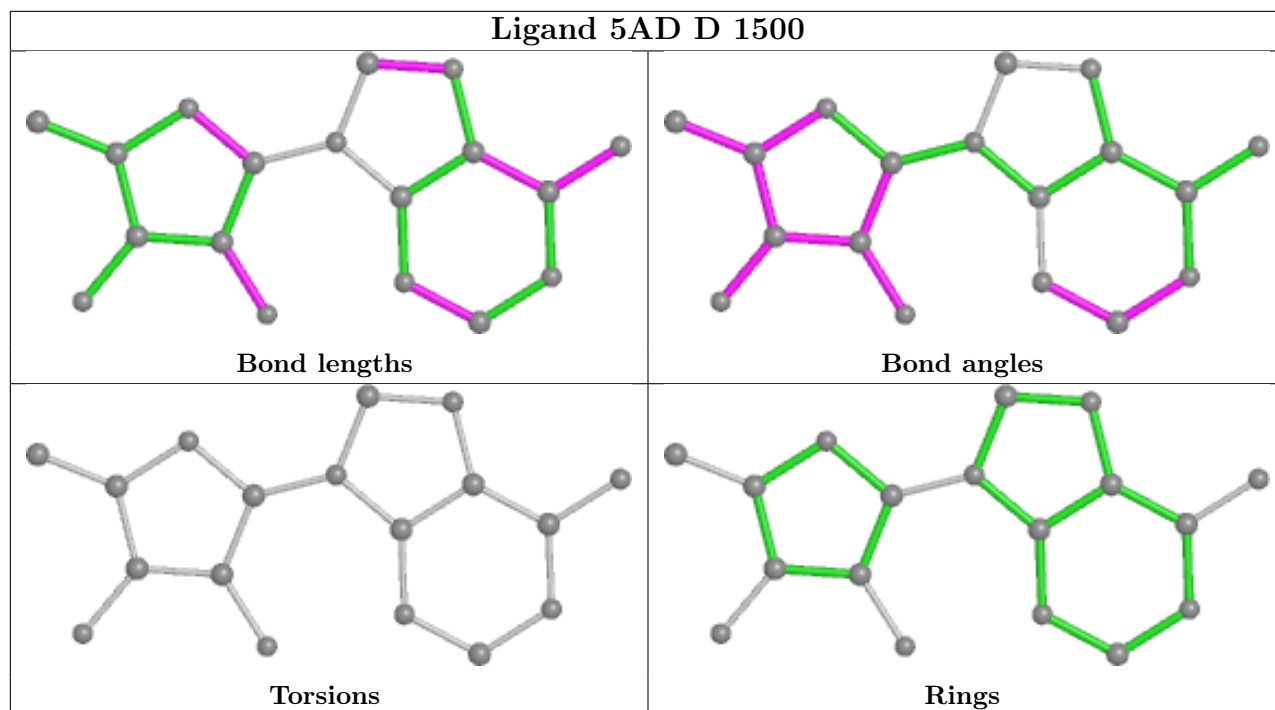
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	767	Z97	3	0
5	C	1500	5AD	2	0
5	D	1500	5AD	2	0
4	B	767	Z97	4	0
3	A	1801	B12	24	0
3	B	1801	B12	22	0
5	A	1500	5AD	3	0
3	D	1801	B12	33	0
5	B	1500	5AD	4	0
3	C	1801	B12	26	0
4	C	767	Z97	2	0

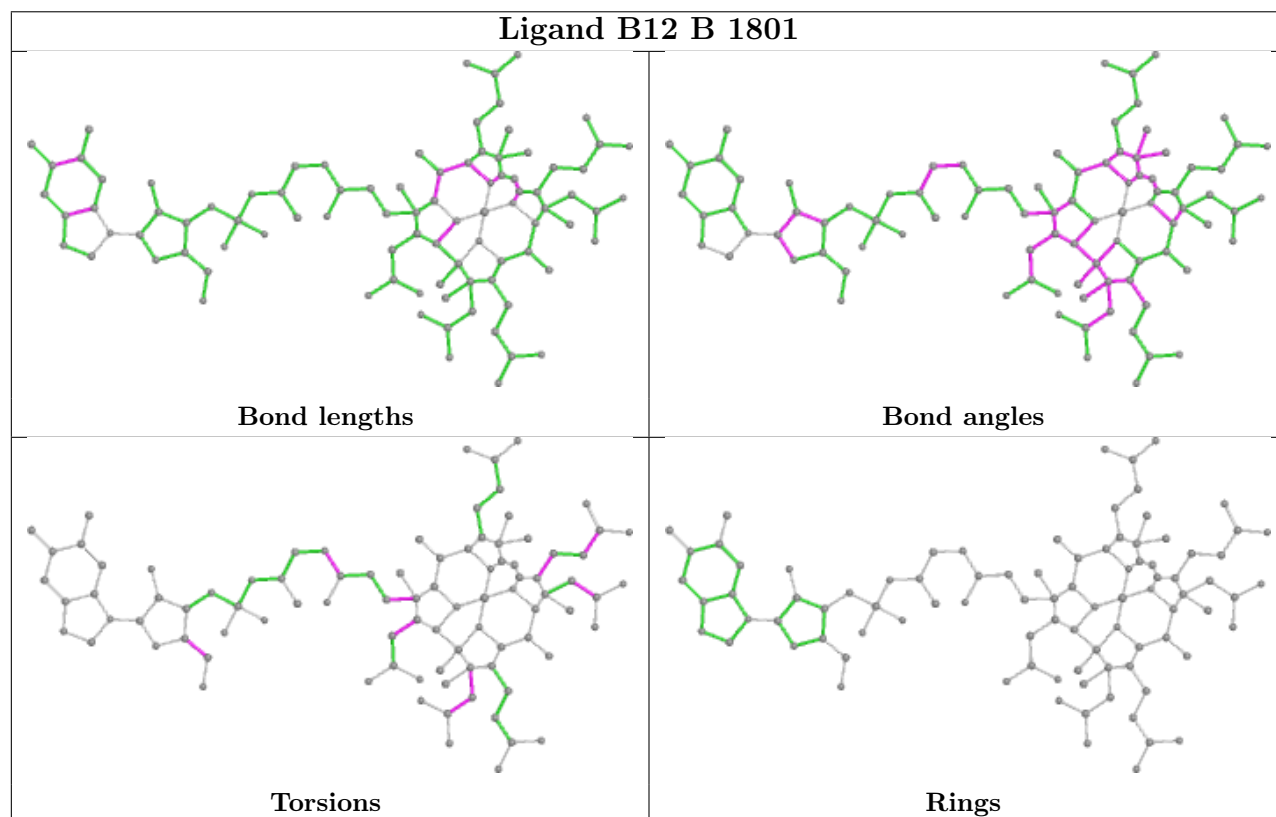
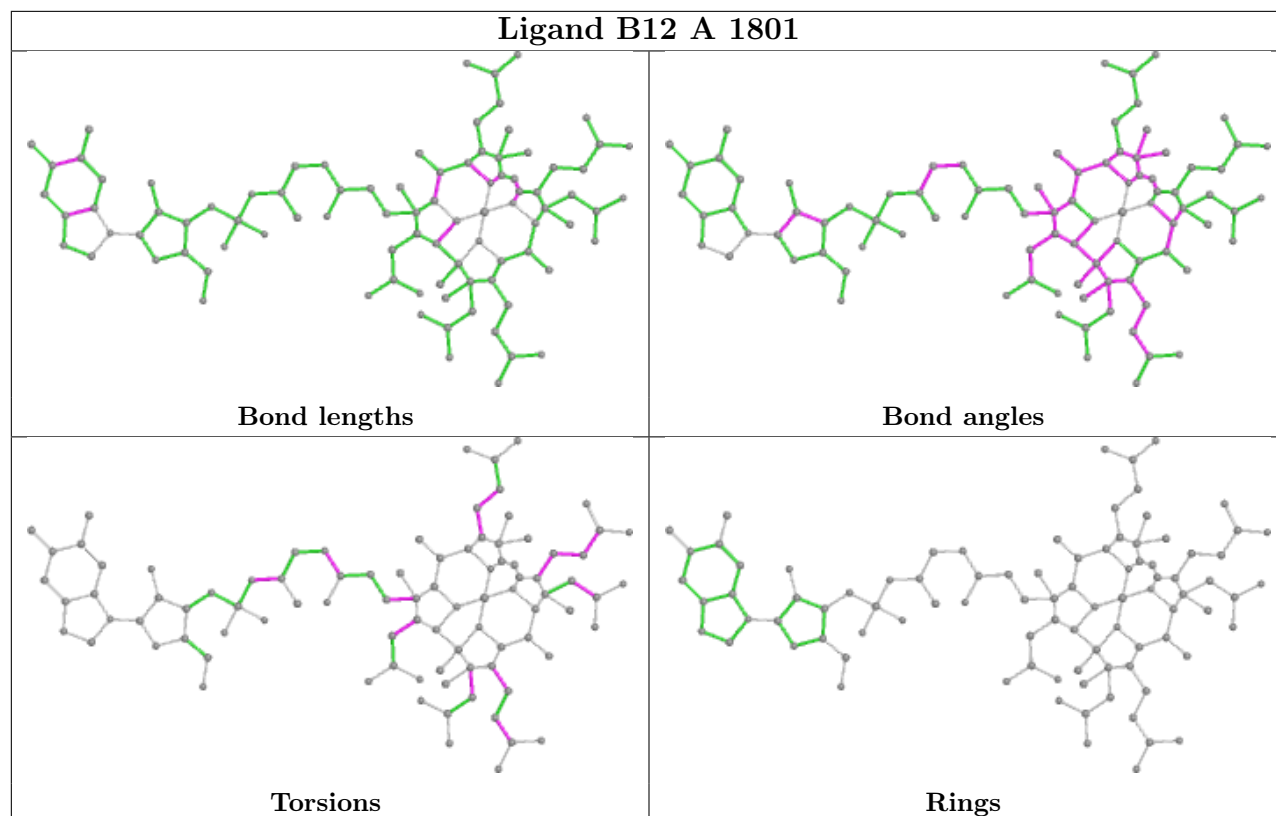
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

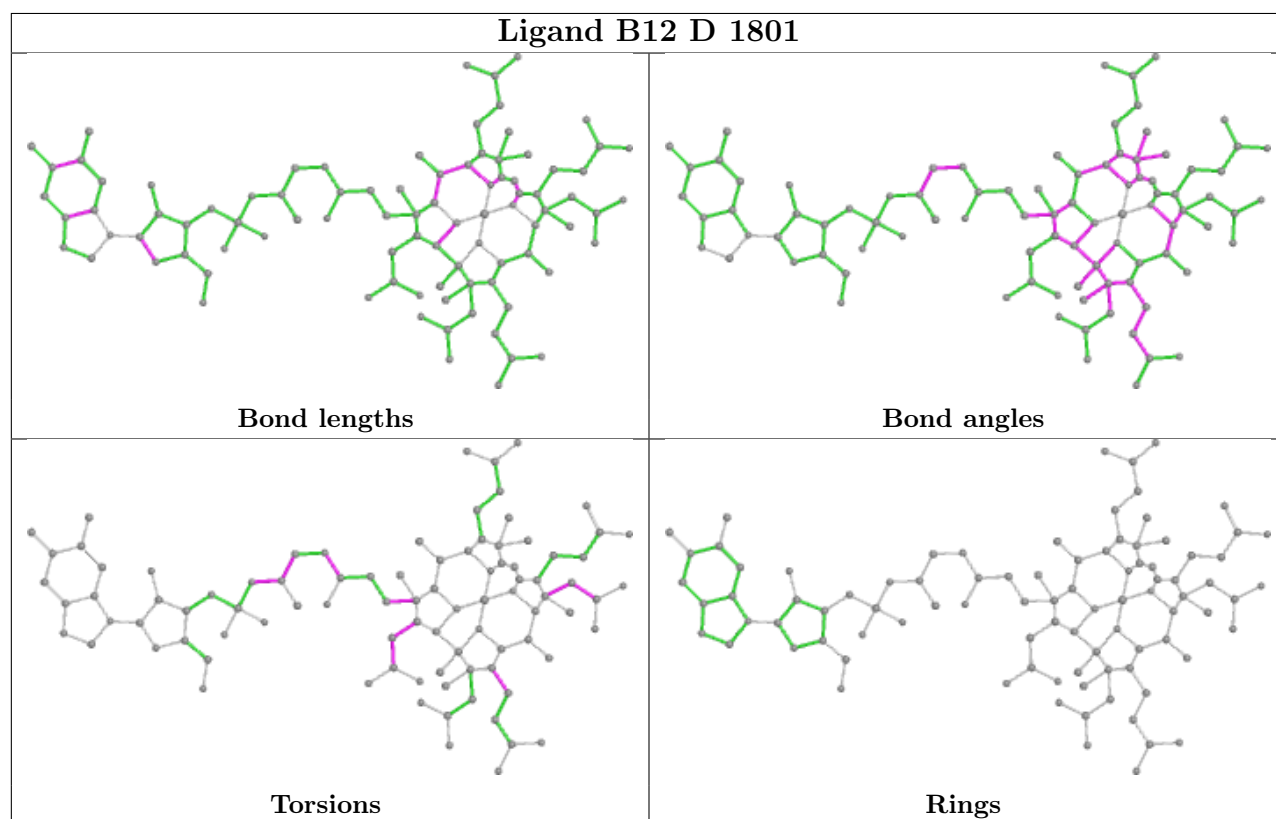
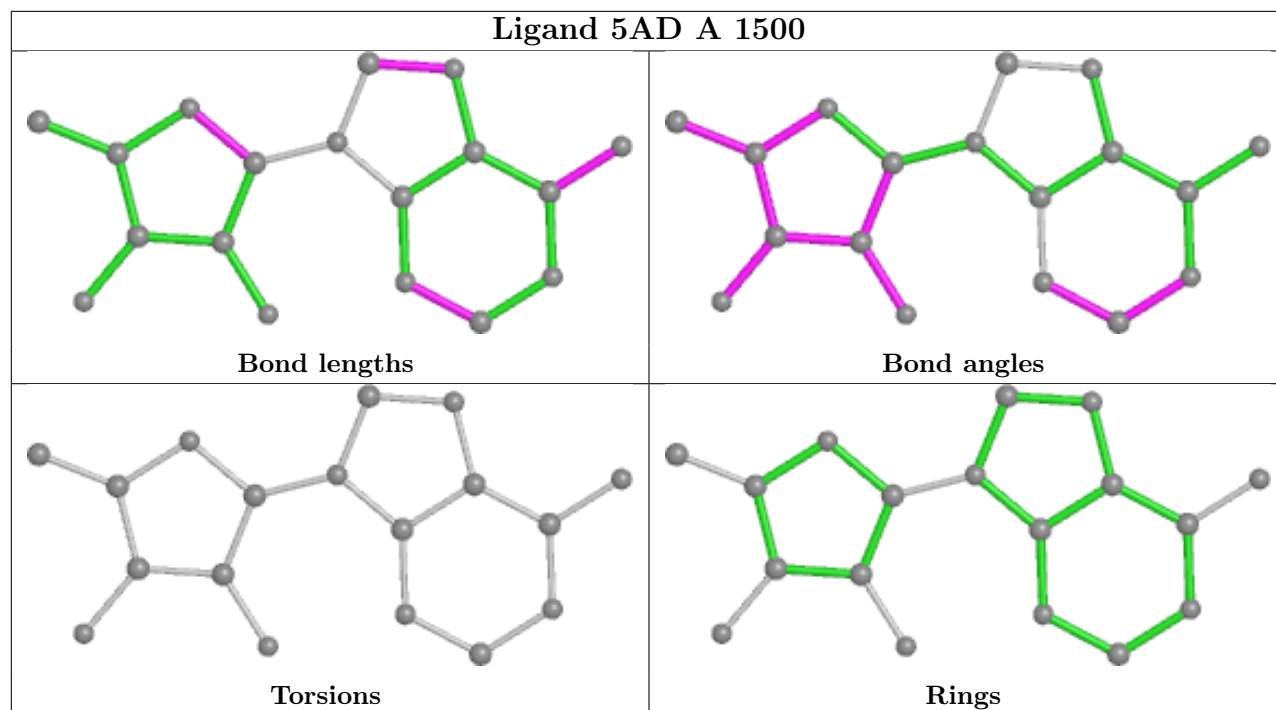
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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

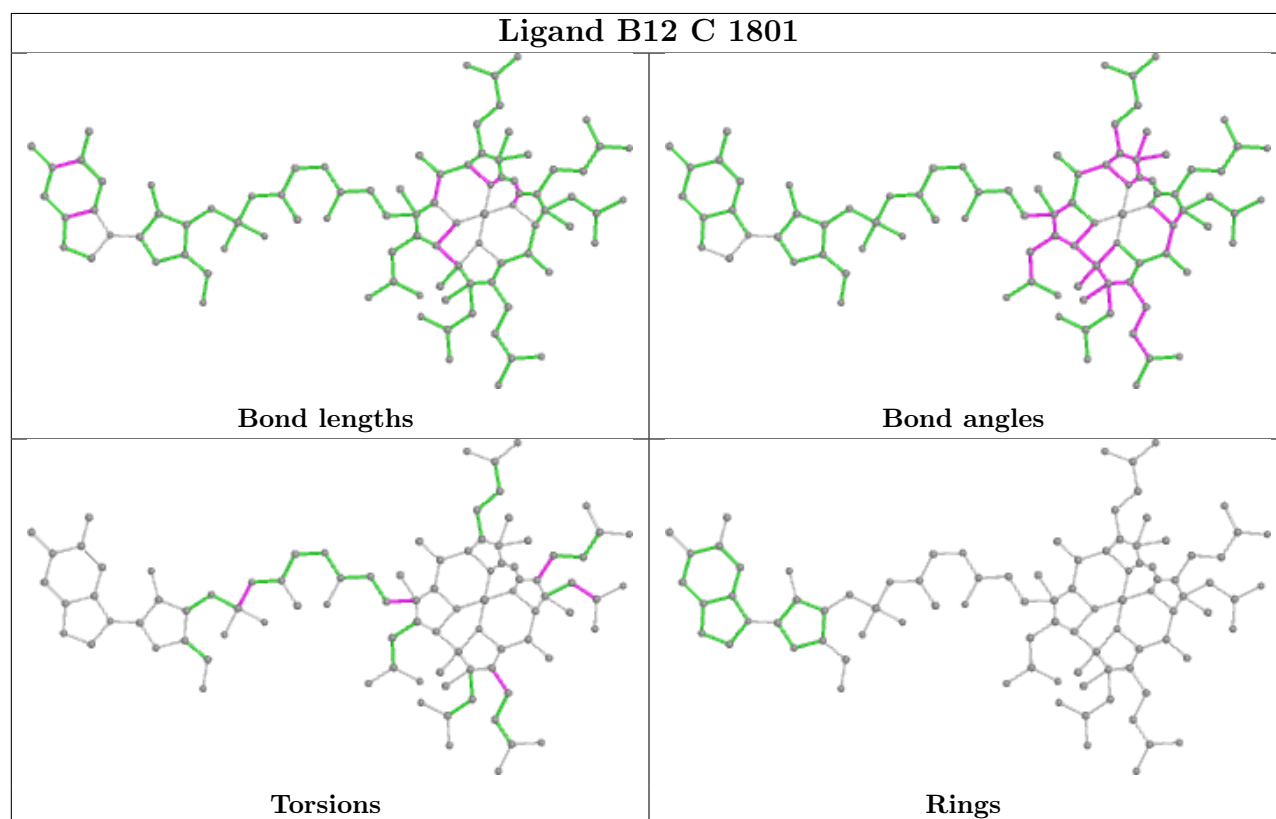
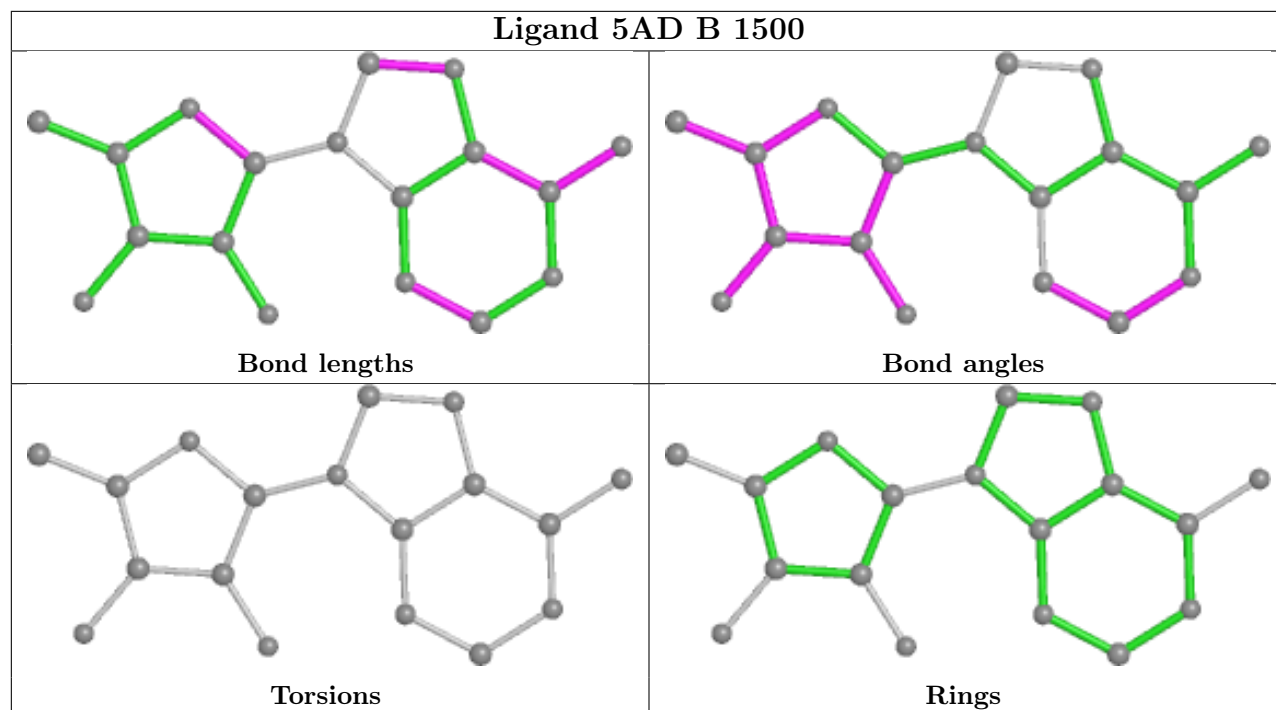


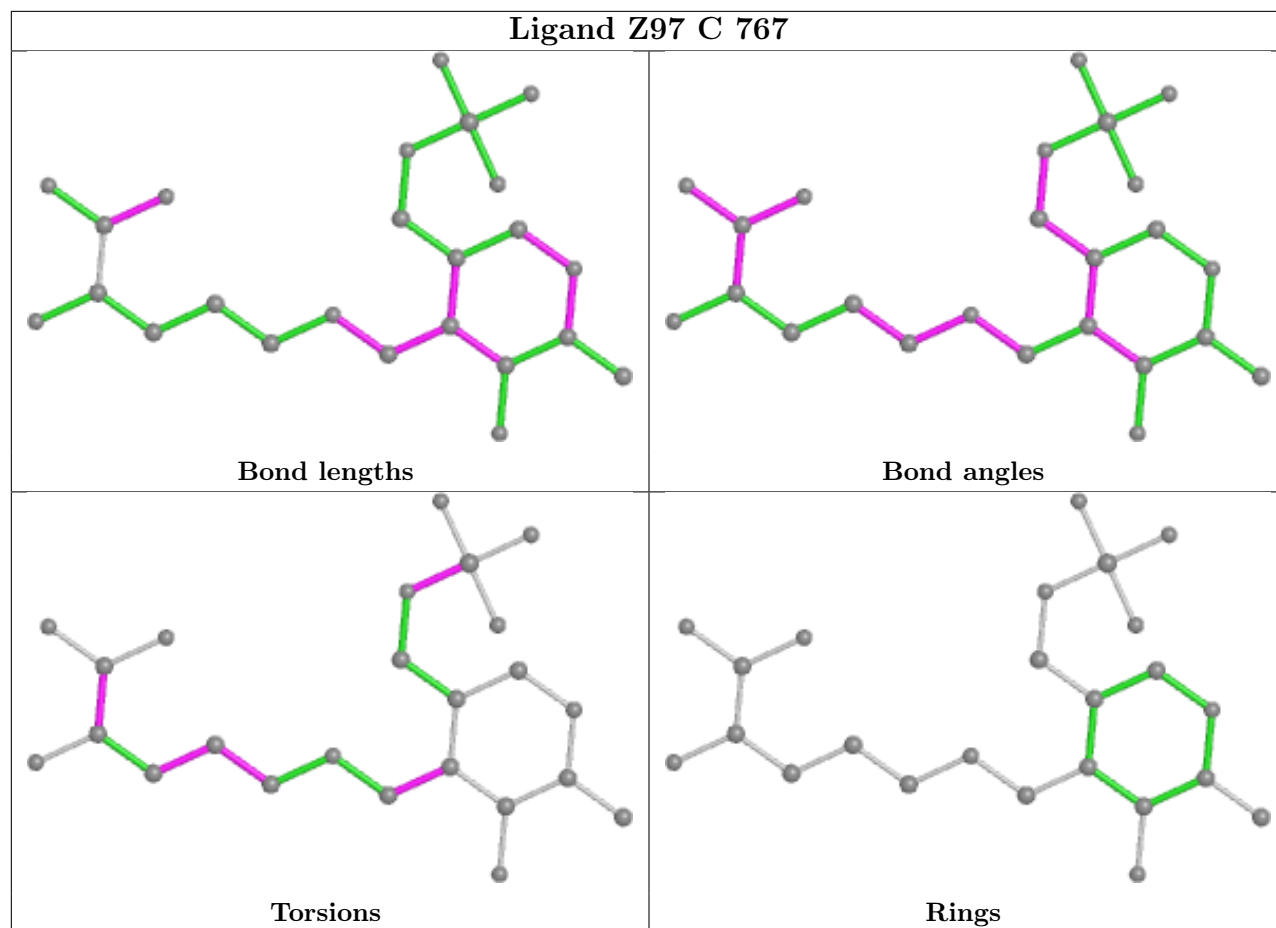












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	728/763 (95%)	-0.41	7 (0%) 82 77	16, 34, 103, 118	0
1	B	728/763 (95%)	-0.59	0 100 100	15, 33, 66, 95	0
1	C	728/763 (95%)	-0.59	0 100 100	19, 38, 61, 83	0
1	D	728/763 (95%)	-0.46	8 (1%) 80 75	17, 32, 89, 104	0
2	E	110/121 (90%)	-0.45	0 100 100	25, 40, 62, 73	0
2	F	110/121 (90%)	-0.60	0 100 100	26, 38, 53, 72	0
2	G	110/121 (90%)	-0.46	0 100 100	32, 45, 69, 80	0
2	H	110/121 (90%)	-0.41	0 100 100	25, 38, 57, 86	0
All	All	3352/3536 (94%)	-0.51	15 (0%) 92 91	15, 36, 83, 118	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	710	ALA	3.4
1	D	647	VAL	2.9
1	D	714	GLY	2.8
1	A	717	ALA	2.6
1	A	617	GLU	2.2
1	D	690	LYS	2.2
1	D	667	SER	2.2
1	A	675	ILE	2.2
1	D	683	ILE	2.1
1	A	716	ASP	2.1
1	A	683	ILE	2.1
1	D	688	VAL	2.1
1	A	661	ALA	2.1
1	A	698	ILE	2.1
1	D	680	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

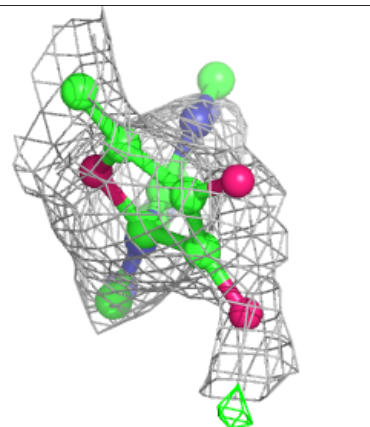
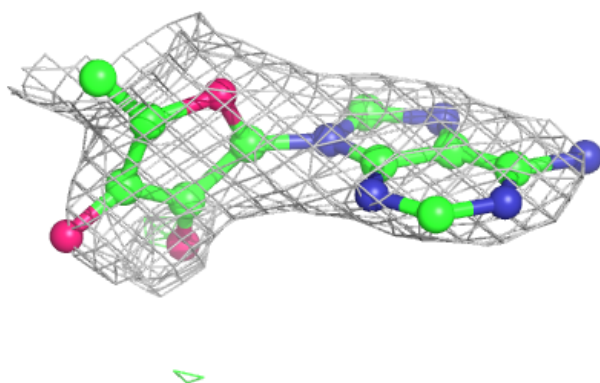
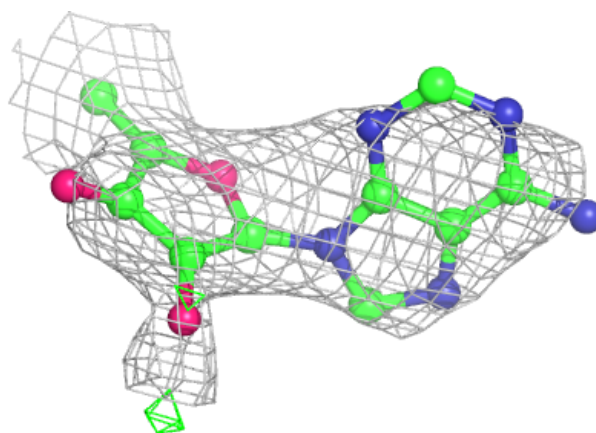
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	5AD	C	1500	18/18	0.86	0.24	78,87,94,97	0
5	5AD	B	1500	18/18	0.88	0.33	64,76,83,84	0
5	5AD	D	1500	18/18	0.92	0.22	48,60,65,66	0
5	5AD	A	1500	18/18	0.93	0.21	37,46,54,55	0
3	B12	A	1801	91/91	0.93	0.27	57,87,98,99	0
3	B12	D	1801	91/91	0.94	0.19	40,73,84,86	0
4	Z97	C	767	24/24	0.97	0.18	35,40,50,56	0
4	Z97	D	767	24/24	0.97	0.17	25,36,41,44	0
3	B12	C	1801	91/91	0.97	0.16	20,34,46,51	0
3	B12	B	1801	91/91	0.97	0.18	35,55,67,70	0
4	Z97	A	767	24/24	0.97	0.18	22,29,36,38	0
4	Z97	B	767	24/24	0.97	0.15	22,32,46,50	0

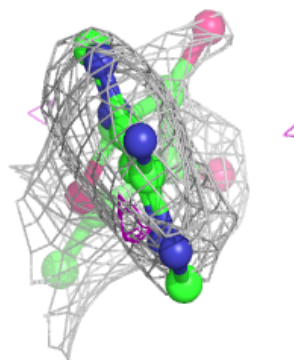
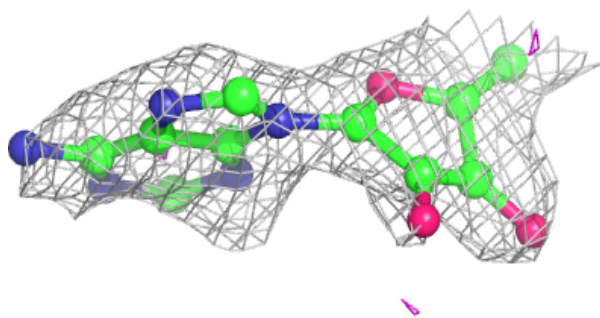
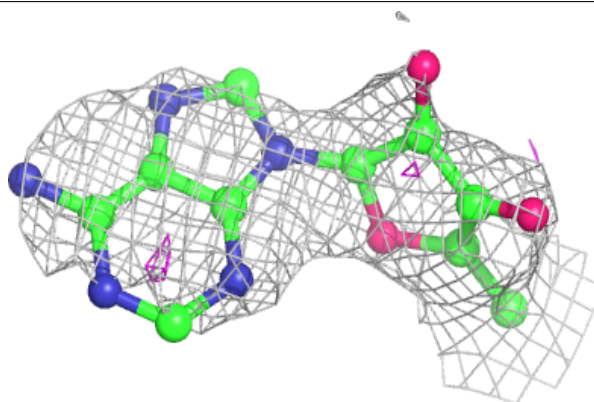
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

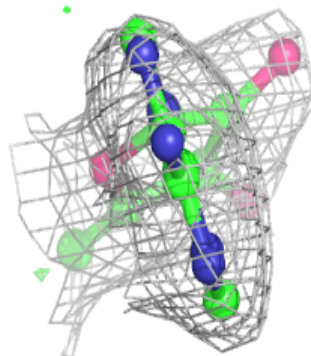
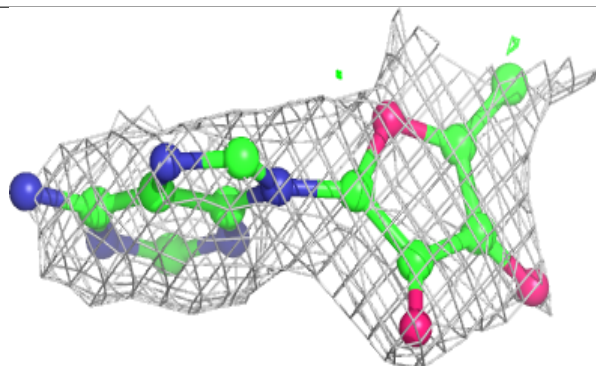
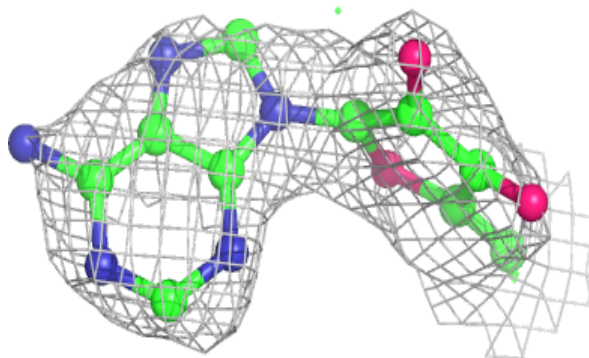
**Electron density around 5AD B 1500:**

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

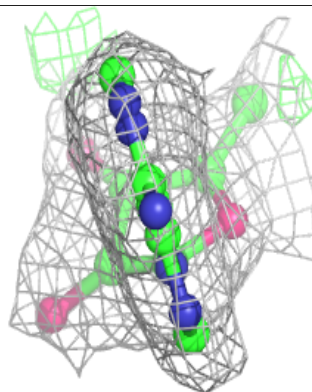
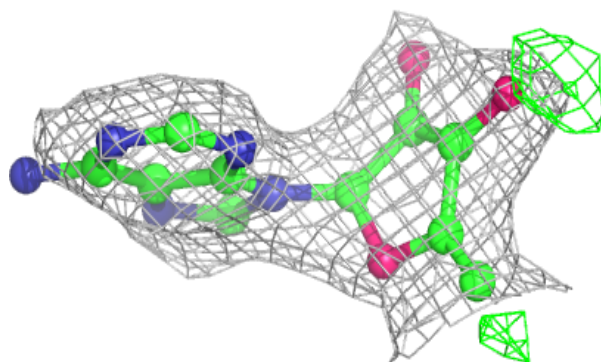
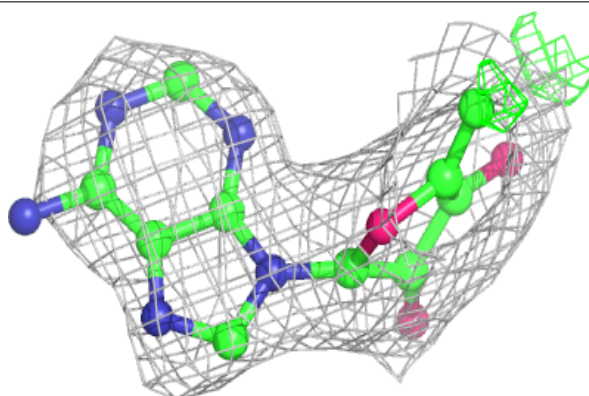


Electron density around 5AD D 1500:

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

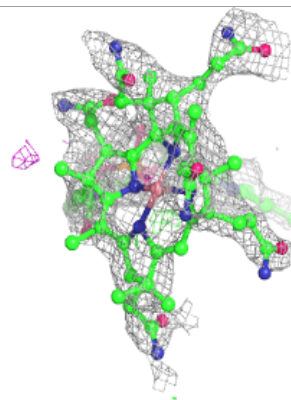
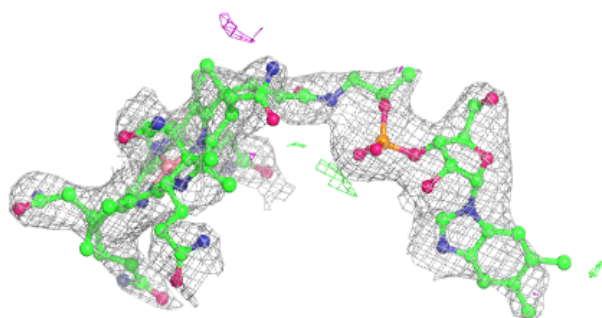
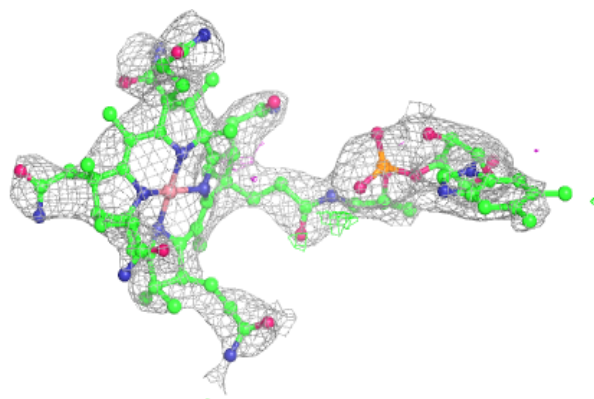
**Electron density around 5AD A 1500:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

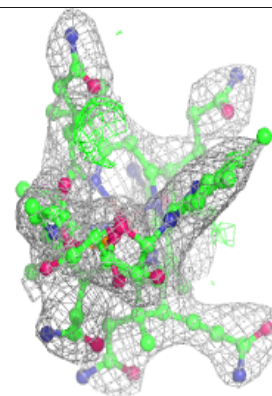
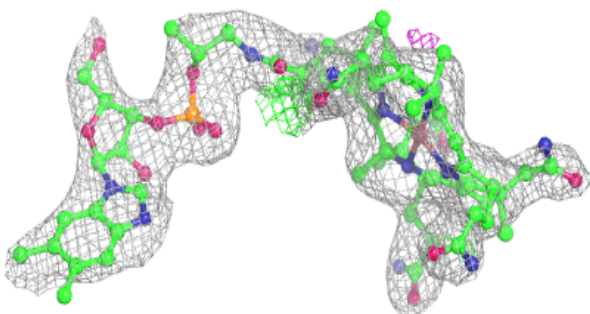
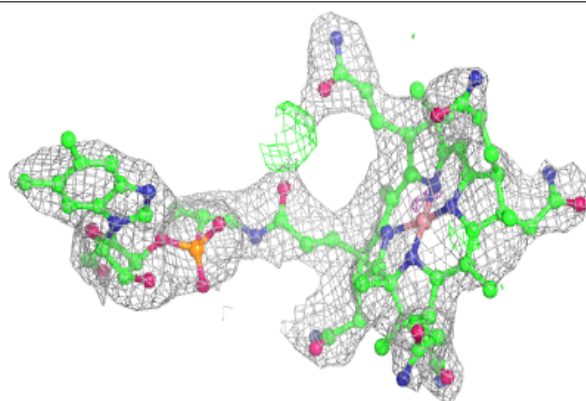


Electron density around B12 A 1801:

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

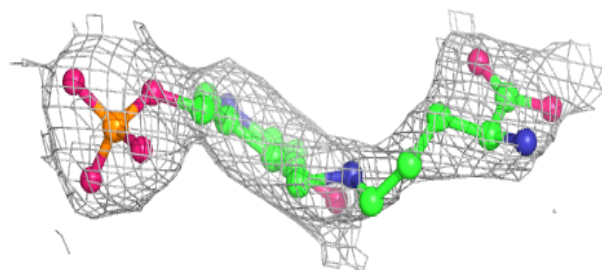
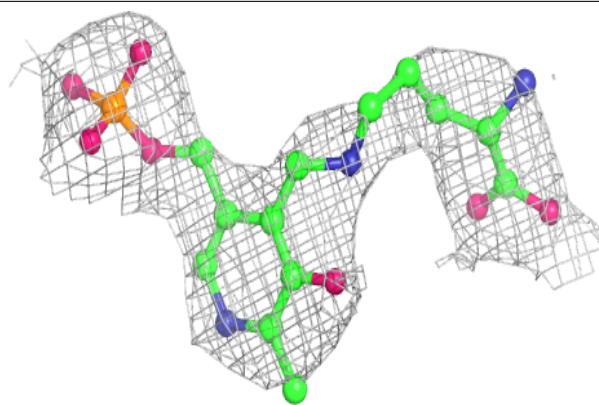
**Electron density around B12 D 1801:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

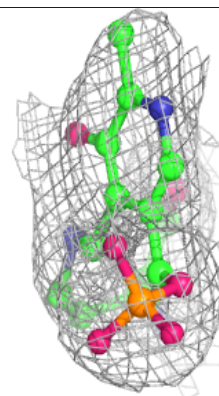
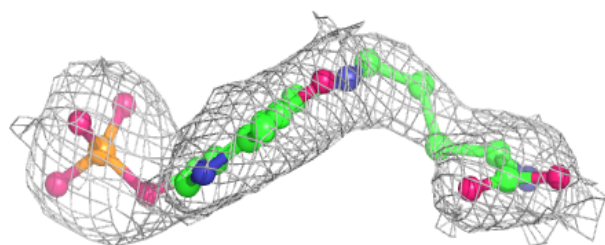


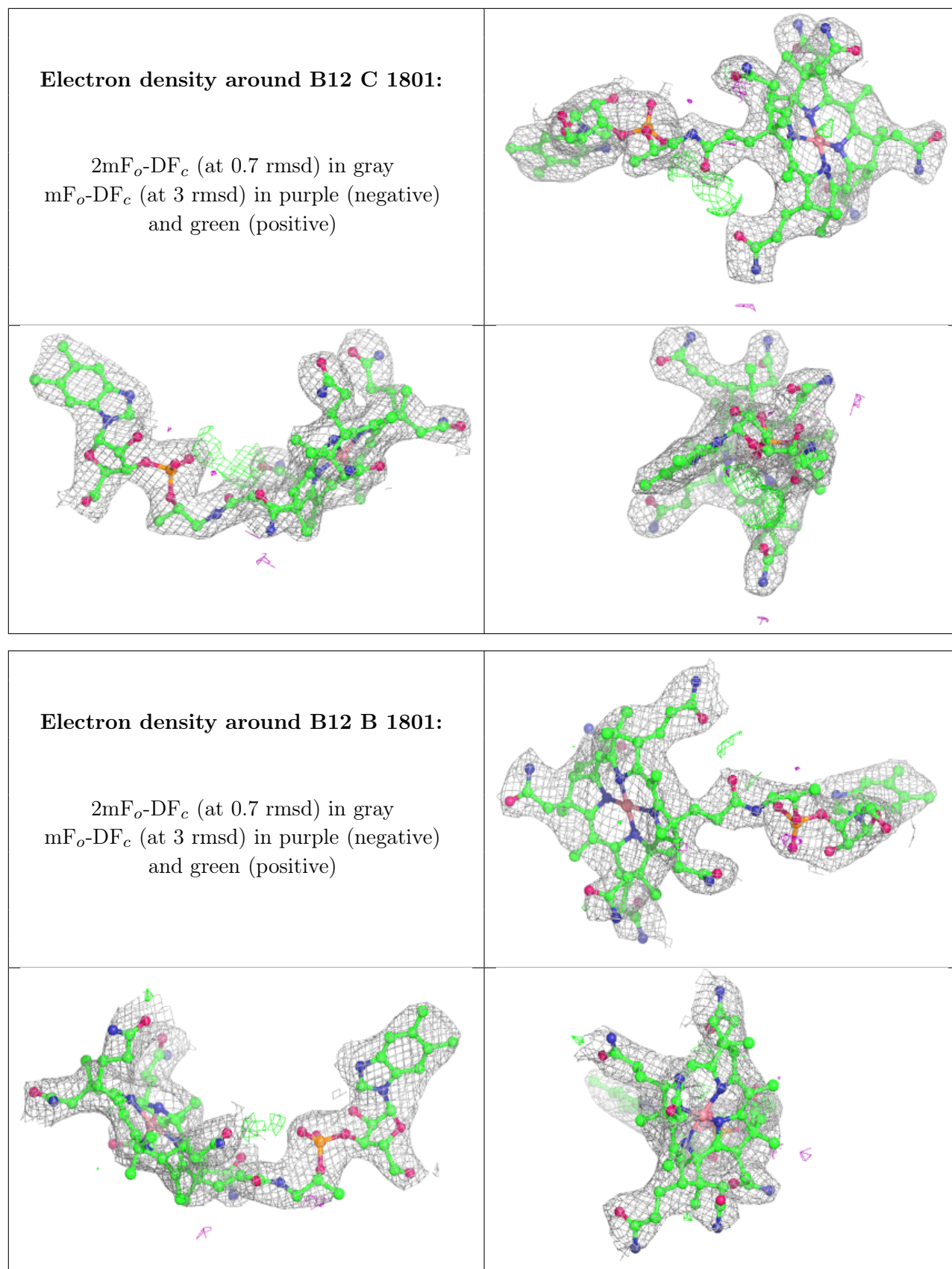
Electron density around Z97 C 767:

$2mF_o-DF_c$ (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:**

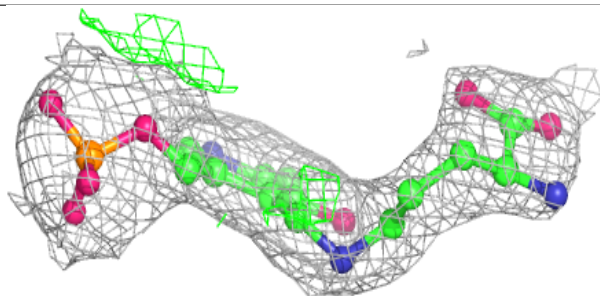
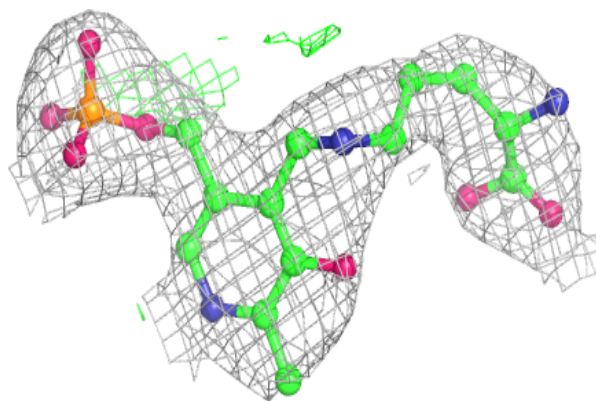
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



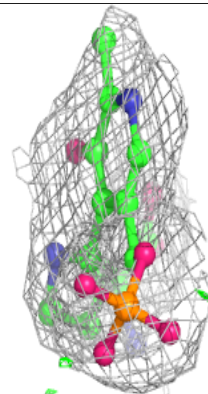
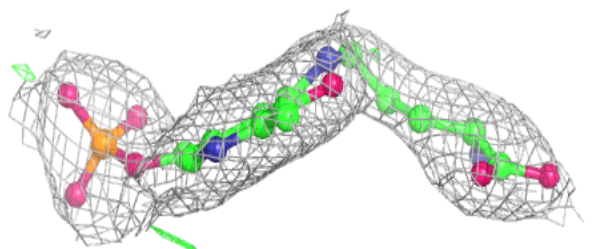
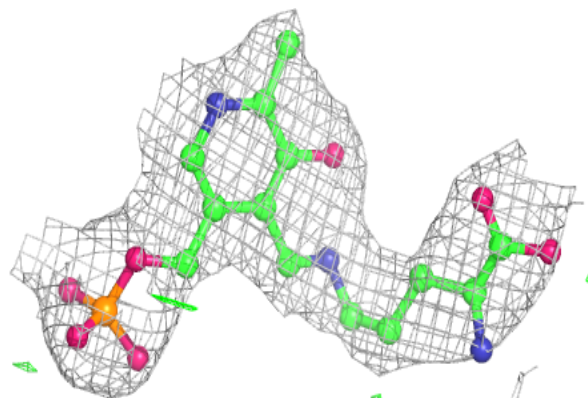


Electron density around Z97 A 767:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.