



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:58 PM UTC

PDB ID : 3KOZ / pdb_00003koz
Title : Crystal Structure of ornithine 4,5 aminomutase in complex with ornithine (Anaerobic)
Authors : Wolthers, K.R.; Levy, C.W.; Scrutton, N.S.; Leys, D.
Deposited on : 2009-11-14
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

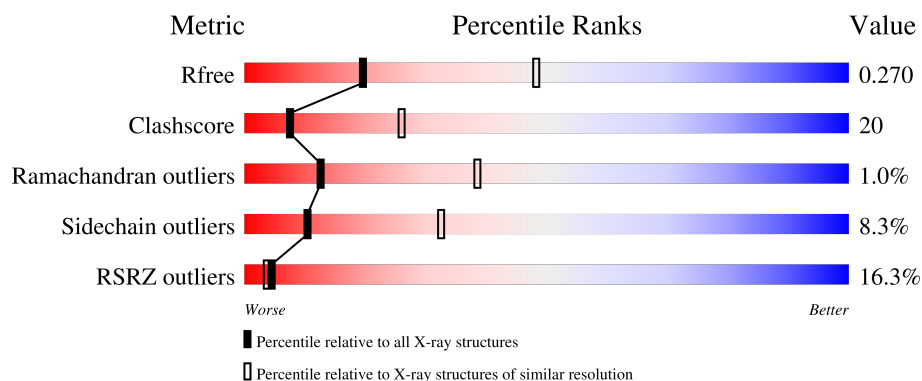
1 Overall quality at a glance

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.



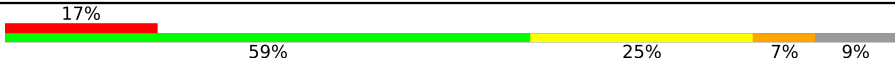
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	15% 59% 31% 5%
1	B	763	21% 56% 35% 5%
1	C	763	9% 58% 33% 5%
1	D	763	20% 60% 31% 5%
2	E	121	6% 45% 40% 6% 9%

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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	-	-	-
3	B12	B	1801	X	-	X	-
3	B12	C	1801	X	-	X	-
3	B12	D	1801	X	-	X	-
4	5AD	A	1500	X	-	-	-
4	5AD	B	1500	X	-	-	-
4	5AD	C	1500	X	-	-	-
4	5AD	D	1500	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26616 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called D-ornithine aminomutase E component.

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

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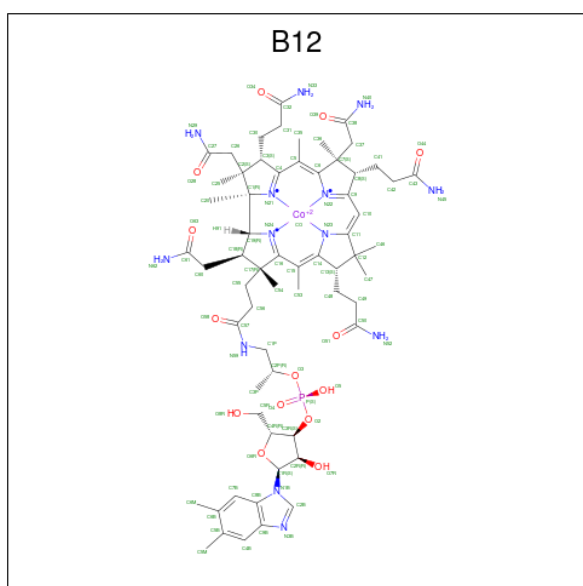
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Chain	Residue	Modelled	Actual	Comment	Reference
C	752	VAL	-	expression tag	UNP Q8VPJ5
C	753	ASP	-	expression tag	UNP Q8VPJ5
C	754	LYS	-	expression tag	UNP Q8VPJ5
C	755	LEU	-	expression tag	UNP Q8VPJ5
C	756	ALA	-	expression tag	UNP Q8VPJ5
C	757	ALA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

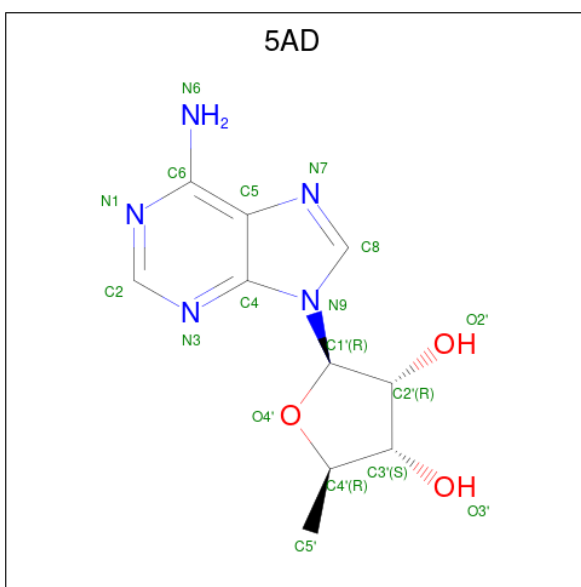
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	110	Total	C	N	O	S	0	0	0
			860	541	153	162	4			
2	F	110	Total	C	N	O	S	0	0	0
			863	542	153	164	4			
2	G	110	Total	C	N	O	S	0	0	0
			860	541	153	162	4			
2	H	110	Total	C	N	O	S	0	0	0
			860	541	153	162	4			

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



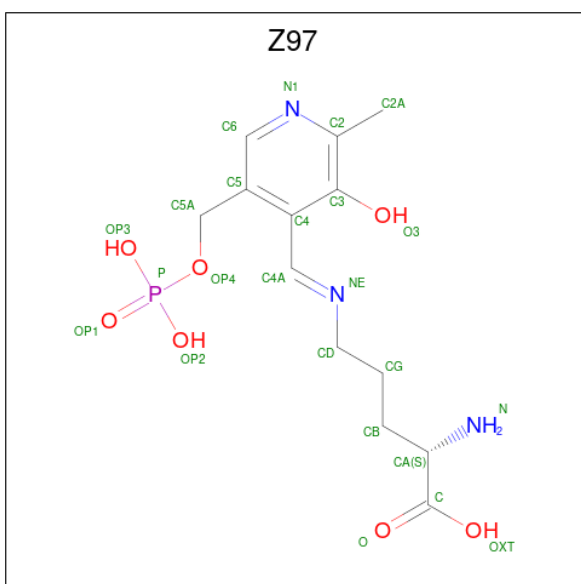
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	C	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	D	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

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



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

- Molecule 5 is (E)-N 5 -({3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene)-L-ornithine (CCD ID: Z97) (formula: $C_{13}H_{20}N_3O_7P$).

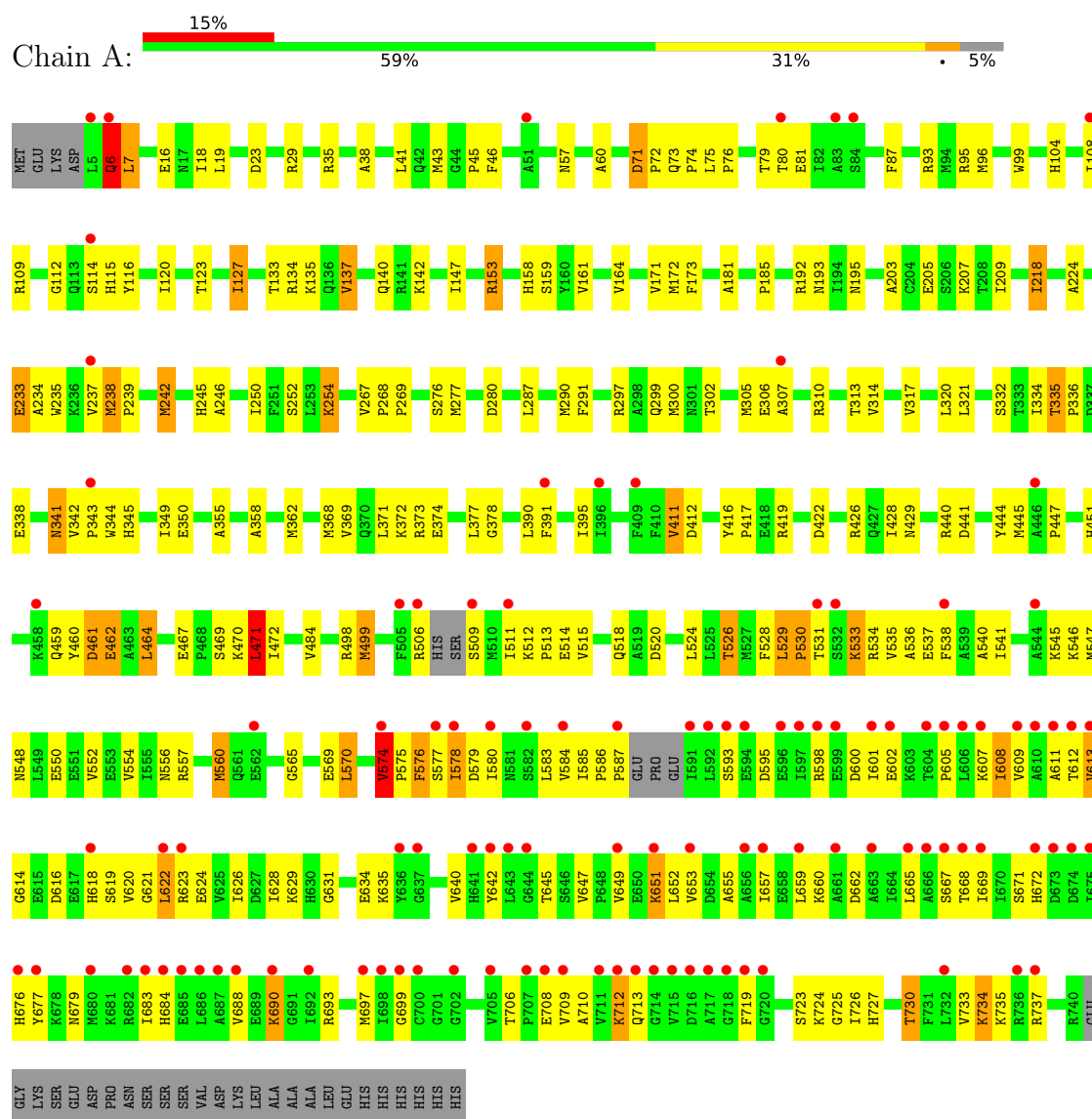


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 24	C 13	N 3	O 7	P 1	0	0
5	B	1	Total 24	C 13	N 3	O 7	P 1	0	0
5	C	1	Total 24	C 13	N 3	O 7	P 1	0	0
5	D	1	Total 24	C 13	N 3	O 7	P 1	0	0

3 Residue-property plots

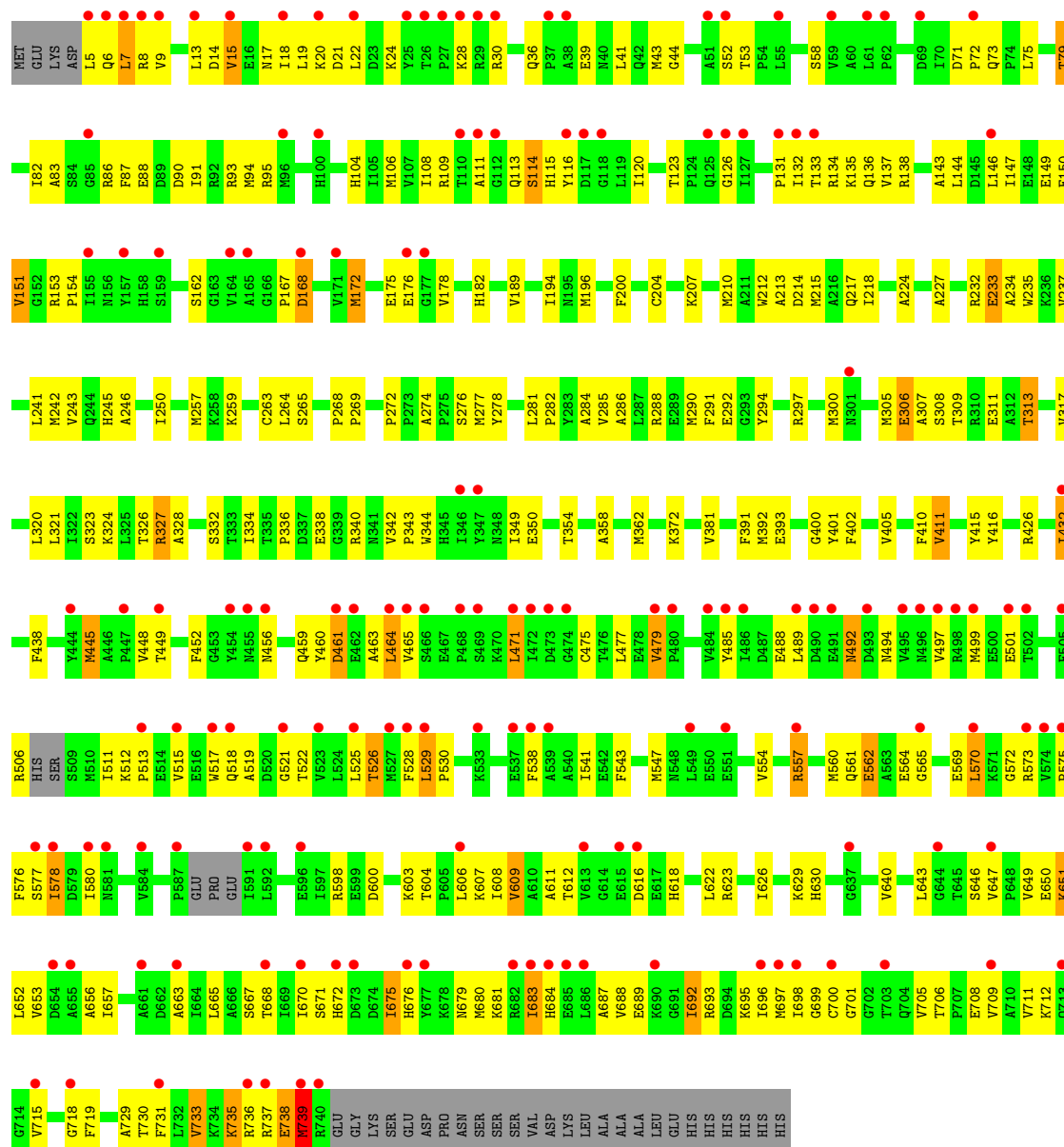
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

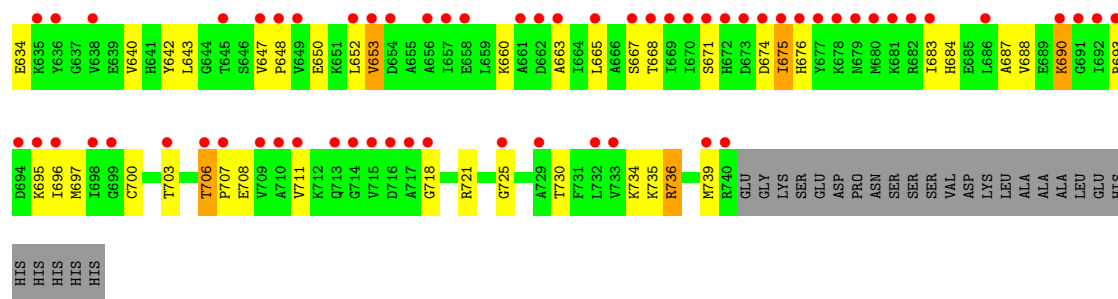
• Molecule 1: D-ornithine aminomutase E component



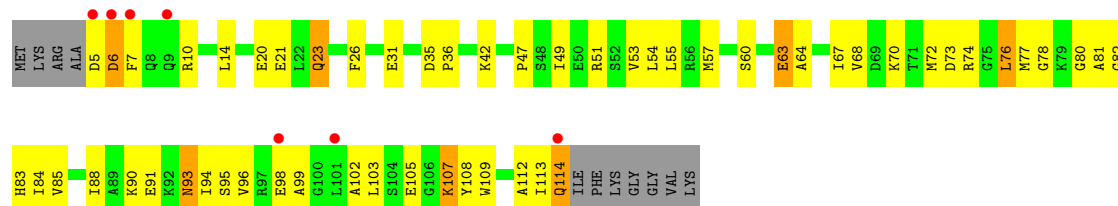
• Molecule 1: D-ornithine aminomutase E component



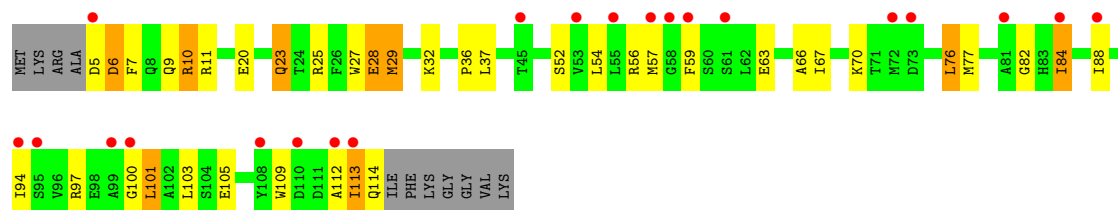




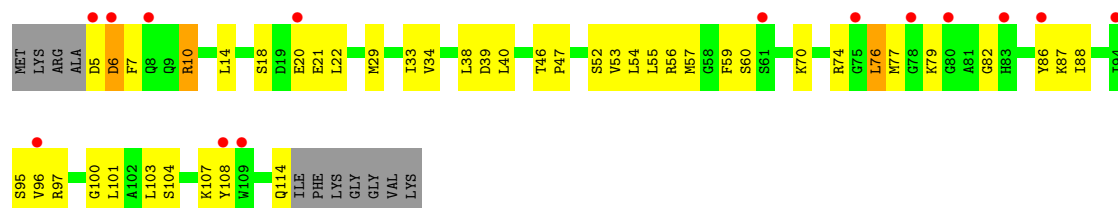
• Molecule 2: D-ornithine aminomutase S component



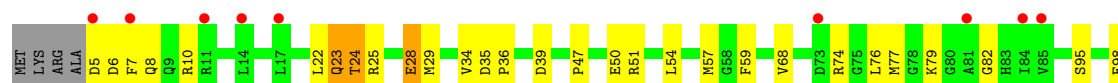
• Molecule 2: D-ornithine aminomutase S component

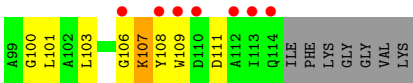


• Molecule 2: D-ornithine aminomutase S component



• Molecule 2: D-ornithine aminomutase S component





4 Data and refinement statistics

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 60.37 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (60.37-2.80) 98.8 (60.37-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.5_2, REFMAC 5.5.0102	Depositor
R, R_{free}	0.185 , 0.254 (Not available) , 0.270	Depositor DCC
R_{free} test set	5217 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	26616	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.59	0/5756	0.97	10/7794 (0.1%)
1	B	0.58	0/5777	0.96	14/7818 (0.2%)
1	C	0.57	0/5759	0.93	14/7796 (0.2%)
1	D	0.59	0/5769	0.93	8/7808 (0.1%)
2	E	0.53	0/872	0.90	0/1170
2	F	0.57	0/875	0.90	0/1174
2	G	0.53	0/872	0.86	1/1170 (0.1%)
2	H	0.58	0/872	0.93	0/1170
All	All	0.58	0/26552	0.94	47/35900 (0.1%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	THR	CA-C-N	8.07	129.93	119.84
1	A	335	THR	C-N-CA	8.07	129.93	119.84
1	A	71	ASP	CA-C-N	7.87	127.87	119.76
1	A	71	ASP	C-N-CA	7.87	127.87	119.76
1	C	238	MET	CA-C-N	-7.34	110.90	119.05
1	C	238	MET	C-N-CA	-7.34	110.90	119.05
1	A	560	MET	N-CA-C	-6.91	102.09	112.04
1	C	585	ILE	CA-C-N	6.80	127.39	120.38
1	C	585	ILE	C-N-CA	6.80	127.39	120.38
1	A	574	VAL	CA-C-N	6.67	126.12	118.85
1	A	574	VAL	C-N-CA	6.67	126.12	118.85
1	B	53	THR	CA-C-N	6.39	126.34	120.21
1	B	53	THR	C-N-CA	6.39	126.34	120.21
1	D	585	ILE	N-CA-C	6.33	114.94	107.73
1	B	479	VAL	CA-C-N	6.17	126.63	119.47
1	B	479	VAL	C-N-CA	6.17	126.63	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	529	LEU	CA-C-N	6.13	127.51	119.84
1	A	529	LEU	C-N-CA	6.13	127.51	119.84
1	C	533	LYS	N-CA-C	5.98	117.59	111.14
1	C	73	GLN	CA-C-N	5.95	126.29	119.92
1	C	73	GLN	C-N-CA	5.95	126.29	119.92
2	G	33	ILE	N-CA-C	5.93	116.71	110.72
1	A	276	SER	N-CA-C	5.92	117.81	111.36
1	B	272	PRO	O-C-N	5.90	124.02	121.31
1	D	272	PRO	CA-C-O	-5.88	116.66	120.90
1	B	44	GLY	CA-C-N	5.79	125.41	119.56
1	B	44	GLY	C-N-CA	5.79	125.41	119.56
1	B	529	LEU	CA-C-N	5.76	127.04	119.84
1	B	529	LEU	C-N-CA	5.76	127.04	119.84
1	C	153	ARG	CA-C-N	5.61	125.62	119.90
1	C	153	ARG	C-N-CA	5.61	125.62	119.90
1	C	161	VAL	CB-CA-C	-5.58	106.97	113.22
1	B	564	GLU	N-CA-C	5.55	118.10	111.71
1	C	107	VAL	CB-CA-C	-5.53	104.35	111.53
1	D	560	MET	N-CA-C	-5.44	104.99	111.03
1	C	276	SER	N-CA-C	5.33	116.89	111.14
1	D	219	ASP	N-CA-C	5.22	117.56	110.35
1	D	272	PRO	O-C-N	5.19	123.70	121.31
1	B	647	VAL	N-CA-C	5.19	113.09	108.63
1	B	194	ILE	N-CA-C	-5.17	104.41	110.05
1	D	53	THR	CA-C-N	5.17	125.15	120.03
1	D	53	THR	C-N-CA	5.17	125.15	120.03
1	D	178	VAL	CB-CA-C	-5.12	105.08	111.08
1	C	511	ILE	N-CA-C	5.12	114.61	108.06
1	C	247	LEU	N-CA-C	5.11	116.54	111.07
1	B	400	GLY	N-CA-C	5.11	117.24	112.08
1	B	113	GLN	N-CA-C	-5.05	106.95	113.01

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5651	0	5584	232	0
1	B	5672	0	5644	251	0
1	C	5654	0	5621	229	0
1	D	5664	0	5636	221	0
2	E	860	0	865	46	0
2	F	863	0	867	37	0
2	G	860	0	865	34	0
2	H	860	0	865	38	0
3	A	91	0	87	19	0
3	B	91	0	87	26	0
3	C	91	0	87	24	0
3	D	91	0	87	31	0
4	A	18	0	7	3	0
4	B	18	0	7	3	0
4	C	18	0	7	3	0
4	D	18	0	7	3	0
5	A	24	0	18	2	0
5	B	24	0	18	3	0
5	C	24	0	18	3	0
5	D	24	0	18	4	0
All	All	26616	0	26395	1076	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 (1076) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:ASP:HA	2:E:7:PHE:N	1.61	1.16
2:F:5:ASP:HA	2:F:7:PHE:N	1.66	1.08
2:G:5:ASP:HA	2:G:7:PHE:N	1.70	1.07
1:D:537:GLU:HG3	1:D:554:VAL:HG21	1.39	1.04
1:A:43:MET:HE1	1:A:72:PRO:HA	1.41	1.00
2:F:5:ASP:HA	2:F:7:PHE:H	1.21	0.99
3:A:1801:B12:H262	3:A:1801:B12:H601	1.45	0.98
2:G:5:ASP:HA	2:G:7:PHE:H	1.26	0.97
1:C:649:VAL:HG13	1:C:683:ILE:HG12	1.47	0.97
1:B:525:LEU:HD23	1:B:570:LEU:HD11	1.45	0.96
1:B:526:THR:HG23	1:B:569:GLU:HG2	1.48	0.94
2:E:5:ASP:HA	2:E:7:PHE:H	1.24	0.93
1:A:134:ARG:HA	1:A:172:MET:HE3	1.48	0.93
3:C:1801:B12:H401	3:C:1801:B12:H8	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ARG:HG2	1:B:132:ILE:HG13	1.54	0.89
1:C:668:THR:HG23	1:C:676:HIS:HB2	1.51	0.89
1:A:127:ILE:HD11	3:C:1801:B12:H1P1	1.54	0.89
1:B:14:ASP:OD2	1:B:17:ASN:HB2	1.72	0.89
2:H:25:ARG:HA	2:H:28:GLU:HG3	1.54	0.89
1:C:43:MET:HE1	1:C:72:PRO:HA	1.55	0.88
3:C:1801:B12:H362	3:C:1801:B12:H351	1.54	0.88
1:B:577:SER:O	1:B:578:ILE:HD12	1.75	0.86
2:H:5:ASP:HA	2:H:7:PHE:N	1.90	0.86
1:D:611:ALA:HB2	1:D:643:LEU:HB2	1.56	0.85
1:B:598:ARG:NH2	1:D:232:ARG:HH21	1.76	0.84
1:C:612:THR:HB	1:C:645:THR:HG22	1.59	0.84
1:B:393:GLU:HG3	2:F:29:MET:HE1	1.60	0.83
1:B:277:MET:HE2	1:B:321:LEU:HD23	1.60	0.83
1:B:393:GLU:HG3	2:F:29:MET:CE	2.09	0.82
1:C:238:MET:HE3	1:C:283:TYR:HB2	1.61	0.82
1:C:525:LEU:HB3	1:C:570:LEU:HD12	1.61	0.82
1:D:109:ARG:NH2	5:D:767:Z97:OP2	2.14	0.81
2:H:57:MET:HE1	2:H:82:GLY:HA2	1.62	0.80
1:C:668:THR:CG2	1:C:676:HIS:HB2	2.10	0.80
1:B:15:VAL:HG22	1:B:499:MET:HE1	1.64	0.80
1:D:88:GLU:OE2	1:D:498:ARG:HD2	1.82	0.80
1:C:213:ALA:HB3	1:C:215:MET:HG3	1.63	0.79
2:F:88:ILE:HG13	2:F:103:LEU:HD11	1.65	0.79
1:A:577:SER:O	1:A:578:ILE:HD12	1.83	0.79
1:B:649:VAL:HG13	1:B:683:ILE:HG12	1.65	0.79
2:G:57:MET:HE1	2:G:82:GLY:HA2	1.64	0.78
3:D:1801:B12:H362	3:D:1801:B12:H351	1.65	0.78
1:B:456:ASN:OD1	1:B:459:GLN:HB3	1.83	0.78
1:C:460:TYR:O	1:C:461:ASP:HB2	1.82	0.78
1:D:394:GLU:HG2	1:D:409:PHE:CE2	2.19	0.78
1:A:267:VAL:HG22	1:A:299:GLN:HB3	1.66	0.77
1:D:394:GLU:HG2	1:D:409:PHE:HE2	1.47	0.77
1:D:5:LEU:HD23	1:D:6:GLN:HB2	1.66	0.77
1:D:652:LEU:HD23	1:D:683:ILE:HD11	1.67	0.76
2:F:57:MET:HE1	2:F:82:GLY:HA2	1.67	0.76
3:B:1801:B12:H291	3:B:1801:B12:H251	1.50	0.76
1:C:96:MET:HE1	1:C:345:HIS:HB3	1.66	0.76
1:A:724:LYS:HB2	1:A:726:ILE:HG22	1.67	0.76
1:C:250:ILE:HG23	2:G:34:VAL:HG21	1.68	0.76
1:D:512:LYS:HB2	1:D:513:PRO:HD2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LEU:HD23	1:B:43:MET:HE2	1.66	0.75
1:C:123:THR:HG23	1:C:135:LYS:HD3	1.67	0.75
1:A:528:PHE:CE1	1:A:565:GLY:HA3	2.20	0.75
1:B:506:ARG:HH11	1:B:518:GLN:HE22	1.32	0.75
1:A:560:MET:HB3	1:C:96:MET:HE3	1.67	0.75
3:B:1801:B12:N40	3:B:1801:B12:H8	2.00	0.74
1:B:233:GLU:HG2	1:B:235:TRP:CH2	2.21	0.74
1:B:651:LYS:HE3	1:B:651:LYS:HA	1.68	0.74
1:C:514:GLU:OE2	1:C:518:GLN:HA	1.88	0.74
3:A:1801:B12:H362	3:A:1801:B12:H351	1.69	0.74
1:C:512:LYS:HB2	1:C:513:PRO:HD2	1.69	0.74
2:F:109:TRP:O	2:F:113:ILE:HG13	1.88	0.73
1:A:18:ILE:HG23	1:A:142:LYS:HD3	1.69	0.73
3:B:1801:B12:H8	3:B:1801:B12:H401	1.53	0.73
1:D:541:ILE:HD11	1:D:554:VAL:HG23	1.71	0.73
3:A:1801:B12:H2B	3:A:1801:B12:O7R	1.89	0.72
1:B:109:ARG:HG2	1:B:132:ILE:CG1	2.19	0.72
1:B:393:GLU:CG	2:F:29:MET:HE1	2.18	0.72
1:D:41:LEU:HD23	1:D:43:MET:HE2	1.71	0.72
3:D:1801:B12:H601	3:D:1801:B12:H262	1.72	0.72
2:F:6:ASP:O	2:F:10:ARG:HG2	1.90	0.72
1:C:540:ALA:HB1	1:C:570:LEU:HD21	1.71	0.72
3:B:1801:B12:H362	3:B:1801:B12:H351	1.69	0.71
1:B:653:VAL:O	1:B:657:ILE:HG13	1.89	0.71
4:B:1500:5AD:H5'3	3:D:1801:B12:C16	2.18	0.71
1:C:577:SER:O	1:C:578:ILE:HD12	1.90	0.71
1:B:207:LYS:HZ2	1:B:217:GLN:NE2	1.87	0.71
1:D:467:GLU:HA	1:D:467:GLU:OE1	1.90	0.71
1:B:137:VAL:HG21	1:B:172:MET:HE1	1.73	0.71
2:H:95:SER:OG	2:H:98:GLU:HG2	1.89	0.71
1:A:254:LYS:HE2	2:E:31:GLU:HG3	1.72	0.70
1:B:600:ASP:OD2	1:B:733:VAL:HG23	1.90	0.70
1:A:712:LYS:HD2	1:A:713:GLN:NE2	2.05	0.70
1:C:467:GLU:HB3	1:C:470:LYS:HG3	1.73	0.70
1:A:79:THR:HB	1:A:332:SER:HA	1.72	0.69
1:A:368:MET:HE3	1:C:278:TYR:CE1	2.27	0.69
1:A:684:HIS:O	1:A:688:VAL:HG23	1.92	0.69
3:A:1801:B12:H401	3:A:1801:B12:H8	1.57	0.69
2:H:59:PHE:CE1	2:H:100:GLY:HA3	2.27	0.69
1:B:207:LYS:HZ2	1:B:217:GLN:HE22	1.41	0.69
3:A:1801:B12:H8	3:A:1801:B12:N40	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ARG:NH1	1:C:378:GLY:HA2	2.08	0.69
3:B:1801:B12:C16	4:D:1500:5AD:H5'3	2.21	0.68
3:C:1801:B12:H8	3:C:1801:B12:N40	2.05	0.68
1:B:688:VAL:HG22	1:B:693:ARG:HG2	1.75	0.68
1:A:74:PRO:HB2	1:A:76:PRO:HD2	1.74	0.68
1:B:8:ARG:HH11	1:B:8:ARG:HB2	1.59	0.67
2:F:63:GLU:O	2:F:67:ILE:HG13	1.93	0.67
1:C:396:ILE:CD1	2:G:29:MET:HG2	2.25	0.67
1:B:82:ILE:HG12	1:B:93:ARG:HD2	1.75	0.67
1:A:626:ILE:O	1:A:634:GLU:HB2	1.94	0.67
1:A:688:VAL:HG22	1:A:693:ARG:HG2	1.77	0.67
3:A:1801:B12:H601	3:A:1801:B12:C26	2.23	0.67
1:C:399:GLY:HA3	1:C:403:ASN:HD22	1.59	0.67
1:A:540:ALA:HB1	1:A:570:LEU:HD11	1.77	0.67
1:B:111:ALA:O	1:D:620:VAL:HG11	1.96	0.66
1:C:543:PHE:O	1:C:547:MET:HG3	1.95	0.66
2:G:6:ASP:O	2:G:10:ARG:HG3	1.95	0.66
1:D:79:THR:HG23	1:D:104:HIS:CG	2.30	0.66
1:A:537:GLU:HG3	1:A:554:VAL:HG21	1.77	0.66
2:H:54:LEU:HD23	2:H:57:MET:CE	2.25	0.66
1:A:158:HIS:HE1	1:A:218:ILE:HG13	1.61	0.66
1:A:440:ARG:NH1	1:A:444:TYR:CE2	2.64	0.66
1:A:43:MET:HE1	1:A:72:PRO:CA	2.23	0.66
1:B:729:ALA:O	1:B:733:VAL:HG12	1.95	0.66
1:B:320:LEU:HD13	1:B:358:ALA:HB3	1.78	0.66
1:A:120:ILE:HG13	1:A:133:THR:HG22	1.78	0.65
1:A:560:MET:CB	1:C:96:MET:HE3	2.26	0.65
3:A:1801:B12:C16	4:C:1500:5AD:H5'3	2.25	0.65
2:F:54:LEU:HD23	2:F:57:MET:CE	2.26	0.65
1:C:259:LYS:HA	1:C:262:ILE:HD12	1.78	0.65
1:B:680:MET:HE1	1:B:705:VAL:HG22	1.79	0.65
1:B:735:LYS:O	1:B:735:LYS:HG3	1.95	0.65
1:B:196:MET:SD	1:B:402:PHE:CD1	2.90	0.65
1:B:393:GLU:OE2	2:F:25:ARG:NH1	2.29	0.65
1:D:671:SER:HB2	1:D:676:HIS:ND1	2.12	0.65
3:D:1801:B12:O2	3:D:1801:B12:H2B	1.97	0.65
2:H:5:ASP:HA	2:H:6:ASP:C	2.19	0.65
2:H:108:TYR:HA	2:H:111:ASP:OD2	1.97	0.65
1:A:112:GLY:HA3	1:C:620:VAL:HG13	1.78	0.65
1:C:550:GLU:HG3	1:C:573:ARG:NH2	2.12	0.65
3:D:1801:B12:N40	3:D:1801:B12:H8	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:MET:HE2	1:B:257:MET:HE1	1.77	0.65
1:D:234:ALA:O	1:D:237:VAL:HG12	1.97	0.65
1:D:464:LEU:HD23	1:D:471:LEU:HD13	1.79	0.65
3:C:1801:B12:H301	3:C:1801:B12:H203	1.78	0.64
1:B:278:TYR:CD1	1:D:368:MET:HE3	2.32	0.64
1:C:394:GLU:HG2	1:C:409:PHE:CE2	2.31	0.64
1:D:652:LEU:HD23	1:D:683:ILE:CD1	2.27	0.64
1:B:607:LYS:C	1:B:608:ILE:HD12	2.23	0.64
1:C:16:GLU:HG3	1:C:499:MET:CE	2.27	0.64
1:B:464:LEU:HD23	1:B:471:LEU:HD13	1.80	0.64
1:D:224:ALA:HB3	1:D:245:HIS:CE1	2.33	0.64
1:B:598:ARG:HH22	1:D:232:ARG:HH21	1.42	0.63
1:C:606:LEU:HB2	1:C:736:ARG:NH2	2.13	0.63
1:A:618:HIS:CD2	3:A:1801:B12:H482	2.33	0.63
1:B:391:PHE:HA	1:B:416:TYR:CZ	2.33	0.63
1:C:593:SER:O	1:C:597:ILE:HG12	1.98	0.63
2:G:59:PHE:CZ	2:G:100:GLY:HA3	2.33	0.63
1:B:687:ALA:HB3	1:B:693:ARG:HD3	1.80	0.63
1:B:115:HIS:CE1	1:D:623:ARG:HD3	2.34	0.63
1:D:123:THR:HG23	1:D:135:LYS:HD3	1.79	0.63
1:B:41:LEU:CD2	1:B:43:MET:HE2	2.28	0.62
1:B:73:GLN:HE21	1:B:153:ARG:HH22	1.47	0.62
1:B:120:ILE:HG13	1:B:133:THR:HG22	1.80	0.62
1:B:300:MET:HB2	1:B:334:ILE:HG12	1.81	0.62
1:A:158:HIS:CE1	1:A:218:ILE:HG13	2.35	0.62
3:A:1801:B12:O7R	3:A:1801:B12:C2B	2.47	0.62
2:E:109:TRP:O	2:E:113:ILE:HG13	1.99	0.62
2:E:107:LYS:O	2:E:108:TYR:HB2	1.99	0.62
1:C:537:GLU:HG3	1:C:554:VAL:HG21	1.82	0.62
1:C:607:LYS:HE2	1:C:639:GLU:OE2	2.00	0.62
1:D:445:MET:HE3	1:D:447:PRO:N	2.14	0.62
1:B:623:ARG:HD3	1:D:115:HIS:CE1	2.35	0.62
1:D:721:ARG:HG3	1:D:721:ARG:HH11	1.63	0.62
2:H:47:PRO:O	2:H:51:ARG:HG3	1.98	0.62
1:B:313:THR:O	1:B:317:VAL:HG23	2.00	0.62
2:F:112:ALA:C	2:F:114:GLN:H	2.08	0.62
1:C:126:GLY:O	1:C:127:ILE:HD13	1.98	0.62
1:D:397:GLU:O	1:D:397:GLU:HG2	1.98	0.62
1:A:620:VAL:HG21	1:C:116:TYR:HE1	1.64	0.62
2:E:5:ASP:HA	2:E:6:ASP:C	2.20	0.62
1:B:232:ARG:NH2	1:D:598:ARG:NH2	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:SER:HB2	1:B:676:HIS:CE1	2.34	0.61
1:B:675:ILE:HD11	1:B:679:ASN:HD21	1.65	0.61
1:D:459:GLN:HG3	1:D:460:TYR:CD2	2.36	0.61
1:C:307:ALA:O	1:C:340:ARG:HD3	2.00	0.61
1:C:560:MET:HE2	1:C:560:MET:HA	1.83	0.61
1:B:79:THR:HA	1:B:104:HIS:HB3	1.82	0.61
1:B:143:ALA:O	1:B:147:ILE:HG13	2.00	0.61
1:B:153:ARG:HG2	1:B:154:PRO:HD2	1.83	0.61
1:B:232:ARG:CZ	1:D:598:ARG:CZ	2.79	0.60
2:E:81:ALA:O	2:E:85:VAL:HG23	2.02	0.60
1:B:207:LYS:NZ	1:B:217:GLN:NE2	2.48	0.60
1:C:158:HIS:CD2	1:C:159:SER:N	2.68	0.60
3:C:1801:B12:H362	3:C:1801:B12:C35	2.27	0.60
1:D:90:ASP:O	1:D:94:MET:HG3	2.00	0.60
1:C:506:ARG:HH11	1:C:518:GLN:HE22	1.50	0.60
2:G:97:ARG:O	2:G:101:LEU:HB2	2.01	0.60
1:A:238:MET:HE3	1:A:269:PRO:HG2	1.83	0.60
3:B:1801:B12:H261	4:D:1500:5AD:H5'2	1.83	0.60
1:A:671:SER:HB2	1:A:676:HIS:CE1	2.37	0.60
1:B:172:MET:HE2	1:B:172:MET:O	2.01	0.60
1:B:344:TRP:CG	1:B:515:VAL:HB	2.37	0.60
1:C:445:MET:HE1	1:C:447:PRO:HB3	1.82	0.60
1:C:626:ILE:HG23	1:C:640:VAL:HG21	1.84	0.60
1:B:372:LYS:HE2	1:D:370:GLN:NE2	2.17	0.60
1:C:475:CYS:HB2	2:G:56:ARG:O	2.02	0.60
1:C:610:ALA:HB1	1:C:622:LEU:HD21	1.84	0.60
1:A:185:PRO:HG3	1:A:203:ALA:CB	2.32	0.60
1:C:397:GLU:HG3	1:C:397:GLU:O	2.02	0.60
2:E:57:MET:HE1	2:E:82:GLY:HA2	1.82	0.59
1:B:290:MET:SD	2:F:23:GLN:HG3	2.41	0.59
2:H:5:ASP:HA	2:H:7:PHE:H	1.62	0.59
1:C:109:ARG:HH21	5:C:767:Z97:P	2.24	0.59
1:D:537:GLU:CG	1:D:554:VAL:HG21	2.26	0.59
1:B:393:GLU:HA	2:F:29:MET:HE1	1.82	0.59
1:C:459:GLN:HG3	1:C:460:TYR:CD2	2.36	0.59
1:B:73:GLN:NE2	1:B:153:ARG:HH22	2.00	0.59
1:A:224:ALA:HB3	1:A:245:HIS:CE1	2.37	0.59
1:A:459:GLN:HG3	1:A:460:TYR:CD2	2.37	0.59
2:H:107:LYS:NZ	2:H:107:LYS:HB3	2.18	0.59
1:D:161:VAL:HG12	1:D:161:VAL:O	2.03	0.59
1:A:619:SER:HB3	1:A:645:THR:CG2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:LEU:HD12	2:G:86:TYR:OH	2.02	0.59
1:A:607:LYS:O	1:A:608:ILE:HD12	2.03	0.59
1:C:373:ARG:HH11	1:C:378:GLY:HA2	1.67	0.59
1:A:541:ILE:O	1:A:545:LYS:HG2	2.03	0.58
1:C:396:ILE:HD11	2:G:29:MET:HG2	1.84	0.58
3:B:1801:B12:H203	3:B:1801:B12:H301	1.85	0.58
1:B:259:LYS:HE3	1:B:294:TYR:CZ	2.39	0.58
1:C:132:ILE:HA	1:C:136:GLN:OE1	2.03	0.58
1:A:161:VAL:HG23	1:A:181:ALA:HB1	1.86	0.58
1:A:621:GLY:O	1:A:624:GLU:HB2	2.04	0.58
1:B:738:GLU:O	1:B:738:GLU:HG2	2.03	0.58
1:B:264:LEU:HD21	1:B:291:PHE:CD1	2.38	0.58
1:B:475:CYS:HB2	2:F:56:ARG:O	2.03	0.58
1:C:41:LEU:HD21	1:C:43:MET:HE2	1.86	0.58
1:C:528:PHE:CE1	1:C:565:GLY:HA3	2.39	0.58
1:C:619:SER:HB3	1:C:645:THR:HG21	1.84	0.58
1:C:649:VAL:HG12	1:C:686:LEU:CD1	2.33	0.58
1:C:679:ASN:O	1:C:683:ILE:HG13	2.03	0.58
1:A:668:THR:HG23	1:A:668:THR:O	2.03	0.58
1:B:506:ARG:HH11	1:B:518:GLN:NE2	1.99	0.58
1:D:236:LYS:HG2	1:D:415:TYR:HB2	1.86	0.58
1:B:217:GLN:O	1:B:263:CYS:HB2	2.03	0.58
3:B:1801:B12:H251	3:B:1801:B12:N29	2.17	0.58
3:B:1801:B12:N23	4:D:1500:5AD:C4'	2.67	0.58
1:C:618:HIS:CE1	3:C:1801:B12:N22	2.72	0.58
1:A:60:ALA:HB2	1:A:71:ASP:HB2	1.86	0.58
1:B:278:TYR:CE1	1:D:368:MET:HE3	2.39	0.57
1:B:120:ILE:HG13	1:B:133:THR:CG2	2.35	0.57
3:D:1801:B12:H203	3:D:1801:B12:H301	1.86	0.57
1:B:115:HIS:HB3	1:D:623:ARG:HH11	1.69	0.57
1:C:428:ILE:HG12	1:C:428:ILE:O	2.04	0.57
2:G:53:VAL:HG12	2:G:57:MET:HE2	1.86	0.57
3:C:1801:B12:H262	3:C:1801:B12:H601	1.86	0.57
1:B:259:LYS:HE3	1:B:294:TYR:CE2	2.40	0.57
1:B:123:THR:HG23	1:B:135:LYS:HD3	1.87	0.57
1:A:612:THR:HG22	1:A:616:ASP:HB3	1.87	0.57
1:B:663:ALA:HB2	1:B:697:MET:HE3	1.87	0.57
1:D:690:LYS:O	1:D:690:LYS:HD3	2.04	0.57
1:A:601:ILE:HG22	1:A:601:ILE:O	2.04	0.57
1:B:511:ILE:CG1	1:D:530:PRO:HD2	2.34	0.57
1:B:668:THR:O	1:B:668:THR:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:PRO:O	1:D:471:LEU:HB2	2.05	0.57
1:A:556:ASN:HB3	1:A:569:GLU:HB2	1.87	0.57
1:B:281:LEU:O	1:B:285:VAL:HG23	2.04	0.57
1:C:320:LEU:HD13	1:C:358:ALA:HB3	1.87	0.57
1:D:232:ARG:HA	1:D:232:ARG:HH11	1.70	0.57
3:D:1801:B12:H601	3:D:1801:B12:H252	1.86	0.57
2:G:59:PHE:CE1	2:G:100:GLY:HA3	2.40	0.56
1:A:290:MET:SD	2:E:23:GLN:HG3	2.46	0.56
1:C:668:THR:CG2	1:C:668:THR:O	2.53	0.56
1:B:286:ALA:HB2	1:B:381:VAL:HG13	1.87	0.56
4:B:1500:5AD:H5'2	3:D:1801:B12:H261	1.87	0.56
1:A:622:LEU:HD21	1:A:642:TYR:HE1	1.70	0.56
1:C:457:VAL:HG13	1:C:471:LEU:HD21	1.87	0.56
1:A:75:LEU:N	1:A:76:PRO:CD	2.68	0.56
1:A:440:ARG:HD2	2:E:42:LYS:O	2.06	0.56
1:B:709:VAL:O	1:B:712:LYS:HB2	2.06	0.56
1:C:5:LEU:C	1:C:5:LEU:HD22	2.31	0.56
1:C:394:GLU:HG2	1:C:409:PHE:HE2	1.71	0.56
1:A:579:ASP:O	1:A:583:LEU:HG	2.06	0.56
1:B:207:LYS:NZ	1:B:217:GLN:HE22	2.04	0.56
1:D:86:ARG:HD3	1:D:498:ARG:HD3	1.87	0.56
2:H:57:MET:CE	2:H:82:GLY:HA2	2.34	0.56
1:A:550:GLU:HG3	1:A:575:PRO:HG3	1.88	0.56
1:D:288:ARG:HA	1:D:296:MET:HE3	1.87	0.56
3:A:1801:B12:C15	4:C:1500:5AD:H5'3	2.37	0.56
1:B:116:TYR:CE1	3:D:1801:B12:H491	2.41	0.56
1:C:5:LEU:HD22	1:C:6:GLN:HB2	1.87	0.56
1:D:688:VAL:HG22	1:D:693:ARG:HG2	1.88	0.56
1:A:277:MET:CE	1:A:321:LEU:HD23	2.35	0.55
1:B:604:THR:HG22	1:B:736:ARG:NH2	2.21	0.55
2:H:24:THR:O	2:H:28:GLU:HG2	2.06	0.55
2:H:5:ASP:CB	2:H:8:GLN:H	2.19	0.55
1:B:95:ARG:HD3	1:D:564:GLU:HG2	1.86	0.55
1:B:126:GLY:CA	1:B:131:PRO:HD3	2.36	0.55
1:B:488:GLU:O	1:B:489:LEU:HD23	2.07	0.55
2:F:5:ASP:CA	2:F:7:PHE:H	2.06	0.55
1:C:191:TYR:CE1	1:C:230:THR:HG21	2.42	0.55
1:D:320:LEU:HD13	1:D:358:ALA:HB3	1.88	0.55
1:A:726:ILE:HG23	1:A:727:HIS:N	2.21	0.55
1:C:226:ASN:O	1:C:230:THR:HG23	2.05	0.55
1:A:277:MET:HE2	1:A:321:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:TYR:O	1:B:461:ASP:HB2	2.06	0.55
1:B:554:VAL:HA	1:B:570:LEU:HB3	1.88	0.55
1:C:74:PRO:HB2	1:C:76:PRO:HD2	1.88	0.55
1:C:5:LEU:O	1:C:6:GLN:HB3	2.07	0.55
1:D:250:ILE:HG23	2:H:34:VAL:HG21	1.87	0.55
1:D:264:LEU:HD21	1:D:291:PHE:CD1	2.41	0.55
1:A:668:THR:OG1	1:A:676:HIS:HB2	2.07	0.55
1:B:464:LEU:N	1:B:464:LEU:HD13	2.21	0.55
1:B:651:LYS:HE3	1:B:651:LYS:CA	2.37	0.55
1:D:79:THR:HG23	1:D:104:HIS:ND1	2.21	0.55
1:D:667:SER:HA	3:D:1801:B12:H4B	1.89	0.55
1:A:233:GLU:HG2	1:A:235:TRP:CH2	2.41	0.55
1:C:213:ALA:CB	1:C:215:MET:HG3	2.35	0.55
1:D:537:GLU:O	1:D:541:ILE:HG12	2.06	0.55
1:A:631:GLY:O	1:A:725:GLY:HA3	2.07	0.55
1:C:444:TYR:C	1:C:444:TYR:CD2	2.85	0.55
1:D:389:VAL:HG13	2:H:29:MET:HE1	1.87	0.55
2:F:97:ARG:O	2:F:101:LEU:HB2	2.07	0.54
3:C:1801:B12:H531	3:C:1801:B12:H543	1.89	0.54
1:A:116:TYR:CE2	1:A:120:ILE:HD13	2.42	0.54
1:D:668:THR:HG23	1:D:668:THR:O	2.07	0.54
1:A:137:VAL:HB	1:A:172:MET:HE1	1.88	0.54
1:B:326:THR:OG1	1:B:327:ARG:N	2.39	0.54
1:A:484:VAL:HG11	2:E:60:SER:HB3	1.89	0.54
1:A:622:LEU:HB2	1:A:667:SER:HB2	1.88	0.54
2:E:49:ILE:O	2:E:53:VAL:HG23	2.07	0.54
1:B:612:THR:HG22	1:B:616:ASP:HB3	1.90	0.54
1:A:668:THR:OG1	1:A:676:HIS:CB	2.56	0.54
1:A:712:LYS:HD2	1:A:713:GLN:HE22	1.70	0.54
1:C:207:LYS:HB3	1:C:257:MET:HE3	1.89	0.54
1:D:632:GLY:HA2	1:D:725:GLY:HA3	1.88	0.54
1:A:416:TYR:CG	1:A:417:PRO:HA	2.43	0.54
1:B:86:ARG:HG3	1:B:517:TRP:NE1	2.23	0.54
2:F:7:PHE:O	2:F:11:ARG:HG2	2.08	0.54
1:C:43:MET:CE	1:C:72:PRO:HA	2.35	0.54
1:C:467:GLU:N	1:C:468:PRO:HD3	2.23	0.54
1:A:41:LEU:CD2	1:A:43:MET:HE2	2.38	0.53
1:A:623:ARG:HD3	1:C:115:HIS:CE1	2.43	0.53
1:B:43:MET:HE1	1:B:72:PRO:HA	1.91	0.53
1:B:132:ILE:HA	1:B:136:GLN:OE1	2.08	0.53
1:C:628:ILE:HD12	1:C:635:LYS:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:THR:CG2	1:A:536:ALA:HB2	2.38	0.53
1:A:628:ILE:HG13	1:A:635:LYS:HB2	1.90	0.53
1:B:86:ARG:HG3	1:B:517:TRP:CE2	2.42	0.53
1:B:393:GLU:HG3	2:F:29:MET:HE2	1.87	0.53
1:B:464:LEU:N	1:B:464:LEU:CD1	2.72	0.53
1:A:57:ASN:HB3	1:A:99:TRP:CH2	2.44	0.53
1:A:237:VAL:HG22	1:A:237:VAL:O	2.08	0.53
1:A:580:ILE:HA	1:A:583:LEU:HD12	1.91	0.53
1:B:7:LEU:HG	1:B:146:LEU:HB3	1.91	0.53
1:A:205:GLU:O	1:A:209:ILE:HD12	2.08	0.53
1:C:217:GLN:NE2	1:C:257:MET:HE1	2.23	0.53
1:D:416:TYR:CG	1:D:417:PRO:HA	2.43	0.53
1:A:585:ILE:HG12	1:C:538:PHE:CD2	2.43	0.53
2:E:20:GLU:H	2:E:20:GLU:CD	2.17	0.53
1:C:649:VAL:CG1	1:C:683:ILE:HG12	2.29	0.53
1:A:19:LEU:HD11	1:A:499:MET:HE2	1.91	0.53
1:B:541:ILE:HD11	1:B:554:VAL:HG23	1.90	0.53
3:B:1801:B12:H531	3:B:1801:B12:C55	2.39	0.53
1:C:277:MET:HE2	1:C:321:LEU:HD23	1.89	0.53
1:B:41:LEU:HD23	1:B:43:MET:CE	2.37	0.53
1:B:147:ILE:O	1:B:151:VAL:HG13	2.09	0.53
1:C:237:VAL:HG13	1:C:241:LEU:HG	1.90	0.53
1:C:614:GLY:O	1:C:646:SER:HA	2.09	0.53
3:D:1801:B12:H262	3:D:1801:B12:C60	2.38	0.53
2:H:50:GLU:HG2	2:H:77:MET:HE1	1.91	0.53
1:B:114:SER:HB2	5:B:767:Z97:OP2	2.09	0.52
1:B:306:GLU:CG	1:D:65:LYS:HE2	2.39	0.52
3:D:1801:B12:O7R	3:D:1801:B12:C2B	2.57	0.52
1:A:123:THR:O	1:A:498:ARG:NH2	2.42	0.52
1:C:541:ILE:HG23	1:C:552:VAL:CG1	2.40	0.52
1:A:416:TYR:CD1	1:A:417:PRO:HA	2.44	0.52
1:A:6:GLN:CG	1:A:7:LEU:H	2.22	0.52
1:B:578:ILE:HD13	1:D:543:PHE:CZ	2.45	0.52
1:C:556:ASN:HB3	1:C:569:GLU:HB2	1.90	0.52
2:H:59:PHE:CZ	2:H:100:GLY:HA3	2.44	0.52
1:A:514:GLU:HA	1:A:520:ASP:OD1	2.08	0.52
1:D:618:HIS:CE1	3:D:1801:B12:N22	2.77	0.52
1:D:277:MET:HE1	1:D:321:LEU:HG	1.90	0.52
1:A:238:MET:O	1:A:239:PRO:C	2.53	0.52
1:A:671:SER:HA	1:A:676:HIS:ND1	2.25	0.52
1:C:701:GLY:HA2	1:C:719:PHE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ILE:HG23	1:A:429:ASN:N	2.25	0.52
1:C:541:ILE:HG23	1:C:552:VAL:HG11	1.92	0.52
1:D:120:ILE:HG13	1:D:133:THR:HG22	1.90	0.52
1:A:373:ARG:HH11	1:A:378:GLY:HA2	1.74	0.52
1:C:427:GLN:C	1:C:429:ASN:H	2.17	0.52
1:D:373:ARG:HD2	1:D:373:ARG:O	2.10	0.52
1:A:313:THR:O	1:A:317:VAL:HG23	2.09	0.52
4:A:1500:5AD:C4'	3:C:1801:B12:N23	2.72	0.52
1:A:613:VAL:HG13	1:A:614:GLY:N	2.25	0.51
1:B:19:LEU:HD12	1:B:499:MET:HE2	1.91	0.51
1:B:153:ARG:HG2	1:B:154:PRO:CD	2.40	0.51
1:C:391:PHE:HA	1:C:416:TYR:CZ	2.45	0.51
1:C:612:THR:CB	1:C:645:THR:HG22	2.37	0.51
1:D:57:ASN:HB3	1:D:99:TRP:CH2	2.45	0.51
1:D:189:VAL:CG2	1:D:196:MET:HA	2.40	0.51
2:E:54:LEU:HD23	2:E:57:MET:HE2	1.92	0.51
2:E:74:ARG:NH2	2:E:109:TRP:HB2	2.25	0.51
1:B:189:VAL:CG2	1:B:196:MET:HA	2.40	0.51
1:C:6:GLN:CG	1:C:7:LEU:N	2.73	0.51
1:C:75:LEU:N	1:C:76:PRO:CD	2.73	0.51
1:C:183:GLN:OE1	1:C:207:LYS:HE2	2.10	0.51
2:H:107:LYS:HB3	2:H:107:LYS:HZ3	1.76	0.51
1:B:675:ILE:HD11	1:B:679:ASN:ND2	2.25	0.51
1:B:737:ARG:O	1:B:739:MET:N	2.40	0.51
1:D:307:ALA:HB1	1:D:340:ARG:HG3	1.91	0.51
1:D:574:VAL:HG13	1:D:576:PHE:CE1	2.46	0.51
1:A:109:ARG:HH21	5:A:767:Z97:P	2.33	0.51
1:A:123:THR:HG23	1:A:135:LYS:HD3	1.91	0.51
1:C:719:PHE:HB3	1:C:723:SER:OG	2.11	0.51
3:C:1801:B12:H531	3:C:1801:B12:C55	2.40	0.51
2:H:35:ASP:HB2	2:H:36:PRO:HD3	1.93	0.51
1:A:611:ALA:HB3	1:A:652:LEU:HD13	1.91	0.51
2:E:72:MET:HG2	2:E:77:MET:HG3	1.93	0.51
1:B:232:ARG:NH2	1:D:598:ARG:CZ	2.74	0.51
1:B:274:ALA:O	1:B:276:SER:N	2.44	0.51
1:B:700:CYS:O	1:B:718:GLY:HA2	2.10	0.51
1:C:36:GLN:O	1:C:52:SER:HB2	2.09	0.51
3:C:1801:B12:H251	3:C:1801:B12:N29	2.25	0.51
1:A:526:THR:HG23	1:A:569:GLU:HG3	1.93	0.51
1:A:560:MET:CG	1:C:96:MET:HE3	2.40	0.51
1:B:618:HIS:HD2	3:B:1801:B12:H482	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:LEU:HA	1:B:699:GLY:O	2.10	0.51
1:C:416:TYR:CD1	1:C:417:PRO:HA	2.46	0.51
1:A:310:ARG:O	1:A:314:VAL:HG23	2.10	0.51
1:B:120:ILE:C	1:B:133:THR:HG22	2.35	0.51
2:F:5:ASP:HA	2:F:6:ASP:C	2.28	0.51
1:A:358:ALA:O	1:A:362:MET:HG3	2.10	0.51
1:A:528:PHE:CZ	1:A:565:GLY:HA3	2.46	0.51
1:C:547:MET:O	1:C:548:ASN:HB2	2.11	0.51
1:C:668:THR:HG23	1:C:676:HIS:CB	2.33	0.51
3:A:1801:B12:H362	3:A:1801:B12:C35	2.39	0.50
1:B:134:ARG:HA	1:B:172:MET:HE3	1.91	0.50
3:B:1801:B12:H362	3:B:1801:B12:C35	2.37	0.50
1:C:525:LEU:HD23	1:C:570:LEU:CD1	2.41	0.50
1:D:663:ALA:HB2	1:D:697:MET:HE3	1.92	0.50
1:A:462:GLU:CD	1:A:462:GLU:H	2.19	0.50
1:B:204:CYS:HB3	1:B:452:PHE:CD2	2.47	0.50
1:C:124:PRO:HA	1:C:493:ASP:O	2.11	0.50
1:D:109:ARG:HG2	1:D:132:ILE:CG1	2.41	0.50
1:D:607:LYS:O	1:D:608:ILE:HD12	2.11	0.50
3:D:1801:B12:H362	3:D:1801:B12:C35	2.37	0.50
3:A:1801:B12:H351	3:A:1801:B12:H372	1.93	0.50
1:B:224:ALA:HB3	1:B:245:HIS:CE1	2.47	0.50
1:B:342:VAL:HG12	1:B:343:PRO:HD2	1.94	0.50
1:C:218:ILE:HD13	1:C:297:ARG:HD2	1.93	0.50
2:G:70:LYS:O	2:G:74:ARG:HG2	2.11	0.50
1:A:662:ASP:O	1:A:697:MET:HE3	2.12	0.50
2:E:51:ARG:HG2	2:E:68:VAL:HG21	1.94	0.50
1:B:13:LEU:HD22	1:B:18:ILE:HD11	1.93	0.50
1:A:688:VAL:HG22	1:A:693:ARG:CG	2.40	0.50
1:B:277:MET:CE	1:B:321:LEU:HD23	2.38	0.50
1:D:7:LEU:HD13	1:D:150:GLU:CD	2.37	0.50
1:D:541:ILE:CD1	1:D:554:VAL:HG23	2.40	0.50
1:A:524:LEU:HB3	1:C:526:THR:HB	1.93	0.50
1:A:719:PHE:HB3	1:A:723:SER:OG	2.11	0.50
1:C:144:LEU:O	1:C:148:GLU:HG2	2.12	0.50
2:H:6:ASP:O	2:H:10:ARG:HG3	2.11	0.50
4:A:1500:5AD:H5'3	3:C:1801:B12:C16	2.41	0.50
1:B:189:VAL:HG22	1:B:196:MET:HA	1.93	0.50
1:C:649:VAL:HG12	1:C:686:LEU:HD13	1.93	0.50
1:C:733:VAL:O	1:C:737:ARG:HG3	2.11	0.50
1:D:290:MET:SD	2:H:23:GLN:HB2	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:THR:CG2	1:A:616:ASP:HB3	2.42	0.50
1:B:671:SER:HA	1:B:676:HIS:ND1	2.26	0.50
3:C:1801:B12:H471	3:C:1801:B12:H492	1.94	0.50
1:D:233:GLU:HG2	1:D:235:TRP:CH2	2.47	0.50
1:D:735:LYS:O	1:D:739:MET:HG3	2.12	0.50
1:A:116:TYR:HE2	1:A:120:ILE:HD13	1.76	0.49
2:E:70:LYS:O	2:E:74:ARG:HG2	2.12	0.49
1:B:8:ARG:HH11	1:B:8:ARG:CB	2.24	0.49
1:B:611:ALA:HB2	1:B:643:LEU:HB2	1.94	0.49
1:D:23:ASP:OD2	1:D:24:LYS:HE3	2.11	0.49
1:D:172:MET:HE3	1:D:176:GLU:HG3	1.94	0.49
1:A:470:LYS:O	1:A:472:ILE:N	2.45	0.49
1:C:622:LEU:HB2	1:C:667:SER:HB2	1.94	0.49
3:C:1801:B12:H492	3:C:1801:B12:C47	2.43	0.49
1:D:671:SER:HB2	1:D:676:HIS:CE1	2.47	0.49
1:A:159:SER:HB3	1:A:173:PHE:CZ	2.48	0.49
1:C:659:LEU:C	1:C:660:LYS:HG2	2.36	0.49
1:A:679:ASN:O	1:A:683:ILE:HG13	2.12	0.49
2:E:64:ALA:O	2:E:68:VAL:HG23	2.12	0.49
1:B:372:LYS:HE2	1:D:370:GLN:HE21	1.76	0.49
1:B:607:LYS:O	1:B:608:ILE:HD12	2.12	0.49
2:G:54:LEU:HD23	2:G:57:MET:CE	2.43	0.49
3:D:1801:B12:H492	3:D:1801:B12:H471	1.95	0.49
1:B:234:ALA:O	1:B:237:VAL:HG12	2.11	0.49
1:B:464:LEU:HD23	1:B:471:LEU:CD1	2.43	0.49
1:C:539:ALA:O	1:C:543:PHE:HD2	1.96	0.49
1:B:512:LYS:HB2	1:B:513:PRO:CD	2.42	0.49
1:B:708:GLU:O	1:B:711:VAL:HG12	2.13	0.49
1:C:116:TYR:CE2	1:C:120:ILE:HD13	2.48	0.49
1:D:510:MET:HE3	1:D:577:SER:HB2	1.94	0.49
1:A:45:PRO:HD2	1:A:46:PHE:CD2	2.48	0.49
2:F:20:GLU:CD	2:F:20:GLU:H	2.21	0.49
1:A:580:ILE:HD12	1:C:535:VAL:CG1	2.42	0.49
3:A:1801:B12:N29	3:A:1801:B12:H251	2.28	0.49
1:C:116:TYR:HE2	1:C:120:ILE:HD13	1.77	0.49
1:D:135:LYS:HG3	1:D:485:TYR:OH	2.12	0.49
1:A:618:HIS:CD2	3:A:1801:B12:N24	2.80	0.49
1:A:619:SER:HB3	1:A:645:THR:HG23	1.94	0.49
1:A:733:VAL:O	1:A:737:ARG:HG3	2.13	0.49
2:E:54:LEU:HD23	2:E:57:MET:CE	2.42	0.49
1:C:43:MET:HE2	1:C:54:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:SER:OG	5:D:767:Z97:OP2	2.22	0.48
1:D:137:VAL:HG11	1:D:172:MET:HE1	1.94	0.48
1:D:204:CYS:HB3	1:D:452:PHE:CD2	2.47	0.48
1:A:690:LYS:HE3	1:A:690:LYS:HA	1.94	0.48
3:A:1801:B12:H251	3:A:1801:B12:H291	1.78	0.48
1:B:432:ILE:N	1:B:432:ILE:HD13	2.27	0.48
1:C:610:ALA:HA	1:C:665:LEU:O	2.12	0.48
1:D:478:GLU:O	1:D:480:PRO:HD3	2.13	0.48
1:B:15:VAL:HG22	1:B:499:MET:CE	2.40	0.48
1:B:511:ILE:HG12	1:D:530:PRO:HD2	1.95	0.48
1:C:8:ARG:HD3	1:C:11:GLU:OE1	2.13	0.48
1:C:406:GLU:HG2	1:C:426:ARG:O	2.13	0.48
1:D:316:HIS:O	1:D:319:ASN:HB2	2.13	0.48
1:D:449:THR:HB	1:D:477:LEU:HD12	1.95	0.48
1:A:218:ILE:HD13	1:A:297:ARG:HG3	1.94	0.48
2:E:80:GLY:O	2:E:84:ILE:HG12	2.14	0.48
1:C:15:VAL:HG22	1:C:499:MET:HE1	1.95	0.48
1:C:668:THR:HG21	1:C:680:MET:HE2	1.95	0.48
1:C:677:TYR:HA	1:C:680:MET:HE3	1.95	0.48
1:A:79:THR:HG22	1:A:80:THR:N	2.29	0.48
1:A:344:TRP:CG	1:A:515:VAL:HB	2.49	0.48
1:A:552:VAL:HG13	1:A:570:LEU:HD23	1.96	0.48
1:B:448:VAL:HB	2:F:56:ARG:HD2	1.96	0.48
1:B:706:THR:HB	1:B:709:VAL:HG23	1.95	0.48
1:C:416:TYR:CG	1:C:417:PRO:HA	2.49	0.48
1:D:684:HIS:O	1:D:687:ALA:HB3	2.12	0.48
1:A:531:THR:HG22	1:A:536:ALA:HB2	1.95	0.48
1:C:61:LEU:O	1:C:62:PRO:C	2.53	0.48
1:A:730:THR:O	1:A:734:LYS:HB2	2.14	0.48
4:A:1500:5AD:H5'2	3:C:1801:B12:H261	1.96	0.48
2:E:63:GLU:O	2:E:67:ILE:HG13	2.14	0.48
1:B:212:TRP:CZ2	1:B:477:LEU:HB3	2.49	0.48
1:C:75:LEU:N	1:C:76:PRO:HD3	2.28	0.48
1:C:355:ALA:O	1:C:359:LEU:HD12	2.14	0.48
1:D:7:LEU:HD23	1:D:7:LEU:HA	1.73	0.48
1:D:438:PHE:CD2	2:H:77:MET:HG3	2.49	0.48
3:D:1801:B12:H421	3:D:1801:B12:C10	2.43	0.48
3:D:1801:B12:H552	3:D:1801:B12:H531	1.96	0.48
1:A:41:LEU:HD21	1:A:43:MET:HE2	1.96	0.48
1:A:287:LEU:HD12	1:A:291:PHE:CD2	2.49	0.48
1:A:526:THR:HG23	1:A:569:GLU:CG	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:MET:HB2	1:B:565:GLY:O	2.14	0.48
1:B:683:ILE:CG2	1:B:698:ILE:HD13	2.44	0.48
2:F:59:PHE:CE1	2:F:100:GLY:HA3	2.49	0.48
1:C:225:HIS:O	1:C:228:ASN:HB2	2.13	0.48
2:G:18:SER:OG	2:G:21:GLU:HG3	2.14	0.48
1:D:281:LEU:HB3	1:D:282:PRO:HD3	1.94	0.48
1:B:137:VAL:CG2	1:B:172:MET:HE1	2.42	0.48
2:F:113:ILE:HG22	2:F:113:ILE:O	2.13	0.48
1:C:335:THR:HG22	1:C:348:ASN:HA	1.96	0.48
2:G:76:LEU:O	2:G:77:MET:C	2.56	0.48
1:D:251:PHE:O	1:D:255:VAL:HG23	2.14	0.48
1:A:628:ILE:O	1:A:629:LYS:C	2.56	0.47
2:E:107:LYS:O	2:E:108:TYR:CB	2.62	0.47
1:B:311:GLU:OE2	1:D:63:SER:HB2	2.14	0.47
1:C:143:ALA:O	1:C:146:LEU:HB2	2.14	0.47
1:D:189:VAL:HG22	1:D:196:MET:HA	1.96	0.47
1:D:337:ASP:O	1:D:338:GLU:C	2.57	0.47
1:A:390:LEU:HD13	2:E:10:ARG:HB3	1.96	0.47
2:E:99:ALA:O	2:E:102:ALA:HB3	2.14	0.47
1:B:123:THR:O	1:B:494:ASN:HA	2.14	0.47
1:B:246:ALA:O	1:B:250:ILE:HG22	2.13	0.47
4:B:1500:5AD:H5'3	3:D:1801:B12:C15	2.39	0.47
1:D:124:PRO:O	1:D:131:PRO:HG2	2.14	0.47
1:D:219:ASP:HB3	1:D:248:ASN:ND2	2.29	0.47
2:H:103:LEU:HD22	2:H:109:TRP:CZ2	2.49	0.47
1:A:584:VAL:C	1:A:585:ILE:HG13	2.40	0.47
1:D:5:LEU:HD23	1:D:5:LEU:C	2.39	0.47
1:D:86:ARG:CD	1:D:498:ARG:HD3	2.44	0.47
1:D:511:ILE:HG22	1:D:578:ILE:O	2.14	0.47
1:A:137:VAL:HB	1:A:172:MET:CE	2.44	0.47
1:A:537:GLU:O	1:A:541:ILE:HG13	2.14	0.47
1:C:458:LYS:HE2	1:C:462:GLU:HG2	1.96	0.47
1:C:466:SER:O	1:C:467:GLU:HG2	2.14	0.47
1:B:90:ASP:O	1:B:94:MET:HG3	2.14	0.47
1:B:309:THR:HG22	1:B:336:PRO:O	2.13	0.47
1:A:137:VAL:CB	1:A:172:MET:HE1	2.44	0.47
2:E:47:PRO:O	2:E:51:ARG:HG3	2.14	0.47
1:B:609:VAL:HG23	1:B:652:LEU:HD11	1.97	0.47
1:B:676:HIS:O	1:B:680:MET:HE3	2.15	0.47
1:C:233:GLU:HG2	1:C:235:TRP:CH2	2.50	0.47
1:C:612:THR:HG22	1:C:616:ASP:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:LYS:HB2	1:C:695:LYS:HE3	1.61	0.47
2:G:107:LYS:HG2	2:G:108:TYR:CD1	2.50	0.47
1:D:25:TYR:HD2	1:D:138:ARG:HG2	1.80	0.47
3:D:1801:B12:H351	3:D:1801:B12:H372	1.97	0.47
3:D:1801:B12:H531	3:D:1801:B12:H543	1.97	0.47
1:A:538:PHE:CD2	1:C:585:ILE:HG12	2.50	0.47
1:B:737:ARG:C	1:B:739:MET:N	2.73	0.47
1:C:467:GLU:O	1:C:469:SER:N	2.48	0.47
1:D:342:VAL:O	1:D:343:PRO:C	2.57	0.47
1:D:374:GLU:HA	1:D:374:GLU:OE1	2.14	0.47
1:D:561:GLN:HB3	1:D:564:GLU:HB2	1.96	0.47
1:A:159:SER:O	1:A:181:ALA:HA	2.15	0.47
1:A:268:PRO:HA	1:A:269:PRO:HD3	1.81	0.47
1:A:341:ASN:ND2	1:A:342:VAL:O	2.45	0.47
1:A:547:MET:O	1:A:548:ASN:HB2	2.15	0.47
1:A:649:VAL:O	1:A:653:VAL:HG23	2.15	0.47
3:A:1801:B12:H531	3:A:1801:B12:H543	1.97	0.47
2:E:23:GLN:O	2:E:26:PHE:HB3	2.15	0.47
1:B:8:ARG:CB	1:B:8:ARG:NH1	2.77	0.47
1:B:324:LYS:HE2	1:B:362:MET:O	2.15	0.47
1:D:396:ILE:C	1:D:398:ALA:H	2.23	0.47
1:D:411:VAL:HG12	1:D:411:VAL:O	2.15	0.47
2:H:50:GLU:CG	2:H:77:MET:HE1	2.45	0.47
1:A:6:GLN:CG	1:A:7:LEU:N	2.77	0.47
1:C:95:ARG:HH21	1:C:150:GLU:CD	2.22	0.47
3:C:1801:B12:C2B	3:C:1801:B12:O7R	2.63	0.47
1:D:416:TYR:CD2	1:D:417:PRO:HA	2.50	0.47
3:D:1801:B12:C49	3:D:1801:B12:C47	2.87	0.47
1:A:622:LEU:HD11	1:A:626:ILE:HD11	1.97	0.46
1:C:117:ASP:HA	1:C:164:VAL:HG23	1.97	0.46
1:C:495:VAL:O	1:C:499:MET:HG2	2.14	0.46
1:D:560:MET:HE2	1:D:560:MET:HA	1.97	0.46
1:C:299:GLN:HG3	1:C:300:MET:N	2.30	0.46
1:C:444:TYR:HA	2:G:79:LYS:O	2.15	0.46
1:C:550:GLU:HB2	1:C:573:ARG:HB3	1.96	0.46
1:D:219:ASP:HB3	1:D:248:ASN:HD22	1.80	0.46
1:A:534:ARG:NH2	1:C:586:PRO:O	2.35	0.46
2:F:5:ASP:N	2:F:6:ASP:HB3	2.30	0.46
1:C:7:LEU:HA	1:C:7:LEU:HD23	1.63	0.46
1:C:158:HIS:HD2	1:C:159:SER:N	2.09	0.46
2:H:24:THR:O	2:H:28:GLU:CG	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASN:C	1:A:341:ASN:HD22	2.23	0.46
1:B:622:LEU:HB2	1:B:667:SER:HB2	1.96	0.46
1:B:684:HIS:O	1:B:688:VAL:HG23	2.15	0.46
1:C:184:ASP:OD1	1:C:186:GLN:HB2	2.15	0.46
2:G:46:THR:HB	2:G:47:PRO:HD2	1.97	0.46
1:D:196:MET:SD	1:D:402:PHE:CD1	3.08	0.46
1:D:736:ARG:O	1:D:736:ARG:HG2	2.15	0.46
1:B:13:LEU:HD13	1:B:91:ILE:HG22	1.96	0.46
1:D:344:TRP:CD1	1:D:515:VAL:HB	2.51	0.46
1:D:444:TYR:C	1:D:444:TYR:CD2	2.93	0.46
1:A:612:THR:HB	1:A:645:THR:HA	1.98	0.46
1:D:510:MET:CE	1:D:577:SER:HB2	2.46	0.46
1:D:721:ARG:HG3	1:D:721:ARG:NH1	2.27	0.46
3:B:1801:B12:H351	3:B:1801:B12:H372	1.98	0.46
1:D:269:PRO:HD2	1:D:280:ASP:CG	2.41	0.46
1:D:561:GLN:O	1:D:562:GLU:C	2.58	0.46
3:D:1801:B12:H552	3:D:1801:B12:C53	2.46	0.46
1:A:305:MET:HE3	1:A:305:MET:HB2	1.73	0.46
1:A:350:GLU:CG	1:C:310:ARG:HD3	2.46	0.46
1:B:79:THR:HB	1:B:332:SER:HA	1.98	0.46
1:B:115:HIS:HB3	1:D:623:ARG:NH1	2.30	0.46
1:B:506:ARG:HD3	1:B:518:GLN:HE22	1.80	0.46
3:B:1801:B12:H531	3:B:1801:B12:H543	1.98	0.46
1:C:50:ASP:O	1:C:75:LEU:HG	2.15	0.46
1:C:173:PHE:CD1	1:C:178:VAL:HG21	2.51	0.46
1:C:281:LEU:HB3	1:C:282:PRO:HD3	1.98	0.46
1:D:459:GLN:CG	1:D:460:TYR:CD2	2.98	0.46
1:D:578:ILE:HD13	1:D:578:ILE:HA	1.76	0.46
1:A:349:ILE:HD12	1:A:349:ILE:N	2.30	0.46
1:A:618:HIS:CG	1:A:669:ILE:HG21	2.51	0.46
1:B:650:GLU:HB3	1:B:651:LYS:HZ2	1.80	0.46
2:F:112:ALA:C	2:F:114:GLN:N	2.72	0.46
1:C:336:PRO:HD2	1:C:347:TYR:HB3	1.97	0.46
1:D:192:ARG:HD3	1:D:192:ARG:HA	1.81	0.46
1:D:445:MET:HE3	1:D:447:PRO:CD	2.46	0.46
1:D:607:LYS:C	1:D:608:ILE:HD12	2.41	0.46
1:B:36:GLN:O	1:B:52:SER:HB2	2.16	0.46
1:B:580:ILE:HD12	1:D:535:VAL:HG11	1.96	0.46
1:D:8:ARG:HG3	1:D:11:GLU:OE1	2.16	0.46
1:A:307:ALA:HB1	1:A:556:ASN:HB2	1.98	0.45
1:A:344:TRP:CD1	1:A:515:VAL:HB	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLU:HG3	1:C:499:MET:HE3	1.98	0.45
1:C:186:GLN:HG2	1:C:401:TYR:OH	2.16	0.45
1:C:396:ILE:HD12	2:G:29:MET:HG2	1.98	0.45
1:D:43:MET:CE	1:D:72:PRO:HB3	2.46	0.45
1:D:399:GLY:HA3	1:D:403:ASN:HD22	1.81	0.45
1:B:7:LEU:HD13	1:B:150:GLU:HB2	1.97	0.45
1:B:82:ILE:HG22	1:B:90:ASP:HB3	1.99	0.45
1:B:86:ARG:O	1:B:87:PHE:C	2.59	0.45
1:B:415:TYR:O	1:B:416:TYR:C	2.59	0.45
1:B:538:PHE:CD2	1:D:585:ILE:HG23	2.51	0.45
1:B:543:PHE:O	1:B:547:MET:HG3	2.17	0.45
1:D:138:ARG:HE	1:D:176:GLU:CD	2.24	0.45
1:D:286:ALA:HB2	1:D:381:VAL:HG13	1.98	0.45
1:A:460:TYR:O	1:A:461:ASP:HB2	2.16	0.45
3:B:1801:B12:H252	3:B:1801:B12:H601	1.99	0.45
1:D:622:LEU:HD23	1:D:642:TYR:HE1	1.81	0.45
1:A:373:ARG:NH1	1:A:378:GLY:HA2	2.31	0.45
1:A:412:ASP:OD1	1:A:419:ARG:HG3	2.17	0.45
1:A:541:ILE:HG23	1:A:552:VAL:CG1	2.47	0.45
1:A:576:PHE:CD2	1:A:576:PHE:N	2.84	0.45
2:E:57:MET:CE	2:E:82:GLY:HA2	2.46	0.45
1:B:668:THR:HG21	1:B:680:MET:HE2	1.97	0.45
1:B:676:HIS:O	1:B:680:MET:HG3	2.16	0.45
2:F:6:ASP:OD1	2:F:10:ARG:HD2	2.17	0.45
1:C:345:HIS:CD2	1:C:515:VAL:O	2.70	0.45
1:D:622:LEU:HB2	1:D:667:SER:HB2	1.98	0.45
1:D:675:ILE:O	1:D:675:ILE:HG13	2.14	0.45
1:B:557:ARG:HG3	1:B:557:ARG:HH11	1.80	0.45
1:C:233:GLU:HB3	1:C:235:TRP:CZ3	2.51	0.45
1:C:654:ASP:OD1	1:C:690:LYS:HE2	2.16	0.45
1:D:622:LEU:HG	1:D:626:ILE:HD12	1.98	0.45
1:D:305:MET:HE3	1:D:305:MET:HB2	1.69	0.45
1:A:445:MET:HE3	2:E:83:HIS:CD2	2.51	0.45
2:E:112:ALA:C	2:E:114:GLN:N	2.74	0.45
1:B:167:PRO:O	1:B:168:ASP:C	2.60	0.45
1:B:237:VAL:O	1:B:237:VAL:HG22	2.17	0.45
1:A:246:ALA:O	1:A:250:ILE:HG22	2.16	0.45
1:A:290:MET:HE3	2:E:26:PHE:CG	2.52	0.45
1:A:300:MET:HB2	1:A:334:ILE:HG12	1.98	0.45
1:A:350:GLU:HG2	1:C:310:ARG:HD3	1.98	0.45
1:A:647:VAL:HG13	1:A:651:LYS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:60:SER:H	2:E:63:GLU:HG3	1.80	0.45
1:B:323:SER:HB3	1:B:328:ALA:HB2	1.98	0.45
1:C:290:MET:HE3	1:C:385:LYS:HG2	1.99	0.45
1:D:109:ARG:HG2	1:D:132:ILE:HG12	1.99	0.45
3:D:1801:B12:H291	3:D:1801:B12:H251	1.81	0.45
1:B:626:ILE:HD13	1:B:640:VAL:HG11	1.99	0.45
1:C:181:ALA:HB3	1:C:210:MET:HE3	1.99	0.45
1:C:547:MET:O	1:C:548:ASN:CB	2.65	0.45
3:D:1801:B12:H601	3:D:1801:B12:C26	2.45	0.45
2:E:60:SER:OG	2:E:63:GLU:HG2	2.17	0.45
1:B:401:TYR:O	1:B:405:VAL:HG23	2.17	0.45
1:B:538:PHE:CE2	1:D:585:ILE:HG23	2.52	0.45
1:C:287:LEU:O	1:C:291:PHE:HD2	2.00	0.45
2:G:38:LEU:HD23	2:G:38:LEU:HA	1.74	0.45
1:D:116:TYR:CD1	1:D:116:TYR:N	2.85	0.45
1:D:158:HIS:HE1	1:D:218:ILE:HG13	1.82	0.45
1:D:172:MET:C	1:D:172:MET:HE2	2.42	0.45
1:B:176:GLU:OE1	1:B:176:GLU:HA	2.17	0.44
1:D:123:THR:O	1:D:494:ASN:HA	2.16	0.44
1:D:250:ILE:HD12	1:D:250:ILE:HA	1.68	0.44
1:D:401:TYR:O	1:D:402:PHE:C	2.60	0.44
1:B:426:ARG:NH1	1:D:634:GLU:OE2	2.32	0.44
1:C:6:GLN:CG	1:C:7:LEU:H	2.30	0.44
1:D:26:THR:HG22	1:D:27:PRO:HD2	2.00	0.44
1:D:162:SER:HB2	5:D:767:Z97:H6	1.98	0.44
1:D:461:ASP:OD1	1:D:463:ALA:HB3	2.17	0.44
1:D:734:LYS:HB3	1:D:734:LYS:HE2	1.78	0.44
1:A:38:ALA:HB1	1:A:41:LEU:HB2	1.99	0.44
1:A:574:VAL:HA	1:A:575:PRO:HD3	1.69	0.44
1:A:671:SER:O	1:A:672:HIS:C	2.59	0.44
3:A:1801:B12:H18	3:A:1801:B12:H561	1.64	0.44
1:B:213:ALA:HB3	1:B:215:MET:HG3	1.98	0.44
1:C:300:MET:HE2	1:C:320:LEU:HD21	2.00	0.44
1:D:116:TYR:N	1:D:116:TYR:HD1	2.15	0.44
1:D:424:ILE:HD13	1:D:424:ILE:HA	1.71	0.44
1:D:610:ALA:HA	1:D:665:LEU:O	2.17	0.44
1:C:23:ASP:OD2	1:C:24:LYS:HE3	2.18	0.44
2:G:95:SER:O	2:G:96:VAL:C	2.61	0.44
1:D:706:THR:O	1:D:707:PRO:C	2.59	0.44
1:A:269:PRO:HD2	1:A:280:ASP:CG	2.43	0.44
1:A:441:ASP:HB2	2:E:78:GLY:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:PHE:C	1:C:411:VAL:HG23	2.43	0.44
1:C:517:TRP:O	1:C:518:GLN:C	2.60	0.44
1:D:290:MET:HE2	1:D:385:LYS:HG2	1.99	0.44
1:D:406:GLU:OE2	1:D:428:ILE:HG23	2.18	0.44
1:A:234:ALA:O	1:A:237:VAL:HG12	2.18	0.44
1:A:470:LYS:O	1:A:471:LEU:C	2.61	0.44
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.76	0.44
2:E:74:ARG:HB2	2:E:76:LEU:HD22	2.00	0.44
1:B:7:LEU:HD12	1:B:146:LEU:C	2.43	0.44
1:B:538:PHE:CZ	1:D:586:PRO:HD2	2.52	0.44
1:B:687:ALA:O	1:B:692:ILE:HG13	2.17	0.44
1:D:31:GLY:O	1:D:179:ASN:HB3	2.17	0.44
1:A:369:VAL:CG1	1:C:369:VAL:HG13	2.47	0.44
1:C:90:ASP:O	1:C:94:MET:HG3	2.17	0.44
2:G:40:LEU:HD23	2:G:40:LEU:HA	1.74	0.44
1:B:126:GLY:HA3	1:B:131:PRO:HD3	1.99	0.44
1:B:178:VAL:O	1:B:215:MET:HE3	2.17	0.44
3:B:1801:B12:H301	3:B:1801:B12:H253	1.75	0.44
1:D:116:TYR:CE2	1:D:120:ILE:HD13	2.53	0.44
1:A:688:VAL:HG22	1:A:693:ARG:CB	2.48	0.43
1:A:735:LYS:O	1:A:735:LYS:HG3	2.18	0.43
1:C:160:TYR:OH	5:C:767:Z97:HBA	2.18	0.43
1:A:195:ASN:ND2	1:A:428:ILE:O	2.50	0.43
1:A:372:LYS:HG2	1:C:370:GLN:NE2	2.33	0.43
1:B:232:ARG:CZ	1:D:598:ARG:NH2	2.80	0.43
1:B:712:LYS:HA	1:B:712:LYS:HD3	1.71	0.43
1:C:344:TRP:CG	1:C:515:VAL:HB	2.54	0.43
1:D:233:GLU:HG2	1:D:235:TRP:CZ2	2.53	0.43
2:H:10:ARG:HE	2:H:10:ARG:HB3	1.57	0.43
1:A:598:ARG:NH1	1:C:232:ARG:HD2	2.34	0.43
1:A:607:LYS:NZ	1:A:659:LEU:O	2.45	0.43
1:C:14:ASP:CG	1:C:17:ASN:HB2	2.44	0.43
1:C:144:LEU:HD23	1:C:147:ILE:HD12	2.00	0.43
1:C:190:LEU:O	1:C:426:ARG:NH2	2.50	0.43
1:C:291:PHE:O	1:C:292:GLU:C	2.60	0.43
1:D:445:MET:HG2	1:D:446:ALA:N	2.32	0.43
1:A:87:PHE:HB2	1:A:140:GLN:NE2	2.34	0.43
1:A:341:ASN:ND2	1:A:341:ASN:C	2.76	0.43
1:A:586:PRO:HA	1:A:587:PRO:HD3	1.85	0.43
2:E:6:ASP:OD1	2:E:10:ARG:HG2	2.19	0.43
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:TRP:C	1:B:214:ASP:H	2.26	0.43
1:B:522:THR:HA	1:B:572:GLY:O	2.18	0.43
1:B:526:THR:HB	1:D:524:LEU:HB3	2.00	0.43
1:B:608:ILE:HG21	1:B:665:LEU:HD12	2.00	0.43
1:B:672:HIS:O	1:B:675:ILE:HG22	2.19	0.43
1:C:94:MET:SD	1:C:105:ILE:HG21	2.58	0.43
1:C:305:MET:HE3	1:C:305:MET:HB2	1.83	0.43
3:C:1801:B12:O7R	3:C:1801:B12:H2B	2.17	0.43
2:G:86:TYR:O	2:G:87:LYS:C	2.59	0.43
1:D:591:ILE:HD12	1:D:591:ILE:N	2.32	0.43
1:A:310:ARG:HD3	1:C:350:GLU:HG2	1.99	0.43
1:A:320:LEU:HD11	1:A:355:ALA:HA	2.01	0.43
1:A:528:PHE:HE1	1:A:565:GLY:HA3	1.79	0.43
1:A:708:GLU:C	1:A:710:ALA:H	2.26	0.43
1:B:297:ARG:O	1:B:297:ARG:HD3	2.18	0.43
1:B:576:PHE:HE1	1:D:543:PHE:HD1	1.67	0.43
1:C:427:GLN:C	1:C:429:ASN:N	2.77	0.43
1:A:726:ILE:CG2	1:A:727:HIS:N	2.82	0.43
1:B:109:ARG:HH21	5:B:767:Z97:P	2.42	0.43
1:D:108:ILE:H	1:D:108:ILE:HG12	1.55	0.43
1:D:110:THR:O	1:D:111:ALA:C	2.61	0.43
2:H:103:LEU:HD22	2:H:109:TRP:CE2	2.53	0.43
1:A:242:MET:HE2	1:A:242:MET:HB3	1.77	0.43
1:B:265:SER:OG	1:B:297:ARG:NH1	2.49	0.43
3:B:1801:B12:H412	3:B:1801:B12:H363	1.48	0.43
1:C:317:VAL:HA	1:C:320:LEU:HD12	2.01	0.43
1:C:723:SER:O	3:C:1801:B12:C5R	2.67	0.43
2:G:14:LEU:HD22	2:G:22:LEU:CD1	2.49	0.43
2:H:74:ARG:HE	2:H:109:TRP:HB3	1.84	0.43
2:H:101:LEU:HD12	2:H:101:LEU:HA	1.88	0.43
1:A:618:HIS:CE1	3:A:1801:B12:N22	2.86	0.43
1:B:561:GLN:O	1:B:562:GLU:C	2.61	0.43
1:B:578:ILE:HD13	1:D:543:PHE:CE1	2.53	0.43
3:B:1801:B12:H2B	3:B:1801:B12:O7R	2.19	0.43
1:C:53:THR:HA	1:C:54:PRO:HD3	1.85	0.43
1:C:670:ILE:HG23	3:C:1801:B12:O34	2.18	0.43
3:D:1801:B12:H421	3:D:1801:B12:H10	2.00	0.43
2:H:51:ARG:HG2	2:H:68:VAL:HG21	2.01	0.43
1:A:310:ARG:HD3	1:C:350:GLU:CG	2.49	0.43
1:B:58:SER:HB2	1:B:71:ASP:OD2	2.18	0.43
1:B:126:GLY:HA2	1:B:131:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1801:B12:H531	3:D:1801:B12:C55	2.49	0.43
1:A:373:ARG:HA	1:A:377:LEU:HD23	2.01	0.43
1:A:391:PHE:O	1:A:395:ILE:HG13	2.19	0.43
1:A:464:LEU:HA	1:A:464:LEU:HD12	1.67	0.43
1:B:689:GLU:O	1:B:689:GLU:HG2	2.19	0.43
1:C:391:PHE:HD2	1:C:391:PHE:O	2.02	0.43
1:D:123:THR:O	1:D:498:ARG:NH2	2.48	0.43
1:D:235:TRP:O	1:D:238:MET:HE3	2.18	0.43
2:H:5:ASP:HA	2:H:6:ASP:CB	2.49	0.43
1:A:533:LYS:HG3	1:A:534:ARG:N	2.33	0.42
1:A:600:ASP:OD1	1:A:733:VAL:HB	2.18	0.42
1:A:611:ALA:CB	1:A:652:LEU:HD13	2.49	0.42
1:A:697:MET:HG2	1:A:735:LYS:HG3	2.01	0.42
2:E:95:SER:O	2:E:96:VAL:C	2.61	0.42
1:B:7:LEU:HA	1:B:7:LEU:HD23	1.28	0.42
3:B:1801:B12:HM63	3:B:1801:B12:HM51	1.87	0.42
1:C:250:ILE:CG2	1:C:251:PHE:N	2.82	0.42
1:C:492:ASN:N	1:C:492:ASN:HD22	2.17	0.42
1:C:575:PRO:HD2	1:C:576:PHE:CE2	2.53	0.42
1:C:626:ILE:HG21	1:C:640:VAL:HG11	2.01	0.42
3:C:1801:B12:H301	3:C:1801:B12:H253	1.83	0.42
2:G:76:LEU:HD12	2:G:76:LEU:HA	1.80	0.42
1:D:650:GLU:O	1:D:653:VAL:HG23	2.19	0.42
3:D:1801:B12:H562	3:D:1801:B12:H18	1.73	0.42
1:B:8:ARG:HB2	1:B:8:ARG:NH1	2.32	0.42
1:B:116:TYR:CE2	1:B:120:ILE:HD13	2.54	0.42
1:B:529:LEU:HA	1:B:530:PRO:HD3	1.64	0.42
1:D:608:ILE:HG13	1:D:663:ALA:HB3	2.01	0.42
1:D:618:HIS:CD2	3:D:1801:B12:N24	2.87	0.42
1:D:700:CYS:O	1:D:718:GLY:HA2	2.19	0.42
1:A:73:GLN:OE1	1:A:153:ARG:NH2	2.49	0.42
1:A:75:LEU:N	1:A:76:PRO:HD3	2.34	0.42
2:E:103:LEU:C	2:E:105:GLU:H	2.27	0.42
1:B:22:LEU:HD23	1:B:22:LEU:HA	1.79	0.42
1:B:138:ARG:NH1	1:B:485:TYR:CD1	2.87	0.42
1:B:268:PRO:HA	1:B:269:PRO:HD3	1.73	0.42
1:B:609:VAL:HG11	1:B:656:ALA:HA	2.00	0.42
2:F:54:LEU:HD23	2:F:57:MET:HE2	1.98	0.42
1:C:224:ALA:HB3	1:C:245:HIS:CE1	2.54	0.42
1:C:238:MET:HE3	1:C:283:TYR:CB	2.41	0.42
1:C:441:ASP:O	1:C:442:GLU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:MET:O	1:D:239:PRO:C	2.62	0.42
1:B:547:MET:HB3	1:D:547:MET:HB3	2.00	0.42
1:B:706:THR:HB	1:B:709:VAL:CG2	2.49	0.42
3:B:1801:B12:H601	3:B:1801:B12:H262	2.01	0.42
1:C:399:GLY:HA3	1:C:403:ASN:ND2	2.30	0.42
1:C:592:LEU:HD22	1:C:596:GLU:CB	2.49	0.42
1:A:19:LEU:CD1	1:A:499:MET:HE2	2.50	0.42
1:A:467:GLU:O	1:A:469:SER:N	2.52	0.42
1:C:109:ARG:NH2	5:C:767:Z97:P	2.91	0.42
1:D:186:GLN:HG2	1:D:401:TYR:OH	2.19	0.42
1:D:307:ALA:O	1:D:340:ARG:HD3	2.20	0.42
1:A:233:GLU:HB3	1:A:235:TRP:CZ3	2.55	0.42
1:A:467:GLU:C	1:A:469:SER:H	2.27	0.42
1:D:684:HIS:O	1:D:688:VAL:HG23	2.19	0.42
1:A:444:TYR:CE1	2:E:80:GLY:HA2	2.55	0.42
1:B:350:GLU:HB3	1:D:310:ARG:HD3	2.02	0.42
1:B:354:THR:OG1	1:D:310:ARG:HD2	2.20	0.42
1:B:521:GLY:O	1:B:573:ARG:HA	2.20	0.42
3:B:1801:B12:C53	3:B:1801:B12:H552	2.49	0.42
1:C:310:ARG:O	1:C:311:GLU:C	2.63	0.42
3:C:1801:B12:N40	3:C:1801:B12:C8	2.81	0.42
2:G:54:LEU:HD23	2:G:57:MET:HE1	2.01	0.42
1:D:352:CYS:O	1:D:353:ASP:C	2.62	0.42
1:D:443:ASP:OD1	2:H:79:LYS:HE3	2.20	0.42
1:D:506:ARG:HD3	1:D:518:GLN:HE22	1.85	0.42
1:D:574:VAL:HG13	1:D:576:PHE:CD1	2.55	0.42
1:A:207:LYS:HD3	1:A:252:SER:OG	2.19	0.42
1:A:467:GLU:C	1:A:469:SER:N	2.76	0.42
1:A:616:ASP:OD2	1:A:669:ILE:HB	2.20	0.42
1:A:655:ALA:C	1:A:657:ILE:N	2.75	0.42
1:A:712:LYS:HG2	1:A:712:LYS:O	2.20	0.42
2:E:55:LEU:HD23	2:E:55:LEU:HA	1.92	0.42
1:C:126:GLY:HA3	1:C:129:GLY:O	2.20	0.42
1:D:528:PHE:CE1	1:D:560:MET:HG3	2.54	0.42
1:A:16:GLU:OE1	1:A:506:ARG:NH2	2.45	0.42
1:A:512:LYS:HB2	1:A:513:PRO:CD	2.50	0.42
1:B:242:MET:HE2	1:B:242:MET:HB3	1.76	0.42
1:C:191:TYR:HE1	1:C:230:THR:HG21	1.85	0.42
1:D:212:TRP:CZ2	1:D:477:LEU:HB3	2.55	0.42
1:D:522:THR:HG22	1:D:523:VAL:N	2.35	0.42
1:A:349:ILE:N	1:A:349:ILE:CD1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LYS:O	1:C:548:ASN:ND2	2.52	0.42
1:A:593:SER:OG	1:A:595:ASP:HB2	2.19	0.42
1:B:86:ARG:C	1:B:88:GLU:N	2.78	0.42
1:B:492:ASN:HD22	1:B:492:ASN:HA	1.53	0.42
1:D:85:GLY:HA2	1:D:129:GLY:O	2.20	0.42
1:D:399:GLY:HA3	1:D:403:ASN:ND2	2.35	0.42
1:A:585:ILE:HA	1:A:586:PRO:HD3	1.81	0.41
1:B:134:ARG:NH2	1:B:175:GLU:OE2	2.44	0.41
1:B:305:MET:HE3	1:B:305:MET:HB2	1.62	0.41
1:B:512:LYS:HD3	1:B:519:ALA:HB1	2.02	0.41
1:B:665:LEU:HB3	3:B:1801:B12:C5M	2.50	0.41
1:C:6:GLN:HG2	1:C:7:LEU:N	2.35	0.41
2:G:88:ILE:HG13	2:G:103:LEU:HD11	2.02	0.41
1:D:320:LEU:HD11	1:D:355:ALA:HA	2.02	0.41
1:A:96:MET:HG2	1:C:560:MET:HB3	2.02	0.41
1:A:115:HIS:CE1	1:C:623:ARG:HD3	2.55	0.41
1:A:302:THR:HG22	1:A:334:ILE:HG21	2.02	0.41
3:A:1801:B12:N23	4:C:1500:5AD:C4'	2.74	0.41
1:B:182:HIS:HA	1:B:218:ILE:O	2.20	0.41
1:B:200:PHE:CD2	2:F:37:LEU:HD13	2.55	0.41
1:B:701:GLY:HA2	1:B:719:PHE:O	2.20	0.41
1:C:53:THR:HG22	1:C:54:PRO:O	2.20	0.41
1:C:393:GLU:O	1:C:397:GLU:HB3	2.20	0.41
1:D:205:GLU:OE2	1:D:451:HIS:HA	2.20	0.41
1:D:397:GLU:O	1:D:397:GLU:CG	2.64	0.41
1:D:454:TYR:CD2	1:D:454:TYR:C	2.98	0.41
1:A:335:THR:HA	1:A:336:PRO:HD3	1.85	0.41
1:B:511:ILE:HD11	1:D:530:PRO:HD2	2.01	0.41
1:C:18:ILE:HD13	1:C:143:ALA:HB2	2.02	0.41
1:C:110:THR:HG22	1:C:131:PRO:HA	2.01	0.41
1:C:250:ILE:HG23	1:C:251:PHE:N	2.34	0.41
1:C:554:VAL:HG22	1:C:570:LEU:HD23	2.02	0.41
1:D:212:TRP:CH2	1:D:477:LEU:HB3	2.55	0.41
1:D:344:TRP:CG	1:D:515:VAL:HB	2.55	0.41
1:D:415:TYR:O	1:D:416:TYR:C	2.63	0.41
1:D:529:LEU:HA	1:D:530:PRO:HD3	1.85	0.41
1:A:95:ARG:HA	1:A:147:ILE:HD13	2.03	0.41
1:A:547:MET:HE2	1:C:574:VAL:CG2	2.50	0.41
1:B:162:SER:CB	5:B:767:Z97:H6	2.50	0.41
1:B:291:PHE:O	1:B:292:GLU:C	2.64	0.41
1:B:411:VAL:HG12	1:B:411:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:TRP:O	1:B:518:GLN:C	2.62	0.41
1:C:57:ASN:HB3	1:C:99:TRP:CH2	2.56	0.41
1:C:153:ARG:HA	1:C:154:PRO:HD3	1.85	0.41
1:C:406:GLU:OE2	1:C:428:ILE:HG22	2.20	0.41
1:C:619:SER:HB3	1:C:645:THR:CG2	2.49	0.41
1:C:620:VAL:HG23	3:C:1801:B12:O51	2.20	0.41
1:A:79:THR:HA	1:A:104:HIS:HB3	2.02	0.41
1:A:193:ASN:HB2	1:A:426:ARG:CZ	2.50	0.41
1:A:447:PRO:HG2	2:E:57:MET:SD	2.61	0.41
1:B:629:LYS:NZ	5:D:767:Z97:HDA	2.35	0.41
1:C:215:MET:HE2	1:C:215:MET:HB3	1.77	0.41
1:C:223:GLY:O	1:C:224:ALA:C	2.62	0.41
1:C:406:GLU:CD	1:C:428:ILE:HG22	2.45	0.41
1:C:484:VAL:HG11	2:G:60:SER:HB3	2.01	0.41
1:D:275:PRO:HD2	1:D:279:LEU:HD11	2.02	0.41
1:D:344:TRP:CE2	1:D:515:VAL:HG11	2.55	0.41
3:D:1801:B12:H2B	3:D:1801:B12:O7R	2.20	0.41
2:H:6:ASP:HB3	2:H:7:PHE:H	1.74	0.41
1:A:224:ALA:CB	1:A:245:HIS:CE1	3.03	0.41
1:B:20:LYS:O	1:B:21:ASP:HB2	2.21	0.41
1:B:438:PHE:CD2	2:F:77:MET:HG3	2.55	0.41
1:C:464:LEU:HD12	1:C:464:LEU:HA	1.80	0.41
1:D:396:ILE:C	1:D:398:ALA:N	2.79	0.41
1:D:416:TYR:HA	1:D:418:GLU:N	2.35	0.41
1:D:628:ILE:HG12	1:D:628:ILE:O	2.20	0.41
1:D:711:VAL:HG12	1:D:711:VAL:O	2.19	0.41
1:A:342:VAL:CG1	1:A:343:PRO:HD2	2.50	0.41
2:E:35:ASP:HB2	2:E:36:PRO:HD3	2.03	0.41
1:B:243:VAL:HG22	1:B:392:MET:HG3	2.03	0.41
1:C:158:HIS:CD2	1:C:158:HIS:C	2.98	0.41
1:C:649:VAL:HG12	1:C:686:LEU:HD12	2.01	0.41
2:G:52:SER:HA	2:G:55:LEU:HD12	2.03	0.41
1:D:109:ARG:HG2	1:D:132:ILE:HG13	2.02	0.41
1:D:492:ASN:O	1:D:497:VAL:HG21	2.20	0.41
1:D:526:THR:HG23	1:D:569:GLU:HG2	2.02	0.41
1:D:574:VAL:HA	1:D:575:PRO:HD3	1.97	0.41
1:A:41:LEU:HD23	1:A:43:MET:HE2	2.02	0.41
1:A:93:ARG:HG3	1:A:345:HIS:ND1	2.36	0.41
1:A:192:ARG:O	1:A:193:ASN:C	2.62	0.41
1:A:512:LYS:HB2	1:A:513:PRO:HD2	2.03	0.41
1:B:86:ARG:HB3	1:B:88:GLU:CD	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LEU:O	1:B:281:LEU:HD12	2.20	0.41
1:B:307:ALA:O	1:B:340:ARG:HD3	2.21	0.41
3:B:1801:B12:N40	3:B:1801:B12:C8	2.80	0.41
1:D:443:ASP:HA	1:D:456:ASN:HD22	1.85	0.41
2:H:35:ASP:CB	2:H:36:PRO:HD3	2.51	0.41
1:A:578:ILE:CG2	1:A:579:ASP:N	2.84	0.41
1:A:665:LEU:HA	1:A:699:GLY:O	2.20	0.41
2:E:90:LYS:HE2	2:E:90:LYS:HB3	1.83	0.41
1:B:79:THR:HG23	1:B:104:HIS:ND1	2.35	0.41
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.89	0.41
1:B:344:TRP:CD1	1:B:515:VAL:HB	2.56	0.41
1:B:461:ASP:OD1	1:B:463:ALA:HB3	2.21	0.41
1:B:528:PHE:CZ	1:B:565:GLY:HA3	2.56	0.41
1:B:530:PRO:HD2	1:D:511:ILE:HD11	2.03	0.41
3:B:1801:B12:O7R	3:B:1801:B12:C2B	2.68	0.41
2:F:27:TRP:O	2:F:28:GLU:C	2.63	0.41
2:F:66:ALA:O	2:F:70:LYS:HG3	2.21	0.41
2:F:76:LEU:HG	2:F:84:ILE:HD11	2.03	0.41
1:C:500:GLU:C	1:C:502:THR:H	2.28	0.41
1:C:728:VAL:HG21	3:C:1801:B12:HM62	2.03	0.41
1:D:305:MET:HE1	1:D:316:HIS:NE2	2.36	0.41
1:D:382:ARG:CZ	2:H:22:LEU:HD22	2.50	0.41
1:D:464:LEU:O	1:D:465:VAL:C	2.64	0.41
1:D:585:ILE:HA	1:D:586:PRO:HD3	1.76	0.41
3:D:1801:B12:H492	3:D:1801:B12:C47	2.51	0.41
1:A:574:VAL:CG2	1:C:547:MET:HE2	2.51	0.41
1:A:709:VAL:HG12	1:A:709:VAL:O	2.21	0.41
1:B:410:PHE:C	1:B:411:VAL:HG23	2.46	0.41
1:A:116:TYR:HE1	1:C:620:VAL:HG21	1.86	0.40
1:A:422:ASP:OD1	1:A:422:ASP:N	2.50	0.40
1:A:440:ARG:HH22	1:A:451:HIS:CE1	2.38	0.40
1:A:677:TYR:CE1	1:A:709:VAL:HB	2.56	0.40
1:B:281:LEU:HB3	1:B:282:PRO:HD3	2.03	0.40
1:B:284:ALA:O	1:B:288:ARG:HD3	2.20	0.40
1:B:730:THR:O	1:B:731:PHE:C	2.64	0.40
2:F:32:LYS:O	2:F:36:PRO:HD3	2.21	0.40
1:C:109:ARG:NH2	1:C:114:SER:OG	2.51	0.40
1:C:537:GLU:O	1:C:540:ALA:HB3	2.20	0.40
1:C:631:GLY:O	1:C:725:GLY:HA3	2.21	0.40
2:G:54:LEU:HA	2:G:57:MET:CE	2.51	0.40
3:D:1801:B12:H412	3:D:1801:B12:H363	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:106:GLY:HA2	2:H:109:TRP:HD1	1.87	0.40
1:B:14:ASP:O	1:B:18:ILE:HG13	2.21	0.40
1:B:479:VAL:HG12	1:B:479:VAL:O	2.20	0.40
2:F:25:ARG:O	2:F:29:MET:HG3	2.21	0.40
1:C:7:LEU:HD12	1:C:146:LEU:HB3	2.04	0.40
2:G:10:ARG:HE	2:G:10:ARG:HB3	1.19	0.40
1:A:35:ARG:HH12	1:A:74:PRO:HD2	1.86	0.40
1:A:81:GLU:OE2	5:A:767:Z97:N	2.52	0.40
1:A:341:ASN:HD22	1:A:342:VAL:C	2.29	0.40
1:A:470:LYS:C	1:A:472:ILE:N	2.79	0.40
1:A:684:HIS:CE1	1:A:693:ARG:HE	2.39	0.40
2:E:6:ASP:O	2:E:7:PHE:C	2.64	0.40
1:B:665:LEU:HB3	3:B:1801:B12:HM52	2.02	0.40
1:C:6:GLN:HB3	1:C:6:GLN:HE21	1.59	0.40
1:C:668:THR:HG23	1:C:668:THR:O	2.21	0.40
1:D:267:VAL:HG12	1:D:268:PRO:O	2.21	0.40
1:D:457:VAL:O	1:D:458:LYS:C	2.64	0.40
1:D:581:ASN:C	1:D:583:LEU:H	2.30	0.40
2:H:5:ASP:CA	2:H:6:ASP:CB	3.00	0.40
1:B:167:PRO:HB2	2:F:52:SER:HB3	2.02	0.40
1:C:79:THR:HG22	1:C:80:THR:N	2.37	0.40
1:D:575:PRO:HG2	1:D:576:PHE:CD2	2.57	0.40
1:A:390:LEU:HD23	2:E:14:LEU:HD11	2.03	0.40
1:A:534:ARG:O	1:A:535:VAL:C	2.63	0.40
1:A:541:ILE:HG23	1:A:552:VAL:HG12	2.04	0.40
1:A:688:VAL:HG22	1:A:693:ARG:HB2	2.04	0.40
2:E:88:ILE:HD13	2:E:88:ILE:HA	1.85	0.40
1:B:227:ALA:HB3	1:B:241:LEU:CD2	2.51	0.40
1:B:445:MET:HE2	1:B:445:MET:HB3	1.94	0.40
1:B:471:LEU:HD12	1:B:471:LEU:HA	1.86	0.40
1:B:629:LYS:HE3	1:B:630:HIS:NE2	2.37	0.40
3:B:1801:B12:C61	3:B:1801:B12:H562	2.51	0.40
1:C:693:ARG:HD2	1:C:693:ARG:HA	1.72	0.40
2:G:20:GLU:CD	2:G:20:GLU:H	2.30	0.40
1:D:132:ILE:HA	1:D:136:GLN:OE1	2.21	0.40
1:D:238:MET:H	1:D:238:MET:HG3	1.55	0.40
1:D:647:VAL:HA	1:D:648:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	722/763 (95%)	664 (92%)	51 (7%)	7 (1%)	12	38
1	B	722/763 (95%)	660 (91%)	54 (8%)	8 (1%)	11	36
1	C	722/763 (95%)	673 (93%)	43 (6%)	6 (1%)	16	44
1	D	722/763 (95%)	663 (92%)	54 (8%)	5 (1%)	18	47
2	E	108/121 (89%)	95 (88%)	11 (10%)	2 (2%)	6	22
2	F	108/121 (89%)	99 (92%)	6 (6%)	3 (3%)	4	14
2	G	108/121 (89%)	98 (91%)	9 (8%)	1 (1%)	14	41
2	H	108/121 (89%)	97 (90%)	11 (10%)	0	100	100
All	All	3320/3536 (94%)	3049 (92%)	239 (7%)	32 (1%)	12	38

All (32) Ramachandran outliers are listed below:

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

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	598/644 (93%)	550 (92%)	48 (8%)	11	34
1	B	604/644 (94%)	552 (91%)	52 (9%)	10	31
1	C	600/644 (93%)	556 (93%)	44 (7%)	13	38
1	D	602/644 (94%)	549 (91%)	53 (9%)	9	29
2	E	89/100 (89%)	78 (88%)	11 (12%)	4	16
2	F	90/100 (90%)	81 (90%)	9 (10%)	7	24
2	G	89/100 (89%)	84 (94%)	5 (6%)	19	50
2	H	89/100 (89%)	83 (93%)	6 (7%)	15	42
All	All	2761/2976 (93%)	2533 (92%)	228 (8%)	10	32

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	LEU
1	A	23	ASP
1	A	29	ARG
1	A	108	ILE
1	A	114	SER
1	A	127	ILE
1	A	137	VAL
1	A	153	ARG
1	A	164	VAL
1	A	171	VAL
1	A	218	ILE
1	A	233	GLU
1	A	238	MET
1	A	242	MET
1	A	254	LYS
1	A	306	GLU
1	A	338	GLU
1	A	341	ASN
1	A	371	LEU
1	A	374	GLU
1	A	411	VAL
1	A	462	GLU
1	A	464	LEU
1	A	471	LEU
1	A	499	MET
1	A	509	SER
1	A	511	ILE
1	A	518	GLN
1	A	526	THR
1	A	533	LYS
1	A	557	ARG
1	A	570	LEU
1	A	574	VAL
1	A	576	PHE
1	A	578	ILE
1	A	602	GLU
1	A	608	ILE
1	A	609	VAL
1	A	613	VAL
1	A	622	LEU
1	A	640	VAL
1	A	651	LYS

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Mol	Chain	Res	Type
1	A	690	LYS
1	A	706	THR
1	A	712	LYS
1	A	730	THR
1	A	734	LYS
2	E	21	GLU
2	E	23	GLN
2	E	63	GLU
2	E	73	ASP
2	E	76	LEU
2	E	91	GLU
2	E	93	ASN
2	E	94	ILE
2	E	98	GLU
2	E	107	LYS
2	E	114	GLN
1	B	5	LEU
1	B	6	GLN
1	B	7	LEU
1	B	9	VAL
1	B	15	VAL
1	B	24	LYS
1	B	28	LYS
1	B	30	ARG
1	B	39	GLU
1	B	79	THR
1	B	106	MET
1	B	108	ILE
1	B	114	SER
1	B	149	GLU
1	B	151	VAL
1	B	172	MET
1	B	233	GLU
1	B	306	GLU
1	B	308	SER
1	B	313	THR
1	B	327	ARG
1	B	338	GLU
1	B	349	ILE
1	B	432	ILE
1	B	445	MET
1	B	449	THR

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Mol	Chain	Res	Type
1	B	464	LEU
1	B	465	VAL
1	B	471	LEU
1	B	492	ASN
1	B	497	VAL
1	B	501	GLU
1	B	526	THR
1	B	557	ARG
1	B	562	GLU
1	B	570	LEU
1	B	578	ILE
1	B	603	LYS
1	B	606	LEU
1	B	609	VAL
1	B	646	SER
1	B	651	LYS
1	B	670	ILE
1	B	675	ILE
1	B	681	LYS
1	B	683	ILE
1	B	692	ILE
1	B	695	LYS
1	B	696	ILE
1	B	715	VAL
1	B	733	VAL
1	B	739	MET
2	F	9	GLN
2	F	10	ARG
2	F	23	GLN
2	F	28	GLU
2	F	29	MET
2	F	76	LEU
2	F	94	ILE
2	F	101	LEU
2	F	105	GLU
1	C	5	LEU
1	C	6	GLN
1	C	13	LEU
1	C	15	VAL
1	C	20	LYS
1	C	33	THR
1	C	39	GLU

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Mol	Chain	Res	Type
1	C	114	SER
1	C	153	ARG
1	C	162	SER
1	C	232	ARG
1	C	238	MET
1	C	301	ASN
1	C	306	GLU
1	C	338	GLU
1	C	360	ILE
1	C	370	GLN
1	C	397	GLU
1	C	428	ILE
1	C	462	GLU
1	C	464	LEU
1	C	471	LEU
1	C	492	ASN
1	C	500	GLU
1	C	509	SER
1	C	511	ILE
1	C	541	ILE
1	C	569	GLU
1	C	570	LEU
1	C	576	PHE
1	C	577	SER
1	C	578	ILE
1	C	584	VAL
1	C	591	ILE
1	C	604	THR
1	C	608	ILE
1	C	609	VAL
1	C	613	VAL
1	C	628	ILE
1	C	643	LEU
1	C	651	LYS
1	C	660	LYS
1	C	668	THR
1	C	736	ARG
2	G	10	ARG
2	G	39	ASP
2	G	76	LEU
2	G	104	SER
2	G	114	GLN

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Mol	Chain	Res	Type
1	D	6	GLN
1	D	7	LEU
1	D	8	ARG
1	D	9	VAL
1	D	15	VAL
1	D	18	ILE
1	D	26	THR
1	D	29	ARG
1	D	39	GLU
1	D	43	MET
1	D	47	ILE
1	D	50	ASP
1	D	53	THR
1	D	63	SER
1	D	79	THR
1	D	91	ILE
1	D	108	ILE
1	D	127	ILE
1	D	153	ARG
1	D	172	MET
1	D	179	ASN
1	D	232	ARG
1	D	250	ILE
1	D	306	GLU
1	D	338	GLU
1	D	369	VAL
1	D	370	GLN
1	D	397	GLU
1	D	424	ILE
1	D	428	ILE
1	D	465	VAL
1	D	471	LEU
1	D	491	GLU
1	D	501	GLU
1	D	502	THR
1	D	577	SER
1	D	584	VAL
1	D	585	ILE
1	D	608	ILE
1	D	628	ILE
1	D	640	VAL
1	D	653	VAL

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Mol	Chain	Res	Type
1	D	660	LYS
1	D	674	ASP
1	D	675	ILE
1	D	690	LYS
1	D	695	LYS
1	D	696	ILE
1	D	703	THR
1	D	706	THR
1	D	708	GLU
1	D	730	THR
1	D	736	ARG
2	H	23	GLN
2	H	24	THR
2	H	28	GLU
2	H	39	ASP
2	H	76	LEU
2	H	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	226	ASN
1	A	245	HIS
1	A	331	GLN
1	A	341	ASN
1	A	348	ASN
1	A	370	GLN
1	A	407	GLN
2	E	114	GLN
1	B	73	GLN
1	B	217	GLN
1	B	228	ASN
1	B	331	GLN
1	B	348	ASN
1	B	370	GLN
1	B	407	GLN
1	B	429	ASN
1	B	492	ASN
1	B	496	ASN
1	B	518	GLN
1	B	679	ASN

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Mol	Chain	Res	Type
1	B	713	GLN
1	C	40	ASN
1	C	217	GLN
1	C	228	ASN
1	C	245	HIS
1	C	331	GLN
1	C	348	ASN
1	C	370	GLN
1	C	403	ASN
1	C	429	ASN
1	C	492	ASN
1	C	518	GLN
2	G	8	GLN
2	G	16	ASN
2	G	83	HIS
1	D	6	GLN
1	D	115	HIS
1	D	226	ASN
1	D	319	ASN
1	D	331	GLN
1	D	370	GLN
1	D	407	GLN
1	D	492	ASN
2	H	16	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	B12	A	1801	4,1	94,101,101	1.47	13 (13%)	149,166,166	2.37	37 (24%)
4	5AD	B	1500	3	20,20,20	2.49	10 (50%)	28,30,30	4.22	16 (57%)
4	5AD	A	1500	3	20,20,20	2.51	9 (45%)	28,30,30	4.17	17 (60%)
5	Z97	C	767	-	23,24,24	2.15	7 (30%)	27,33,33	1.79	8 (29%)
5	Z97	D	767	-	23,24,24	2.24	8 (34%)	27,33,33	1.87	5 (18%)
3	B12	D	1801	4,1	94,101,101	1.51	13 (13%)	149,166,166	2.31	35 (23%)
3	B12	C	1801	4,1	94,101,101	1.59	10 (10%)	149,166,166	2.43	39 (26%)
4	5AD	D	1500	3	20,20,20	2.45	9 (45%)	28,30,30	4.11	17 (60%)
4	5AD	C	1500	3	20,20,20	2.57	11 (55%)	28,30,30	4.09	17 (60%)
5	Z97	A	767	-	23,24,24	2.17	6 (26%)	27,33,33	1.86	7 (25%)
5	Z97	B	767	-	23,24,24	2.09	6 (26%)	27,33,33	1.92	5 (18%)
3	B12	B	1801	4,1	94,101,101	1.52	12 (12%)	149,166,166	2.25	34 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B12	A	1801	4,1	1/1/36/38	23/56/223/223	0/3/11/11
4	5AD	B	1500	3	2/2/4/4	0/4/20/20	0/3/3/3
4	5AD	A	1500	3	3/3/4/4	1/4/20/20	0/3/3/3
5	Z97	C	767	-	-	9/18/18/18	0/1/1/1
5	Z97	D	767	-	-	9/18/18/18	0/1/1/1
3	B12	D	1801	4,1	1/1/36/38	24/56/223/223	0/3/11/11
3	B12	C	1801	4,1	1/1/36/38	11/56/223/223	0/3/11/11
4	5AD	D	1500	3	3/3/4/4	0/4/20/20	0/3/3/3
4	5AD	C	1500	3	2/2/4/4	1/4/20/20	0/3/3/3
5	Z97	A	767	-	-	6/18/18/18	0/1/1/1
5	Z97	B	767	-	-	8/18/18/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B12	B	1801	4,1	1/1/36/38	17/56/223/223	0/3/11/11

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1801	B12	C19-N24	-7.88	1.39	1.49
3	B	1801	B12	C19-N24	-6.63	1.40	1.49
3	D	1801	B12	C19-N24	-5.77	1.41	1.49
3	A	1801	B12	C19-N24	-5.42	1.42	1.49
4	A	1500	5AD	C8-N7	5.33	1.41	1.31
5	D	767	Z97	C4A-NE	5.33	1.45	1.27
3	D	1801	B12	C8B-C9B	5.30	1.48	1.40
5	D	767	Z97	C4-C5	5.28	1.49	1.42
3	C	1801	B12	C8B-C9B	5.28	1.48	1.40
4	D	1500	5AD	C8-N7	5.24	1.41	1.31
3	A	1801	B12	C8B-C9B	5.20	1.48	1.40
3	B	1801	B12	C8B-C9B	5.15	1.48	1.40
3	B	1801	B12	C14-N23	5.03	1.41	1.35
5	B	767	Z97	C4A-NE	5.01	1.43	1.27
5	C	767	Z97	C4-C5	4.93	1.48	1.42
5	A	767	Z97	C4-C5	4.92	1.48	1.42
3	C	1801	B12	C14-N23	4.83	1.41	1.35
5	A	767	Z97	C4A-NE	4.81	1.43	1.27
5	C	767	Z97	C4A-NE	4.79	1.43	1.27
4	C	1500	5AD	C8-N7	4.73	1.40	1.31
3	B	1801	B12	C9-N22	4.69	1.42	1.30
5	B	767	Z97	C4-C5	4.68	1.48	1.42
4	C	1500	5AD	O4'-C4'	-4.61	1.30	1.44
3	C	1801	B12	C9-N22	4.50	1.41	1.30
3	A	1801	B12	C9-N22	4.44	1.41	1.30
4	B	1500	5AD	O4'-C4'	-4.38	1.31	1.44
3	D	1801	B12	C9-N22	4.26	1.41	1.30
4	B	1500	5AD	C6-N6	4.23	1.45	1.34
3	A	1801	B12	C14-N23	4.12	1.40	1.35
3	D	1801	B12	C14-N23	4.07	1.40	1.35
4	C	1500	5AD	C6-N6	4.04	1.44	1.34
4	C	1500	5AD	C2-N3	3.98	1.41	1.33
4	A	1500	5AD	C2-N3	3.96	1.41	1.33
4	B	1500	5AD	C2-N3	3.93	1.40	1.33
3	A	1801	B12	C11-N23	3.87	1.44	1.36
3	D	1801	B12	C11-N23	3.86	1.44	1.36
5	D	767	Z97	C4-C4A	3.81	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1500	5AD	C5-C4	3.81	1.45	1.39
4	A	1500	5AD	C6-N6	3.80	1.43	1.34
4	D	1500	5AD	C5-C4	3.78	1.45	1.39
5	A	767	Z97	C4-C4A	3.76	1.54	1.46
4	D	1500	5AD	C6-N6	3.74	1.43	1.34
3	C	1801	B12	C16-C15	-3.72	1.34	1.44
5	B	767	Z97	C4-C4A	3.71	1.54	1.46
3	B	1801	B12	C11-N23	3.69	1.43	1.36
3	D	1801	B12	C16-C15	-3.68	1.34	1.44
4	B	1500	5AD	C8-N7	3.65	1.38	1.31
5	C	767	Z97	C2-N1	3.65	1.40	1.33
4	B	1500	5AD	C5-N7	-3.64	1.32	1.39
3	B	1801	B12	C16-C15	-3.62	1.34	1.44
4	C	1500	5AD	C5-C4	3.61	1.45	1.39
4	D	1500	5AD	C2-N3	3.59	1.40	1.33
5	C	767	Z97	C4-C4A	3.53	1.54	1.46
4	A	1500	5AD	O4'-C4'	-3.45	1.34	1.44
3	D	1801	B12	C6B-C5B	3.44	1.49	1.40
3	A	1801	B12	C6B-C5B	3.43	1.49	1.40
3	C	1801	B12	C11-N23	3.42	1.43	1.36
4	B	1500	5AD	C5-C4	3.40	1.45	1.39
3	A	1801	B12	C16-C15	-3.40	1.34	1.44
3	C	1801	B12	C6B-C5B	3.37	1.49	1.40
4	D	1500	5AD	C5-N7	-3.31	1.33	1.39
3	B	1801	B12	C6B-C5B	3.29	1.48	1.40
5	A	767	Z97	C3-C2	3.12	1.44	1.41
5	A	767	Z97	C2-N1	3.08	1.39	1.33
5	B	767	Z97	C2-N1	3.07	1.39	1.33
3	A	1801	B12	C10-C9	2.99	1.47	1.39
3	D	1801	B12	C10-C9	2.99	1.47	1.39
4	D	1500	5AD	O4'-C4'	-2.95	1.35	1.44
5	D	767	Z97	C2-N1	2.95	1.39	1.33
4	C	1500	5AD	C5-N7	-2.89	1.33	1.39
3	D	1801	B12	C8B-N1B	-2.87	1.33	1.39
5	B	767	Z97	C4-C3	-2.84	1.36	1.41
5	D	767	Z97	OXT-C	2.79	1.39	1.30
5	A	767	Z97	OXT-C	2.76	1.39	1.30
3	C	1801	B12	C2B-N3B	2.73	1.36	1.31
3	C	1801	B12	C8B-N1B	-2.71	1.34	1.39
4	A	1500	5AD	O3'-C3'	-2.70	1.36	1.43
3	B	1801	B12	C9B-N3B	-2.64	1.34	1.39
4	D	1500	5AD	O3'-C3'	-2.64	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1500	5AD	C5-N7	-2.63	1.34	1.39
3	D	1801	B12	C9B-N3B	-2.60	1.34	1.39
4	C	1500	5AD	O3'-C3'	-2.54	1.36	1.43
4	C	1500	5AD	C2-N1	2.54	1.38	1.33
3	B	1801	B12	C8B-N1B	-2.54	1.34	1.39
4	B	1500	5AD	O3'-C3'	-2.52	1.36	1.43
5	C	767	Z97	OXT-C	2.47	1.38	1.30
3	A	1801	B12	C8B-N1B	-2.44	1.34	1.39
5	D	767	Z97	C3-C2	2.44	1.43	1.41
3	B	1801	B12	C10-C9	2.41	1.46	1.39
4	D	1500	5AD	C5-C6	-2.38	1.34	1.41
5	D	767	Z97	C6-N1	2.37	1.39	1.34
4	C	1500	5AD	C6-N1	2.37	1.42	1.35
3	A	1801	B12	C9B-N3B	-2.36	1.35	1.39
4	B	1500	5AD	C5-C6	-2.35	1.34	1.41
5	C	767	Z97	C6-N1	2.35	1.39	1.34
3	D	1801	B12	C2B-N3B	2.33	1.36	1.31
4	B	1500	5AD	C6-N1	2.31	1.42	1.35
3	A	1801	B12	C2B-N3B	2.31	1.36	1.31
5	B	767	Z97	OXT-C	2.30	1.38	1.30
3	C	1801	B12	C10-C9	2.30	1.45	1.39
5	C	767	Z97	C4-C3	-2.29	1.37	1.41
3	D	1801	B12	C14-C15	2.26	1.48	1.38
4	D	1500	5AD	C6-N1	2.26	1.42	1.35
4	A	1500	5AD	C5-C6	-2.18	1.34	1.41
3	B	1801	B12	C14-C15	2.18	1.47	1.38
3	D	1801	B12	C1-C2	-2.15	1.53	1.58
3	A	1801	B12	C14-C15	2.12	1.47	1.38
4	C	1500	5AD	C5-C6	-2.11	1.35	1.41
4	A	1500	5AD	C2-N1	2.11	1.37	1.33
5	D	767	Z97	C4-C3	-2.11	1.37	1.41
3	B	1801	B12	C2B-N3B	2.09	1.35	1.31
4	B	1500	5AD	C4-N3	2.06	1.38	1.34
3	A	1801	B12	C20-C1	-2.01	1.49	1.53
4	C	1500	5AD	C8-N9	2.00	1.40	1.37

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1500	5AD	C5'-C4'-C3'	11.37	127.64	115.70
4	C	1500	5AD	C5'-C4'-C3'	11.25	127.51	115.70
4	D	1500	5AD	C5'-C4'-C3'	10.68	126.91	115.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	B12	C1-C19-N24	9.94	117.31	106.25
3	D	1801	B12	C1-C19-N24	9.82	117.17	106.25
4	A	1500	5AD	C5'-C4'-C3'	9.73	125.92	115.70
4	A	1500	5AD	C2'-C1'-N9	8.91	135.44	113.30
3	B	1801	B12	C13-C12-C11	-8.86	91.07	100.97
3	B	1801	B12	C1-C19-N24	8.70	115.92	106.25
3	C	1801	B12	C20-C1-C19	-8.68	101.00	109.35
4	D	1500	5AD	C2'-C1'-N9	8.41	134.21	113.30
4	B	1500	5AD	C2'-C1'-N9	8.31	133.96	113.30
3	A	1801	B12	C13-C12-C11	-8.21	91.79	100.97
3	C	1801	B12	C13-C12-C11	-8.05	91.97	100.97
3	D	1801	B12	C13-C12-C11	-8.00	92.03	100.97
3	D	1801	B12	C46-C12-C13	-7.85	80.93	112.74
3	D	1801	B12	C47-C12-C46	7.80	122.32	109.41
3	C	1801	B12	C46-C12-C13	-7.79	81.18	112.74
3	C	1801	B12	C1-C19-N24	7.69	114.81	106.25
4	C	1500	5AD	C2'-C1'-N9	7.65	132.31	113.30
3	A	1801	B12	C12-C11-N23	7.56	122.25	111.83
3	A	1801	B12	C47-C12-C46	7.45	121.75	109.41
3	B	1801	B12	C1-C19-C18	7.25	133.65	121.90
3	C	1801	B12	C47-C12-C46	7.24	121.39	109.41
3	A	1801	B12	C46-C12-C13	-7.14	83.80	112.74
3	C	1801	B12	C1-C19-C18	7.13	133.46	121.90
5	D	767	Z97	OP4-C5A-C5	6.97	122.42	109.36
3	A	1801	B12	C12-C11-C10	-6.75	114.70	123.40
3	D	1801	B12	C12-C11-N23	6.70	121.05	111.83
3	C	1801	B12	C55-C17-C16	-6.53	103.82	116.59
4	A	1500	5AD	N3-C2-N1	-6.45	118.81	128.58
3	D	1801	B12	C12-C11-C10	-6.41	115.13	123.40
3	B	1801	B12	C46-C12-C13	-6.40	86.81	112.74
3	B	1801	B12	C47-C12-C46	6.36	119.94	109.41
4	C	1500	5AD	N3-C2-N1	-6.21	119.19	128.58
4	D	1500	5AD	C5-C4-N3	-6.09	118.34	126.72
4	D	1500	5AD	O3'-C3'-C4'	6.04	125.27	110.47
3	A	1801	B12	C47-C12-C13	-6.04	88.27	112.74
3	D	1801	B12	C1-C19-C18	5.98	131.60	121.90
4	A	1500	5AD	C5-C4-N3	-5.95	118.53	126.72
4	B	1500	5AD	O2'-C2'-C3'	5.94	130.86	111.82
4	B	1500	5AD	O3'-C3'-C4'	5.91	124.94	110.47
3	A	1801	B12	C1-C19-C18	5.89	131.46	121.90
4	A	1500	5AD	O2'-C2'-C3'	5.88	130.67	111.82
4	B	1500	5AD	N3-C2-N1	-5.88	119.68	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	767	Z97	OP4-C5A-C5	5.88	120.37	109.36
4	D	1500	5AD	N3-C2-N1	-5.84	119.74	128.58
3	A	1801	B12	C18-C19-N24	5.75	110.97	102.33
5	B	767	Z97	OP4-C5A-C5	5.72	120.07	109.36
3	B	1801	B12	C12-C11-N23	5.70	119.68	111.83
3	D	1801	B12	C18-C19-N24	5.69	110.88	102.33
3	B	1801	B12	C12-C11-C10	-5.67	116.09	123.40
4	A	1500	5AD	O3'-C3'-C4'	5.66	124.33	110.47
4	A	1500	5AD	O3'-C3'-C2'	5.63	129.88	111.82
3	B	1801	B12	C47-C12-C13	-5.59	90.09	112.74
4	C	1500	5AD	O2'-C2'-C1'	5.58	129.31	110.10
3	C	1801	B12	C18-C19-N24	5.51	110.61	102.33
4	B	1500	5AD	C5-C4-N3	-5.51	119.13	126.72
3	C	1801	B12	C12-C11-C10	-5.49	116.32	123.40
5	C	767	Z97	OP4-C5A-C5	5.43	119.53	109.36
4	C	1500	5AD	C5-C4-N3	-5.18	119.59	126.72
4	C	1500	5AD	O3'-C3'-C4'	5.13	123.04	110.47
3	D	1801	B12	C47-C12-C13	-5.12	91.97	112.74
3	C	1801	B12	C12-C11-N23	5.04	118.78	111.83
3	B	1801	B12	C18-C19-N24	5.01	109.86	102.33
3	B	1801	B12	C20-C1-C19	-5.00	104.54	109.35
3	C	1801	B12	C8B-C9B-N3B	-4.89	104.71	110.00
3	C	1801	B12	C47-C12-C13	-4.86	93.03	112.74
4	B	1500	5AD	O2'-C2'-C1'	4.80	126.65	110.10
4	B	1500	5AD	O4'-C1'-N9	4.80	117.31	108.09
3	A	1801	B12	C20-C1-C19	-4.79	104.74	109.35
3	C	1801	B12	C26-C2-C1	4.72	117.30	110.00
3	C	1801	B12	C9B-C8B-N1B	4.70	107.39	105.30
4	D	1500	5AD	O2'-C2'-C1'	4.65	126.11	110.10
3	A	1801	B12	C15-C14-N23	-4.65	120.66	126.26
4	D	1500	5AD	O2'-C2'-C3'	4.63	126.65	111.82
4	C	1500	5AD	O2'-C2'-C3'	4.61	126.61	111.82
3	B	1801	B12	C2P-C1P-N59	-4.61	106.14	112.92
3	B	1801	B12	C55-C17-C16	-4.59	107.61	116.59
3	A	1801	B12	C13-C14-N23	4.58	115.29	109.09
4	C	1500	5AD	C2'-C3'-C4'	4.54	109.07	102.36
4	C	1500	5AD	O3'-C3'-C2'	4.52	126.31	111.82
4	D	1500	5AD	O3'-C3'-C2'	4.44	126.05	111.82
3	C	1801	B12	C2-C1-C19	4.42	125.49	118.61
4	C	1500	5AD	N9-C8-N7	-4.38	107.72	113.94
3	A	1801	B12	C26-C2-C1	4.38	116.78	110.00
3	D	1801	B12	C55-C17-C16	-4.27	108.23	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1801	B12	C20-C1-C19	-4.25	105.26	109.35
4	A	1500	5AD	O2'-C2'-C1'	4.24	124.71	110.10
3	B	1801	B12	C19-C1-N21	4.21	106.47	102.14
4	D	1500	5AD	O4'-C1'-N9	4.20	116.17	108.09
4	A	1500	5AD	N9-C8-N7	-4.18	108.00	113.94
4	A	1500	5AD	O4'-C1'-N9	4.15	116.05	108.09
3	C	1801	B12	C19-C1-N21	4.13	106.40	102.14
4	B	1500	5AD	O3'-C3'-C2'	4.08	124.89	111.82
3	C	1801	B12	C15-C14-N23	-4.04	121.39	126.26
3	D	1801	B12	C15-C14-N23	-4.00	121.43	126.26
3	B	1801	B12	C15-C14-N23	-3.93	121.53	126.26
4	B	1500	5AD	N9-C8-N7	-3.91	108.39	113.94
3	B	1801	B12	C47-C12-C11	3.90	124.03	110.08
3	D	1801	B12	C30-C3-C2	-3.88	110.45	119.00
4	D	1500	5AD	C2-N3-C4	3.86	121.27	111.83
4	A	1500	5AD	C2-N3-C4	3.81	121.14	111.83
3	C	1801	B12	C9B-N3B-C2B	3.78	109.04	104.40
3	C	1801	B12	C2-C1-N21	3.76	107.00	101.78
3	D	1801	B12	C13-C14-N23	3.75	114.18	109.09
3	C	1801	B12	C13-C14-N23	3.72	114.13	109.09
3	A	1801	B12	C55-C17-C16	-3.71	109.33	116.59
4	D	1500	5AD	N9-C8-N7	-3.70	108.69	113.94
4	C	1500	5AD	C2-N3-C4	3.69	120.84	111.83
3	A	1801	B12	C8B-C9B-N3B	-3.64	106.06	110.00
5	B	767	Z97	C5-C6-N1	-3.62	117.94	123.83
4	B	1500	5AD	C5-N7-C8	3.59	109.09	103.45
3	D	1801	B12	C2-C1-N21	3.54	106.69	101.78
3	C	1801	B12	C25-C2-C1	-3.51	108.51	113.75
3	D	1801	B12	C19-C1-N21	3.49	105.73	102.14
3	A	1801	B12	C9-C10-C11	-3.48	121.00	125.97
4	B	1500	5AD	C2-N3-C4	3.48	120.33	111.83
5	B	767	Z97	OXT-C-O	-3.46	116.23	124.08
4	C	1500	5AD	O4'-C1'-N9	3.45	114.71	108.09
4	B	1500	5AD	O4'-C4'-C5'	3.45	127.08	110.28
3	D	1801	B12	C8B-C9B-N3B	-3.44	106.27	110.00
4	C	1500	5AD	O4'-C4'-C5'	3.43	127.01	110.28
3	D	1801	B12	C26-C2-C1	3.40	115.26	110.00
4	B	1500	5AD	N3-C4-N9	3.39	132.93	127.17
4	A	1500	5AD	O4'-C4'-C5'	3.35	126.61	110.28
3	B	1801	B12	C2-C1-N21	3.30	106.36	101.78
3	D	1801	B12	C25-C2-C1	-3.28	108.85	113.75
3	B	1801	B12	C8B-C9B-N3B	-3.25	106.48	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1801	B12	C26-C2-C1	3.24	115.02	110.00
3	C	1801	B12	C18-C60-C61	-3.23	105.83	114.04
4	D	1500	5AD	O4'-C4'-C5'	3.23	126.00	110.28
3	A	1801	B12	C2-C1-N21	3.21	106.24	101.78
4	A	1500	5AD	N3-C4-N9	3.19	132.60	127.17
3	D	1801	B12	C12-C13-C14	3.16	107.46	102.26
3	A	1801	B12	C9B-C8B-N1B	3.15	106.70	105.30
4	C	1500	5AD	N3-C4-N9	3.15	132.52	127.17
4	D	1500	5AD	N3-C4-N9	3.14	132.50	127.17
4	D	1500	5AD	C4-C5-N7	-3.13	107.00	110.58
3	A	1801	B12	C30-C3-C2	-3.11	112.13	119.00
4	C	1500	5AD	C5-N7-C8	3.11	108.34	103.45
3	B	1801	B12	C2-C26-C27	-3.11	106.54	115.19
3	A	1801	B12	C2-C1-C19	3.11	123.45	118.61
4	D	1500	5AD	C5-N7-C8	3.11	108.33	103.45
4	D	1500	5AD	C5-C4-N9	3.08	109.16	105.81
3	A	1801	B12	C19-C1-N21	3.06	105.29	102.14
4	B	1500	5AD	C2'-C3'-C4'	3.05	106.87	102.36
3	A	1801	B12	C12-C13-C14	3.04	107.25	102.26
3	B	1801	B12	C13-C14-N23	3.03	113.19	109.09
4	A	1500	5AD	C5-N7-C8	3.02	108.19	103.45
4	A	1500	5AD	C4-C5-N7	-3.00	107.16	110.58
3	B	1801	B12	C20-C1-C2	-2.97	108.39	113.28
3	B	1801	B12	C1-C2-C3	2.93	105.28	101.60
3	D	1801	B12	C9B-C8B-N1B	2.90	106.59	105.30
3	B	1801	B12	C30-C3-C2	-2.86	112.69	119.00
3	C	1801	B12	O6R-C4R-C5R	-2.83	103.24	109.22
3	B	1801	B12	C1P-N59-C57	-2.81	116.65	122.69
3	C	1801	B12	C4B-C9B-N3B	2.81	135.24	130.51
4	B	1500	5AD	C4-C5-N7	-2.81	107.37	110.58
4	A	1500	5AD	C5-C4-N9	2.81	108.87	105.81
3	B	1801	B12	C12-C13-C14	2.81	106.87	102.26
3	B	1801	B12	C2-C1-C19	2.81	122.98	118.61
3	C	1801	B12	C47-C12-C11	2.80	120.09	110.08
3	A	1801	B12	C1-C2-C3	2.78	105.10	101.60
3	B	1801	B12	C9-N22-C6	-2.77	101.94	105.28
3	B	1801	B12	C25-C2-C1	-2.77	109.62	113.75
3	D	1801	B12	C9-N22-C6	-2.75	101.96	105.28
3	A	1801	B12	C18-C60-C61	-2.72	107.12	114.04
5	B	767	Z97	CD-NE-C4A	-2.66	110.21	118.72
3	D	1801	B12	C46-C12-C11	2.65	119.55	110.08
3	D	1801	B12	C54-C17-C55	2.64	113.66	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	B12	C9B-N3B-C2B	2.64	107.64	104.40
3	A	1801	B12	C47-C12-C11	2.64	119.50	110.08
5	A	767	Z97	OP4-P-OP1	2.63	113.55	106.44
3	C	1801	B12	N1B-C2B-N3B	-2.62	110.22	113.94
3	C	1801	B12	C8B-N1B-C2B	2.62	108.63	106.26
5	A	767	Z97	CD-NE-C4A	-2.58	110.45	118.72
3	A	1801	B12	C20-C1-C2	-2.56	109.07	113.28
5	A	767	Z97	C5-C6-N1	-2.56	119.67	123.83
5	C	767	Z97	C2A-C2-N1	2.55	122.45	117.64
3	D	1801	B12	C7-C6-N22	2.55	112.57	107.94
5	C	767	Z97	CD-NE-C4A	-2.54	110.59	118.72
3	A	1801	B12	C3R-C2R-C1R	2.53	105.45	99.89
5	C	767	Z97	C5-C6-N1	-2.52	119.73	123.83
3	A	1801	B12	C54-C17-C18	-2.47	109.44	112.99
5	D	767	Z97	CD-NE-C4A	-2.45	110.86	118.72
3	B	1801	B12	C9B-N3B-C2B	2.45	107.41	104.40
4	C	1500	5AD	C4-C5-N7	-2.45	107.79	110.58
5	A	767	Z97	C5-C4-C4A	-2.43	117.72	121.47
3	C	1801	B12	C20-C1-C2	-2.42	109.29	113.28
3	A	1801	B12	C7-C6-N22	2.42	112.35	107.94
5	D	767	Z97	CG-CD-NE	2.42	117.23	110.83
3	C	1801	B12	C20-C1-N21	-2.42	106.27	110.26
5	B	767	Z97	C6-N1-C2	2.41	123.57	119.20
4	C	1500	5AD	C4-N9-C8	2.40	108.26	105.74
3	D	1801	B12	C30-C31-C32	-2.38	104.47	112.55
3	D	1801	B12	C18-C60-C61	-2.38	108.00	114.04
3	C	1801	B12	C12-C13-C14	2.37	106.16	102.26
3	D	1801	B12	C20-C1-C2	-2.37	109.38	113.28
3	C	1801	B12	C30-C3-C2	-2.37	113.78	119.00
3	B	1801	B12	C3R-C2R-C1R	2.36	105.09	99.89
4	D	1500	5AD	C2'-C3'-C4'	2.36	105.84	102.36
5	D	767	Z97	CB-CA-N	2.35	116.26	110.12
3	D	1801	B12	C9B-N3B-C2B	2.34	107.27	104.40
3	D	1801	B12	C9-C10-C11	-2.34	122.63	125.97
3	C	1801	B12	C46-C12-C11	2.32	118.38	110.08
3	A	1801	B12	C18-C17-C16	2.32	103.49	100.69
3	A	1801	B12	C46-C12-C11	2.32	118.36	110.08
3	D	1801	B12	C56-C55-C17	-2.29	111.17	115.58
3	D	1801	B12	C18-C17-C16	2.29	103.45	100.69
5	C	767	Z97	C2A-C2-C3	-2.27	118.14	120.80
5	C	767	Z97	OXT-C-O	-2.23	119.01	124.08
5	A	767	Z97	CG-CD-NE	2.22	116.71	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1801	B12	C48-C13-C14	2.22	114.03	108.51
3	C	1801	B12	C9-N22-C6	-2.22	102.61	105.28
4	A	1500	5AD	C6-C5-C4	2.22	120.20	117.18
3	C	1801	B12	C2-C26-C27	-2.21	109.04	115.19
3	D	1801	B12	C1-C2-C3	2.20	104.37	101.60
5	D	767	Z97	C5-C6-N1	-2.20	120.25	123.83
3	D	1801	B12	C47-C12-C11	2.17	117.84	110.08
3	C	1801	B12	C54-C17-C55	2.15	112.84	109.27
3	C	1801	B12	C7-C6-N22	2.14	111.84	107.94
3	A	1801	B12	C9-N22-C6	-2.14	102.70	105.28
3	C	1801	B12	C8B-N1B-C1R	-2.14	121.79	125.41
5	C	767	Z97	CB-CA-N	2.11	115.61	110.12
3	D	1801	B12	C7-C6-C5	-2.08	124.82	128.07
3	B	1801	B12	C7B-C8B-C9B	-2.06	120.01	122.47
3	A	1801	B12	C7-C6-C5	-2.05	124.86	128.07
3	B	1801	B12	C18-C17-C16	2.05	103.16	100.69
5	A	767	Z97	C3-C4-C4A	2.04	124.09	120.40
3	A	1801	B12	C4B-C9B-N3B	2.04	133.95	130.51
3	A	1801	B12	C25-C2-C1	-2.04	110.70	113.75
5	C	767	Z97	CG-CD-NE	2.02	116.19	110.83
3	B	1801	B12	C8B-N1B-C2B	2.02	108.09	106.26
3	B	1801	B12	C9-C10-C11	-2.02	123.09	125.97
3	A	1801	B12	C7B-C8B-C9B	-2.01	120.07	122.47
3	C	1801	B12	C2P-C1P-N59	-2.01	109.97	112.92

All (14) chirality outliers are listed below:

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

All (109) 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	B	1801	B12	C42-C41-C8-C9
3	B	1801	B12	C16-C17-C55-C56
3	B	1801	B12	C54-C17-C55-C56
3	B	1801	B12	C18-C17-C55-C56
3	C	1801	B12	C16-C17-C55-C56
3	C	1801	B12	C54-C17-C55-C56
3	C	1801	B12	C18-C17-C55-C56
3	D	1801	B12	C16-C17-C55-C56
3	D	1801	B12	C54-C17-C55-C56
3	D	1801	B12	C18-C17-C55-C56
3	D	1801	B12	C3P-C2P-O3-P
5	B	767	Z97	C5A-OP4-P-OP2
5	B	767	Z97	C5A-OP4-P-OP3
5	B	767	Z97	N-CA-CB-CG
5	C	767	Z97	C5A-OP4-P-OP1
3	D	1801	B12	O6R-C4R-C5R-O8R
3	D	1801	B12	C3R-C4R-C5R-O8R
3	A	1801	B12	O58-C57-N59-C1P
3	B	1801	B12	C42-C41-C8-C7
3	A	1801	B12	C4-C3-C30-C31
5	A	767	Z97	NE-CD-CG-CB
5	C	767	Z97	NE-CD-CG-CB
3	C	1801	B12	C7-C37-C38-N40
5	A	767	Z97	OXT-C-CA-N
3	A	1801	B12	C2-C3-C30-C31
5	D	767	Z97	CG-CD-NE-C4A
3	A	1801	B12	C2R-C1R-N1B-C2B
3	A	1801	B12	C8-C41-C42-C43
3	A	1801	B12	C12-C13-C48-C49
5	B	767	Z97	NE-CD-CG-CB
3	B	1801	B12	C2-C26-C27-N29
3	C	1801	B12	C7-C37-C38-O39
3	A	1801	B12	C2R-C1R-N1B-C8B
5	D	767	Z97	OXT-C-CA-CB
3	D	1801	B12	C2-C3-C30-C31
5	D	767	Z97	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C3P-C2P-O3-P
3	D	1801	B12	C1P-C2P-O3-P
5	C	767	Z97	CA-CB-CG-CD
5	D	767	Z97	NE-CD-CG-CB
3	B	1801	B12	C2-C26-C27-O28
3	B	1801	B12	C7-C37-C38-O39
3	B	1801	B12	C7-C37-C38-N40
3	D	1801	B12	C2-C26-C27-N29
3	C	1801	B12	O6R-C4R-C5R-O8R
5	D	767	Z97	O-C-CA-CB
3	D	1801	B12	O58-C57-N59-C1P
3	A	1801	B12	C42-C41-C8-C9
3	B	1801	B12	C2R-C1R-N1B-C2B
3	C	1801	B12	C2R-C1R-N1B-C2B
3	C	1801	B12	C2R-C1R-N1B-C8B
3	A	1801	B12	C13-C48-C49-C50
3	D	1801	B12	C38-C37-C7-C6
5	C	767	Z97	OXT-C-CA-N
5	D	767	Z97	OXT-C-CA-N
3	D	1801	B12	C56-C57-N59-C1P
3	D	1801	B12	C2-C26-C27-O28
5	A	767	Z97	O-C-CA-N
3	D	1801	B12	C4-C3-C30-C31
3	D	1801	B12	C18-C60-C61-O63
3	D	1801	B12	C18-C60-C61-N62
3	B	1801	B12	C14-C13-C48-C49
5	C	767	Z97	C5A-OP4-P-OP2
3	C	1801	B12	O6R-C1R-N1B-C8B
5	A	767	Z97	O-C-CA-CB
3	D	1801	B12	C38-C37-C7-C8
3	D	1801	B12	C2R-C1R-N1B-C2B
5	B	767	Z97	CA-CB-CG-CD
3	A	1801	B12	C41-C42-C43-N45
3	B	1801	B12	C3-C2-C26-C27
3	D	1801	B12	C3-C2-C26-C27
5	D	767	Z97	C5A-OP4-P-OP1
5	A	767	Z97	OXT-C-CA-CB
5	B	767	Z97	OXT-C-CA-CB
3	A	1801	B12	O6R-C1R-N1B-C8B
3	B	1801	B12	C2R-C1R-N1B-C8B
3	B	1801	B12	O6R-C1R-N1B-C8B
3	D	1801	B12	C2R-C1R-N1B-C8B

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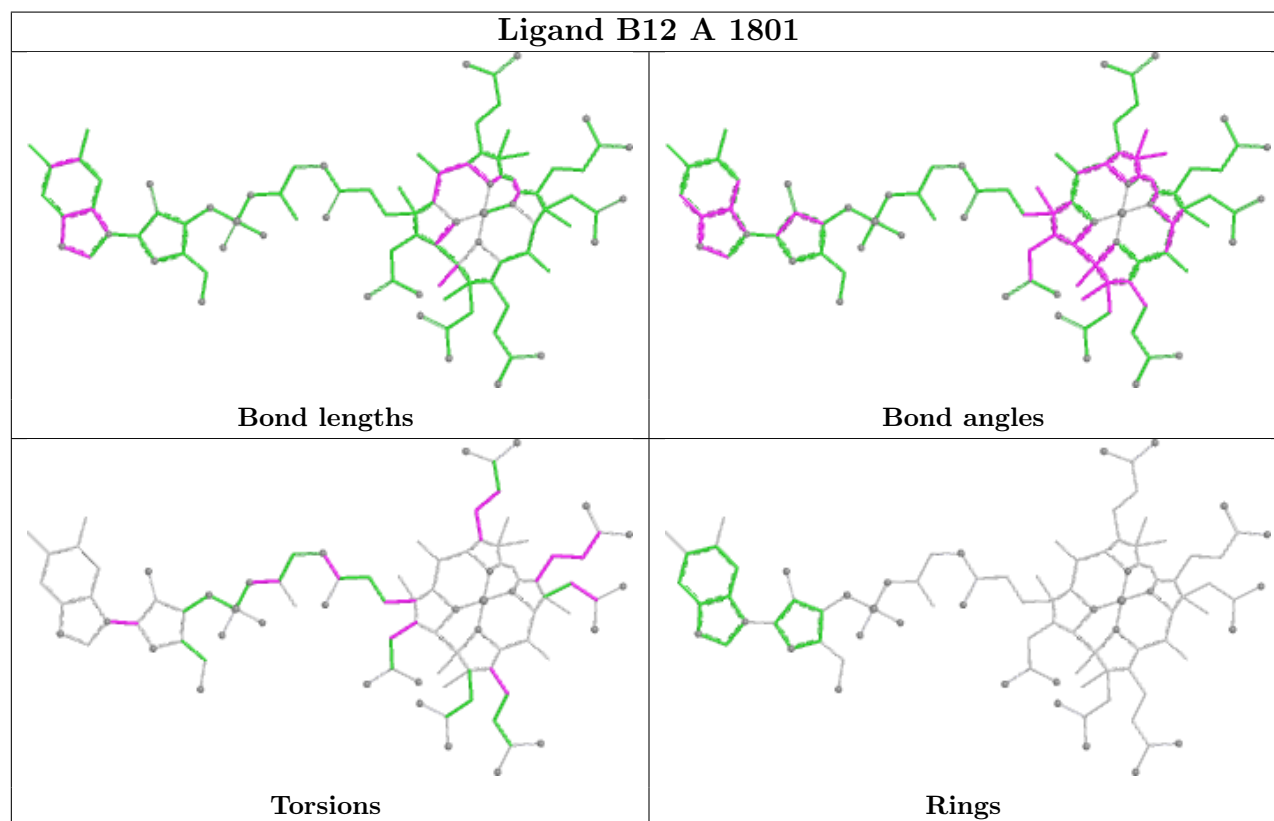
Mol	Chain	Res	Type	Atoms
3	D	1801	B12	O6R-C1R-N1B-C8B
3	A	1801	B12	C41-C42-C43-O44
5	D	767	Z97	O-C-CA-N
3	D	1801	B12	O6R-C1R-N1B-C2B
5	C	767	Z97	C3-C4-C4A-NE
3	D	1801	B12	C25-C2-C26-C27
5	D	767	Z97	C5A-OP4-P-OP2
3	B	1801	B12	O6R-C1R-N1B-C2B
3	A	1801	B12	C7-C37-C38-O39
5	C	767	Z97	O-C-CA-CB
3	A	1801	B12	C19-C18-C60-C61
3	C	1801	B12	C19-C18-C60-C61
5	C	767	Z97	OXT-C-CA-CB
3	A	1801	B12	C7-C37-C38-N40
3	B	1801	B12	C2P-O3-P-O5
3	D	1801	B12	C2P-O3-P-O5
3	C	1801	B12	O6R-C1R-N1B-C2B
5	B	767	Z97	OXT-C-CA-N
5	A	767	Z97	C4-C4A-NE-CD
3	A	1801	B12	C17-C18-C60-C61
4	A	1500	5AD	O4'-C1'-N9-C8
4	C	1500	5AD	O4'-C1'-N9-C8
5	B	767	Z97	O-C-CA-CB
5	C	767	Z97	O-C-CA-N
3	B	1801	B12	C38-C37-C7-C8

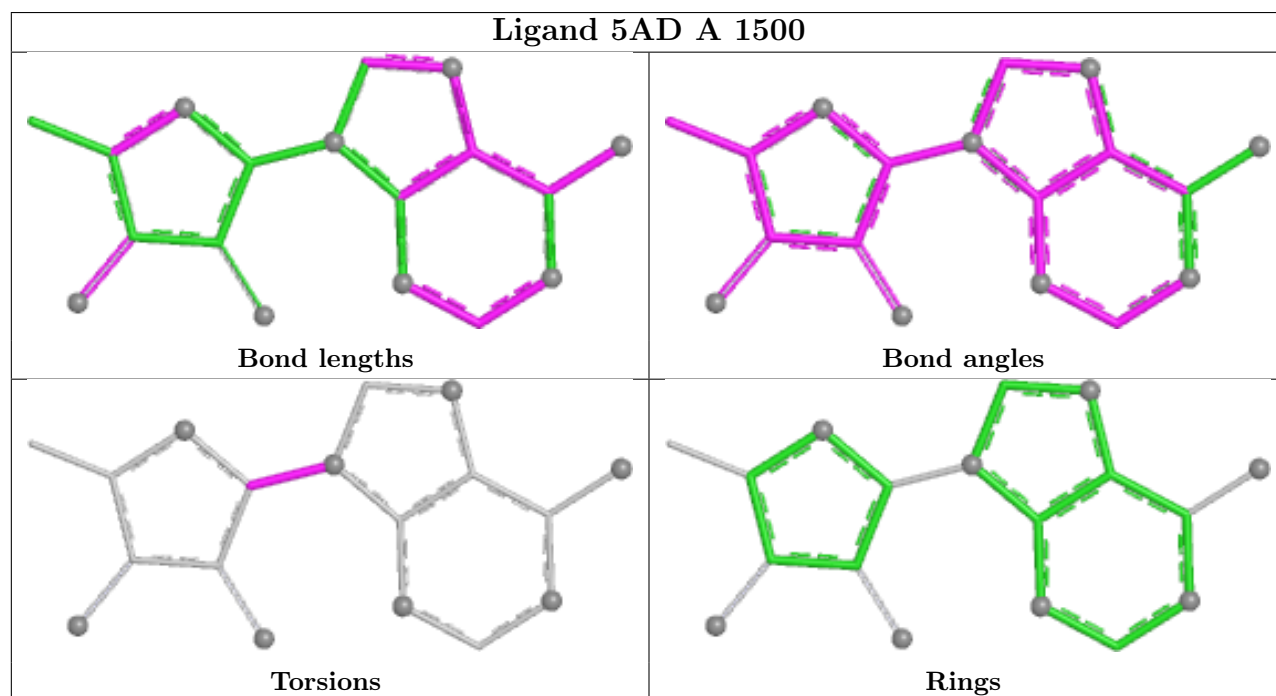
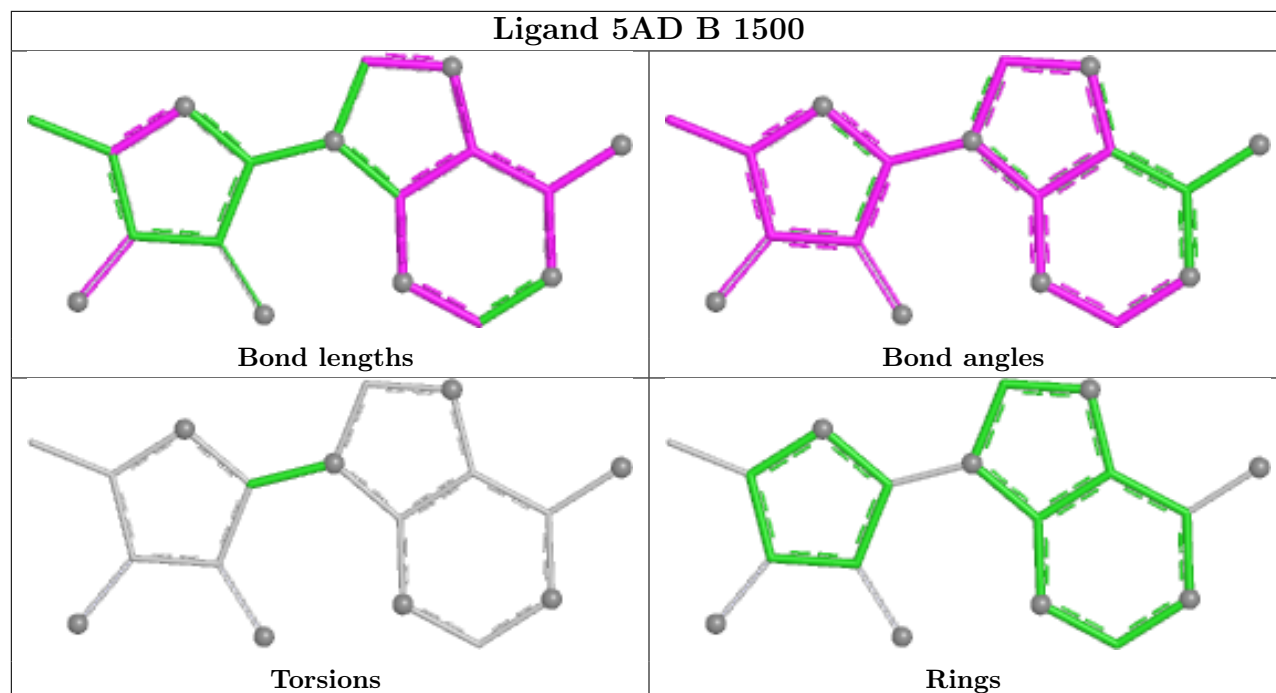
There are no ring outliers.

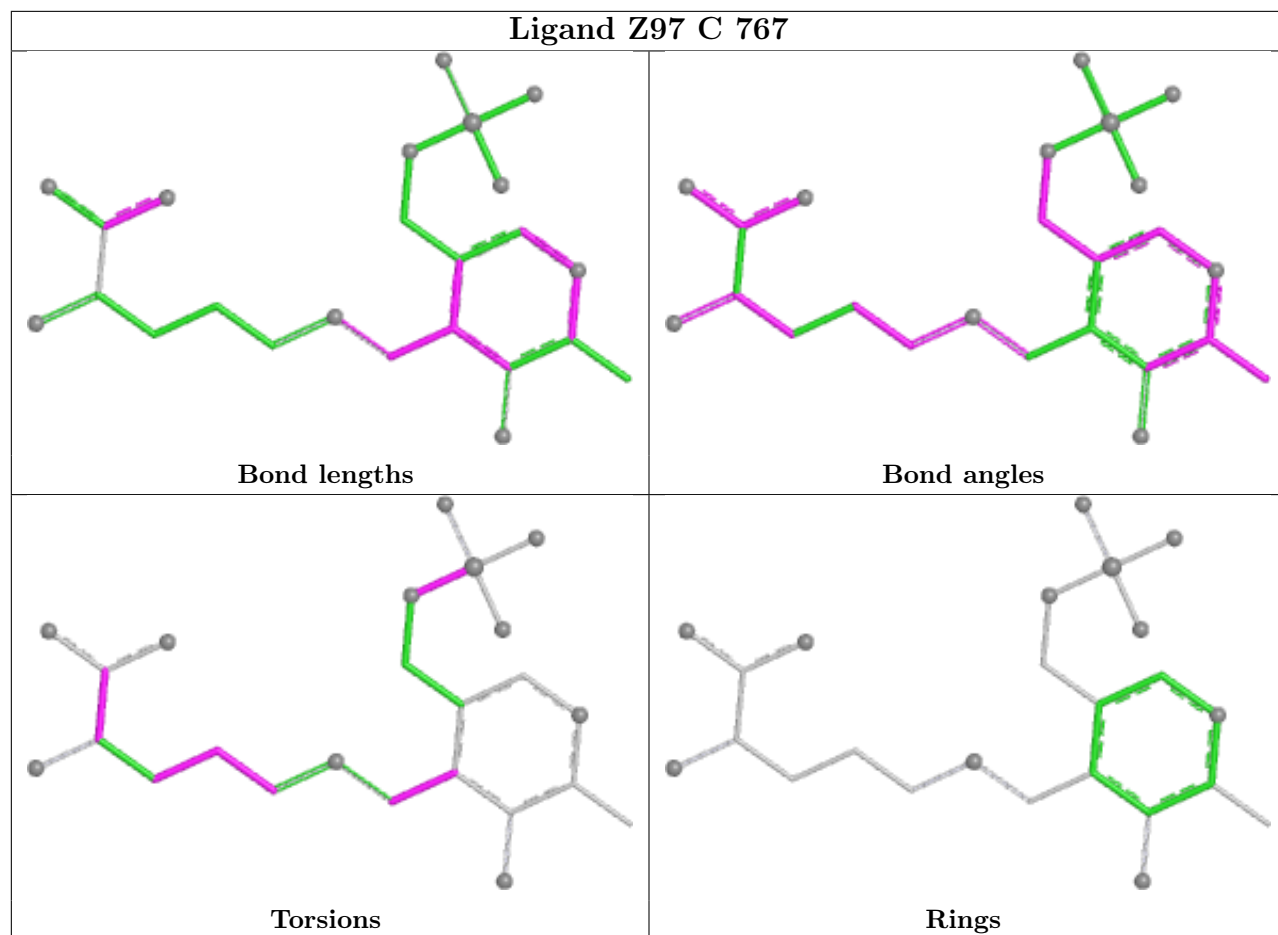
12 monomers are involved in 112 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1801	B12	19	0
4	B	1500	5AD	3	0
4	A	1500	5AD	3	0
5	C	767	Z97	3	0
5	D	767	Z97	4	0
3	D	1801	B12	31	0
3	C	1801	B12	24	0
4	D	1500	5AD	3	0
4	C	1500	5AD	3	0
5	A	767	Z97	2	0
5	B	767	Z97	3	0
3	B	1801	B12	26	0

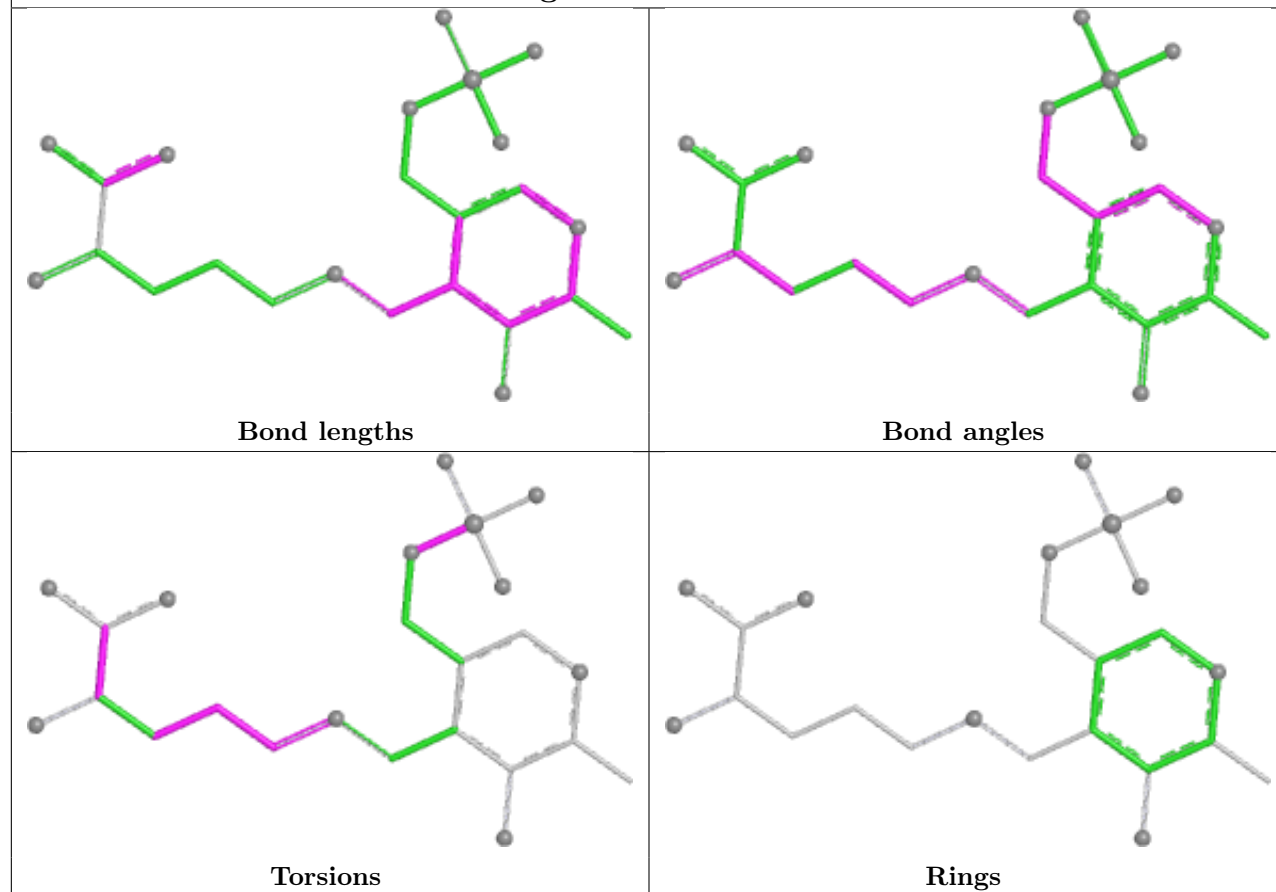
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



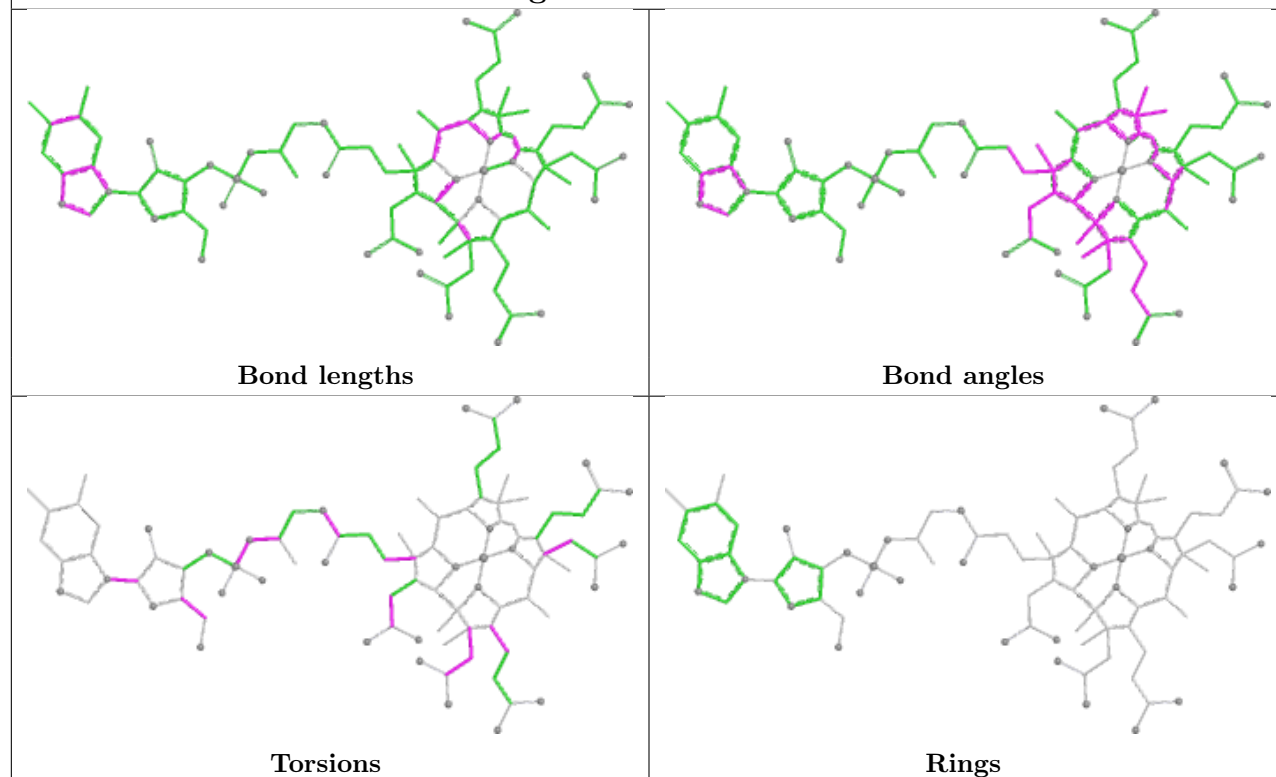


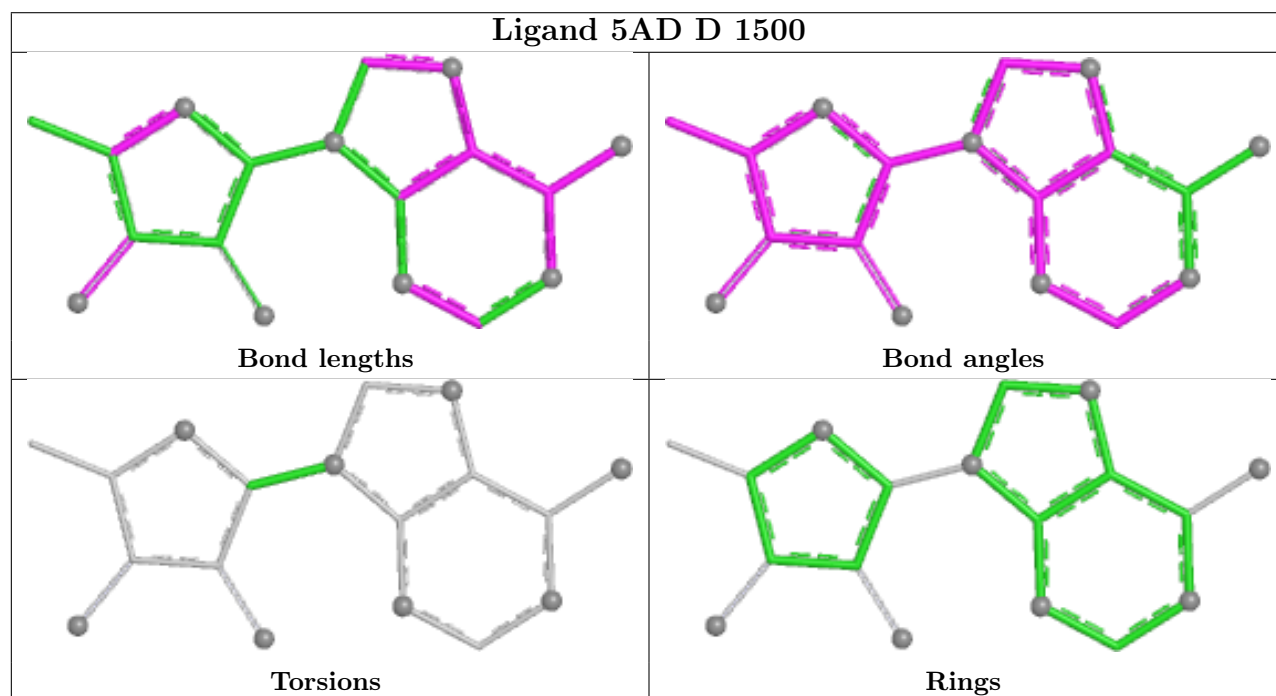
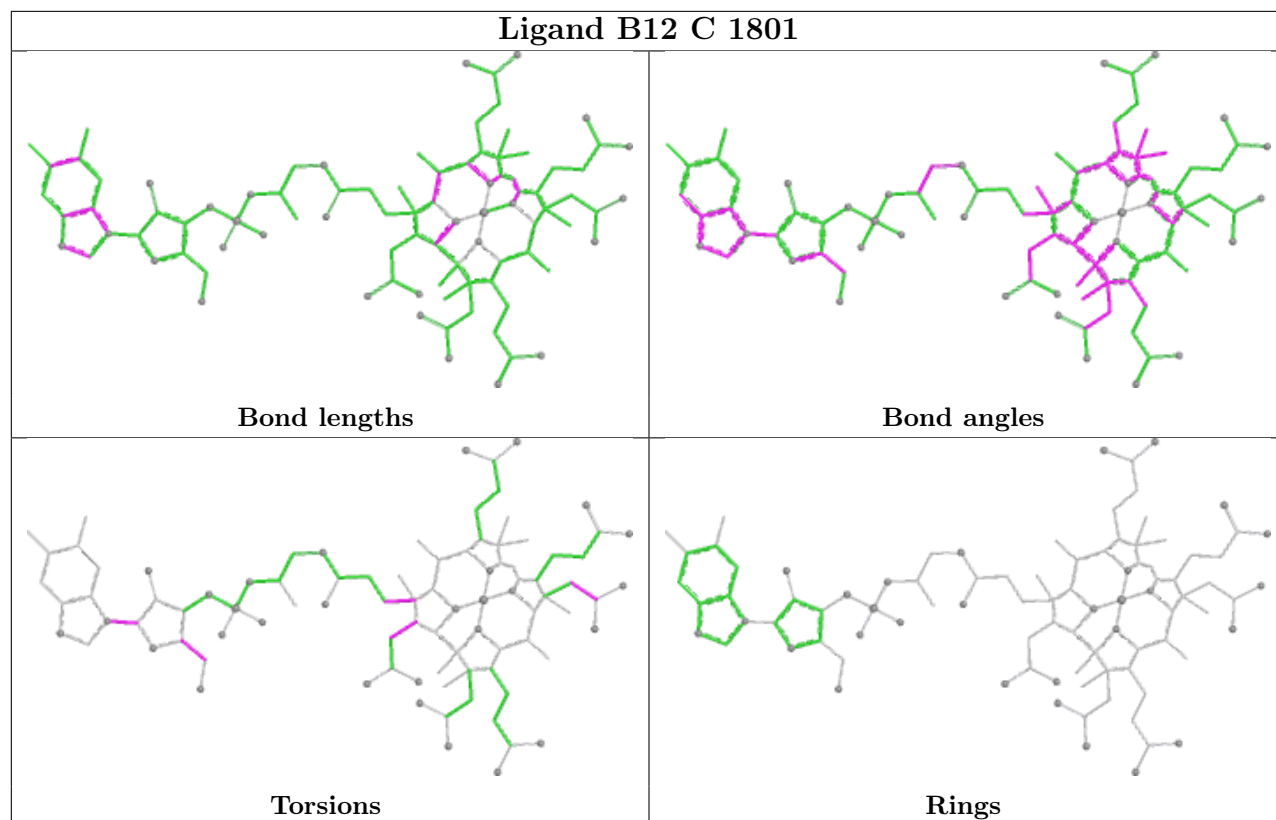


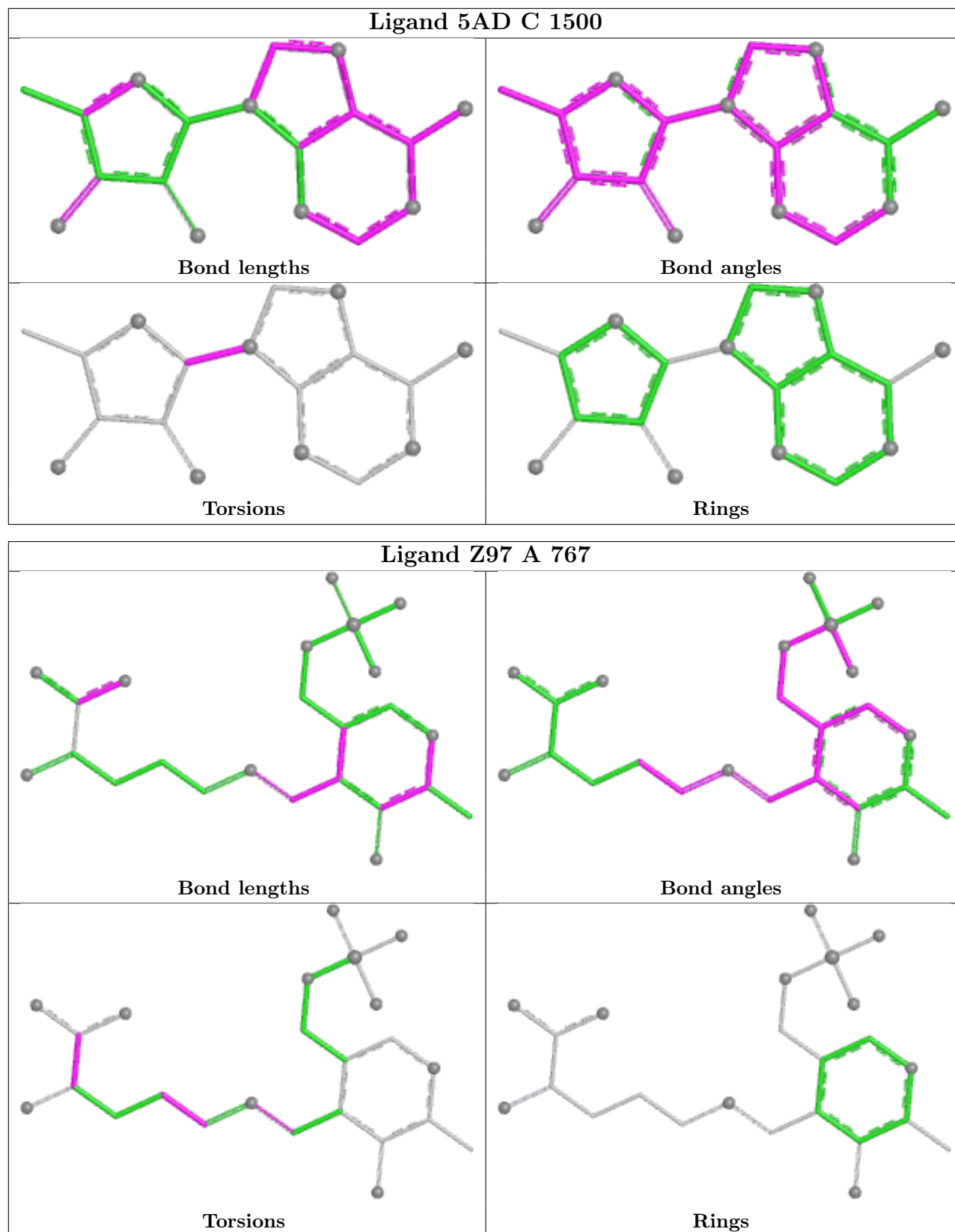
Ligand Z97 D 767



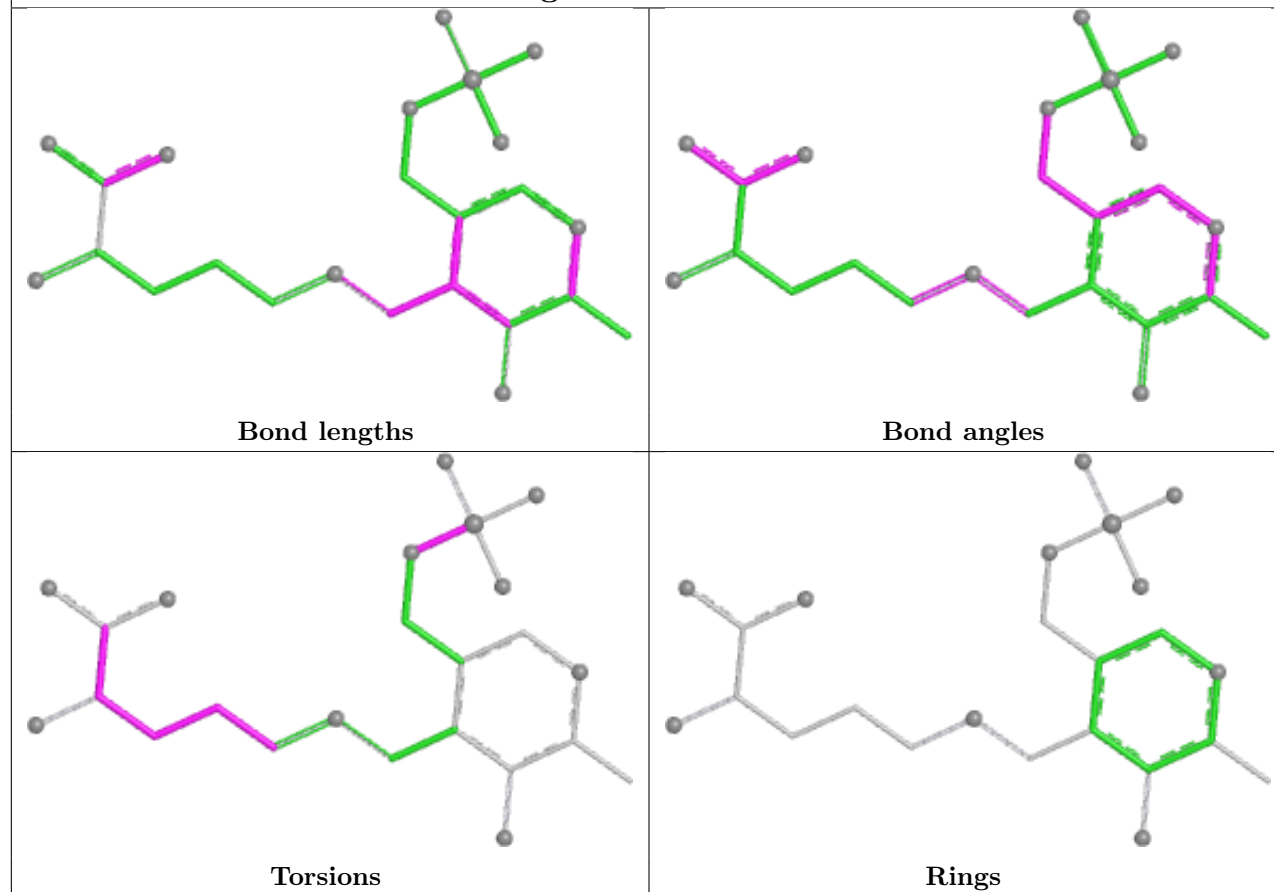
Ligand B12 D 1801



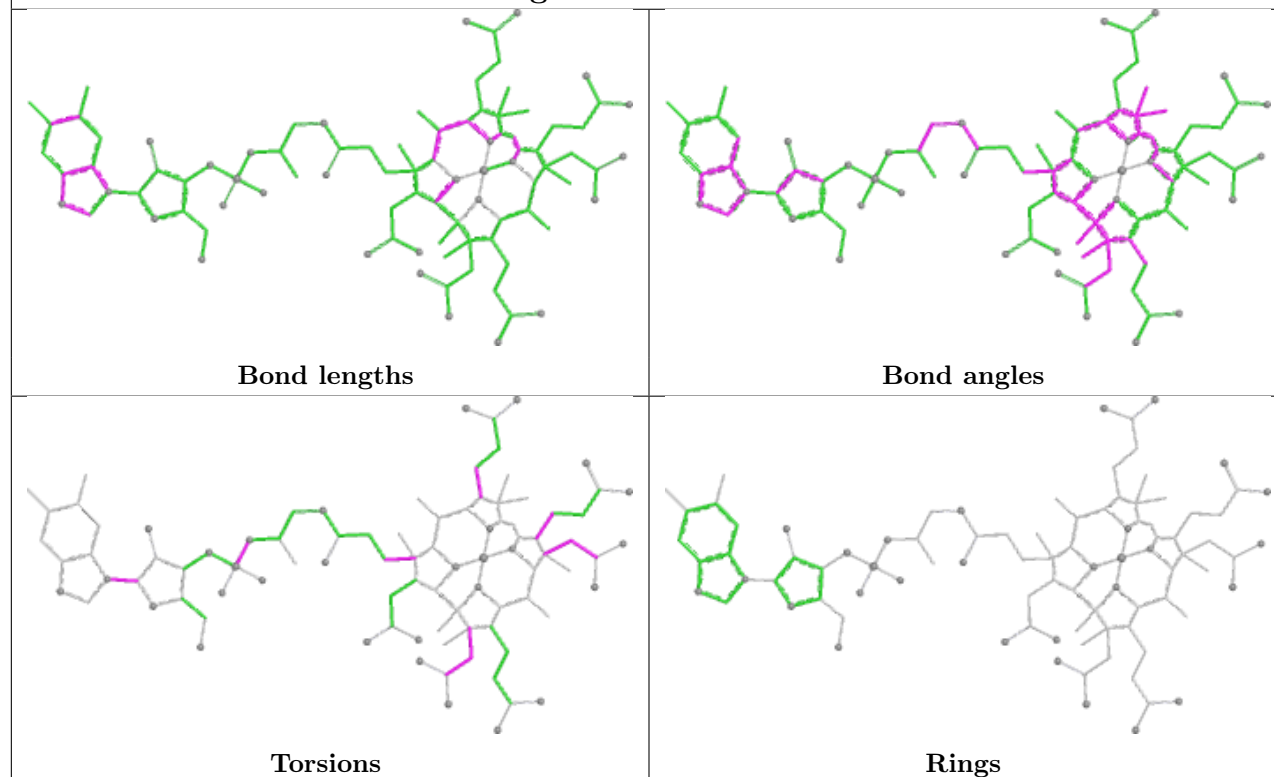




Ligand Z97 B 767



Ligand B12 B 1801



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	1.05	111 (15%) 5 4	16, 33, 93, 108	0
1	B	728/763 (95%)	1.33	157 (21%) 2 2	16, 33, 65, 81	0
1	C	728/763 (95%)	1.09	71 (9%) 13 9	18, 37, 62, 79	0
1	D	728/763 (95%)	1.31	150 (20%) 2 2	16, 32, 91, 116	0
2	E	110/121 (90%)	0.89	7 (6%) 25 18	25, 41, 62, 74	0
2	F	110/121 (90%)	1.16	21 (19%) 3 2	24, 38, 54, 59	0
2	G	110/121 (90%)	1.16	14 (12%) 8 6	32, 45, 64, 73	0
2	H	110/121 (90%)	1.24	16 (14%) 6 4	23, 39, 58, 80	0
All	All	3352/3536 (94%)	1.18	547 (16%) 4 4	16, 36, 80, 116	0

All (547) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	683	ILE	5.9
1	C	163	GLY	5.6
1	A	668	THR	5.1
1	B	69	ASP	4.7
1	A	667	SER	4.7
1	A	717	ALA	4.6
1	C	5	LEU	4.4
1	D	696	ILE	4.3
1	D	717	ALA	4.2
1	D	668	THR	4.2
1	D	658	GLU	4.1
1	A	672	HIS	4.1
1	A	610	ALA	4.0
2	F	5	ASP	4.0
1	C	429	ASN	3.9
1	D	670	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	686	LEU	3.9
1	C	13	LEU	3.9
1	D	678	LYS	3.9
1	B	513	PRO	3.8
1	D	647	VAL	3.7
1	D	672	HIS	3.7
1	D	733	VAL	3.7
1	D	122	GLY	3.7
1	D	714	GLY	3.7
1	A	716	ASP	3.7
1	D	223	GLY	3.7
1	D	657	ILE	3.7
1	D	671	SER	3.7
1	A	651	LYS	3.6
1	D	669	ILE	3.6
1	C	683	ILE	3.6
1	D	695	LYS	3.6
2	F	112	ALA	3.6
1	A	669	ILE	3.6
1	D	10	ASN	3.5
2	H	110	ASP	3.5
1	A	677	TYR	3.5
1	B	8	ARG	3.5
1	B	6	GLN	3.5
1	A	711	VAL	3.5
1	A	666	ALA	3.5
1	B	715	VAL	3.5
1	B	471	LEU	3.4
1	D	665	LEU	3.4
1	D	234	ALA	3.4
1	D	683	ILE	3.4
1	B	468	PRO	3.4
2	H	112	ALA	3.4
1	A	636	TYR	3.4
1	A	715	VAL	3.4
1	D	649	VAL	3.4
1	C	111	ALA	3.4
1	C	509	SER	3.4
1	D	108	ILE	3.4
1	B	116	TYR	3.4
1	B	538	PHE	3.4
1	B	465	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	118	GLY	3.3
1	A	532	SER	3.3
1	A	531	THR	3.3
1	C	484	VAL	3.3
2	H	85	VAL	3.3
1	D	690	LYS	3.3
1	B	127	ILE	3.3
1	B	502	THR	3.3
1	C	506	ARG	3.3
2	G	75	GLY	3.3
1	B	132	ILE	3.2
1	B	346	ILE	3.2
1	A	592	LEU	3.2
1	B	59	VAL	3.2
1	D	587	PRO	3.2
1	D	231	ALA	3.2
1	B	575	PRO	3.2
1	D	224	ALA	3.2
1	A	609	VAL	3.2
1	B	587	PRO	3.2
1	D	602	GLU	3.2
2	H	5	ASP	3.1
1	A	649	VAL	3.1
1	A	732	LEU	3.1
1	B	117	ASP	3.1
1	B	125	GLN	3.1
1	A	656	ALA	3.1
1	B	159	SER	3.1
1	A	692	ILE	3.1
2	G	5	ASP	3.1
1	D	8	ARG	3.1
1	D	686	LEU	3.1
1	B	676	HIS	3.0
1	A	683	ILE	3.0
1	B	591	ILE	3.0
1	B	495	VAL	3.0
1	C	479	VAL	3.0
2	G	96	VAL	3.0
1	B	677	TYR	3.0
1	B	521	GLY	3.0
1	B	696	ILE	3.0
1	B	37	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	13	LEU	3.0
1	C	448	VAL	3.0
1	C	116	TYR	3.0
1	D	692	ILE	3.0
1	D	694	ASP	3.0
1	B	111	ALA	3.0
1	A	613	VAL	3.0
1	B	177	GLY	2.9
1	C	6	GLN	2.9
1	B	131	PRO	2.9
1	C	16	GLU	2.9
1	D	547	MET	2.9
1	C	486	ILE	2.9
1	B	577	SER	2.9
1	D	528	PHE	2.9
1	A	675	ILE	2.9
2	H	84	ILE	2.9
1	B	51	ALA	2.9
1	B	700	CYS	2.9
1	A	659	LEU	2.9
1	B	489	LEU	2.9
1	D	527	MET	2.9
1	D	707	PRO	2.9
1	A	688	VAL	2.9
1	D	715	VAL	2.9
1	B	672	HIS	2.9
1	A	690	LYS	2.8
1	B	491	GLU	2.8
1	C	444	TYR	2.8
2	F	99	ALA	2.8
1	D	673	ASP	2.8
1	A	591	ILE	2.8
1	B	146	LEU	2.8
1	C	464	LEU	2.8
1	D	675	ILE	2.8
1	D	703	THR	2.8
1	C	587	PRO	2.8
1	B	20	LYS	2.8
1	A	601	ILE	2.8
1	A	673	ASP	2.8
1	B	673	ASP	2.8
1	B	698	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	667	SER	2.8
1	B	62	PRO	2.8
1	D	653	VAL	2.8
1	A	409	PHE	2.8
1	A	719	PHE	2.8
1	B	655	ALA	2.8
1	C	100	HIS	2.8
1	B	110	THR	2.8
1	D	565	GLY	2.8
1	C	468	PRO	2.8
1	C	445	MET	2.8
1	D	681	LYS	2.8
1	C	453	GLY	2.8
1	C	134	ARG	2.7
1	A	307	ALA	2.7
1	A	446	ALA	2.7
1	A	699	GLY	2.7
1	A	718	GLY	2.7
1	B	72	PRO	2.7
1	D	711	VAL	2.7
1	C	446	ALA	2.7
2	F	113	ILE	2.7
1	D	680	MET	2.7
1	C	69	ASP	2.7
1	C	461	ASP	2.7
1	D	662	ASP	2.7
1	D	682	ARG	2.7
1	A	562	GLU	2.7
1	C	505	PHE	2.7
1	D	343	PRO	2.7
1	D	414	GLY	2.7
1	B	497	VAL	2.7
1	B	5	LEU	2.7
1	D	524	LEU	2.7
1	B	27	PRO	2.7
1	B	112	GLY	2.7
1	D	631	GLY	2.7
2	G	80	GLY	2.7
2	F	73	ASP	2.7
1	A	713	GLN	2.7
1	A	709	VAL	2.7
1	B	486	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	652	LEU	2.7
2	H	11	ARG	2.6
1	D	129	GLY	2.6
1	C	110	THR	2.6
1	D	706	THR	2.6
1	D	348	ASN	2.6
1	B	15	VAL	2.6
1	B	515	VAL	2.6
1	B	713	GLN	2.6
1	C	489	LEU	2.6
1	A	505	PHE	2.6
1	A	577	SER	2.6
1	A	611	ALA	2.6
1	A	661	ALA	2.6
1	B	684	HIS	2.6
1	D	718	GLY	2.6
1	D	133	THR	2.6
1	D	645	THR	2.6
1	D	237	VAL	2.6
1	D	492	ASN	2.6
1	B	462	GLU	2.6
1	B	551	GLU	2.6
1	D	537	GLU	2.6
1	D	613	VAL	2.6
1	D	576	PHE	2.6
2	H	7	PHE	2.6
1	C	469	SER	2.6
1	B	30	ARG	2.6
1	A	720	GLY	2.6
1	D	605	PRO	2.6
1	C	108	ILE	2.6
1	B	527	MET	2.6
1	D	594	GLU	2.6
2	E	5	ASP	2.6
1	A	676	HIS	2.6
1	C	160	TYR	2.6
1	D	529	LEU	2.6
1	D	606	LEU	2.6
1	A	80	THR	2.6
1	D	526	THR	2.6
2	F	94	ILE	2.6
1	A	602	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	110	ASP	2.6
1	A	684	HIS	2.5
1	B	736	ARG	2.5
1	C	109	ARG	2.5
1	D	740	ARG	2.5
1	A	665	LEU	2.5
1	B	570	LEU	2.5
1	A	511	ILE	2.5
1	A	657	ILE	2.5
1	B	537	GLU	2.5
1	A	687	ALA	2.5
1	B	493	ASP	2.5
1	B	737	ARG	2.5
2	G	83	HIS	2.5
1	A	593	SER	2.5
1	B	469	SER	2.5
1	A	5	LEU	2.5
1	A	702	GLY	2.5
1	B	96	MET	2.5
1	A	6	GLN	2.5
1	D	505	PHE	2.5
1	D	543	PHE	2.5
1	B	661	ALA	2.5
1	D	656	ALA	2.5
1	A	618	HIS	2.5
1	B	616	ASP	2.5
1	B	690	LYS	2.5
2	E	6	ASP	2.5
1	B	61	LEU	2.5
1	B	739	MET	2.5
1	C	18	ILE	2.5
1	C	120	ILE	2.5
1	A	642	TYR	2.5
1	B	347	TYR	2.5
1	B	731	PHE	2.5
1	D	11	GLU	2.5
1	A	598	ARG	2.5
1	A	682	ARG	2.5
1	D	693	ARG	2.5
1	A	458	LYS	2.5
1	A	700	CYS	2.5
1	D	225	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	168	ASP	2.5
1	B	22	LEU	2.5
1	A	605	PRO	2.5
1	C	480	PRO	2.5
1	A	580	ILE	2.5
1	B	155	ILE	2.5
1	B	474	GLY	2.5
1	C	127	ILE	2.5
1	A	705	VAL	2.5
1	A	596	GLU	2.5
1	B	740	ARG	2.5
1	C	270	THR	2.5
1	A	641	HIS	2.5
1	B	496	ASN	2.5
1	B	525	LEU	2.4
1	B	697	MET	2.4
1	D	510	MET	2.4
1	B	484	VAL	2.4
1	B	647	VAL	2.4
1	C	159	SER	2.4
1	D	535	VAL	2.4
1	D	625	VAL	2.4
1	B	528	PHE	2.4
1	A	83	ALA	2.4
1	B	518	GLN	2.4
1	B	456	ASN	2.4
1	B	606	LEU	2.4
1	D	549	LEU	2.4
1	C	201	ILE	2.4
1	D	674	ASP	2.4
1	D	691	GLY	2.4
2	F	58	GLY	2.4
1	A	114	SER	2.4
1	A	685	GLU	2.4
1	D	88	GLU	2.4
1	C	710	ALA	2.4
1	D	710	ALA	2.4
2	H	109	TRP	2.4
2	F	108	TYR	2.4
1	D	604	THR	2.4
1	A	643	LEU	2.4
1	B	686	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	560	MET	2.4
1	B	18	ILE	2.4
1	D	648	PRO	2.4
1	B	461	ASP	2.4
1	C	152	GLY	2.4
1	D	550	GLU	2.4
2	F	61	SER	2.4
1	B	38	ALA	2.4
1	D	425	ALA	2.4
1	D	676	HIS	2.4
2	F	57	MET	2.4
1	B	592	LEU	2.4
1	A	237	VAL	2.4
2	F	53	VAL	2.4
1	B	28	LYS	2.4
1	B	505	PHE	2.4
1	D	538	PHE	2.4
1	A	663	ALA	2.4
1	C	32	TRP	2.4
1	D	677	TYR	2.4
2	G	108	TYR	2.4
1	B	584	VAL	2.3
1	D	556	ASN	2.3
1	D	638	VAL	2.3
1	C	520	ASP	2.3
2	H	81	ALA	2.3
1	B	52	SER	2.3
1	B	466	SER	2.3
1	A	606	LEU	2.3
1	B	703	THR	2.3
2	F	45	THR	2.3
1	A	506	ARG	2.3
1	D	232	ARG	2.3
1	B	85	GLY	2.3
1	D	521	GLY	2.3
1	D	699	GLY	2.3
1	A	708	GLU	2.3
1	C	579	ASP	2.3
1	B	663	ALA	2.3
1	A	680	MET	2.3
2	E	114	GLN	2.3
1	A	84	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	100	HIS	2.3
1	B	449	THR	2.3
1	A	707	PRO	2.3
1	B	498	ARG	2.3
1	B	171	VAL	2.3
1	B	613	VAL	2.3
1	B	709	VAL	2.3
1	C	137	VAL	2.3
1	B	565	GLY	2.3
1	D	725	GLY	2.3
2	H	106	GLY	2.3
1	B	473	ASP	2.3
1	B	654	ASP	2.3
1	C	493	ASP	2.3
1	B	7	LEU	2.3
1	A	582	SER	2.3
1	B	454	TYR	2.3
2	G	86	TYR	2.3
1	B	574	VAL	2.3
1	C	497	VAL	2.3
1	D	709	VAL	2.3
1	C	101	GLY	2.3
1	D	177	GLY	2.3
2	E	7	PHE	2.3
1	B	176	GLU	2.3
1	D	551	GLU	2.3
1	D	661	ALA	2.3
1	D	739	MET	2.3
1	D	600	ASP	2.3
2	H	73	ASP	2.3
1	A	712	LYS	2.3
1	D	608	ILE	2.3
1	B	25	TYR	2.3
1	B	485	TYR	2.3
1	B	615	GLU	2.2
1	B	685	GLU	2.2
1	C	216	ALA	2.2
1	B	464	LEU	2.2
1	B	549	LEU	2.2
1	D	732	LEU	2.2
1	A	108	ILE	2.2
1	D	424	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	623	ARG	2.2
1	A	604	THR	2.2
1	A	653	VAL	2.2
1	D	497	VAL	2.2
1	B	444	TYR	2.2
1	D	430	GLY	2.2
1	A	594	GLU	2.2
1	A	599	GLU	2.2
1	B	529	LEU	2.2
1	D	622	LEU	2.2
1	B	682	ARG	2.2
1	D	23	ASP	2.2
1	B	668	THR	2.2
1	C	554	VAL	2.2
1	D	513	PRO	2.2
1	D	501	GLU	2.2
2	E	98	GLU	2.2
1	A	698	ILE	2.2
1	B	472	ILE	2.2
1	C	585	ILE	2.2
1	D	557	ARG	2.2
1	D	578	ILE	2.2
2	H	113	ILE	2.2
1	B	26	THR	2.2
1	D	266	THR	2.2
1	D	499	MET	2.2
2	F	95	SER	2.2
1	B	55	LEU	2.2
1	D	540	ALA	2.2
1	A	597	ILE	2.2
1	D	132	ILE	2.2
2	F	84	ILE	2.2
1	B	581	ASN	2.2
1	B	9	VAL	2.2
1	B	479	VAL	2.2
1	B	480	PRO	2.2
1	C	490	ASP	2.2
1	D	716	ASP	2.2
1	B	718	GLY	2.2
1	D	114	SER	2.2
1	D	544	ALA	2.2
2	F	81	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	580	ILE	2.1
1	D	713	GLN	2.1
1	B	301	ASN	2.1
1	A	574	VAL	2.1
1	B	133	THR	2.1
1	D	572	GLY	2.1
1	C	525	LEU	2.1
2	H	14	LEU	2.1
1	C	485	TYR	2.1
1	D	636	TYR	2.1
1	B	539	ALA	2.1
1	B	501	GLU	2.1
1	D	462	GLU	2.1
1	C	483	ILE	2.1
1	C	696	ILE	2.1
1	C	10	ASN	2.1
1	D	679	ASN	2.1
1	A	584	VAL	2.1
1	D	9	VAL	2.1
1	A	607	LYS	2.1
1	A	674	ASP	2.1
1	D	654	ASP	2.1
1	A	612	THR	2.1
2	F	59	PHE	2.1
2	G	109	TRP	2.1
1	A	51	ALA	2.1
1	A	544	ALA	2.1
1	A	736	ARG	2.1
1	C	498	ARG	2.1
1	A	396	ILE	2.1
1	D	698	ILE	2.1
2	F	88	ILE	2.1
2	G	61	SER	2.1
2	G	8	GLN	2.1
1	A	697	MET	2.1
1	B	164	VAL	2.1
1	B	499	MET	2.1
1	C	495	VAL	2.1
1	A	637	GLY	2.1
1	B	637	GLY	2.1
2	F	100	GLY	2.1
1	A	391	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	538	PHE	2.1
1	C	26	THR	2.1
1	D	92	ARG	2.1
1	A	578	ILE	2.1
1	D	82	ILE	2.1
1	D	174	ALA	2.1
1	B	157	TYR	2.1
1	D	591	ILE	2.1
1	A	509	SER	2.1
1	D	635	LYS	2.1
1	D	226	ASN	2.1
1	A	622	LEU	2.1
1	D	384	LEU	2.1
2	E	101	LEU	2.1
1	A	644	GLY	2.1
1	C	85	GLY	2.1
1	B	490	ASP	2.1
1	C	53	THR	2.1
1	D	534	ARG	2.1
1	D	127	ILE	2.1
1	D	555	ILE	2.1
2	G	20	GLU	2.1
1	B	533	LYS	2.0
1	C	582	SER	2.0
2	F	72	MET	2.0
2	H	114	GLN	2.0
1	C	465	VAL	2.0
1	D	523	VAL	2.0
1	A	587	PRO	2.0
1	C	54	PRO	2.0
2	F	55	LEU	2.0
1	A	737	ARG	2.0
1	B	29	ARG	2.0
1	B	126	GLY	2.0
1	B	557	ARG	2.0
1	B	573	ARG	2.0
1	C	430	GLY	2.0
1	B	432	ILE	2.0
1	B	578	ILE	2.0
1	C	580	ILE	2.0
1	D	313	THR	2.0
1	D	568	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	597	ILE	2.0
1	D	729	ALA	2.0
1	D	504	GLU	2.0
1	C	510	MET	2.0
2	E	9	GLN	2.0
1	A	343	PRO	2.0
1	B	447	PRO	2.0
1	C	549	LEU	2.0
2	H	17	LEU	2.0
1	B	455	ASN	2.0
1	A	714	GLY	2.0
1	B	644	GLY	2.0
2	G	78	GLY	2.0
1	B	670	ILE	2.0
2	G	94	ILE	2.0
1	B	165	ALA	2.0
1	C	544	ALA	2.0
1	D	229	ALA	2.0
1	D	522	THR	2.0
1	D	663	ALA	2.0
1	B	596	GLU	2.0
1	D	500	GLU	2.0
2	G	6	ASP	2.0
1	B	517	TRP	2.0
2	H	108	TYR	2.0
1	B	523	VAL	2.0
1	D	381	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

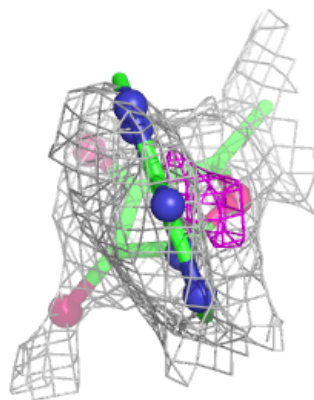
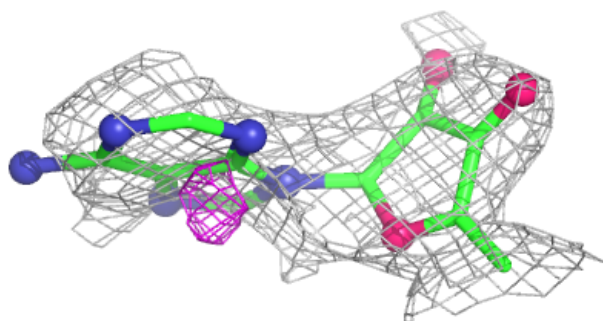
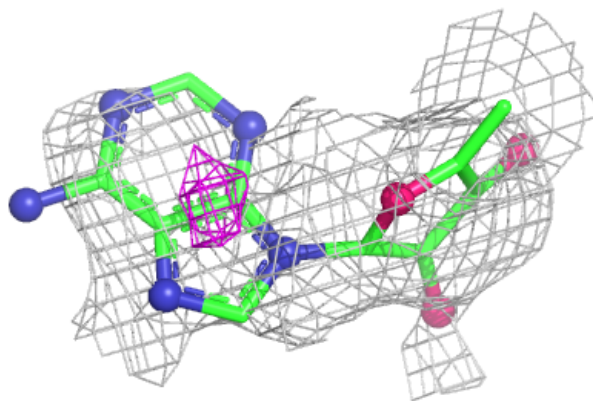
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	5AD	C	1500	18/18	0.60	0.18	70,80,87,88	0
4	5AD	B	1500	18/18	0.62	0.21	60,79,87,91	0
4	5AD	D	1500	18/18	0.79	0.17	51,62,69,77	0
3	B12	D	1801	91/91	0.81	0.17	44,73,81,91	0
3	B12	A	1801	91/91	0.81	0.18	55,78,88,92	0
5	Z97	D	767	24/24	0.82	0.18	24,34,44,46	0
4	5AD	A	1500	18/18	0.84	0.13	37,45,51,52	0
5	Z97	B	767	24/24	0.85	0.16	23,30,47,48	0
3	B12	B	1801	91/91	0.85	0.17	33,52,61,64	0
5	Z97	C	767	24/24	0.86	0.15	33,40,49,50	0
5	Z97	A	767	24/24	0.88	0.14	22,30,36,38	0
3	B12	C	1801	91/91	0.93	0.12	18,34,43,49	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.

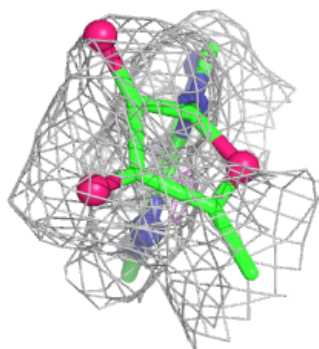
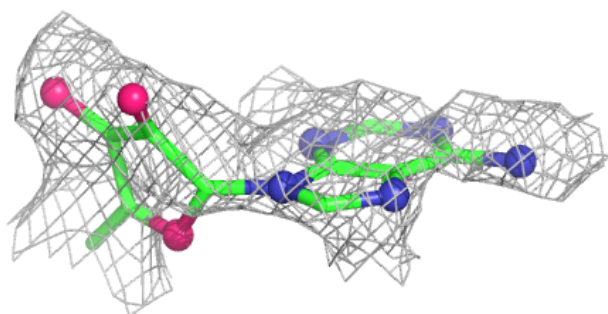
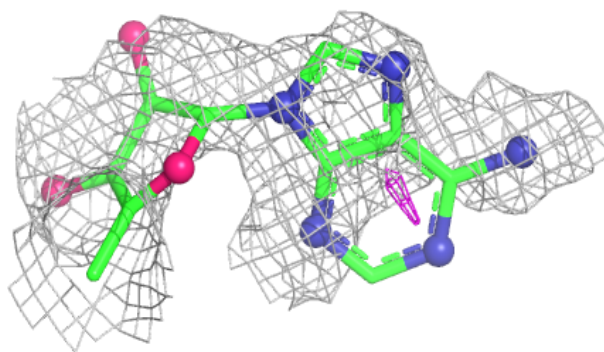
Electron density around 5AD C 1500:

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

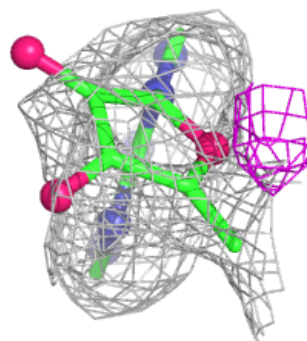
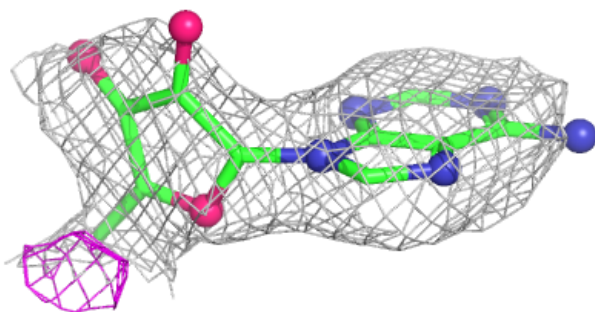
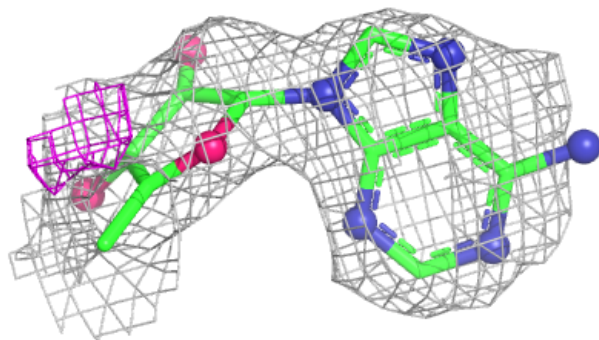


Electron density around 5AD B 1500:

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

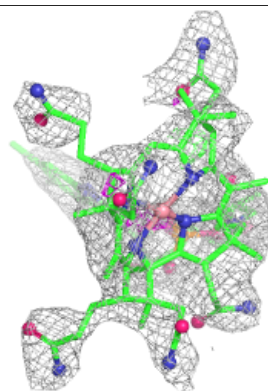
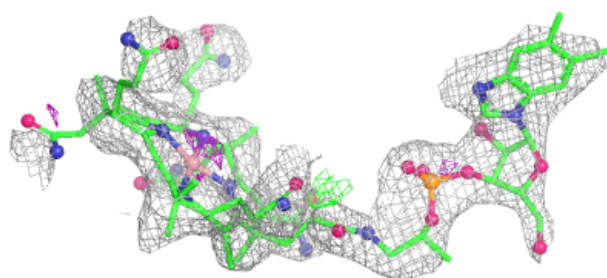
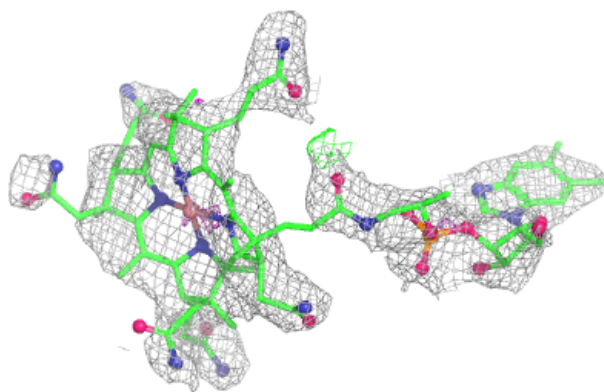
**Electron density around 5AD D 1500:**

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

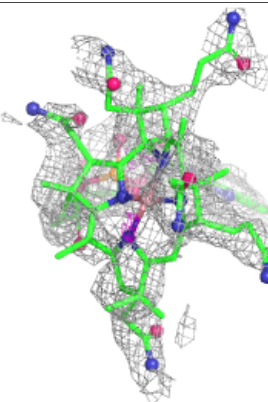
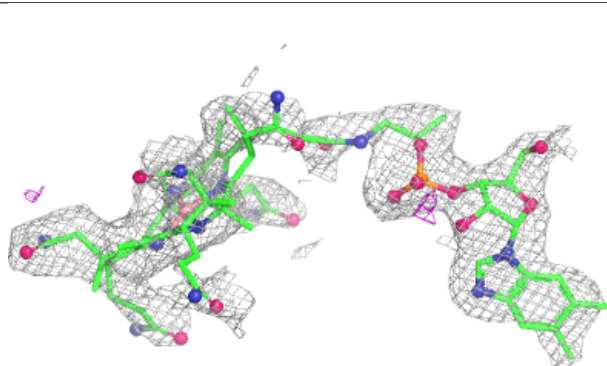
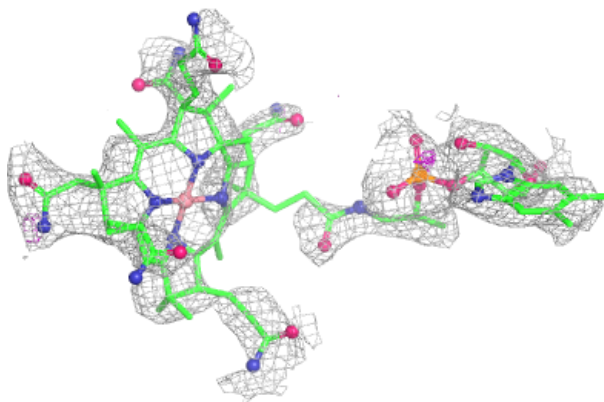


Electron density around B12 D 1801:

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and green (positive)

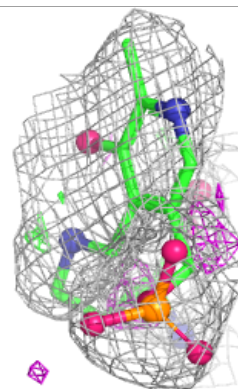
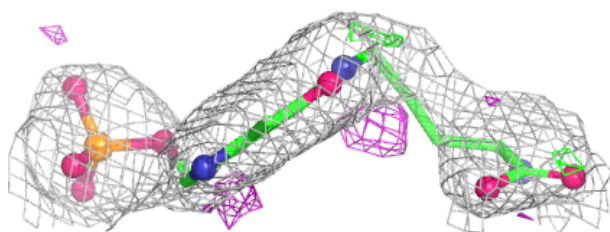
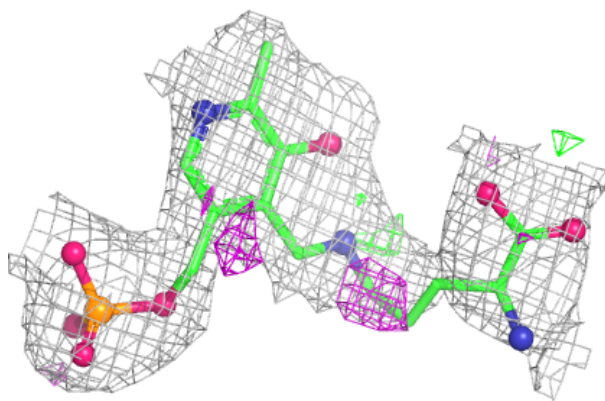
**Electron density around B12 A 1801:**

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

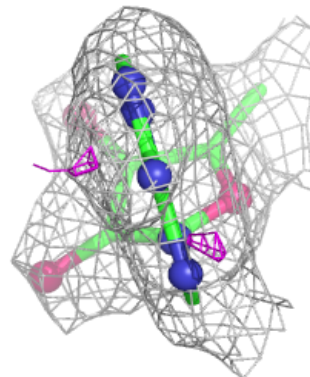
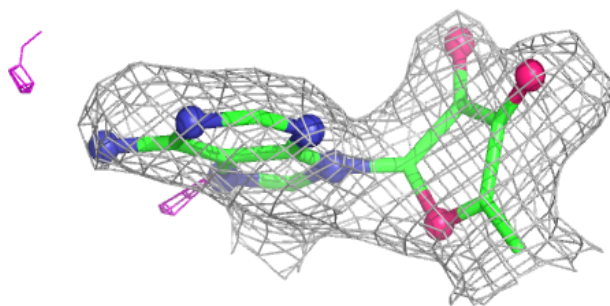
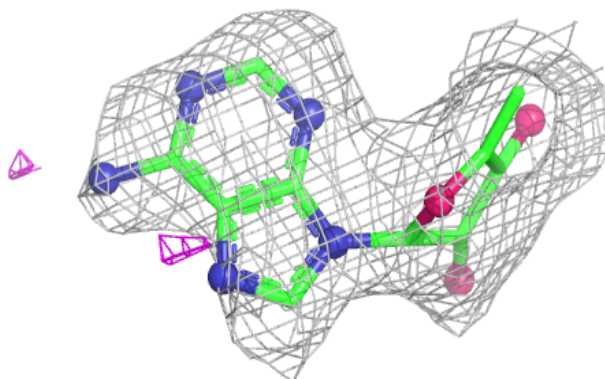


Electron density around Z97 D 767:

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

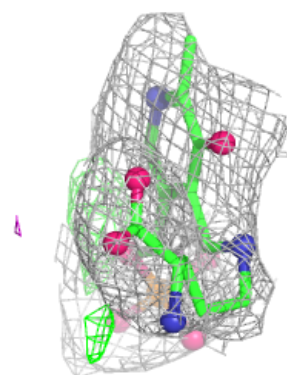
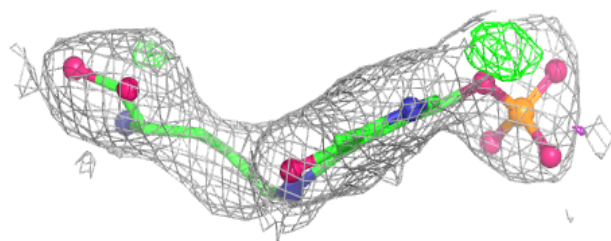
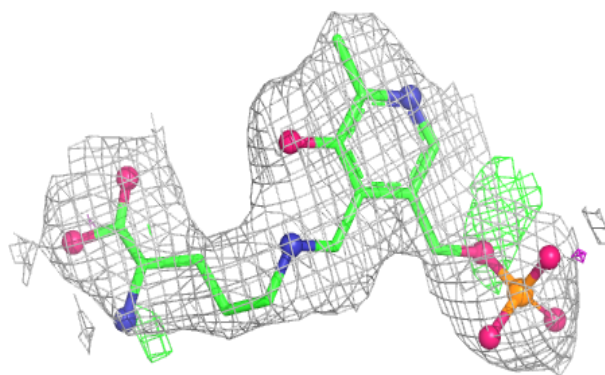
**Electron density around 5AD A 1500:**

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

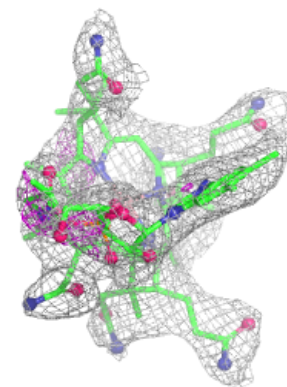
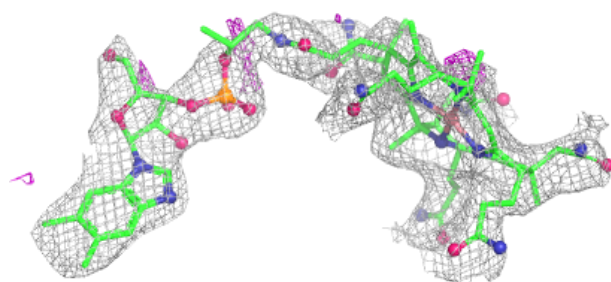
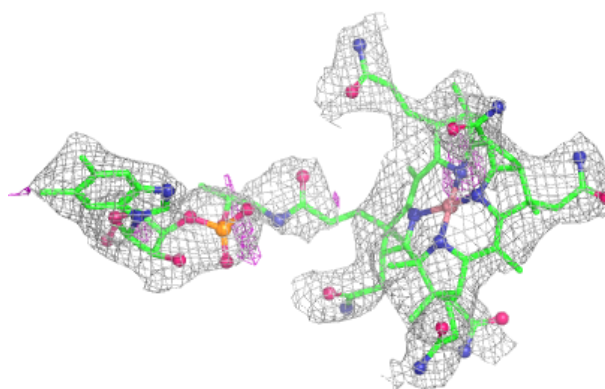


Electron density around Z97 B 767:

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

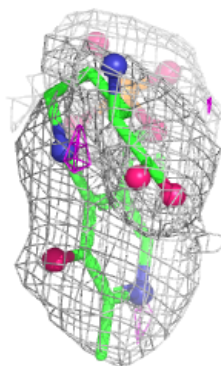
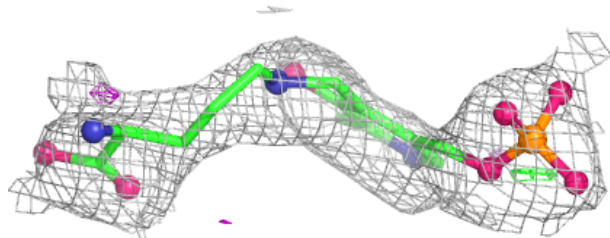
**Electron density around B12 B 1801:**

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

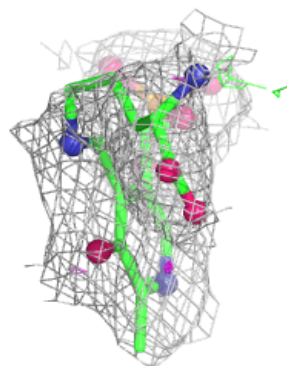
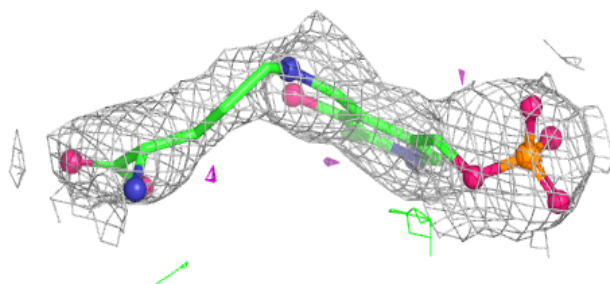
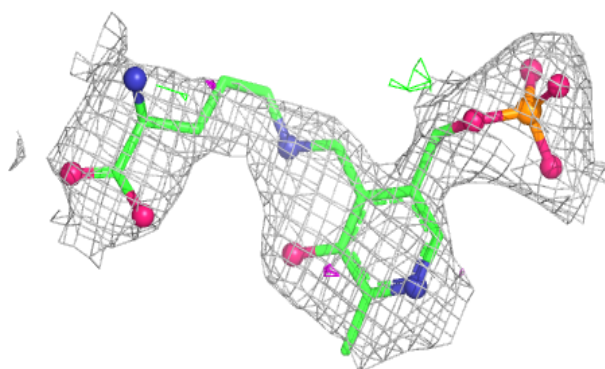


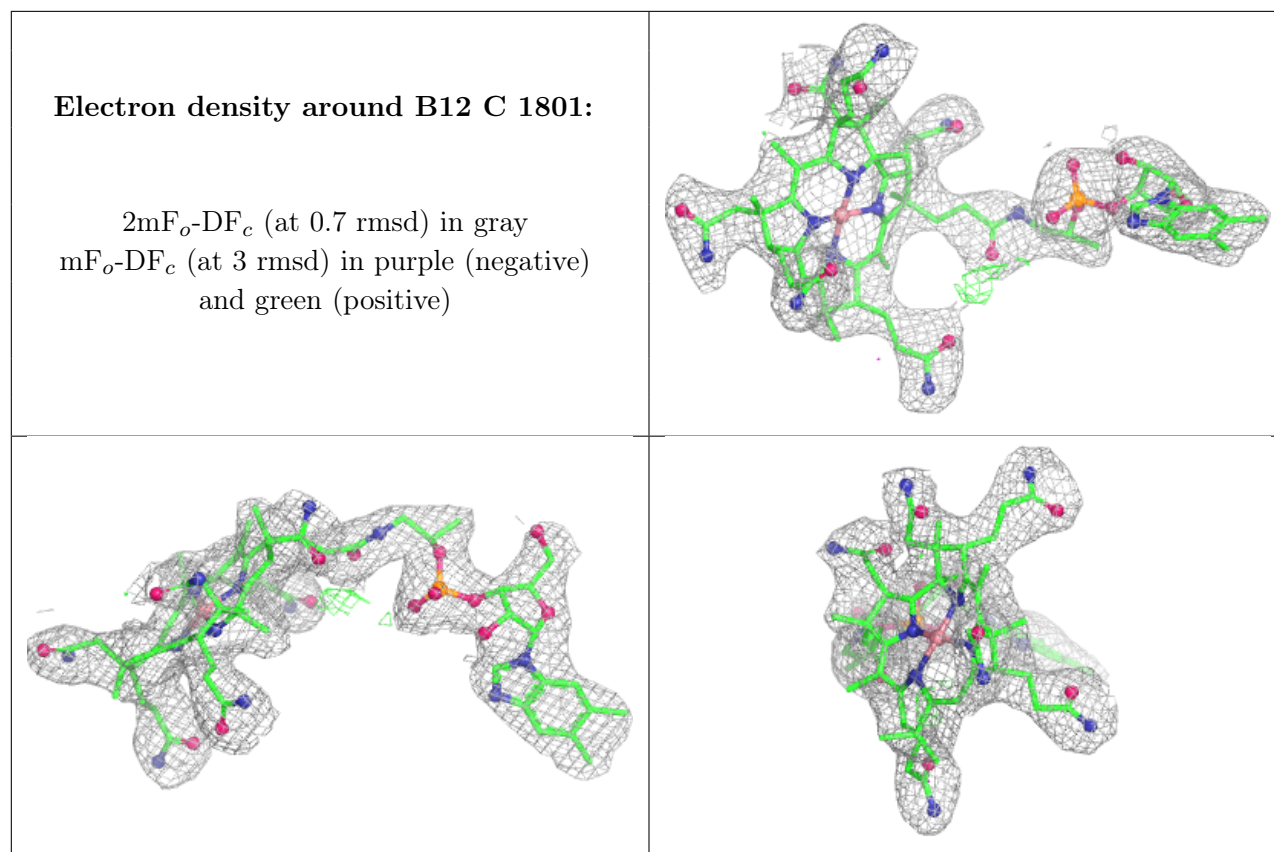
Electron density around Z97 C 767:

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

**Electron density around Z97 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.