



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 07:00 AM EDT

PDB ID : 3KOW  
Title : Crystal Structure of ornithine 4,5 aminomutase backsoaked complex  
Authors : Wolthers, K.R.; Levy, C.W.; Scrutton, N.S.; Leys, D.  
Deposited on : 2009-11-14  
Resolution : 2.90 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

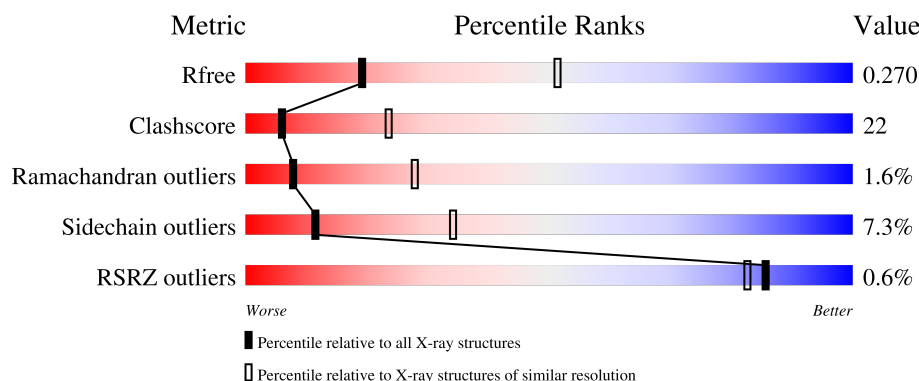
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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  $\geq 3$ , 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	<div> <div>2%</div> <div>53% 38% 5%</div> </div>
1	B	763	<div> <div>58% 35% 5%</div> </div>
1	C	763	<div> <div>52% 39% 5%</div> </div>
1	D	763	<div> <div>2%</div> <div>55% 36% 5%</div> </div>
2	E	121	<div> <div>50% 36% 10%</div> </div>

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

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

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

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26527 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	727	Total	C	N	O	S	0	0	0
			5646	3558	980	1074	34			
1	B	728	Total	C	N	O	S	0	0	0
			5672	3579	984	1075	34			
1	C	727	Total	C	N	O	S	0	0	0
			5649	3567	980	1068	34			
1	D	727	Total	C	N	O	S	0	0	0
			5659	3572	983	1070	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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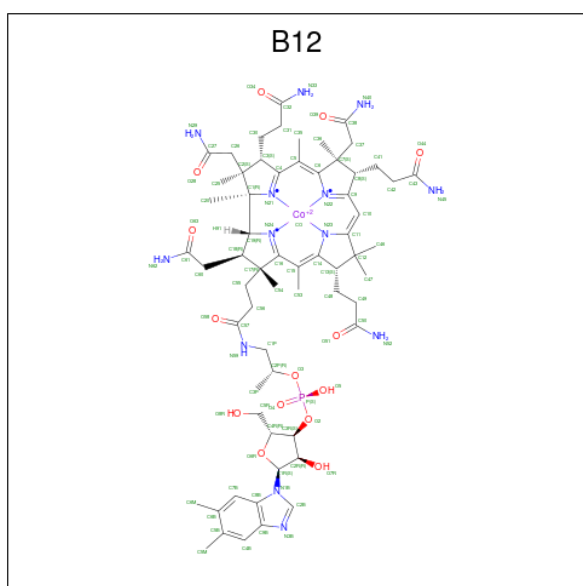
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Chain	Residue	Modelled	Actual	Comment	Reference
C	752	VAL	-	expression tag	UNP Q8VPJ5
C	753	ASP	-	expression tag	UNP Q8VPJ5
C	754	LYS	-	expression tag	UNP Q8VPJ5
C	755	LEU	-	expression tag	UNP Q8VPJ5
C	756	ALA	-	expression tag	UNP Q8VPJ5
C	757	ALA	-	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.

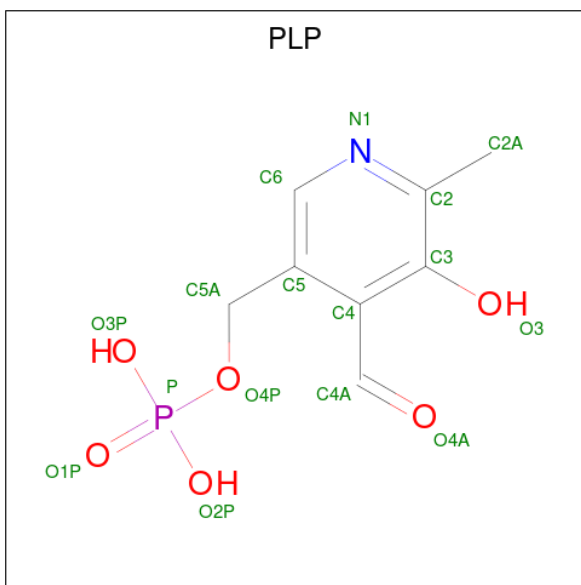
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			
2	F	109	Total	C	N	O	S	0	0	0
			858	539	152	163	4			
2	G	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			
2	H	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			

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



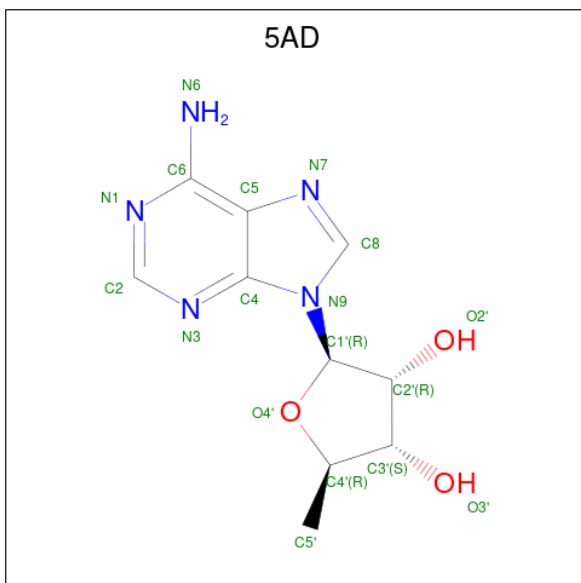
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	C	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	D	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

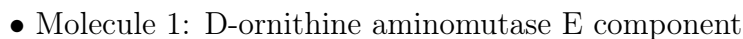
- Molecule 5 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula:  $C_{10}H_{13}N_5O_3$ ).



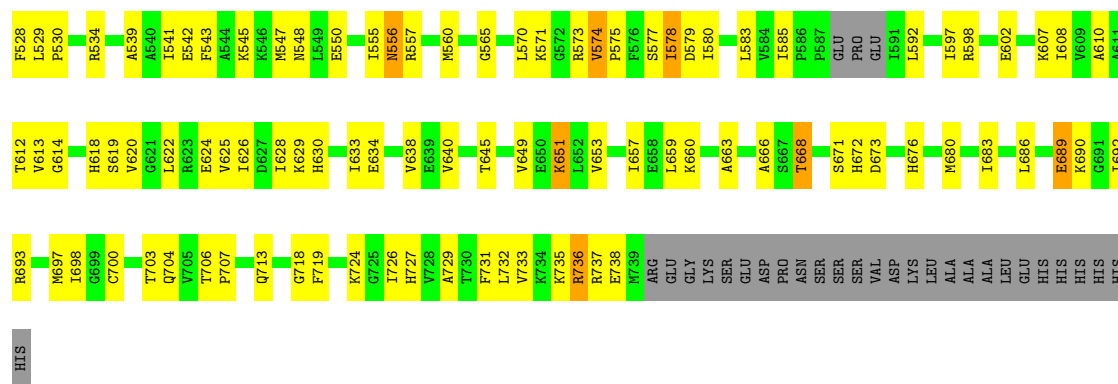


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	10	5	3		
5	C	1	Total	C	N	O	0	0
			18	10	5	3		
5	D	1	Total	C	N	O	0	0
			18	10	5	3		

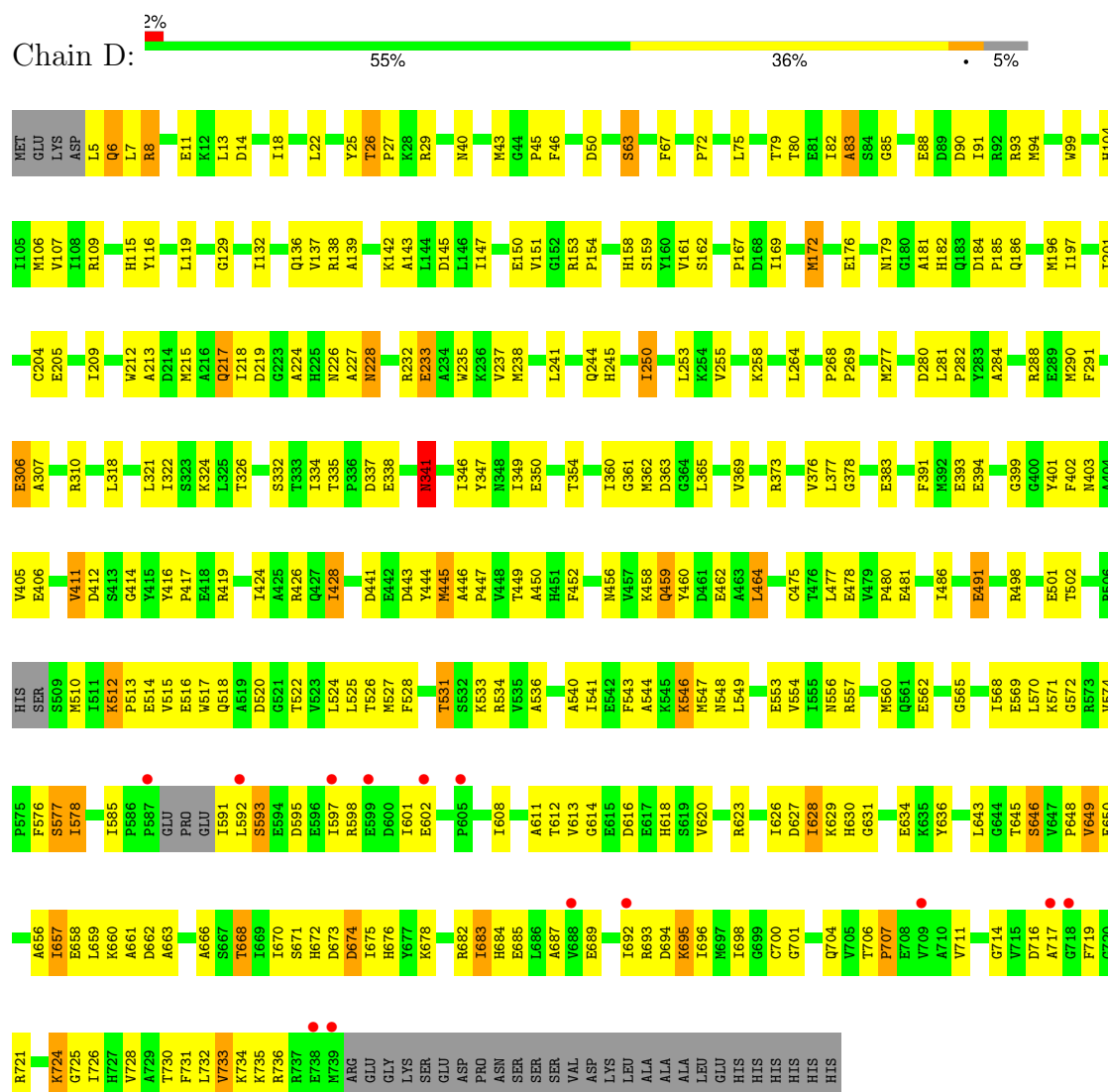
- Molecule 1: D-ornithine aminomutase E component





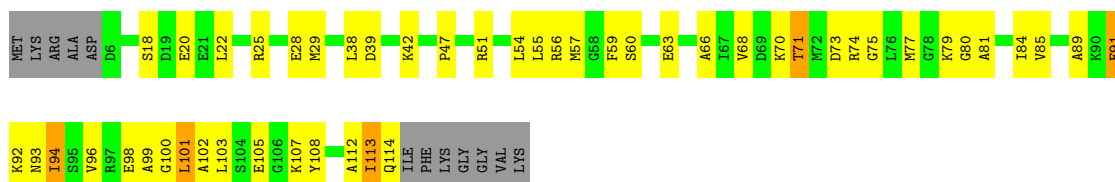


• Molecule 1: D-ornithine aminomutase E component



• Molecule 2: D-ornithine aminomutase S component

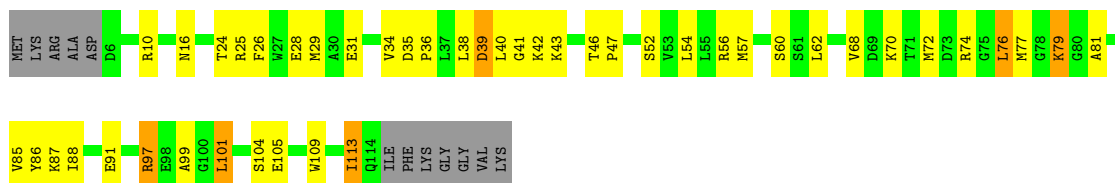




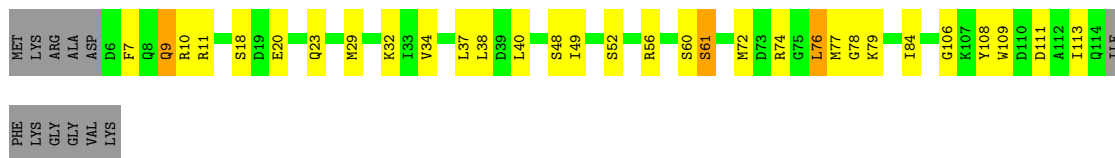
• Molecule 2: D-ornithine aminomutase S component



• 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, $\alpha$ , $\beta$ , $\gamma$	65.18Å 229.01Å 123.92Å 90.00° 102.76° 90.00°	Depositor
Resolution (Å)	120.86 – 2.90 120.86 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (120.86-2.90) 97.9 (120.86-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.191 , 0.279 0.181 , 0.270	Depositor DCC
$R_{free}$ test set	3837 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.7	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	26527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.45	0/5751	0.60	0/7787
1	B	0.50	0/5777	0.63	0/7818
1	C	0.45	0/5754	0.59	0/7789
1	D	0.48	0/5764	0.62	0/7801
2	E	0.46	0/867	0.58	0/1163
2	F	0.53	0/870	0.64	0/1167
2	G	0.47	0/867	0.56	0/1163
2	H	0.50	0/867	0.60	0/1163
All	All	0.47	0/26517	0.61	0/35851

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5646	0	5580	256	0
1	B	5672	0	5642	242	0
1	C	5649	0	5616	282	0
1	D	5659	0	5632	260	0
2	E	855	0	863	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	858	0	865	38	0
2	G	855	0	863	44	0
2	H	855	0	863	24	0
3	A	91	0	87	25	0
3	B	91	0	87	27	0
3	C	91	0	87	29	0
3	D	91	0	87	18	0
4	A	15	0	6	2	0
4	B	15	0	7	2	0
4	C	15	0	7	0	0
4	D	15	0	6	2	0
5	A	18	0	9	3	0
5	C	18	0	9	2	0
5	D	18	0	10	2	0
All	All	26527	0	26326	1183	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 22.

All (1183) 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:F:74:ARG:HG3	2:F:74:ARG:HH11	0.95	1.08
1:A:82:ILE:HG12	1:A:93:ARG:HD2	1.39	1.05
1:B:528:PHE:HE1	1:B:560:MET:HG3	1.22	1.04
1:A:120:ILE:HG13	1:A:133:THR:HG22	1.48	0.96
2:F:74:ARG:HH11	2:F:74:ARG:CG	1.78	0.95
3:A:1801:B12:O28	3:A:1801:B12:H3	1.66	0.94
1:C:612:THR:HB	1:C:645:THR:HG22	1.49	0.93
2:F:74:ARG:HG3	2:F:74:ARG:NH1	1.77	0.92
5:A:1500:5AD:H5'2	3:C:1801:B12:H261	1.53	0.90
1:A:628:ILE:HG13	1:A:635:LYS:HB2	1.54	0.89
1:C:613:VAL:HG11	1:C:649:VAL:HG22	1.54	0.88
1:D:82:ILE:HG12	1:D:93:ARG:HD2	1.54	0.88
3:B:1801:B12:H601	3:B:1801:B12:H262	1.55	0.87
2:E:60:SER:OG	2:E:63:GLU:HG3	1.74	0.87
1:D:491:GLU:OE2	1:D:491:GLU:HA	1.72	0.87
3:A:1801:B12:H262	3:A:1801:B12:H601	1.56	0.86
1:C:610:ALA:HB1	1:C:622:LEU:HD21	1.57	0.85
1:D:684:HIS:CE1	1:D:693:ARG:HE	1.94	0.85
1:B:528:PHE:CE1	1:B:560:MET:HG3	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ARG:HB3	1:D:8:ARG:CZ	2.05	0.84
1:B:238:MET:CE	1:B:269:PRO:HG2	2.07	0.83
1:D:288:ARG:HG3	1:D:288:ARG:HH11	1.43	0.83
3:D:1801:B12:H362	3:D:1801:B12:H351	1.60	0.83
1:A:123:THR:HG23	1:A:135:LYS:HD3	1.61	0.81
1:A:233:GLU:HB3	1:A:235:TRP:CH2	2.15	0.81
5:A:1500:5AD:H5'3	3:C:1801:B12:C16	2.11	0.81
2:F:88:ILE:HG13	2:F:103:LEU:HD11	1.60	0.81
1:D:526:THR:HG23	1:D:569:GLU:HG2	1.60	0.81
1:D:611:ALA:HB2	1:D:643:LEU:HB2	1.60	0.81
1:C:197:ILE:HG22	1:C:437:VAL:HG21	1.61	0.81
1:D:8:ARG:HB3	1:D:8:ARG:NH1	1.96	0.81
1:A:5:LEU:O	1:A:6:GLN:HB2	1.82	0.80
1:D:592:LEU:HB2	1:D:597:ILE:HD11	1.64	0.80
1:D:161:VAL:HG22	1:D:169:ILE:HG22	1.64	0.80
1:D:132:ILE:HA	1:D:136:GLN:OE1	1.82	0.79
1:C:79:THR:HB	1:C:332:SER:HA	1.65	0.79
1:D:716:ASP:HB3	1:D:735:LYS:HE2	1.63	0.78
3:D:1801:B12:N40	3:D:1801:B12:H8	1.98	0.78
3:B:1801:B12:H531	3:B:1801:B12:H552	1.66	0.78
2:H:20:GLU:CD	2:H:20:GLU:H	1.85	0.78
1:D:406:GLU:OE2	1:D:428:ILE:HG22	1.83	0.78
1:B:534:ARG:HG3	1:B:534:ARG:HH11	1.46	0.78
1:A:218:ILE:HD13	1:A:297:ARG:HD2	1.66	0.78
1:C:264:LEU:HD21	1:C:291:PHE:CD1	2.18	0.77
3:C:1801:B12:H203	3:C:1801:B12:H302	1.63	0.77
1:B:238:MET:HE3	1:B:269:PRO:HG2	1.65	0.77
1:B:116:TYR:CE2	1:B:120:ILE:HD13	2.18	0.77
1:A:83:ALA:HB3	1:A:108:ILE:HD12	1.65	0.76
2:E:47:PRO:O	2:E:51:ARG:HG3	1.84	0.76
1:A:735:LYS:HE3	1:A:739:MET:SD	2.24	0.76
1:C:335:THR:HG21	1:C:343:PRO:HB3	1.67	0.76
1:C:120:ILE:HG13	1:C:133:THR:HG22	1.68	0.76
1:A:269:PRO:HD2	1:A:280:ASP:OD1	1.86	0.76
1:C:344:TRP:CG	1:C:515:VAL:HB	2.21	0.76
1:A:610:ALA:HB1	1:A:622:LEU:HD21	1.68	0.75
1:A:79:THR:HB	1:A:332:SER:HA	1.66	0.75
1:C:13:LEU:HD13	1:C:91:ILE:HG22	1.67	0.75
3:B:1801:B12:H492	3:B:1801:B12:H471	1.68	0.74
1:B:113:GLN:HE22	1:B:132:ILE:HB	1.52	0.74
3:C:1801:B12:H471	3:C:1801:B12:H492	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:HB	1:B:332:SER:HA	1.69	0.74
1:D:269:PRO:HD2	1:D:280:ASP:OD1	1.87	0.74
1:B:82:ILE:HG12	1:B:93:ARG:HD2	1.69	0.73
1:C:668:THR:HG23	1:C:676:HIS:HB2	1.70	0.73
1:C:495:VAL:O	1:C:499:MET:HG2	1.88	0.73
1:C:8:ARG:NH1	1:C:11:GLU:HG3	2.03	0.73
1:C:43:MET:HB2	1:C:48:TYR:CE2	2.24	0.72
1:A:424:ILE:HD11	1:C:628:ILE:HD12	1.69	0.72
1:C:633:ILE:HD12	1:C:638:VAL:HG11	1.72	0.72
3:B:1801:B12:H362	3:B:1801:B12:H351	1.70	0.72
1:A:219:ASP:HB3	1:A:248:ASN:ND2	2.04	0.72
1:A:233:GLU:OE1	1:A:236:LYS:HD2	1.90	0.72
1:B:577:SER:O	1:B:578:ILE:HD12	1.89	0.71
1:D:401:TYR:O	1:D:405:VAL:HG23	1.90	0.71
1:B:259:LYS:HA	1:B:262:ILE:HD12	1.72	0.71
3:A:1801:B12:H8	3:A:1801:B12:N40	2.05	0.71
2:E:20:GLU:H	2:E:20:GLU:CD	1.94	0.71
1:B:623:ARG:HD3	1:D:115:HIS:CE1	2.26	0.71
1:C:324:LYS:HE2	1:C:362:MET:O	1.91	0.71
2:E:25:ARG:HG2	2:E:29:MET:HE2	1.73	0.70
1:C:607:LYS:O	1:C:608:ILE:HD12	1.90	0.70
1:D:334:ILE:HG22	1:D:335:THR:O	1.91	0.70
3:C:1801:B12:N40	3:C:1801:B12:H8	2.03	0.70
1:D:597:ILE:HG23	1:D:733:VAL:HG11	1.73	0.70
1:B:172:MET:HE2	1:B:172:MET:C	2.12	0.70
1:C:5:LEU:HG	1:C:6:GLN:HB2	1.74	0.70
1:D:704:GLN:HE22	1:D:721:ARG:HH21	1.40	0.70
1:C:207:LYS:HE3	1:C:251:PHE:HD2	1.56	0.69
1:C:668:THR:CG2	1:C:676:HIS:HB2	2.22	0.69
1:D:528:PHE:HE1	1:D:560:MET:HG3	1.57	0.69
1:B:259:LYS:HE2	1:B:294:TYR:CE2	2.27	0.69
1:C:86:ARG:HB3	1:C:88:GLU:OE2	1.92	0.69
1:C:79:THR:HG21	1:C:106:MET:HE3	1.74	0.69
1:A:89:ASP:OD2	1:A:517:TRP:HA	1.92	0.69
3:A:1801:B12:H362	3:A:1801:B12:H351	1.72	0.69
1:B:113:GLN:HG3	1:B:116:TYR:CD2	2.27	0.69
1:D:186:GLN:HG2	1:D:401:TYR:OH	1.93	0.69
1:B:668:THR:HG23	1:B:676:HIS:HB2	1.74	0.69
1:C:201:ILE:HG23	2:G:41:GLY:HA2	1.75	0.69
1:C:598:ARG:O	1:C:602:GLU:HB2	1.92	0.69
1:D:531:THR:H	1:D:565:GLY:HA2	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ILE:HB	1:A:580:ILE:HD11	1.73	0.68
2:E:25:ARG:HG2	2:E:29:MET:CE	2.23	0.68
2:E:99:ALA:O	2:E:102:ALA:HB3	1.92	0.68
1:C:511:ILE:HG13	1:C:580:ILE:HD11	1.75	0.68
1:D:531:THR:HG23	1:D:536:ALA:HB2	1.75	0.68
1:A:520:ASP:O	1:A:573:ARG:HD2	1.92	0.68
1:C:126:GLY:C	1:C:127:ILE:HD13	2.13	0.68
1:C:397:GLU:O	1:C:397:GLU:HG2	1.92	0.68
3:C:1801:B12:O28	3:C:1801:B12:H3	1.93	0.68
1:D:412:ASP:OD2	1:D:414:GLY:N	2.26	0.68
1:B:607:LYS:O	1:B:608:ILE:HD12	1.94	0.68
1:C:43:MET:HE2	1:C:54:PRO:HG3	1.74	0.68
3:C:1801:B12:H362	3:C:1801:B12:H351	1.76	0.68
1:A:212:TRP:CH2	1:A:477:LEU:HB3	2.28	0.68
3:A:1801:B12:H2B	3:A:1801:B12:O7R	1.94	0.68
1:C:207:LYS:HE3	1:C:251:PHE:CD2	2.29	0.68
1:B:552:VAL:HG13	1:B:570:LEU:HD23	1.75	0.67
1:D:673:ASP:O	1:D:674:ASP:HB2	1.94	0.67
1:B:238:MET:HE2	1:B:269:PRO:HG2	1.76	0.67
2:E:91:GLU:HB3	2:E:92:LYS:HD3	1.75	0.67
1:A:234:ALA:O	1:A:237:VAL:HG12	1.94	0.67
1:C:393:GLU:HG3	2:G:29:MET:SD	2.34	0.67
1:A:267:VAL:HG22	1:A:299:GLN:HB3	1.74	0.67
1:C:95:ARG:HA	1:C:147:ILE:HD13	1.77	0.66
2:G:70:LYS:O	2:G:74:ARG:HG2	1.94	0.66
1:D:445:MET:HE2	1:D:446:ALA:C	2.16	0.66
2:F:69:ASP:HA	2:F:72:MET:HE2	1.77	0.66
1:D:22:LEU:HD11	1:D:139:ALA:HB2	1.77	0.66
1:C:43:MET:HB2	1:C:48:TYR:HE2	1.60	0.66
1:C:232:ARG:HA	1:C:232:ARG:HH11	1.61	0.66
1:D:227:ALA:HB3	1:D:241:LEU:HD21	1.77	0.66
1:A:391:PHE:HD1	1:A:416:TYR:CD1	2.14	0.66
1:B:686:LEU:HD23	1:B:686:LEU:O	1.95	0.66
1:B:514:GLU:HA	1:B:520:ASP:OD1	1.96	0.66
1:C:525:LEU:HD23	1:C:570:LEU:HD13	1.77	0.66
1:B:612:THR:HG22	1:B:616:ASP:HB3	1.77	0.65
1:B:671:SER:OG	1:B:704:GLN:HG3	1.95	0.65
1:A:604:THR:HB	1:A:736:ARG:NH1	2.11	0.65
1:D:668:THR:HG23	1:D:676:HIS:HB2	1.78	0.65
1:C:254:LYS:HB2	2:G:38:LEU:HD11	1.79	0.65
1:A:289:GLU:CD	1:A:373:ARG:HH21	2.00	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:PHE:CE1	1:D:560:MET:HG3	2.30	0.65
1:A:608:ILE:HD11	1:A:663:ALA:HB3	1.77	0.65
1:C:460:TYR:CE1	2:G:86:TYR:HE2	2.13	0.65
3:B:1801:B12:H262	3:B:1801:B12:C60	2.26	0.64
1:B:41:LEU:HD21	1:B:54:PRO:HG3	1.79	0.64
2:F:67:ILE:HG13	2:F:104:SER:HB3	1.78	0.64
1:C:161:VAL:HG23	1:C:181:ALA:HB1	1.79	0.64
1:A:109:ARG:O	1:A:129:GLY:HA3	1.96	0.64
1:B:161:VAL:HG23	1:B:181:ALA:HB1	1.79	0.64
2:F:54:LEU:HD23	2:F:57:MET:CE	2.28	0.64
1:A:698:ILE:O	1:A:716:ASP:HB2	1.98	0.64
1:C:250:ILE:HG23	2:G:34:VAL:HG21	1.79	0.64
1:D:510:MET:HE3	1:D:577:SER:HB2	1.79	0.64
1:B:50:ASP:HB2	1:B:363:ASP:OD1	1.98	0.64
1:A:126:GLY:C	1:A:127:ILE:HD13	2.19	0.64
3:A:1801:B12:O7R	3:A:1801:B12:C2B	2.46	0.64
2:G:52:SER:OG	2:G:56:ARG:NH2	2.29	0.64
1:D:104:HIS:HE2	1:D:158:HIS:CG	2.15	0.64
1:B:534:ARG:HG3	1:B:534:ARG:NH1	2.13	0.64
1:D:648:PRO:C	1:D:650:GLU:H	2.00	0.64
1:A:610:ALA:HA	1:A:665:LEU:O	1.99	0.63
1:B:537:GLU:HG3	1:B:554:VAL:HG21	1.79	0.63
1:D:132:ILE:HG22	1:D:132:ILE:O	1.97	0.63
1:C:228:ASN:O	1:C:303:LYS:HD2	1.98	0.63
1:C:277:MET:CE	1:C:321:LEU:HD23	2.28	0.63
1:A:243:VAL:HG21	1:A:391:PHE:CD2	2.32	0.63
1:B:217:GLN:O	1:B:263:CYS:HB2	1.97	0.63
1:B:233:GLU:HG2	1:B:235:TRP:CH2	2.33	0.63
1:B:607:LYS:HE2	1:B:639:GLU:OE2	1.98	0.63
2:G:88:ILE:HG22	2:G:99:ALA:HB1	1.80	0.63
1:B:168:ASP:N	1:B:168:ASP:OD2	2.32	0.63
1:C:443:ASP:OD2	2:G:79:LYS:HE3	1.99	0.63
1:A:245:HIS:O	1:A:249:SER:HB2	1.99	0.62
1:B:552:VAL:CG1	1:B:570:LEU:HD23	2.29	0.62
1:B:668:THR:O	1:B:668:THR:CG2	2.47	0.62
2:H:18:SER:HB2	2:H:20:GLU:OE1	1.99	0.62
1:A:264:LEU:N	1:A:264:LEU:HD12	2.14	0.62
1:B:619:SER:HB3	1:B:645:THR:HG21	1.82	0.62
1:C:541:ILE:HG22	1:C:545:LYS:NZ	2.15	0.62
1:B:205:GLU:O	1:B:209:ILE:HD12	1.99	0.62
2:G:24:THR:O	2:G:28:GLU:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:514:GLU:HA	1:D:520:ASP:OD1	2.00	0.62
1:C:108:ILE:H	1:C:108:ILE:HD12	1.64	0.62
1:C:432:ILE:HD13	1:C:432:ILE:N	2.13	0.62
1:B:264:LEU:HD21	1:B:291:PHE:CD1	2.34	0.62
1:D:238:MET:CE	1:D:269:PRO:HG2	2.29	0.62
1:D:475:CYS:HB2	2:H:56:ARG:O	2.00	0.62
1:B:350:GLU:HG2	1:D:310:ARG:HD3	1.80	0.62
1:C:402:PHE:HB3	1:C:428:ILE:HD12	1.81	0.62
1:A:193:ASN:O	1:A:432:ILE:HG12	1.99	0.62
1:C:456:ASN:ND2	1:C:459:GLN:HE21	1.96	0.62
1:C:649:VAL:O	1:C:653:VAL:HG23	2.00	0.62
1:D:79:THR:HA	1:D:104:HIS:HB3	1.81	0.62
1:D:224:ALA:HB3	1:D:245:HIS:CE1	2.34	0.62
4:A:1802:PLP:H2A2	1:C:182:HIS:HB3	1.80	0.61
1:A:14:ASP:HB3	1:A:17:ASN:HB3	1.81	0.61
1:A:730:THR:O	1:A:734:LYS:HG3	2.00	0.61
1:B:693:ARG:HG3	1:B:693:ARG:O	1.99	0.61
1:D:233:GLU:HB3	1:D:235:TRP:CH2	2.35	0.61
1:A:515:VAL:HG13	1:A:522:THR:HB	1.82	0.61
1:A:415:TYR:N	1:A:418:GLU:OE1	2.33	0.61
3:B:1801:B12:C49	3:B:1801:B12:C47	2.73	0.61
1:A:198:ARG:HG3	1:A:198:ARG:HH11	1.65	0.61
1:C:284:ALA:O	1:C:288:ARG:HD2	2.00	0.61
1:C:555:ILE:HG21	1:C:571:LYS:HG2	1.82	0.61
1:D:5:LEU:HD23	1:D:5:LEU:O	2.00	0.61
2:G:97:ARG:O	2:G:101:LEU:HB2	2.01	0.61
1:A:682:ARG:O	1:A:686:LEU:HB2	1.99	0.61
1:C:133:THR:O	1:C:137:VAL:HG23	2.00	0.61
1:A:172:MET:HE2	1:A:176:GLU:HG3	1.83	0.61
3:B:1801:B12:C16	5:D:1500:5AD:H5'3	2.31	0.60
1:C:219:ASP:HB3	1:C:248:ASN:ND2	2.16	0.60
2:G:25:ARG:HG2	2:G:29:MET:CE	2.30	0.60
1:D:204:CYS:HB3	1:D:452:PHE:CD2	2.36	0.60
1:D:277:MET:SD	1:D:322:ILE:HD11	2.40	0.60
1:A:608:ILE:CD1	1:A:663:ALA:HB3	2.30	0.60
1:C:28:LYS:HE2	1:C:145:ASP:HB3	1.82	0.60
1:B:578:ILE:HD13	1:D:543:PHE:CE1	2.36	0.60
2:F:74:ARG:CG	2:F:74:ARG:NH1	2.47	0.60
1:A:159:SER:HB3	1:A:173:PHE:CZ	2.36	0.60
1:A:528:PHE:CE1	1:A:560:MET:HG3	2.35	0.60
1:A:243:VAL:HG21	1:A:391:PHE:HD2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:VAL:O	1:C:423:GLY:HA2	2.02	0.60
1:D:516:GLU:HG3	1:D:517:TRP:CD1	2.36	0.60
1:A:683:ILE:HG22	1:A:698:ILE:HD13	1.81	0.60
1:B:172:MET:HE2	1:B:173:PHE:HD1	1.66	0.60
1:C:657:ILE:HD11	1:C:692:ILE:HD13	1.82	0.60
3:C:1801:B12:C2B	3:C:1801:B12:O7R	2.49	0.60
1:A:93:ARG:HA	1:A:96:MET:HE2	1.84	0.60
2:E:80:GLY:O	2:E:84:ILE:HG12	2.01	0.60
1:B:116:TYR:HE2	1:B:120:ILE:HD13	1.64	0.60
3:D:1801:B12:H10	3:D:1801:B12:H422	1.84	0.60
1:A:109:ARG:HG2	1:A:132:ILE:CG1	2.31	0.60
1:D:341:ASN:HD22	1:D:341:ASN:C	2.05	0.60
1:B:459:GLN:HG3	1:B:460:TYR:CD2	2.37	0.59
1:B:481:GLU:H	1:B:481:GLU:CD	2.05	0.59
1:B:475:CYS:HB2	2:F:56:ARG:O	2.02	0.59
1:C:555:ILE:O	1:C:556:ASN:HB2	2.02	0.59
1:A:574:VAL:HG11	1:C:543:PHE:CE1	2.37	0.59
1:C:135:LYS:HG3	1:C:485:TYR:OH	2.02	0.59
1:C:335:THR:HG22	1:C:348:ASN:ND2	2.17	0.59
1:D:373:ARG:NH1	1:D:378:GLY:HA2	2.17	0.59
1:C:649:VAL:HG12	1:C:686:LEU:HD12	1.85	0.59
1:D:593:SER:O	1:D:597:ILE:HG12	2.02	0.59
1:B:17:ASN:HA	1:B:20:LYS:HE2	1.83	0.59
2:F:107:LYS:O	2:F:108:TYR:HB2	2.02	0.59
1:C:7:LEU:HD12	1:C:146:LEU:HB3	1.84	0.59
1:C:613:VAL:CG1	1:C:649:VAL:HG22	2.31	0.59
1:D:547:MET:O	1:D:548:ASN:HB2	2.02	0.59
1:D:684:HIS:CE1	1:D:693:ARG:NE	2.69	0.59
1:A:416:TYR:CG	1:A:417:PRO:HA	2.37	0.59
1:B:541:ILE:HD11	1:B:554:VAL:HG23	1.84	0.59
1:D:137:VAL:HG21	1:D:172:MET:HE1	1.84	0.59
1:B:688:VAL:HG13	1:B:688:VAL:O	2.03	0.59
1:D:568:ILE:HG22	1:D:570:LEU:CD1	2.32	0.59
1:A:134:ARG:NH1	1:A:175:GLU:OE2	2.29	0.59
1:B:239:PRO:O	1:B:243:VAL:HG23	2.01	0.59
3:C:1801:B12:H262	3:C:1801:B12:H601	1.84	0.59
1:D:416:TYR:CD1	1:D:417:PRO:HA	2.38	0.59
3:D:1801:B12:H252	3:D:1801:B12:H601	1.84	0.59
1:A:264:LEU:HD21	1:A:291:PHE:CD1	2.38	0.59
1:C:732:LEU:O	1:C:736:ARG:HB3	2.03	0.59
3:D:1801:B12:H362	3:D:1801:B12:C35	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:THR:HG22	1:B:450:ALA:N	2.18	0.58
1:C:197:ILE:CG2	1:C:437:VAL:HG21	2.32	0.58
1:D:233:GLU:HB3	1:D:235:TRP:CZ2	2.37	0.58
1:C:82:ILE:HG22	1:C:82:ILE:O	2.02	0.58
1:B:401:TYR:O	1:B:405:VAL:HG23	2.04	0.58
1:D:90:ASP:O	1:D:94:MET:HG3	2.02	0.58
1:A:187:TYR:OH	1:C:629:LYS:HD3	2.04	0.58
3:B:1801:B12:H552	3:B:1801:B12:C53	2.30	0.58
1:D:5:LEU:O	1:D:6:GLN:HB2	2.03	0.58
1:D:719:PHE:CD2	3:D:1801:B12:HM63	2.38	0.58
1:A:161:VAL:CG1	1:A:161:VAL:O	2.50	0.58
1:B:445:MET:HA	1:B:455:ASN:OD1	2.03	0.58
1:C:288:ARG:HD3	1:C:326:THR:HB	1.85	0.58
1:A:55:LEU:HD21	1:A:153:ARG:CZ	2.33	0.58
1:B:207:LYS:NZ	1:B:217:GLN:NE2	2.51	0.58
1:D:668:THR:HG23	1:D:668:THR:O	2.02	0.58
1:D:730:THR:O	1:D:734:LYS:HB2	2.02	0.58
1:C:110:THR:HG22	1:C:131:PRO:HA	1.86	0.58
1:C:267:VAL:HG22	1:C:299:GLN:HB3	1.86	0.58
1:A:675:ILE:HG13	1:A:675:ILE:O	2.03	0.58
2:E:28:GLU:HB2	1:D:40:ASN:ND2	2.19	0.58
1:D:393:GLU:HG3	2:H:29:MET:SD	2.44	0.58
1:D:533:LYS:HG3	1:D:534:ARG:N	2.19	0.58
1:A:237:VAL:HG22	1:A:237:VAL:O	2.04	0.57
1:A:735:LYS:HA	1:A:738:GLU:HB2	1.86	0.57
1:B:172:MET:HE2	1:B:173:PHE:N	2.19	0.57
1:B:281:LEU:HB3	1:B:282:PRO:HD3	1.86	0.57
1:B:392:MET:HB3	2:F:29:MET:HE3	1.85	0.57
3:C:1801:B12:H422	3:C:1801:B12:C10	2.33	0.57
1:A:396:ILE:HD12	2:E:29:MET:HG2	1.84	0.57
4:A:1802:PLP:O3P	1:C:114:SER:HB2	2.04	0.57
1:B:124:PRO:O	1:B:131:PRO:HG2	2.03	0.57
1:B:668:THR:HG23	1:B:668:THR:O	2.04	0.57
1:C:689:GLU:HG2	1:C:690:LYS:N	2.18	0.57
1:D:724:LYS:HD2	1:D:726:ILE:HG22	1.84	0.57
1:A:93:ARG:HA	1:A:96:MET:CE	2.34	0.57
1:B:476:THR:HB	1:B:483:ILE:HG13	1.86	0.57
1:C:550:GLU:HB2	1:C:573:ARG:HB3	1.85	0.57
1:C:697:MET:HG2	1:C:735:LYS:HG2	1.86	0.57
1:D:416:TYR:CG	1:D:417:PRO:HA	2.39	0.57
1:D:574:VAL:HG12	1:D:576:PHE:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:PHE:O	1:A:506:ARG:HB2	2.03	0.57
1:D:288:ARG:HH11	1:D:288:ARG:CG	2.17	0.57
1:D:541:ILE:HD11	1:D:554:VAL:HG23	1.87	0.57
1:D:649:VAL:O	1:D:649:VAL:HG12	2.05	0.57
3:A:1801:B12:H552	3:A:1801:B12:H531	1.85	0.57
1:D:399:GLY:HA3	1:D:403:ASN:HD22	1.69	0.57
1:A:278:TYR:OH	1:A:376:VAL:HG21	2.05	0.57
1:A:547:MET:O	1:A:548:ASN:HB2	2.04	0.57
1:A:620:VAL:HG21	1:C:116:TYR:HE1	1.68	0.57
1:C:109:ARG:HG2	1:C:132:ILE:CG1	2.35	0.57
1:C:486:ILE:CD1	2:G:62:LEU:HD12	2.35	0.57
1:A:302:THR:HG22	1:A:334:ILE:HG21	1.86	0.57
1:A:679:ASN:O	1:A:683:ILE:HG13	2.04	0.57
1:D:648:PRO:O	1:D:650:GLU:N	2.38	0.57
3:A:1801:B12:H261	5:C:1500:5AD:H5'2	1.86	0.57
1:B:612:THR:HA	1:B:667:SER:HB3	1.87	0.57
3:B:1801:B12:H203	3:B:1801:B12:H301	1.86	0.57
3:C:1801:B12:O7R	3:C:1801:B12:H2B	2.03	0.57
1:A:619:SER:HB3	1:A:645:THR:HG21	1.87	0.56
1:D:675:ILE:O	1:D:675:ILE:HG13	2.04	0.56
1:C:109:ARG:HA	1:C:130:VAL:O	2.03	0.56
1:C:134:ARG:HD3	1:C:138:ARG:HH21	1.69	0.56
1:D:269:PRO:HD2	1:D:280:ASP:CG	2.26	0.56
2:H:37:LEU:HA	2:H:40:LEU:HD12	1.86	0.56
1:A:543:PHE:O	1:A:547:MET:HG3	2.06	0.56
1:C:29:ARG:O	1:C:30:ARG:HG2	2.05	0.56
1:C:108:ILE:HD12	1:C:108:ILE:N	2.20	0.56
1:C:358:ALA:O	1:C:362:MET:HG3	2.05	0.56
1:C:479:VAL:HG12	1:C:482:LYS:HG3	1.87	0.56
1:C:578:ILE:HG23	1:C:579:ASP:N	2.19	0.56
2:G:87:LYS:O	2:G:91:GLU:HG2	2.04	0.56
1:D:462:GLU:CD	1:D:462:GLU:H	2.08	0.56
2:E:89:ALA:HA	2:E:94:ILE:HG13	1.87	0.56
1:B:211:ALA:HB2	1:B:257:MET:HG2	1.88	0.56
3:B:1801:B12:H492	3:B:1801:B12:C47	2.35	0.56
3:D:1801:B12:H531	3:D:1801:B12:H543	1.88	0.56
1:A:426:ARG:HH12	1:C:634:GLU:CD	2.07	0.56
1:B:333:THR:HB	1:B:351:ALA:HB1	1.86	0.56
1:A:233:GLU:HB3	1:A:235:TRP:CZ3	2.41	0.56
1:A:300:MET:HE2	1:A:320:LEU:HG	1.88	0.56
2:F:54:LEU:HD12	2:F:68:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:633:ILE:O	1:C:638:VAL:HB	2.06	0.56
1:C:95:ARG:CA	1:C:147:ILE:HD13	2.35	0.56
1:C:613:VAL:HG12	1:C:614:GLY:N	2.20	0.56
1:A:6:GLN:CD	1:A:7:LEU:H	2.08	0.55
1:A:391:PHE:CD1	1:A:416:TYR:CD1	2.95	0.55
2:E:54:LEU:HD23	2:E:57:MET:HE2	1.88	0.55
1:C:204:CYS:HB3	1:C:452:PHE:CD2	2.40	0.55
1:C:212:TRP:CZ2	1:C:477:LEU:HB3	2.41	0.55
1:D:394:GLU:OE2	1:D:416:TYR:HE1	1.90	0.55
1:A:95:ARG:NH2	1:A:150:GLU:OE2	2.34	0.55
3:B:1801:B12:N40	3:B:1801:B12:H8	2.21	0.55
1:C:79:THR:HG21	1:C:106:MET:CE	2.36	0.55
1:B:269:PRO:HD2	1:B:280:ASP:OD1	2.07	0.55
3:B:1801:B12:H421	3:B:1801:B12:C10	2.35	0.55
3:C:1801:B12:C49	3:C:1801:B12:C47	2.75	0.55
1:A:438:PHE:CE2	2:E:77:MET:HG3	2.41	0.55
2:F:57:MET:HE1	2:F:82:GLY:HA2	1.89	0.55
1:C:267:VAL:CG2	1:C:299:GLN:HB3	2.37	0.55
1:D:613:VAL:HG13	1:D:649:VAL:HG22	1.88	0.55
1:A:82:ILE:HG22	1:A:82:ILE:O	2.06	0.55
1:B:138:ARG:HE	1:B:176:GLU:CD	2.10	0.55
1:B:286:ALA:HB2	1:B:381:VAL:HG13	1.89	0.55
1:B:541:ILE:O	1:B:545:LYS:HG2	2.07	0.55
1:C:286:ALA:HB2	1:C:381:VAL:HG13	1.86	0.55
1:A:115:HIS:HB2	1:C:620:VAL:HG22	1.89	0.55
3:A:1801:B12:H363	3:A:1801:B12:C42	2.35	0.55
1:B:449:THR:HG22	1:B:450:ALA:H	1.70	0.55
1:C:289:GLU:OE2	1:C:373:ARG:NH2	2.40	0.55
1:D:631:GLY:O	1:D:725:GLY:HA3	2.06	0.55
1:A:448:VAL:HB	2:E:56:ARG:HD2	1.88	0.55
1:C:626:ILE:HD13	1:C:640:VAL:HG11	1.87	0.55
1:A:573:ARG:HB3	1:A:573:ARG:CZ	2.36	0.55
3:A:1801:B12:H362	3:A:1801:B12:C35	2.37	0.55
2:F:95:SER:OG	2:F:98:GLU:HG2	2.07	0.55
3:C:1801:B12:H422	3:C:1801:B12:H10	1.89	0.55
1:A:525:LEU:HD23	1:A:570:LEU:HD13	1.89	0.55
3:A:1801:B12:H351	3:A:1801:B12:H372	1.88	0.55
1:D:205:GLU:O	1:D:209:ILE:HD12	2.07	0.55
1:B:478:GLU:C	1:B:480:PRO:HD3	2.26	0.54
1:C:171:VAL:HG23	1:C:209:ILE:HD12	1.89	0.54
1:D:683:ILE:O	1:D:698:ILE:HD13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:GLU:C	1:B:551:GLU:HG3	2.26	0.54
1:C:240:GLU:OE2	1:C:244:GLN:NE2	2.40	0.54
1:A:628:ILE:HG12	1:A:628:ILE:O	2.05	0.54
1:D:441:ASP:HB2	2:H:78:GLY:O	2.07	0.54
1:A:25:TYR:OH	1:A:145:ASP:OD2	2.21	0.54
1:A:674:ASP:O	1:A:678:LYS:HG3	2.08	0.54
1:B:115:HIS:CE1	1:D:623:ARG:HD3	2.41	0.54
1:C:197:ILE:O	1:C:201:ILE:HG13	2.06	0.54
2:G:74:ARG:CB	2:G:76:LEU:HD22	2.37	0.54
1:A:604:THR:HB	1:A:736:ARG:HH12	1.72	0.54
1:D:119:LEU:HD12	2:H:61:SER:HB3	1.90	0.54
1:B:207:LYS:NZ	1:B:217:GLN:HE22	2.06	0.54
1:D:449:THR:HG22	1:D:450:ALA:N	2.23	0.54
1:C:651:LYS:HZ3	1:C:651:LYS:HB2	1.73	0.54
1:D:394:GLU:OE1	1:D:419:ARG:NH2	2.38	0.54
1:A:5:LEU:O	1:A:6:GLN:CB	2.56	0.53
1:A:369:VAL:HG13	1:C:369:VAL:CG1	2.38	0.53
1:A:406:GLU:OE2	1:A:428:ILE:HG22	2.08	0.53
1:B:444:TYR:HA	2:F:79:LYS:O	2.07	0.53
1:D:591:ILE:O	1:D:591:ILE:HG22	2.08	0.53
2:H:20:GLU:CD	2:H:20:GLU:N	2.59	0.53
1:A:130:VAL:HG12	1:A:131:PRO:O	2.08	0.53
2:E:107:LYS:O	2:E:108:TYR:HB2	2.07	0.53
1:B:246:ALA:O	1:B:250:ILE:HG22	2.08	0.53
1:D:394:GLU:OE2	1:D:416:TYR:CE1	2.61	0.53
1:C:608:ILE:HG13	1:C:663:ALA:HB3	1.90	0.53
1:A:109:ARG:HG2	1:A:132:ILE:HG13	1.88	0.53
1:B:108:ILE:HA	1:B:160:TYR:HE2	1.73	0.53
1:C:377:LEU:O	1:C:381:VAL:HG23	2.08	0.53
3:C:1801:B12:H531	3:C:1801:B12:H543	1.90	0.53
1:D:25:TYR:OH	1:D:145:ASP:OD2	2.26	0.53
1:D:684:HIS:CD2	1:D:714:GLY:HA3	2.44	0.53
2:F:67:ILE:CG1	2:F:104:SER:HB3	2.38	0.53
1:A:186:GLN:HG2	1:A:401:TYR:OH	2.08	0.53
1:A:524:LEU:CD1	1:A:555:ILE:HD11	2.38	0.53
1:B:391:PHE:HA	1:B:416:TYR:CZ	2.44	0.53
1:C:436:THR:O	2:G:47:PRO:HD3	2.09	0.53
1:A:116:TYR:CE1	1:C:620:VAL:HG21	2.43	0.53
4:B:1802:PLP:N1	1:D:162:SER:OG	2.37	0.53
1:C:676:HIS:O	1:C:680:MET:HG3	2.08	0.53
1:D:628:ILE:HG12	1:D:628:ILE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLY:HA2	1:A:129:GLY:O	2.09	0.53
1:A:528:PHE:HE1	1:A:560:MET:HG3	1.73	0.53
1:C:302:THR:HG22	1:C:334:ILE:HG13	1.91	0.53
1:A:577:SER:O	1:A:578:ILE:HD12	2.09	0.53
3:C:1801:B12:H353	3:C:1801:B12:C31	2.39	0.53
1:D:79:THR:HB	1:D:332:SER:HA	1.90	0.53
1:D:264:LEU:HD21	1:D:291:PHE:CD1	2.43	0.53
1:D:512:LYS:HB2	1:D:513:PRO:HD2	1.91	0.53
1:C:168:ASP:OD2	1:C:168:ASP:N	2.41	0.52
3:B:1801:B12:H261	5:D:1500:5AD:H5'2	1.90	0.52
2:E:18:SER:HB2	2:E:20:GLU:OE1	2.09	0.52
4:B:1802:PLP:H2A2	1:D:182:HIS:HB3	1.90	0.52
1:C:61:LEU:HD13	1:C:357:GLN:HG3	1.91	0.52
1:C:391:PHE:HD1	1:C:416:TYR:CG	2.27	0.52
1:C:578:ILE:CG2	1:C:579:ASP:N	2.72	0.52
2:G:25:ARG:HG2	2:G:29:MET:HE1	1.92	0.52
1:D:228:ASN:N	1:D:228:ASN:OD1	2.42	0.52
1:A:126:GLY:HA3	1:A:131:PRO:HD3	1.91	0.52
1:A:693:ARG:O	1:A:693:ARG:HG3	2.10	0.52
1:A:161:VAL:HG12	1:A:183:GLN:HG2	1.91	0.52
1:A:284:ALA:O	1:A:288:ARG:HD2	2.08	0.52
1:B:479:VAL:HG12	1:B:482:LYS:HG3	1.92	0.52
1:B:642:TYR:C	1:B:643:LEU:HD23	2.30	0.52
1:B:250:ILE:HD11	2:F:31:GLU:HG2	1.90	0.52
1:B:568:ILE:HG22	1:B:570:LEU:CD1	2.39	0.52
1:D:14:ASP:O	1:D:18:ILE:HG13	2.10	0.52
1:A:650:GLU:HG3	1:A:686:LEU:HD21	1.90	0.52
1:B:445:MET:HE1	1:B:447:PRO:HB3	1.90	0.52
1:A:626:ILE:HD13	1:A:640:VAL:HG11	1.92	0.52
3:A:1801:B12:H531	3:A:1801:B12:H543	1.92	0.52
1:B:445:MET:O	2:F:83:HIS:HB2	2.10	0.52
2:G:35:ASP:N	2:G:36:PRO:HD2	2.25	0.52
1:C:109:ARG:HG2	1:C:132:ILE:HG13	1.91	0.52
2:G:25:ARG:HG2	2:G:29:MET:HE2	1.92	0.52
1:D:406:GLU:HG2	1:D:426:ARG:O	2.10	0.52
1:B:378:GLY:O	1:B:381:VAL:HB	2.09	0.52
1:C:719:PHE:CD2	3:C:1801:B12:HM63	2.45	0.52
1:B:258:LYS:HB2	1:B:261:ASN:HD22	1.75	0.51
3:A:1801:B12:H601	3:A:1801:B12:C26	2.34	0.51
2:F:109:TRP:O	2:F:113:ILE:HG13	2.10	0.51
1:C:438:PHE:CD2	2:G:77:MET:HG3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:MET:HE2	1:D:447:PRO:N	2.24	0.51
1:B:620:VAL:HG21	1:D:116:TYR:HE1	1.75	0.51
1:D:456:ASN:ND2	1:D:459:GLN:HG2	2.25	0.51
1:B:111:ALA:HB2	1:B:127:ILE:HG22	1.92	0.51
3:B:1801:B12:H531	3:B:1801:B12:C55	2.33	0.51
1:D:321:LEU:HD13	1:D:362:MET:HE2	1.93	0.51
1:D:491:GLU:OE2	1:D:491:GLU:CA	2.50	0.51
1:D:592:LEU:HB2	1:D:597:ILE:CD1	2.38	0.51
1:C:13:LEU:HD13	1:C:91:ILE:CG2	2.40	0.51
1:D:264:LEU:HD21	1:D:291:PHE:CE1	2.45	0.51
1:D:510:MET:CE	1:D:577:SER:HB2	2.41	0.51
1:A:424:ILE:HG21	1:A:426:ARG:CZ	2.41	0.51
5:A:1500:5AD:C5'	3:C:1801:B12:C16	2.88	0.51
1:B:445:MET:HE1	1:B:447:PRO:CB	2.41	0.51
1:C:93:ARG:HD3	1:C:348:ASN:OD1	2.09	0.51
1:B:207:LYS:HZ3	1:B:217:GLN:NE2	2.09	0.51
1:C:269:PRO:HD2	1:C:280:ASP:OD2	2.11	0.51
1:C:649:VAL:HG12	1:C:686:LEU:CD1	2.40	0.51
1:D:649:VAL:HG13	1:D:683:ILE:CG1	2.41	0.51
1:A:41:LEU:HD12	1:A:42:GLN:N	2.26	0.51
1:A:122:GLY:HA2	1:A:487:ASP:O	2.11	0.51
1:B:478:GLU:O	1:B:480:PRO:HD3	2.11	0.51
1:C:668:THR:CG2	1:C:668:THR:O	2.59	0.51
1:A:198:ARG:HG3	1:A:198:ARG:NH1	2.26	0.51
1:A:224:ALA:HB3	1:A:245:HIS:CE1	2.46	0.51
1:A:541:ILE:HD11	1:A:554:VAL:HG23	1.91	0.51
1:C:13:LEU:CD2	1:C:18:ILE:HD11	2.41	0.51
2:G:68:VAL:O	2:G:72:MET:HE2	2.11	0.51
1:A:345:HIS:CE1	1:A:516:GLU:HA	2.45	0.51
1:A:613:VAL:CG1	1:A:614:GLY:N	2.73	0.51
1:B:172:MET:CE	1:B:173:PHE:HD1	2.24	0.51
1:B:606:LEU:HD13	1:B:736:ARG:NH2	2.26	0.51
1:B:710:ALA:O	1:B:715:VAL:HG22	2.11	0.51
1:C:13:LEU:HD22	1:C:18:ILE:HD11	1.93	0.51
1:C:706:THR:O	1:C:707:PRO:C	2.48	0.51
1:D:26:THR:HG22	1:D:27:PRO:HD2	1.92	0.51
1:D:568:ILE:HG22	1:D:570:LEU:HD11	1.93	0.51
3:D:1801:B12:H8	3:D:1801:B12:H401	1.75	0.51
1:A:90:ASP:O	1:A:94:MET:HG3	2.11	0.50
3:A:1801:B12:H471	3:A:1801:B12:C49	2.40	0.50
1:C:528:PHE:HE1	1:C:560:MET:HG3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:MET:HE3	1:D:72:PRO:HG3	1.92	0.50
1:D:668:THR:O	1:D:668:THR:CG2	2.59	0.50
1:A:193:ASN:HB2	1:A:426:ARG:CZ	2.42	0.50
1:B:223:GLY:O	1:B:226:ASN:HB2	2.11	0.50
1:B:224:ALA:HB3	1:B:245:HIS:CE1	2.46	0.50
1:B:692:ILE:C	1:B:694:ASP:H	2.15	0.50
2:G:54:LEU:HD23	2:G:57:MET:CE	2.41	0.50
2:E:20:GLU:CD	2:E:20:GLU:N	2.64	0.50
1:B:90:ASP:O	1:B:94:MET:HG3	2.11	0.50
1:B:207:LYS:HZ2	1:B:217:GLN:HE22	1.59	0.50
1:D:201:ILE:HG22	2:H:49:ILE:HD11	1.93	0.50
1:D:238:MET:HE2	1:D:269:PRO:HG2	1.91	0.50
1:A:161:VAL:O	1:A:161:VAL:HG12	2.11	0.50
1:B:132:ILE:HA	1:B:136:GLN:OE1	2.11	0.50
1:D:591:ILE:HD12	1:D:591:ILE:N	2.26	0.50
1:B:8:ARG:NH1	1:B:11:GLU:HG3	2.26	0.50
1:B:692:ILE:O	1:B:694:ASP:N	2.44	0.50
1:D:672:HIS:O	1:D:675:ILE:HG22	2.12	0.50
1:A:123:THR:O	1:A:498:ARG:NH2	2.45	0.50
1:A:461:ASP:CG	1:A:464:LEU:HD13	2.32	0.50
1:B:310:ARG:HD2	1:D:354:THR:OG1	2.11	0.50
1:B:447:PRO:O	1:B:469:SER:HA	2.12	0.50
1:C:233:GLU:HB3	1:C:235:TRP:CH2	2.46	0.50
1:C:479:VAL:CG1	1:C:482:LYS:HG3	2.41	0.50
1:C:527:MET:SD	1:C:529:LEU:HD11	2.52	0.50
1:C:729:ALA:O	1:C:733:VAL:HG13	2.11	0.50
1:C:736:ARG:HG2	1:C:737:ARG:N	2.26	0.50
1:A:608:ILE:CG2	1:A:640:VAL:HG13	2.41	0.50
1:B:467:GLU:N	1:B:468:PRO:HD3	2.26	0.50
1:C:649:VAL:HG13	1:C:683:ILE:HG12	1.94	0.50
1:A:608:ILE:HG22	1:A:640:VAL:HA	1.93	0.50
1:C:406:GLU:HG2	1:C:426:ARG:O	2.12	0.50
1:D:456:ASN:CG	1:D:459:GLN:HG2	2.32	0.50
1:C:117:ASP:HA	1:C:164:VAL:HG23	1.94	0.50
1:D:106:MET:HG3	1:D:158:HIS:CD2	2.47	0.49
1:A:671:SER:HG	3:A:1801:B12:H332	1.56	0.49
1:D:50:ASP:HB2	1:D:363:ASP:OD1	2.12	0.49
1:D:238:MET:HE3	1:D:269:PRO:HG2	1.93	0.49
1:A:467:GLU:N	1:A:468:PRO:HD3	2.27	0.49
1:C:651:LYS:HB2	1:C:651:LYS:NZ	2.27	0.49
2:H:7:PHE:O	2:H:11:ARG:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:GLU:OE2	1:C:111:ALA:HB1	2.12	0.49
3:A:1801:B12:H363	3:A:1801:B12:H421	1.94	0.49
1:B:528:PHE:O	1:B:528:PHE:CD2	2.65	0.49
2:G:113:ILE:O	2:G:113:ILE:CG2	2.60	0.49
1:D:648:PRO:C	1:D:650:GLU:N	2.65	0.49
1:B:608:ILE:HG22	1:B:640:VAL:HG13	1.95	0.49
1:C:16:GLU:O	1:C:20:LYS:HG3	2.12	0.49
1:D:172:MET:HE2	1:D:172:MET:O	2.13	0.49
3:D:1801:B12:C10	3:D:1801:B12:C42	2.91	0.49
1:A:415:TYR:O	1:A:418:GLU:HB3	2.13	0.49
1:A:608:ILE:HG22	1:A:640:VAL:HG13	1.95	0.49
1:A:646:SER:O	1:A:648:PRO:HD3	2.12	0.49
1:B:14:ASP:O	1:B:18:ILE:HG13	2.12	0.49
1:B:277:MET:HE3	1:D:365:LEU:HD11	1.95	0.49
1:D:613:VAL:CG1	1:D:649:VAL:HG22	2.41	0.49
1:D:670:ILE:O	1:D:676:HIS:HB3	2.12	0.49
1:A:685:GLU:HA	1:A:688:VAL:HB	1.94	0.49
3:A:1801:B12:H1P1	1:C:127:ILE:HG13	1.94	0.49
2:F:98:GLU:OE1	2:F:98:GLU:HA	2.11	0.49
1:C:209:ILE:O	1:C:212:TRP:HB3	2.13	0.49
1:A:219:ASP:HB3	1:A:248:ASN:HD22	1.78	0.49
2:E:28:GLU:HB2	1:D:40:ASN:HD21	1.78	0.49
1:B:207:LYS:HE3	1:B:251:PHE:HD2	1.78	0.49
3:B:1801:B12:H362	3:B:1801:B12:C35	2.40	0.49
1:C:376:VAL:HG13	1:C:377:LEU:N	2.28	0.49
3:C:1801:B12:H471	3:C:1801:B12:C49	2.32	0.49
1:D:568:ILE:HG22	1:D:570:LEU:HD12	1.94	0.49
1:A:264:LEU:N	1:A:264:LEU:CD1	2.76	0.48
1:A:396:ILE:CD1	2:E:29:MET:HG2	2.43	0.48
1:B:182:HIS:HB3	4:D:1802:PLP:H2A2	1.94	0.48
1:D:524:LEU:HD12	1:D:570:LEU:O	2.13	0.48
1:C:122:GLY:O	1:C:133:THR:HG21	2.13	0.48
1:C:158:HIS:CD2	1:C:159:SER:N	2.82	0.48
1:A:173:PHE:CD1	1:A:178:VAL:HG21	2.48	0.48
1:B:479:VAL:CG1	1:B:482:LYS:HG3	2.43	0.48
1:C:123:THR:O	1:C:498:ARG:NH2	2.46	0.48
1:C:456:ASN:ND2	1:C:459:GLN:NE2	2.61	0.48
1:A:134:ARG:HG3	1:A:176:GLU:OE2	2.14	0.48
1:A:374:GLU:HG3	1:A:375:GLY:N	2.28	0.48
1:A:550:GLU:CG	1:A:575:PRO:HG3	2.43	0.48
1:B:81:GLU:OE1	1:B:108:ILE:HD11	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:ARG:NH2	1:D:232:ARG:NH2	2.60	0.48
1:C:250:ILE:HD12	1:C:250:ILE:HA	1.75	0.48
1:A:616:ASP:OD1	1:A:669:ILE:HB	2.14	0.48
1:B:668:THR:CG2	1:B:676:HIS:HB2	2.43	0.48
1:D:197:ILE:HD11	1:D:428:ILE:CG1	2.43	0.48
1:A:94:MET:SD	1:A:144:LEU:HD21	2.53	0.48
1:B:55:LEU:HD12	1:B:58:SER:HB3	1.95	0.48
1:C:449:THR:HG22	1:C:450:ALA:N	2.28	0.48
1:C:700:CYS:O	1:C:718:GLY:HA2	2.13	0.48
2:G:74:ARG:HB3	2:G:76:LEU:HD22	1.94	0.48
1:D:45:PRO:HD2	1:D:46:PHE:CD2	2.48	0.48
2:H:74:ARG:HG3	2:H:74:ARG:HH11	1.79	0.48
1:A:135:LYS:HE2	1:A:495:VAL:HG11	1.94	0.48
1:A:441:ASP:OD2	2:E:79:LYS:HE3	2.14	0.48
1:B:21:ASP:OD1	1:B:21:ASP:N	2.46	0.48
1:C:196:MET:SD	1:C:402:PHE:CD1	3.06	0.48
1:A:103:ASP:HB3	1:A:153:ARG:NH1	2.28	0.48
1:A:394:GLU:HG2	1:A:409:PHE:CE2	2.48	0.48
1:A:606:LEU:HD12	1:A:662:ASP:OD2	2.14	0.48
3:B:1801:B12:C10	3:B:1801:B12:C42	2.92	0.48
1:D:601:ILE:HD12	1:D:636:TYR:HB3	1.96	0.48
1:D:656:ALA:HA	1:D:661:ALA:CB	2.43	0.48
3:D:1801:B12:H311	3:D:1801:B12:H353	1.96	0.48
1:A:631:GLY:HA2	1:A:635:LYS:HD3	1.95	0.48
2:E:103:LEU:C	2:E:105:GLU:H	2.17	0.48
1:B:447:PRO:HG2	2:F:57:MET:SD	2.54	0.48
1:C:55:LEU:HD21	1:C:153:ARG:CZ	2.43	0.48
3:C:1801:B12:H362	3:C:1801:B12:C35	2.42	0.48
1:D:213:ALA:HB3	1:D:215:MET:HG3	1.96	0.48
1:D:671:SER:HB2	1:D:676:HIS:CE1	2.49	0.48
1:A:6:GLN:O	1:A:7:LEU:HB2	2.14	0.48
1:B:612:THR:CG2	1:B:616:ASP:HB3	2.44	0.48
2:F:29:MET:O	2:F:33:ILE:HD12	2.13	0.48
1:C:183:GLN:OE1	1:C:207:LYS:HE2	2.13	0.48
1:C:300:MET:HB2	1:C:334:ILE:HG12	1.95	0.48
1:C:438:PHE:CE2	2:G:77:MET:HG3	2.48	0.48
1:D:218:ILE:HG22	1:D:219:ASP:O	2.14	0.48
2:H:108:TYR:O	2:H:111:ASP:HB2	2.14	0.48
1:A:693:ARG:O	1:A:693:ARG:CG	2.63	0.47
1:B:301:ASN:O	1:B:305:MET:HE3	2.14	0.47
1:B:525:LEU:HD12	1:B:526:THR:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:ILE:CD1	1:B:663:ALA:HB3	2.44	0.47
2:F:74:ARG:HE	2:F:109:TRP:CB	2.27	0.47
2:E:66:ALA:O	2:E:70:LYS:HD2	2.14	0.47
1:C:121:GLU:HG3	1:C:486:ILE:HD12	1.97	0.47
1:C:238:MET:HG3	1:C:283:TYR:CD1	2.48	0.47
1:A:180:GLY:HA2	1:A:215:MET:HB3	1.96	0.47
1:A:505:PHE:O	1:A:506:ARG:CB	2.62	0.47
1:A:538:PHE:CD2	1:C:585:ILE:HG23	2.49	0.47
1:A:609:VAL:HG23	1:A:609:VAL:O	2.14	0.47
1:B:311:GLU:CD	1:D:63:SER:HG	2.17	0.47
1:B:597:ILE:HG23	1:B:733:VAL:HG11	1.97	0.47
1:B:665:LEU:HB3	3:B:1801:B12:HM52	1.96	0.47
1:C:460:TYR:O	1:C:461:ASP:HB2	2.14	0.47
1:D:288:ARG:HG3	1:D:288:ARG:NH1	2.20	0.47
1:D:324:LYS:HE2	1:D:362:MET:O	2.14	0.47
1:A:116:TYR:HE1	1:C:620:VAL:HG21	1.80	0.47
1:A:303:LYS:HD3	1:A:304:TYR:CE2	2.49	0.47
1:A:346:ILE:HG13	1:A:347:TYR:N	2.30	0.47
1:B:236:LYS:O	1:B:415:TYR:HD1	1.98	0.47
1:B:313:THR:O	1:B:317:VAL:HG23	2.14	0.47
1:B:424:ILE:HD13	1:B:424:ILE:HA	1.76	0.47
1:A:533:LYS:HG3	1:A:534:ARG:N	2.28	0.47
1:C:618:HIS:NE2	3:C:1801:B12:N22	2.63	0.47
1:A:517:TRP:O	1:A:518:GLN:C	2.51	0.47
1:B:396:ILE:CD1	2:F:29:MET:HB3	2.44	0.47
1:B:531:THR:H	1:B:565:GLY:HA2	1.79	0.47
2:F:86:TYR:CZ	2:F:90:LYS:HD3	2.49	0.47
1:C:396:ILE:HG22	1:C:397:GLU:N	2.30	0.47
1:C:550:GLU:HG3	1:C:575:PRO:HB3	1.96	0.47
1:D:728:VAL:O	1:D:732:LEU:HG	2.14	0.47
1:A:172:MET:O	1:A:176:GLU:HG2	2.14	0.47
1:A:414:GLY:CA	1:A:418:GLU:OE1	2.62	0.47
1:A:645:THR:C	1:A:647:VAL:H	2.18	0.47
1:A:663:ALA:HB1	1:A:697:MET:O	2.15	0.47
1:A:694:ASP:OD1	1:A:694:ASP:N	2.45	0.47
1:B:250:ILE:HD11	2:F:31:GLU:CG	2.44	0.47
1:B:277:MET:SD	1:B:322:ILE:HD11	2.55	0.47
1:B:307:ALA:HB3	1:B:556:ASN:OD1	2.14	0.47
1:B:386:GLU:O	1:B:390:LEU:HG	2.14	0.47
1:C:8:ARG:O	1:C:10:ASN:N	2.48	0.47
1:C:8:ARG:HH11	1:C:11:GLU:HG3	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:TRP:CD1	1:C:515:VAL:HB	2.47	0.47
1:C:574:VAL:HG12	1:C:574:VAL:O	2.13	0.47
1:C:618:HIS:CE1	3:C:1801:B12:N22	2.83	0.47
1:D:394:GLU:CD	1:D:419:ARG:HH22	2.17	0.47
1:D:693:ARG:HG3	1:D:693:ARG:O	2.14	0.47
1:A:505:PHE:N	1:A:505:PHE:CD1	2.83	0.47
1:A:583:LEU:HD11	1:C:539:ALA:HA	1.96	0.47
1:A:650:GLU:HG3	1:A:686:LEU:HD11	1.95	0.47
1:A:654:ASP:O	1:A:658:GLU:N	2.43	0.47
1:C:224:ALA:HB3	1:C:245:HIS:CE1	2.50	0.47
1:A:268:PRO:HA	1:A:269:PRO:HD3	1.62	0.47
1:A:416:TYR:CD2	1:A:417:PRO:HA	2.50	0.47
1:A:620:VAL:HG23	3:A:1801:B12:O51	2.15	0.47
1:B:115:HIS:HB3	1:D:623:ARG:HH11	1.80	0.47
1:C:231:ALA:O	1:C:303:LYS:HE2	2.15	0.47
1:C:254:LYS:HE2	2:G:31:GLU:HG3	1.96	0.47
1:C:416:TYR:HA	1:C:417:PRO:C	2.35	0.47
3:D:1801:B12:H351	3:D:1801:B12:H372	1.96	0.47
1:B:311:GLU:OE2	1:D:63:SER:OG	2.32	0.47
1:C:607:LYS:C	1:C:608:ILE:HD12	2.35	0.47
1:D:288:ARG:HD2	1:D:326:THR:HB	1.96	0.47
1:D:734:LYS:C	1:D:736:ARG:H	2.19	0.47
1:A:158:HIS:HE2	1:A:182:HIS:CE1	2.32	0.46
1:A:505:PHE:O	1:A:506:ARG:HD3	2.15	0.46
2:E:38:LEU:O	2:E:42:LYS:HG3	2.15	0.46
1:B:65:LYS:HD3	1:D:306:GLU:OE2	2.15	0.46
1:B:106:MET:HE3	1:B:106:MET:HB2	1.85	0.46
1:B:224:ALA:CB	1:B:245:HIS:CE1	2.99	0.46
3:B:1801:B12:H473	3:B:1801:B12:H481	1.11	0.46
1:C:342:VAL:HG12	1:C:343:PRO:HD2	1.97	0.46
1:D:85:GLY:HA2	1:D:129:GLY:O	2.15	0.46
1:D:556:ASN:HB3	1:D:569:GLU:HB2	1.98	0.46
1:A:10:ASN:OD1	1:A:10:ASN:N	2.48	0.46
1:A:447:PRO:HG2	2:E:57:MET:SD	2.55	0.46
1:B:212:TRP:CE3	1:B:477:LEU:HD13	2.51	0.46
1:B:578:ILE:HD13	1:D:543:PHE:CD1	2.50	0.46
1:C:88:GLU:HG2	1:C:89:ASP:N	2.30	0.46
1:C:320:LEU:HD13	1:C:358:ALA:HB3	1.97	0.46
2:G:76:LEU:HD23	2:G:109:TRP:HZ3	1.79	0.46
2:H:52:SER:OG	2:H:56:ARG:NH2	2.48	0.46
1:A:178:VAL:HG12	1:A:215:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:GLU:HG3	1:A:554:VAL:HG21	1.96	0.46
1:B:122:GLY:O	1:B:133:THR:HG21	2.15	0.46
1:B:157:TYR:CD2	1:B:178:VAL:HG22	2.50	0.46
1:B:172:MET:C	1:B:172:MET:CE	2.83	0.46
2:F:69:ASP:HA	2:F:72:MET:CE	2.44	0.46
1:C:668:THR:HG23	1:C:668:THR:O	2.16	0.46
1:D:611:ALA:CB	1:D:643:LEU:HB2	2.38	0.46
1:D:685:GLU:C	1:D:687:ALA:H	2.18	0.46
1:A:541:ILE:O	1:A:545:LYS:HG2	2.16	0.46
1:B:116:TYR:CD2	1:B:120:ILE:HD13	2.49	0.46
1:B:578:ILE:O	1:B:578:ILE:HG22	2.15	0.46
3:B:1801:B12:H2B	3:B:1801:B12:O2	2.14	0.46
1:C:163:GLY:O	1:C:165:ALA:N	2.49	0.46
1:D:153:ARG:HG2	1:D:154:PRO:HD2	1.97	0.46
1:A:274:ALA:O	1:A:276:SER:N	2.49	0.46
1:B:96:MET:SD	1:D:560:MET:HB3	2.56	0.46
1:B:321:LEU:HD21	1:D:321:LEU:HD13	1.97	0.46
1:B:449:THR:O	2:F:56:ARG:NH1	2.48	0.46
1:D:109:ARG:HG2	1:D:132:ILE:HD13	1.96	0.46
1:D:666:ALA:HB3	1:D:700:CYS:SG	2.56	0.46
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.80	0.46
1:A:687:ALA:C	1:A:693:ARG:HB2	2.36	0.46
2:E:113:ILE:O	2:E:113:ILE:HG22	2.16	0.46
1:C:382:ARG:NE	1:C:386:GLU:OE2	2.48	0.46
1:A:79:THR:HG21	1:A:106:MET:HE3	1.97	0.46
1:A:697:MET:HG2	1:A:735:LYS:HG2	1.97	0.46
1:B:157:TYR:HD2	1:B:178:VAL:HG22	1.79	0.46
1:A:8:ARG:NH1	1:A:11:GLU:OE2	2.49	0.46
1:A:542:GLU:O	1:A:546:LYS:HG2	2.16	0.46
1:B:8:ARG:HB2	1:B:11:GLU:HB2	1.97	0.46
1:D:549:LEU:HD13	1:D:572:GLY:HA3	1.97	0.46
1:A:84:SER:HB2	1:A:516:GLU:OE1	2.16	0.46
1:A:542:GLU:O	1:A:545:LYS:HB2	2.16	0.46
1:A:631:GLY:HA2	1:A:635:LYS:CD	2.46	0.46
1:B:13:LEU:HD13	1:B:91:ILE:HG22	1.98	0.46
1:C:237:VAL:O	1:C:237:VAL:HG13	2.15	0.46
1:C:529:LEU:HA	1:C:530:PRO:HD3	1.68	0.46
1:D:541:ILE:CD1	1:D:554:VAL:HG23	2.45	0.46
1:A:178:VAL:HG12	1:A:215:MET:CE	2.46	0.46
1:B:160:TYR:CD1	1:B:182:HIS:HB2	2.51	0.46
1:C:543:PHE:O	1:C:547:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:GLN:O	1:D:136:GLN:HG2	2.15	0.46
1:A:730:THR:CG2	1:A:734:LYS:HD2	2.46	0.45
2:E:81:ALA:O	2:E:85:VAL:HG23	2.15	0.45
1:B:277:MET:HE3	1:D:365:LEU:CD1	2.46	0.45
1:B:610:ALA:HB1	1:B:622:LEU:HD21	1.97	0.45
1:B:684:HIS:O	1:B:688:VAL:HB	2.16	0.45
2:F:25:ARG:O	2:F:29:MET:HG3	2.16	0.45
1:C:276:SER:O	1:C:280:ASP:OD1	2.33	0.45
1:C:668:THR:HG23	1:C:676:HIS:CB	2.42	0.45
1:D:268:PRO:HA	1:D:269:PRO:HD3	1.64	0.45
1:B:224:ALA:C	1:B:226:ASN:H	2.20	0.45
2:F:106:GLY:O	2:F:109:TRP:HD1	1.99	0.45
1:C:592:LEU:HB2	1:C:597:ILE:HD11	1.98	0.45
1:D:99:TRP:NE1	1:D:150:GLU:OE1	2.48	0.45
1:A:472:ILE:O	1:A:473:ASP:HB2	2.16	0.45
1:A:709:VAL:HA	1:A:712:LYS:HE2	1.99	0.45
1:B:340:ARG:NH2	1:B:347:TYR:CE2	2.85	0.45
1:B:606:LEU:HD12	1:B:606:LEU:HA	1.74	0.45
1:B:608:ILE:HD11	1:B:663:ALA:HB3	1.98	0.45
1:C:417:PRO:O	1:C:418:GLU:C	2.54	0.45
1:C:432:ILE:N	1:C:432:ILE:CD1	2.79	0.45
1:D:288:ARG:CG	1:D:288:ARG:NH1	2.77	0.45
1:D:546:LYS:HD2	1:D:546:LYS:HA	1.82	0.45
1:D:614:GLY:O	1:D:646:SER:HA	2.16	0.45
1:A:580:ILE:HG22	1:A:580:ILE:O	2.16	0.45
1:A:628:ILE:O	1:A:629:LYS:C	2.54	0.45
2:E:74:ARG:O	2:E:75:GLY:C	2.52	0.45
1:B:95:ARG:HA	1:B:147:ILE:HD13	1.98	0.45
1:B:629:LYS:HE3	1:D:226:ASN:OD1	2.15	0.45
1:C:619:SER:HB3	1:C:645:THR:HG21	1.99	0.45
2:G:76:LEU:HD23	2:G:109:TRP:CZ3	2.52	0.45
1:D:79:THR:HG21	1:D:106:MET:CE	2.47	0.45
1:D:224:ALA:C	1:D:226:ASN:N	2.69	0.45
3:D:1801:B12:O7R	3:D:1801:B12:C2B	2.64	0.45
1:A:233:GLU:HB3	1:A:235:TRP:CZ2	2.50	0.45
1:B:26:THR:O	1:B:27:PRO:C	2.55	0.45
1:B:610:ALA:HA	1:B:665:LEU:O	2.16	0.45
1:D:13:LEU:HD22	1:D:18:ILE:HD11	1.97	0.45
1:D:307:ALA:HB3	1:D:556:ASN:OD1	2.16	0.45
1:D:694:ASP:CG	1:D:695:LYS:HE2	2.37	0.45
1:A:528:PHE:CZ	1:A:565:GLY:HA3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:HA	1:B:104:HIS:HB3	1.98	0.45
1:A:161:VAL:CG1	1:A:183:GLN:HG2	2.47	0.45
1:B:273:PRO:HD2	1:D:67:PHE:CD2	2.52	0.45
1:B:693:ARG:O	1:B:693:ARG:CG	2.64	0.45
3:B:1801:B12:O28	3:B:1801:B12:H3	2.17	0.45
1:C:512:LYS:HB2	1:C:513:PRO:HD2	1.99	0.45
1:D:104:HIS:HE2	1:D:158:HIS:CB	2.29	0.45
1:D:107:VAL:HG12	1:D:107:VAL:O	2.15	0.45
1:D:335:THR:HB	1:D:337:ASP:OD1	2.17	0.45
3:A:1801:B12:C30	3:A:1801:B12:H203	2.46	0.45
1:B:277:MET:HE1	1:B:321:LEU:CD2	2.47	0.45
1:B:337:ASP:HB3	1:B:347:TYR:CD2	2.51	0.45
1:C:183:GLN:O	1:C:217:GLN:NE2	2.49	0.45
1:C:185:PRO:O	1:C:188:ASN:HB2	2.16	0.45
1:C:264:LEU:HD21	1:C:291:PHE:CE1	2.50	0.45
1:D:184:ASP:HA	1:D:185:PRO:HD2	1.81	0.45
1:D:196:MET:SD	1:D:402:PHE:CD1	3.09	0.45
1:D:411:VAL:HB	1:D:424:ILE:HG12	1.98	0.45
1:D:540:ALA:CB	1:D:568:ILE:HG21	2.47	0.45
1:A:373:ARG:HG3	1:A:373:ARG:NH1	2.31	0.45
1:B:241:LEU:HA	1:B:241:LEU:HD23	1.73	0.45
1:C:335:THR:HB	1:C:337:ASP:OD1	2.16	0.45
2:G:54:LEU:HD23	2:G:57:MET:HE3	1.97	0.45
2:H:106:GLY:O	2:H:109:TRP:HD1	2.00	0.45
2:E:55:LEU:HD23	2:E:59:PHE:O	2.17	0.45
2:E:70:LYS:O	2:E:73:ASP:N	2.50	0.45
2:E:112:ALA:O	2:E:114:GLN:N	2.50	0.45
1:B:277:MET:HE1	1:B:321:LEU:HD23	1.98	0.45
1:A:19:LEU:HD12	1:A:499:MET:HE3	1.99	0.44
1:A:57:ASN:O	1:A:58:SER:HB3	2.15	0.44
1:B:87:PHE:O	1:B:91:ILE:HG13	2.17	0.44
2:F:91:GLU:O	2:F:92:LYS:HD3	2.17	0.44
1:C:514:GLU:OE2	1:C:518:GLN:HA	2.17	0.44
2:G:113:ILE:O	2:G:113:ILE:HG22	2.17	0.44
1:D:227:ALA:HB3	1:D:241:LEU:CD2	2.46	0.44
1:D:678:LYS:CB	1:D:682:ARG:HH21	2.30	0.44
1:A:172:MET:CE	1:A:176:GLU:HG3	2.45	0.44
1:A:631:GLY:O	1:A:725:GLY:HA3	2.16	0.44
1:B:212:TRP:CD2	1:B:477:LEU:HD13	2.52	0.44
1:B:441:ASP:OD2	2:F:79:LYS:HE3	2.17	0.44
1:C:14:ASP:CG	1:C:17:ASN:HB2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ALA:HB3	1:C:556:ASN:OD1	2.17	0.44
1:C:541:ILE:HG22	1:C:545:LYS:HZ1	1.81	0.44
1:C:545:LYS:O	1:C:548:ASN:N	2.50	0.44
1:D:224:ALA:C	1:D:226:ASN:H	2.20	0.44
1:A:13:LEU:HD13	1:A:91:ILE:HG22	1.98	0.44
1:B:14:ASP:OD1	1:B:16:GLU:HB3	2.17	0.44
1:B:467:GLU:O	1:B:469:SER:N	2.51	0.44
1:C:20:LYS:O	1:C:21:ASP:HB2	2.17	0.44
1:C:462:GLU:C	1:C:464:LEU:H	2.21	0.44
1:D:512:LYS:HB2	1:D:513:PRO:CD	2.47	0.44
1:B:624:GLU:OE2	1:B:624:GLU:HA	2.18	0.44
3:B:1801:B12:H471	3:B:1801:B12:C49	2.35	0.44
2:F:13:HIS:CD2	2:F:14:LEU:HG	2.52	0.44
1:C:683:ILE:HG22	1:C:698:ILE:HD13	1.99	0.44
3:C:1801:B12:H353	3:C:1801:B12:H312	2.00	0.44
1:D:598:ARG:O	1:D:602:GLU:CB	2.66	0.44
3:A:1801:B12:N23	5:C:1500:5AD:C4'	2.80	0.44
1:C:263:CYS:SG	1:C:295:ARG:HB2	2.57	0.44
1:C:492:ASN:HD22	1:C:492:ASN:HA	1.63	0.44
1:D:692:ILE:HD12	1:D:696:ILE:HD12	1.99	0.44
3:D:1801:B12:H253	3:D:1801:B12:H301	1.63	0.44
2:H:32:LYS:HE2	2:H:32:LYS:HB3	1.79	0.44
2:H:72:MET:HG2	2:H:77:MET:HG3	1.99	0.44
1:A:15:VAL:HG22	1:A:15:VAL:O	2.17	0.44
1:A:337:ASP:OD2	1:A:347:TYR:CD2	2.71	0.44
1:B:672:HIS:O	1:B:673:ASP:HB3	2.18	0.44
1:C:196:MET:HE2	1:C:405:VAL:HG11	2.00	0.44
2:G:10:ARG:HE	2:G:10:ARG:HB3	1.56	0.44
1:D:88:GLU:OE1	1:D:498:ARG:NH1	2.50	0.44
1:D:578:ILE:HD13	1:D:578:ILE:HA	1.66	0.44
3:D:1801:B12:H351	3:D:1801:B12:C36	2.33	0.44
1:A:488:GLU:O	1:A:489:LEU:HD23	2.17	0.44
2:E:25:ARG:HG2	2:E:29:MET:HE1	1.98	0.44
1:B:521:GLY:O	1:B:573:ARG:HA	2.17	0.44
2:F:18:SER:OG	2:F:21:GLU:HG3	2.17	0.44
1:C:81:GLU:O	1:C:82:ILE:HG13	2.18	0.44
1:C:486:ILE:HD13	2:G:62:LEU:HD12	1.99	0.44
1:C:693:ARG:O	1:C:693:ARG:NH1	2.50	0.44
1:D:284:ALA:O	1:D:288:ARG:HG3	2.18	0.44
1:A:22:LEU:HA	1:A:22:LEU:HD23	1.63	0.44
1:A:53:THR:HA	1:A:54:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:CG2	1:A:135:LYS:HD3	2.40	0.44
1:C:109:ARG:NH2	1:C:162:SER:HB2	2.33	0.44
1:C:335:THR:HG22	1:C:348:ASN:HD22	1.80	0.44
1:C:406:GLU:OE2	1:C:428:ILE:HG22	2.17	0.44
1:C:459:GLN:O	1:C:459:GLN:HG3	2.18	0.44
1:C:467:GLU:N	1:C:468:PRO:HD3	2.32	0.44
1:D:250:ILE:HG23	2:H:34:VAL:HG21	1.99	0.44
1:D:346:ILE:O	1:D:350:GLU:HG3	2.18	0.44
1:D:373:ARG:HA	1:D:377:LEU:HD23	2.00	0.44
2:H:9:GLN:HG2	2:H:10:ARG:N	2.32	0.44
1:C:346:ILE:HG13	1:C:347:TYR:N	2.33	0.44
1:C:666:ALA:O	1:C:700:CYS:HA	2.17	0.44
2:G:101:LEU:HD12	2:G:101:LEU:HA	1.86	0.44
1:D:444:TYR:HA	2:H:79:LYS:O	2.17	0.44
1:D:689:GLU:O	1:D:689:GLU:HG2	2.17	0.44
2:H:76:LEU:HG	2:H:84:ILE:HD11	1.99	0.44
1:A:446:ALA:HA	1:A:447:PRO:HD3	1.82	0.43
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.63	0.43
1:C:394:GLU:CG	1:C:409:PHE:CE2	3.01	0.43
1:C:671:SER:OG	1:C:704:GLN:HG3	2.18	0.43
3:C:1801:B12:H601	3:C:1801:B12:H252	2.00	0.43
2:G:54:LEU:HA	2:G:57:MET:HE3	2.01	0.43
1:D:8:ARG:NH1	1:D:8:ARG:CB	2.73	0.43
1:D:264:LEU:N	1:D:264:LEU:HD12	2.32	0.43
1:D:525:LEU:HD21	1:D:547:MET:HE3	2.00	0.43
1:A:475:CYS:HB2	2:E:56:ARG:O	2.18	0.43
2:E:92:LYS:HD3	2:E:92:LYS:N	2.32	0.43
1:B:162:SER:OG	4:D:1802:PLP:N1	2.43	0.43
1:B:568:ILE:HG22	1:B:570:LEU:HD12	1.99	0.43
1:C:8:ARG:NH1	1:C:10:ASN:OD1	2.51	0.43
1:C:250:ILE:CG2	2:G:34:VAL:HG21	2.48	0.43
1:C:345:HIS:CE1	1:C:516:GLU:O	2.70	0.43
1:C:392:MET:O	1:C:395:ILE:HB	2.18	0.43
1:C:659:LEU:O	1:C:660:LYS:C	2.56	0.43
3:C:1801:B12:H561	3:C:1801:B12:H18	1.73	0.43
1:D:612:THR:HB	1:D:645:THR:HA	2.00	0.43
1:D:656:ALA:HA	1:D:661:ALA:HB3	2.00	0.43
1:A:241:LEU:HA	1:A:241:LEU:HD23	1.63	0.43
1:A:461:ASP:O	1:A:462:GLU:C	2.56	0.43
1:B:541:ILE:CD1	1:B:552:VAL:HG12	2.47	0.43
1:C:264:LEU:HD13	1:C:296:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:GLU:CG	1:C:517:TRP:N	2.81	0.43
1:C:633:ILE:CD1	1:C:638:VAL:HG11	2.47	0.43
1:D:608:ILE:HG13	1:D:663:ALA:HB3	1.99	0.43
1:A:63:SER:HB2	1:C:311:GLU:OE2	2.18	0.43
1:A:160:TYR:N	1:A:160:TYR:CD2	2.87	0.43
1:A:386:GLU:HG3	2:E:22:LEU:HD21	1.99	0.43
2:E:51:ARG:HG2	2:E:68:VAL:HG21	2.01	0.43
1:B:534:ARG:NH1	1:B:534:ARG:CG	2.80	0.43
2:F:54:LEU:HD23	2:F:57:MET:HE1	1.99	0.43
1:C:456:ASN:CG	1:C:459:GLN:HE21	2.21	0.43
1:D:626:ILE:O	1:D:634:GLU:HB2	2.18	0.43
1:D:683:ILE:O	1:D:683:ILE:HG22	2.18	0.43
1:A:391:PHE:HD1	1:A:416:TYR:CG	2.36	0.43
1:B:108:ILE:HA	1:B:160:TYR:CE2	2.53	0.43
1:B:116:TYR:CE1	3:D:1801:B12:H491	2.54	0.43
1:B:547:MET:HB3	1:D:547:MET:HB3	2.00	0.43
1:C:79:THR:HA	1:C:104:HIS:HB3	1.99	0.43
1:C:189:VAL:HG22	1:C:196:MET:HA	2.00	0.43
1:C:348:ASN:HD22	1:C:348:ASN:HA	1.66	0.43
1:C:516:GLU:HG2	1:C:517:TRP:H	1.82	0.43
2:E:63:GLU:OE1	2:E:101:LEU:HD11	2.18	0.43
1:B:688:VAL:HG23	1:B:693:ARG:HG2	2.01	0.43
3:B:1801:B12:O7R	3:B:1801:B12:C2B	2.65	0.43
1:C:17:ASN:O	1:C:20:LYS:HB2	2.19	0.43
1:D:255:VAL:HG23	2:H:38:LEU:HD21	2.00	0.43
1:D:612:THR:CG2	1:D:616:ASP:HB3	2.49	0.43
1:A:539:ALA:HB2	1:C:583:LEU:HD11	2.01	0.43
1:A:657:ILE:CD1	1:A:690:LYS:HD2	2.49	0.43
2:E:25:ARG:O	2:E:29:MET:HE2	2.19	0.43
1:B:643:LEU:HD23	1:B:643:LEU:N	2.33	0.43
1:D:464:LEU:HA	1:D:464:LEU:HD12	1.68	0.43
1:A:134:ARG:HD3	1:A:138:ARG:HH21	1.83	0.43
1:A:232:ARG:HD3	1:A:232:ARG:HA	1.75	0.43
1:A:381:VAL:HG12	1:A:385:LYS:HE3	2.01	0.43
1:B:115:HIS:HB3	1:D:623:ARG:NH1	2.34	0.43
1:B:277:MET:O	1:B:281:LEU:HB2	2.19	0.43
1:B:489:LEU:HD23	1:B:489:LEU:HA	1.83	0.43
1:C:653:VAL:HG21	1:C:686:LEU:HB3	1.99	0.43
3:C:1801:B12:N40	3:C:1801:B12:C8	2.77	0.43
1:D:613:VAL:HG11	1:D:683:ILE:HD11	2.01	0.43
1:A:416:TYR:CD1	1:A:417:PRO:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:MET:SD	1:B:402:PHE:CD1	3.11	0.43
1:B:369:VAL:HG13	1:D:369:VAL:HG13	2.00	0.43
1:B:561:GLN:O	1:B:562:GLU:C	2.57	0.43
1:C:340:ARG:O	1:C:341:ASN:HB3	2.18	0.43
1:C:464:LEU:HG	1:C:470:LYS:HB2	2.01	0.43
1:C:668:THR:HG21	1:C:676:HIS:HB2	2.00	0.43
1:D:186:GLN:OE1	1:D:244:GLN:HG2	2.18	0.43
1:A:547:MET:O	1:A:548:ASN:CB	2.67	0.43
1:A:682:ARG:O	1:A:686:LEU:CB	2.65	0.43
1:C:93:ARG:NH1	1:C:348:ASN:OD1	2.52	0.43
1:C:471:LEU:HD12	1:C:471:LEU:HA	1.67	0.43
1:D:657:ILE:C	1:D:659:LEU:H	2.22	0.43
1:A:13:LEU:HD13	1:A:91:ILE:CG2	2.49	0.42
1:A:561:GLN:O	1:A:562:GLU:C	2.57	0.42
1:B:6:GLN:CG	1:B:7:LEU:H	2.30	0.42
1:B:100:HIS:CD2	1:B:349:ILE:HG13	2.54	0.42
1:B:570:LEU:HD12	1:B:570:LEU:N	2.34	0.42
1:B:593:SER:O	1:B:596:GLU:N	2.52	0.42
2:G:81:ALA:O	2:G:85:VAL:HG23	2.18	0.42
1:D:253:LEU:HD12	1:D:253:LEU:HA	1.86	0.42
1:A:321:LEU:HD13	1:A:362:MET:HE1	2.01	0.42
1:A:618:HIS:CD2	3:A:1801:B12:N24	2.87	0.42
1:B:522:THR:HA	1:B:572:GLY:O	2.19	0.42
1:B:619:SER:HB3	1:B:645:THR:CG2	2.48	0.42
1:C:271:ALA:O	1:C:274:ALA:HB3	2.19	0.42
1:C:360:ILE:HD13	1:C:360:ILE:HA	1.69	0.42
1:C:394:GLU:HG3	1:C:409:PHE:CE2	2.54	0.42
1:D:662:ASP:O	1:D:696:ILE:HA	2.19	0.42
1:A:13:LEU:O	1:A:15:VAL:N	2.52	0.42
1:A:87:PHE:CD1	1:A:87:PHE:C	2.92	0.42
2:E:100:GLY:C	2:E:102:ALA:N	2.73	0.42
1:B:43:MET:HE1	1:B:72:PRO:HA	2.01	0.42
1:B:538:PHE:CE2	1:D:585:ILE:HG23	2.55	0.42
1:B:597:ILE:HG21	1:B:729:ALA:HB1	2.00	0.42
1:C:8:ARG:HH12	1:C:11:GLU:HG3	1.83	0.42
1:D:277:MET:CE	1:D:321:LEU:HD23	2.48	0.42
3:D:1801:B12:H422	3:D:1801:B12:C10	2.48	0.42
1:A:583:LEU:HD21	1:C:542:GLU:HG2	2.02	0.42
1:A:616:ASP:OD2	1:A:670:ILE:HG12	2.19	0.42
1:A:620:VAL:HG13	1:C:112:GLY:HA3	2.01	0.42
1:B:53:THR:HA	1:B:54:PRO:HD3	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1801:B12:H363	3:C:1801:B12:H412	1.58	0.42
1:D:82:ILE:O	1:D:83:ALA:HB2	2.19	0.42
1:D:91:ILE:HD13	1:D:143:ALA:CB	2.49	0.42
1:D:458:LYS:C	1:D:460:TYR:H	2.23	0.42
1:C:28:LYS:HG3	1:C:145:ASP:OD2	2.20	0.42
1:C:207:LYS:NZ	1:C:217:GLN:NE2	2.67	0.42
1:D:138:ARG:NE	1:D:176:GLU:OE1	2.49	0.42
1:A:335:THR:HB	1:A:337:ASP:OD1	2.19	0.42
1:B:344:TRP:CG	1:B:515:VAL:HB	2.55	0.42
1:C:102:ALA:HB2	1:C:352:CYS:SG	2.59	0.42
1:C:251:PHE:CE1	2:G:38:LEU:HD23	2.55	0.42
2:G:46:THR:HB	2:G:47:PRO:HD2	2.02	0.42
1:D:22:LEU:HD22	1:D:138:ARG:HB3	2.00	0.42
1:D:147:ILE:O	1:D:151:VAL:HG22	2.20	0.42
1:D:217:GLN:HG2	1:D:218:ILE:N	2.33	0.42
1:A:438:PHE:CD2	2:E:77:MET:HG3	2.54	0.42
1:B:123:THR:O	1:B:494:ASN:HA	2.20	0.42
1:B:660:LYS:HG3	1:B:660:LYS:O	2.20	0.42
3:B:1801:B12:H312	3:B:1801:B12:C25	2.49	0.42
1:C:388:ALA:HB1	2:G:26:PHE:HE1	1.85	0.42
1:D:335:THR:O	1:D:338:GLU:HB2	2.20	0.42
1:B:46:PHE:HE2	1:B:67:PHE:CD1	2.38	0.42
2:G:39:ASP:O	2:G:40:LEU:C	2.57	0.42
1:D:159:SER:O	1:D:181:ALA:HA	2.20	0.42
1:A:121:GLU:HG3	1:A:486:ILE:HB	2.02	0.42
1:A:227:ALA:HB3	1:A:241:LEU:HD21	2.01	0.42
1:A:650:GLU:HG2	1:A:654:ASP:OD2	2.19	0.42
1:B:79:THR:CB	1:B:332:SER:HA	2.46	0.42
1:B:416:TYR:CD1	1:B:417:PRO:HA	2.55	0.42
1:B:426:ARG:HH22	1:D:634:GLU:CD	2.23	0.42
1:C:424:ILE:HG21	1:C:426:ARG:CZ	2.50	0.42
1:C:577:SER:O	1:C:578:ILE:HD12	2.20	0.42
1:D:25:TYR:CE1	1:D:142:LYS:HB2	2.55	0.42
1:D:629:LYS:HG3	1:D:630:HIS:CD2	2.55	0.42
1:A:626:ILE:O	1:A:634:GLU:HB2	2.20	0.42
1:A:726:ILE:HD12	1:A:726:ILE:HA	1.89	0.42
1:B:44:GLY:HA3	1:B:45:PRO:HD3	1.79	0.42
1:B:194:ILE:O	1:B:195:ASN:C	2.58	0.42
1:B:465:VAL:HG12	1:B:465:VAL:O	2.19	0.42
1:C:134:ARG:O	1:C:138:ARG:HG3	2.19	0.42
1:C:488:GLU:O	1:C:489:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:ILE:HD13	1:D:360:ILE:HA	1.90	0.42
1:D:481:GLU:H	1:D:481:GLU:CD	2.22	0.42
1:D:734:LYS:HB3	1:D:734:LYS:HE2	1.87	0.42
1:A:513:PRO:HA	1:C:528:PHE:O	2.20	0.41
1:A:671:SER:O	1:A:672:HIS:C	2.57	0.41
3:A:1801:B12:O28	3:A:1801:B12:C3	2.49	0.41
2:F:90:LYS:HB3	2:F:90:LYS:HE2	1.69	0.41
1:C:476:THR:HG23	2:G:56:ARG:O	2.20	0.41
1:D:8:ARG:HG3	1:D:11:GLU:OE1	2.20	0.41
1:D:167:PRO:HD2	2:H:48:SER:HB2	2.02	0.41
1:D:441:ASP:HB3	1:D:443:ASP:OD1	2.20	0.41
1:A:471:LEU:HD13	1:A:471:LEU:HA	1.93	0.41
1:B:322:ILE:HD13	1:B:322:ILE:HA	1.85	0.41
1:C:234:ALA:O	1:C:237:VAL:HG12	2.20	0.41
2:G:38:LEU:O	2:G:42:LYS:HG3	2.20	0.41
1:D:281:LEU:HB3	1:D:282:PRO:HD3	2.02	0.41
1:D:318:LEU:HD23	1:D:318:LEU:HA	1.79	0.41
2:H:37:LEU:O	2:H:40:LEU:HB2	2.21	0.41
2:H:74:ARG:HD3	2:H:113:ILE:HD11	2.01	0.41
1:A:533:LYS:HB2	1:A:533:LYS:HE3	1.55	0.41
1:B:111:ALA:O	1:D:620:VAL:HG11	2.20	0.41
1:B:172:MET:CE	1:B:172:MET:O	2.68	0.41
1:B:224:ALA:C	1:B:226:ASN:N	2.73	0.41
1:B:232:ARG:HD3	1:B:232:ARG:HA	1.80	0.41
1:B:512:LYS:HB2	1:B:512:LYS:HE3	1.75	0.41
1:C:505:PHE:CD1	1:C:505:PHE:N	2.88	0.41
1:D:623:ARG:HB3	1:D:627:ASP:OD2	2.20	0.41
1:D:704:GLN:NE2	1:D:721:ARG:HH21	2.13	0.41
1:A:636:TYR:OH	1:A:726:ILE:HD13	2.21	0.41
1:A:663:ALA:HB2	1:A:697:MET:HB2	2.02	0.41
1:B:26:THR:HG22	1:B:27:PRO:O	2.20	0.41
1:B:651:LYS:O	1:B:654:ASP:HB2	2.20	0.41
1:C:86:ARG:HB3	1:C:88:GLU:CD	2.41	0.41
1:C:300:MET:CE	1:C:316:HIS:HB3	2.51	0.41
1:C:306:GLU:HB3	1:C:307:ALA:H	1.66	0.41
1:C:458:LYS:C	1:C:460:TYR:H	2.24	0.41
2:G:74:ARG:HB2	2:G:76:LEU:HD22	2.01	0.41
1:D:82:ILE:CG2	1:D:90:ASP:HB3	2.51	0.41
1:D:138:ARG:HE	1:D:176:GLU:CD	2.22	0.41
1:D:335:THR:CB	1:D:337:ASP:OD1	2.67	0.41
1:A:731:PHE:CD2	1:A:732:LEU:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLN:NE2	1:B:132:ILE:HB	2.29	0.41
2:F:59:PHE:CE1	2:F:100:GLY:HA3	2.56	0.41
1:D:347:TYR:HA	1:D:350:GLU:HB2	2.03	0.41
1:D:553:GLU:OE2	1:D:571:LYS:HE3	2.20	0.41
1:D:711:VAL:CG2	1:D:717:ALA:HA	2.50	0.41
1:A:609:VAL:HG22	1:A:663:ALA:O	2.20	0.41
1:A:617:GLU:HB2	3:A:1801:B12:O44	2.20	0.41
1:A:730:THR:HG22	1:A:731:PHE:N	2.35	0.41
1:B:531:THR:HG23	1:B:536:ALA:HB2	2.03	0.41
1:B:592:LEU:HD12	1:B:730:THR:HG23	2.02	0.41
1:C:171:VAL:HG12	1:C:172:MET:N	2.36	0.41
1:C:264:LEU:HD13	1:C:296:MET:HE1	2.01	0.41
1:C:430:GLY:O	1:C:434:ALA:HB2	2.21	0.41
1:C:521:GLY:O	1:C:573:ARG:HA	2.20	0.41
1:C:624:GLU:OE1	1:C:630:HIS:ND1	2.53	0.41
3:C:1801:B12:H473	3:C:1801:B12:H481	1.07	0.41
1:D:399:GLY:CA	1:D:403:ASN:HD22	2.32	0.41
1:A:344:TRP:CG	1:A:515:VAL:HB	2.56	0.41
1:A:731:PHE:CE2	1:A:732:LEU:HD23	2.55	0.41
1:B:31:GLY:O	1:B:179:ASN:ND2	2.49	0.41
1:B:575:PRO:HD2	1:B:576:PHE:CD2	2.55	0.41
1:C:137:VAL:HG13	1:C:157:TYR:HE2	1.86	0.41
1:C:475:CYS:HB2	2:G:56:ARG:O	2.20	0.41
1:C:713:GLN:NE2	1:C:713:GLN:N	2.68	0.41
1:D:255:VAL:O	1:D:255:VAL:CG1	2.68	0.41
1:D:478:GLU:O	1:D:480:PRO:HD3	2.20	0.41
1:D:701:GLY:HA3	3:D:1801:B12:C9B	2.50	0.41
1:A:373:ARG:HD2	1:A:373:ARG:HA	1.88	0.41
1:B:523:VAL:HG11	1:D:527:MET:HE1	2.03	0.41
1:B:620:VAL:HG12	3:B:1801:B12:H3P3	2.02	0.41
3:B:1801:B12:H312	3:B:1801:B12:H251	2.03	0.41
1:C:335:THR:CG2	1:C:348:ASN:ND2	2.82	0.41
1:D:515:VAL:HG13	1:D:522:THR:HB	2.02	0.41
1:A:263:CYS:HA	1:A:295:ARG:O	2.21	0.41
2:E:70:LYS:O	2:E:71:THR:C	2.58	0.41
1:B:55:LEU:CD1	1:B:58:SER:HB3	2.49	0.41
1:B:153:ARG:HA	1:B:154:PRO:HD3	1.90	0.41
1:B:198:ARG:HD2	2:F:46:THR:HG21	2.02	0.41
1:B:233:GLU:OE1	1:B:235:TRP:CZ2	2.74	0.41
1:B:439:GLU:HG2	1:B:440:ARG:N	2.35	0.41
1:B:555:ILE:CG2	1:B:571:LYS:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:VAL:HG13	1:B:683:ILE:HG12	2.02	0.41
1:C:7:LEU:HA	1:C:7:LEU:HD23	1.75	0.41
1:C:184:ASP:HA	1:C:185:PRO:HD2	1.90	0.41
1:C:649:VAL:HG13	1:C:683:ILE:CG1	2.51	0.41
1:C:726:ILE:HG23	1:C:727:HIS:N	2.36	0.41
1:D:8:ARG:H	1:D:8:ARG:HG2	1.48	0.41
1:D:197:ILE:O	1:D:201:ILE:HD12	2.21	0.41
1:D:516:GLU:HG2	1:D:517:TRP:N	2.36	0.41
1:D:568:ILE:CG2	1:D:570:LEU:HD11	2.51	0.41
1:D:678:LYS:HB2	1:D:682:ARG:HH21	1.86	0.41
1:D:706:THR:HA	1:D:707:PRO:HD3	1.87	0.41
1:A:464:LEU:HD12	1:A:464:LEU:N	2.36	0.41
1:A:676:HIS:O	1:A:680:MET:HG3	2.21	0.41
2:E:94:ILE:HG13	2:E:99:ALA:HB2	2.03	0.41
1:B:409:PHE:N	1:B:409:PHE:HD1	2.19	0.41
1:B:479:VAL:HG12	1:B:479:VAL:O	2.21	0.41
3:B:1801:B12:H363	3:B:1801:B12:H412	1.62	0.41
1:A:698:ILE:HG21	1:A:715:VAL:HG12	2.02	0.40
1:B:196:MET:SD	1:B:402:PHE:HD1	2.45	0.40
1:C:316:HIS:CE1	1:C:334:ILE:HB	2.56	0.40
1:C:619:SER:HB3	1:C:645:THR:CG2	2.51	0.40
1:D:458:LYS:O	1:D:460:TYR:N	2.54	0.40
1:D:544:ALA:HB2	1:D:570:LEU:HD22	2.03	0.40
1:A:613:VAL:HG12	1:A:679:ASN:HD22	1.86	0.40
3:A:1801:B12:H471	3:A:1801:B12:H492	2.02	0.40
2:E:98:GLU:HA	2:E:101:LEU:HB2	2.03	0.40
1:B:409:PHE:N	1:B:409:PHE:CD1	2.89	0.40
1:B:528:PHE:CD2	1:B:528:PHE:C	2.94	0.40
3:B:1801:B12:H601	3:B:1801:B12:C26	2.38	0.40
1:C:462:GLU:O	1:C:464:LEU:N	2.54	0.40
1:C:528:PHE:CZ	1:C:565:GLY:HA3	2.55	0.40
1:C:613:VAL:CG1	1:C:614:GLY:N	2.84	0.40
3:C:1801:B12:H541	3:C:1801:B12:H602	1.82	0.40
1:D:613:VAL:HG21	1:D:683:ILE:CD1	2.52	0.40
1:A:445:MET:HG2	1:A:446:ALA:N	2.37	0.40
2:E:18:SER:CB	2:E:20:GLU:OE1	2.68	0.40
1:B:467:GLU:N	1:B:468:PRO:CD	2.85	0.40
1:B:672:HIS:O	1:B:675:ILE:HG22	2.20	0.40
1:C:618:HIS:CE1	3:C:1801:B12:H421	2.56	0.40
1:D:212:TRP:CZ2	1:D:477:LEU:HB3	2.56	0.40
1:A:192:ARG:HA	1:A:192:ARG:HD3	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ARG:NH1	1:C:232:ARG:HD2	2.37	0.40
1:A:707:PRO:HG3	1:A:718:GLY:O	2.22	0.40
1:A:719:PHE:HB3	1:A:723:SER:OG	2.21	0.40
2:E:63:GLU:OE1	2:E:101:LEU:CD1	2.69	0.40
1:B:42:GLN:HA	1:B:46:PHE:O	2.22	0.40
1:C:672:HIS:O	1:C:673:ASP:HB3	2.21	0.40
1:C:713:GLN:N	1:C:713:GLN:HE21	2.18	0.40
1:D:618:HIS:NE2	3:D:1801:B12:N22	2.69	0.40
1:A:184:ASP:HA	1:A:185:PRO:HD2	1.82	0.40
1:A:342:VAL:O	1:A:343:PRO:C	2.59	0.40
3:A:1801:B12:H473	3:A:1801:B12:H481	0.98	0.40
1:B:205:GLU:OE2	1:B:451:HIS:HA	2.22	0.40
1:C:94:MET:CE	1:C:140:GLN:NE2	2.85	0.40
1:C:305:MET:HE2	1:C:305:MET:HB2	1.92	0.40
1:C:424:ILE:CG2	1:C:426:ARG:CZ	2.99	0.40
1:C:463:ALA:C	1:C:464:LEU:HD13	2.42	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	721/763 (94%)	633 (88%)	75 (10%)	13 (2%)	7	25
1	B	722/763 (95%)	658 (91%)	56 (8%)	8 (1%)	12	37
1	C	721/763 (94%)	629 (87%)	79 (11%)	13 (2%)	7	25
1	D	721/763 (94%)	643 (89%)	64 (9%)	14 (2%)	6	24
2	E	107/121 (88%)	93 (87%)	11 (10%)	3 (3%)	4	16
2	F	107/121 (88%)	95 (89%)	11 (10%)	1 (1%)	14	43
2	G	107/121 (88%)	97 (91%)	9 (8%)	1 (1%)	14	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	107/121 (88%)	102 (95%)	5 (5%)	0	100	100
All	All	3313/3536 (94%)	2950 (89%)	310 (9%)	53 (2%)	8	28

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	12	LYS
1	A	69	ASP
1	B	162	SER
1	D	6	GLN
1	A	255	VAL
1	A	473	ASP
2	E	113	ILE
1	B	6	GLN
1	B	66	TYR
1	B	693	ARG
1	C	6	GLN
1	C	21	ASP
1	C	461	ASP
1	C	556	ASN
1	D	649	VAL
1	B	225	HIS
1	C	738	GLU
1	D	63	SER
1	D	83	ALA
1	D	361	GLY
1	D	459	GLN
1	A	40	ASN
1	A	672	HIS
1	A	738	GLU
2	E	71	THR
2	E	93	ASN
1	B	195	ASN
1	B	474	GLY
1	C	39	GLU
1	C	164	VAL
1	C	505	PHE
2	G	113	ILE
1	D	674	ASP
1	A	649	VAL
1	A	694	ASP

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Mol	Chain	Res	Type
1	B	487	ASP
2	F	15	ALA
1	D	562	GLU
1	D	593	SER
1	D	658	GLU
1	D	683	ILE
1	A	537	GLU
1	A	601	ILE
1	C	189	VAL
1	C	463	ALA
1	D	341	ASN
1	A	707	PRO
1	C	9	VAL
1	D	411	VAL
1	D	707	PRO
1	C	453	GLY
1	C	417	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	598/644 (93%)	547 (92%)	51 (8%)	8	27
1	B	604/644 (94%)	561 (93%)	43 (7%)	12	36
1	C	600/644 (93%)	562 (94%)	38 (6%)	15	42
1	D	602/644 (94%)	557 (92%)	45 (8%)	11	33
2	E	89/100 (89%)	84 (94%)	5 (6%)	17	47
2	F	90/100 (90%)	86 (96%)	4 (4%)	24	57
2	G	89/100 (89%)	79 (89%)	10 (11%)	5	16
2	H	89/100 (89%)	84 (94%)	5 (6%)	17	47
All	All	2761/2976 (93%)	2560 (93%)	201 (7%)	11	34

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	GLN
1	A	24	LYS
1	A	29	ARG
1	A	33	THR
1	A	42	GLN
1	A	47	ILE
1	A	61	LEU
1	A	69	ASP
1	A	148	GLU
1	A	153	ARG
1	A	159	SER
1	A	168	ASP
1	A	172	MET
1	A	183	GLN
1	A	198	ARG
1	A	249	SER
1	A	259	LYS
1	A	260	SER
1	A	264	LEU
1	A	276	SER
1	A	301	ASN
1	A	306	GLU
1	A	311	GLU
1	A	338	GLU
1	A	341	ASN
1	A	376	VAL
1	A	380	THR
1	A	418	GLU
1	A	442	GLU
1	A	465	VAL
1	A	471	LEU
1	A	486	ILE
1	A	505	PHE
1	A	509	SER
1	A	531	THR
1	A	550	GLU
1	A	557	ARG
1	A	570	LEU
1	A	578	ILE
1	A	591	ILE
1	A	592	LEU
1	A	604	THR

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Mol	Chain	Res	Type
1	A	608	ILE
1	A	624	GLU
1	A	651	LYS
1	A	668	THR
1	A	674	ASP
1	A	696	ILE
1	A	731	PHE
1	A	736	ARG
2	E	39	ASP
2	E	91	GLU
2	E	94	ILE
2	E	96	VAL
2	E	101	LEU
1	B	6	GLN
1	B	7	LEU
1	B	9	VAL
1	B	21	ASP
1	B	69	ASP
1	B	92	ARG
1	B	127	ILE
1	B	153	ARG
1	B	162	SER
1	B	168	ASP
1	B	172	MET
1	B	232	ARG
1	B	270	THR
1	B	301	ASN
1	B	306	GLU
1	B	338	GLU
1	B	341	ASN
1	B	383	GLU
1	B	391	PHE
1	B	424	ILE
1	B	442	GLU
1	B	457	VAL
1	B	471	LEU
1	B	477	LEU
1	B	489	LEU
1	B	492	ASN
1	B	501	GLU
1	B	509	SER
1	B	525	LEU

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Mol	Chain	Res	Type
1	B	532	SER
1	B	551	GLU
1	B	591	ILE
1	B	603	LYS
1	B	616	ASP
1	B	628	ILE
1	B	651	LYS
1	B	668	THR
1	B	674	ASP
1	B	688	VAL
1	B	696	ILE
1	B	703	THR
1	B	731	PHE
1	B	736	ARG
2	F	28	GLU
2	F	74	ARG
2	F	91	GLU
2	F	101	LEU
1	C	5	LEU
1	C	6	GLN
1	C	13	LEU
1	C	15	VAL
1	C	26	THR
1	C	110	THR
1	C	125	GLN
1	C	159	SER
1	C	168	ASP
1	C	171	VAL
1	C	182	HIS
1	C	232	ARG
1	C	238	MET
1	C	280	ASP
1	C	288	ARG
1	C	289	GLU
1	C	306	GLU
1	C	313	THR
1	C	362	MET
1	C	394	GLU
1	C	396	ILE
1	C	432	ILE
1	C	464	LEU
1	C	469	SER

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Mol	Chain	Res	Type
1	C	471	LEU
1	C	526	THR
1	C	534	ARG
1	C	557	ARG
1	C	574	VAL
1	C	578	ILE
1	C	625	VAL
1	C	651	LYS
1	C	668	THR
1	C	689	GLU
1	C	703	THR
1	C	724	LYS
1	C	731	PHE
1	C	736	ARG
2	G	16	ASN
2	G	39	ASP
2	G	43	LYS
2	G	60	SER
2	G	76	LEU
2	G	79	LYS
2	G	97	ARG
2	G	101	LEU
2	G	104	SER
2	G	105	GLU
1	D	7	LEU
1	D	8	ARG
1	D	26	THR
1	D	29	ARG
1	D	75	LEU
1	D	80	THR
1	D	172	MET
1	D	179	ASN
1	D	217	GLN
1	D	228	ASN
1	D	233	GLU
1	D	237	VAL
1	D	250	ILE
1	D	258	LYS
1	D	290	MET
1	D	306	GLU
1	D	341	ASN
1	D	349	ILE

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Mol	Chain	Res	Type
1	D	376	VAL
1	D	383	GLU
1	D	391	PHE
1	D	428	ILE
1	D	445	MET
1	D	464	LEU
1	D	486	ILE
1	D	491	GLU
1	D	501	GLU
1	D	502	THR
1	D	512	LYS
1	D	518	GLN
1	D	531	THR
1	D	546	LYS
1	D	557	ARG
1	D	577	SER
1	D	578	ILE
1	D	595	ASP
1	D	628	ILE
1	D	646	SER
1	D	657	ILE
1	D	660	LYS
1	D	668	THR
1	D	695	LYS
1	D	724	LYS
1	D	731	PHE
1	D	733	VAL
2	H	9	GLN
2	H	23	GLN
2	H	60	SER
2	H	61	SER
2	H	76	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	244	GLN
1	A	248	ASN
1	A	341	ASN
1	A	456	ASN
1	A	518	GLN

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Mol	Chain	Res	Type
1	A	672	HIS
1	A	679	ASN
1	B	217	GLN
1	B	261	ASN
1	B	331	GLN
1	B	341	ASN
1	B	403	ASN
1	B	459	GLN
1	C	217	GLN
1	C	370	GLN
1	C	459	GLN
1	C	492	ASN
1	C	518	GLN
1	C	713	GLN
2	G	16	ASN
2	G	93	ASN
1	D	40	ASN
1	D	331	GLN
1	D	341	ASN
1	D	348	ASN
1	D	370	GLN
1	D	403	ASN
1	D	459	GLN
1	D	518	GLN
1	D	704	GLN
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

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	5AD	A	1500	3	16,20,20	2.38	7 (43%)	14,30,30	4.08	7 (50%)
4	PLP	B	1802	1	15,15,16	1.80	3 (20%)	21,22,23	1.96	7 (33%)
4	PLP	C	1802	1	15,15,16	1.81	3 (20%)	21,22,23	1.69	3 (14%)
4	PLP	D	1802	1	15,15,16	1.48	1 (6%)	21,22,23	1.37	4 (19%)
3	B12	D	1801	1	91,101,101	1.42	8 (8%)	140,166,166	2.37	33 (23%)
3	B12	B	1801	1,5	91,101,101	1.50	11 (12%)	140,166,166	2.36	31 (22%)
5	5AD	D	1500	3	16,20,20	2.32	7 (43%)	14,30,30	4.53	7 (50%)
3	B12	C	1801	1,5	91,101,101	1.42	9 (9%)	140,166,166	2.48	33 (23%)
3	B12	A	1801	1,5	91,101,101	1.47	10 (10%)	140,166,166	2.40	36 (25%)
5	5AD	C	1500	3	16,20,20	2.30	6 (37%)	14,30,30	4.36	7 (50%)
4	PLP	A	1802	1	15,15,16	2.04	3 (20%)	21,22,23	1.64	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	5AD	A	1500	3	3/3/4/4	0/0/20/20	0/3/3/3
4	PLP	B	1802	1	-	0/6/6/8	0/1/1/1
4	PLP	C	1802	1	-	0/6/6/8	0/1/1/1
5	5AD	D	1500	3	3/3/4/4	0/0/20/20	0/3/3/3
3	B12	D	1801	1	1/1/36/38	21/52/223/223	0/3/11/11
3	B12	B	1801	1,5	1/1/36/38	3/52/223/223	0/3/11/11
4	PLP	D	1802	1	-	0/6/6/8	0/1/1/1
3	B12	C	1801	1,5	1/1/36/38	12/52/223/223	0/3/11/11
3	B12	A	1801	1,5	1/1/36/38	11/52/223/223	0/3/11/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	5AD	C	1500	3	3/3/4/4	0/0/20/20	0/3/3/3
4	PLP	A	1802	1	-	0/6/6/8	0/1/1/1

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1801	B12	C19-N24	-6.70	1.40	1.49
3	D	1801	B12	C19-N24	-6.29	1.41	1.49
3	C	1801	B12	C19-N24	-5.92	1.41	1.49
3	B	1801	B12	C14-N23	5.82	1.42	1.35
3	A	1801	B12	C14-N23	5.76	1.42	1.35
3	A	1801	B12	C19-N24	-5.66	1.42	1.49
3	C	1801	B12	C14-N23	5.26	1.42	1.35
4	B	1802	PLP	C6-N1	5.10	1.44	1.34
4	A	1802	PLP	C6-N1	4.78	1.44	1.34
3	D	1801	B12	C14-N23	4.77	1.41	1.35
4	D	1802	PLP	C6-N1	4.75	1.44	1.34
3	A	1801	B12	C9-N22	4.59	1.41	1.30
5	C	1500	5AD	C2-N3	4.58	1.39	1.32
3	C	1801	B12	C9-N22	4.57	1.41	1.30
5	D	1500	5AD	C2-N3	4.54	1.39	1.32
5	A	1500	5AD	C2-N3	4.54	1.39	1.32
5	D	1500	5AD	O4'-C1'	4.33	1.46	1.40
4	C	1802	PLP	C6-N1	4.31	1.43	1.34
4	A	1802	PLP	C5-C4	-4.20	1.35	1.40
3	D	1801	B12	C9-N22	4.19	1.40	1.30
3	B	1801	B12	C9-N22	4.18	1.40	1.30
5	C	1500	5AD	O4'-C1'	4.08	1.46	1.40
3	A	1801	B12	C8B-C9B	3.95	1.48	1.40
5	A	1500	5AD	C8-N7	3.90	1.41	1.34
5	A	1500	5AD	O4'-C1'	3.89	1.46	1.40
3	B	1801	B12	C16-C15	-3.84	1.33	1.44
3	D	1801	B12	C8B-C9B	3.83	1.48	1.40
3	B	1801	B12	C8B-C9B	3.82	1.48	1.40
3	C	1801	B12	C16-C15	-3.77	1.33	1.44
5	C	1500	5AD	C8-N7	3.66	1.41	1.34
3	A	1801	B12	C16-C15	-3.62	1.34	1.44
3	D	1801	B12	C16-C15	-3.59	1.34	1.44
3	A	1801	B12	C6B-C5B	3.54	1.49	1.40
5	D	1500	5AD	C8-N7	3.50	1.41	1.34
3	A	1801	B12	C11-N23	3.40	1.43	1.36
4	C	1802	PLP	C5-C4	-3.32	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1801	B12	C6B-C5B	3.25	1.48	1.40
3	C	1801	B12	C8B-C9B	3.23	1.47	1.40
5	A	1500	5AD	C4-N3	3.16	1.39	1.35
3	D	1801	B12	C11-N23	3.15	1.42	1.36
4	C	1802	PLP	C4A-C4	-3.02	1.45	1.51
3	A	1801	B12	C10-C9	2.97	1.47	1.39
3	C	1801	B12	C6B-C5B	2.89	1.47	1.40
3	C	1801	B12	C11-N23	2.88	1.42	1.36
3	B	1801	B12	C6B-C5B	2.77	1.47	1.40
4	A	1802	PLP	C4A-C4	-2.77	1.46	1.51
5	A	1500	5AD	C6-N6	2.62	1.43	1.34
5	D	1500	5AD	C6-N6	2.61	1.43	1.34
4	B	1802	PLP	C4A-C4	-2.61	1.46	1.51
5	C	1500	5AD	C6-N6	2.61	1.43	1.34
3	C	1801	B12	C10-C9	2.58	1.46	1.39
4	B	1802	PLP	C5-C4	-2.55	1.37	1.40
5	D	1500	5AD	C4-N3	2.55	1.39	1.35
5	A	1500	5AD	C2-N1	2.53	1.38	1.33
5	C	1500	5AD	C4-N3	2.41	1.38	1.35
5	C	1500	5AD	C2-N1	2.31	1.38	1.33
3	D	1801	B12	C10-C9	2.30	1.45	1.39
5	D	1500	5AD	C1'-N9	-2.29	1.44	1.49
3	B	1801	B12	C11-N23	2.29	1.41	1.36
3	A	1801	B12	O6R-C1R	2.25	1.43	1.40
5	A	1500	5AD	C1'-N9	-2.24	1.44	1.49
3	B	1801	B12	C10-C9	2.21	1.45	1.39
3	B	1801	B12	C1-C19	-2.18	1.50	1.55
5	D	1500	5AD	C2-N1	2.18	1.37	1.33
3	C	1801	B12	O6R-C1R	2.17	1.43	1.40
3	B	1801	B12	C1-C2	-2.09	1.54	1.58
3	B	1801	B12	C14-C15	2.07	1.47	1.38
3	A	1801	B12	C2-C3	-2.00	1.51	1.57

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1500	5AD	C5'-C4'-C3'	10.91	127.15	115.70
5	D	1500	5AD	C5'-C4'-C3'	10.72	126.96	115.70
3	B	1801	B12	C47-C12-C46	9.01	124.33	109.41
3	A	1801	B12	C47-C12-C46	9.01	124.32	109.41
5	A	1500	5AD	C5'-C4'-C3'	8.83	124.97	115.70
3	C	1801	B12	C1-C19-N24	8.82	116.06	106.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1801	B12	C13-C12-C11	-8.69	91.26	100.97
3	A	1801	B12	C1-C19-N24	8.68	115.91	106.25
3	D	1801	B12	C1-C19-N24	8.56	115.77	106.25
3	C	1801	B12	C47-C12-C46	8.24	123.05	109.41
3	A	1801	B12	C46-C12-C13	-8.07	80.03	112.74
3	C	1801	B12	C46-C12-C13	-7.92	80.62	112.74
3	B	1801	B12	C20-C1-C19	-7.87	101.77	109.35
5	D	1500	5AD	N3-C2-N1	-7.87	117.99	128.67
3	C	1801	B12	C20-C1-C19	-7.71	101.92	109.35
3	B	1801	B12	C1-C19-N24	7.57	114.67	106.25
3	D	1801	B12	C47-C12-C46	7.48	121.79	109.41
3	B	1801	B12	C12-C11-C10	-7.35	113.92	123.40
5	A	1500	5AD	N3-C2-N1	-7.29	118.77	128.67
3	D	1801	B12	C12-C11-N23	7.25	121.81	111.83
3	A	1801	B12	C12-C11-N23	6.96	121.41	111.83
5	C	1500	5AD	N3-C2-N1	-6.92	119.28	128.67
3	D	1801	B12	C46-C12-C13	-6.88	84.84	112.74
3	D	1801	B12	C1-C19-C18	6.77	132.88	121.90
3	D	1801	B12	C12-C11-C10	-6.71	114.75	123.40
3	B	1801	B12	C13-C12-C11	-6.69	93.49	100.97
5	D	1500	5AD	O3'-C3'-C4'	6.68	126.84	110.47
5	C	1500	5AD	O3'-C3'-C4'	6.67	126.80	110.47
3	B	1801	B12	C12-C11-N23	6.63	120.96	111.83
3	B	1801	B12	C18-C19-N24	6.55	112.18	102.33
3	C	1801	B12	C13-C12-C11	-6.41	93.81	100.97
3	A	1801	B12	C18-C19-N24	6.39	111.93	102.33
3	C	1801	B12	C12-C11-N23	6.37	120.61	111.83
3	C	1801	B12	C12-C11-C10	-6.31	115.26	123.40
4	B	1802	PLP	O4P-C5A-C5	6.27	121.11	109.36
3	B	1801	B12	C1-C19-C18	6.18	131.92	121.90
3	C	1801	B12	C18-C19-N24	6.17	111.60	102.33
3	A	1801	B12	C1-C19-C18	6.12	131.82	121.90
5	A	1500	5AD	O3'-C3'-C4'	6.02	125.22	110.47
3	C	1801	B12	C2P-C1P-N59	-6.02	104.07	112.92
3	C	1801	B12	C1-C19-C18	6.01	131.65	121.90
3	B	1801	B12	C47-C12-C13	-5.99	88.48	112.74
3	B	1801	B12	C46-C12-C13	-5.98	88.49	112.74
3	A	1801	B12	C47-C12-C13	-5.92	88.73	112.74
4	C	1802	PLP	O4P-C5A-C5	5.73	120.09	109.36
4	A	1802	PLP	O4P-C5A-C5	5.70	120.04	109.36
3	A	1801	B12	C12-C11-C10	-5.67	116.09	123.40
3	D	1801	B12	C18-C19-N24	5.60	110.75	102.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1801	B12	C47-C12-C13	-5.60	90.05	112.74
3	C	1801	B12	C26-C2-C1	5.52	118.53	110.00
3	A	1801	B12	C20-C1-C19	-5.47	104.08	109.35
3	D	1801	B12	C55-C17-C16	-5.45	105.94	116.59
3	C	1801	B12	C47-C12-C13	-5.33	91.15	112.74
3	A	1801	B12	C13-C12-C11	-5.20	95.15	100.97
3	D	1801	B12	C20-C1-C19	-5.14	104.41	109.35
3	C	1801	B12	C55-C17-C16	-4.99	106.84	116.59
3	A	1801	B12	C26-C2-C1	4.75	117.34	110.00
5	A	1500	5AD	O3'-C3'-C2'	4.62	126.62	111.82
5	D	1500	5AD	O2'-C2'-C3'	4.61	126.58	111.82
5	A	1500	5AD	O2'-C2'-C3'	4.52	126.30	111.82
3	C	1801	B12	C2-C1-C19	4.45	125.53	118.61
3	C	1801	B12	C2-C1-N21	4.33	107.80	101.78
3	A	1801	B12	C19-C1-N21	4.29	106.55	102.14
3	D	1801	B12	C19-C1-N21	4.24	106.51	102.14
3	A	1801	B12	C54-C17-C18	-4.22	106.93	112.99
5	C	1500	5AD	O2'-C2'-C3'	4.22	125.34	111.82
3	C	1801	B12	C30-C3-C2	-4.21	109.72	119.00
3	B	1801	B12	C2-C1-N21	4.20	107.62	101.78
5	C	1500	5AD	O3'-C3'-C2'	4.19	125.26	111.82
3	D	1801	B12	C26-C2-C1	4.05	116.26	110.00
3	B	1801	B12	C18-C17-C16	4.01	105.52	100.69
3	B	1801	B12	C54-C17-C18	-4.00	107.25	112.99
4	D	1802	PLP	O4P-C5A-C5	3.97	116.79	109.36
5	D	1500	5AD	O3'-C3'-C2'	3.96	124.52	111.82
3	B	1801	B12	C12-C13-C14	3.88	108.64	102.26
3	C	1801	B12	C12-C13-C14	3.78	108.48	102.26
3	A	1801	B12	C13-C14-N23	3.76	114.19	109.09
3	A	1801	B12	C12-C13-C14	3.73	108.39	102.26
3	B	1801	B12	C19-C1-N21	3.72	105.97	102.14
3	D	1801	B12	C15-C14-N23	-3.66	121.84	126.26
3	C	1801	B12	C18-C17-C16	3.63	105.06	100.69
3	D	1801	B12	C2-C1-N21	3.61	106.80	101.78
3	D	1801	B12	C13-C14-N23	3.53	113.88	109.09
3	B	1801	B12	C2-C1-C19	3.43	123.96	118.61
5	D	1500	5AD	C2'-C3'-C4'	3.40	107.38	102.36
3	A	1801	B12	C2-C1-N21	3.32	106.40	101.78
3	C	1801	B12	C19-C1-N21	3.30	105.54	102.14
3	D	1801	B12	C12-C13-C14	3.30	107.68	102.26
3	B	1801	B12	C55-C17-C16	-3.25	110.23	116.59
3	A	1801	B12	C7-C6-N22	3.22	113.81	107.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	B12	C20-C1-C2	-3.19	108.02	113.28
3	A	1801	B12	C30-C3-C2	-3.17	112.00	119.00
3	A	1801	B12	C9-C10-C11	-3.17	121.44	125.97
3	C	1801	B12	C13-C14-N23	3.17	113.38	109.09
3	A	1801	B12	C2-C26-C27	-3.12	106.52	115.19
3	A	1801	B12	C2-C1-C19	3.10	123.44	118.61
3	C	1801	B12	C20-C1-C2	-3.09	108.19	113.28
3	D	1801	B12	C7-C6-N22	3.06	113.52	107.94
5	A	1500	5AD	C2'-C3'-C4'	3.06	106.88	102.36
5	D	1500	5AD	O4'-C4'-C5'	3.05	125.15	110.28
5	A	1500	5AD	O4'-C4'-C5'	3.03	125.06	110.28
3	C	1801	B12	C54-C17-C18	-3.01	108.67	112.99
3	B	1801	B12	C55-C56-C57	-2.97	104.63	111.25
5	C	1500	5AD	O4'-C4'-C5'	2.96	124.70	110.28
3	B	1801	B12	C15-C14-N23	-2.94	122.72	126.26
4	A	1802	PLP	C4A-C4-C5	-2.93	117.92	120.94
3	D	1801	B12	C30-C3-C2	-2.93	112.54	119.00
3	A	1801	B12	C10-C9-N22	-2.92	122.41	125.74
3	A	1801	B12	C18-C17-C16	2.90	104.19	100.69
3	D	1801	B12	C25-C2-C1	-2.89	109.44	113.75
4	B	1802	PLP	C5-C6-N1	-2.87	119.16	123.83
3	B	1801	B12	C25-C2-C1	-2.85	109.50	113.75
3	B	1801	B12	C18-C60-C61	-2.84	106.82	114.04
3	D	1801	B12	C46-C12-C11	2.83	120.20	110.08
3	C	1801	B12	C46-C12-C11	2.78	120.00	110.08
4	B	1802	PLP	O3P-P-O4P	2.77	113.90	106.67
3	C	1801	B12	C25-C2-C1	-2.76	109.62	113.75
3	D	1801	B12	C7-C6-C5	-2.73	123.80	128.07
5	C	1500	5AD	C2'-C3'-C4'	2.73	106.39	102.36
3	B	1801	B12	C2P-C1P-N59	-2.72	108.92	112.92
3	D	1801	B12	C2-C1-C19	2.71	122.83	118.61
3	B	1801	B12	C30-C3-C2	-2.66	113.12	119.00
3	D	1801	B12	C20-C1-C2	-2.65	108.91	113.28
3	A	1801	B12	C7-C6-C5	-2.64	123.95	128.07
3	B	1801	B12	C20-C1-C2	-2.64	108.93	113.28
3	D	1801	B12	C18-C17-C16	2.63	103.86	100.69
3	A	1801	B12	C15-C14-N23	-2.61	123.11	126.26
3	D	1801	B12	C9-C10-C11	-2.55	122.32	125.97
3	A	1801	B12	C3R-C2R-C1R	2.52	105.43	99.89
3	C	1801	B12	C2-C26-C27	-2.51	108.21	115.19
3	A	1801	B12	C2-C3-C4	-2.49	98.84	101.64
3	B	1801	B12	C26-C2-C1	2.48	113.83	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	B12	C2P-C1P-N59	-2.48	109.28	112.92
3	B	1801	B12	C47-C12-C11	2.46	118.88	110.08
3	D	1801	B12	C16-C15-C14	-2.45	117.53	121.26
3	C	1801	B12	C18-C60-C61	-2.45	107.83	114.04
3	C	1801	B12	C54-C17-C55	2.40	113.25	109.27
3	D	1801	B12	C9-N22-C6	-2.39	102.40	105.28
3	C	1801	B12	C15-C14-N23	-2.39	123.39	126.26
3	A	1801	B12	C46-C12-C11	2.37	118.56	110.08
3	C	1801	B12	C7-C6-N22	2.37	112.25	107.94
3	C	1801	B12	C7-C6-C5	-2.37	124.37	128.07
3	D	1801	B12	C20-C1-N21	-2.35	106.37	110.26
4	B	1802	PLP	C2A-C2-C3	2.33	123.53	120.80
3	C	1801	B12	C55-C56-C57	-2.30	106.11	111.25
3	A	1801	B12	C7-C8-C9	2.30	103.81	100.89
3	D	1801	B12	C53-C15-C16	2.29	124.26	120.36
3	C	1801	B12	C20-C1-N21	-2.29	106.48	110.26
3	A	1801	B12	C55-C17-C16	-2.26	112.18	116.59
4	C	1802	PLP	O2P-P-O4P	2.25	112.55	106.67
3	B	1801	B12	C1-C2-C3	2.25	104.43	101.60
3	B	1801	B12	C2-C26-C27	-2.24	108.97	115.19
3	A	1801	B12	C16-C15-C14	-2.23	117.86	121.26
3	A	1801	B12	C37-C7-C6	2.22	113.99	107.11
4	D	1802	PLP	C6-C5-C4	2.21	119.91	118.10
3	A	1801	B12	C1-C2-C3	2.20	104.37	101.60
3	D	1801	B12	C3R-C2R-C1R	2.20	104.73	99.89
4	D	1802	PLP	C5-C6-N1	-2.19	120.27	123.83
3	D	1801	B12	C55-C56-C57	-2.18	106.38	111.25
3	D	1801	B12	C47-C12-C11	2.17	117.85	110.08
3	C	1801	B12	C2R-C3R-C4R	2.15	107.00	103.24
4	B	1802	PLP	O2P-P-O4P	2.14	112.25	106.67
4	B	1802	PLP	C3-C4-C5	2.12	121.14	118.59
4	C	1802	PLP	C6-N1-C2	-2.05	115.48	119.20
3	B	1801	B12	C7-C6-N22	2.04	111.65	107.94
4	D	1802	PLP	O2P-P-O4P	2.03	111.97	106.67
4	B	1802	PLP	C4A-C4-C5	-2.03	118.85	120.94
3	B	1801	B12	C13-C14-N23	2.02	111.82	109.09
3	A	1801	B12	C26-C2-C3	-2.01	103.91	107.42
3	B	1801	B12	C8-C7-C6	2.00	104.31	100.92

All (13) chirality outliers are listed below:

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

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C4-C3-C30-C31
3	A	1801	B12	N59-C1P-C2P-O3
3	A	1801	B12	C3R-C4R-C5R-O8R
3	A	1801	B12	O6R-C4R-C5R-O8R
3	B	1801	B12	C16-C17-C55-C56
3	B	1801	B12	C18-C17-C55-C56
3	C	1801	B12	C38-C37-C7-C6
3	C	1801	B12	C38-C37-C7-C36
3	C	1801	B12	C38-C37-C7-C8
3	C	1801	B12	C42-C41-C8-C9
3	C	1801	B12	C16-C17-C55-C56
3	C	1801	B12	C54-C17-C55-C56
3	C	1801	B12	C18-C17-C55-C56
3	D	1801	B12	C16-C17-C55-C56
3	D	1801	B12	C54-C17-C55-C56
3	D	1801	B12	C18-C17-C55-C56
3	D	1801	B12	C56-C57-N59-C1P
3	D	1801	B12	C1P-C2P-O3-P
3	D	1801	B12	C3P-C2P-O3-P
3	D	1801	B12	O58-C57-N59-C1P
3	D	1801	B12	C4-C3-C30-C31
3	A	1801	B12	C8-C41-C42-C43
3	C	1801	B12	C56-C57-N59-C1P
3	C	1801	B12	C42-C41-C8-C7

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Mol	Chain	Res	Type	Atoms
3	C	1801	B12	O58-C57-N59-C1P
3	D	1801	B12	C3-C2-C26-C27
3	A	1801	B12	C2-C3-C30-C31
3	D	1801	B12	C42-C41-C8-C9
3	B	1801	B12	C54-C17-C55-C56
3	A	1801	B12	N59-C1P-C2P-C3P
3	D	1801	B12	C42-C41-C8-C7
3	D	1801	B12	C38-C37-C7-C6
3	D	1801	B12	C2-C3-C30-C31
3	A	1801	B12	C41-C42-C43-O44
3	D	1801	B12	C1-C2-C26-C27
3	D	1801	B12	C38-C37-C7-C8
3	D	1801	B12	C14-C13-C48-C49
3	A	1801	B12	C41-C42-C43-N45
3	D	1801	B12	C25-C2-C26-C27
3	A	1801	B12	C38-C37-C7-C8
3	D	1801	B12	C18-C60-C61-O63
3	D	1801	B12	C2-C26-C27-N29
3	D	1801	B12	C2-C26-C27-O28
3	C	1801	B12	C19-C18-C60-C61
3	D	1801	B12	C18-C60-C61-N62
3	A	1801	B12	C2P-O3-P-O5
3	C	1801	B12	C17-C18-C60-C61

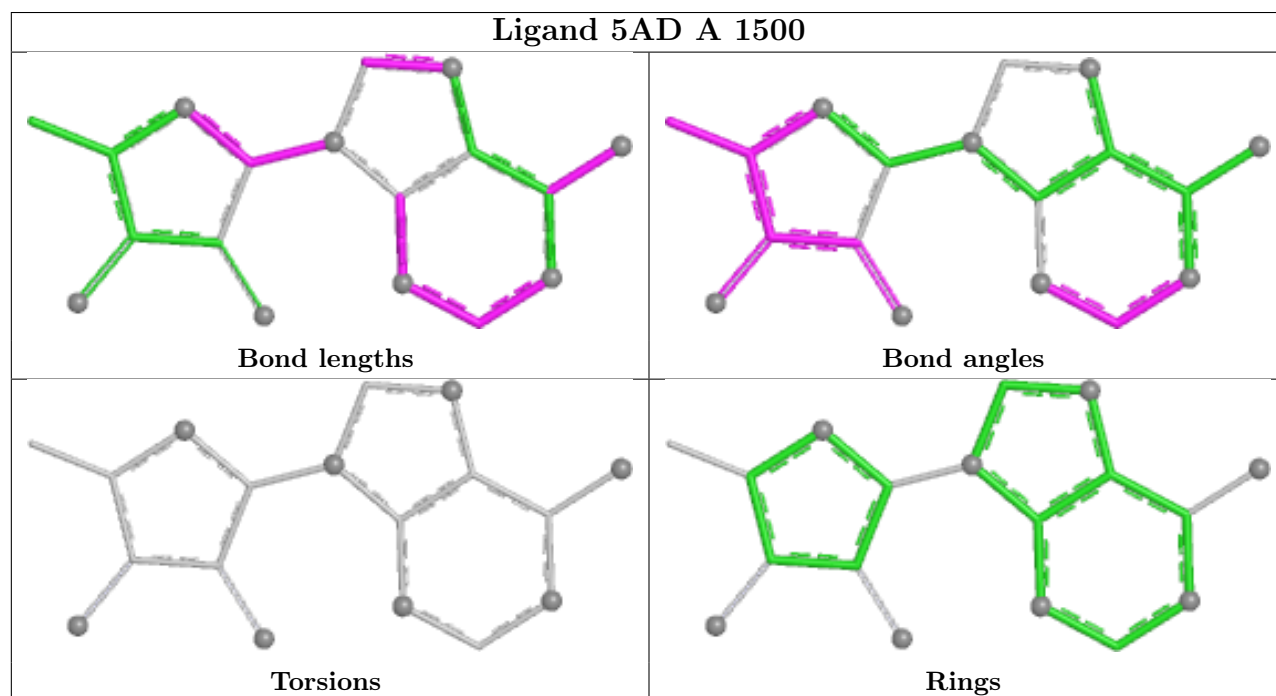
There are no ring outliers.

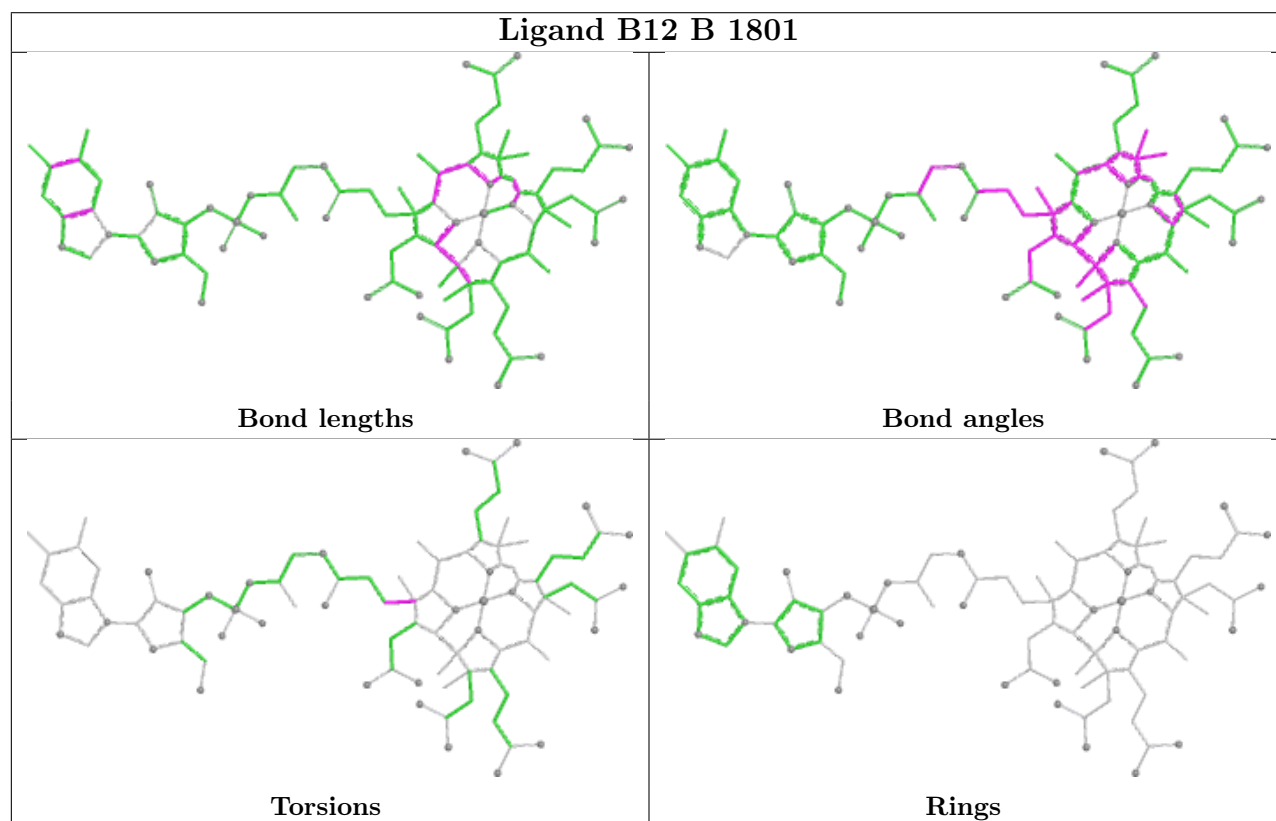
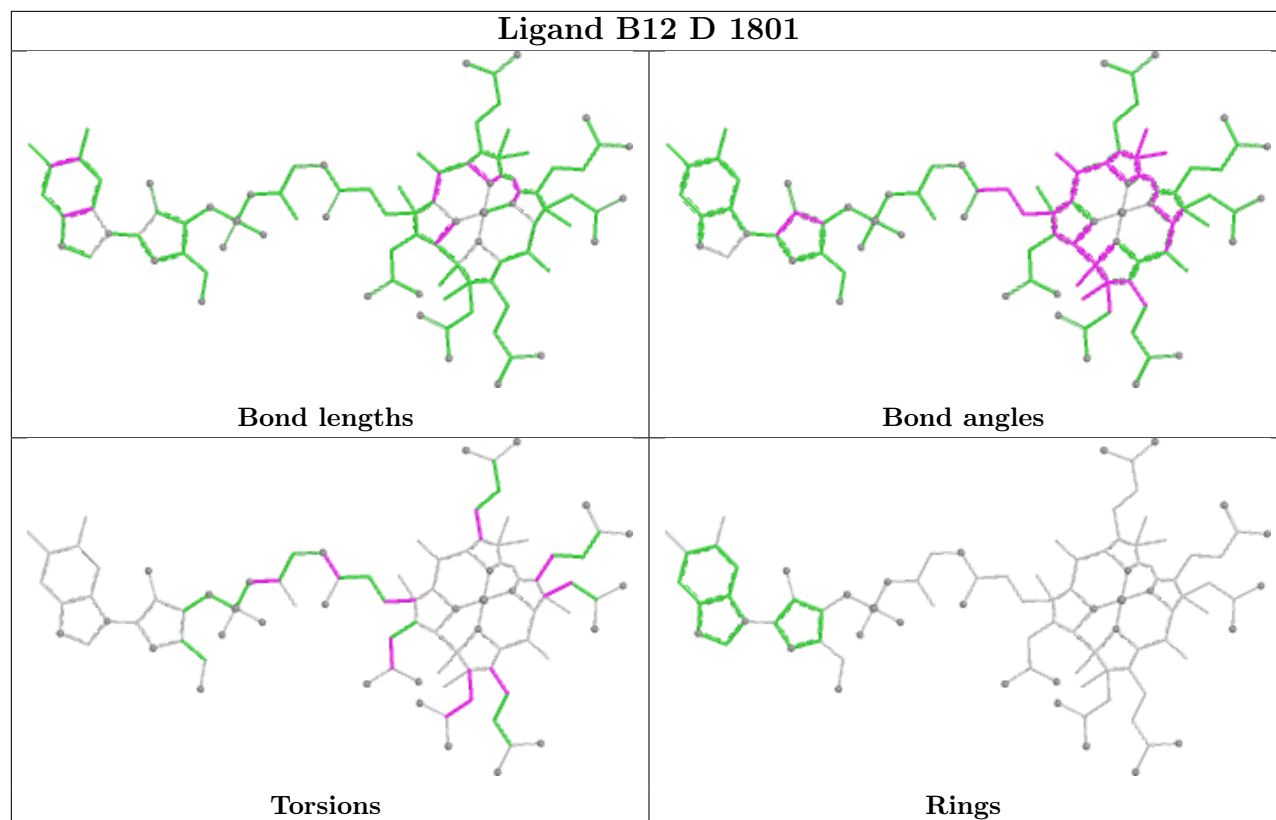
10 monomers are involved in 105 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1500	5AD	3	0
4	B	1802	PLP	2	0
4	D	1802	PLP	2	0
3	D	1801	B12	18	0
3	B	1801	B12	27	0
5	D	1500	5AD	2	0
3	C	1801	B12	29	0
3	A	1801	B12	25	0
5	C	1500	5AD	2	0
4	A	1802	PLP	2	0

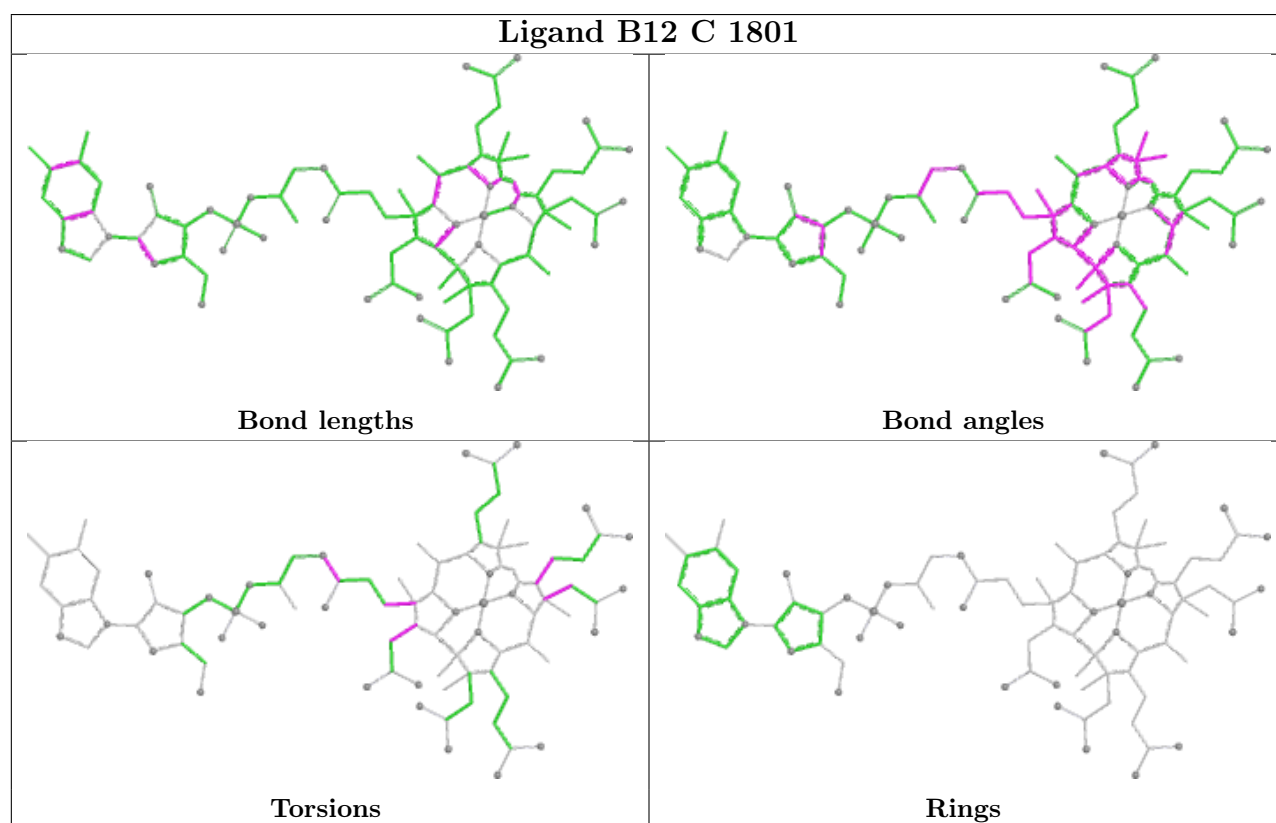
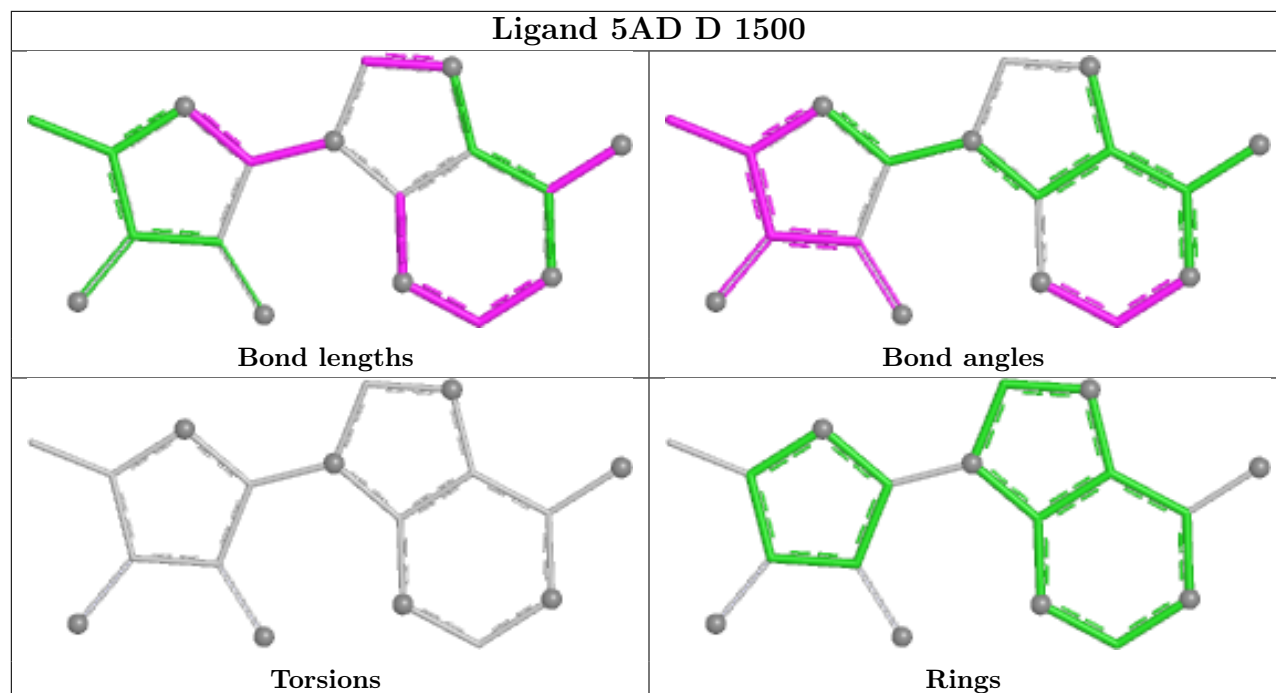
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

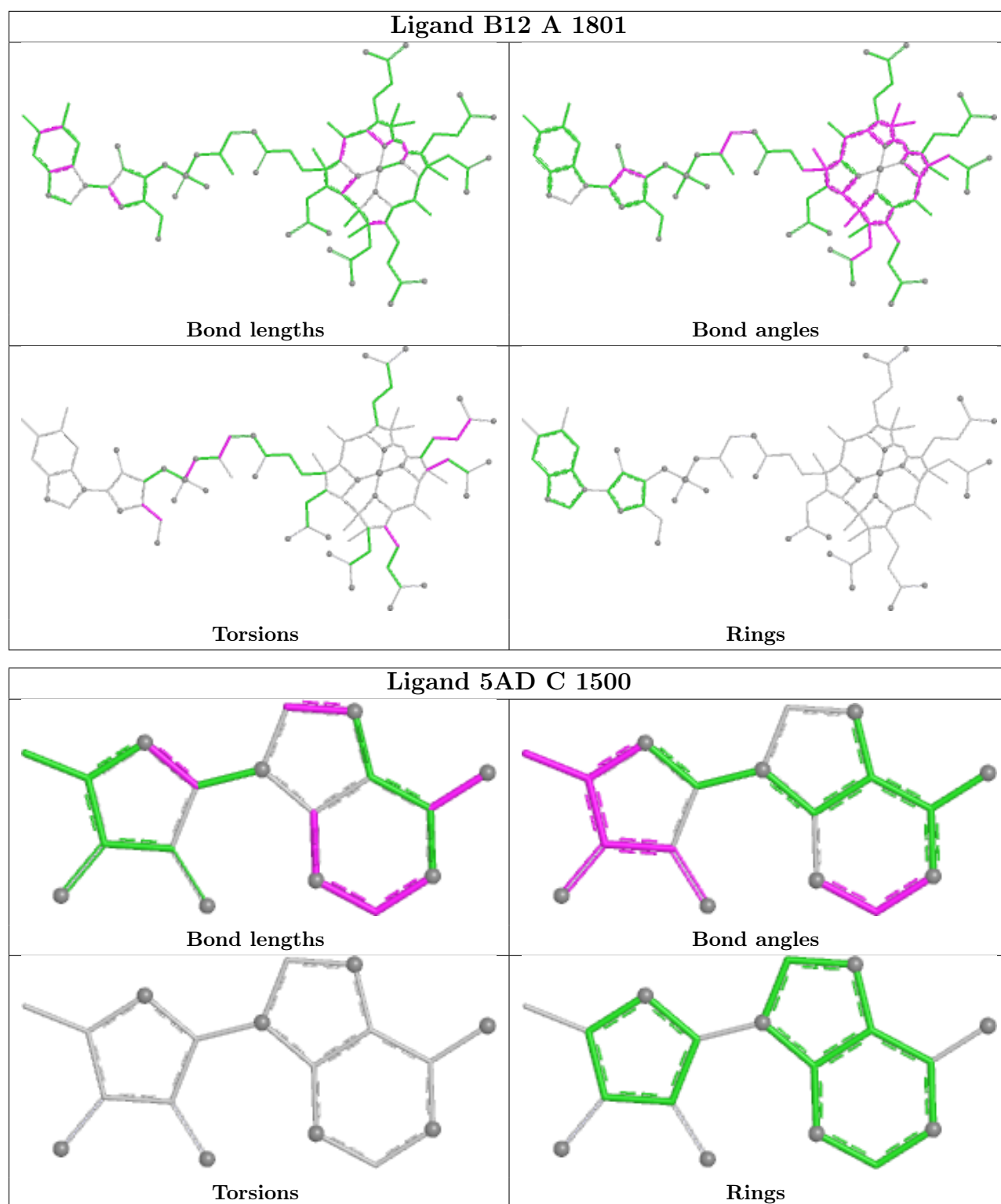
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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











## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	727/763 (95%)	-0.33	5 (0%) 84 80	16, 37, 90, 105	0
1	B	728/763 (95%)	-0.57	1 (0%) 92 92	15, 32, 54, 72	0
1	C	727/763 (95%)	-0.45	2 (0%) 90 88	17, 38, 65, 84	0
1	D	727/763 (95%)	-0.40	13 (1%) 67 61	15, 30, 93, 118	0
2	E	109/121 (90%)	-0.44	0 100 100	22, 39, 59, 75	0
2	F	109/121 (90%)	-0.47	0 100 100	19, 32, 53, 69	0
2	G	109/121 (90%)	-0.37	0 100 100	25, 44, 62, 68	0
2	H	109/121 (90%)	-0.48	0 100 100	15, 31, 55, 72	0
All	All	3345/3536 (94%)	-0.44	21 (0%) 85 82	15, 35, 79, 118	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	LEU	3.6
1	D	599	GLU	3.4
1	D	717	ALA	3.0
1	D	692	ILE	2.8
1	C	5	LEU	2.8
1	D	688	VAL	2.8
1	D	587	PRO	2.6
1	D	597	ILE	2.6
1	D	738	GLU	2.5
1	D	602	GLU	2.4
1	D	709	VAL	2.2
1	A	688	VAL	2.2
1	A	614	GLY	2.2
1	A	692	ILE	2.2
1	D	718	GLY	2.1
1	C	14	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	605	PRO	2.1
1	A	739	MET	2.1
1	D	739	MET	2.1
1	D	592	LEU	2.0
1	A	672	HIS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

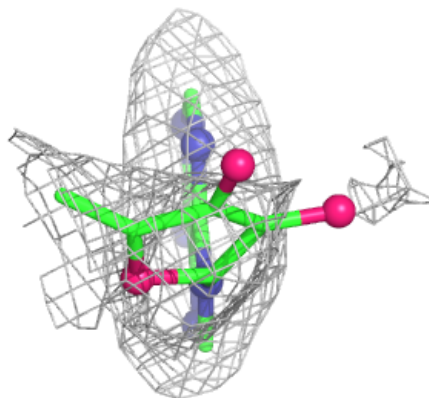
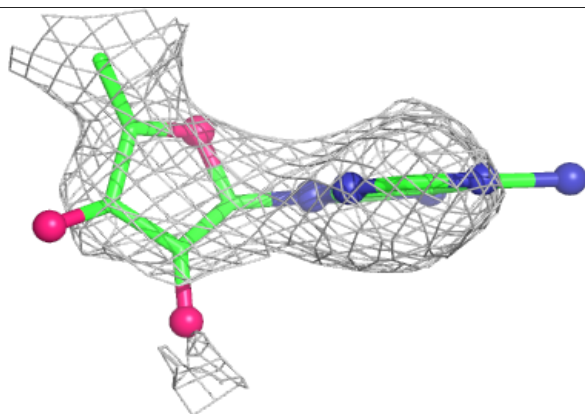
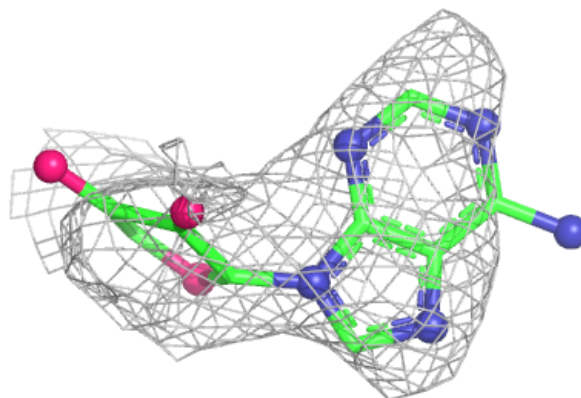
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	5AD	C	1500	18/18	0.76	0.13	68,80,83,86	0
5	5AD	A	1500	18/18	0.85	0.11	37,56,61,65	0
5	5AD	D	1500	18/18	0.91	0.09	27,44,50,51	0
3	B12	A	1801	91/91	0.93	0.11	41,65,75,82	0
3	B12	D	1801	91/91	0.94	0.10	37,56,69,77	0
4	PLP	D	1802	15/16	0.95	0.07	25,32,38,43	0
4	PLP	B	1802	15/16	0.96	0.07	18,27,36,37	0
4	PLP	C	1802	15/16	0.96	0.07	27,29,36,37	0
4	PLP	A	1802	15/16	0.96	0.07	30,37,49,52	0
3	B12	B	1801	91/91	0.97	0.07	16,28,35,38	0
3	B12	C	1801	91/91	0.97	0.09	17,35,43,50	0

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

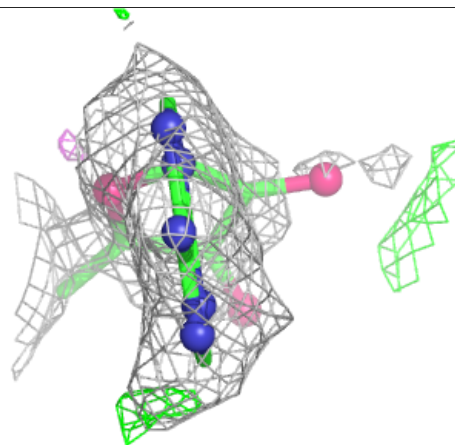
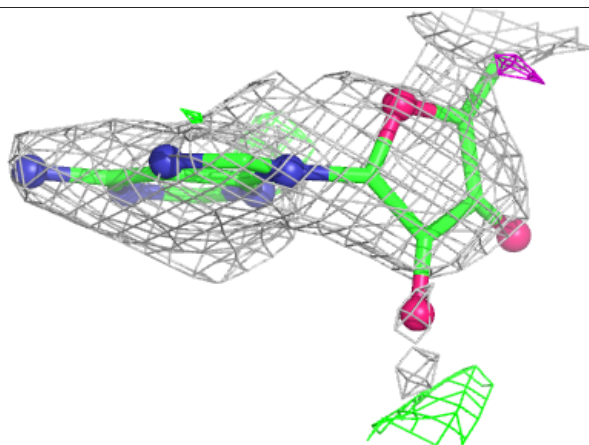
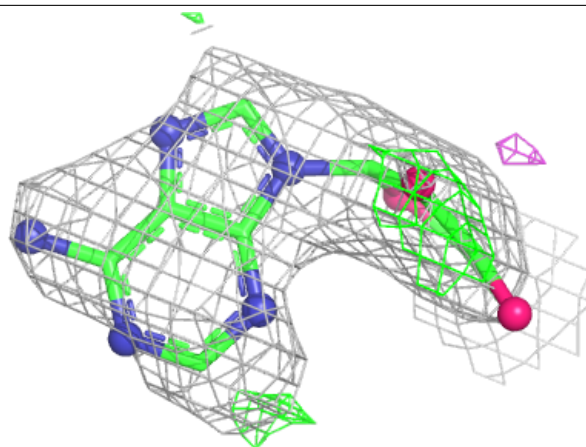
**Electron density around 5AD C 1500:**

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

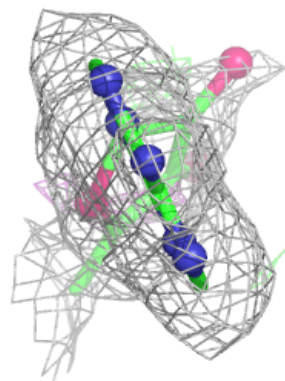
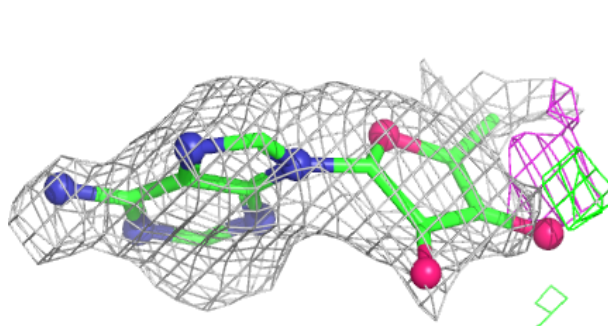
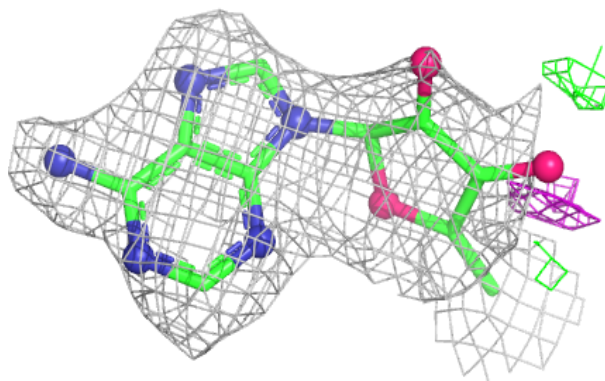


**Electron density around 5AD A 1500:**

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

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

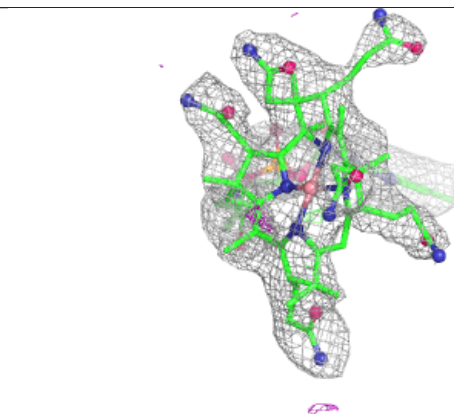
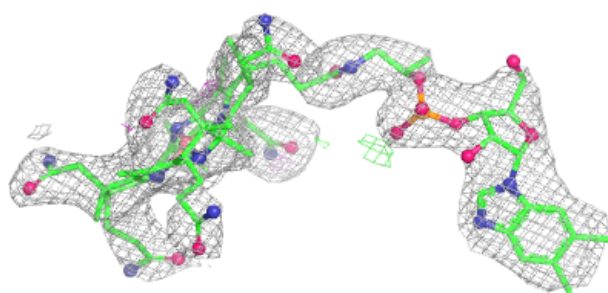
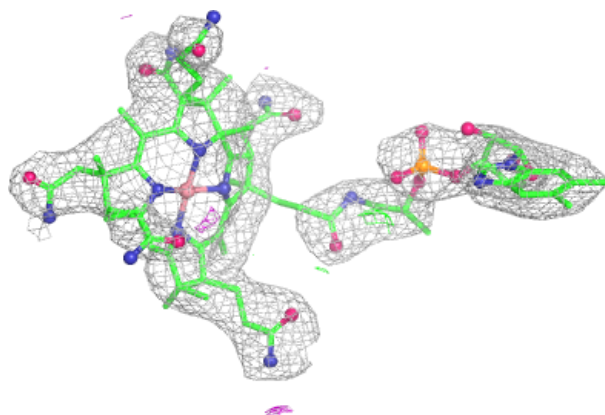
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



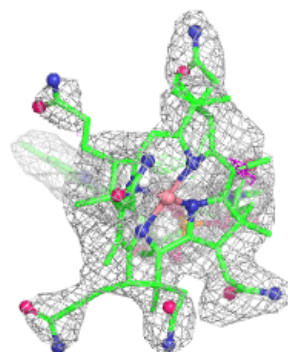
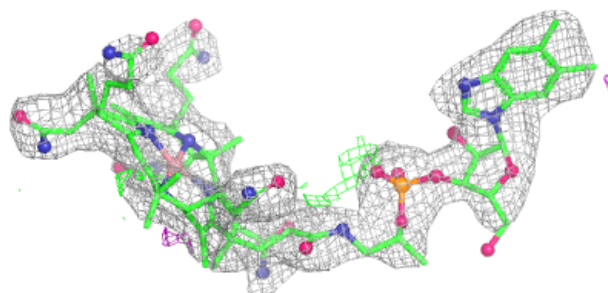
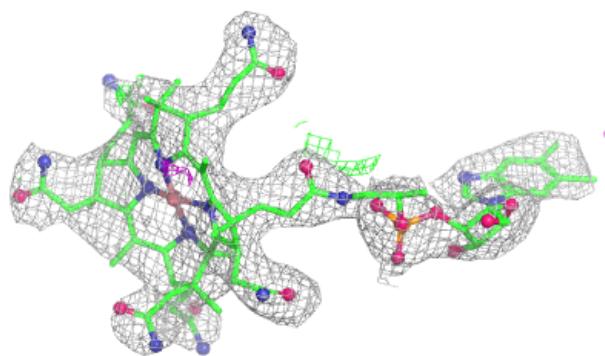


**Electron density around B12 A 1801:**

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

**Electron density around B12 D 1801:**

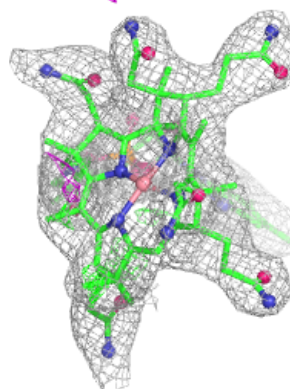
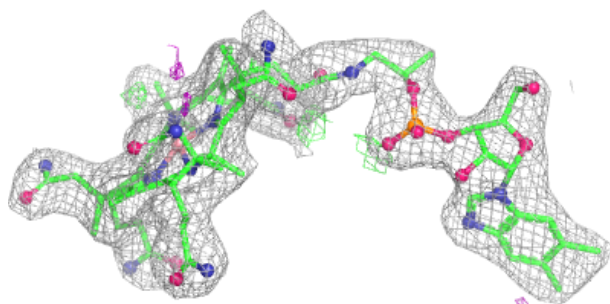
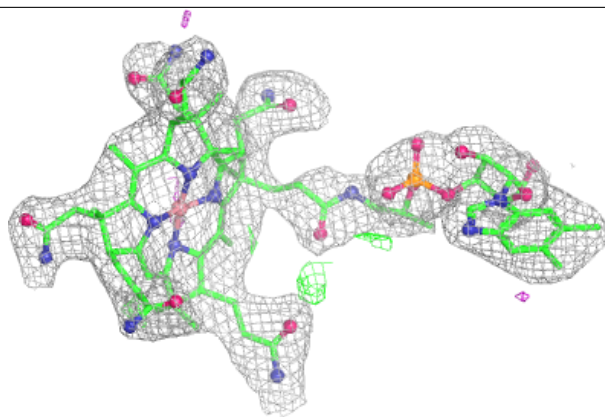
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



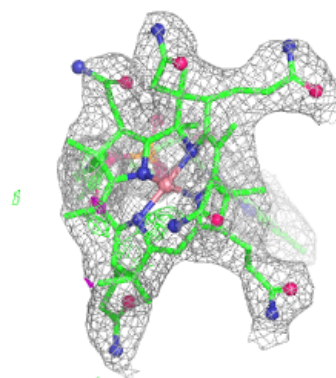
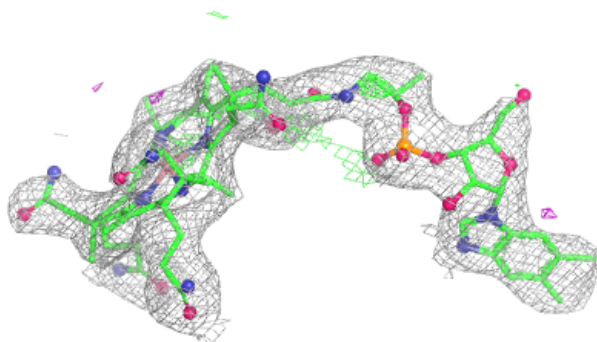
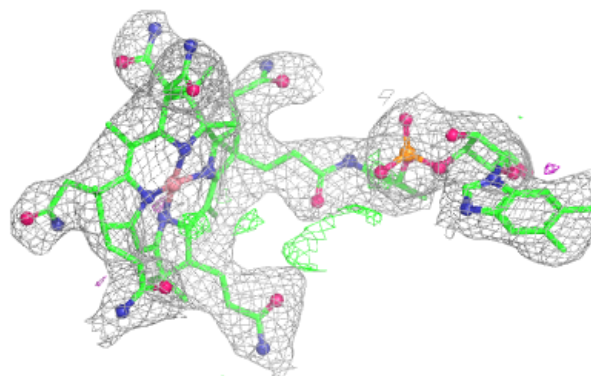


**Electron density around B12 B 1801:**

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

**Electron density around B12 C 1801:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.