



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:28 am BST

PDB ID : 4JUC  
Title : Crystal Structure of the Ser26Met mutant of Benzoylformate Decarboxylase from *Pseudomonas putida*  
Authors : McLeish, M.J.; Brodtkin, H.R.  
Deposited on : 2013-03-24  
Resolution : 2.30 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

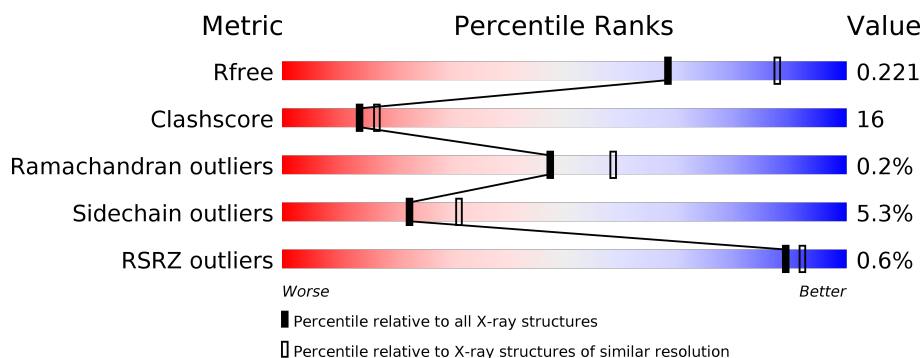
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	534	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>• •</div> </div> </div>
1	B	534	<div> <div>74%</div> <div>22%</div> <div>• •</div> </div>
1	C	534	<div> <div>74%</div> <div>22%</div> <div>• •</div> </div>
1	D	534	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>28%</div> <div>• •</div> </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
4	GOL	B	604	-	-	X	-
4	GOL	C	604	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16657 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 Benzoylformate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	1	0
			3944	2495	682	747	20			
1	B	526	Total	C	N	O	S	0	0	0
			3950	2499	684	747	20			
1	C	526	Total	C	N	O	S	6	3	0
			3966	2512	685	747	22			
1	D	525	Total	C	N	O	S	0	4	0
			3969	2512	689	747	21			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	SER	ENGINEERED MUTATION	UNP P20906
A	529	HIS	-	EXPRESSION TAG	UNP P20906
A	530	HIS	-	EXPRESSION TAG	UNP P20906
A	531	HIS	-	EXPRESSION TAG	UNP P20906
A	532	HIS	-	EXPRESSION TAG	UNP P20906
A	533	HIS	-	EXPRESSION TAG	UNP P20906
A	534	HIS	-	EXPRESSION TAG	UNP P20906
B	26	MET	SER	ENGINEERED MUTATION	UNP P20906
B	529	HIS	-	EXPRESSION TAG	UNP P20906
B	530	HIS	-	EXPRESSION TAG	UNP P20906
B	531	HIS	-	EXPRESSION TAG	UNP P20906
B	532	HIS	-	EXPRESSION TAG	UNP P20906
B	533	HIS	-	EXPRESSION TAG	UNP P20906
B	534	HIS	-	EXPRESSION TAG	UNP P20906
C	26	MET	SER	ENGINEERED MUTATION	UNP P20906
C	529	HIS	-	EXPRESSION TAG	UNP P20906
C	530	HIS	-	EXPRESSION TAG	UNP P20906
C	531	HIS	-	EXPRESSION TAG	UNP P20906
C	532	HIS	-	EXPRESSION TAG	UNP P20906
C	533	HIS	-	EXPRESSION TAG	UNP P20906
C	534	HIS	-	EXPRESSION TAG	UNP P20906

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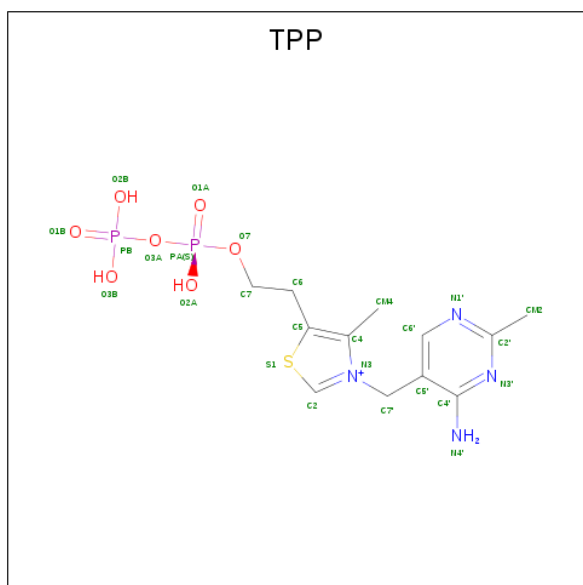
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Chain	Residue	Modelled	Actual	Comment	Reference
D	26	MET	SER	ENGINEERED MUTATION	UNP P20906
D	529	HIS	-	EXPRESSION TAG	UNP P20906
D	530	HIS	-	EXPRESSION TAG	UNP P20906
D	531	HIS	-	EXPRESSION TAG	UNP P20906
D	532	HIS	-	EXPRESSION TAG	UNP P20906
D	533	HIS	-	EXPRESSION TAG	UNP P20906
D	534	HIS	-	EXPRESSION TAG	UNP P20906

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 26 12 4 7 2 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

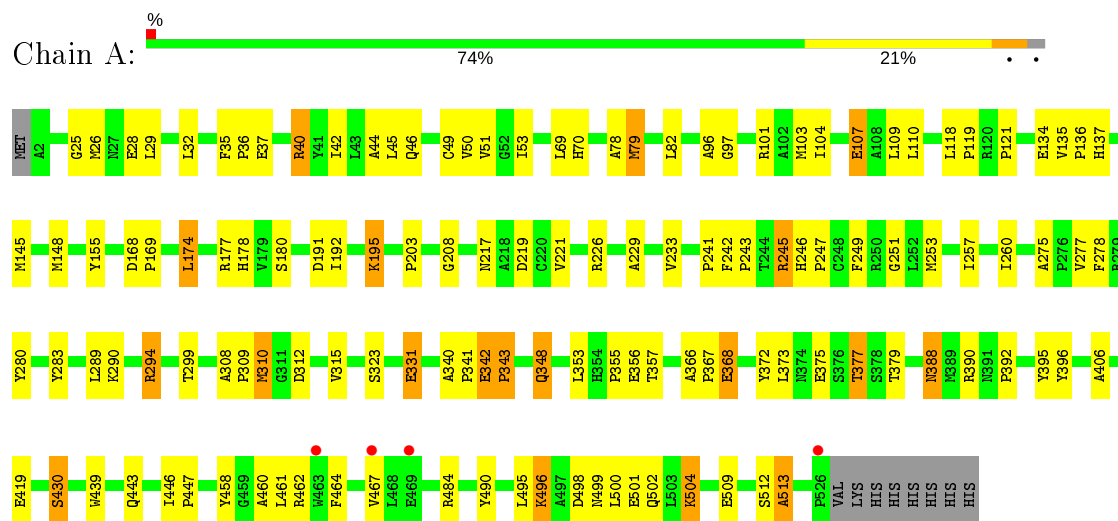
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total 173	O 173	0	0
5	B	189	Total 189	O 189	0	0
5	C	171	Total 171	O 171	0	0
5	D	151	Total 151	O 151	0	0

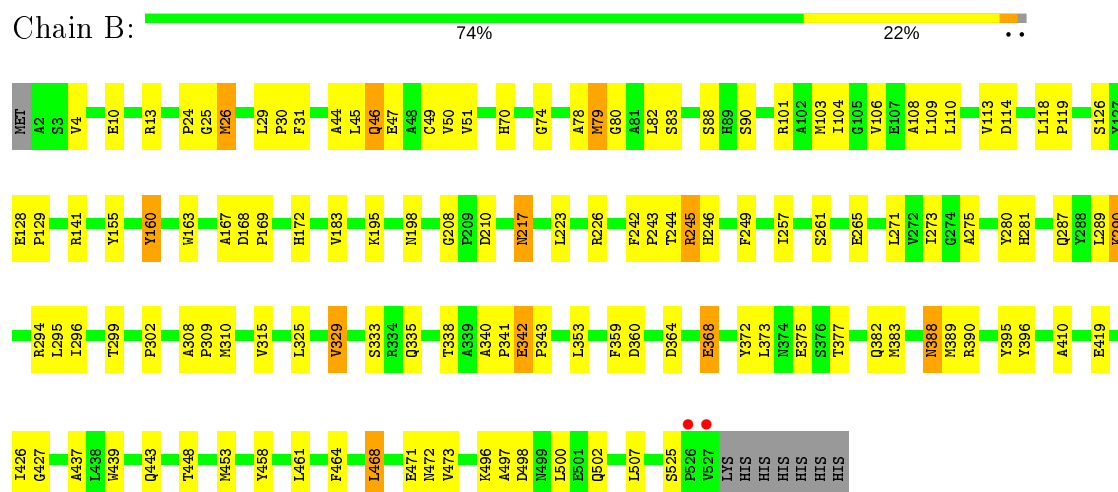
### 3 Residue-property plots

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: Benzoylformate decarboxylase



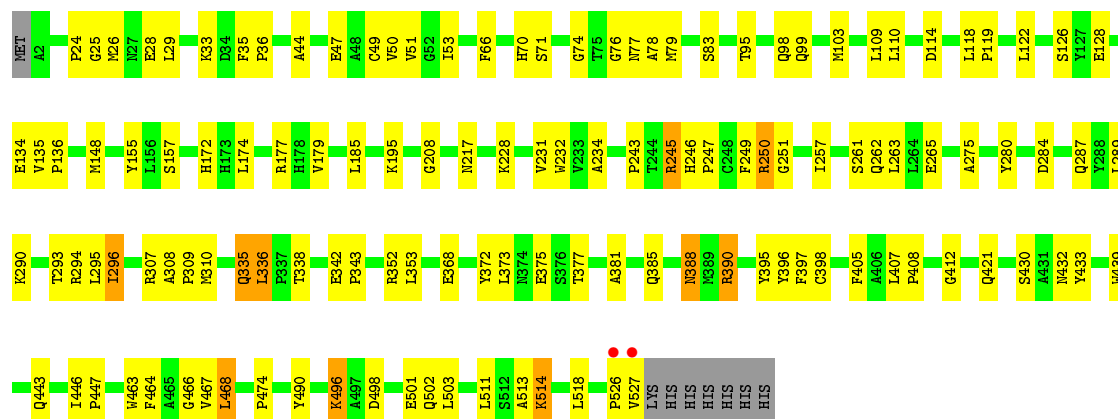
#### • Molecule 1: Benzoylformate decarboxylase



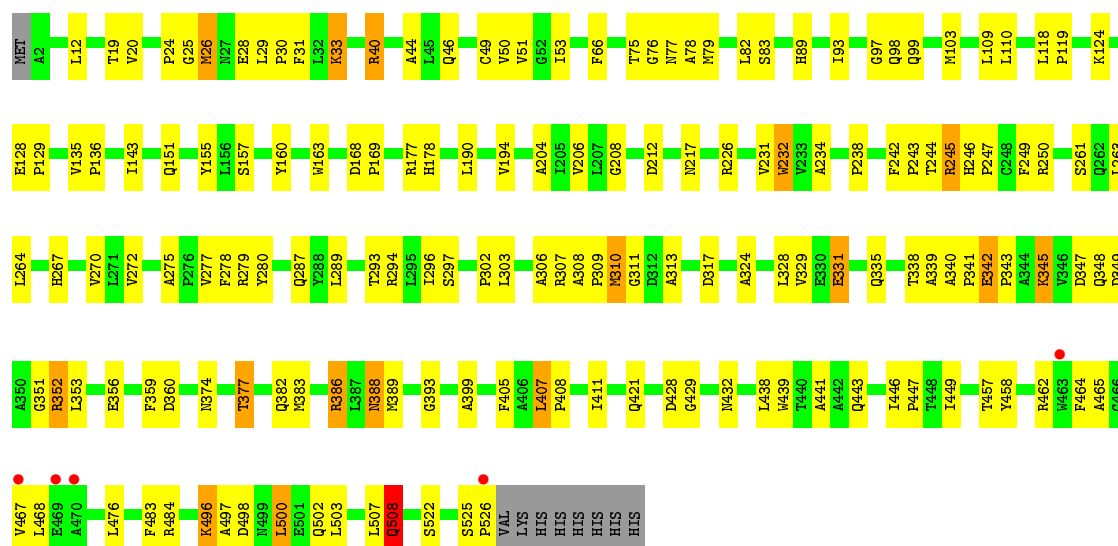
#### • Molecule 1: Benzoylformate decarboxylase







• Molecule 1: Benzoylformate decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.88 Å   163.83 Å   175.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	42.40 – 2.30 42.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.7 (42.40-2.30) 89.7 (42.40-2.30)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.32 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.196   ,   0.228 0.190   ,   0.221	Depositor DCC
$R_{free}$ test set	1984 reflections (2.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 32.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16657	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: GOL, CA, TPP

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	0.40	0/4043	0.49	0/5528
1	B	0.41	0/4046	0.48	0/5532
1	C	0.42	0/4071	0.49	0/5563
1	D	0.42	0/4078	0.49	2/5573 (0.0%)
All	All	0.41	0/16238	0.49	2/22196 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	508[A]	GLN	CB-CA-C	5.77	121.94	110.40
1	D	508[B]	GLN	CB-CA-C	5.77	121.94	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	508[A]	GLN	Mainchain
1	D	508[B]	GLN	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3944	0	3872	148	0
1	B	3950	0	3883	113	0
1	C	3966	0	3914	124	0
1	D	3969	0	3911	169	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	26	0	16	8	0
3	B	26	0	16	5	0
3	C	26	0	16	0	0
3	D	26	0	16	5	0
4	A	12	0	16	1	0
4	B	12	0	16	6	0
4	C	12	0	16	7	0
5	A	173	0	0	15	0
5	B	189	0	0	9	0
5	C	171	0	0	12	0
5	D	151	0	0	9	0
All	All	16657	0	15692	502	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 16.

All (502) 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:D:382:GLN:NE2	1:D:386:ARG:HE	1.05	1.52
1:D:382:GLN:NE2	1:D:386:ARG:NE	1.83	1.27
1:A:496:LYS:HE2	1:A:502:GLN:NE2	1.51	1.26
4:B:604:GOL:H32	5:B:838:HOH:O	1.27	1.25
1:D:294:ARG:NH1	5:D:737:HOH:O	1.71	1.21
1:A:145:MET:HE1	1:D:303:LEU:HA	1.37	1.01
1:A:496:LYS:HD3	1:A:496:LYS:O	1.59	1.00
1:A:462:ARG:HG2	1:A:462:ARG:HH11	1.28	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ALA:HB3	1:B:50:VAL:HG22	1.43	0.99
1:A:145:MET:CE	1:D:303:LEU:HA	1.94	0.97
1:C:421:GLN:OE1	4:C:604:GOL:H2	1.64	0.97
1:A:208:GLY:HA3	1:A:275:ALA:HB2	1.46	0.95
1:D:464:PHE:O	1:D:468:LEU:HD12	1.65	0.95
1:B:498:ASP:H	1:B:502:GLN:NE2	1.62	0.95
1:D:382:GLN:HE21	1:D:386:ARG:NE	1.54	0.94
1:A:348:GLN:HG3	1:A:357:THR:OG1	1.68	0.93
1:A:464:PHE:CE2	1:C:26[B]:MET:HG3	2.04	0.92
1:A:496:LYS:HE2	1:A:502:GLN:HE22	1.07	0.92
1:A:246:HIS:CG	1:A:247:PRO:HD2	2.08	0.89
1:D:226[A]:ARG:HH11	1:D:331:GLU:HG3	1.38	0.86
1:B:44:ALA:HB3	1:B:50:VAL:CG2	2.05	0.86
1:C:118:LEU:HB3	1:C:119:PRO:HD3	1.59	0.85
1:A:331:GLU:OE2	5:A:744:HOH:O	1.95	0.85
1:B:281:HIS:NE2	1:D:26:MET:HE2	1.92	0.84
1:D:498:ASP:H	1:D:502:GLN:NE2	1.74	0.84
1:D:128:GLU:OE1	1:D:157:SER:OG	1.94	0.84
1:D:464:PHE:CE2	1:D:468:LEU:HD11	2.11	0.84
1:D:349:ASP:OD1	1:D:351:GLY:N	2.10	0.83
1:C:208:GLY:HA3	1:C:275:ALA:HB2	1.60	0.83
1:D:352:ARG:NH1	1:D:522:SER:HB3	1.94	0.82
1:D:342:GLU:HG3	1:D:343:PRO:HD2	1.60	0.82
1:D:496:LYS:HE3	1:D:502:GLN:HE22	1.42	0.81
1:A:348:GLN:OE1	1:A:353:LEU:HA	1.79	0.81
1:D:388:ASN:C	1:D:388:ASN:HD22	1.85	0.80
1:C:26[A]:MET:HG3	5:C:718:HOH:O	1.81	0.80
1:C:172:HIS:HD2	5:C:870:HOH:O	1.64	0.79
1:A:245:ARG:HB2	5:A:873:HOH:O	1.81	0.79
1:A:496:LYS:CE	1:A:502:GLN:HE22	1.92	0.79
1:C:47:GLU:HG2	1:C:74:GLY:O	1.82	0.79
1:D:382:GLN:HE22	1:D:386:ARG:HE	0.80	0.78
1:B:464:PHE:CZ	1:B:468:LEU:HD21	2.20	0.77
1:B:325:LEU:O	1:B:329:VAL:HG22	1.86	0.76
1:C:287:GLN:OE1	1:C:290:LYS:NZ	2.18	0.76
1:A:145:MET:HE1	1:D:303:LEU:CA	2.14	0.75
1:B:342:GLU:HG3	1:B:343:PRO:HD2	1.69	0.75
1:D:464:PHE:CD2	1:D:468:LEU:HD11	2.21	0.75
1:B:368:GLU:HG2	1:B:390:ARG:NH1	2.00	0.75
1:A:462:ARG:NH1	1:A:462:ARG:HG2	2.02	0.75
1:D:382:GLN:HE21	1:D:386:ARG:CD	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ARG:HH22	4:B:604:GOL:H11	1.50	0.74
1:C:228:LYS:HD2	1:C:336:LEU:CD1	2.17	0.74
1:A:464:PHE:HD2	1:C:29:LEU:HD12	1.52	0.74
1:B:172:HIS:HD2	5:B:873:HOH:O	1.71	0.73
1:A:496:LYS:HD3	1:A:496:LYS:C	2.07	0.73
1:A:134:GLU:HA	4:A:604:GOL:H11	1.70	0.73
1:D:226[A]:ARG:NH1	1:D:331:GLU:HG3	2.04	0.73
1:D:382:GLN:HE22	1:D:386:ARG:NE	1.63	0.72
1:C:174:LEU:HA	1:C:177:ARG:HG3	1.71	0.72
1:C:135:VAL:HB	1:C:136:PRO:HD3	1.71	0.72
1:A:461:LEU:HD11	3:A:602:TPP:HM43	1.70	0.71
1:A:499:ASN:HB2	5:A:850:HOH:O	1.88	0.71
1:D:109:LEU:O	1:D:110:LEU:HB2	1.89	0.71
1:C:228:LYS:CD	1:C:336:LEU:CD1	2.67	0.71
1:C:390:ARG:CD	5:C:705:HOH:O	2.38	0.71
1:C:513:ALA:O	4:C:604:GOL:H31	1.91	0.71
1:D:345:LYS:O	1:D:345:LYS:HG3	1.90	0.71
1:C:232:TRP:CE2	1:C:250:ARG:HB3	2.26	0.71
1:A:191:ASP:O	1:A:195:LYS:HG3	1.91	0.71
1:A:496:LYS:CE	1:A:502:GLN:NE2	2.44	0.71
1:C:118:LEU:HB3	1:C:119:PRO:CD	2.21	0.70
1:B:439:TRP:CZ2	1:B:443:GLN:HG3	2.26	0.70
1:B:458:TYR:CD1	3:B:602:TPP:H61	2.27	0.69
1:D:317:ASP:OD2	5:D:842:HOH:O	2.08	0.69
1:B:464:PHE:CD1	1:B:468:LEU:HD11	2.28	0.69
1:C:353:LEU:HD22	1:C:503:LEU:HD22	1.75	0.69
1:D:234:ALA:HB1	5:D:703:HOH:O	1.92	0.69
1:B:281:HIS:NE2	1:D:26:MET:CE	2.54	0.69
1:B:464:PHE:CE1	1:B:468:LEU:HD11	2.27	0.69
1:C:289:LEU:HD22	1:C:293:THR:HG21	1.74	0.69
1:A:145:MET:HE2	1:D:306:ALA:HB3	1.75	0.68
1:B:210:ASP:OD2	5:B:788:HOH:O	2.10	0.68
1:C:498:ASP:H	1:C:502:GLN:NE2	1.92	0.68
1:D:30:PRO:HG2	1:D:160:TYR:HB2	1.74	0.68
1:A:135:VAL:HB	1:A:136:PRO:HD3	1.74	0.68
1:B:80:GLY:O	1:B:83:SER:HB3	1.93	0.68
1:C:284:ASP:OD2	5:C:823:HOH:O	2.12	0.68
1:D:353:LEU:HD21	1:D:500:LEU:HA	1.76	0.68
1:D:77:ASN:OD1	5:D:717:HOH:O	2.11	0.68
1:D:496:LYS:HE3	1:D:502:GLN:NE2	2.09	0.68
1:D:135:VAL:HB	1:D:136:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:MET:HA	1:B:79:MET:CE	2.25	0.67
1:D:464:PHE:CZ	1:D:468:LEU:HD11	2.29	0.67
1:B:25:GLY:HA2	3:D:602:TPP:H7'1	1.77	0.67
1:A:243:PRO:HG2	1:A:246:HIS:HB2	1.76	0.66
1:A:51:VAL:HG21	1:A:78:ALA:HB1	1.76	0.66
1:A:464:PHE:CE1	1:C:26[B]:MET:HE3	2.30	0.66
1:B:26:MET:HE2	1:D:464:PHE:HB2	1.75	0.66
1:B:243:PRO:HB2	1:B:246:HIS:HB2	1.78	0.66
1:C:250:ARG:NH2	1:C:338:THR:O	2.22	0.66
1:D:208:GLY:HA3	1:D:275:ALA:HB2	1.78	0.66
1:D:247:PRO:HA	1:D:339:ALA:HB2	1.79	0.65
1:A:109:LEU:O	1:A:110:LEU:HB2	1.97	0.65
1:D:29:LEU:HB2	1:D:30:PRO:HD3	1.77	0.65
1:D:118:LEU:HB3	1:D:119:PRO:HD3	1.79	0.65
1:A:79:MET:HB2	1:C:76:GLY:O	1.96	0.65
1:A:464:PHE:CD2	1:C:26[B]:MET:HG3	2.32	0.65
1:B:26:MET:CE	1:D:464:PHE:HB2	2.27	0.65
1:B:281:HIS:CE1	1:D:26:MET:HE1	2.32	0.64
1:C:246:HIS:CG	1:C:247:PRO:HD2	2.32	0.64
1:C:390:ARG:HD2	5:C:705:HOH:O	1.96	0.64
1:D:289:LEU:HD13	1:D:293:THR:HG22	1.78	0.64
1:C:405:PHE:O	1:C:408:PRO:HD2	1.98	0.64
1:C:228:LYS:HD2	1:C:336:LEU:HD13	1.80	0.64
1:D:353:LEU:HD21	1:D:500:LEU:CA	2.28	0.64
1:D:458:TYR:CD1	3:D:602:TPP:H61	2.33	0.63
1:A:377:THR:HG21	3:A:602:TPP:S1	2.38	0.63
1:C:47:GLU:HB3	1:C:78:ALA:HB2	1.81	0.63
1:A:430:SER:OG	3:A:602:TPP:O1A	2.14	0.63
1:C:511:LEU:O	4:C:604:GOL:H32	1.98	0.63
1:A:499:ASN:CB	5:A:850:HOH:O	2.44	0.62
1:C:390:ARG:HD3	5:C:705:HOH:O	1.99	0.62
1:D:407:LEU:HB3	1:D:408:PRO:HD3	1.80	0.62
1:B:108:ALA:HB1	1:D:280:TYR:O	1.99	0.62
1:C:439:TRP:CZ2	1:C:443:GLN:HG3	2.35	0.62
1:A:145:MET:HE2	1:D:306:ALA:CB	2.30	0.62
1:D:360:ASP:OD1	1:D:386:ARG:HG2	2.00	0.61
1:D:382:GLN:NE2	1:D:386:ARG:CD	2.62	0.61
3:B:602:TPP:HM43	1:D:24:PRO:O	2.00	0.61
1:D:352:ARG:HH11	1:D:522:SER:HB3	1.63	0.61
1:A:353:LEU:HD21	1:A:500:LEU:HA	1.81	0.61
1:D:407:LEU:HB3	1:D:408:PRO:CD	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508[B]:GLN:HA	1:D:508[B]:GLN:OE1	1.99	0.61
1:A:439:TRP:CZ2	1:A:443:GLN:HG3	2.34	0.61
1:D:226[B]:ARG:NH1	1:D:329:VAL:O	2.34	0.61
1:B:198:ASN:O	5:B:730:HOH:O	2.16	0.60
1:A:278:PHE:HB2	1:A:280:TYR:CZ	2.36	0.60
1:B:377:THR:OG1	3:B:602:TPP:H71	2.01	0.60
1:D:28:GLU:OE2	1:D:97:GLY:HA3	2.02	0.60
1:C:265:GLU:HG3	1:C:290:LYS:HD3	1.84	0.60
1:C:526:PRO:O	1:C:527:VAL:O	2.20	0.60
1:C:51:VAL:HG21	1:C:78:ALA:HB1	1.83	0.60
1:A:283:TYR:OH	5:A:867:HOH:O	2.09	0.60
1:B:29:LEU:HB2	1:B:30:PRO:HD3	1.85	0.59
1:A:109:LEU:O	1:A:110:LEU:CB	2.51	0.59
1:D:244:THR:HA	1:D:249:PHE:CD2	2.37	0.59
1:B:79:MET:HB2	1:D:76:GLY:O	2.02	0.59
1:D:464:PHE:O	1:D:467:VAL:HG22	2.02	0.59
3:B:602:TPP:H7'1	1:D:25:GLY:HA2	1.85	0.59
1:A:464:PHE:CZ	1:C:26[B]:MET:HE2	2.38	0.59
1:D:388:ASN:C	1:D:388:ASN:ND2	2.54	0.59
1:B:168:ASP:OD1	1:B:169:PRO:HD2	2.02	0.58
1:A:29:LEU:HD12	1:C:464:PHE:HD2	1.67	0.58
1:D:267:HIS:O	1:D:293:THR:OG1	2.14	0.58
1:B:183:VAL:HG12	1:C:185:LEU:HA	1.84	0.58
1:B:289:LEU:HD11	1:B:295:LEU:HB2	1.85	0.58
1:D:388:ASN:HD22	1:D:389:MET:N	2.02	0.58
1:A:245:ARG:HG2	1:A:388:ASN:CG	2.24	0.58
1:A:79:MET:HG3	1:C:79[B]:MET:HB2	1.86	0.57
1:A:464:PHE:CD2	1:C:29:LEU:HD12	2.38	0.57
1:D:109:LEU:O	1:D:110:LEU:CB	2.50	0.57
1:D:386:ARG:HG2	1:D:386:ARG:HH11	1.68	0.57
1:A:277:VAL:HG13	1:A:278:PHE:CE2	2.40	0.57
1:C:109:LEU:O	1:C:110:LEU:HB2	2.04	0.57
1:C:498:ASP:H	1:C:502:GLN:HE21	1.51	0.57
1:B:294:ARG:HH22	4:B:604:GOL:C1	2.17	0.57
1:D:428:ASP:HB2	1:D:483:PHE:HZ	1.69	0.57
1:B:353:LEU:HD21	1:B:500:LEU:HA	1.87	0.57
1:C:228:LYS:HD3	1:C:336:LEU:CD1	2.34	0.57
1:B:101:ARG:HA	1:B:104:ILE:HD12	1.87	0.56
1:A:499:ASN:CA	5:A:850:HOH:O	2.53	0.56
1:B:24:PRO:O	3:D:602:TPP:HM43	2.05	0.56
1:A:464:PHE:CE1	1:C:26[B]:MET:CE	2.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HG2	1:C:307:ARG:HA	1.87	0.56
1:A:168:ASP:OD1	1:A:169:PRO:HD2	2.06	0.56
1:A:79:MET:HG3	1:C:79[A]:MET:HB2	1.87	0.56
1:D:129:PRO:HD2	1:D:157:SER:O	2.06	0.56
1:A:203:PRO:HG2	1:A:229:ALA:HB2	1.87	0.56
1:D:356:GLU:HG3	1:D:382:GLN:HG3	1.86	0.56
1:A:340:ALA:HB1	1:A:341:PRO:HD2	1.88	0.55
1:C:28:GLU:OE2	1:C:70:HIS:HA	2.07	0.55
1:D:421:GLN:NE2	1:D:449:ILE:HG13	2.20	0.55
1:A:377:THR:OG1	3:A:602:TPP:H71	2.07	0.55
1:C:208:GLY:CA	1:C:275:ALA:HB2	2.33	0.55
1:B:368:GLU:HG2	1:B:390:ARG:CZ	2.36	0.55
1:C:511:LEU:O	4:C:604:GOL:C3	2.55	0.55
1:D:377:THR:OG1	3:D:602:TPP:H71	2.06	0.55
1:A:134:GLU:HG2	1:A:134:GLU:O	2.07	0.55
1:A:44:ALA:HB3	1:A:50:VAL:HG22	1.87	0.55
1:C:308:ALA:O	5:C:703:HOH:O	2.18	0.55
1:C:335:GLN:HG3	1:C:336:LEU:N	2.21	0.55
1:A:312:ASP:OD1	1:D:178[B]:HIS:HB2	2.07	0.55
1:A:299:THR:O	1:A:315:VAL:HA	2.05	0.55
1:A:499:ASN:HA	5:A:850:HOH:O	2.06	0.55
1:D:243:PRO:HB2	1:D:246:HIS:HB2	1.89	0.55
1:A:208:GLY:CA	1:A:275:ALA:HB2	2.30	0.55
1:A:219:ASP:OD2	1:A:323:SER:HB2	2.07	0.55
1:D:503:LEU:HD12	1:D:503:LEU:O	2.07	0.54
1:A:249:PHE:CE2	1:A:251:GLY:HA2	2.42	0.54
1:D:428:ASP:HB2	1:D:483:PHE:CZ	2.42	0.54
1:B:464:PHE:CD1	1:D:29:LEU:HD12	2.42	0.54
1:A:246:HIS:CD2	1:A:247:PRO:HD2	2.42	0.54
1:A:458:TYR:CD1	3:A:602:TPP:H61	2.42	0.54
1:B:464:PHE:HD1	1:D:29:LEU:HD12	1.73	0.54
1:A:246:HIS:ND1	1:A:247:PRO:HD2	2.23	0.54
1:A:392:PRO:HD3	5:A:813:HOH:O	2.07	0.53
1:B:160:TYR:CD1	1:B:160:TYR:C	2.81	0.53
1:B:208:GLY:HA3	1:B:275:ALA:HB2	1.89	0.53
1:A:203:PRO:O	1:A:229:ALA:HB1	2.08	0.53
1:A:233:VAL:O	1:A:253:MET:HG3	2.09	0.53
1:A:121:PRO:HG3	1:C:114:ASP:HB3	1.90	0.53
1:B:160:TYR:HD1	1:B:160:TYR:O	1.91	0.53
1:B:364:ASP:OD1	4:B:603:GOL:H2	2.09	0.53
1:B:79:MET:HA	1:B:79:MET:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:O	1:A:309:PRO:HD3	2.09	0.53
1:A:353:LEU:HD21	1:A:500:LEU:CA	2.38	0.53
1:D:89:HIS:O	1:D:151:GLN:HB2	2.08	0.53
1:D:498:ASP:H	1:D:502:GLN:HE21	1.52	0.53
1:B:45:LEU:HD13	1:D:432:ASN:CG	2.30	0.52
1:C:148:MET:SD	1:C:179:VAL:HG11	2.49	0.52
1:C:289:LEU:HD22	1:C:293:THR:CG2	2.39	0.52
1:D:232:TRP:CE2	1:D:250:ARG:HB3	2.45	0.52
1:D:44:ALA:HB3	1:D:50:VAL:HG22	1.92	0.52
1:A:145:MET:HE2	1:D:302:PRO:O	2.10	0.52
1:C:232:TRP:CD2	1:C:250:ARG:HB3	2.44	0.52
1:B:281:HIS:CE1	1:D:26:MET:CE	2.93	0.52
1:A:40:ARG:HD2	1:A:42:ILE:HD11	1.92	0.52
1:A:419:GLU:HB2	5:A:750:HOH:O	2.10	0.52
1:B:51:VAL:HG21	1:B:78:ALA:HB1	1.91	0.52
1:B:29:LEU:HD12	1:D:464:PHE:CD2	2.46	0.51
1:B:498:ASP:H	1:B:502:GLN:HE21	1.52	0.51
1:A:145:MET:CE	1:D:306:ALA:HB3	2.40	0.51
1:A:348:GLN:CG	1:A:357:THR:OG1	2.52	0.51
1:C:172:HIS:CD2	5:C:870:HOH:O	2.50	0.51
1:D:405:PHE:HB2	5:D:722:HOH:O	2.09	0.51
1:D:51:VAL:HG21	1:D:78:ALA:HB1	1.92	0.51
1:D:261:SER:HB3	1:D:287:GLN:O	2.08	0.51
1:B:373:LEU:HG	1:B:396:TYR:HB2	1.92	0.51
1:B:79:MET:CE	1:B:82:LEU:HD12	2.41	0.51
1:D:429:GLY:HA3	1:D:458:TYR:HE1	1.76	0.51
1:A:79:MET:CE	1:A:82:LEU:HD12	2.41	0.51
1:C:245:ARG:HG2	1:C:388:ASN:CG	2.31	0.51
1:B:4:VAL:HA	1:B:167:ALA:HB2	1.93	0.51
1:C:397:PHE:O	1:C:398:CYS:C	2.49	0.51
1:C:511:LEU:C	4:C:604:GOL:H32	2.31	0.51
1:A:118:LEU:HB3	1:A:119:PRO:HD3	1.93	0.51
1:A:373:LEU:HG	1:A:396:TYR:HB2	1.92	0.51
1:B:265:GLU:OE2	1:B:290:LYS:HG2	2.11	0.51
1:B:439:TRP:CE2	1:B:443:GLN:HG3	2.46	0.51
1:C:257:ILE:HA	1:C:280:TYR:CE1	2.45	0.51
1:A:137:HIS:NE2	1:D:307:ARG:O	2.34	0.51
1:D:496:LYS:CE	1:D:502:GLN:NE2	2.74	0.51
1:D:79[A]:MET:HA	1:D:82:LEU:HB2	1.92	0.51
1:D:168:ASP:OD1	1:D:169:PRO:HD2	2.11	0.50
1:D:19:THR:HG23	1:D:40:ARG:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:MET:CE	1:A:79:MET:HA	2.41	0.50
1:B:160:TYR:CD1	1:B:160:TYR:O	2.64	0.50
1:C:228:LYS:HD3	1:C:336:LEU:HD11	1.93	0.50
1:A:119:PRO:HG3	1:A:155:TYR:CD2	2.46	0.50
1:A:79:MET:HG3	1:C:79[B]:MET:CB	2.42	0.50
1:B:388:ASN:HD22	1:B:389:MET:N	2.10	0.50
1:D:118:LEU:HB3	1:D:119:PRO:CD	2.41	0.50
1:C:526:PRO:O	1:C:527:VAL:C	2.49	0.50
1:D:348:GLN:NE2	1:D:352:ARG:O	2.41	0.50
1:A:512:SER:O	1:A:513:ALA:O	2.30	0.50
1:A:28:GLU:OE2	1:A:97:GLY:HA3	2.12	0.50
1:D:462:ARG:O	1:D:465:ALA:HB3	2.12	0.50
1:A:260:ILE:HD12	1:A:280:TYR:CE1	2.47	0.50
1:D:439:TRP:CZ2	1:D:443:GLN:HG3	2.47	0.50
1:C:439:TRP:CE2	1:C:443:GLN:HG3	2.47	0.50
1:D:264:LEU:HD12	1:D:289:LEU:HD21	1.93	0.49
1:B:242:PHE:CD2	1:B:243:PRO:HD2	2.47	0.49
1:B:360:ASP:OD1	5:B:792:HOH:O	2.20	0.49
1:B:70:HIS:NE2	1:B:110:LEU:HD22	2.27	0.49
1:C:234:ALA:HB1	5:C:741:HOH:O	2.12	0.49
1:C:243:PRO:HB2	1:C:246:HIS:HB2	1.95	0.49
1:A:145:MET:CE	1:D:303:LEU:HD23	2.43	0.49
1:D:464:PHE:HA	1:D:467:VAL:HG22	1.94	0.49
1:B:245:ARG:HG2	1:B:388:ASN:CG	2.33	0.49
1:B:79:MET:HA	1:B:79:MET:HE2	1.93	0.49
1:B:103:MET:CE	5:D:809:HOH:O	2.60	0.49
1:D:324:ALA:O	1:D:328:LEU:HG	2.11	0.49
1:B:244:THR:HA	1:B:249:PHE:CD2	2.48	0.49
1:A:280:TYR:HB2	1:C:103:MET:HE1	1.94	0.49
1:D:160:TYR:C	1:D:160:TYR:CD1	2.86	0.49
1:A:342:GLU:O	1:A:343:PRO:C	2.51	0.49
1:B:294:ARG:NH1	5:B:826:HOH:O	2.33	0.49
1:B:368:GLU:CG	1:B:390:ARG:NH1	2.72	0.49
1:B:388:ASN:HD22	1:B:388:ASN:C	2.15	0.49
1:D:119:PRO:HG3	1:D:155:TYR:CD2	2.47	0.49
1:D:278:PHE:HB2	1:D:280:TYR:CZ	2.48	0.49
1:D:484:ARG:HD2	1:D:496:LYS:HB3	1.95	0.49
1:B:461:LEU:HD11	3:B:602:TPP:HM43	1.95	0.48
1:C:421:GLN:OE1	4:C:604:GOL:C2	2.51	0.48
1:A:46:GLN:HG3	1:C:433:TYR:HA	1.95	0.48
1:A:500:LEU:O	1:A:504:LYS:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLU:HG2	1:B:74:GLY:CA	2.42	0.48
1:A:26:MET:HG3	1:C:464:PHE:CE2	2.47	0.48
1:A:101:ARG:HA	1:A:104:ILE:HD12	1.95	0.48
1:B:47:GLU:HG2	1:B:74:GLY:O	2.13	0.48
1:D:177:ARG:HB2	5:D:756:HOH:O	2.14	0.48
1:D:226[A]:ARG:HH11	1:D:331:GLU:CG	2.19	0.48
1:A:462:ARG:NH1	1:A:462:ARG:CG	2.68	0.48
1:B:168:ASP:OD1	1:B:169:PRO:CD	2.61	0.48
1:B:257:ILE:HA	1:B:280:TYR:CE1	2.49	0.48
1:B:49:CYS:HB3	1:B:437:ALA:HB2	1.95	0.48
1:C:109:LEU:O	1:C:110:LEU:CB	2.61	0.48
1:C:134:GLU:HG2	1:C:134:GLU:O	2.14	0.48
1:C:119:PRO:HG3	1:C:155:TYR:CG	2.48	0.48
1:D:439:TRP:CH2	1:D:443:GLN:HG3	2.47	0.48
1:B:473:VAL:HG22	1:D:33:LYS:HA	1.96	0.48
1:A:119:PRO:HG3	1:A:155:TYR:CG	2.49	0.48
1:B:299:THR:O	1:B:315:VAL:HA	2.14	0.48
1:A:464:PHE:CZ	1:C:26[B]:MET:CE	2.97	0.48
1:C:289:LEU:HD11	1:C:295:LEU:HB2	1.96	0.48
1:D:464:PHE:CG	1:D:468:LEU:HD11	2.48	0.48
1:C:265:GLU:CG	1:C:290:LYS:HD3	2.43	0.47
1:C:308:ALA:HA	1:C:309:PRO:HD3	1.76	0.47
1:D:353:LEU:HD21	1:D:500:LEU:N	2.29	0.47
1:D:411:ILE:HG12	1:D:441:ALA:HB2	1.95	0.47
1:D:46:GLN:O	1:D:50:VAL:HG23	2.14	0.47
1:B:471:GLU:O	1:B:472:ASN:HB2	2.15	0.47
3:A:602:TPP:H7'1	1:C:25:GLY:HA2	1.96	0.47
1:C:119:PRO:HG3	1:C:155:TYR:CD2	2.49	0.47
1:C:261:SER:HB3	1:C:287:GLN:O	2.15	0.47
1:A:294:ARG:HG2	5:A:839:HOH:O	2.14	0.47
1:A:32:LEU:HB3	1:C:474:PRO:HD2	1.96	0.47
1:A:69:LEU:O	1:A:96:ALA:HA	2.15	0.47
1:B:26:MET:HG3	1:D:464:PHE:CD2	2.49	0.47
1:C:375:GLU:OE1	1:C:430:SER:HB3	2.14	0.47
1:C:407:LEU:HB3	1:C:408:PRO:HD3	1.97	0.47
1:D:118:LEU:N	1:D:119:PRO:HD2	2.30	0.47
1:C:373:LEU:HG	1:C:396:TYR:HB2	1.97	0.47
1:B:294:ARG:NH1	4:B:604:GOL:O3	2.32	0.46
1:C:249:PHE:CE2	1:C:251:GLY:HA2	2.50	0.46
1:D:347:ASP:HA	5:D:815:HOH:O	2.14	0.46
1:A:79:MET:HE1	1:A:119:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:N	1:B:30:PRO:CD	2.79	0.46
1:A:495:LEU:HD11	1:A:509:GLU:HG2	1.98	0.46
1:D:212:ASP:OD2	1:D:393:GLY:HA2	2.15	0.46
1:C:439:TRP:HB2	1:C:490:TYR:CD1	2.50	0.46
1:D:497:ALA:HA	1:D:502:GLN:HE21	1.81	0.46
1:A:242:PHE:CG	1:A:243:PRO:HD2	2.50	0.46
1:B:497:ALA:HA	1:B:502:GLN:HB3	1.97	0.46
1:C:446:ILE:HA	1:C:447:PRO:HD3	1.59	0.46
1:D:246:HIS:CG	1:D:247:PRO:HD2	2.51	0.46
1:A:312:ASP:CG	1:D:178[B]:HIS:HB2	2.36	0.46
1:A:348:GLN:OE1	1:A:353:LEU:CA	2.59	0.46
1:C:128:GLU:HG3	1:C:157:SER:O	2.16	0.45
1:D:261:SER:CB	1:D:287:GLN:O	2.64	0.45
1:D:294:ARG:NH2	1:D:296:ILE:HD11	2.31	0.45
1:D:310:MET:SD	1:D:310:MET:N	2.89	0.45
1:A:135:VAL:CB	1:A:136:PRO:HD3	2.46	0.45
1:A:257:ILE:HG13	5:A:746:HOH:O	2.15	0.45
1:A:446:ILE:HA	1:A:447:PRO:HD3	1.76	0.45
1:B:295:LEU:HD23	1:B:296:ILE:N	2.31	0.45
1:C:294:ARG:NH2	1:C:296:ILE:HD11	2.31	0.45
1:A:375:GLU:HB2	1:A:406:ALA:CB	2.46	0.45
1:B:10:GLU:OE1	1:B:13:ARG:HD2	2.17	0.45
1:D:49:CYS:O	1:D:53:ILE:HG13	2.16	0.45
1:A:79:MET:HE3	1:A:79:MET:HA	1.99	0.45
1:B:245:ARG:HB2	5:B:709:HOH:O	2.15	0.45
1:B:410:ALA:HB1	1:B:448:THR:HG21	1.99	0.45
3:A:602:TPP:HM43	1:C:24:PRO:O	2.16	0.45
1:C:44:ALA:HB3	1:C:50:VAL:CG2	2.47	0.45
1:A:368:GLU:HG3	1:A:390:ARG:NH1	2.31	0.45
1:C:496:LYS:HD3	1:C:496:LYS:O	2.17	0.45
1:D:457:THR:OG1	1:D:476:LEU:O	2.30	0.45
1:B:498:ASP:N	1:B:502:GLN:NE2	2.46	0.45
1:D:31:PHE:HB2	1:D:163:TRP:CE2	2.52	0.45
1:A:464:PHE:CE2	1:C:26[B]:MET:CG	2.91	0.45
1:C:342:GLU:HG3	1:C:343:PRO:HD2	1.99	0.45
1:B:223:LEU:HD12	1:B:329:VAL:HG21	1.99	0.44
1:B:46:GLN:O	1:B:50:VAL:HG23	2.18	0.44
1:C:388:ASN:HD22	1:C:388:ASN:C	2.20	0.44
1:D:246:HIS:ND1	1:D:247:PRO:HD2	2.32	0.44
1:A:277:VAL:HA	1:A:278:PHE:HA	1.74	0.44
1:D:44:ALA:HB3	1:D:50:VAL:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:HIS:HE1	1:A:180:SER:HB2	1.82	0.44
1:A:290:LYS:HE2	5:A:827:HOH:O	2.17	0.44
1:A:103:MET:CE	5:A:844:HOH:O	2.66	0.44
1:A:257:ILE:HA	1:A:280:TYR:CE1	2.53	0.44
1:A:277:VAL:HG13	1:A:278:PHE:CD2	2.53	0.44
1:C:49:CYS:O	1:C:53:ILE:HG13	2.18	0.44
3:D:602:TPP:HM42	3:D:602:TPP:C6'	2.47	0.44
1:A:226:ARG:HD3	1:A:331:GLU:HB2	1.99	0.44
1:A:388:ASN:HD22	1:A:388:ASN:C	2.21	0.44
1:C:135:VAL:CB	1:C:136:PRO:HD3	2.46	0.44
1:A:245:ARG:HD3	1:A:245:ARG:HA	1.54	0.44
1:A:512:SER:O	1:A:513:ALA:C	2.56	0.44
1:D:124:LYS:HE2	1:D:124:LYS:HB3	1.66	0.44
1:C:47:GLU:HB2	1:C:77:ASN:CB	2.48	0.44
1:D:245:ARG:HB2	5:D:716:HOH:O	2.17	0.44
1:A:289:LEU:HG	1:A:310:MET:HG3	2.00	0.43
1:B:109:LEU:O	1:B:110:LEU:HB2	2.17	0.43
1:D:308:ALA:HA	1:D:309:PRO:HD3	1.84	0.43
1:B:88:SER:OG	1:B:90:SER:OG	2.30	0.43
1:D:206:VAL:HB	1:D:272:VAL:HG22	2.01	0.43
1:B:359:PHE:CZ	1:B:383:MET:HB2	2.53	0.43
1:C:35:PHE:HA	1:C:36:PRO:HD3	1.92	0.43
1:A:148:MET:HE1	1:D:302:PRO:O	2.19	0.43
1:A:355:PRO:HG2	1:A:356:GLU:OE1	2.19	0.43
1:B:128:GLU:HA	1:B:129:PRO:HD3	1.84	0.43
1:B:427:GLY:HA2	1:B:453:MET:HB2	2.01	0.43
1:C:514:LYS:HA	1:C:514:LYS:HE3	2.00	0.43
1:D:374:ASN:HB2	1:D:383:MET:SD	2.59	0.43
1:B:372:TYR:O	1:B:395:TYR:HA	2.19	0.43
1:B:47:GLU:HB3	1:B:78:ALA:HB2	2.00	0.43
1:B:79:MET:HE1	1:B:82:LEU:HD12	2.00	0.43
1:C:250:ARG:HD2	1:C:250:ARG:HA	1.64	0.43
1:D:245:ARG:HG2	1:D:388:ASN:CG	2.39	0.43
1:D:407:LEU:CB	1:D:408:PRO:CD	2.95	0.43
1:A:439:TRP:CE2	1:A:443:GLN:HG3	2.54	0.43
1:D:279:ARG:HD3	1:D:279:ARG:HA	1.88	0.43
1:A:25:GLY:HA3	1:A:70:HIS:ND1	2.34	0.43
1:C:466:GLY:C	1:C:468:LEU:H	2.22	0.43
1:C:518:LEU:C	1:C:518:LEU:HD23	2.39	0.42
1:D:250:ARG:HA	1:D:250:ARG:HD3	1.71	0.42
1:A:107:GLU:HG2	5:A:720:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ARG:NH2	4:B:604:GOL:H11	2.28	0.42
1:A:35:PHE:HA	1:A:36:PRO:HD3	1.90	0.42
1:A:353:LEU:HD21	1:A:500:LEU:N	2.34	0.42
1:B:308:ALA:HA	1:B:309:PRO:HD3	1.85	0.42
1:D:12:LEU:HD23	1:D:143:ILE:HD11	2.01	0.42
1:D:190:LEU:O	1:D:194:VAL:HG23	2.19	0.42
1:D:231:VAL:O	1:D:250:ARG:HB2	2.20	0.42
1:D:242:PHE:CD2	1:D:243:PRO:HD2	2.54	0.42
1:B:26:MET:HE3	1:D:464:PHE:HB2	2.01	0.42
1:C:245:ARG:HB2	5:C:709:HOH:O	2.18	0.42
1:D:359:PHE:CZ	1:D:383:MET:HB2	2.55	0.42
1:D:20:VAL:HG22	1:D:66:PHE:CD1	2.55	0.42
1:D:297:SER:O	1:D:313:ALA:HA	2.18	0.42
1:D:503:LEU:HD12	1:D:503:LEU:C	2.40	0.42
1:B:119:PRO:HG3	1:B:155:TYR:CD2	2.54	0.42
1:C:372:TYR:O	1:C:395:TYR:HA	2.19	0.42
1:C:514:LYS:CE	1:C:514:LYS:HA	2.49	0.42
1:D:75:THR:O	1:D:79[A]:MET:HG3	2.20	0.42
1:A:355:PRO:HB3	1:A:379:THR:HG21	2.01	0.42
1:B:183:VAL:HG12	1:C:185:LEU:CA	2.49	0.42
1:B:294:ARG:CG	5:B:826:HOH:O	2.68	0.42
1:D:29:LEU:N	1:D:30:PRO:CD	2.83	0.42
1:D:464:PHE:CE1	1:D:468:LEU:HD11	2.53	0.42
1:A:366:ALA:HB1	1:A:367:PRO:HD2	2.02	0.42
1:B:113:VAL:O	1:B:114:ASP:C	2.55	0.42
1:C:53:ILE:O	1:C:412:GLY:HA3	2.18	0.42
1:C:463:TRP:O	1:C:467:VAL:HG13	2.20	0.42
1:B:30:PRO:HG2	1:B:160:TYR:CD1	2.54	0.42
1:B:375:GLU:HB3	1:B:426:ILE:HG23	2.02	0.42
1:C:98:GLN:HG3	1:C:99:GLN:N	2.35	0.42
1:D:128:GLU:OE1	1:D:157:SER:CB	2.68	0.42
1:D:245:ARG:HA	1:D:245:ARG:HD2	1.88	0.42
1:D:30:PRO:HG2	1:D:160:TYR:CD1	2.55	0.42
1:D:446:ILE:HA	1:D:447:PRO:HD3	1.79	0.42
1:A:168:ASP:OD1	1:A:169:PRO:CD	2.68	0.42
1:C:231:VAL:O	1:C:250:ARG:HB2	2.20	0.42
1:C:439:TRP:CH2	1:C:443:GLN:HG3	2.55	0.42
1:C:511:LEU:O	4:C:604:GOL:O3	2.35	0.42
1:A:44:ALA:HB3	1:A:50:VAL:CG2	2.48	0.41
1:B:217:ASN:OD1	1:B:217:ASN:N	2.53	0.41
1:C:44:ALA:HB3	1:C:50:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:SER:HB3	1:B:287:GLN:O	2.20	0.41
1:C:352:ARG:HD3	5:C:848:HOH:O	2.20	0.41
1:B:30:PRO:HG2	1:B:160:TYR:HB2	2.01	0.41
1:B:242:PHE:CG	1:B:243:PRO:HD2	2.56	0.41
1:B:118:LEU:O	5:B:702:HOH:O	2.22	0.41
1:C:245:ARG:HD2	1:C:245:ARG:HA	1.78	0.41
1:A:177:ARG:NE	1:D:311:GLY:O	2.50	0.41
1:A:49:CYS:O	1:A:53:ILE:HG13	2.21	0.41
1:B:507:LEU:HA	1:B:507:LEU:HD23	1.88	0.41
1:C:381:ALA:O	1:C:385:GLN:HG3	2.21	0.41
1:D:238:PRO:HB3	1:D:399:ALA:HB2	2.01	0.41
1:B:302:PRO:O	1:C:148:MET:HE1	2.21	0.41
1:A:145:MET:CE	1:D:302:PRO:O	2.69	0.41
1:A:308:ALA:HA	1:A:309:PRO:HD3	1.90	0.41
1:D:93:ILE:HD13	1:D:143:ILE:HG12	2.03	0.41
1:D:277:VAL:HA	1:D:278:PHE:HA	1.77	0.41
1:D:525:SER:HA	1:D:526:PRO:HD3	1.90	0.41
1:A:118:LEU:HB3	1:A:119:PRO:CD	2.50	0.41
1:A:342:GLU:HG3	1:A:343:PRO:HD2	2.02	0.41
1:A:342:GLU:O	1:A:343:PRO:O	2.38	0.41
1:A:461:LEU:HD11	3:A:602:TPP:CM4	2.45	0.41
1:D:204:ALA:HB3	1:D:270:VAL:HG22	2.03	0.41
1:A:372:TYR:O	1:A:395:TYR:HA	2.20	0.41
1:A:45:LEU:HD13	1:C:432:ASN:CG	2.41	0.41
1:C:83:SER:CA	1:C:122:LEU:HD13	2.50	0.41
1:D:226[B]:ARG:HD3	1:D:329:VAL:HG23	2.03	0.41
1:A:145:MET:HE1	1:D:303:LEU:HD23	2.01	0.41
1:A:377:THR:HB	1:A:460:ALA:HB2	2.03	0.41
1:A:498:ASP:H	1:A:502:GLN:NE2	2.19	0.41
1:B:340:ALA:HA	1:B:341:PRO:HD3	1.90	0.41
1:C:368:GLU:CB	5:C:846:HOH:O	2.69	0.41
1:D:340:ALA:HA	1:D:341:PRO:HD3	1.96	0.41
1:B:31:PHE:HB2	1:B:163:TRP:CE2	2.56	0.40
1:C:66:PHE:CZ	1:C:95:THR:HG21	2.56	0.40
1:D:79[B]:MET:HA	1:D:82:LEU:HB2	2.02	0.40
1:D:98:GLN:HG3	1:D:99:GLN:N	2.35	0.40
1:A:174:LEU:HA	1:A:177:ARG:HG3	2.03	0.40
1:A:439:TRP:HB2	1:A:490:TYR:CD1	2.57	0.40
1:C:249:PHE:CZ	1:C:251:GLY:HA2	2.56	0.40
1:D:407:LEU:HD21	1:D:438:LEU:HG	2.02	0.40
1:A:484:ARG:HD3	5:A:851:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LEU:CD2	1:B:273:ILE:HD11	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	524/534 (98%)	505 (96%)	16 (3%)	3 (1%)	25	31
1	B	524/534 (98%)	503 (96%)	21 (4%)	0	100	100
1	C	527/534 (99%)	514 (98%)	12 (2%)	1 (0%)	47	58
1	D	527/534 (99%)	508 (96%)	19 (4%)	0	100	100
All	All	2102/2136 (98%)	2030 (97%)	68 (3%)	4 (0%)	47	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	513	ALA
1	A	343	PRO
1	A	241	PRO
1	C	71	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	411/420 (98%)	388 (94%)	23 (6%)	21	29
1	B	412/420 (98%)	388 (94%)	24 (6%)	20	27
1	C	415/420 (99%)	396 (95%)	19 (5%)	27	38
1	D	415/420 (99%)	393 (95%)	22 (5%)	22	31
All	All	1653/1680 (98%)	1565 (95%)	88 (5%)	22	31

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	40	ARG
1	A	79	MET
1	A	107	GLU
1	A	174	LEU
1	A	192	ILE
1	A	195	LYS
1	A	217	ASN
1	A	221	VAL
1	A	245	ARG
1	A	294	ARG
1	A	310	MET
1	A	331	GLU
1	A	342	GLU
1	A	348	GLN
1	A	368	GLU
1	A	377	THR
1	A	388	ASN
1	A	430	SER
1	A	467	VAL
1	A	496	LYS
1	A	501	GLU
1	A	504	LYS
1	B	26	MET
1	B	46	GLN
1	B	79	MET
1	B	106	VAL
1	B	126	SER
1	B	160	TYR
1	B	195	LYS
1	B	217	ASN
1	B	226	ARG
1	B	245	ARG

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Mol	Chain	Res	Type
1	B	290	LYS
1	B	310	MET
1	B	329	VAL
1	B	333	SER
1	B	335	GLN
1	B	338	THR
1	B	342	GLU
1	B	368	GLU
1	B	382	GLN
1	B	388	ASN
1	B	419	GLU
1	B	468	LEU
1	B	496	LYS
1	B	525	SER
1	C	33	LYS
1	C	126	SER
1	C	195	LYS
1	C	217	ASN
1	C	245	ARG
1	C	250	ARG
1	C	262	GLN
1	C	263	LEU
1	C	296	ILE
1	C	310	MET
1	C	335	GLN
1	C	336	LEU
1	C	377	THR
1	C	388	ASN
1	C	390	ARG
1	C	468	LEU
1	C	496	LYS
1	C	501	GLU
1	C	514	LYS
1	D	26	MET
1	D	33	LYS
1	D	40	ARG
1	D	83	SER
1	D	103	MET
1	D	217	ASN
1	D	232	TRP
1	D	245	ARG
1	D	263	LEU

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Mol	Chain	Res	Type
1	D	310	MET
1	D	331	GLU
1	D	335	GLN
1	D	338	THR
1	D	342	GLU
1	D	345	LYS
1	D	352	ARG
1	D	377	THR
1	D	386	ARG
1	D	388	ASN
1	D	407	LEU
1	D	496	LYS
1	D	500	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	HIS
1	A	388	ASN
1	A	502	GLN
1	B	172	HIS
1	B	388	ASN
1	B	502	GLN
1	C	172	HIS
1	C	335	GLN
1	C	388	ASN
1	C	391	ASN
1	C	502	GLN
1	D	172	HIS
1	D	335	GLN
1	D	382	GLN
1	D	388	ASN
1	D	421	GLN
1	D	502	GLN

### 5.3.3 RNA ⓘ

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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	GOL	A	604	-	5,5,5	0.26	0	5,5,5	0.27	0
3	TPP	D	602	2	22,27,27	1.50	2 (9%)	29,40,40	2.04	6 (20%)
3	TPP	B	602	2	22,27,27	1.51	2 (9%)	29,40,40	2.03	6 (20%)
3	TPP	C	602	2	22,27,27	1.50	5 (22%)	29,40,40	2.18	8 (27%)
3	TPP	A	602	2	22,27,27	1.51	2 (9%)	29,40,40	2.04	6 (20%)
4	GOL	B	604	-	5,5,5	0.26	0	5,5,5	0.27	0
4	GOL	B	603	-	5,5,5	0.26	0	5,5,5	0.26	0
4	GOL	A	603	-	5,5,5	0.26	0	5,5,5	0.26	0
4	GOL	C	604	-	5,5,5	0.25	0	5,5,5	0.29	0
4	GOL	C	603	-	5,5,5	0.25	0	5,5,5	0.29	0

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	GOL	A	604	-	-	4/4/4/4	-
3	TPP	D	602	2	-	6/16/17/17	0/2/2/2
3	TPP	B	602	2	-	5/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	C	602	2	-	0/16/17/17	0/2/2/2
3	TPP	A	602	2	-	3/16/17/17	0/2/2/2
4	GOL	B	604	-	-	4/4/4/4	-
4	GOL	B	603	-	-	2/4/4/4	-
4	GOL	A	603	-	-	2/4/4/4	-
4	GOL	C	604	-	-	4/4/4/4	-
4	GOL	C	603	-	-	2/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	TPP	C4-N3	-5.42	1.35	1.39
3	B	602	TPP	C4-N3	-5.38	1.35	1.39
3	D	602	TPP	C4-N3	-5.33	1.35	1.39
3	B	602	TPP	C5'-C4'	3.38	1.48	1.42
3	A	602	TPP	C5'-C4'	3.35	1.48	1.42
3	D	602	TPP	C5'-C4'	3.34	1.48	1.42
3	C	602	TPP	C4-N3	-3.02	1.37	1.39
3	C	602	TPP	C2'-N3'	2.79	1.39	1.34
3	C	602	TPP	C2'-N1'	2.69	1.38	1.34
3	C	602	TPP	C4'-N3'	2.60	1.38	1.35
3	C	602	TPP	C6'-N1'	2.17	1.39	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	TPP	C6-C5-C4	7.96	133.82	127.43
3	A	602	TPP	C6-C5-C4	6.55	132.69	127.43
3	D	602	TPP	C6-C5-C4	6.52	132.67	127.43
3	B	602	TPP	C6-C5-C4	6.37	132.54	127.43
3	B	602	TPP	C6'-N1'-C2'	3.57	122.04	115.96
3	A	602	TPP	C6'-N1'-C2'	3.56	122.01	115.96
3	D	602	TPP	C6'-N1'-C2'	3.55	122.01	115.96
3	C	602	TPP	N1'-C2'-N3'	-3.52	119.48	125.54
3	B	602	TPP	PA-O3A-PB	-3.49	120.86	132.83
3	D	602	TPP	PA-O3A-PB	-3.46	120.94	132.83
3	A	602	TPP	PA-O3A-PB	-3.37	121.25	132.83
3	C	602	TPP	CM2-C2'-N1'	2.92	120.35	117.14
3	A	602	TPP	N4'-C4'-N3'	2.68	120.82	117.03
3	D	602	TPP	N4'-C4'-N3'	2.63	120.75	117.03
3	B	602	TPP	N4'-C4'-N3'	2.62	120.73	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	TPP	C5'-C6'-N1'	-2.61	119.47	123.82
3	D	602	TPP	C5'-C6'-N1'	-2.60	119.48	123.82
3	A	602	TPP	C5'-C6'-N1'	-2.57	119.53	123.82
3	C	602	TPP	C6'-N1'-C2'	2.53	120.26	115.96
3	C	602	TPP	C6'-C5'-C4'	2.51	119.13	115.72
3	C	602	TPP	O2B-PB-O3A	2.37	112.57	104.64
3	A	602	TPP	N1'-C2'-N3'	-2.26	121.65	125.54
3	B	602	TPP	N1'-C2'-N3'	-2.25	121.66	125.54
3	D	602	TPP	N1'-C2'-N3'	-2.25	121.67	125.54
3	C	602	TPP	CM4-C4-N3	2.08	125.19	122.53
3	C	602	TPP	PA-O3A-PB	-2.00	125.96	132.83

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	GOL	O1-C1-C2-C3
3	A	602	TPP	C4-C5-C6-C7
3	A	602	TPP	PA-O3A-PB-O2B
3	A	602	TPP	PA-O3A-PB-O3B
3	D	602	TPP	C4-C5-C6-C7
3	D	602	TPP	C7-O7-PA-O2A
3	D	602	TPP	PB-O3A-PA-O7
3	B	602	TPP	C4-C5-C6-C7
3	B	602	TPP	C7-O7-PA-O2A
3	B	602	TPP	PB-O3A-PA-O7
4	A	603	GOL	C1-C2-C3-O3
4	B	604	GOL	O1-C1-C2-C3
4	B	603	GOL	O1-C1-C2-C3
4	A	603	GOL	O2-C2-C3-O3
4	B	603	GOL	O1-C1-C2-O2
4	A	604	GOL	C1-C2-C3-O3
4	B	604	GOL	C1-C2-C3-O3
4	C	604	GOL	C1-C2-C3-O3
4	C	603	GOL	C1-C2-C3-O3
4	A	604	GOL	O1-C1-C2-O2
4	B	604	GOL	O1-C1-C2-O2
4	C	604	GOL	O2-C2-C3-O3
4	B	604	GOL	O2-C2-C3-O3
4	C	604	GOL	O1-C1-C2-O2
3	D	602	TPP	C7-O7-PA-O3A
3	B	602	TPP	C7-O7-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	D	602	TPP	C7-O7-PA-O1A
4	C	603	GOL	O2-C2-C3-O3
4	A	604	GOL	O2-C2-C3-O3
4	C	604	GOL	O1-C1-C2-C3
3	D	602	TPP	C5-C6-C7-O7
3	B	602	TPP	C7-O7-PA-O1A

There are no ring outliers.

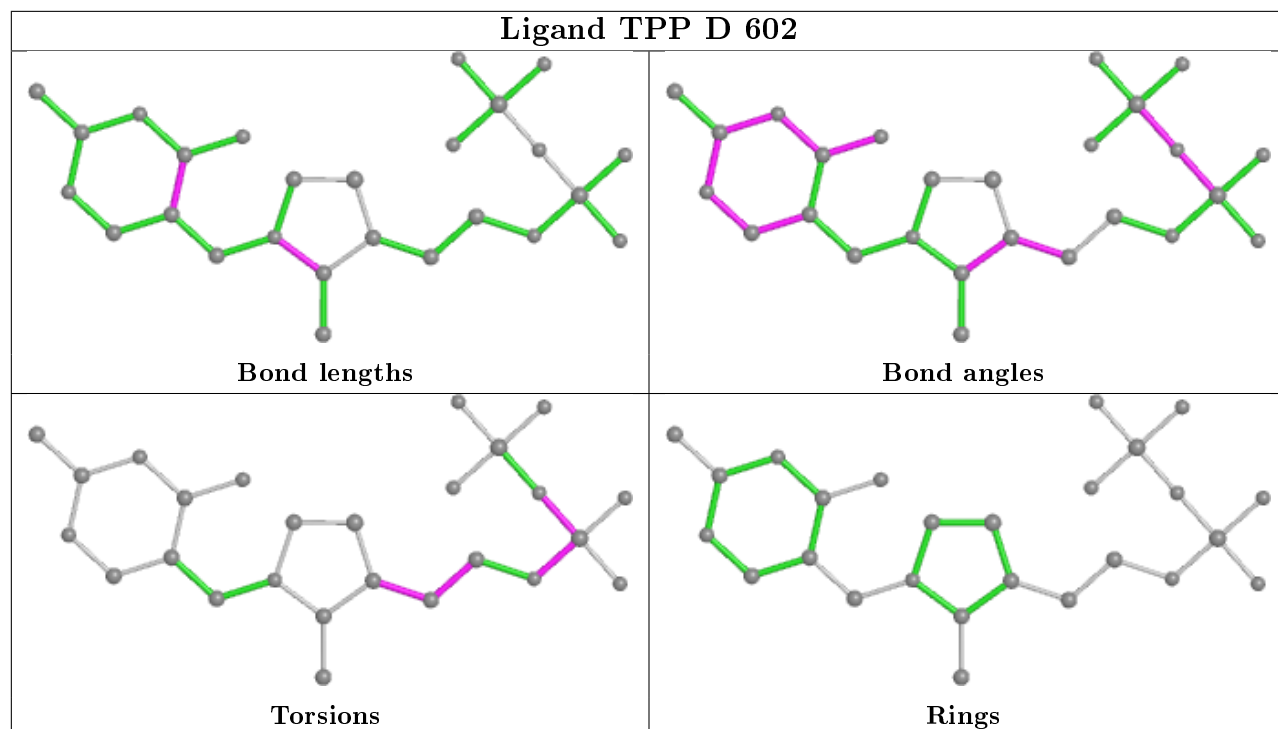
7 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	GOL	1	0
3	D	602	TPP	5	0
3	B	602	TPP	5	0
3	A	602	TPP	8	0
4	B	604	GOL	5	0
4	B	603	GOL	1	0
4	C	604	GOL	7	0

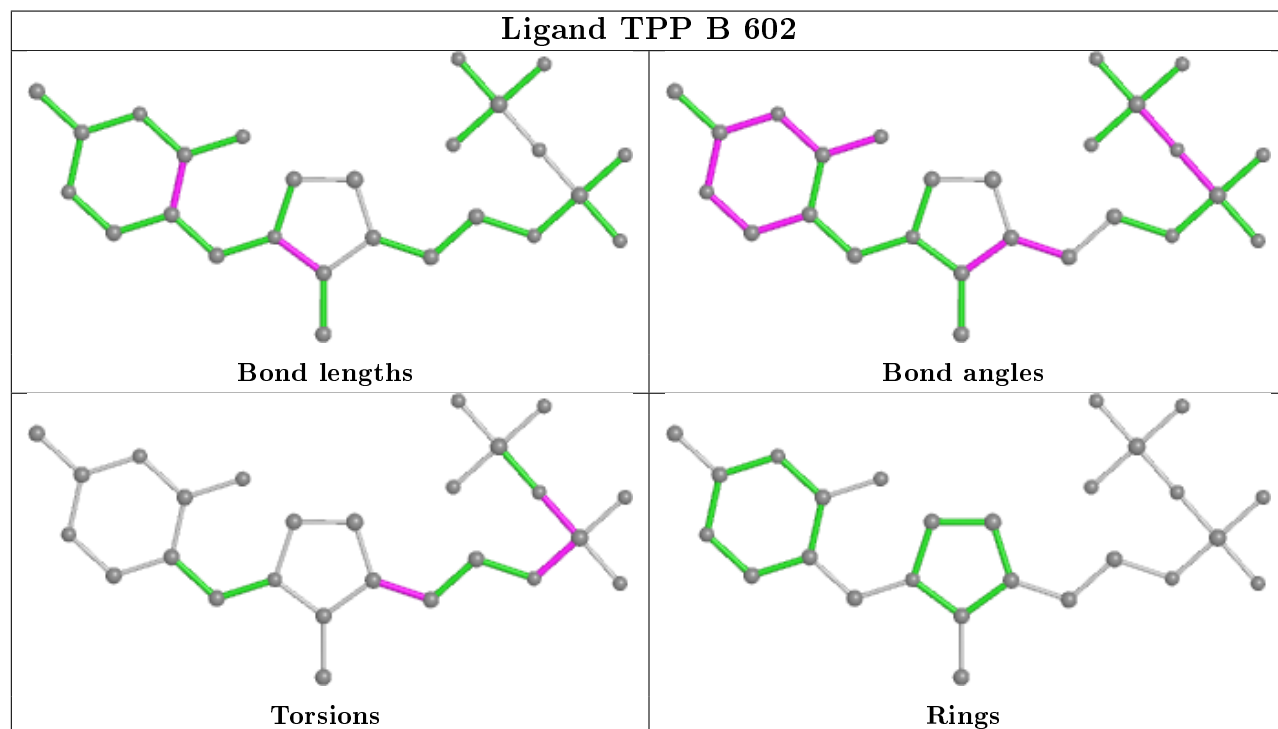
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

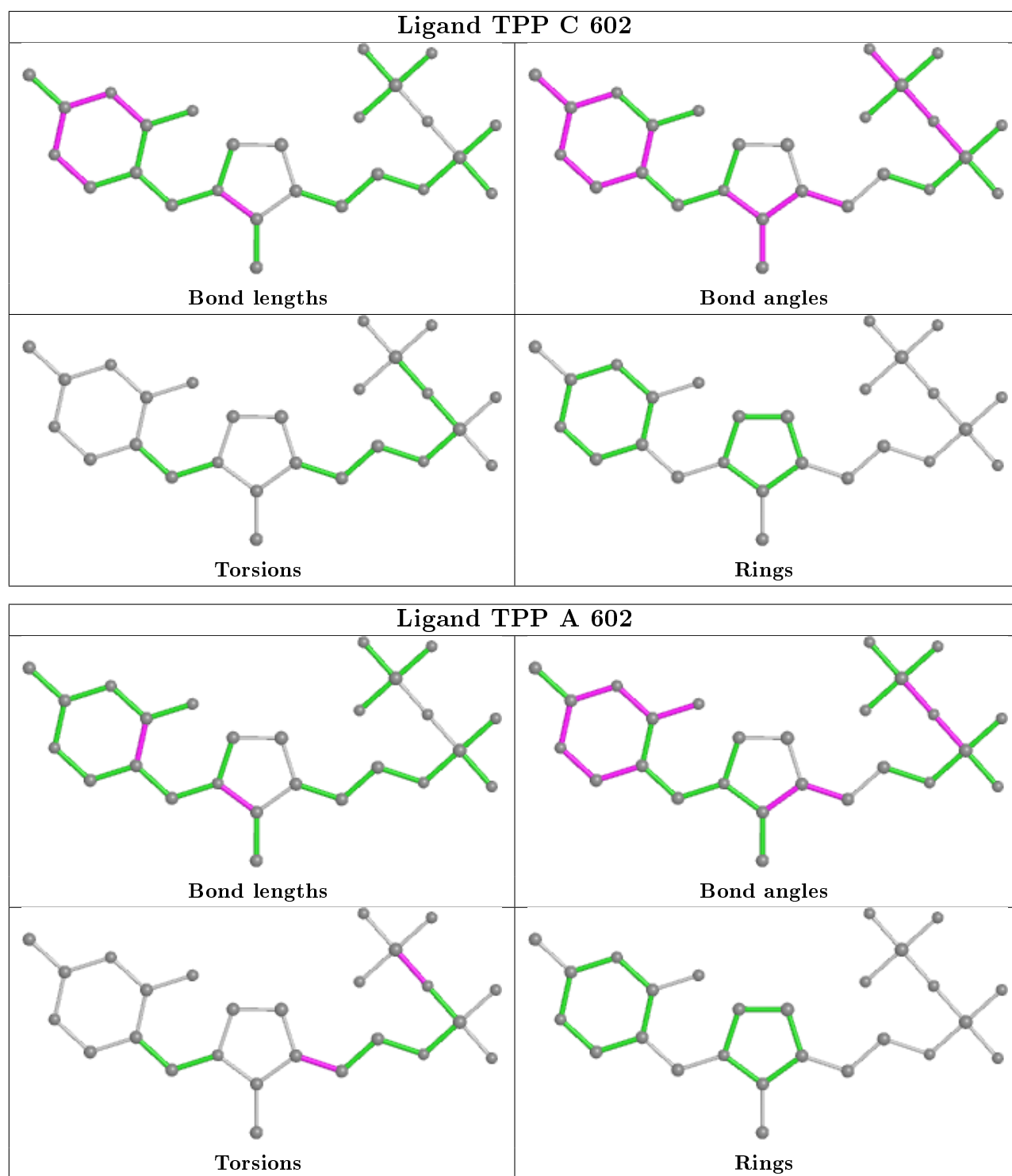


## Ligand TPP D 602



## Ligand TPP B 602





## 5.7 Other polymers [\(i\)](#)

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	525/534 (98%)	-0.28	4 (0%) 86 89	18, 25, 39, 67	2 (0%)
1	B	526/534 (98%)	-0.40	2 (0%) 92 95	17, 24, 38, 61	2 (0%)
1	C	526/534 (98%)	-0.35	2 (0%) 92 95	16, 23, 36, 77	4 (0%)
1	D	525/534 (98%)	-0.15	5 (0%) 82 86	19, 26, 43, 70	2 (0%)
All	All	2102/2136 (98%)	-0.30	13 (0%) 89 92	16, 24, 40, 77	10 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	527	VAL	5.0
1	C	526	PRO	4.4
1	B	527	VAL	3.6
1	B	526	PRO	3.6
1	A	526	PRO	3.2
1	A	467	VAL	3.0
1	A	469	GLU	2.9
1	D	469	GLU	2.7
1	A	463	TRP	2.5
1	D	463	TRP	2.3
1	D	470	ALA	2.3
1	D	526	PRO	2.3
1	D	467	VAL	2.2

### 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 ⓘ

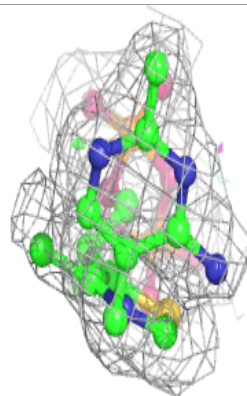
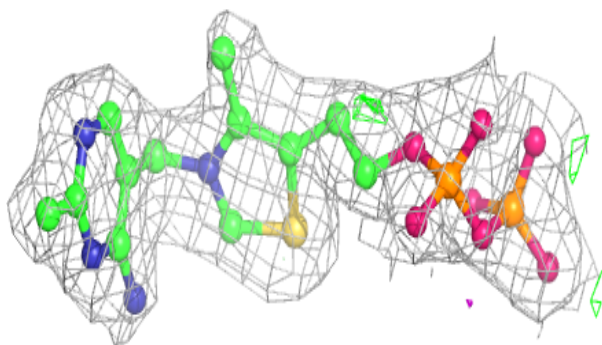
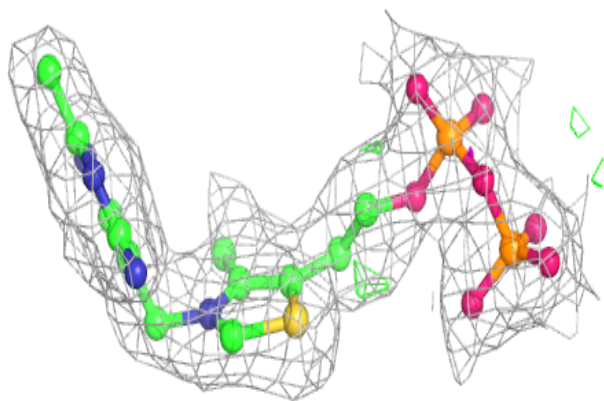
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	GOL	B	603	6/6	0.71	0.19	41,53,54,57	0
4	GOL	C	603	6/6	0.79	0.18	38,42,46,52	0
4	GOL	C	604	6/6	0.85	0.14	41,44,45,45	0
4	GOL	A	603	6/6	0.85	0.15	30,37,39,44	0
4	GOL	A	604	6/6	0.86	0.22	38,43,46,51	0
2	CA	A	601	1/1	0.89	0.08	38,38,38,38	0
4	GOL	B	604	6/6	0.90	0.21	36,36,41,44	0
2	CA	D	601	1/1	0.92	0.09	37,37,37,37	0
3	TPP	B	602	26/26	0.95	0.17	20,27,32,33	4
3	TPP	C	602	26/26	0.95	0.14	23,28,31,34	3
3	TPP	A	602	26/26	0.95	0.13	22,28,33,34	0
3	TPP	D	602	26/26	0.96	0.18	24,31,34,37	6
2	CA	B	601	1/1	0.96	0.10	35,35,35,35	0
2	CA	C	601	1/1	0.98	0.06	32,32,32,32	0

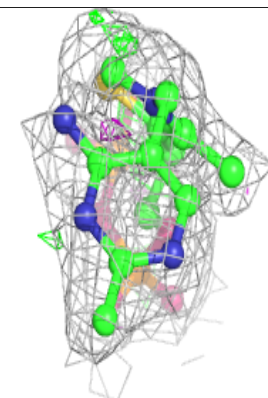
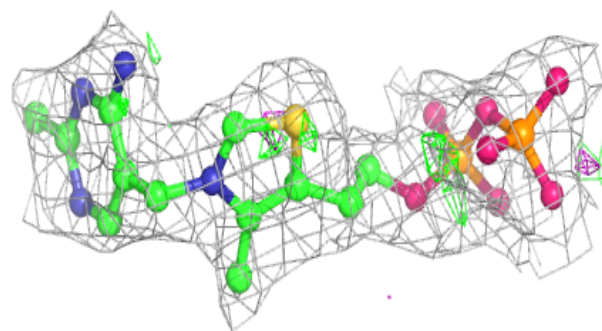
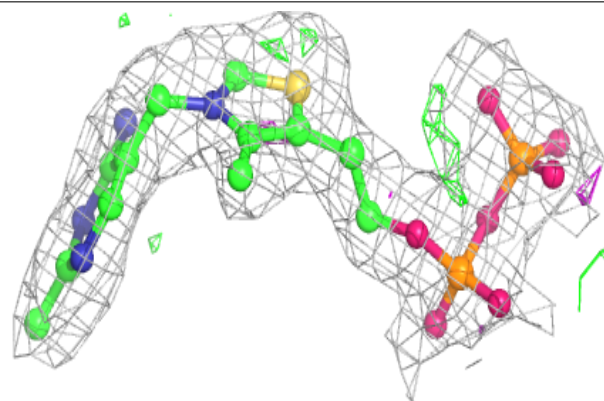
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TPP B 602:**

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

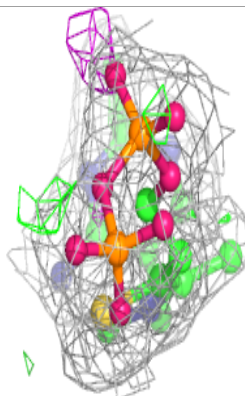
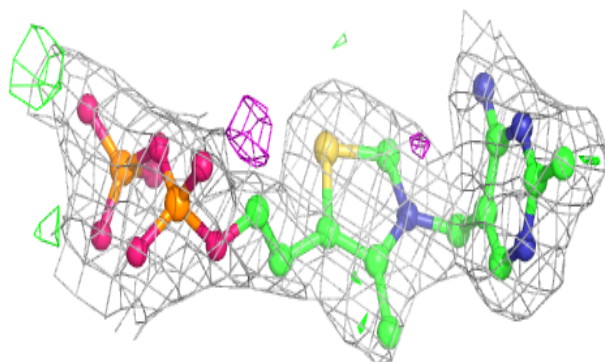
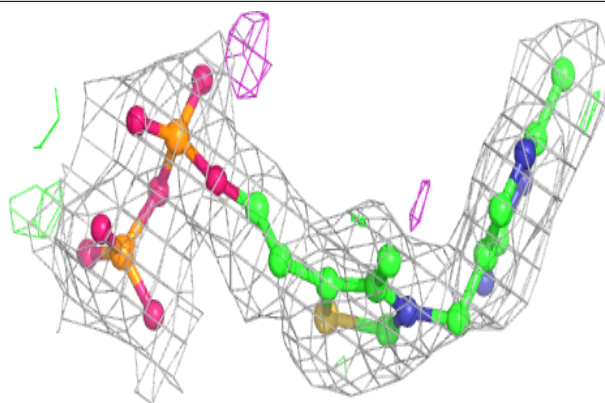
**Electron density around TPP C 602:**

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

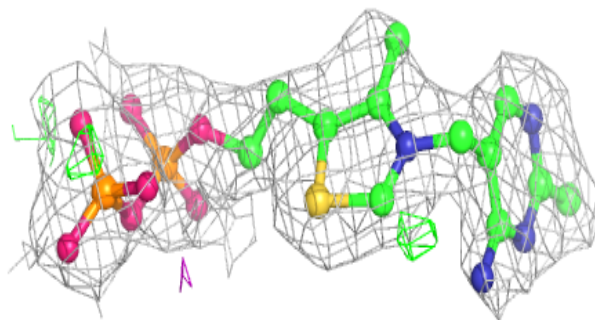
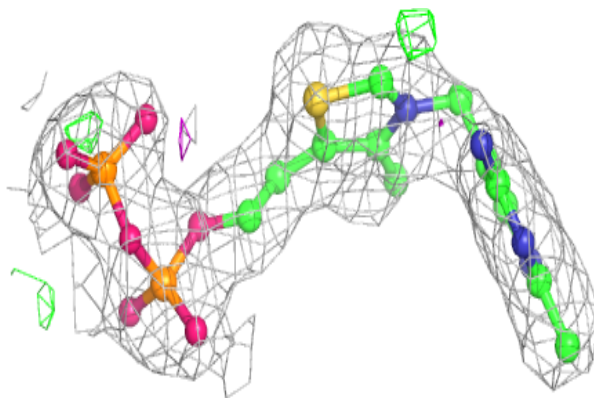


**Electron density around TPP A 602:**

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

**Electron density around TPP D 602:**

$2mF_o-DF_c$  (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.