



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:22 pm BST

PDB ID : 1RG9  
Title : S-Adenosylmethionine synthetase complexed with SAM and PPNP  
Authors : Komoto, J.; Yamada, T.; Takata, Y.; Markham, G.D.; Takusagawa, F.  
Deposited on : 2003-11-11  
Resolution : 2.50 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.

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

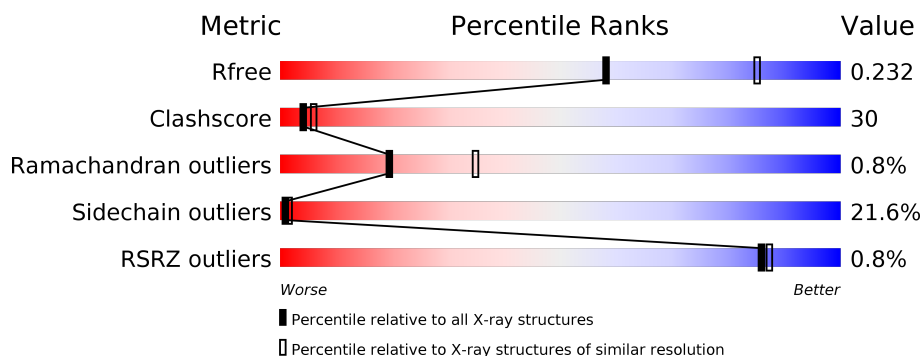
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	383	<div> <div>52%</div> <div>37%</div> <div>11%</div> </div>
1	B	383	<div> <div>50%</div> <div>39%</div> <div>11%</div> </div>
1	C	383	<div> <div>49%</div> <div>38%</div> <div>13%</div> </div>
1	D	383	<div> <div>51%</div> <div>37%</div> <div>11%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PPK	A	384	-	-	X	-
5	PPK	B	484	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11960 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 S-adenosylmethionine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			2942	1856	503	570	13			
1	B	383	Total	C	N	O	S	0	0	0
			2942	1856	503	570	13			
1	C	383	Total	C	N	O	S	0	0	0
			2942	1856	503	570	13			
1	D	383	Total	C	N	O	S	0	0	0
			2942	1856	503	570	13			

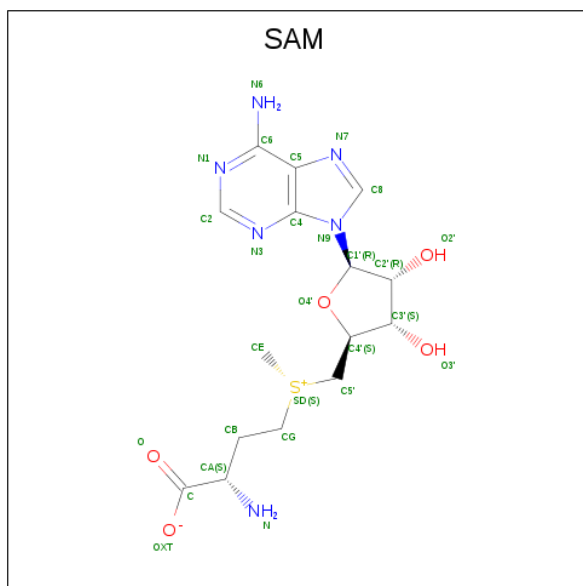
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

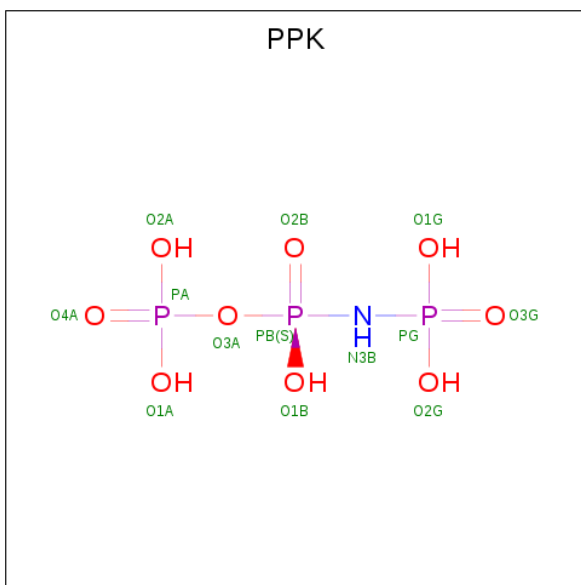
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula:  $C_{15}H_{22}N_6O_5S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 5 is (DIPHOSPHONO)AMINOPHOSPHONIC ACID (three-letter code: PPK) (formula:  $H_6NO_9P_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	N	O	P	0	0
			13	1	9	3		
5	B	1	Total	N	O	P	0	0
			13	1	9	3		
5	C	1	Total	N	O	P	0	0
			13	1	9	3		
5	D	1	Total	N	O	P	0	0
			13	1	9	3		

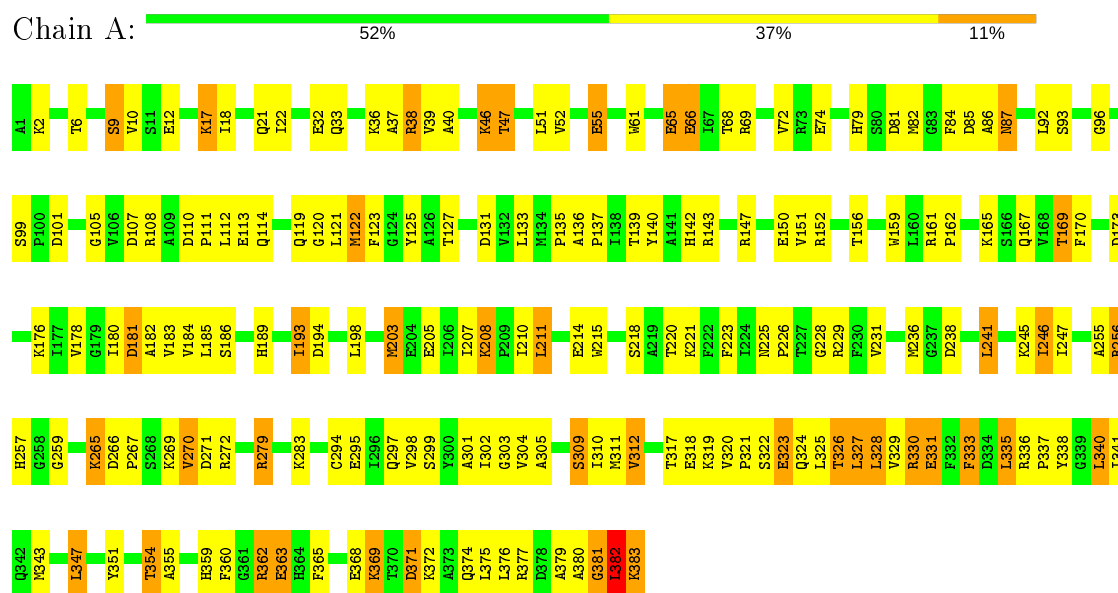
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	3	Total	O	0	0
			3	3		
6	C	7	Total	O	0	0
			7	7		
6	D	4	Total	O	0	0
			4	4		

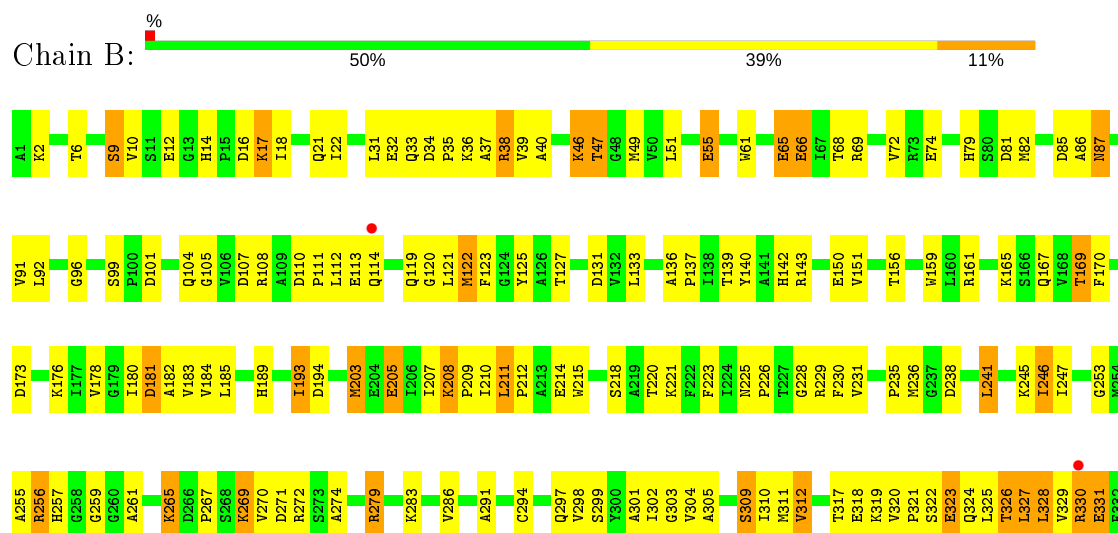
### 3 Residue-property plots

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

#### • Molecule 1: S-adenosylmethionine synthetase

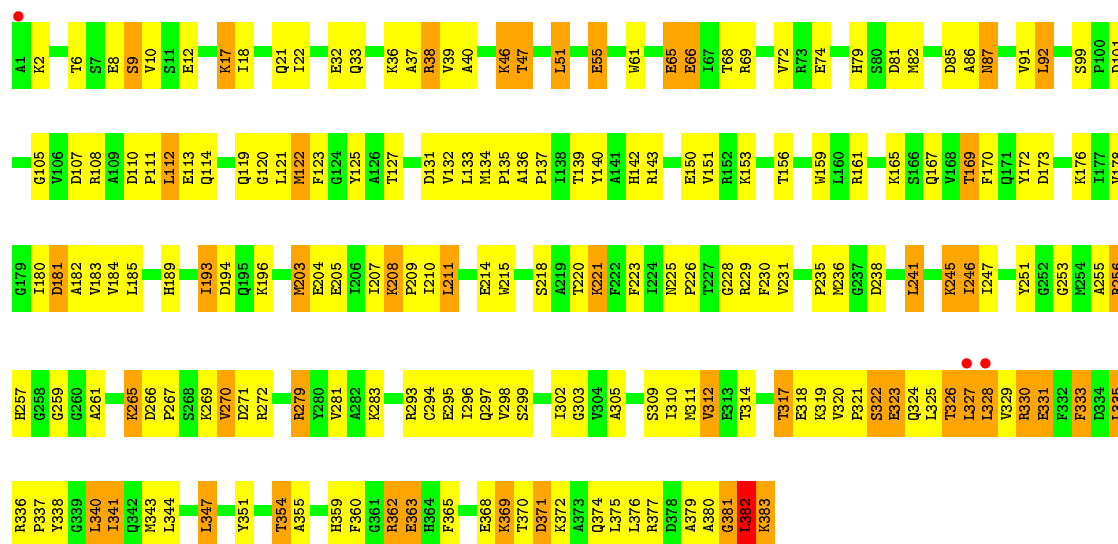


#### • Molecule 1: S-adenosylmethionine synthetase

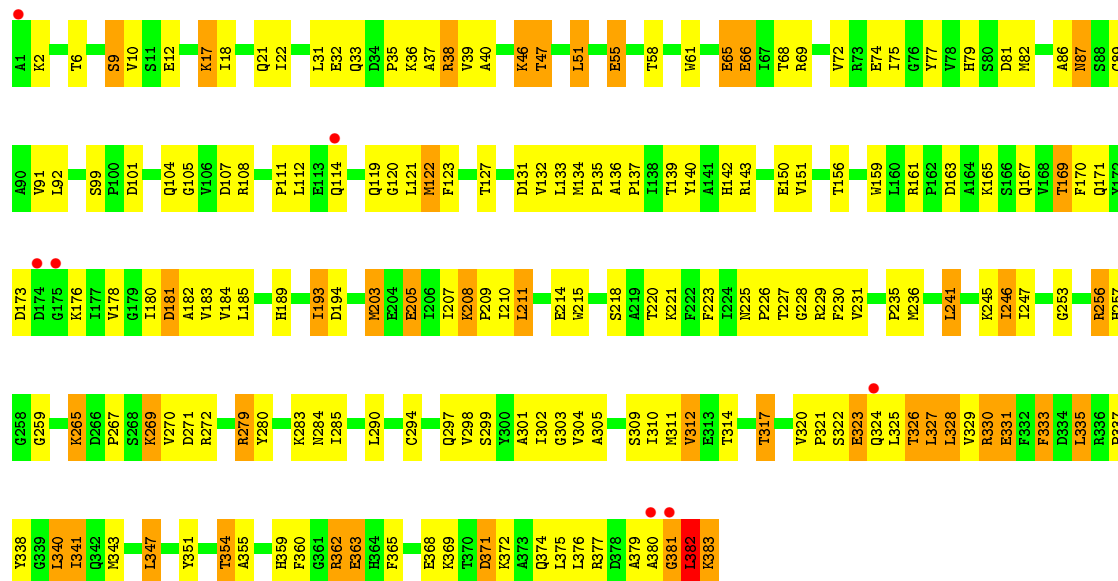




• Molecule 1: S-adenosylmethionine synthetase



• Molecule 1: S-adenosylmethionine synthetase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	225.82Å 69.13Å 118.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.99 – 2.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 71.3 (10.99-2.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.39 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.211 , 0.241 0.205 , 0.232	Depositor DCC
$R_{free}$ test set	4574 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8888e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PPK, K, MG, SAM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.43	0/3001	0.65	0/4068
1	B	0.41	0/3001	0.64	0/4068
1	C	0.40	0/3001	0.63	0/4068
1	D	0.39	0/3001	0.63	0/4068
All	All	0.41	0/12004	0.64	0/16272

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	2942	0	2908	181	0
1	B	2942	0	2908	184	0
1	C	2942	0	2908	197	0
1	D	2942	0	2908	180	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	27	0	22	2	0
4	B	27	0	22	2	0
4	C	54	0	44	2	0
5	A	13	0	1	4	0
5	B	13	0	1	4	0
5	C	13	0	1	3	0
5	D	13	0	1	3	0
6	A	6	0	0	0	0
6	B	3	0	0	0	0
6	C	7	0	0	1	0
6	D	4	0	0	1	0
All	All	11960	0	11724	705	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 30.

All (705) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:LEU:HD11	1:D:241:LEU:HD11	1.34	1.06
1:A:10:VAL:HG12	1:A:165:LYS:HG2	1.43	0.99
1:B:122:MET:HG2	1:B:298:VAL:HG23	1.46	0.98
1:B:10:VAL:HG12	1:B:165:LYS:HG2	1.45	0.97
1:D:10:VAL:HG12	1:D:165:LYS:HG2	1.47	0.96
1:C:107:ASP:HA	1:C:114:GLN:HE21	1.34	0.93
1:A:241:LEU:HD11	1:B:241:LEU:HD11	1.50	0.92
1:B:267:PRO:HB2	1:B:341:ILE:HD13	1.52	0.92
1:B:72:VAL:HG12	1:B:86:ALA:HB2	1.51	0.92
1:D:72:VAL:HG12	1:D:86:ALA:HB2	1.52	0.92
1:A:122:MET:HG2	1:A:298:VAL:HG23	1.51	0.90
1:D:107:ASP:HA	1:D:114:GLN:HE21	1.36	0.90
1:C:10:VAL:HG12	1:C:165:LYS:HG2	1.53	0.90
1:A:107:ASP:HA	1:A:114:GLN:HE21	1.34	0.89
5:C:584:PPK:H3B	1:D:265:LYS:NZ	1.71	0.88
1:B:107:ASP:HA	1:B:114:GLN:HE21	1.37	0.88
1:D:122:MET:HG2	1:D:298:VAL:HG23	1.56	0.88
1:B:79:HIS:HD2	1:B:81:ASP:H	1.19	0.87
1:B:167:GLN:HB3	1:B:184:VAL:HB	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLN:NE2	1:B:61:TRP:H	1.73	0.86
1:D:267:PRO:HB2	1:D:341:ILE:HD13	1.58	0.86
1:C:122:MET:HG2	1:C:298:VAL:HG23	1.56	0.85
1:C:267:PRO:HB2	1:C:341:ILE:HD13	1.57	0.85
1:A:330:ARG:HH21	1:A:331:GLU:HA	1.40	0.85
1:A:72:VAL:HG12	1:A:86:ALA:HB2	1.57	0.85
1:B:330:ARG:HH21	1:B:331:GLU:HA	1.41	0.85
1:A:267:PRO:HB2	1:A:341:ILE:HD13	1.59	0.85
1:B:33:GLN:HE22	1:B:61:TRP:H	1.20	0.85
1:D:330:ARG:HH21	1:D:331:GLU:HA	1.40	0.84
1:C:330:ARG:HH21	1:C:331:GLU:HA	1.40	0.84
1:A:33:GLN:NE2	1:A:61:TRP:H	1.76	0.84
1:C:139:THR:O	1:C:143:ARG:HG3	1.77	0.84
1:C:79:HIS:HD2	1:C:81:ASP:H	1.22	0.84
1:A:33:GLN:HE22	1:A:61:TRP:H	1.24	0.83
1:C:72:VAL:HG12	1:C:86:ALA:HB2	1.60	0.83
1:A:167:GLN:HB3	1:A:184:VAL:HB	1.58	0.83
1:A:382:LEU:HG	1:A:383:LYS:N	1.92	0.82
1:D:79:HIS:HD2	1:D:81:ASP:H	1.26	0.82
1:C:167:GLN:HB3	1:C:184:VAL:HB	1.62	0.82
1:C:265:LYS:NZ	5:D:684:PPK:H3B	1.78	0.81
1:B:257:HIS:HD2	1:B:259:GLY:H	1.28	0.81
1:C:151:VAL:HG23	1:C:156:THR:HB	1.61	0.81
1:C:257:HIS:HD2	1:C:259:GLY:H	1.28	0.81
1:B:79:HIS:CD2	1:B:81:ASP:H	1.98	0.81
1:D:12:GLU:HB2	1:D:21:GLN:HE22	1.45	0.80
1:D:257:HIS:HD2	1:D:259:GLY:H	1.29	0.80
1:D:167:GLN:HB3	1:D:184:VAL:HB	1.64	0.79
1:B:12:GLU:HB2	1:B:21:GLN:HE22	1.48	0.79
1:C:382:LEU:HG	1:C:383:LYS:N	1.96	0.79
1:D:139:THR:O	1:D:143:ARG:HG3	1.83	0.79
1:A:312:VAL:HG13	1:A:326:THR:HG23	1.64	0.78
1:A:330:ARG:HE	1:A:331:GLU:N	1.80	0.78
1:A:79:HIS:HD2	1:A:81:ASP:H	1.28	0.78
1:C:79:HIS:CD2	1:C:81:ASP:H	2.01	0.78
1:A:257:HIS:HD2	1:A:259:GLY:H	1.30	0.77
1:B:151:VAL:HG23	1:B:156:THR:HB	1.64	0.77
1:D:33:GLN:NE2	1:D:61:TRP:H	1.82	0.77
1:C:351:TYR:O	1:C:354:THR:HG22	1.84	0.77
1:D:382:LEU:HG	1:D:383:LYS:N	1.97	0.77
1:A:151:VAL:HG23	1:A:156:THR:HB	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:GLU:HB2	1:C:21:GLN:HE22	1.47	0.77
1:B:139:THR:O	1:B:143:ARG:HG3	1.85	0.77
1:B:133:LEU:HD23	1:B:283:LYS:HE2	1.66	0.77
1:D:330:ARG:HE	1:D:331:GLU:N	1.82	0.77
1:D:33:GLN:HE22	1:D:61:TRP:H	1.30	0.76
1:C:330:ARG:HE	1:C:331:GLU:N	1.83	0.76
1:D:22:ILE:HD13	1:D:68:THR:HG23	1.68	0.76
1:C:121:LEU:HD13	1:D:6:THR:O	1.86	0.76
1:B:330:ARG:HE	1:B:331:GLU:N	1.84	0.75
5:C:584:PPK:H3B	1:D:265:LYS:HZ2	1.33	0.75
1:B:22:ILE:HD13	1:B:68:THR:HG23	1.67	0.75
1:D:79:HIS:CD2	1:D:81:ASP:H	2.04	0.75
1:A:79:HIS:CD2	1:A:81:ASP:H	2.04	0.75
1:B:312:VAL:HG13	1:B:326:THR:HG23	1.69	0.75
1:A:139:THR:O	1:A:143:ARG:HG3	1.87	0.75
1:B:347:LEU:HD22	1:B:347:LEU:H	1.50	0.74
1:C:33:GLN:HE22	1:C:61:TRP:H	1.31	0.74
1:C:226:PRO:HB2	1:D:302:ILE:O	1.87	0.74
1:C:312:VAL:HG13	1:C:326:THR:HG23	1.69	0.74
1:A:12:GLU:HB2	1:A:21:GLN:HE22	1.51	0.74
1:D:133:LEU:HD23	1:D:283:LYS:HE2	1.68	0.74
1:C:33:GLN:NE2	1:C:61:TRP:H	1.85	0.73
1:C:241:LEU:HG	1:D:241:LEU:HG	1.70	0.73
1:B:351:TYR:O	1:B:354:THR:HG22	1.89	0.73
1:D:351:TYR:O	1:D:354:THR:HG22	1.89	0.72
1:A:351:TYR:O	1:A:354:THR:HG22	1.88	0.72
1:C:6:THR:O	1:D:121:LEU:HD13	1.88	0.72
1:B:382:LEU:HG	1:B:383:LYS:N	2.02	0.72
1:D:320:VAL:HB	1:D:324:GLN:NE2	2.05	0.72
1:D:330:ARG:HH21	1:D:331:GLU:CA	2.02	0.72
1:C:302:ILE:O	1:D:226:PRO:HB2	1.90	0.72
1:A:22:ILE:HD13	1:A:68:THR:HG23	1.70	0.71
1:C:22:ILE:HD13	1:C:68:THR:HG23	1.72	0.71
1:B:330:ARG:HH21	1:B:331:GLU:CA	2.02	0.71
1:B:17:LYS:O	1:B:21:GLN:HG3	1.89	0.71
1:D:151:VAL:HG23	1:D:156:THR:HB	1.73	0.71
1:C:328:LEU:HD23	1:C:376:LEU:HD22	1.73	0.70
1:A:265:LYS:NZ	5:B:484:PPK:H3B	1.90	0.69
1:C:305:ALA:O	1:C:337:PRO:HD2	1.92	0.69
1:C:133:LEU:HD23	1:C:283:LYS:HE2	1.74	0.69
1:A:69:ARG:HD3	1:A:86:ALA:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ILE:HG12	1:C:194:ASP:N	2.07	0.69
1:C:184:VAL:HG22	1:C:223:PHE:HB2	1.75	0.69
1:D:337:PRO:HB2	1:D:338:TYR:CD1	2.27	0.69
1:B:6:THR:HG23	1:B:169:THR:HG22	1.74	0.69
1:A:330:ARG:HH21	1:A:331:GLU:CA	2.06	0.68
1:D:312:VAL:HG13	1:D:326:THR:HG23	1.74	0.68
1:B:69:ARG:HD3	1:B:86:ALA:O	1.93	0.68
1:C:330:ARG:HH21	1:C:331:GLU:CA	2.04	0.68
1:D:305:ALA:O	1:D:337:PRO:HD2	1.94	0.68
1:C:257:HIS:CD2	1:C:259:GLY:H	2.12	0.67
1:B:305:ALA:O	1:B:337:PRO:HD2	1.95	0.67
1:A:305:ALA:O	1:A:337:PRO:HD2	1.94	0.67
1:C:328:LEU:HD11	1:C:379:ALA:CB	2.24	0.67
1:C:320:VAL:HB	1:C:324:GLN:NE2	2.10	0.66
1:A:347:LEU:H	1:A:347:LEU:HD22	1.59	0.66
1:B:184:VAL:HG22	1:B:223:PHE:HB2	1.75	0.66
5:C:584:PPK:N3B	1:D:265:LYS:NZ	2.43	0.66
1:D:330:ARG:NH2	1:D:331:GLU:HG3	2.09	0.66
1:D:257:HIS:CD2	1:D:259:GLY:H	2.13	0.66
1:D:328:LEU:HD23	1:D:376:LEU:HD22	1.77	0.66
1:D:298:VAL:HG12	1:D:310:ILE:HG12	1.77	0.66
1:B:257:HIS:CD2	1:B:259:GLY:H	2.11	0.66
1:B:328:LEU:HD23	1:B:376:LEU:HD22	1.78	0.66
1:C:225:ASN:N	1:C:226:PRO:HD3	2.10	0.66
1:D:225:ASN:N	1:D:226:PRO:HD3	2.11	0.65
1:A:17:LYS:O	1:A:21:GLN:HG3	1.96	0.65
1:D:184:VAL:HG22	1:D:223:PHE:HB2	1.78	0.65
1:B:320:VAL:HB	1:B:324:GLN:NE2	2.11	0.65
1:A:133:LEU:HD23	1:A:283:LYS:HE2	1.77	0.65
1:A:184:VAL:HG22	1:A:223:PHE:HB2	1.78	0.65
1:B:225:ASN:N	1:B:226:PRO:HD3	2.12	0.65
1:D:46:LYS:HD3	1:D:47:THR:HG23	1.79	0.65
1:C:17:LYS:O	1:C:21:GLN:HG3	1.96	0.65
1:B:279:ARG:HD3	1:B:368:GLU:OE1	1.96	0.64
1:B:362:ARG:HG3	1:B:365:PHE:CE2	2.31	0.64
1:C:279:ARG:HD3	1:C:368:GLU:OE1	1.97	0.64
1:A:320:VAL:HB	1:A:324:GLN:NE2	2.13	0.64
1:C:241:LEU:HD11	1:D:241:LEU:CD1	2.22	0.64
1:D:328:LEU:HD11	1:D:379:ALA:CB	2.26	0.64
1:A:354:THR:HG23	1:A:359:HIS:CE1	2.33	0.64
1:C:328:LEU:HD11	1:C:379:ALA:HB1	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:PRO:HB2	1:D:338:TYR:HD1	1.61	0.64
1:C:165:LYS:HE2	1:D:119:GLN:HG2	1.80	0.64
1:A:279:ARG:HD3	1:A:368:GLU:OE1	1.97	0.63
1:D:18:ILE:O	1:D:22:ILE:HG13	1.99	0.63
1:D:327:LEU:HA	1:D:330:ARG:HD3	1.80	0.63
1:B:298:VAL:HG12	1:B:310:ILE:HG12	1.80	0.63
1:B:337:PRO:HB2	1:B:338:TYR:CD1	2.33	0.63
1:C:265:LYS:HZ2	5:D:684:PPK:H3B	1.43	0.63
1:C:181:ASP:O	1:C:220:THR:HA	1.98	0.63
1:C:337:PRO:HB2	1:C:338:TYR:CD1	2.34	0.63
1:B:46:LYS:HD3	1:B:47:THR:HG23	1.80	0.63
1:C:298:VAL:HG12	1:C:310:ILE:HG12	1.80	0.63
1:A:337:PRO:HB2	1:A:338:TYR:CD1	2.33	0.62
1:A:111:PRO:HA	1:A:114:GLN:HG3	1.80	0.62
1:A:6:THR:HG23	1:A:169:THR:HG22	1.81	0.62
1:B:33:GLN:HE22	1:B:61:TRP:N	1.96	0.62
1:D:328:LEU:HD11	1:D:379:ALA:HB1	1.80	0.62
1:A:225:ASN:N	1:A:226:PRO:HD3	2.14	0.62
1:D:143:ARG:HB3	1:D:210:ILE:HD12	1.82	0.62
1:C:327:LEU:HA	1:C:330:ARG:HD3	1.81	0.62
1:C:151:VAL:CG2	1:C:156:THR:HB	2.28	0.62
1:D:17:LYS:O	1:D:21:GLN:HG3	1.99	0.62
1:D:69:ARG:HD3	1:D:86:ALA:O	1.98	0.62
1:A:257:HIS:CD2	1:A:259:GLY:H	2.14	0.62
1:B:354:THR:HG23	1:B:359:HIS:CE1	2.34	0.62
1:A:328:LEU:HD23	1:A:376:LEU:HD22	1.81	0.62
4:A:385:SAM:H4'	5:A:384:PPK:O4A	2.00	0.62
1:A:121:LEU:HD13	1:B:6:THR:O	2.00	0.61
1:B:246:ILE:HG23	1:B:257:HIS:CE1	2.34	0.61
1:A:238:ASP:OD2	4:A:385:SAM:H5'2	1.99	0.61
1:B:111:PRO:HA	1:B:114:GLN:HG3	1.80	0.61
5:A:384:PPK:H3B	1:B:265:LYS:NZ	1.98	0.61
1:B:18:ILE:O	1:B:22:ILE:HG13	2.01	0.61
1:B:347:LEU:N	1:B:347:LEU:HD22	2.16	0.61
1:B:327:LEU:HA	1:B:330:ARG:HD3	1.83	0.61
1:D:363:GLU:HA	1:D:368:GLU:HB3	1.83	0.61
1:A:327:LEU:HA	1:A:330:ARG:HD3	1.83	0.61
1:C:105:GLY:O	1:C:303:GLY:HA2	2.01	0.60
1:B:207:ILE:HG23	1:B:211:LEU:HD22	1.82	0.60
1:A:46:LYS:HD3	1:A:47:THR:HG23	1.82	0.60
1:A:321:PRO:HD2	1:A:324:GLN:NE2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ILE:HG12	1:D:194:ASP:N	2.16	0.60
1:C:38:ARG:N	1:C:38:ARG:HD2	2.16	0.60
1:C:265:LYS:NZ	5:D:684:PPK:N3B	2.49	0.60
1:A:105:GLY:O	1:A:303:GLY:HA2	2.01	0.60
1:C:324:GLN:O	1:C:328:LEU:HB2	2.02	0.59
1:A:143:ARG:HB3	1:A:210:ILE:HD12	1.83	0.59
1:A:193:ILE:HG12	1:A:194:ASP:N	2.17	0.59
1:C:207:ILE:HG23	1:C:211:LEU:HD22	1.82	0.59
1:B:105:GLY:O	1:B:303:GLY:HA2	2.01	0.59
1:B:38:ARG:HD2	1:B:38:ARG:N	2.16	0.59
1:C:253:GLY:O	1:D:256:ARG:HG2	2.02	0.59
1:A:272:ARG:HH21	1:A:354:THR:HG21	1.68	0.59
1:D:333:PHE:HZ	1:D:376:LEU:HD11	1.67	0.59
1:C:38:ARG:NH1	1:C:107:ASP:OD1	2.36	0.59
1:B:193:ILE:HG12	1:B:194:ASP:N	2.17	0.58
1:D:279:ARG:HD3	1:D:368:GLU:OE1	2.03	0.58
1:A:183:VAL:HG11	1:A:207:ILE:HD13	1.85	0.58
1:D:105:GLY:O	1:D:303:GLY:HA2	2.04	0.58
1:D:203:MET:O	1:D:208:LYS:HB2	2.03	0.58
1:B:267:PRO:HB2	1:B:341:ILE:CD1	2.31	0.58
1:B:324:GLN:O	1:B:328:LEU:HB2	2.03	0.58
1:C:246:ILE:HG22	1:C:247:ILE:N	2.18	0.58
1:D:347:LEU:H	1:D:347:LEU:HD22	1.69	0.58
1:D:38:ARG:N	1:D:38:ARG:HD2	2.18	0.58
1:C:362:ARG:HG3	1:C:365:PHE:CE2	2.39	0.58
1:A:137:PRO:HA	1:A:170:PHE:CE1	2.39	0.58
1:A:328:LEU:HD11	1:A:379:ALA:CB	2.34	0.58
1:B:203:MET:O	1:B:208:LYS:HB2	2.04	0.58
1:C:183:VAL:HG11	1:C:207:ILE:HD13	1.86	0.58
1:D:135:PRO:O	1:D:139:THR:HG23	2.04	0.58
1:C:256:ARG:HG2	1:D:253:GLY:O	2.04	0.57
1:C:101:ASP:CG	1:D:229:ARG:HG2	2.25	0.57
1:D:111:PRO:HA	1:D:114:GLN:HG3	1.86	0.57
1:D:9:SER:OG	1:D:142:HIS:ND1	2.37	0.57
1:A:324:GLN:O	1:A:328:LEU:HB2	2.04	0.57
1:D:181:ASP:O	1:D:220:THR:HA	2.04	0.57
1:A:127:THR:O	1:A:133:LEU:HA	2.04	0.57
1:B:238:ASP:OD2	4:B:485:SAM:H5'2	2.04	0.57
1:B:143:ARG:HB3	1:B:210:ILE:HD12	1.86	0.57
1:C:111:PRO:HA	1:C:114:GLN:HG3	1.87	0.57
1:B:159:TRP:CE2	1:B:193:ILE:HD12	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ASP:O	1:B:220:THR:HA	2.04	0.56
1:B:328:LEU:HD11	1:B:379:ALA:CB	2.35	0.56
1:C:347:LEU:HD22	1:C:347:LEU:H	1.70	0.56
1:D:246:ILE:HG22	1:D:247:ILE:HG12	1.86	0.56
1:C:143:ARG:HB3	1:C:210:ILE:HD12	1.87	0.56
1:A:302:ILE:O	1:B:226:PRO:HB2	2.06	0.56
1:D:246:ILE:HG22	1:D:247:ILE:N	2.20	0.56
1:C:6:THR:HG23	1:C:169:THR:HG22	1.88	0.56
1:D:38:ARG:NH1	1:D:107:ASP:OD1	2.39	0.56
1:A:246:ILE:HG23	1:A:257:HIS:CE1	2.41	0.56
1:A:363:GLU:HA	1:A:368:GLU:HB3	1.88	0.56
1:A:328:LEU:HD11	1:A:379:ALA:HB1	1.87	0.56
1:B:363:GLU:HA	1:B:368:GLU:HB3	1.88	0.56
1:C:69:ARG:HD3	1:C:86:ALA:O	2.06	0.56
1:D:324:GLN:O	1:D:328:LEU:HB2	2.06	0.56
1:D:323:GLU:HG2	1:D:324:GLN:N	2.19	0.56
1:A:337:PRO:HB2	1:A:338:TYR:HD1	1.71	0.56
1:C:321:PRO:HD2	1:C:324:GLN:NE2	2.21	0.56
1:C:330:ARG:NH2	1:C:331:GLU:HG3	2.21	0.55
1:C:363:GLU:HA	1:C:368:GLU:HB3	1.89	0.55
1:C:203:MET:O	1:C:208:LYS:HB2	2.06	0.55
1:D:362:ARG:HG3	1:D:365:PHE:CE2	2.41	0.55
1:D:371:ASP:OD1	1:D:371:ASP:N	2.37	0.55
1:A:39:VAL:O	1:A:265:LYS:HA	2.06	0.55
1:C:39:VAL:O	1:C:265:LYS:HA	2.06	0.55
1:B:328:LEU:HD11	1:B:379:ALA:HB1	1.88	0.55
1:C:18:ILE:O	1:C:22:ILE:HG13	2.07	0.55
1:B:127:THR:O	1:B:133:LEU:HA	2.06	0.55
1:B:151:VAL:CG2	1:B:156:THR:HB	2.36	0.55
1:A:151:VAL:CG2	1:A:156:THR:HB	2.36	0.55
1:B:272:ARG:HH21	1:B:354:THR:HG21	1.72	0.55
1:B:46:LYS:HD3	1:B:47:THR:H	1.72	0.54
1:D:330:ARG:HH21	1:D:331:GLU:HG3	1.69	0.54
1:B:38:ARG:NH1	1:B:107:ASP:OD1	2.40	0.54
1:D:127:THR:O	1:D:133:LEU:HA	2.06	0.54
1:A:38:ARG:N	1:A:38:ARG:HD2	2.22	0.54
1:C:272:ARG:HH21	1:C:354:THR:HG21	1.72	0.54
1:A:135:PRO:O	1:A:139:THR:HG23	2.06	0.54
1:B:333:PHE:HZ	1:B:376:LEU:HD11	1.73	0.54
1:D:321:PRO:HD2	1:D:324:GLN:NE2	2.22	0.54
1:A:203:MET:O	1:A:208:LYS:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:NH2	1:A:331:GLU:HG3	2.23	0.54
1:D:46:LYS:HD3	1:D:47:THR:H	1.71	0.54
1:A:347:LEU:N	1:A:347:LEU:HD22	2.23	0.54
1:B:137:PRO:HA	1:B:170:PHE:CE1	2.43	0.54
1:B:340:LEU:HA	1:B:343:MET:HB3	1.89	0.54
1:B:337:PRO:HB2	1:B:338:TYR:HD1	1.73	0.54
1:C:151:VAL:HG23	1:C:156:THR:CB	2.33	0.54
1:C:46:LYS:HD3	1:C:47:THR:HG23	1.90	0.54
1:C:337:PRO:HB2	1:C:338:TYR:HD1	1.71	0.54
1:C:51:LEU:HD12	1:D:51:LEU:HD12	1.90	0.54
1:A:38:ARG:NH1	1:A:107:ASP:OD1	2.41	0.53
1:B:114:GLN:HB2	1:B:338:TYR:CD1	2.43	0.53
1:D:9:SER:HG	1:D:142:HIS:HD1	1.53	0.53
1:A:2:LYS:HG2	1:A:173:ASP:HB2	1.90	0.53
1:A:182:ALA:HB1	1:A:223:PHE:HE2	1.73	0.53
1:B:33:GLN:NE2	1:B:61:TRP:N	2.52	0.53
1:C:182:ALA:HB1	1:C:223:PHE:HE2	1.72	0.53
1:D:180:ILE:HG13	1:D:215:TRP:HB3	1.89	0.53
1:D:207:ILE:HG23	1:D:211:LEU:HD22	1.90	0.53
1:A:110:ASP:O	1:A:113:GLU:HG2	2.09	0.53
1:A:189:HIS:CE1	1:A:231:VAL:HG22	2.44	0.53
1:A:362:ARG:HG3	1:A:365:PHE:CE2	2.43	0.53
1:D:6:THR:HG23	1:D:169:THR:HG22	1.91	0.53
1:D:327:LEU:HA	1:D:330:ARG:CD	2.38	0.53
1:C:127:THR:O	1:C:133:LEU:HA	2.08	0.53
1:B:246:ILE:HG22	1:B:247:ILE:N	2.24	0.53
1:A:340:LEU:HA	1:A:343:MET:HB3	1.91	0.53
1:B:330:ARG:NH2	1:B:331:GLU:HG3	2.23	0.53
1:D:39:VAL:O	1:D:265:LYS:HA	2.08	0.53
1:A:181:ASP:O	1:A:220:THR:HA	2.09	0.53
1:B:39:VAL:O	1:B:265:LYS:HA	2.09	0.53
1:D:338:TYR:CD1	1:D:338:TYR:N	2.76	0.53
1:A:323:GLU:HG2	1:A:324:GLN:N	2.23	0.53
1:C:333:PHE:HZ	1:C:376:LEU:HD11	1.73	0.53
1:A:107:ASP:CA	1:A:114:GLN:HE21	2.16	0.52
1:B:159:TRP:CE3	1:B:193:ILE:HG21	2.44	0.52
1:B:301:ALA:O	1:B:304:VAL:HB	2.08	0.52
1:A:61:TRP:CE3	1:C:61:TRP:CE3	2.97	0.52
1:A:18:ILE:O	1:A:22:ILE:HG13	2.09	0.52
1:A:267:PRO:HB2	1:A:341:ILE:CD1	2.37	0.52
1:A:180:ILE:HG13	1:A:215:TRP:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ALA:HB1	1:B:223:PHE:HE2	1.74	0.52
1:D:159:TRP:CE3	1:D:193:ILE:HG21	2.45	0.52
1:B:107:ASP:CA	1:B:114:GLN:HE21	2.17	0.52
1:C:135:PRO:O	1:C:139:THR:HG23	2.10	0.52
1:C:246:ILE:HG23	1:C:257:HIS:CE1	2.44	0.52
1:C:371:ASP:N	1:C:371:ASP:OD1	2.41	0.52
1:D:354:THR:HG23	1:D:359:HIS:CE1	2.43	0.52
1:C:123:PHE:CE2	1:C:297:GLN:HB2	2.45	0.52
1:D:327:LEU:HD12	1:D:330:ARG:HD2	1.92	0.52
1:D:272:ARG:HH21	1:D:354:THR:HG21	1.73	0.52
1:D:183:VAL:HG11	1:D:207:ILE:HD13	1.92	0.52
1:A:123:PHE:CD1	1:A:256:ARG:HB3	2.45	0.51
1:D:151:VAL:CG2	1:D:156:THR:HB	2.39	0.51
1:A:151:VAL:HG23	1:A:156:THR:CB	2.38	0.51
1:C:323:GLU:HG2	1:C:324:GLN:N	2.24	0.51
1:B:17:LYS:HD2	1:B:355:ALA:O	2.09	0.51
1:B:183:VAL:HG11	1:B:207:ILE:HD13	1.93	0.51
1:B:246:ILE:HG22	1:B:247:ILE:HG12	1.92	0.51
1:A:338:TYR:N	1:A:338:TYR:CD1	2.79	0.51
4:B:485:SAM:H4'	5:B:484:PPK:O4A	2.11	0.51
1:C:9:SER:OG	1:C:142:HIS:ND1	2.44	0.51
1:B:323:GLU:HG2	1:B:324:GLN:N	2.26	0.51
1:B:159:TRP:CZ2	1:B:193:ILE:HD12	2.46	0.50
1:B:341:ILE:HG21	1:B:347:LEU:HD11	1.93	0.50
1:C:123:PHE:CD1	1:C:256:ARG:HB3	2.46	0.50
1:A:120:GLY:O	1:A:299:SER:HA	2.11	0.50
1:B:327:LEU:HA	1:B:330:ARG:CD	2.40	0.50
1:C:136:ALA:HB3	1:C:137:PRO:HD3	1.92	0.50
1:C:87:ASN:H	1:C:87:ASN:ND2	2.09	0.50
1:C:229:ARG:HB3	1:D:104:GLN:NE2	2.26	0.50
1:A:298:VAL:HG12	1:A:310:ILE:HG12	1.92	0.50
1:B:151:VAL:HG23	1:B:156:THR:CB	2.38	0.50
1:C:318:GLU:O	1:C:319:LYS:HD3	2.11	0.50
1:D:123:PHE:CD1	1:D:256:ARG:HB3	2.46	0.50
1:D:327:LEU:CA	1:D:330:ARG:HD3	2.41	0.50
1:A:107:ASP:OD2	1:A:114:GLN:NE2	2.45	0.50
1:A:17:LYS:O	1:A:21:GLN:CG	2.59	0.50
1:B:338:TYR:CD1	1:B:338:TYR:N	2.79	0.50
1:B:327:LEU:CA	1:B:330:ARG:HD3	2.42	0.50
1:C:338:TYR:CD1	1:C:338:TYR:N	2.80	0.50
1:C:328:LEU:CD2	1:C:376:LEU:HD22	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ALA:HB3	1:C:55:GLU:HG2	1.92	0.50
1:C:107:ASP:CA	1:C:114:GLN:HE21	2.17	0.50
1:C:114:GLN:HB2	1:C:338:TYR:CD1	2.47	0.50
1:D:87:ASN:H	1:D:87:ASN:ND2	2.09	0.50
1:A:246:ILE:HG22	1:A:247:ILE:N	2.27	0.50
1:B:72:VAL:CG1	1:B:86:ALA:HB2	2.32	0.50
1:C:131:ASP:O	1:C:133:LEU:HD22	2.11	0.50
1:C:33:GLN:HE22	1:C:61:TRP:N	2.06	0.50
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.77	0.49
1:A:122:MET:CE	1:A:271:ASP:HA	2.42	0.49
1:A:241:LEU:HG	1:B:241:LEU:HG	1.94	0.49
1:B:114:GLN:HB3	1:B:338:TYR:CE1	2.47	0.49
1:B:123:PHE:CD1	1:B:256:ARG:HB3	2.47	0.49
1:B:326:THR:O	1:B:330:ARG:HD3	2.13	0.49
1:A:327:LEU:HA	1:A:330:ARG:CD	2.42	0.49
1:A:333:PHE:HZ	1:A:376:LEU:HD11	1.77	0.49
1:B:189:HIS:CE1	1:B:231:VAL:HG22	2.48	0.49
1:A:226:PRO:HB2	1:B:302:ILE:O	2.13	0.49
1:D:107:ASP:CA	1:D:114:GLN:HE21	2.19	0.49
1:D:137:PRO:HA	1:D:170:PHE:CE1	2.47	0.49
1:A:119:GLN:HG2	1:B:165:LYS:HE2	1.94	0.49
1:B:87:ASN:H	1:B:87:ASN:ND2	2.09	0.49
1:D:132:VAL:HG23	1:D:134:MET:HB2	1.95	0.49
1:A:371:ASP:N	1:A:371:ASP:OD1	2.43	0.49
1:B:210:ILE:HG22	1:B:211:LEU:HD13	1.93	0.49
1:C:125:TYR:CG	1:C:255:ALA:HB2	2.48	0.49
1:D:189:HIS:CE1	1:D:231:VAL:HG22	2.47	0.49
1:B:87:ASN:H	1:B:87:ASN:HD22	1.61	0.49
1:D:159:TRP:CE2	1:D:193:ILE:HD12	2.48	0.49
1:A:246:ILE:HG22	1:A:247:ILE:HG12	1.95	0.49
1:B:212:PRO:HG2	1:B:215:TRP:CZ3	2.48	0.49
1:B:17:LYS:O	1:B:21:GLN:CG	2.60	0.49
1:A:265:LYS:HZ2	5:B:484:PPK:H3B	1.57	0.49
1:C:122:MET:N	1:C:122:MET:SD	2.85	0.49
1:C:314:THR:O	1:C:317:THR:HG23	2.13	0.49
1:A:265:LYS:NZ	5:B:484:PPK:N3B	2.59	0.48
1:C:132:VAL:HG23	1:C:134:MET:HB2	1.95	0.48
1:C:2:LYS:HG2	1:C:173:ASP:HB2	1.94	0.48
1:A:226:PRO:C	1:A:228:GLY:N	2.65	0.48
1:A:125:TYR:HD1	1:A:295:GLU:HG3	1.78	0.48
1:A:380:ALA:O	1:A:381:GLY:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:MET:SD	1:D:122:MET:N	2.86	0.48
1:D:225:ASN:N	1:D:226:PRO:CD	2.75	0.48
1:A:207:ILE:HG23	1:A:211:LEU:HD22	1.95	0.48
1:A:125:TYR:CD1	1:A:295:GLU:HG3	2.48	0.48
1:D:205:GLU:O	1:D:209:PRO:HG2	2.13	0.48
1:A:327:LEU:CA	1:A:330:ARG:HD3	2.44	0.48
1:B:371:ASP:OD1	1:B:371:ASP:N	2.45	0.48
1:C:180:ILE:HG13	1:C:215:TRP:HB3	1.94	0.48
1:A:136:ALA:HB3	1:A:137:PRO:HD3	1.95	0.48
1:A:159:TRP:CE2	1:A:193:ILE:HD12	2.49	0.48
1:C:267:PRO:HB2	1:C:341:ILE:CD1	2.37	0.48
1:C:328:LEU:HD11	1:C:379:ALA:HB3	1.94	0.48
1:C:340:LEU:HA	1:C:343:MET:HB3	1.94	0.48
1:B:298:VAL:HA	1:B:309:SER:O	2.14	0.48
1:B:327:LEU:O	1:B:330:ARG:NE	2.46	0.48
1:C:354:THR:HG23	1:C:359:HIS:CE1	2.48	0.48
1:D:131:ASP:O	1:D:133:LEU:HD22	2.14	0.48
1:A:108:ARG:H	1:A:114:GLN:HG2	1.77	0.48
1:A:159:TRP:CE3	1:A:193:ILE:HG21	2.49	0.48
1:A:66:GLU:HA	1:A:66:GLU:OE1	2.14	0.48
1:B:136:ALA:HB3	1:B:137:PRO:HD3	1.96	0.48
1:B:79:HIS:HD2	1:B:81:ASP:N	1.99	0.48
1:C:120:GLY:O	1:C:299:SER:HA	2.13	0.48
1:C:189:HIS:CE1	1:C:231:VAL:HG22	2.49	0.48
1:D:47:THR:HG22	1:D:236:MET:HA	1.95	0.48
1:D:173:ASP:HB3	1:D:178:VAL:HG11	1.95	0.47
1:D:340:LEU:HA	1:D:343:MET:HB3	1.94	0.47
1:D:79:HIS:HD2	1:D:81:ASP:N	2.05	0.47
1:B:335:LEU:HA	1:B:340:LEU:HD23	1.96	0.47
1:C:327:LEU:CA	1:C:330:ARG:HD3	2.44	0.47
1:D:17:LYS:HD2	1:D:355:ALA:O	2.14	0.47
1:A:327:LEU:HD12	1:A:330:ARG:HD2	1.95	0.47
1:C:37:ALA:C	1:C:38:ARG:HD2	2.33	0.47
1:A:114:GLN:HB2	1:A:338:TYR:CD1	2.49	0.47
1:B:9:SER:OG	1:B:142:HIS:ND1	2.47	0.47
1:A:318:GLU:O	1:A:319:LYS:HD3	2.14	0.47
1:D:114:GLN:HB2	1:D:338:TYR:CD1	2.49	0.47
1:A:131:ASP:O	1:A:133:LEU:HD22	2.15	0.47
1:C:229:ARG:HG2	1:D:101:ASP:CG	2.34	0.47
1:C:327:LEU:HD12	1:C:330:ARG:HD2	1.97	0.47
1:C:325:LEU:O	1:C:329:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ASN:H	1:C:87:ASN:HD22	1.62	0.47
1:A:225:ASN:N	1:A:226:PRO:CD	2.77	0.47
1:A:46:LYS:HD3	1:A:47:THR:H	1.80	0.47
1:B:225:ASN:N	1:B:226:PRO:CD	2.77	0.47
1:B:330:ARG:NE	1:B:331:GLU:N	2.58	0.47
1:C:47:THR:HG22	1:C:236:MET:HA	1.95	0.47
1:A:123:PHE:CE2	1:A:297:GLN:HB2	2.49	0.47
1:C:330:ARG:HH21	1:C:331:GLU:HG3	1.79	0.47
1:C:114:GLN:HB3	1:C:338:TYR:CE1	2.49	0.47
1:A:114:GLN:HB3	1:A:338:TYR:CE1	2.50	0.47
1:C:121:LEU:HA	1:C:299:SER:HA	1.97	0.47
1:C:225:ASN:N	1:C:226:PRO:CD	2.77	0.47
1:D:330:ARG:NE	1:D:331:GLU:N	2.58	0.47
1:A:40:ALA:HB3	1:A:55:GLU:HG2	1.97	0.46
1:D:246:ILE:CG2	1:D:247:ILE:N	2.78	0.46
1:D:335:LEU:HA	1:D:340:LEU:HD23	1.96	0.46
1:B:110:ASP:O	1:B:113:GLU:HG2	2.15	0.46
1:B:325:LEU:O	1:B:329:VAL:HG23	2.14	0.46
1:C:327:LEU:HA	1:C:330:ARG:CD	2.43	0.46
1:C:137:PRO:HA	1:C:170:PHE:CE1	2.50	0.46
1:C:330:ARG:NE	1:C:331:GLU:N	2.59	0.46
1:D:108:ARG:H	1:D:114:GLN:HG2	1.81	0.46
1:D:279:ARG:HD2	1:D:360:PHE:CG	2.51	0.46
1:A:173:ASP:HB3	1:A:178:VAL:HG11	1.96	0.46
1:B:17:LYS:HA	1:B:17:LYS:HD3	1.57	0.46
1:B:327:LEU:HD12	1:B:330:ARG:HD2	1.96	0.46
1:C:110:ASP:O	1:C:113:GLU:HG2	2.15	0.46
1:C:321:PRO:O	1:C:322:SER:C	2.54	0.46
1:C:382:LEU:O	1:C:383:LYS:OXT	2.33	0.46
1:D:210:ILE:HG22	1:D:211:LEU:HD13	1.97	0.46
1:A:17:LYS:HD2	1:A:355:ALA:O	2.15	0.46
1:C:122:MET:CE	1:C:271:ASP:HA	2.46	0.46
1:D:120:GLY:O	1:D:299:SER:HA	2.15	0.46
1:A:193:ILE:HD13	1:A:198:LEU:HB2	1.98	0.46
1:D:327:LEU:O	1:D:330:ARG:NE	2.48	0.46
1:A:6:THR:O	1:B:121:LEU:HD13	2.16	0.46
1:C:108:ARG:H	1:C:114:GLN:HG2	1.81	0.46
1:C:229:ARG:CZ	1:C:231:VAL:HG21	2.46	0.46
1:A:152:ARG:NH1	1:A:162:PRO:HA	2.31	0.46
1:A:327:LEU:O	1:A:331:GLU:HB2	2.16	0.46
1:B:261:ALA:O	1:B:265:LYS:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ALA:O	1:D:139:THR:OG1	2.28	0.46
1:A:301:ALA:O	1:A:304:VAL:HB	2.16	0.46
1:B:169:THR:O	1:B:180:ILE:HG23	2.15	0.46
1:C:293:ARG:HG3	1:C:293:ARG:O	2.15	0.46
1:A:335:LEU:HA	1:A:340:LEU:HD23	1.98	0.45
1:B:85:ASP:OD1	1:B:87:ASN:ND2	2.38	0.45
1:C:335:LEU:HA	1:C:340:LEU:HD23	1.98	0.45
1:A:101:ASP:CG	1:B:229:ARG:HG2	2.37	0.45
1:B:341:ILE:HG22	1:B:347:LEU:CD2	2.46	0.45
1:B:2:LYS:HG2	1:B:173:ASP:HB2	1.99	0.45
1:B:65:GLU:OE1	1:B:69:ARG:NE	2.42	0.45
1:C:66:GLU:HA	1:C:66:GLU:OE1	2.16	0.45
1:D:325:LEU:O	1:D:329:VAL:HG23	2.16	0.45
1:B:378:ASP:OD2	1:B:382:LEU:HD13	2.16	0.45
1:C:159:TRP:CE3	1:C:193:ILE:HG21	2.52	0.45
1:D:326:THR:O	1:D:330:ARG:HD3	2.17	0.45
1:A:9:SER:OG	1:A:142:HIS:ND1	2.48	0.45
1:A:330:ARG:NE	1:A:330:ARG:C	2.70	0.45
1:B:107:ASP:OD2	1:B:114:GLN:NE2	2.50	0.45
1:B:122:MET:CE	1:B:271:ASP:HA	2.46	0.45
1:D:327:LEU:HA	1:D:327:LEU:HD12	1.79	0.45
1:D:330:ARG:C	1:D:330:ARG:NE	2.70	0.45
1:C:173:ASP:HB3	1:C:178:VAL:HG11	1.98	0.45
1:B:351:TYR:O	1:B:352:LYS:C	2.54	0.45
1:C:12:GLU:OE2	1:C:153:LYS:NZ	2.49	0.45
1:C:176:LYS:HA	1:C:176:LYS:HD2	1.63	0.45
1:C:343:MET:HG2	1:C:344:LEU:HG	1.98	0.45
1:C:382:LEU:O	1:C:383:LYS:C	2.54	0.45
1:A:122:MET:HG2	1:A:298:VAL:CG2	2.36	0.45
1:C:246:ILE:HG22	1:C:247:ILE:HG12	1.98	0.45
1:D:123:PHE:CE2	1:D:297:GLN:HB2	2.52	0.45
1:D:328:LEU:HD11	1:D:379:ALA:HB3	1.96	0.45
1:D:2:LYS:HG2	1:D:173:ASP:HB2	1.98	0.45
1:D:280:TYR:O	1:D:284:ASN:HB2	2.17	0.45
1:D:40:ALA:HB3	1:D:55:GLU:HG2	1.98	0.45
1:B:321:PRO:HD2	1:B:324:GLN:NE2	2.32	0.45
1:C:279:ARG:HD2	1:C:360:PHE:CG	2.52	0.45
1:C:120:GLY:N	1:D:167:GLN:OE1	2.50	0.45
1:D:341:ILE:HG22	1:D:347:LEU:HD21	1.97	0.44
1:B:341:ILE:HG22	1:B:347:LEU:HD21	1.98	0.44
1:A:330:ARG:NE	1:A:331:GLU:N	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:PRO:C	1:C:228:GLY:N	2.69	0.44
1:D:285:ILE:HG23	1:D:290:LEU:HB2	1.98	0.44
1:D:31:LEU:HD22	1:D:35:PRO:HA	2.00	0.44
1:D:65:GLU:HA	1:D:91:VAL:HG11	1.99	0.44
1:A:140:TYR:CE2	1:A:215:TRP:HZ3	2.35	0.44
1:B:176:LYS:HD2	1:B:176:LYS:HA	1.62	0.44
1:B:328:LEU:CD2	1:B:376:LEU:HD22	2.47	0.44
1:D:323:GLU:CG	1:D:324:GLN:N	2.81	0.44
1:D:87:ASN:H	1:D:87:ASN:HD22	1.65	0.44
1:D:176:LYS:HD2	1:D:176:LYS:HA	1.62	0.44
1:B:140:TYR:CE2	1:B:215:TRP:HZ3	2.34	0.44
1:C:321:PRO:HD2	1:C:324:GLN:HE21	1.81	0.44
1:D:362:ARG:H	1:D:362:ARG:HG2	1.66	0.44
1:A:176:LYS:HD2	1:A:176:LYS:HA	1.61	0.44
1:A:325:LEU:O	1:A:329:VAL:HG23	2.16	0.44
1:A:369:LYS:CE	1:A:369:LYS:HA	2.45	0.44
1:A:37:ALA:C	1:A:38:ARG:HD2	2.38	0.44
1:B:279:ARG:HD2	1:B:360:PHE:CG	2.52	0.44
1:B:382:LEU:O	1:B:383:LYS:C	2.56	0.44
1:C:246:ILE:CG2	1:C:247:ILE:N	2.77	0.44
1:C:330:ARG:NE	1:C:330:ARG:C	2.71	0.44
1:C:362:ARG:HG2	1:C:362:ARG:H	1.67	0.44
1:D:151:VAL:HG23	1:D:156:THR:CB	2.43	0.44
1:B:136:ALA:O	1:B:139:THR:OG1	2.27	0.44
1:B:31:LEU:HD22	1:B:35:PRO:HA	1.98	0.44
1:B:37:ALA:C	1:B:38:ARG:HD2	2.38	0.44
1:C:159:TRP:CE2	1:C:193:ILE:HD12	2.53	0.44
1:D:37:ALA:C	1:D:38:ARG:HD2	2.37	0.44
1:A:61:TRP:HE3	1:C:61:TRP:CE3	2.34	0.44
1:A:330:ARG:HE	1:A:330:ARG:C	2.21	0.43
1:B:180:ILE:HG13	1:B:215:TRP:HB3	2.00	0.43
1:C:17:LYS:O	1:C:21:GLN:CG	2.66	0.43
1:C:326:THR:O	1:C:330:ARG:HD3	2.18	0.43
1:B:173:ASP:HB3	1:B:178:VAL:HG11	2.00	0.43
1:C:38:ARG:HA	1:C:266:ASP:OD2	2.19	0.43
1:C:85:ASP:OD1	1:C:87:ASN:ND2	2.34	0.43
1:B:226:PRO:C	1:B:228:GLY:N	2.69	0.43
1:D:107:ASP:OD2	1:D:114:GLN:NE2	2.50	0.43
1:A:226:PRO:C	1:A:228:GLY:H	2.20	0.43
1:B:65:GLU:HA	1:B:91:VAL:HG11	1.99	0.43
1:B:66:GLU:HA	1:B:66:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:ALA:O	1:C:381:GLY:C	2.56	0.43
1:D:69:ARG:NH1	1:D:89:CYS:O	2.43	0.43
1:A:125:TYR:CG	1:A:255:ALA:HB2	2.54	0.43
1:B:14:HIS:CE1	1:B:16:ASP:HB2	2.54	0.43
1:B:121:LEU:HA	1:B:299:SER:HA	1.99	0.43
1:B:31:LEU:HA	1:B:34:ASP:O	2.19	0.43
1:B:380:ALA:O	1:B:381:GLY:C	2.56	0.43
1:C:33:GLN:NE2	1:C:61:TRP:N	2.62	0.43
1:A:87:ASN:H	1:A:87:ASN:ND2	2.15	0.43
1:A:121:LEU:HA	1:A:299:SER:HA	1.99	0.43
1:A:122:MET:HE2	1:A:270:VAL:O	2.18	0.43
1:A:169:THR:O	1:A:180:ILE:HG23	2.18	0.43
1:B:330:ARG:HH21	1:B:331:GLU:HG3	1.82	0.43
1:D:122:MET:CE	1:D:271:ASP:HA	2.49	0.43
1:D:182:ALA:HB1	1:D:223:PHE:HE2	1.81	0.43
1:A:298:VAL:HA	1:A:309:SER:O	2.19	0.43
1:A:382:LEU:O	1:A:383:LYS:OXT	2.36	0.43
1:B:108:ARG:HH11	1:B:108:ARG:HG2	1.84	0.43
1:C:369:LYS:HA	1:C:369:LYS:CE	2.47	0.43
1:A:147:ARG:O	1:A:151:VAL:HG12	2.18	0.43
1:B:40:ALA:HB3	1:B:55:GLU:HG2	2.01	0.42
1:C:65:GLU:HA	1:C:91:VAL:HG11	2.01	0.42
1:D:347:LEU:N	1:D:347:LEU:HD22	2.32	0.42
1:A:38:ARG:HA	1:A:266:ASP:OD2	2.19	0.42
1:A:79:HIS:HD2	1:A:81:ASP:N	2.06	0.42
1:B:49:MET:SD	1:C:92:LEU:HD21	2.59	0.42
1:C:119:GLN:HG2	1:D:165:LYS:HE2	1.99	0.42
1:D:226:PRO:C	1:D:228:GLY:N	2.71	0.42
1:A:302:ILE:HG23	1:A:302:ILE:O	2.19	0.42
1:A:55:GLU:HA	1:A:96:GLY:O	2.20	0.42
1:B:347:LEU:H	1:B:347:LEU:CD2	2.24	0.42
1:C:245:LYS:HA	6:C:731:HOH:O	2.18	0.42
1:D:72:VAL:O	1:D:75:ILE:HB	2.20	0.42
1:B:318:GLU:O	1:B:319:LYS:HD3	2.19	0.42
1:C:210:ILE:HG22	1:C:211:LEU:HD13	2.01	0.42
1:D:341:ILE:HG21	1:D:347:LEU:HD11	2.02	0.42
1:D:314:THR:O	1:D:317:THR:HG23	2.20	0.42
1:B:122:MET:CG	1:B:298:VAL:HG23	2.32	0.42
1:C:221:LYS:NZ	1:C:221:LYS:HB3	2.34	0.42
1:C:46:LYS:HE2	1:C:235:PRO:O	2.20	0.42
1:D:17:LYS:HA	1:D:17:LYS:HD3	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASP:HA	1:A:111:PRO:HD3	1.90	0.42
1:A:382:LEU:O	1:A:383:LYS:C	2.58	0.42
1:A:9:SER:HG	1:A:142:HIS:HD1	1.66	0.42
1:C:204:GLU:OE2	1:C:208:LYS:HE2	2.20	0.42
4:C:585:SAM:C2	1:D:302:ILE:HD13	2.50	0.42
1:D:65:GLU:O	1:D:69:ARG:HG3	2.20	0.42
1:A:159:TRP:CZ2	1:A:193:ILE:HD12	2.55	0.42
1:C:330:ARG:CZ	1:C:330:ARG:HB2	2.49	0.42
1:C:8:GLU:HG2	1:D:121:LEU:CD2	2.50	0.42
1:D:321:PRO:HD2	1:D:324:GLN:HE21	1.84	0.42
1:D:382:LEU:O	1:D:383:LYS:C	2.57	0.42
1:A:279:ARG:HD2	1:A:360:PHE:CG	2.54	0.42
1:A:65:GLU:OE1	1:A:69:ARG:NE	2.45	0.42
1:A:165:LYS:HE2	1:B:119:GLN:HG2	2.01	0.42
1:B:123:PHE:CE2	1:B:297:GLN:HB2	2.55	0.42
1:B:46:LYS:HE2	1:B:235:PRO:O	2.19	0.42
1:B:122:MET:SD	1:B:122:MET:N	2.93	0.42
1:B:267:PRO:C	1:B:269:LYS:H	2.23	0.42
1:C:121:LEU:C	1:C:122:MET:SD	2.98	0.42
1:C:337:PRO:O	1:C:340:LEU:HD12	2.19	0.42
1:C:167:GLN:OE1	1:D:120:GLY:N	2.53	0.42
1:D:169:THR:O	1:D:180:ILE:HG23	2.20	0.42
1:A:327:LEU:HA	1:A:327:LEU:HD12	1.79	0.41
1:A:47:THR:HG22	1:A:236:MET:HA	2.02	0.41
1:B:133:LEU:HD22	1:B:133:LEU:N	2.34	0.41
1:B:205:GLU:O	1:B:209:PRO:HG2	2.20	0.41
1:A:256:ARG:HG2	1:B:253:GLY:O	2.20	0.41
1:B:323:GLU:CG	1:B:324:GLN:N	2.83	0.41
1:C:17:LYS:HD3	1:C:17:LYS:HA	1.63	0.41
1:C:281:VAL:HB	1:C:333:PHE:CE2	2.55	0.41
1:C:125:TYR:CD1	1:C:295:GLU:HG3	2.55	0.41
1:C:336:ARG:O	1:C:337:PRO:C	2.57	0.41
1:A:46:LYS:O	1:A:84:PHE:HE1	2.03	0.41
1:A:229:ARG:HG2	1:B:101:ASP:CG	2.41	0.41
1:B:120:GLY:O	1:B:299:SER:HA	2.20	0.41
1:C:108:ARG:HG2	1:C:108:ARG:HH11	1.85	0.41
1:D:17:LYS:O	1:D:21:GLN:CG	2.68	0.41
1:A:108:ARG:NH1	1:A:108:ARG:HG2	2.34	0.41
1:A:52:VAL:O	1:A:93:SER:HA	2.20	0.41
1:C:140:TYR:CE2	1:C:215:TRP:HZ3	2.38	0.41
1:C:208:LYS:N	1:C:209:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:ILE:HG22	1:D:347:LEU:CD2	2.50	0.41
1:A:226:PRO:O	1:A:228:GLY:N	2.52	0.41
1:B:330:ARG:NE	1:B:330:ARG:C	2.74	0.41
1:C:341:ILE:HG22	1:C:347:LEU:HD21	2.01	0.41
1:D:140:TYR:CE2	1:D:215:TRP:HZ3	2.38	0.41
1:A:323:GLU:CG	1:A:324:GLN:N	2.83	0.41
5:A:384:PPK:H3B	1:B:265:LYS:HZ1	1.68	0.41
1:B:122:MET:HG3	1:B:274:ALA:CB	2.51	0.41
1:B:362:ARG:HG2	1:B:362:ARG:H	1.72	0.41
1:C:122:MET:HE2	1:C:270:VAL:O	2.21	0.41
1:C:323:GLU:CG	1:C:324:GLN:N	2.83	0.41
1:D:77:TYR:OH	1:D:163:ASP:HB2	2.21	0.41
1:D:46:LYS:HE2	1:D:235:PRO:O	2.21	0.41
1:A:101:ASP:OD1	1:B:229:ARG:HG2	2.20	0.41
1:C:327:LEU:HD12	1:C:327:LEU:HA	1.85	0.41
1:D:333:PHE:CZ	1:D:376:LEU:HD11	2.51	0.41
1:B:104:GLN:H	1:B:104:GLN:HG2	1.73	0.41
1:B:47:THR:HG22	1:B:236:MET:HA	2.03	0.41
1:B:79:HIS:NE2	1:C:79:HIS:NE2	2.68	0.41
1:C:101:ASP:HB3	1:D:229:ARG:O	2.21	0.41
1:D:320:VAL:O	1:D:321:PRO:C	2.57	0.41
1:A:321:PRO:HD2	1:A:324:GLN:HE21	1.81	0.41
1:A:328:LEU:HD11	1:A:379:ALA:HB3	2.02	0.41
1:A:320:VAL:O	1:A:321:PRO:C	2.58	0.41
1:A:362:ARG:H	1:A:362:ARG:HG2	1.67	0.41
1:A:72:VAL:CG1	1:A:86:ALA:HB2	2.41	0.41
1:B:125:TYR:CG	1:B:255:ALA:HB2	2.56	0.41
1:B:114:GLN:O	1:B:337:PRO:HG2	2.21	0.41
1:C:333:PHE:CZ	1:C:376:LEU:HD11	2.54	0.41
1:D:121:LEU:HA	1:D:299:SER:HA	2.03	0.41
1:D:171:GLN:NE2	1:D:181:ASP:OD2	2.54	0.41
1:D:37:ALA:HB1	1:D:58:THR:HB	2.02	0.41
1:A:326:THR:O	1:A:330:ARG:HD3	2.21	0.41
1:A:330:ARG:HH21	1:A:331:GLU:HG3	1.86	0.41
1:A:85:ASP:OD1	1:A:87:ASN:ND2	2.37	0.41
1:B:327:LEU:HA	1:B:327:LEU:HD12	1.80	0.41
1:C:101:ASP:HB2	6:D:916:HOH:O	2.20	0.41
1:C:335:LEU:HA	1:C:335:LEU:HD12	1.90	0.41
1:D:330:ARG:C	1:D:330:ARG:HE	2.24	0.41
1:A:336:ARG:O	1:A:337:PRO:C	2.59	0.41
1:A:61:TRP:CE3	1:C:61:TRP:HE3	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:384:PPK:N3B	1:B:265:LYS:NZ	2.66	0.41
1:B:267:PRO:C	1:B:269:LYS:N	2.73	0.41
1:C:261:ALA:O	1:C:265:LYS:HE3	2.21	0.41
1:D:380:ALA:O	1:D:381:GLY:C	2.58	0.41
1:B:61:TRP:CE3	1:D:61:TRP:CE3	3.09	0.40
1:A:186:SER:HA	1:A:225:ASN:OD1	2.21	0.40
1:B:286:VAL:HG22	1:B:291:ALA:O	2.21	0.40
1:B:333:PHE:CZ	1:B:376:LEU:HD11	2.53	0.40
1:B:55:GLU:HA	1:B:96:GLY:O	2.22	0.40
1:C:17:LYS:HD2	1:C:355:ALA:O	2.21	0.40
1:D:328:LEU:CD2	1:D:376:LEU:HD22	2.45	0.40
1:D:9:SER:HG	1:D:142:HIS:CE1	2.38	0.40
1:B:131:ASP:O	1:B:133:LEU:HD22	2.21	0.40
1:C:169:THR:O	1:C:180:ILE:HG23	2.21	0.40
1:C:382:LEU:HG	1:C:383:LYS:H	1.81	0.40
1:C:46:LYS:HD3	1:C:47:THR:H	1.85	0.40
1:D:267:PRO:C	1:D:269:LYS:H	2.24	0.40
1:D:330:ARG:CZ	1:D:330:ARG:HB2	2.51	0.40
1:D:283:LYS:NZ	1:D:368:GLU:O	2.47	0.40
1:A:229:ARG:HG2	1:B:101:ASP:OD1	2.21	0.40
1:C:112:LEU:HD13	1:C:112:LEU:N	2.36	0.40
1:C:296:ILE:CG2	1:C:297:GLN:N	2.84	0.40
1:C:238:ASP:OD2	4:C:585:SAM:H5'2	2.22	0.40
1:C:101:ASP:OD1	1:D:229:ARG:HG2	2.20	0.40
1:A:210:ILE:HG22	1:A:211:LEU:HD13	2.03	0.40
1:A:122:MET:CG	1:A:298:VAL:HG23	2.36	0.40
1:C:2:LYS:HA	1:C:172:TYR:O	2.22	0.40
1:C:125:TYR:HB3	1:C:251:TYR:CE1	2.57	0.40
1:D:301:ALA:O	1:D:304:VAL:HB	2.22	0.40
1:D:66:GLU:OE1	1:D:66:GLU:HA	2.22	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	381/383 (100%)	355 (93%)	23 (6%)	3 (1%)	19	35
1	B	381/383 (100%)	355 (93%)	23 (6%)	3 (1%)	19	35
1	C	381/383 (100%)	351 (92%)	27 (7%)	3 (1%)	19	35
1	D	381/383 (100%)	348 (91%)	30 (8%)	3 (1%)	19	35
All	All	1524/1532 (100%)	1409 (92%)	103 (7%)	12 (1%)	19	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	THR
1	B	47	THR
1	C	47	THR
1	D	47	THR
1	A	382	LEU
1	B	382	LEU
1	C	382	LEU
1	D	382	LEU
1	A	381	GLY
1	B	381	GLY
1	C	381	GLY
1	D	381	GLY

### 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	311/311 (100%)	246 (79%)	65 (21%)	1	2
1	B	311/311 (100%)	244 (78%)	67 (22%)	1	1
1	C	311/311 (100%)	242 (78%)	69 (22%)	1	1
1	D	311/311 (100%)	243 (78%)	68 (22%)	1	1
All	All	1244/1244 (100%)	975 (78%)	269 (22%)	1	1

All (269) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	17	LYS
1	A	32	GLU
1	A	36	LYS
1	A	38	ARG
1	A	46	LYS
1	A	51	LEU
1	A	55	GLU
1	A	65	GLU
1	A	66	GLU
1	A	74	GLU
1	A	82	MET
1	A	87	ASN
1	A	92	LEU
1	A	99	SER
1	A	112	LEU
1	A	122	MET
1	A	150	GLU
1	A	161	ARG
1	A	169	THR
1	A	181	ASP
1	A	185	LEU
1	A	193	ILE
1	A	203	MET
1	A	205	GLU
1	A	208	LYS
1	A	211	LEU
1	A	214	GLU
1	A	218	SER
1	A	221	LYS
1	A	241	LEU
1	A	245	LYS
1	A	246	ILE
1	A	256	ARG
1	A	265	LYS
1	A	269	LYS
1	A	270	VAL
1	A	279	ARG
1	A	294	CYS
1	A	309	SER
1	A	311	MET
1	A	312	VAL

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Mol	Chain	Res	Type
1	A	317	THR
1	A	322	SER
1	A	323	GLU
1	A	326	THR
1	A	327	LEU
1	A	328	LEU
1	A	330	ARG
1	A	331	GLU
1	A	333	PHE
1	A	335	LEU
1	A	340	LEU
1	A	347	LEU
1	A	354	THR
1	A	362	ARG
1	A	363	GLU
1	A	369	LYS
1	A	371	ASP
1	A	372	LYS
1	A	374	GLN
1	A	375	LEU
1	A	377	ARG
1	A	382	LEU
1	A	383	LYS
1	B	9	SER
1	B	17	LYS
1	B	32	GLU
1	B	36	LYS
1	B	38	ARG
1	B	46	LYS
1	B	51	LEU
1	B	55	GLU
1	B	65	GLU
1	B	66	GLU
1	B	74	GLU
1	B	82	MET
1	B	87	ASN
1	B	92	LEU
1	B	99	SER
1	B	112	LEU
1	B	122	MET
1	B	150	GLU
1	B	161	ARG

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Mol	Chain	Res	Type
1	B	169	THR
1	B	181	ASP
1	B	185	LEU
1	B	193	ILE
1	B	203	MET
1	B	205	GLU
1	B	208	LYS
1	B	211	LEU
1	B	214	GLU
1	B	218	SER
1	B	221	LYS
1	B	230	PHE
1	B	241	LEU
1	B	245	LYS
1	B	246	ILE
1	B	256	ARG
1	B	265	LYS
1	B	269	LYS
1	B	270	VAL
1	B	279	ARG
1	B	294	CYS
1	B	309	SER
1	B	311	MET
1	B	312	VAL
1	B	317	THR
1	B	322	SER
1	B	323	GLU
1	B	326	THR
1	B	327	LEU
1	B	328	LEU
1	B	330	ARG
1	B	331	GLU
1	B	333	PHE
1	B	335	LEU
1	B	340	LEU
1	B	341	ILE
1	B	347	LEU
1	B	354	THR
1	B	362	ARG
1	B	363	GLU
1	B	369	LYS
1	B	371	ASP

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Mol	Chain	Res	Type
1	B	372	LYS
1	B	374	GLN
1	B	375	LEU
1	B	377	ARG
1	B	382	LEU
1	B	383	LYS
1	C	9	SER
1	C	17	LYS
1	C	32	GLU
1	C	36	LYS
1	C	38	ARG
1	C	46	LYS
1	C	51	LEU
1	C	55	GLU
1	C	65	GLU
1	C	66	GLU
1	C	74	GLU
1	C	82	MET
1	C	87	ASN
1	C	92	LEU
1	C	99	SER
1	C	112	LEU
1	C	122	MET
1	C	150	GLU
1	C	161	ARG
1	C	169	THR
1	C	181	ASP
1	C	185	LEU
1	C	193	ILE
1	C	196	LYS
1	C	203	MET
1	C	205	GLU
1	C	208	LYS
1	C	211	LEU
1	C	214	GLU
1	C	218	SER
1	C	221	LYS
1	C	230	PHE
1	C	241	LEU
1	C	245	LYS
1	C	246	ILE
1	C	256	ARG

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Mol	Chain	Res	Type
1	C	265	LYS
1	C	269	LYS
1	C	270	VAL
1	C	279	ARG
1	C	294	CYS
1	C	309	SER
1	C	311	MET
1	C	312	VAL
1	C	317	THR
1	C	322	SER
1	C	323	GLU
1	C	326	THR
1	C	327	LEU
1	C	328	LEU
1	C	330	ARG
1	C	331	GLU
1	C	333	PHE
1	C	335	LEU
1	C	340	LEU
1	C	341	ILE
1	C	347	LEU
1	C	354	THR
1	C	362	ARG
1	C	363	GLU
1	C	369	LYS
1	C	370	THR
1	C	371	ASP
1	C	372	LYS
1	C	374	GLN
1	C	375	LEU
1	C	377	ARG
1	C	382	LEU
1	C	383	LYS
1	D	9	SER
1	D	17	LYS
1	D	32	GLU
1	D	36	LYS
1	D	38	ARG
1	D	46	LYS
1	D	51	LEU
1	D	55	GLU
1	D	65	GLU

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Mol	Chain	Res	Type
1	D	66	GLU
1	D	74	GLU
1	D	82	MET
1	D	87	ASN
1	D	92	LEU
1	D	99	SER
1	D	112	LEU
1	D	122	MET
1	D	150	GLU
1	D	161	ARG
1	D	169	THR
1	D	181	ASP
1	D	185	LEU
1	D	193	ILE
1	D	203	MET
1	D	205	GLU
1	D	208	LYS
1	D	211	LEU
1	D	214	GLU
1	D	218	SER
1	D	221	LYS
1	D	227	THR
1	D	230	PHE
1	D	241	LEU
1	D	245	LYS
1	D	246	ILE
1	D	256	ARG
1	D	265	LYS
1	D	269	LYS
1	D	270	VAL
1	D	279	ARG
1	D	294	CYS
1	D	309	SER
1	D	311	MET
1	D	312	VAL
1	D	317	THR
1	D	322	SER
1	D	323	GLU
1	D	326	THR
1	D	327	LEU
1	D	328	LEU
1	D	330	ARG

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Mol	Chain	Res	Type
1	D	331	GLU
1	D	333	PHE
1	D	335	LEU
1	D	340	LEU
1	D	341	ILE
1	D	347	LEU
1	D	354	THR
1	D	362	ARG
1	D	363	GLU
1	D	369	LYS
1	D	371	ASP
1	D	372	LYS
1	D	374	GLN
1	D	375	LEU
1	D	377	ARG
1	D	382	LEU
1	D	383	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	21	GLN
1	A	33	GLN
1	A	79	HIS
1	A	114	GLN
1	A	119	GLN
1	A	146	GLN
1	A	257	HIS
1	A	297	GLN
1	A	324	GLN
1	B	21	GLN
1	B	33	GLN
1	B	79	HIS
1	B	114	GLN
1	B	119	GLN
1	B	146	GLN
1	B	257	HIS
1	B	297	GLN
1	B	324	GLN
1	C	3	HIS
1	C	21	GLN

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Mol	Chain	Res	Type
1	C	33	GLN
1	C	79	HIS
1	C	114	GLN
1	C	119	GLN
1	C	146	GLN
1	C	257	HIS
1	C	324	GLN
1	D	3	HIS
1	D	21	GLN
1	D	33	GLN
1	D	79	HIS
1	D	104	GLN
1	D	114	GLN
1	D	119	GLN
1	D	146	GLN
1	D	257	HIS
1	D	324	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SAM	A	385	-	21,29,29	1.19	3 (14%)	18,42,42	0.99	1 (5%)
5	PPK	B	484	3,2	11,12,12	2.79	3 (27%)	15,20,20	4.16	6 (40%)
4	SAM	C	685	-	21,29,29	1.15	3 (14%)	18,42,42	1.03	1 (5%)
5	PPK	C	584	3,2	11,12,12	2.84	4 (36%)	15,20,20	4.29	7 (46%)
4	SAM	C	585	-	21,29,29	1.17	3 (14%)	18,42,42	1.01	1 (5%)
5	PPK	D	684	3,2	11,12,12	2.61	3 (27%)	15,20,20	4.24	7 (46%)
4	SAM	B	485	-	21,29,29	0.97	2 (9%)	18,42,42	1.07	1 (5%)
5	PPK	A	384	3,2	11,12,12	2.86	4 (36%)	15,20,20	4.13	6 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAM	A	385	-	-	1/8/33/33	0/3/3/3
5	PPK	B	484	3,2	-	2/8/12/12	-
4	SAM	C	685	-	-	1/8/33/33	0/3/3/3
5	PPK	C	584	3,2	-	2/8/12/12	-
4	SAM	C	585	-	-	2/8/33/33	0/3/3/3
5	PPK	D	684	3,2	-	2/8/12/12	-
4	SAM	B	485	-	-	1/8/33/33	0/3/3/3
5	PPK	A	384	3,2	-	2/8/12/12	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	384	PPK	PG-O3G	7.29	1.57	1.46
5	B	484	PPK	PG-O3G	7.13	1.57	1.46
5	D	684	PPK	PG-O3G	6.24	1.56	1.46
5	C	584	PPK	PG-O3G	6.20	1.56	1.46
5	C	584	PPK	PB-O2B	5.76	1.55	1.46
5	B	484	PPK	PB-O2B	4.57	1.53	1.46
5	D	684	PPK	PB-O2B	4.52	1.53	1.46
5	A	384	PPK	PB-O2B	4.33	1.53	1.46
5	B	484	PPK	PA-O4A	3.32	1.61	1.50
5	A	384	PPK	PA-O4A	3.19	1.60	1.50
5	C	584	PPK	PA-O4A	3.13	1.60	1.50
5	D	684	PPK	PA-O4A	3.06	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	685	SAM	C2-N3	2.94	1.36	1.32
4	A	385	SAM	C2-N3	2.78	1.36	1.32
4	C	585	SAM	C2-N3	2.76	1.36	1.32
4	C	585	SAM	C4-N3	2.60	1.39	1.35
5	A	384	PPK	PB-O3A	2.59	1.62	1.59
4	A	385	SAM	C4-N3	2.44	1.39	1.35
4	B	485	SAM	C2-N3	2.28	1.35	1.32
4	A	385	SAM	C8-N7	-2.21	1.30	1.34
4	B	485	SAM	C8-N7	-2.17	1.30	1.34
4	C	685	SAM	C8-N7	-2.16	1.30	1.34
5	C	584	PPK	PB-O3A	2.15	1.61	1.59
4	C	585	SAM	C8-N7	-2.14	1.30	1.34
4	C	685	SAM	C4-N3	2.08	1.38	1.35

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	584	PPK	O3G-PG-N3B	-10.64	96.10	111.77
5	D	684	PPK	O3G-PG-N3B	-10.08	96.92	111.77
5	D	684	PPK	O2G-PG-O3G	-10.08	88.12	113.45
5	B	484	PPK	O2G-PG-O3G	-9.73	89.00	113.45
5	A	384	PPK	O2G-PG-O3G	-9.66	89.16	113.45
5	C	584	PPK	O2G-PG-O3G	-9.61	89.30	113.45
5	A	384	PPK	O3G-PG-N3B	-9.37	97.97	111.77
5	B	484	PPK	O3G-PG-N3B	-9.34	98.02	111.77
5	B	484	PPK	O2B-PB-N3B	-5.01	104.39	111.77
5	A	384	PPK	O2B-PB-N3B	-4.83	104.66	111.77
5	A	384	PPK	O2G-PG-O1G	4.80	120.41	107.64
5	D	684	PPK	O2G-PG-O1G	4.74	120.27	107.64
5	B	484	PPK	O2G-PG-O1G	4.72	120.21	107.64
5	C	584	PPK	O2B-PB-N3B	-4.69	104.86	111.77
5	C	584	PPK	O2G-PG-O1G	4.48	119.56	107.64
5	D	684	PPK	O2B-PB-N3B	-4.24	105.53	111.77
5	B	484	PPK	O3A-PB-N3B	3.76	117.03	106.59
5	A	384	PPK	O3A-PB-N3B	3.56	116.46	106.59
5	D	684	PPK	O3A-PB-N3B	3.32	115.80	106.59
5	C	584	PPK	O3A-PB-N3B	3.20	115.46	106.59
5	A	384	PPK	O1G-PG-O3G	-2.96	106.01	113.45
5	C	584	PPK	O1G-PG-O3G	-2.74	106.57	113.45
5	D	684	PPK	O1G-PG-O3G	-2.69	106.69	113.45
5	B	484	PPK	O1G-PG-O3G	-2.64	106.83	113.45
4	C	685	SAM	O2'-C2'-C3'	2.54	120.03	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	485	SAM	O2'-C2'-C3'	2.47	119.80	111.82
4	A	385	SAM	O2'-C2'-C3'	2.37	119.49	111.82
4	C	585	SAM	O2'-C2'-C3'	2.36	119.44	111.82
5	C	584	PPK	O1A-PA-O3A	2.26	112.20	104.64
5	D	684	PPK	O1A-PA-O3A	2.17	111.90	104.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	484	PPK	PB-N3B-PG-O3G
5	B	484	PPK	PG-N3B-PB-O2B
4	A	385	SAM	O4'-C4'-C5'-SD
5	A	384	PPK	PB-N3B-PG-O3G
5	A	384	PPK	PG-N3B-PB-O2B
5	C	584	PPK	PB-N3B-PG-O3G
5	C	584	PPK	PG-N3B-PB-O2B
5	D	684	PPK	PB-N3B-PG-O3G
5	D	684	PPK	PG-N3B-PB-O2B
4	B	485	SAM	O4'-C4'-C5'-SD
4	C	585	SAM	CA-CB-CG-SD
4	C	685	SAM	CA-CB-CG-SD
4	C	585	SAM	O4'-C4'-C5'-SD

There are no ring outliers.

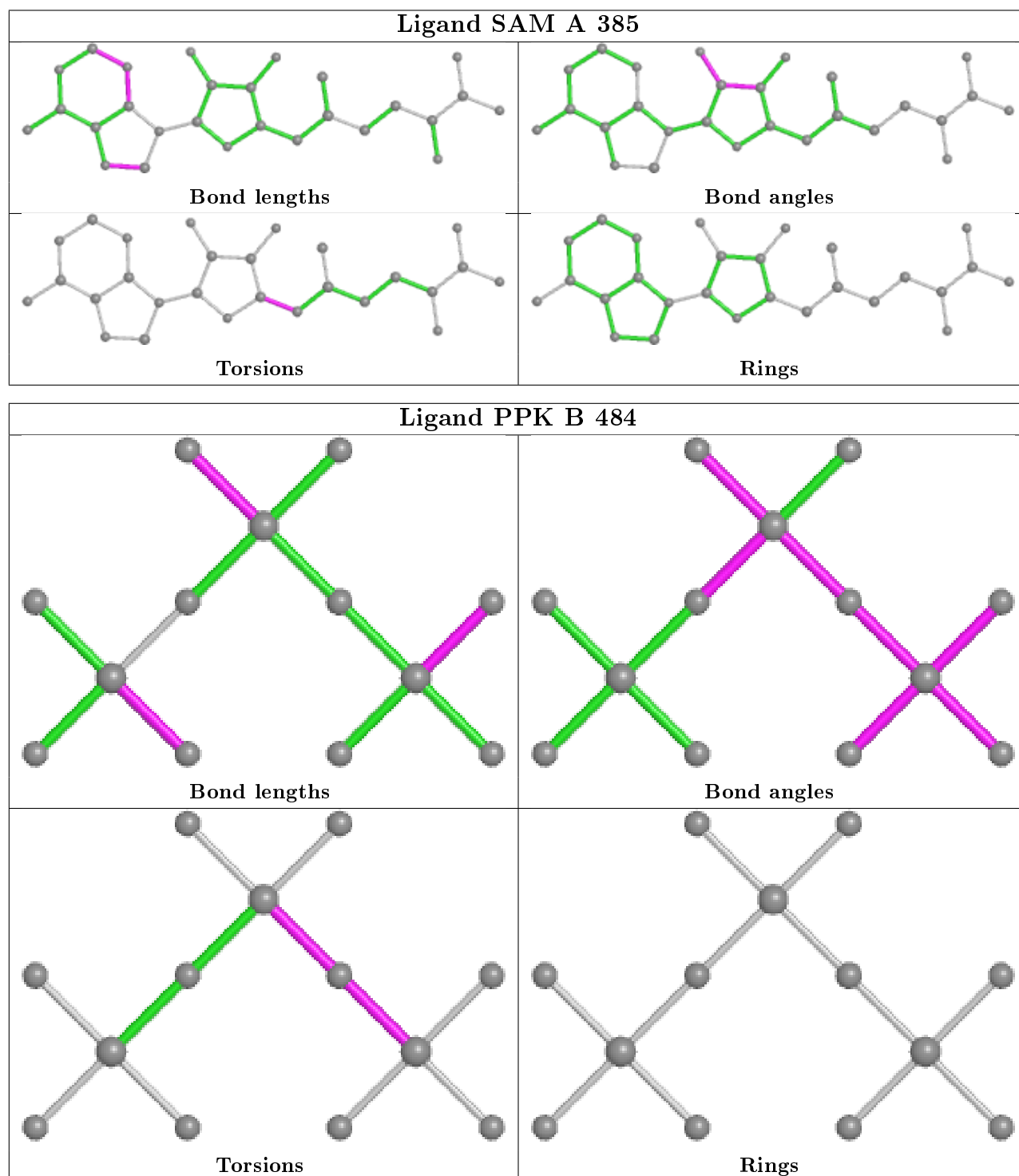
7 monomers are involved in 18 short contacts:

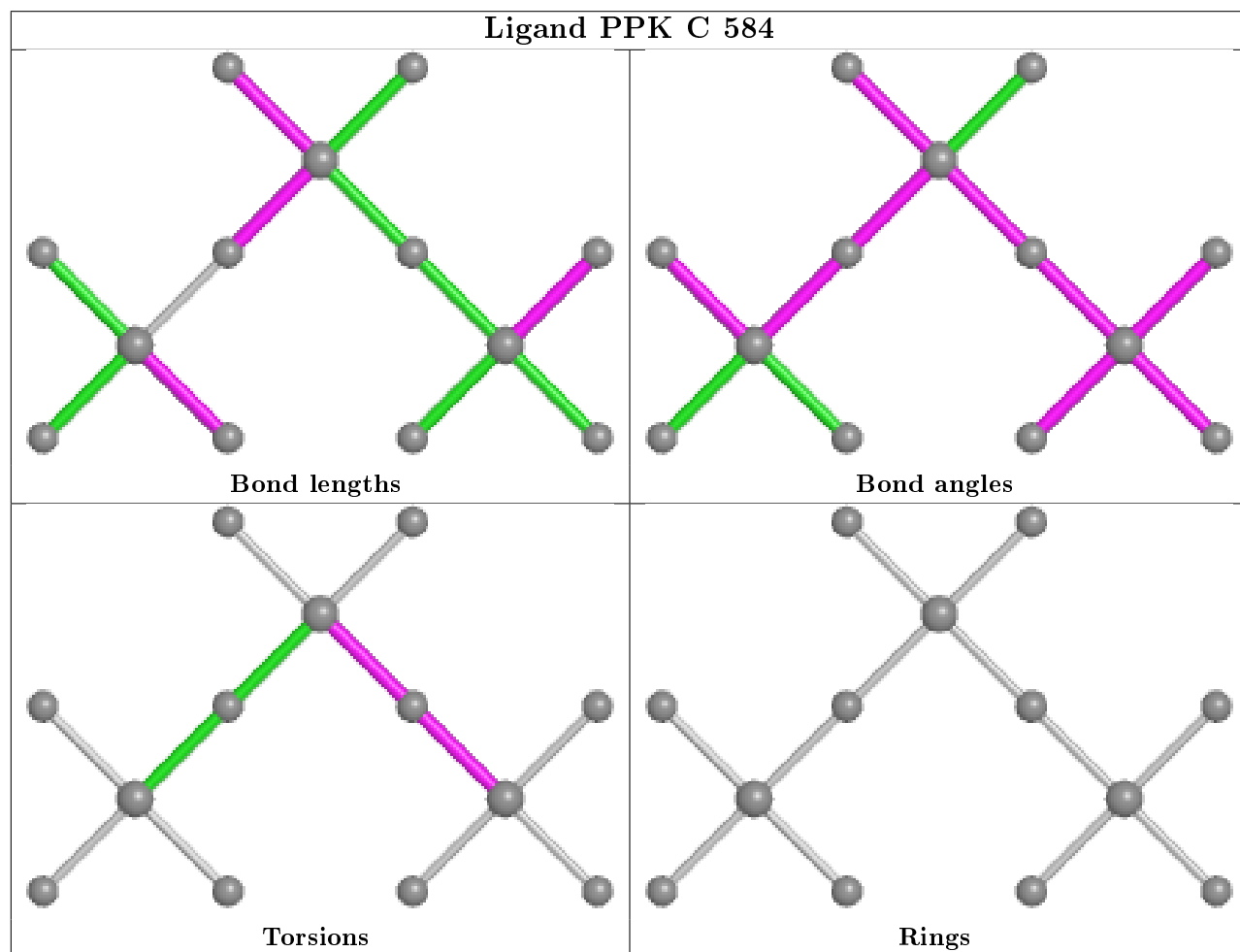
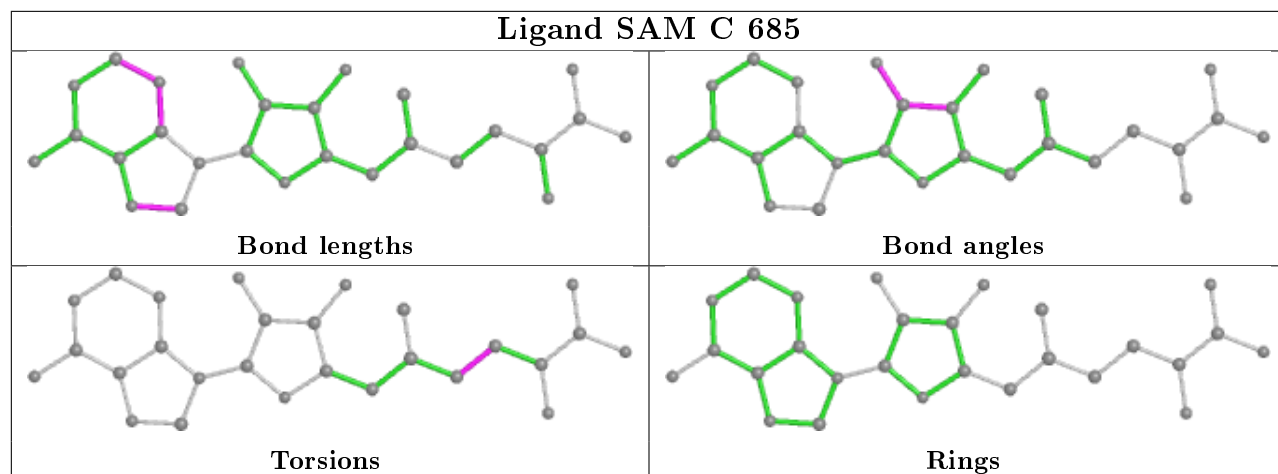
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	385	SAM	2	0
5	B	484	PPK	4	0
5	C	584	PPK	3	0
4	C	585	SAM	2	0
5	D	684	PPK	3	0
4	B	485	SAM	2	0
5	A	384	PPK	4	0

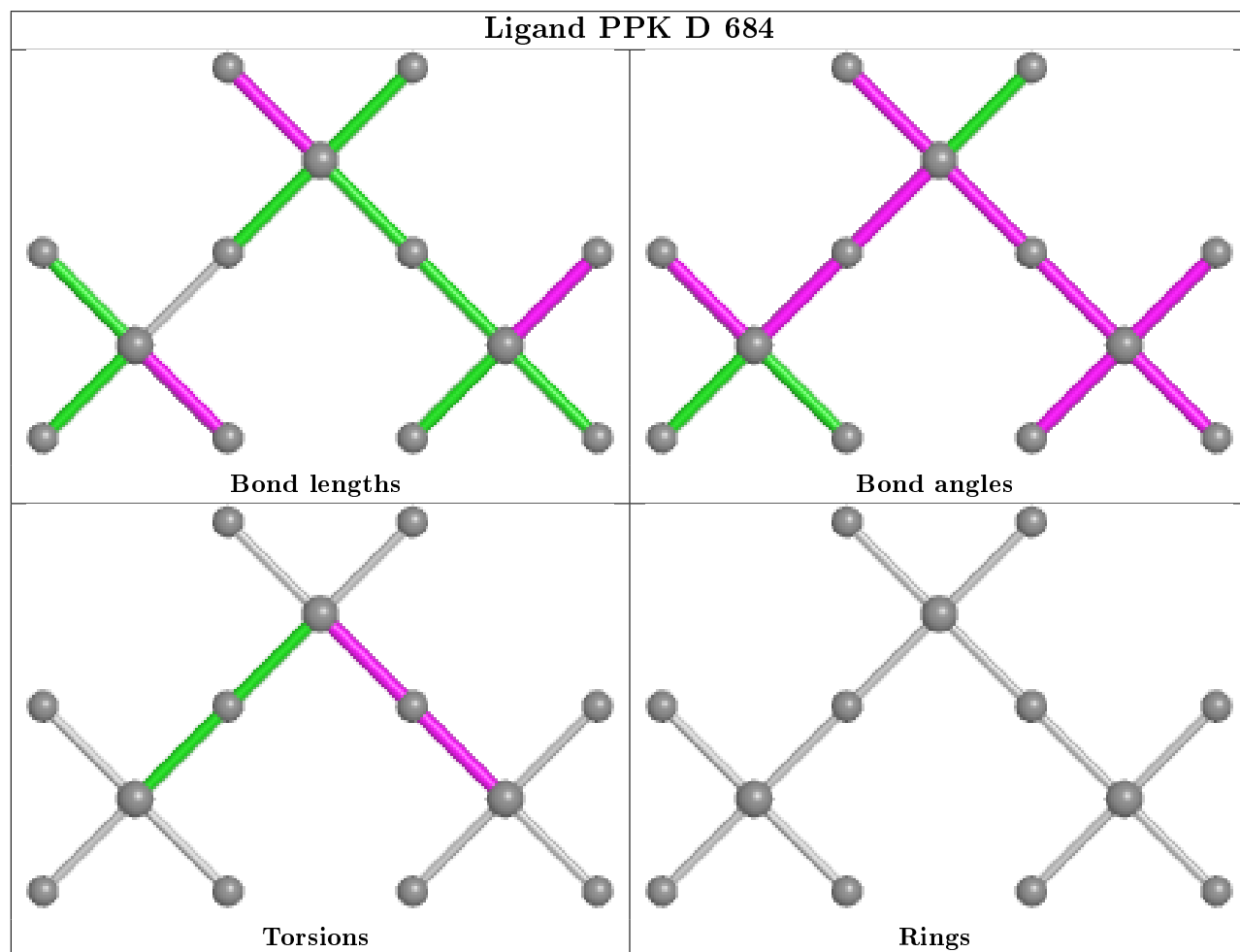
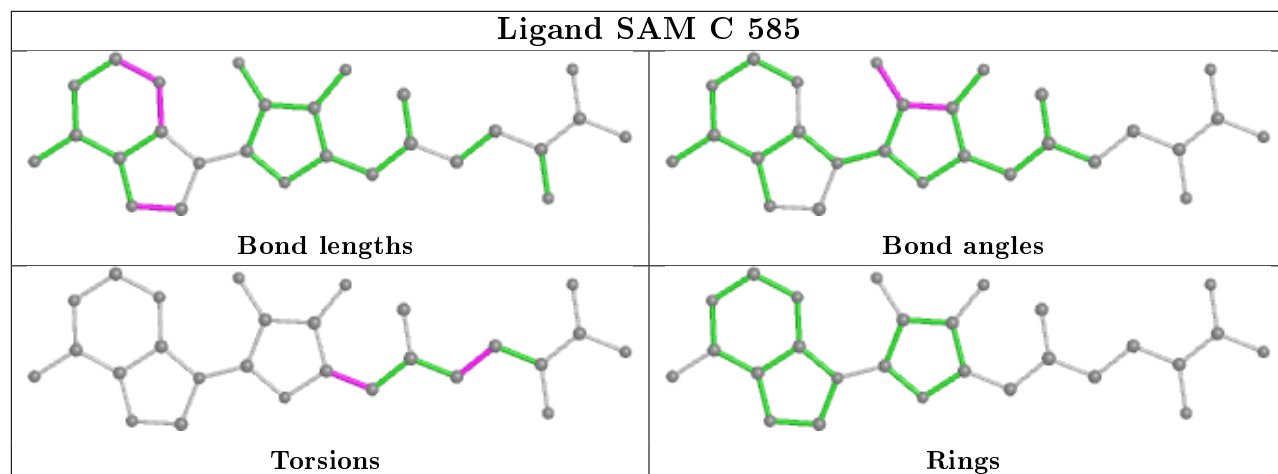
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

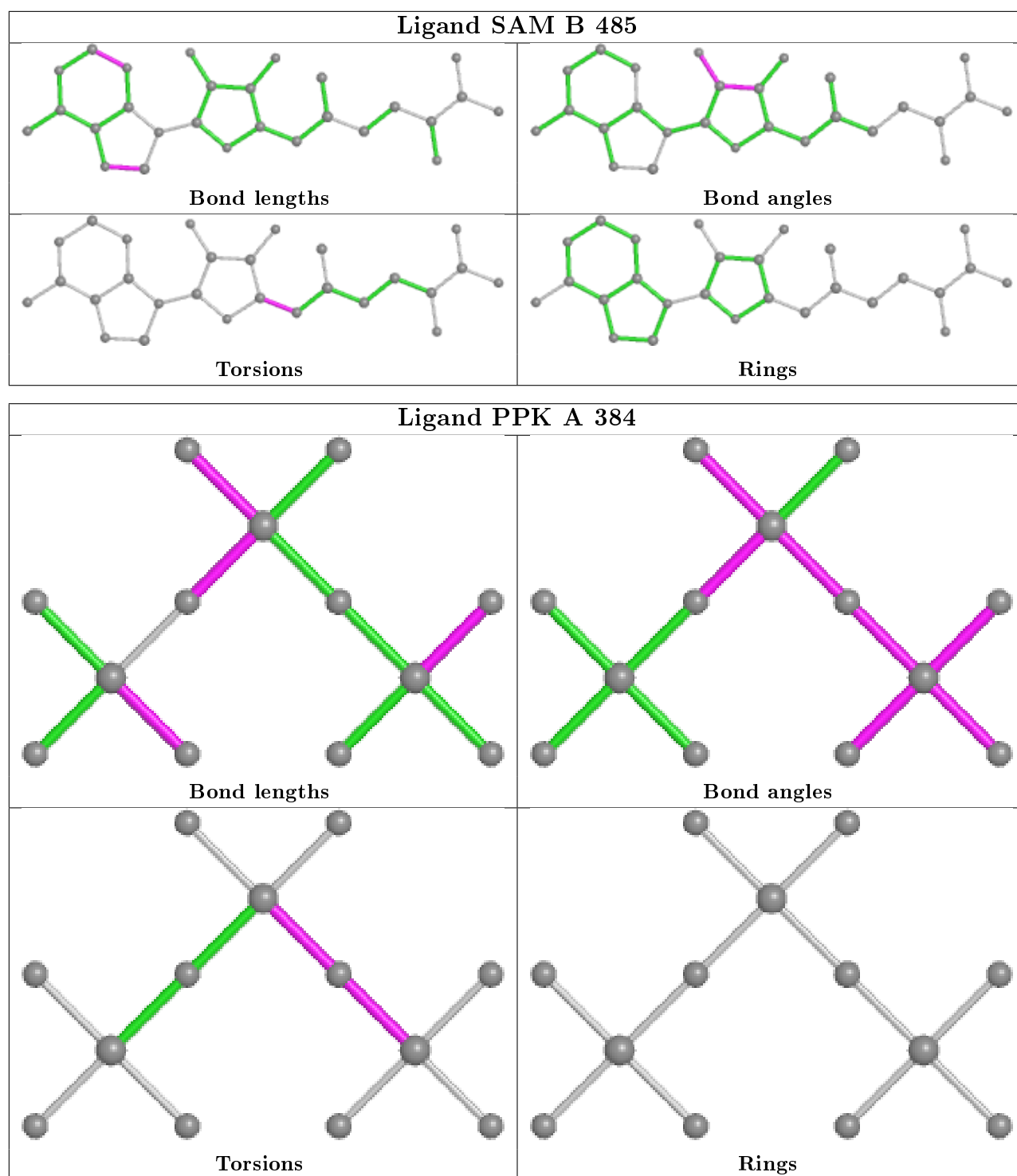


highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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	383/383 (100%)	-0.80	0 100 100	2, 11, 41, 64	0
1	B	383/383 (100%)	-0.83	3 (0%) 86 87	2, 12, 45, 73	0
1	C	383/383 (100%)	-0.57	3 (0%) 86 87	3, 19, 47, 74	0
1	D	383/383 (100%)	-0.49	7 (1%) 68 71	3, 23, 51, 77	0
All	All	1532/1532 (100%)	-0.67	13 (0%) 86 87	2, 15, 47, 77	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	ALA	5.9
1	C	327	LEU	3.7
1	C	1	ALA	3.3
1	D	381	GLY	2.8
1	D	175	GLY	2.7
1	D	174	ASP	2.6
1	D	380	ALA	2.5
1	B	114	GLN	2.3
1	B	330	ARG	2.3
1	D	324	GLN	2.2
1	B	382	LEU	2.1
1	C	328	LEU	2.0
1	D	114	GLN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

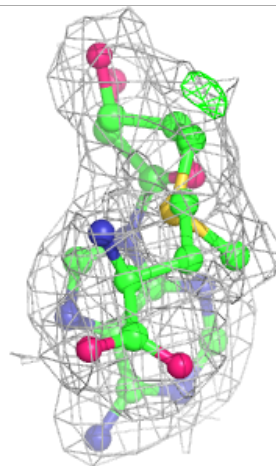
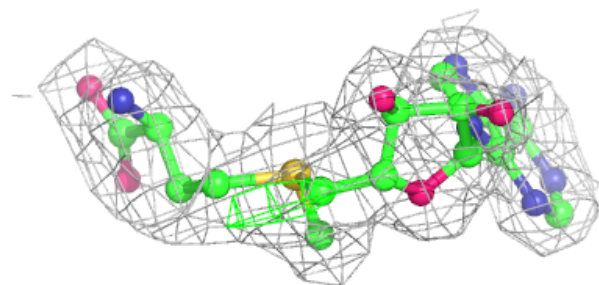
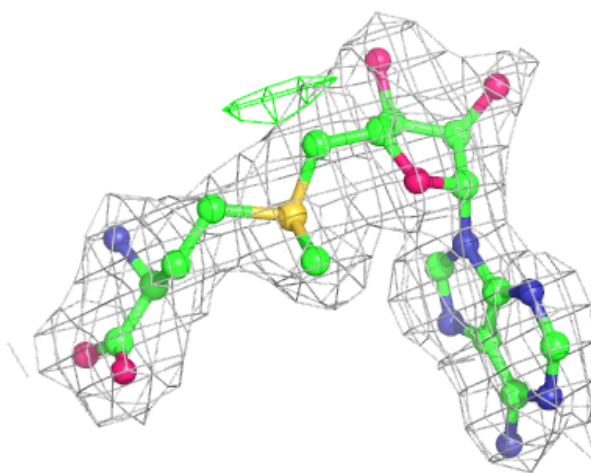
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	MG	C	687	1/1	0.87	0.23	41,41,41,41	0
3	MG	C	588	1/1	0.89	0.25	40,40,40,40	0
3	MG	A	388	1/1	0.89	0.19	24,24,24,24	0
3	MG	B	487	1/1	0.90	0.21	27,27,27,27	0
3	MG	D	587	1/1	0.91	0.16	17,17,17,17	0
3	MG	A	387	1/1	0.93	0.11	23,23,23,23	0
3	MG	D	688	1/1	0.93	0.18	23,23,23,23	0
2	K	D	686	1/1	0.95	0.12	41,41,41,41	0
3	MG	B	488	1/1	0.96	0.10	8,8,8,8	0
4	SAM	C	585	27/27	0.97	0.09	2,14,19,22	0
4	SAM	A	385	27/27	0.97	0.09	2,12,20,21	0
5	PPK	C	584	13/13	0.97	0.10	4,19,25,29	0
4	SAM	C	685	27/27	0.97	0.09	7,13,18,19	0
5	PPK	B	484	13/13	0.98	0.09	2,8,15,17	0
5	PPK	A	384	13/13	0.98	0.09	6,11,18,19	0
5	PPK	D	684	13/13	0.98	0.08	2,9,24,24	0
4	SAM	B	485	27/27	0.98	0.08	2,5,25,30	0
2	K	C	586	1/1	0.99	0.04	18,18,18,18	0
2	K	A	386	1/1	0.99	0.08	4,4,4,4	0
2	K	B	486	1/1	1.00	0.02	2,2,2,2	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 SAM C 585:**

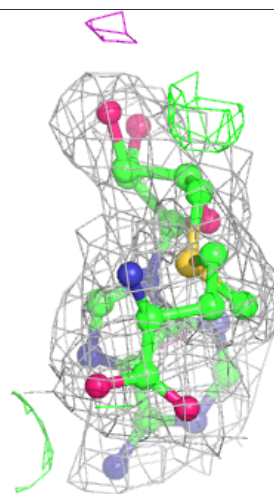
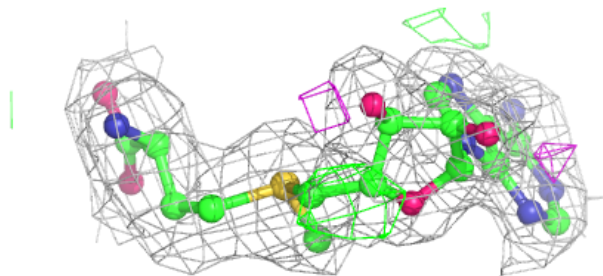
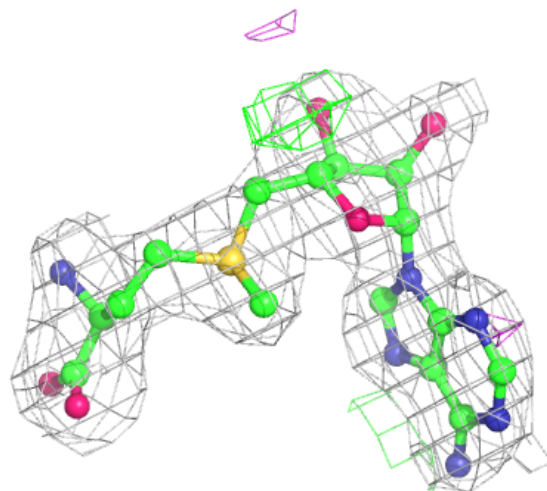
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





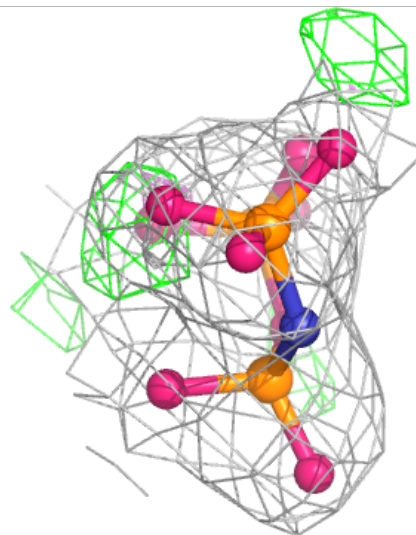
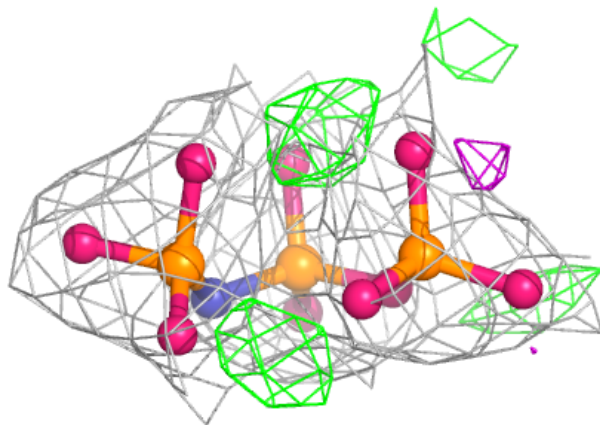
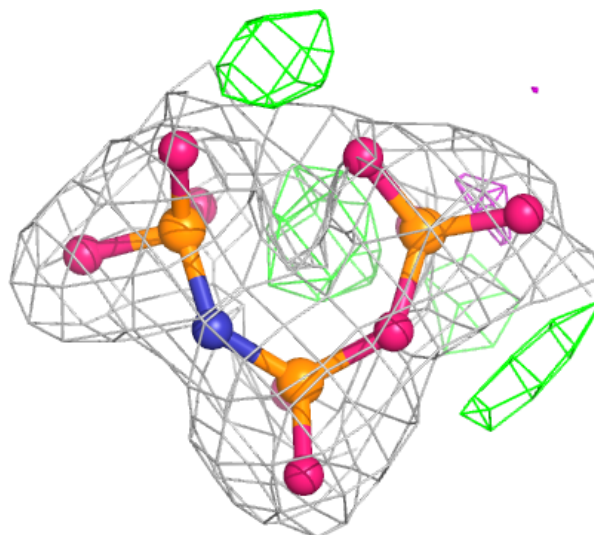
**Electron density around SAM A 385:**

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



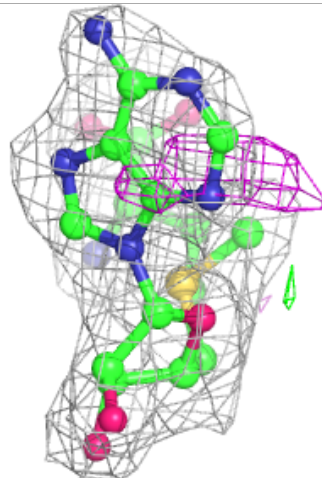
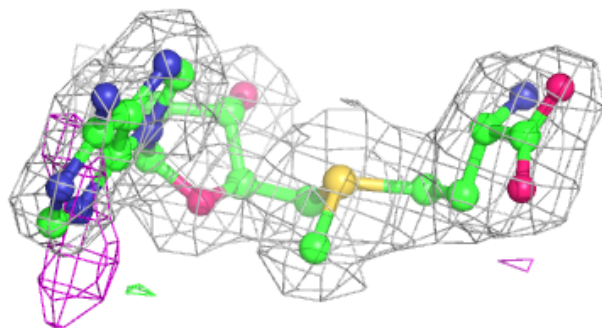
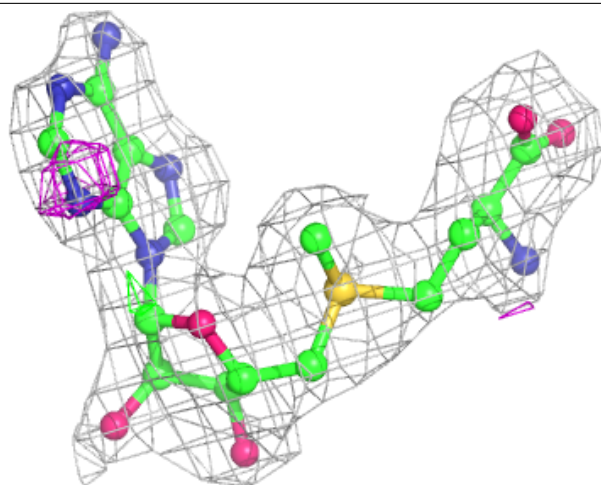
**Electron density around PPK C 584:**

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



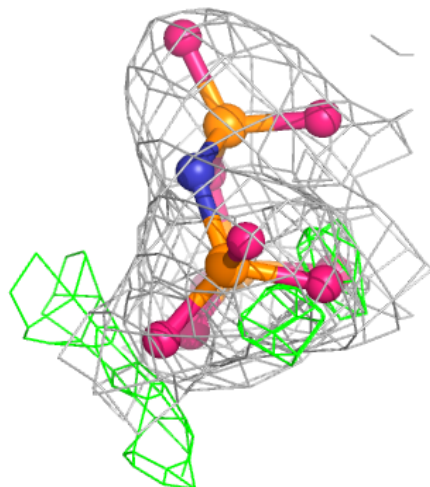
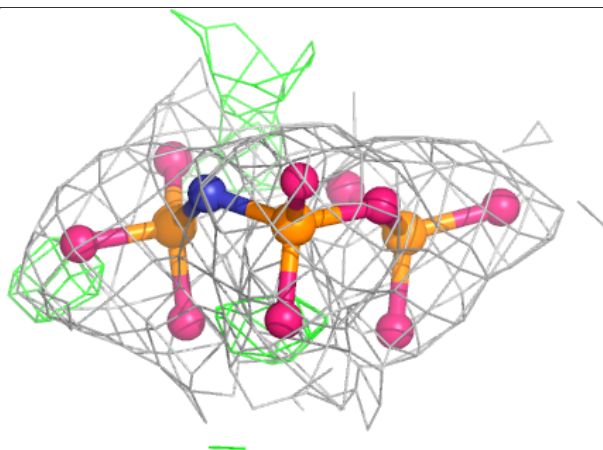
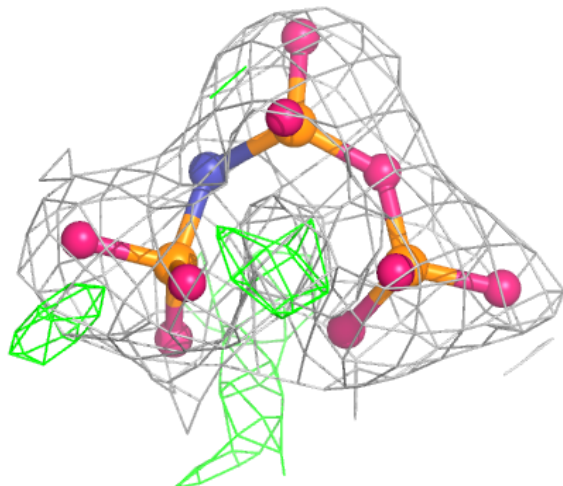
**Electron density around SAM C 685:**

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



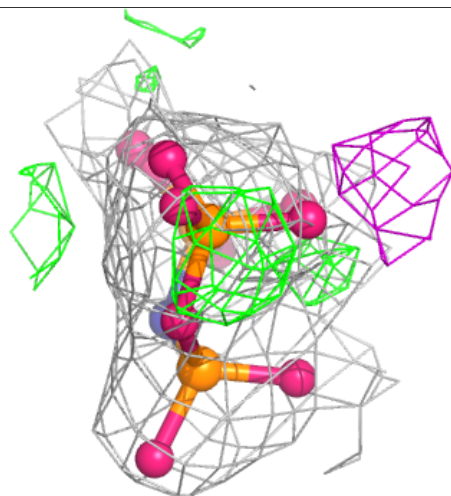
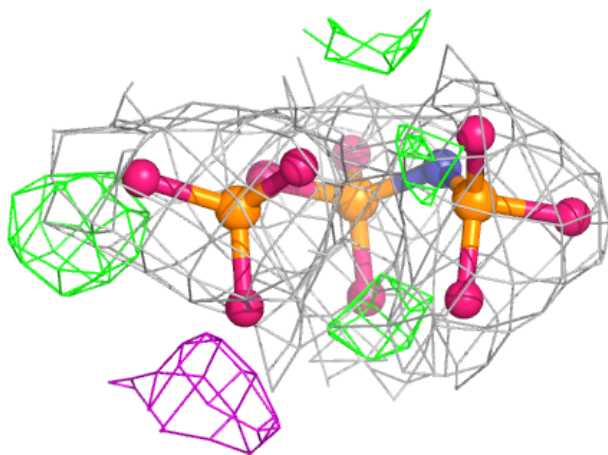
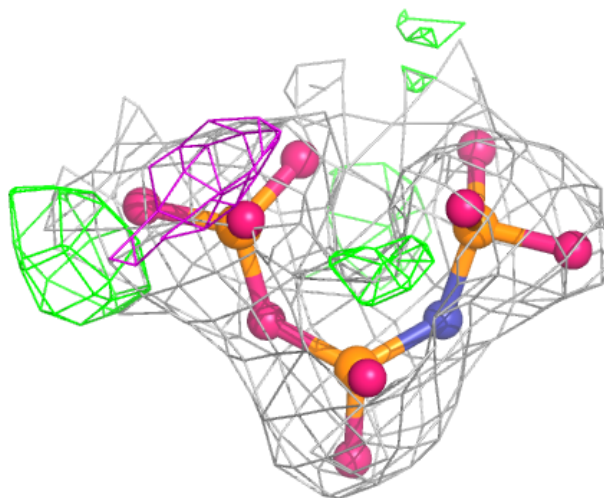
**Electron density around PPK B 484:**

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



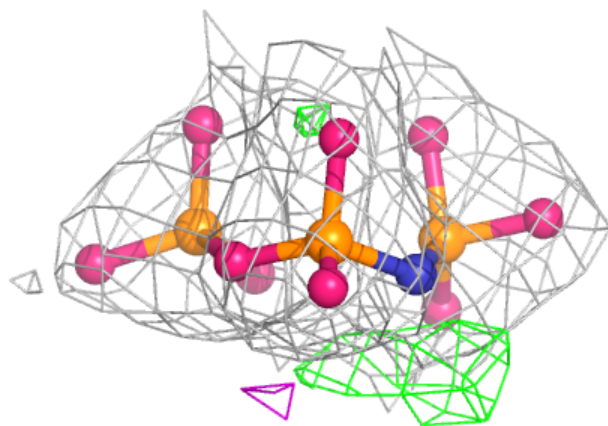
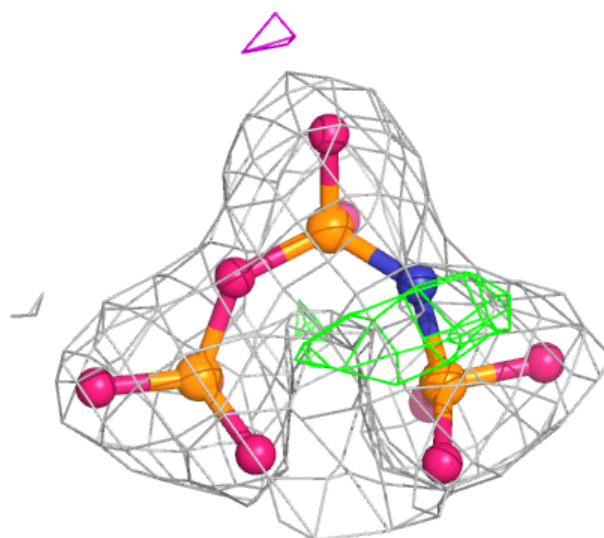
**Electron density around PPK A 384:**

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

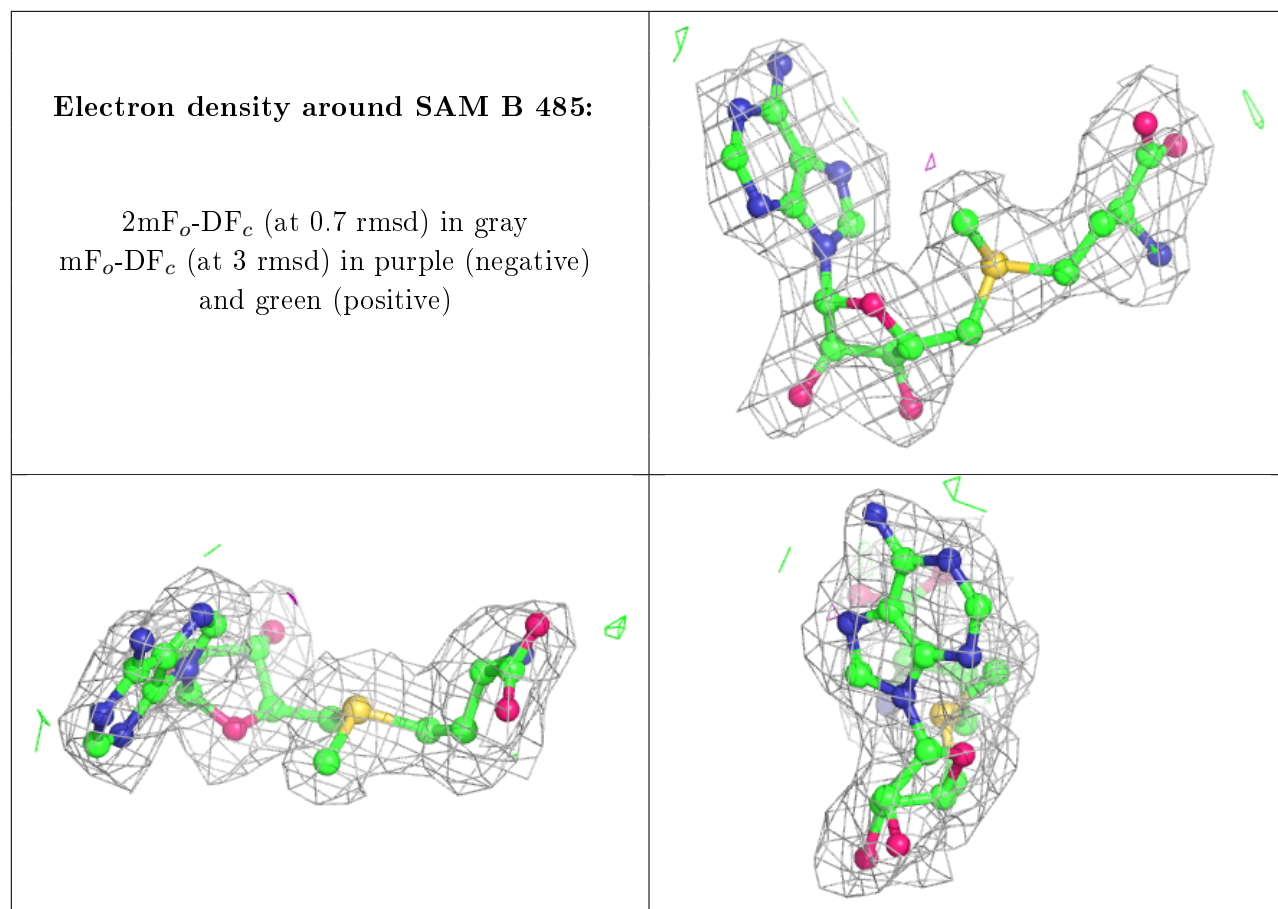


**Electron density around PPK D 684:**

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







## 6.5 Other polymers ⓘ

There are no such residues in this entry.