Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 09:49 AM EDT

PDB ID	:	4K9P
Title	:	Crystal Structure of the His281Tyr/Ala460Ile Double Mutant of Benzoylformate Decarboxylase from Pseudomonas putida
Authors	:	Brodkin, H.R.; McLeish, M.J.
Deposited on	:	2013-04-20
Resolution	:	2.24 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

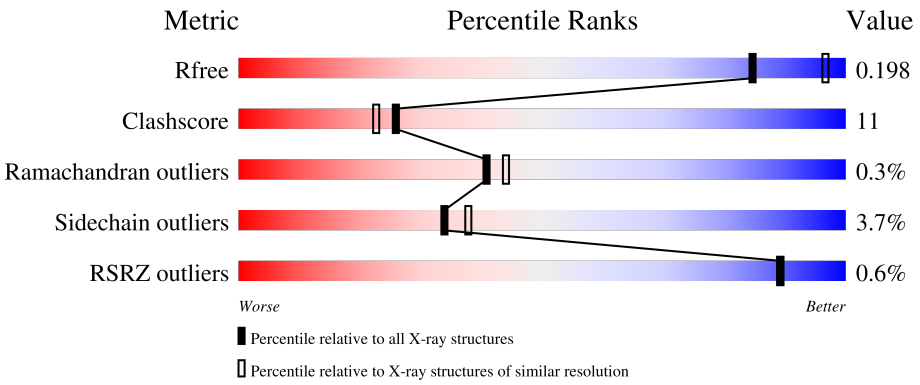
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	533	.% 79% 18% • •
1	B	533	77% 20% • •
1	C	533	.% 80% 16% • •
1	D	533	.% 78% 19% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16968 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
			Total	C	N	O	S			
1	A	525	3987	2528	686	752	21	0	8	0
1	B	525	3968	2513	682	752	21	1	6	0
1	C	524	3976	2521	685	749	21	0	6	0
1	D	524	3974	2520	683	751	20	0	7	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	TYR	HIS	engineered mutation	UNP P20906
A	460	ILE	ALA	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	281	TYR	HIS	engineered mutation	UNP P20906
B	460	ILE	ALA	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	281	TYR	HIS	engineered mutation	UNP P20906
C	460	ILE	ALA	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

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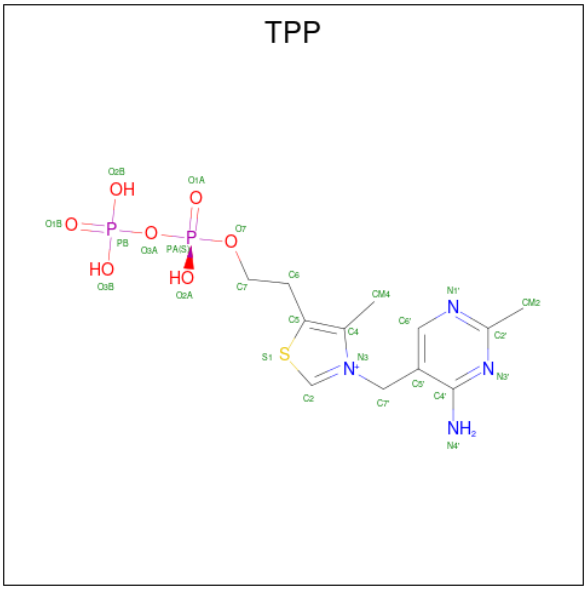
Chain	Residue	Modelled	Actual	Comment	Reference
C	532	HIS	-	expression tag	UNP P20906
C	533	HIS	-	expression tag	UNP P20906
C	534	HIS	-	expression tag	UNP P20906
D	281	TYR	HIS	engineered mutation	UNP P20906
D	460	ILE	ALA	engineered mutation	UNP P20906
D	529	HIS	-	expression tag	UNP P20906
D	530	HIS	-	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	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).

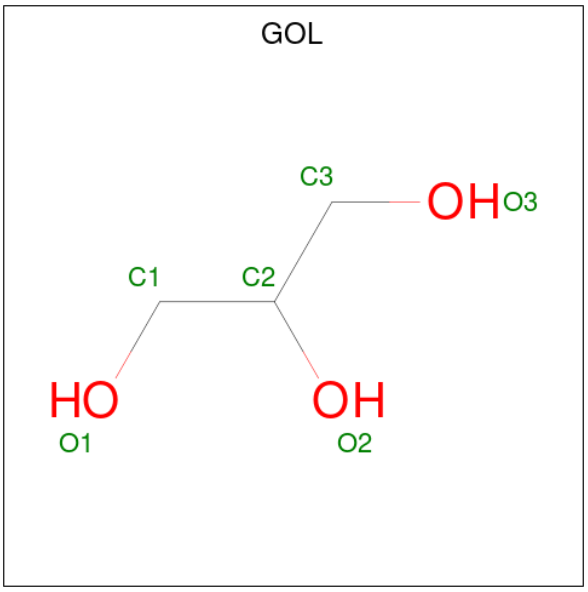


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	26	12	4	7	2	1	0	0
3	B	1	26	12	4	7	2	1	0	0
3	C	1	26	12	4	7	2	1	0	0
3	D	1	26	12	4	7	2	1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
4	B	1	1	1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	C	1	6	3	3	0	0
			Total	C	O		
5	D	1	6	3	3	0	0

- Molecule 6 is water.

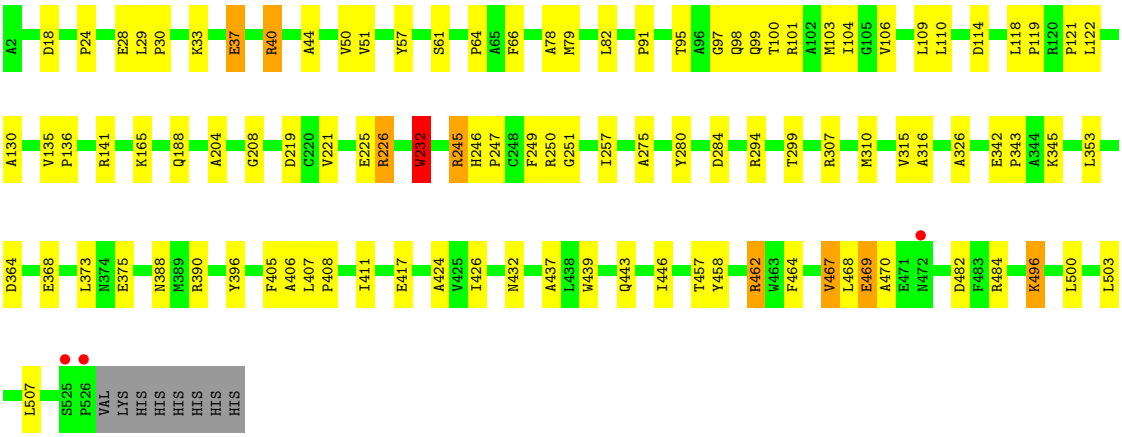
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	250	250	250	0	0
			Total	O		
6	B	227	227	227	0	0
			Total	O		
6	C	212	212	212	0	0
			Total	O		
6	D	228	228	228	0	0

3 Residue-property plots (i)

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

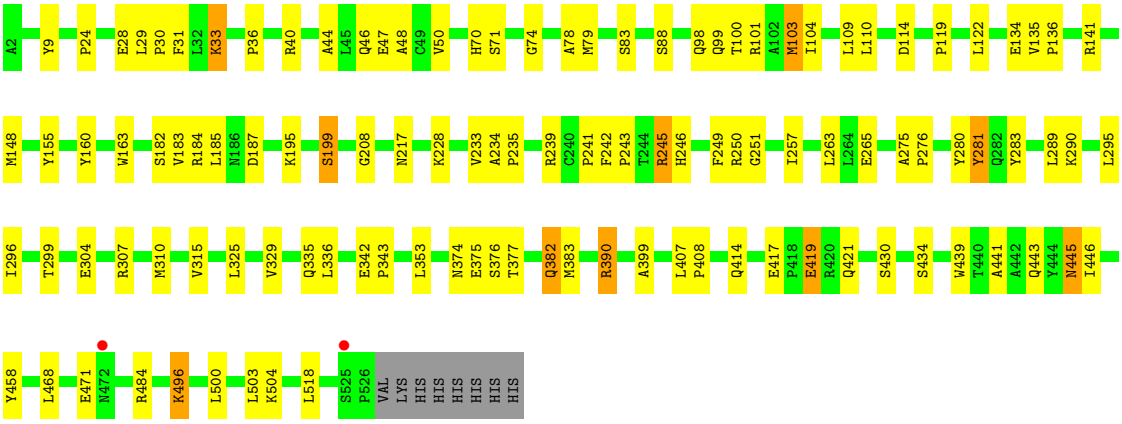
• Molecule 1: Benzoylformate decarboxylase

Chain A:



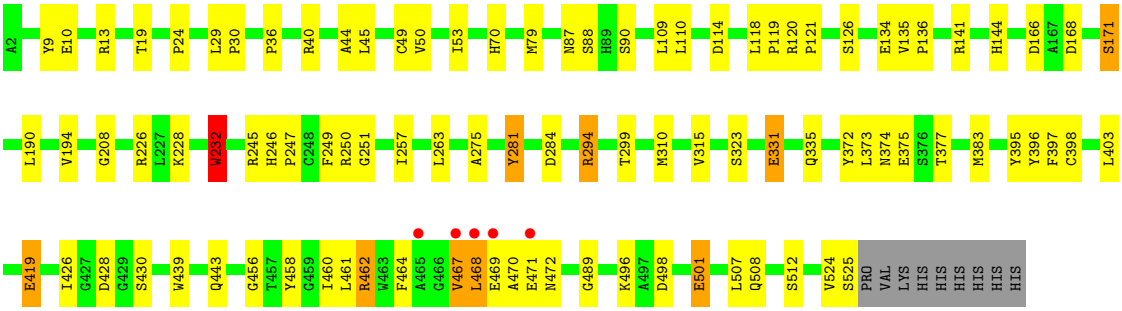
• Molecule 1: Benzoylformate decarboxylase

Chain B:



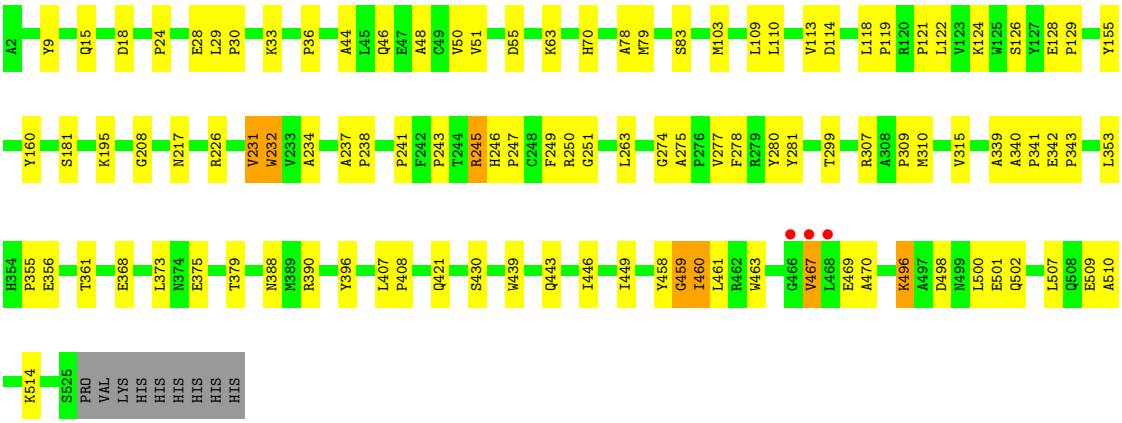
• Molecule 1: Benzoylformate decarboxylase

Chain C:



- Molecule 1: Benzoylformate decarboxylase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.77Å 164.55Å 175.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.14 – 2.24 41.14 – 2.24	Depositor EDS
% Data completeness (in resolution range)	96.8 (41.14-2.24) 96.8 (41.14-2.24)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.173 , 0.201 0.172 , 0.198	Depositor DCC
R_{free} test set	2008 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16968	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: TPP, GOL, MG, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.45	2/4113 (0.0%)	0.51	0/5622
1	B	0.39	0/4084	0.45	0/5582
1	C	0.44	0/4093	0.52	2/5594 (0.0%)
1	D	0.45	4/4095 (0.1%)	0.50	1/5597 (0.0%)
All	All	0.43	6/16385 (0.0%)	0.50	3/22395 (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	A	0	3
1	C	0	3
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232[A]	TRP	N-CA	-9.77	1.26	1.46
1	A	232[B]	TRP	N-CA	-9.77	1.26	1.46
1	D	232[A]	TRP	N-CA	-7.04	1.32	1.46
1	D	232[B]	TRP	N-CA	-7.04	1.32	1.46
1	D	181[A]	SER	N-CA	-5.47	1.35	1.46
1	D	181[B]	SER	N-CA	-5.47	1.35	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	232[A]	TRP	CB-CA-C	5.87	122.13	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	232[B]	TRP	CB-CA-C	5.87	122.13	110.40
1	D	231	VAL	C-N-CA	5.10	134.44	121.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188[A]	GLN	Mainchain
1	A	188[B]	GLN	Mainchain
1	A	232[A]	TRP	Mainchain
1	C	226[A]	ARG	Mainchain
1	C	232[A]	TRP	Mainchain
1	C	232[B]	TRP	Mainchain

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	3987	0	3928	94	0
1	B	3968	0	3909	101	0
1	C	3976	0	3919	77	0
1	D	3974	0	3915	75	1
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	2	0
3	B	26	0	16	3	0
3	C	26	0	16	6	0
3	D	26	0	16	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	18	0	24	3	1
5	B	6	0	8	2	0
5	C	6	0	8	0	0
5	D	6	0	8	1	0
6	A	250	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	227	0	0	10	0
6	C	212	0	0	9	0
6	D	228	0	0	10	0
All	All	16968	0	15783	335	1

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 11.

All (335) 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:A:37:GLU:HG2	6:A:947:HOH:O	1.13	1.26
1:A:462:ARG:CG	1:A:462:ARG:HH11	1.65	1.08
1:B:421:GLN:OE1	5:B:604:GOL:H11	1.53	1.07
1:A:226[A]:ARG:HH21	1:A:226[A]:ARG:CG	1.69	1.06
1:C:228:LYS:NZ	1:C:331:GLU:OE1	1.89	1.05
1:C:462:ARG:HH11	1:C:462:ARG:HG2	1.19	1.04
1:A:462:ARG:HH11	1:A:462:ARG:HG2	1.24	0.98
1:A:294:ARG:HD3	6:A:879:HOH:O	1.64	0.98
1:A:226[A]:ARG:NH2	1:A:226[A]:ARG:HG3	1.55	0.96
1:A:226[A]:ARG:HH21	1:A:226[A]:ARG:HG3	0.80	0.94
1:A:226[A]:ARG:NH2	1:A:326:ALA:O	2.03	0.91
1:D:208:GLY:HA3	1:D:275:ALA:HB2	1.53	0.91
1:D:496:LYS:HE2	1:D:498:ASP:OD2	1.71	0.90
1:B:228:LYS:HD2	1:B:336:LEU:HD12	1.51	0.89
1:B:228:LYS:HD2	1:B:336:LEU:CD1	2.03	0.88
1:A:106:VAL:HG13	6:A:875:HOH:O	1.77	0.85
1:B:375:GLU:HG2	1:B:430:SER:HB3	1.59	0.84
1:B:100:THR:CG2	1:B:103[A]:MET:HG3	2.09	0.83
1:B:44:ALA:HB3	1:B:50:VAL:HG22	1.59	0.83
1:B:110:LEU:HD12	1:D:281:TYR:HE1	1.42	0.83
1:B:375:GLU:HG2	1:B:430:SER:CB	2.08	0.83
1:A:464:PHE:O	1:A:467:VAL:HG13	1.79	0.83
1:C:144:HIS:HE1	6:C:864:HOH:O	1.61	0.82
1:A:462:ARG:HG2	1:A:462:ARG:NH1	1.95	0.81
1:B:421:GLN:OE1	5:B:604:GOL:C1	2.29	0.80
1:A:284:ASP:OD1	6:A:729:HOH:O	1.99	0.79
1:B:439:TRP:CZ2	1:B:443:GLN:HG3	2.19	0.78
1:C:462:ARG:HG2	1:C:462:ARG:NH1	1.89	0.77
1:D:15:GLN:OE1	6:D:911:HOH:O	2.05	0.75
1:A:100:THR:CG2	1:A:103[B]:MET:HG2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:HD12	1:D:281:TYR:CE1	2.23	0.74
1:B:208:GLY:HA3	1:B:275:ALA:HB2	1.70	0.73
1:A:221:VAL:O	1:A:225:GLU:HG3	1.89	0.73
1:A:208:GLY:HA3	1:A:275:ALA:HB2	1.69	0.73
1:A:462:ARG:HH11	1:A:462:ARG:HG3	1.51	0.72
1:B:100:THR:CG2	1:B:103[B]:MET:HB2	2.20	0.72
1:A:100:THR:HG22	1:A:103[B]:MET:HG2	1.71	0.72
1:A:219:ASP:OD2	6:A:735:HOH:O	2.07	0.72
1:D:439:TRP:CZ2	1:D:443:GLN:HG3	2.24	0.71
1:A:101:ARG:HA	1:A:104:ILE:HD12	1.72	0.70
1:B:390:ARG:HD3	6:B:702:HOH:O	1.90	0.70
1:B:353:LEU:HD21	1:B:500:LEU:HA	1.73	0.70
1:B:100:THR:HG22	1:B:103[B]:MET:HB2	1.74	0.70
1:B:44:ALA:HB3	1:B:50:VAL:CG2	2.22	0.69
1:C:109:LEU:O	1:C:110:LEU:HB2	1.93	0.69
1:A:457:THR:OG1	1:A:462:ARG:HD2	1.91	0.69
1:A:118:LEU:HB3	1:A:119:PRO:HD3	1.73	0.69
1:C:461:LEU:HD11	3:C:602:TPP:HM43	1.75	0.69
1:A:33:LYS:HD3	6:A:914:HOH:O	1.92	0.68
1:D:109:LEU:O	1:D:110:LEU:HB2	1.94	0.68
1:B:28:GLU:OE2	1:B:70:HIS:HA	1.95	0.67
1:B:79[A]:MET:HE3	1:B:122:LEU:HD12	1.76	0.67
1:A:468:LEU:O	1:A:470:ALA:N	2.28	0.67
1:D:246:HIS:CG	1:D:247:PRO:HD2	2.30	0.67
1:C:232[A]:TRP:CZ3	1:C:263:LEU:HD21	2.30	0.67
1:C:375:GLU:HG2	1:C:430:SER:HB3	1.76	0.67
1:D:461:LEU:HD11	3:D:602:TPP:HM43	1.77	0.67
1:A:109:LEU:O	1:A:110:LEU:HB2	1.96	0.66
1:C:464:PHE:O	1:C:467:VAL:HG13	1.96	0.66
1:A:468:LEU:C	1:A:470:ALA:H	1.99	0.66
1:C:208:GLY:HA3	1:C:275:ALA:HB2	1.78	0.65
1:A:28:GLU:OE2	1:A:97:GLY:HA3	1.96	0.64
1:C:135:VAL:HB	1:C:136:PRO:HD3	1.78	0.64
1:D:63:LYS:HG3	6:D:902:HOH:O	1.96	0.64
1:C:166:ASP:OD2	6:C:860:HOH:O	2.15	0.64
1:A:29:LEU:HB2	1:A:30:PRO:HD3	1.79	0.64
1:D:496:LYS:HD2	1:D:502:GLN:OE1	1.99	0.63
1:B:135:VAL:HB	1:B:136:PRO:HD3	1.81	0.63
1:A:464:PHE:HA	1:A:467:VAL:CG1	2.28	0.62
1:B:245:ARG:NH1	6:B:891:HOH:O	2.11	0.62
1:A:439:TRP:CZ2	1:A:443:GLN:HG3	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLN:HG3	1:A:99:GLN:N	2.14	0.62
1:A:342:GLU:HG3	1:A:343:PRO:HD2	1.82	0.62
1:A:135:VAL:HB	1:A:136:PRO:HD3	1.81	0.62
1:B:239:ARG:NH1	6:B:926:HOH:O	2.20	0.62
1:A:245:ARG:HG2	1:A:388:ASN:ND2	2.14	0.61
1:D:353:LEU:HD21	1:D:500:LEU:HA	1.82	0.61
1:C:87:ASN:ND2	6:C:871:HOH:O	2.16	0.61
1:B:47:GLU:HG2	1:B:74:GLY:O	2.01	0.60
1:C:375:GLU:HG2	1:C:430:SER:CB	2.31	0.60
1:B:439:TRP:CH2	1:B:443:GLN:HG3	2.36	0.60
1:C:168:ASP:O	1:C:171:SER:HB2	2.02	0.60
1:A:405:PHE:HB2	6:A:840:HOH:O	2.01	0.59
1:A:458:TYR:CD1	3:A:602:TPP:H61	2.37	0.59
1:B:110:LEU:CD1	1:D:281:TYR:CE1	2.85	0.59
1:B:414:GLN:CG	1:B:446:ILE:HG23	2.32	0.59
1:A:417:GLU:OE2	6:A:779:HOH:O	2.16	0.59
1:A:468:LEU:C	1:A:470:ALA:N	2.55	0.59
1:A:353:LEU:HD22	1:A:503:LEU:HD22	1.85	0.59
1:D:30:PRO:HG2	1:D:160:TYR:HB2	1.83	0.59
1:B:265:GLU:HB2	1:B:290:LYS:HD3	1.85	0.58
1:D:421:GLN:NE2	1:D:449:ILE:HG13	2.18	0.58
1:B:100:THR:HG22	1:B:103[A]:MET:HG3	1.85	0.58
1:C:462:ARG:HH11	1:C:462:ARG:CG	2.03	0.58
3:B:602:TPP:HM43	1:D:24:PRO:O	2.04	0.58
1:D:208:GLY:CA	1:D:275:ALA:HB2	2.30	0.58
1:C:439:TRP:CH2	1:C:443:GLN:HG3	2.39	0.57
1:B:30:PRO:HG2	1:B:160:TYR:HB2	1.86	0.57
1:B:46:GLN:O	1:B:50:VAL:HG23	2.04	0.57
1:C:428:ASP:OD1	1:C:428:ASP:N	2.37	0.57
1:B:484:ARG:HD2	1:B:496:LYS:HB2	1.86	0.57
1:B:376:SER:OG	6:B:733:HOH:O	2.16	0.57
1:A:364:ASP:OD1	5:A:606:GOL:H32	2.05	0.57
1:B:29:LEU:HB2	1:B:30:PRO:HD3	1.86	0.57
1:B:417:GLU:OE2	6:B:803:HOH:O	2.17	0.57
1:C:373:LEU:HG	1:C:396:TYR:HB2	1.87	0.57
1:D:79[A]:MET:CE	1:D:122:LEU:HD12	2.35	0.57
1:D:458:TYR:CD1	3:D:602:TPP:H61	2.40	0.57
1:D:245:ARG:HB2	6:D:769:HOH:O	2.05	0.56
1:D:439:TRP:CH2	1:D:443:GLN:HG3	2.40	0.56
1:D:55:ASP:OD2	6:D:836:HOH:O	2.18	0.56
1:A:79[A]:MET:HE3	1:A:122:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LYS:HB2	1:D:470:ALA:HB1	1.88	0.56
1:D:226:ARG:NH1	6:D:809:HOH:O	2.38	0.56
1:A:114:ASP:HB3	1:C:121:PRO:HG3	1.88	0.56
1:C:462:ARG:NH1	1:C:462:ARG:CG	2.64	0.56
1:B:101:ARG:HA	1:B:104:ILE:HD12	1.87	0.56
1:C:419:GLU:HB2	6:C:813:HOH:O	2.05	0.56
1:B:100:THR:HG21	1:B:103[A]:MET:HG3	1.88	0.55
1:B:484:ARG:HD3	6:B:754:HOH:O	2.06	0.55
1:A:249:PHE:CE2	1:A:251:GLY:HA2	2.41	0.55
1:C:461:LEU:HD11	3:C:602:TPP:CM4	2.36	0.55
1:C:496:LYS:HE2	1:C:498:ASP:OD1	2.06	0.55
1:B:390:ARG:CD	6:B:702:HOH:O	2.50	0.55
1:A:24:PRO:O	3:C:602:TPP:HM43	2.07	0.55
1:A:40:ARG:HB3	5:A:604:GOL:O2	2.07	0.55
1:B:208:GLY:CA	1:B:275:ALA:HB2	2.35	0.55
3:D:602:TPP:O2B	6:D:721:HOH:O	2.18	0.54
1:A:368:GLU:HG2	1:A:390:ARG:NH1	2.22	0.54
1:A:57:TYR:O	1:A:61[B]:SER:HB2	2.08	0.54
1:D:231:VAL:O	1:D:250:ARG:N	2.37	0.54
1:B:283:TYR:HA	1:D:103:MET:HE2	1.90	0.54
1:B:299:THR:O	1:B:315:VAL:HA	2.08	0.54
1:B:374:ASN:HB2	1:B:383:MET:SD	2.48	0.54
1:A:484:ARG:HD3	6:A:883:HOH:O	2.07	0.54
5:A:606:GOL:O2	6:A:788:HOH:O	1.92	0.54
1:A:439:TRP:CH2	1:A:443:GLN:HG3	2.43	0.54
1:A:432:ASN:CG	1:C:45:LEU:HD13	2.29	0.53
1:B:295:LEU:C	1:B:295:LEU:HD23	2.29	0.53
1:D:119:PRO:HG3	1:D:155:TYR:CD2	2.43	0.53
1:D:226:ARG:NH2	6:D:809:HOH:O	2.38	0.53
1:A:118:LEU:HB3	1:A:119:PRO:CD	2.38	0.53
1:A:121:PRO:HG3	1:C:114:ASP:HB3	1.91	0.53
1:D:278:PHE:HB2	1:D:280:TYR:CZ	2.44	0.53
1:B:114:ASP:HB3	1:D:121:PRO:HG3	1.91	0.53
1:D:119:PRO:HG3	1:D:155:TYR:CG	2.44	0.53
1:A:33:LYS:CD	6:A:914:HOH:O	2.55	0.52
1:A:316:ALA:HB2	1:B:183:VAL:HG11	1.92	0.52
1:C:464:PHE:HA	1:C:467:VAL:CG1	2.40	0.51
1:D:449:ILE:HD13	1:D:510:ALA:HB1	1.93	0.51
1:A:51:VAL:HG21	1:A:78:ALA:HB1	1.91	0.51
1:C:374:ASN:HB2	1:C:383:MET:SD	2.50	0.51
1:C:375:GLU:HB3	1:C:426:ILE:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:TYR:CD1	3:B:602:TPP:H61	2.45	0.51
1:C:190:LEU:O	1:C:194:VAL:HG23	2.11	0.51
1:A:37:GLU:CG	6:A:947:HOH:O	1.99	0.51
1:B:353:LEU:HD22	1:B:503:LEU:HD22	1.92	0.51
1:C:9:TYR:CD1	1:C:36:PRO:HG2	2.46	0.51
1:D:109:LEU:O	1:D:110:LEU:CB	2.59	0.50
1:B:245:ARG:HB2	6:B:714:HOH:O	2.11	0.50
1:B:439:TRP:CZ2	1:B:443:GLN:CG	2.94	0.50
1:C:118:LEU:N	1:C:119:PRO:HD2	2.26	0.50
1:C:524:VAL:HG12	1:C:525:SER:N	2.26	0.50
1:D:46:GLN:OE1	1:D:48:ALA:HB3	2.11	0.50
1:D:29:LEU:HB2	1:D:30:PRO:HD3	1.92	0.50
1:B:414:GLN:HB3	1:B:446:ILE:CG2	2.42	0.50
1:C:44:ALA:HB3	1:C:50:VAL:HG22	1.94	0.50
1:B:295:LEU:HD23	1:B:296:ILE:N	2.27	0.49
1:B:441:ALA:O	1:B:445[B]:ASN:HA	2.12	0.49
1:B:342:GLU:HG3	1:B:343:PRO:HD2	1.95	0.49
1:D:79[A]:MET:HE3	1:D:122:LEU:HD12	1.94	0.49
3:D:602:TPP:H2	3:D:602:TPP:HN42	1.77	0.49
1:A:482:ASP:OD1	6:A:883:HOH:O	2.20	0.49
1:C:70:HIS:CE1	1:C:110:LEU:HD13	2.48	0.49
1:A:245:ARG:HG2	1:A:388:ASN:CG	2.32	0.49
3:A:602:TPP:HM43	1:C:24:PRO:O	2.12	0.49
1:B:434:SER:HB2	6:B:901:HOH:O	2.13	0.49
1:A:424:ALA:HB1	1:A:426:ILE:HD11	1.95	0.48
1:B:29:LEU:N	1:B:30:PRO:CD	2.76	0.48
1:D:342:GLU:HG3	1:D:343:PRO:HD2	1.95	0.48
1:B:439:TRP:CE2	1:B:443:GLN:CG	2.97	0.48
1:D:243:PRO:HG2	1:D:246:HIS:HB2	1.95	0.48
1:A:66:PHE:CZ	1:A:95:THR:HG21	2.49	0.48
1:B:47:GLU:HB3	1:B:78:ALA:HB2	1.96	0.48
1:D:29:LEU:N	1:D:30:PRO:CD	2.76	0.48
1:A:432:ASN:ND2	1:C:45:LEU:HD13	2.29	0.48
1:C:144:HIS:CE1	6:C:864:HOH:O	2.48	0.48
1:A:44:ALA:HB3	1:A:50:VAL:CG2	2.44	0.47
1:A:411:ILE:CG2	1:A:446:ILE:HD12	2.44	0.47
1:A:407:LEU:HD22	1:A:437:ALA:HB3	1.96	0.47
1:B:250:ARG:HD2	1:B:250:ARG:N	2.28	0.47
1:C:294:ARG:HD2	6:C:865:HOH:O	2.14	0.47
1:B:249:PHE:C	1:B:250:ARG:HD2	2.34	0.47
1:C:281:TYR:CD1	1:C:281:TYR:C	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ARG:CG	1:A:462:ARG:NH1	2.38	0.47
1:B:233:VAL:HG23	1:B:249:PHE:HE1	1.79	0.47
1:A:79[A]:MET:CE	1:A:122:LEU:HD12	2.44	0.47
1:A:373:LEU:HG	1:A:396:TYR:HB2	1.97	0.47
1:B:195:LYS:O	1:B:199:SER:OG	2.30	0.47
1:D:9:TYR:CD1	1:D:36:PRO:HG2	2.50	0.47
1:B:9:TYR:CD1	1:B:36:PRO:HG2	2.49	0.47
1:A:484:ARG:HD2	1:A:496:LYS:HB3	1.97	0.47
1:C:109:LEU:O	1:C:110:LEU:CB	2.62	0.47
1:B:119:PRO:HG3	1:B:155:TYR:CG	2.51	0.46
1:D:356:GLU:OE1	1:D:356:GLU:N	2.39	0.46
1:A:106:VAL:HG11	6:C:884:HOH:O	2.15	0.46
1:C:134:GLU:OE2	6:C:722:HOH:O	2.20	0.46
1:D:247:PRO:HA	1:D:339:ALA:HB2	1.98	0.46
1:B:249:PHE:CE2	1:B:251:GLY:HA2	2.51	0.46
1:C:299:THR:O	1:C:315:VAL:HA	2.16	0.46
1:D:79[A]:MET:HE1	1:D:122:LEU:HD12	1.98	0.46
1:B:184:ARG:NH1	1:B:187:ASP:OD1	2.48	0.45
1:C:246:HIS:CG	1:C:247:PRO:HD2	2.51	0.45
1:C:135:VAL:CB	1:C:136:PRO:HD3	2.46	0.45
1:C:397:PHE:O	1:C:398:CYS:C	2.55	0.45
1:D:28:GLU:OE2	1:D:70:HIS:HA	2.16	0.45
1:A:44:ALA:HB3	1:A:50:VAL:HG22	1.99	0.45
1:A:165:LYS:HA	1:A:165:LYS:HD3	1.84	0.45
1:D:277:VAL:O	1:D:309:PRO:HD2	2.16	0.45
1:B:160:TYR:C	1:B:160:TYR:CD1	2.90	0.45
1:B:276:PRO:HG3	1:B:304:GLU:OE2	2.17	0.45
1:D:51:VAL:HG21	1:D:78:ALA:HB1	1.98	0.45
1:D:237:ALA:HA	1:D:238:PRO:HD3	1.81	0.45
1:B:234:ALA:HB1	1:B:235:PRO:HD2	1.99	0.45
1:C:10:GLU:OE1	1:C:13:ARG:NH1	2.50	0.45
1:C:249:PHE:CE2	1:C:251:GLY:HA2	2.52	0.45
1:A:204:ALA:HB1	1:A:232[B]:TRP:HZ3	1.81	0.45
1:A:353:LEU:HD21	1:A:500:LEU:HA	1.98	0.45
1:B:79[B]:MET:HE3	1:B:119:PRO:HA	1.97	0.45
1:B:382:GLN:H	1:B:382:GLN:HE21	1.65	0.45
1:B:518:LEU:C	1:B:518:LEU:HD23	2.37	0.45
1:D:355:PRO:HB3	1:D:379:THR:HG21	1.98	0.45
1:C:377:THR:HG21	3:C:602:TPP:S1	2.57	0.44
1:D:373:LEU:HG	1:D:396:TYR:HB2	1.98	0.44
1:A:33:LYS:HE3	1:C:470:ALA:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:THR:HG23	1:C:40:ARG:HG3	1.99	0.44
1:C:501:GLU:HB2	6:C:856:HOH:O	2.17	0.44
1:D:245:ARG:HG2	1:D:388:ASN:CG	2.38	0.44
1:B:325:LEU:O	1:B:329:VAL:HG22	2.17	0.44
1:D:340:ALA:HB1	1:D:341:PRO:HD2	1.99	0.44
1:A:29:LEU:N	1:A:30:PRO:CD	2.81	0.44
1:A:109:LEU:O	1:A:110:LEU:CB	2.64	0.44
1:B:407:LEU:HB3	1:B:408:PRO:CD	2.47	0.44
1:C:88:SER:OG	1:C:90:SER:OG	2.30	0.44
1:D:439:TRP:CE2	1:D:443:GLN:HG3	2.52	0.44
1:D:461:LEU:HD11	3:D:602:TPP:CM4	2.46	0.44
1:A:507:LEU:HD23	1:A:507:LEU:HA	1.84	0.44
1:B:109:LEU:O	1:B:110:LEU:HB2	2.18	0.44
1:D:263:LEU:HD13	6:D:767:HOH:O	2.18	0.44
1:D:463:TRP:O	1:D:467:VAL:HG13	2.18	0.44
1:B:184:ARG:HD2	1:B:185:LEU:O	2.17	0.43
1:B:289:LEU:HD11	1:B:295:LEU:HB2	2.00	0.43
1:D:118:LEU:HB3	1:D:119:PRO:HD3	2.00	0.43
1:D:274:GLY:HA2	6:D:729:HOH:O	2.18	0.43
1:A:64:PRO:HA	1:A:91:PRO:O	2.18	0.43
1:A:375:GLU:HB2	1:A:406:ALA:HB2	2.00	0.43
1:B:24:PRO:O	3:D:602:TPP:HM43	2.18	0.43
1:D:368:GLU:HG2	1:D:390:ARG:NH1	2.33	0.43
1:B:98:GLN:HG3	1:B:99:GLN:N	2.33	0.43
1:B:414:GLN:CG	1:B:446:ILE:CG2	2.97	0.43
1:C:507:LEU:HD23	1:C:507:LEU:HA	1.85	0.43
1:A:257:ILE:HA	1:A:280:TYR:CE1	2.54	0.43
1:B:148:MET:HB2	1:B:148:MET:HE3	1.92	0.43
1:B:419:GLU:HB2	6:B:761:HOH:O	2.18	0.43
1:A:208:GLY:CA	1:A:275:ALA:HB2	2.42	0.43
1:A:246:HIS:CG	1:A:247:PRO:HD2	2.54	0.43
1:D:460:ILE:CG2	1:D:461:LEU:N	2.81	0.43
1:C:439:TRP:CZ2	1:C:443:GLN:CG	3.01	0.43
1:B:374:ASN:HB2	1:B:383:MET:CE	2.49	0.43
1:C:439:TRP:CE2	1:C:443:GLN:HG2	2.54	0.43
1:B:134:GLU:O	1:B:134:GLU:HG2	2.19	0.42
1:C:49:CYS:O	1:C:53:ILE:HG13	2.19	0.42
1:B:414:GLN:HG3	1:B:446:ILE:HG23	2.00	0.42
1:C:372:TYR:O	1:C:395:TYR:HA	2.19	0.42
1:A:407:LEU:HB3	1:A:408:PRO:HD3	2.00	0.42
1:D:375:GLU:OE2	1:D:430:SER:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ARG:HA	1:B:141:ARG:HG2	2.00	0.42
1:B:88:SER:HB3	1:B:399:ALA:HB2	2.01	0.42
1:B:335:GLN:HG3	1:B:336:LEU:O	2.19	0.42
1:B:243:PRO:HG2	1:B:246:HIS:HB2	2.02	0.42
1:C:468:LEU:C	1:C:470:ALA:N	2.71	0.42
1:A:250:ARG:HD3	1:A:250:ARG:HA	1.83	0.42
1:B:281:TYR:C	1:B:281:TYR:CD2	2.91	0.42
1:B:439:TRP:CE2	1:B:443:GLN:HG3	2.52	0.42
1:C:118:LEU:N	1:C:119:PRO:CD	2.82	0.42
1:A:464:PHE:HA	1:A:467:VAL:HG12	2.02	0.42
1:C:250:ARG:HD3	1:C:250:ARG:HA	1.89	0.42
1:C:403:LEU:HD22	1:C:430:SER:OG	2.20	0.42
1:D:460:ILE:HG23	1:D:461:LEU:N	2.33	0.42
1:A:79[B]:MET:SD	1:C:79[B]:MET:SD	3.17	0.42
1:C:439:TRP:CZ2	1:C:443:GLN:HG3	2.54	0.42
1:D:249:PHE:CE2	1:D:251:GLY:HA2	2.55	0.42
1:D:44:ALA:HB3	1:D:50:VAL:HG22	2.01	0.42
1:D:113:VAL:O	1:D:114:ASP:C	2.57	0.42
1:D:299:THR:O	1:D:315:VAL:HA	2.20	0.42
1:D:463:TRP:CZ3	1:D:467:VAL:HG11	2.55	0.42
1:B:242:PHE:CG	1:B:243:PRO:HD2	2.55	0.41
1:C:428:ASP:OD2	1:C:456:GLY:N	2.53	0.41
1:C:120:ARG:HA	1:C:121:PRO:HA	1.75	0.41
1:C:257:ILE:HB	1:C:284:ASP:O	2.20	0.41
1:D:234:ALA:HB3	6:D:771:HOH:O	2.19	0.41
1:A:141:ARG:HG2	1:B:307:ARG:HA	2.02	0.41
1:B:100:THR:HB	1:B:160:TYR:CZ	2.56	0.41
1:B:46:GLN:OE1	1:B:48:ALA:HB3	2.20	0.41
1:C:79[A]:MET:SD	1:C:119:PRO:HA	2.60	0.41
1:C:524:VAL:CG1	1:C:525:SER:N	2.83	0.41
1:A:28:GLU:OE2	1:A:97:GLY:CA	2.66	0.41
1:A:462:ARG:NH1	1:A:462:ARG:HG3	2.22	0.41
1:B:31:PHE:HB2	1:B:163:TRP:CE2	2.55	0.41
1:C:460:ILE:HD12	1:C:460:ILE:HA	1.89	0.41
1:D:232[A]:TRP:CE2	1:D:250:ARG:HB3	2.55	0.41
1:A:299:THR:O	1:A:315:VAL:HA	2.20	0.41
3:B:602:TPP:HN42	3:B:602:TPP:H2	1.86	0.41
1:A:79[A]:MET:SD	1:A:82:LEU:HD12	2.60	0.41
1:B:407:LEU:HB3	1:B:408:PRO:HD3	2.03	0.41
1:D:361:THR:HG22	1:D:507:LEU:HD12	2.03	0.41
1:D:458:TYR:O	1:D:459:GLY:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ASP:HB3	1:C:489:GLY:HA2	2.03	0.41
1:B:119:PRO:HG3	1:B:155:TYR:CD2	2.56	0.41
1:B:257:ILE:HA	1:B:280:TYR:CE1	2.56	0.41
1:C:460:ILE:HG13	1:C:464:PHE:CE2	2.56	0.41
1:D:342:GLU:HA	1:D:343:PRO:HD3	1.98	0.41
1:A:18:ASP:C	1:A:18:ASP:OD1	2.59	0.40
1:D:250:ARG:HA	1:D:250:ARG:HD3	1.58	0.40
1:A:130:ALA:HA	5:D:603:GOL:O1	2.21	0.40
1:B:79[A]:MET:CE	1:B:122:LEU:HD12	2.49	0.40
1:C:29:LEU:HB2	1:C:30:PRO:HD3	2.02	0.40
1:C:458:TYR:CD1	3:C:602:TPP:H61	2.57	0.40
1:C:468:LEU:C	1:C:470:ALA:H	2.24	0.40
1:D:128:GLU:HA	1:D:129:PRO:HD3	1.86	0.40
1:B:382:GLN:H	1:B:382:GLN:NE2	2.19	0.40
1:C:471:GLU:O	1:C:472:ASN:HB2	2.21	0.40
3:C:602:TPP:H2	3:C:602:TPP:HN42	1.87	0.40
1:D:407:LEU:HB3	1:D:408:PRO:HD3	2.03	0.40
1:C:141:ARG:HG2	1:D:307:ARG:HA	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ASP:OD2	5:A:605:GOL:C1[2_455]	1.41	0.79

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	531/533 (100%)	518 (98%)	12 (2%)	1 (0%)	47 53
1	B	529/533 (99%)	516 (98%)	7 (1%)	6 (1%)	14 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	528/533 (99%)	519 (98%)	9 (2%)	0	100	100
1	D	529/533 (99%)	517 (98%)	10 (2%)	2 (0%)	34	35
All	All	2117/2132 (99%)	2070 (98%)	38 (2%)	9 (0%)	41	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	GLU
1	B	182[A]	SER
1	B	182[B]	SER
1	B	71	SER
1	B	445[A]	ASN
1	B	445[B]	ASN
1	D	241	PRO
1	D	459	GLY
1	B	241	PRO

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	420/420 (100%)	409 (97%)	11 (3%)	46	52
1	B	418/420 (100%)	399 (96%)	19 (4%)	27	29
1	C	417/420 (99%)	400 (96%)	17 (4%)	30	33
1	D	418/420 (100%)	401 (96%)	17 (4%)	30	33
All	All	1673/1680 (100%)	1609 (96%)	64 (4%)	34	36

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	40	ARG
1	A	226[A]	ARG

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Mol	Chain	Res	Type
1	A	226[B]	ARG
1	A	245	ARG
1	A	310	MET
1	A	345	LYS
1	A	462	ARG
1	A	467	VAL
1	A	469	GLU
1	A	496	LYS
1	B	33	LYS
1	B	40	ARG
1	B	83	SER
1	B	103[A]	MET
1	B	103[B]	MET
1	B	199	SER
1	B	217	ASN
1	B	245	ARG
1	B	263	LEU
1	B	281	TYR
1	B	310	MET
1	B	377	THR
1	B	382	GLN
1	B	390	ARG
1	B	419	GLU
1	B	468	LEU
1	B	471	GLU
1	B	496	LYS
1	B	504	LYS
1	C	126	SER
1	C	171	SER
1	C	245	ARG
1	C	281	TYR
1	C	294	ARG
1	C	310	MET
1	C	323	SER
1	C	331	GLU
1	C	335	GLN
1	C	419	GLU
1	C	462	ARG
1	C	467	VAL
1	C	468	LEU
1	C	469	GLU
1	C	501	GLU

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Mol	Chain	Res	Type
1	C	508	GLN
1	C	512	SER
1	D	33	LYS
1	D	83	SER
1	D	124	LYS
1	D	126	SER
1	D	195[A]	LYS
1	D	195[B]	LYS
1	D	217	ASN
1	D	245	ARG
1	D	310	MET
1	D	446	ILE
1	D	460	ILE
1	D	467	VAL
1	D	469	GLU
1	D	496	LYS
1	D	501	GLU
1	D	509	GLU
1	D	514	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	ASN
1	B	262	GLN
1	B	382	GLN
1	C	144	HIS
1	C	178	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
3	TPP	A	602	2	22,27,27	1.50	2 (9%)	29,40,40	1.94	6 (20%)
5	GOL	A	606	-	5,5,5	0.25	0	5,5,5	0.26	0
3	TPP	D	602	2	22,27,27	1.51	2 (9%)	29,40,40	2.00	6 (20%)
5	GOL	B	604	-	5,5,5	0.24	0	5,5,5	0.31	0
3	TPP	B	602	2	22,27,27	1.53	2 (9%)	29,40,40	2.01	6 (20%)
5	GOL	A	604	-	5,5,5	0.25	0	5,5,5	0.25	0
5	GOL	D	603	-	5,5,5	0.25	0	5,5,5	0.31	0
3	TPP	C	602	2	22,27,27	1.50	2 (9%)	29,40,40	2.01	6 (20%)
5	GOL	A	605	-	5,5,5	0.24	0	5,5,5	0.27	0
5	GOL	C	603	-	5,5,5	0.24	0	5,5,5	0.28	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
3	TPP	A	602	2	-	2/16/17/17	0/2/2/2
5	GOL	A	606	-	-	4/4/4/4	-
3	TPP	D	602	2	-	2/16/17/17	0/2/2/2
5	GOL	B	604	-	-	2/4/4/4	-
3	TPP	B	602	2	-	1/16/17/17	0/2/2/2
5	GOL	A	604	-	-	2/4/4/4	-
5	GOL	D	603	-	-	4/4/4/4	-
3	TPP	C	602	2	-	1/16/17/17	0/2/2/2
5	GOL	A	605	-	-	2/4/4/4	-
5	GOL	C	603	-	-	4/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	TPP	C4-N3	-5.46	1.35	1.39
3	A	602	TPP	C4-N3	-5.44	1.35	1.39
3	B	602	TPP	C4-N3	-5.43	1.35	1.39
3	D	602	TPP	C4-N3	-5.37	1.35	1.39
3	B	602	TPP	C5'-C4'	3.32	1.48	1.42
3	D	602	TPP	C5'-C4'	3.31	1.48	1.42
3	A	602	TPP	C5'-C4'	3.25	1.48	1.42
3	C	602	TPP	C5'-C4'	3.23	1.48	1.42

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	602	TPP	C6-C5-C4	6.46	132.62	127.43
3	B	602	TPP	C6-C5-C4	6.43	132.59	127.43
3	C	602	TPP	C6-C5-C4	6.41	132.58	127.43
3	A	602	TPP	C6-C5-C4	5.82	132.10	127.43
3	B	602	TPP	C6'-N1'-C2'	3.60	122.08	115.96
3	C	602	TPP	C6'-N1'-C2'	3.57	122.03	115.96
3	A	602	TPP	C6'-N1'-C2'	3.56	122.01	115.96
3	D	602	TPP	C6'-N1'-C2'	3.53	121.96	115.96
3	C	602	TPP	PA-O3A-PB	-3.20	121.83	132.83
3	B	602	TPP	PA-O3A-PB	-3.14	122.04	132.83
3	D	602	TPP	PA-O3A-PB	-3.13	122.08	132.83
3	A	602	TPP	PA-O3A-PB	-3.06	122.34	132.83
3	C	602	TPP	C5'-C6'-N1'	-2.66	119.38	123.82
3	A	602	TPP	C5'-C6'-N1'	-2.65	119.40	123.82
3	B	602	TPP	C5'-C6'-N1'	-2.63	119.44	123.82
3	D	602	TPP	N4'-C4'-N3'	2.61	120.72	117.03
3	D	602	TPP	C5'-C6'-N1'	-2.60	119.48	123.82
3	C	602	TPP	N4'-C4'-N3'	2.60	120.71	117.03
3	B	602	TPP	N4'-C4'-N3'	2.58	120.68	117.03
3	A	602	TPP	N4'-C4'-N3'	2.57	120.67	117.03
3	B	602	TPP	N1'-C2'-N3'	-2.25	121.67	125.54
3	C	602	TPP	N1'-C2'-N3'	-2.24	121.68	125.54
3	D	602	TPP	N1'-C2'-N3'	-2.24	121.68	125.54
3	A	602	TPP	N1'-C2'-N3'	-2.22	121.72	125.54

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	TPP	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	B	602	TPP	C4-C5-C6-C7
3	C	602	TPP	C4-C5-C6-C7
3	D	602	TPP	PA-O3A-PB-O2B
5	A	606	GOL	O1-C1-C2-C3
5	A	606	GOL	C1-C2-C3-O3
5	B	604	GOL	O1-C1-C2-C3
5	C	603	GOL	O1-C1-C2-O2
5	C	603	GOL	O1-C1-C2-C3
5	C	603	GOL	C1-C2-C3-O3
5	D	603	GOL	C1-C2-C3-O3
5	C	603	GOL	O2-C2-C3-O3
5	A	604	GOL	O1-C1-C2-C3
5	A	605	GOL	O1-C1-C2-C3
5	D	603	GOL	O1-C1-C2-C3
5	A	606	GOL	O1-C1-C2-O2
5	B	604	GOL	O1-C1-C2-O2
3	A	602	TPP	PB-O3A-PA-O7
5	A	604	GOL	O1-C1-C2-O2
5	A	605	GOL	O1-C1-C2-O2
5	A	606	GOL	O2-C2-C3-O3
5	D	603	GOL	O2-C2-C3-O3
3	D	602	TPP	C4-C5-C6-C7
5	D	603	GOL	O1-C1-C2-O2

There are no ring outliers.

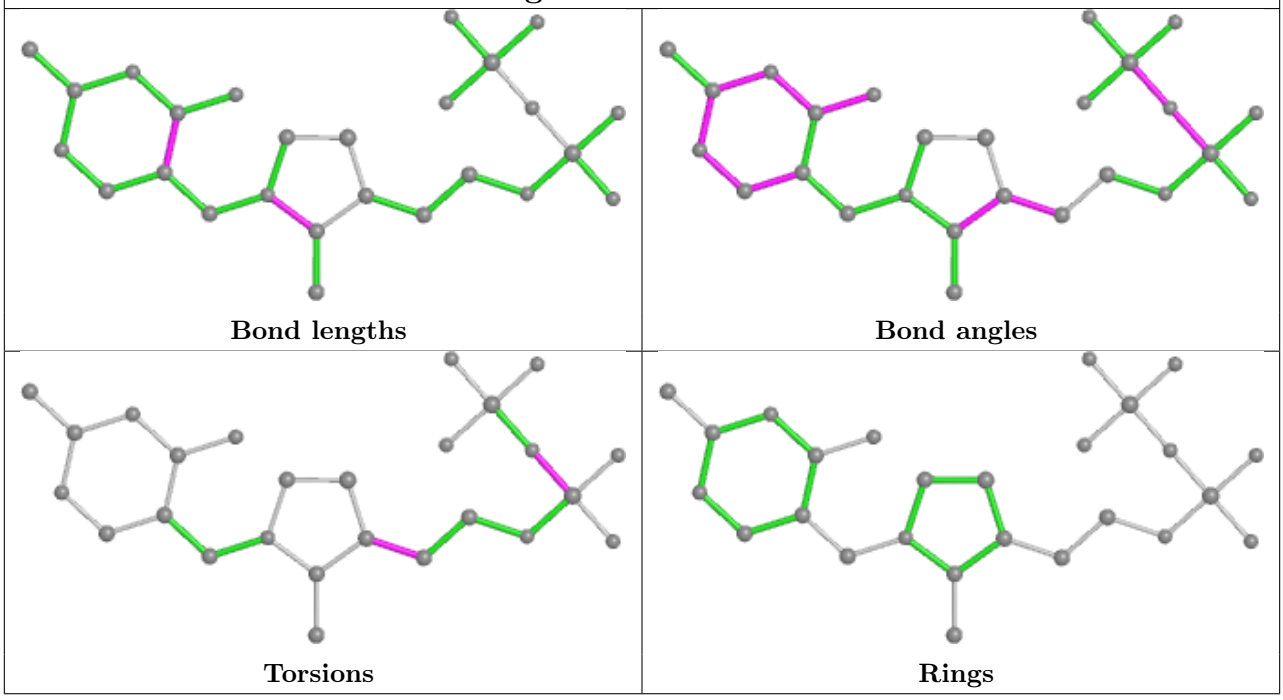
9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	TPP	2	0
5	A	606	GOL	2	0
3	D	602	TPP	6	0
5	B	604	GOL	2	0
3	B	602	TPP	3	0
5	A	604	GOL	1	0
5	D	603	GOL	1	0
3	C	602	TPP	6	0
5	A	605	GOL	0	1

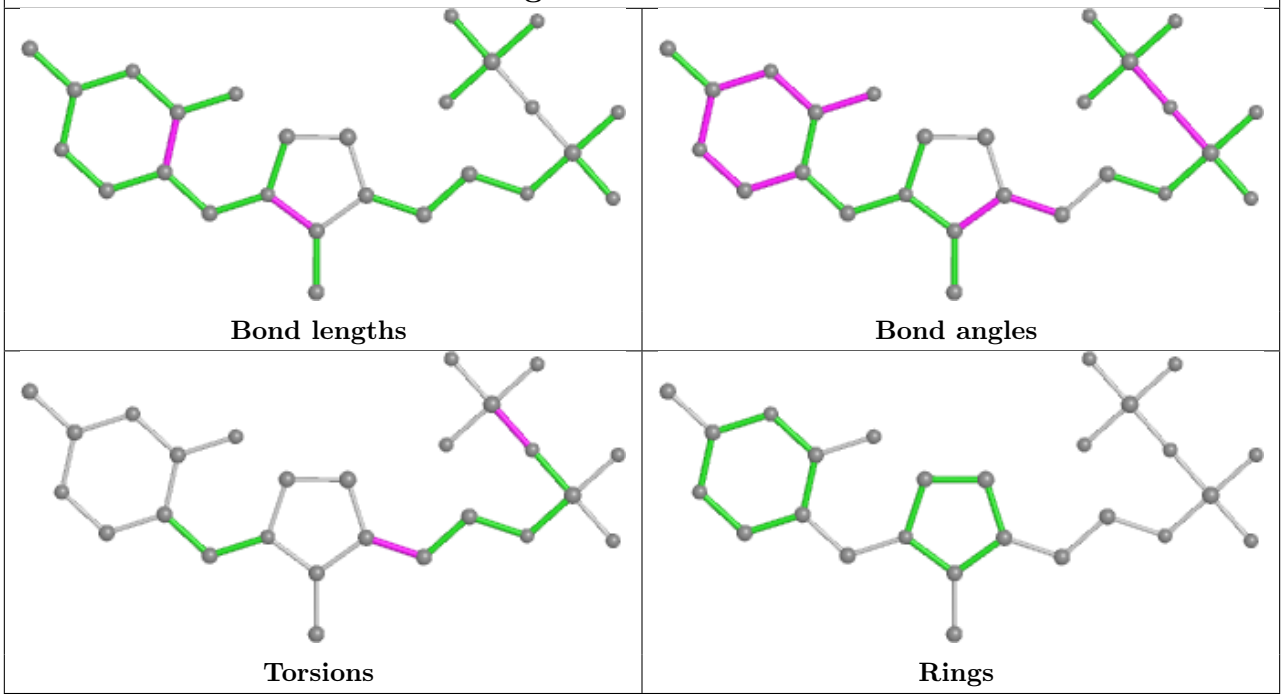
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

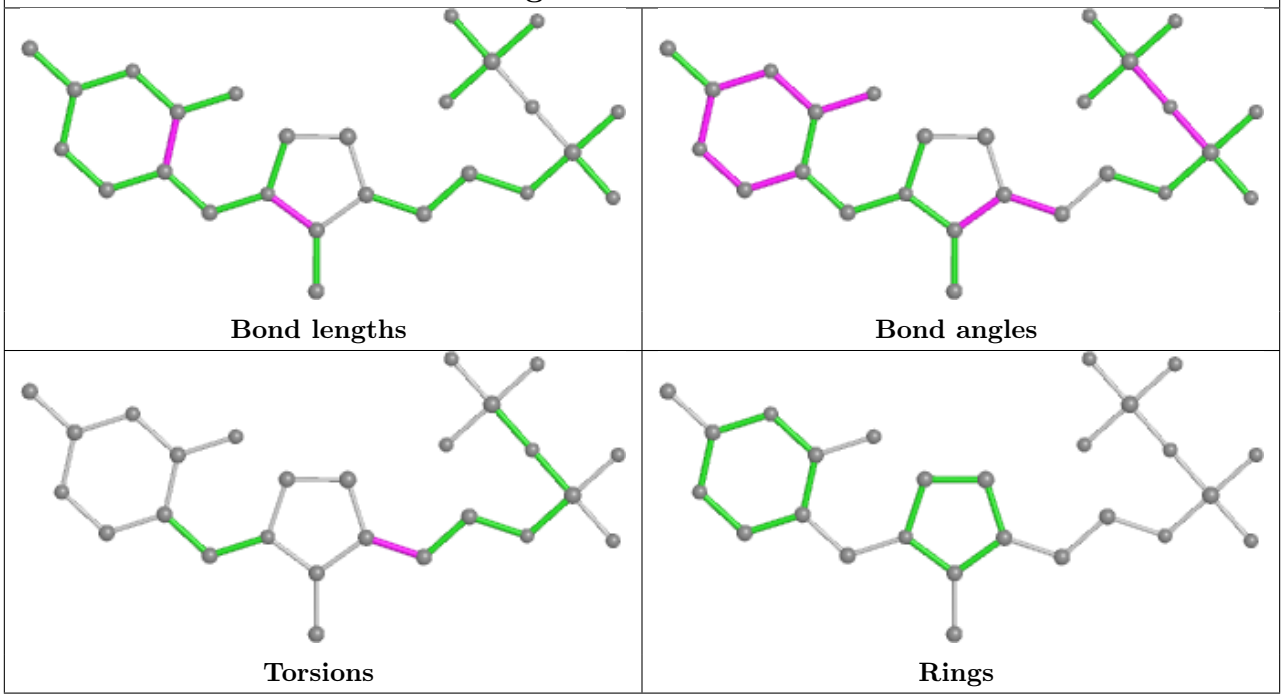
Ligand TPP A 602



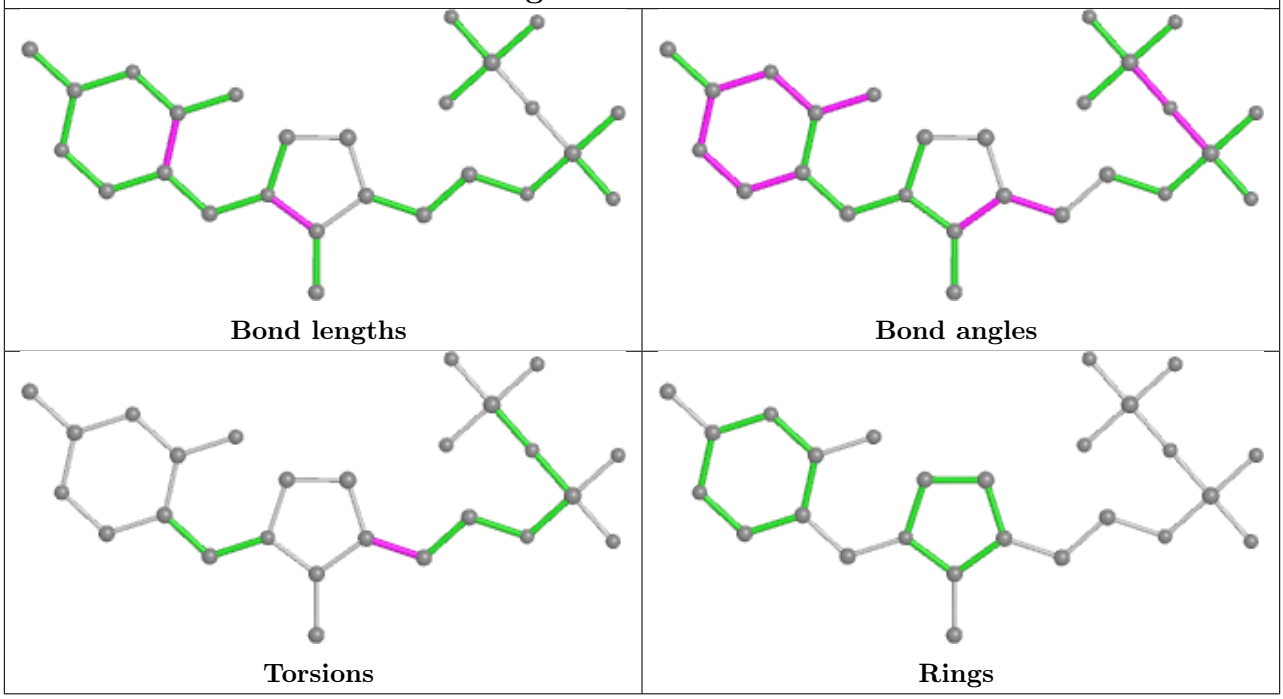
Ligand TPP D 602



Ligand TPP B 602



Ligand TPP C 602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	525/533 (98%)	-0.62	3 (0%)	89	89	15, 24, 38, 72	7 (1%)
1	B	525/533 (98%)	-0.51	2 (0%)	92	93	16, 24, 37, 68	8 (1%)
1	C	524/533 (98%)	-0.45	5 (0%)	82	83	17, 26, 42, 69	9 (1%)
1	D	524/533 (98%)	-0.48	3 (0%)	89	89	16, 25, 41, 64	9 (1%)
All	All	2098/2132 (98%)	-0.51	13 (0%)	89	89	15, 24, 40, 72	33 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	467	VAL	3.5
1	C	468	LEU	2.5
1	A	525	SER	2.4
1	C	471	GLU	2.4
1	C	469	GLU	2.3
1	C	467	VAL	2.3
1	A	526	PRO	2.3
1	C	465	ALA	2.3
1	D	468	LEU	2.3
1	B	472	ASN	2.2
1	A	472	ASN	2.1
1	B	525	SER	2.1
1	D	466	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

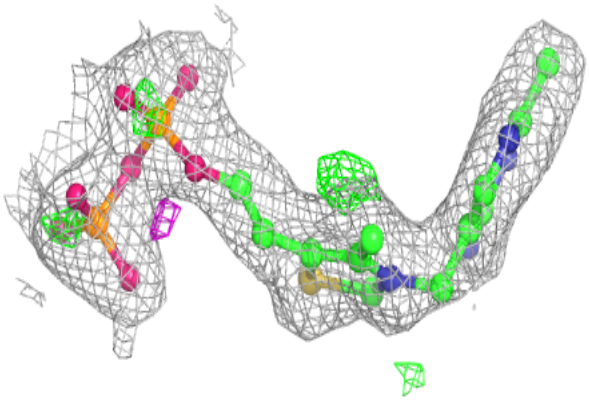
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

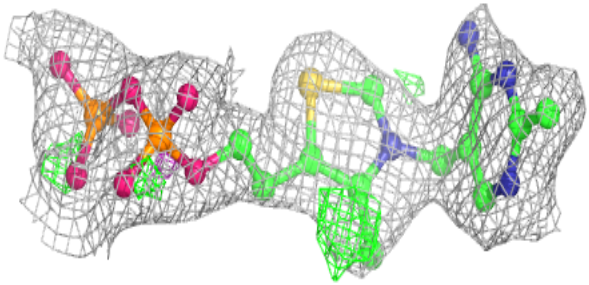
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	604	6/6	0.80	0.25	43,49,53,55	0
5	GOL	A	605	6/6	0.81	0.15	50,54,60,61	0
5	GOL	A	606	6/6	0.81	0.14	56,60,67,74	0
5	GOL	D	603	6/6	0.81	0.20	36,45,47,53	0
5	GOL	B	604	6/6	0.83	0.14	41,47,54,58	0
5	GOL	C	603	6/6	0.89	0.16	38,42,48,52	2
3	TPP	C	602	26/26	0.95	0.16	20,33,38,43	3
3	TPP	B	602	26/26	0.96	0.12	19,29,32,34	5
2	CA	A	601	1/1	0.97	0.11	25,25,25,25	0
2	CA	D	601	1/1	0.97	0.06	30,30,30,30	0
3	TPP	D	602	26/26	0.97	0.11	24,31,34,38	5
4	MG	A	603	1/1	0.97	0.16	14,14,14,14	0
3	TPP	A	602	26/26	0.97	0.14	18,29,35,39	5
2	CA	B	601	1/1	0.98	0.06	25,25,25,25	0
2	CA	C	601	1/1	0.98	0.09	31,31,31,31	0
4	MG	B	603	1/1	0.98	0.18	14,14,14,14	0

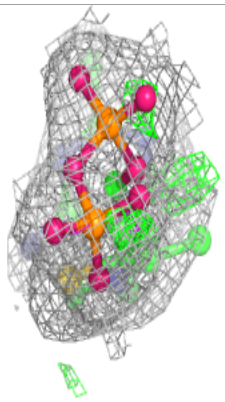
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP 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)

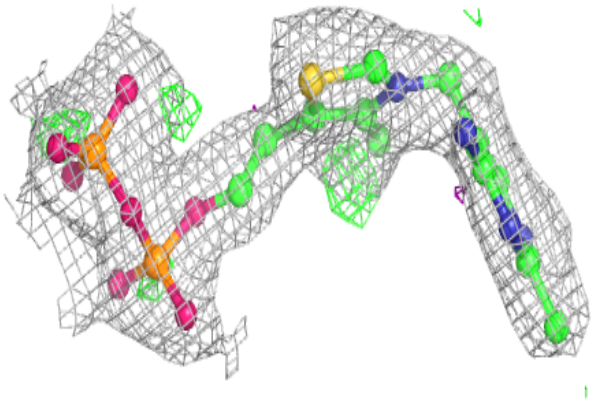


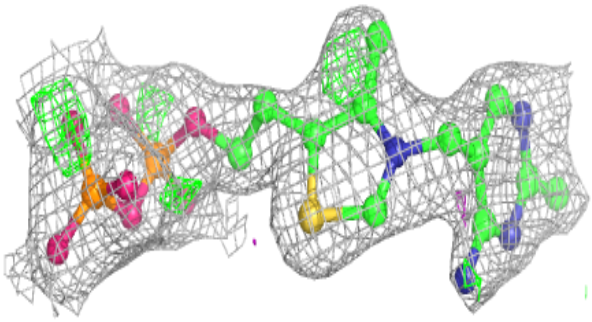


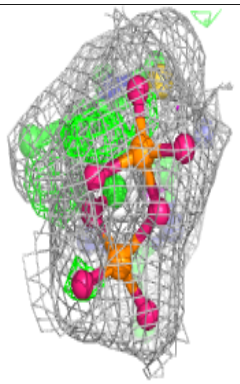


Electron density around TPP B 602:

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

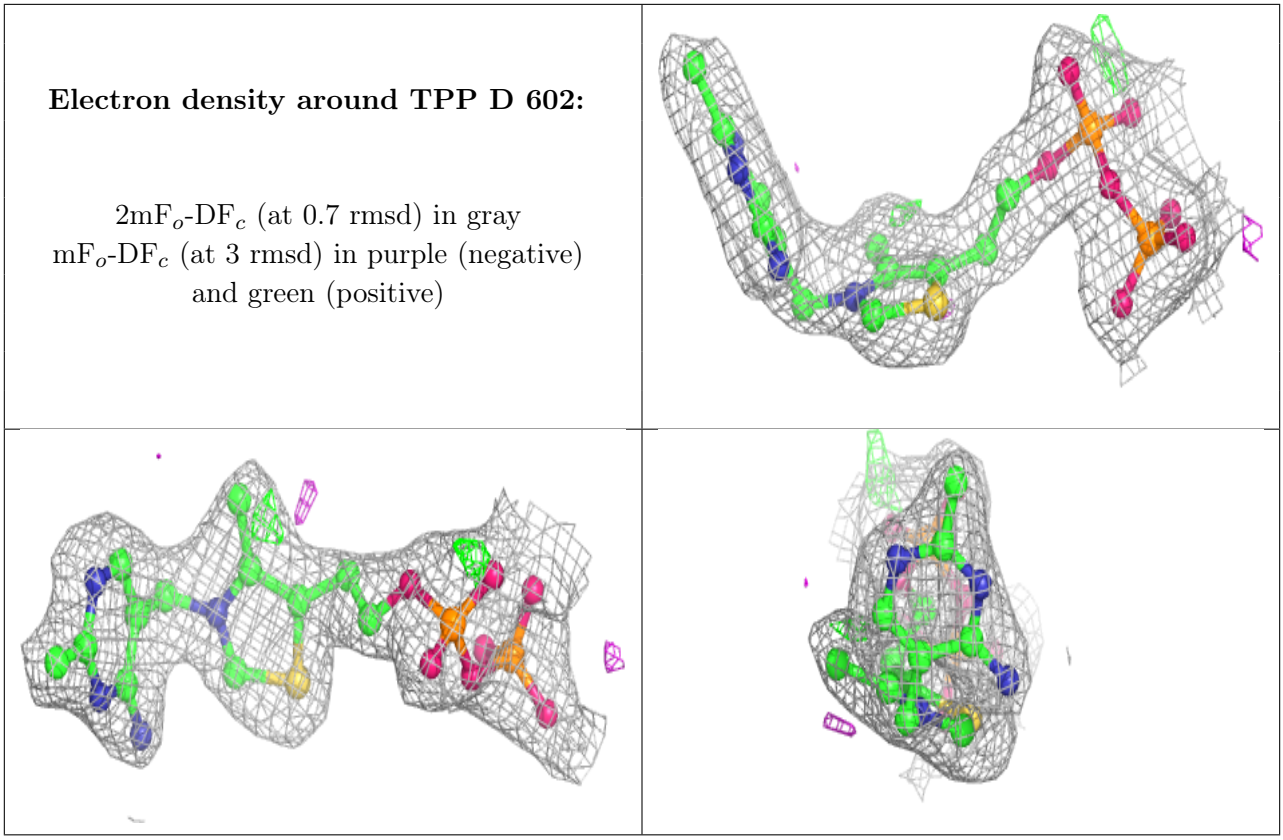






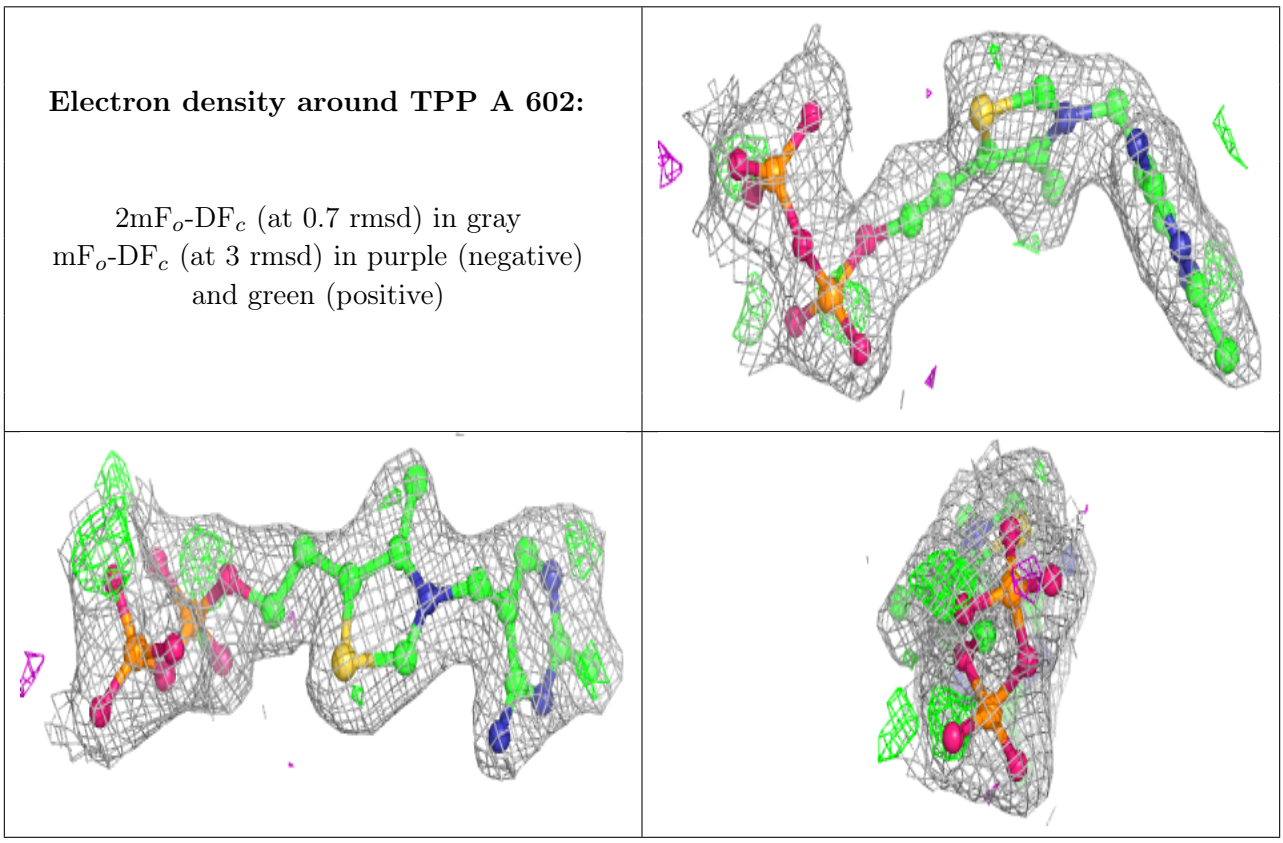
Electron density around TPP D 602:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.