Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 08:45 AM EST

PDB ID	:	3EZ3
Title	:	Crystal Structure of Plasmodium vivax geranylgeranylpyrophosphate synthase PVX_092040 with zoledronate and IPP bound
Authors	:	Wernimont, A.K.; Lew, J.; Zhao, Y.; Kozieradzki, I.; Cossar, D.; Schapira, M.; Bochkarev, A.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Hui, R.; Artz, J.D.; Structural Genomics Consortium (SGC)
Deposited on	:	2008-10-22
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*
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 (1)) were used in the production of this report:

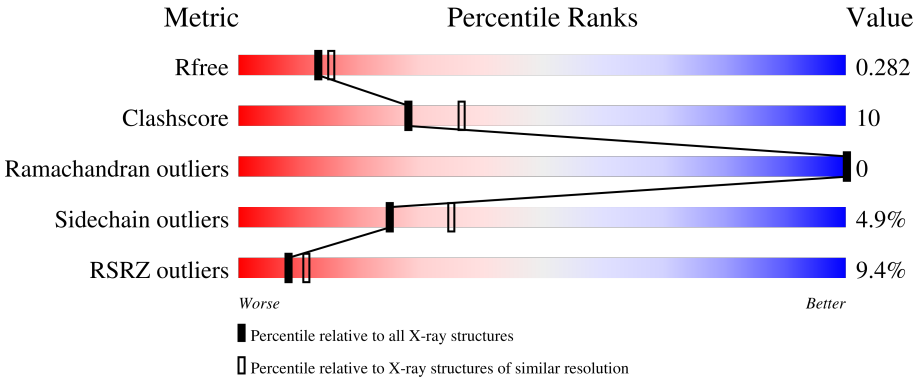
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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 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	396	9% 71% 18% • 10%
1	B	396	7% 67% 21% • 11%
1	C	396	9% 69% 19% • 10%
1	D	396	10% 65% 21% • 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	B	1106	-	-	X	X
6	GOL	A	1106	-	-	X	X
6	GOL	B	1105	-	-	X	-
6	GOL	D	1105	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12384 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 Farnesyl pyrophosphate synthase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	14	4	0
			2931	1909	465	541	16			
1	B	353	Total	C	N	O	S	11	3	0
			2910	1902	460	533	15			
1	C	357	Total	C	N	O	S	12	6	0
			2937	1917	467	538	15			
1	D	351	Total	C	N	O	S	14	4	0
			2887	1882	457	533	15			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A5K4U6
A	2	GLY	-	expression tag	UNP A5K4U6
A	3	SER	-	expression tag	UNP A5K4U6
A	4	SER	-	expression tag	UNP A5K4U6
A	5	HIS	-	expression tag	UNP A5K4U6
A	6	HIS	-	expression tag	UNP A5K4U6
A	7	HIS	-	expression tag	UNP A5K4U6
A	8	HIS	-	expression tag	UNP A5K4U6
A	9	HIS	-	expression tag	UNP A5K4U6
A	10	HIS	-	expression tag	UNP A5K4U6
A	11	SER	-	expression tag	UNP A5K4U6
A	12	SER	-	expression tag	UNP A5K4U6
A	13	GLY	-	expression tag	UNP A5K4U6
A	14	ARG	-	expression tag	UNP A5K4U6
A	15	GLU	-	expression tag	UNP A5K4U6
A	16	ASN	-	expression tag	UNP A5K4U6
A	17	LEU	-	expression tag	UNP A5K4U6
A	18	TYR	-	expression tag	UNP A5K4U6
A	19	PHE	-	expression tag	UNP A5K4U6
A	20	GLN	-	expression tag	UNP A5K4U6
A	21	GLY	-	expression tag	UNP A5K4U6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	134	MET	THR	SEE REMARK 999	UNP A5K4U6
A	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
B	1	MET	-	expression tag	UNP A5K4U6
B	2	GLY	-	expression tag	UNP A5K4U6
B	3	SER	-	expression tag	UNP A5K4U6
B	4	SER	-	expression tag	UNP A5K4U6
B	5	HIS	-	expression tag	UNP A5K4U6
B	6	HIS	-	expression tag	UNP A5K4U6
B	7	HIS	-	expression tag	UNP A5K4U6
B	8	HIS	-	expression tag	UNP A5K4U6
B	9	HIS	-	expression tag	UNP A5K4U6
B	10	HIS	-	expression tag	UNP A5K4U6
B	11	SER	-	expression tag	UNP A5K4U6
B	12	SER	-	expression tag	UNP A5K4U6
B	13	GLY	-	expression tag	UNP A5K4U6
B	14	ARG	-	expression tag	UNP A5K4U6
B	15	GLU	-	expression tag	UNP A5K4U6
B	16	ASN	-	expression tag	UNP A5K4U6
B	17	LEU	-	expression tag	UNP A5K4U6
B	18	TYR	-	expression tag	UNP A5K4U6
B	19	PHE	-	expression tag	UNP A5K4U6
B	20	GLN	-	expression tag	UNP A5K4U6
B	21	GLY	-	expression tag	UNP A5K4U6
B	134	MET	THR	SEE REMARK 999	UNP A5K4U6
B	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
C	1	MET	-	expression tag	UNP A5K4U6
C	2	GLY	-	expression tag	UNP A5K4U6
C	3	SER	-	expression tag	UNP A5K4U6
C	4	SER	-	expression tag	UNP A5K4U6
C	5	HIS	-	expression tag	UNP A5K4U6
C	6	HIS	-	expression tag	UNP A5K4U6
C	7	HIS	-	expression tag	UNP A5K4U6
C	8	HIS	-	expression tag	UNP A5K4U6
C	9	HIS	-	expression tag	UNP A5K4U6
C	10	HIS	-	expression tag	UNP A5K4U6
C	11	SER	-	expression tag	UNP A5K4U6
C	12	SER	-	expression tag	UNP A5K4U6
C	13	GLY	-	expression tag	UNP A5K4U6
C	14	ARG	-	expression tag	UNP A5K4U6
C	15	GLU	-	expression tag	UNP A5K4U6
C	16	ASN	-	expression tag	UNP A5K4U6
C	17	LEU	-	expression tag	UNP A5K4U6

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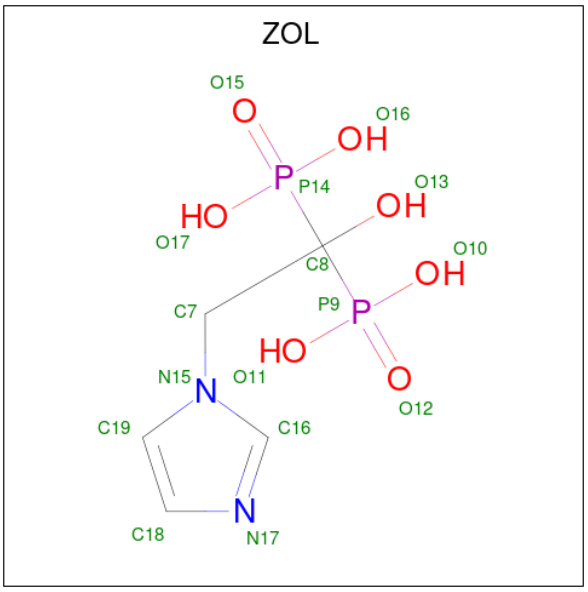
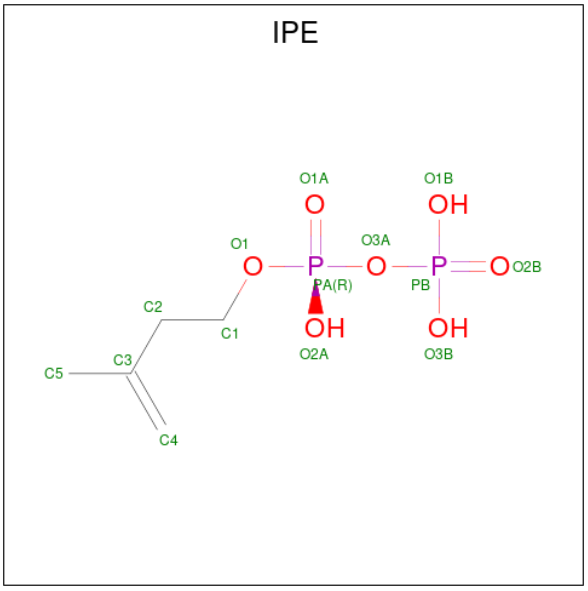
Chain	Residue	Modelled	Actual	Comment	Reference
C	18	TYR	-	expression tag	UNP A5K4U6
C	19	PHE	-	expression tag	UNP A5K4U6
C	20	GLN	-	expression tag	UNP A5K4U6
C	21	GLY	-	expression tag	UNP A5K4U6
C	134	MET	THR	SEE REMARK 999	UNP A5K4U6
C	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
D	1	MET	-	expression tag	UNP A5K4U6
D	2	GLY	-	expression tag	UNP A5K4U6
D	3	SER	-	expression tag	UNP A5K4U6
D	4	SER	-	expression tag	UNP A5K4U6
D	5	HIS	-	expression tag	UNP A5K4U6
D	6	HIS	-	expression tag	UNP A5K4U6
D	7	HIS	-	expression tag	UNP A5K4U6
D	8	HIS	-	expression tag	UNP A5K4U6
D	9	HIS	-	expression tag	UNP A5K4U6
D	10	HIS	-	expression tag	UNP A5K4U6
D	11	SER	-	expression tag	UNP A5K4U6
D	12	SER	-	expression tag	UNP A5K4U6
D	13	GLY	-	expression tag	UNP A5K4U6
D	14	ARG	-	expression tag	UNP A5K4U6
D	15	GLU	-	expression tag	UNP A5K4U6
D	16	ASN	-	expression tag	UNP A5K4U6
D	17	LEU	-	expression tag	UNP A5K4U6
D	18	TYR	-	expression tag	UNP A5K4U6
D	19	PHE	-	expression tag	UNP A5K4U6
D	20	GLN	-	expression tag	UNP A5K4U6
D	21	GLY	-	expression tag	UNP A5K4U6
D	134	MET	THR	SEE REMARK 999	UNP A5K4U6
D	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6

- Molecule 2 is ZOLEDRONIC ACID (three-letter code: ZOL) (formula: $C_5H_{10}N_2O_7P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	5	2	7	2		
2	B	1	Total	C	N	O	P	0	0
			16	5	2	7	2		
2	C	1	Total	C	N	O	P	0	0
			16	5	2	7	2		
2	D	1	Total	C	N	O	P	0	0
			16	5	2	7	2		

- Molecule 3 is 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (three-letter code: IPE) (formula: $C_5H_{12}O_7P_2$).

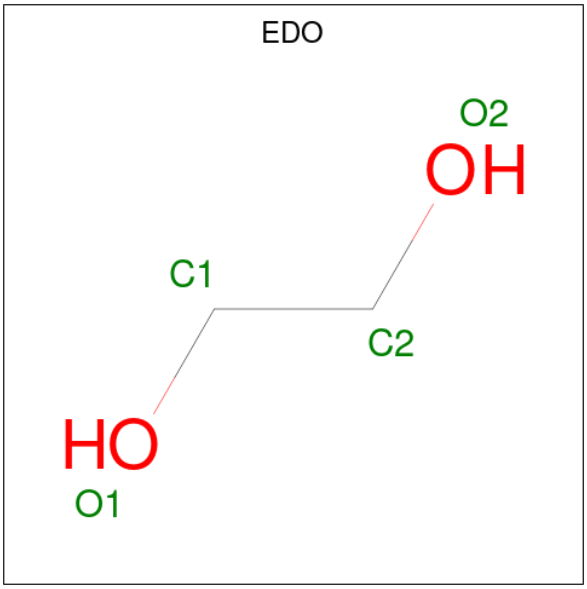


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 14 5 7 2	0	0
3	B	1	Total C O P 14 5 7 2	0	0
3	C	1	Total C O P 14 5 7 2	0	0
3	D	1	Total C O P 14 5 7 2	0	0

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

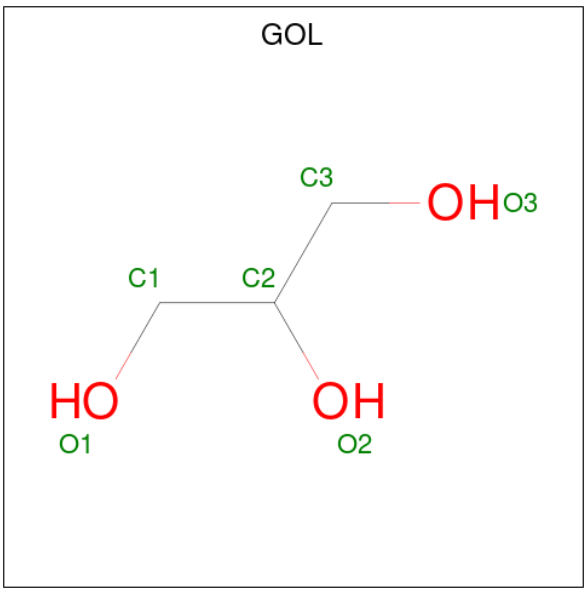
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Mg 3 3	0	0
4	B	3	Total Mg 3 3	0	0
4	C	3	Total Mg 3 3	0	0
4	D	3	Total Mg 3 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

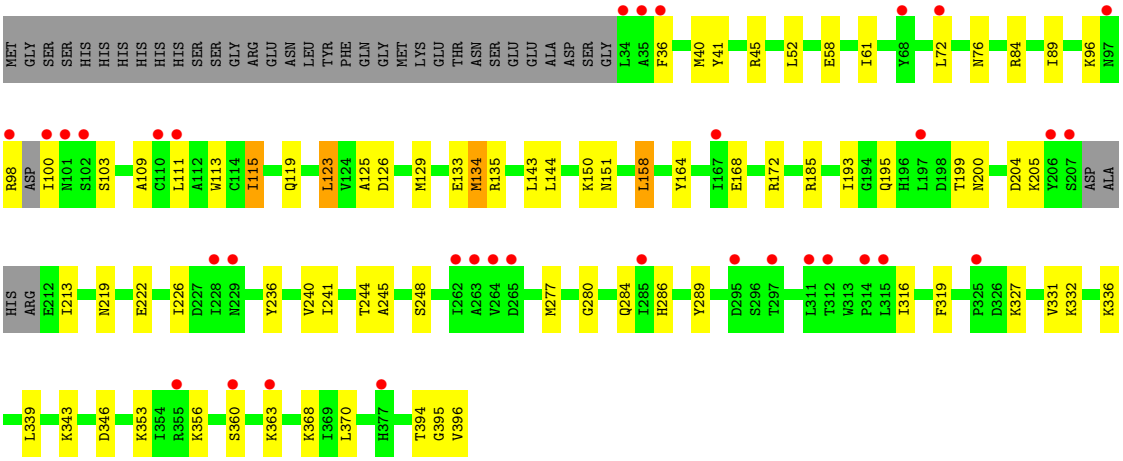
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	149	Total O 149 149	0	0
7	B	140	Total O 140 140	0	0
7	C	140	Total O 140 140	0	0
7	D	132	Total O 132 132	0	0

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.

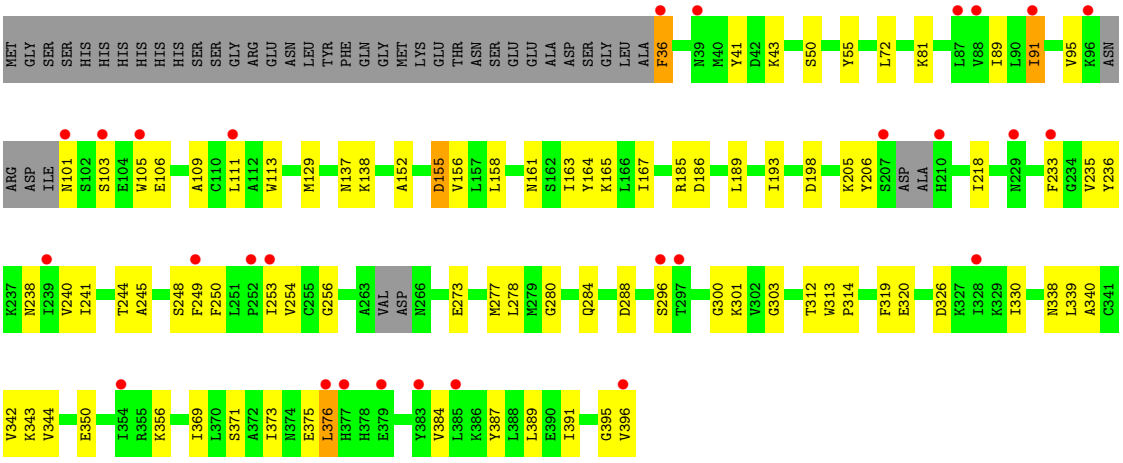
• Molecule 1: Farnesyl pyrophosphate synthase, putative

Chain A:



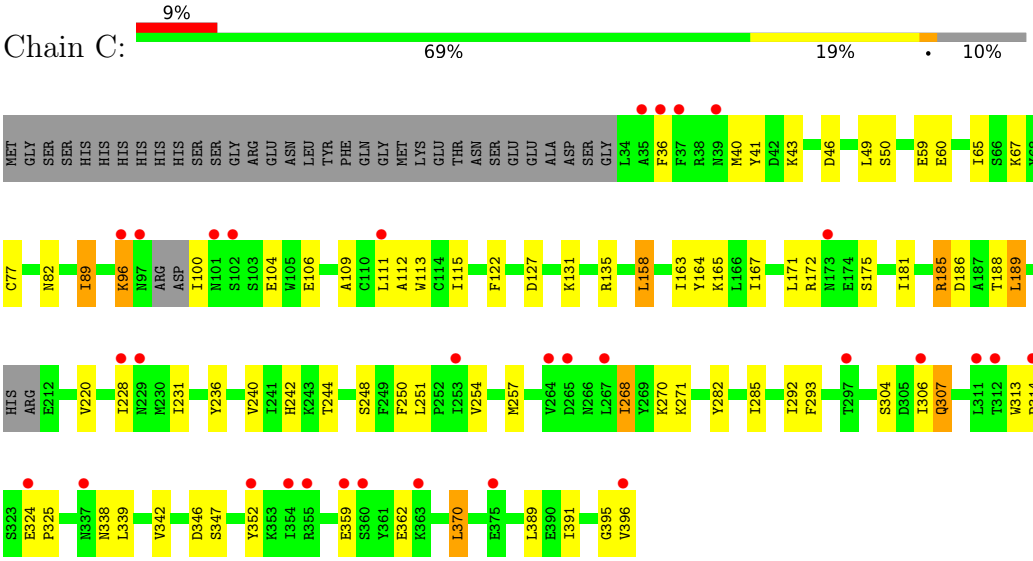
• Molecule 1: Farnesyl pyrophosphate synthase, putative

Chain B:



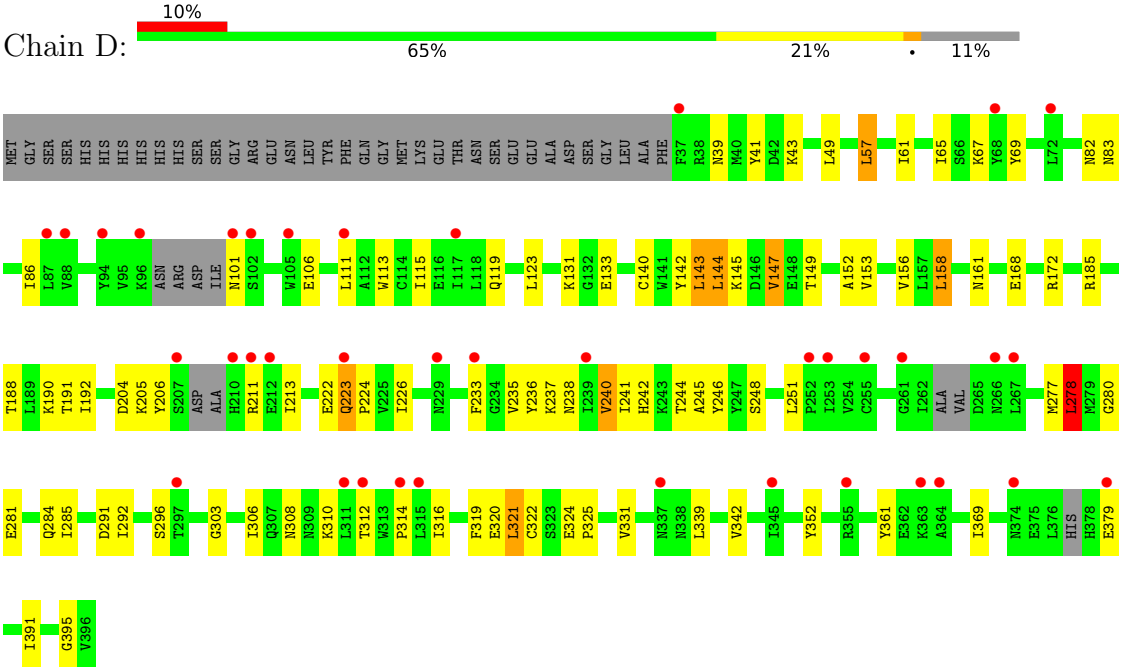
• Molecule 1: Farnesyl pyrophosphate synthase, putative

Chain C:



• Molecule 1: Farnesyl pyrophosphate synthase, putative

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	111.27Å 109.70Å 139.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.43 – 2.30 24.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.1 (24.43-2.30) 95.1 (24.43-2.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.291 0.221 , 0.282	Depositor DCC
R_{free} test set	3633 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12384	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7001e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: ZOL, IPE, GOL, EDO, MG

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	0.76	5/3000 (0.2%)	0.78	5/4053 (0.1%)
1	B	0.79	2/2981 (0.1%)	0.90	7/4027 (0.2%)
1	C	1.30	6/3015 (0.2%)	1.12	9/4075 (0.2%)
1	D	0.73	1/2956 (0.0%)	0.81	4/3993 (0.1%)
All	All	0.92	14/11952 (0.1%)	0.91	25/16148 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	172	ARG	NE-CZ	-39.70	0.81	1.33
1	C	67	LYS	CD-CE	-31.96	0.71	1.51
1	C	59	GLU	CG-CD	-24.89	1.14	1.51
1	B	375	GLU	CG-CD	-14.97	1.29	1.51
1	C	60	GLU	CG-CD	-13.15	1.32	1.51
1	B	350	GLU	CD-OE2	-11.43	1.13	1.25
1	D	39	ASN	CA-CB	10.92	1.81	1.53
1	A	346	ASP	CG-OD2	-9.07	1.04	1.25
1	A	353	LYS	CG-CD	-8.97	1.22	1.52
1	C	307[A]	GLN	CD-OE1	-7.92	1.06	1.24
1	C	307[B]	GLN	CD-OE1	-7.92	1.06	1.24
1	A	368	LYS	CG-CD	-6.85	1.29	1.52
1	A	394	THR	CB-CG2	-6.67	1.30	1.52
1	A	356	LYS	CG-CD	-5.37	1.34	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	172	ARG	NE-CZ-NH2	-33.98	103.31	120.30
1	C	172	ARG	NE-CZ-NH1	33.04	136.82	120.30
1	B	350	GLU	CG-CD-OE1	-21.96	74.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	67	LYS	CG-CD-CE	17.05	163.06	111.90
1	B	350	GLU	OE1-CD-OE2	13.27	139.22	123.30
1	B	350	GLU	CG-CD-OE2	12.41	143.12	118.30
1	C	59	GLU	CB-CG-CD	8.98	138.44	114.20
1	C	59	GLU	CG-CD-OE2	8.97	136.23	118.30
1	C	59	GLU	CG-CD-OE1	-8.94	100.42	118.30
1	D	39	ASN	N-CA-CB	-7.51	97.08	110.60
1	D	39	ASN	CB-CA-C	-7.15	96.10	110.40
1	C	60	GLU	CB-CG-CD	7.05	133.23	114.20
1	B	155	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	171	LEU	CA-CB-CG	6.19	129.53	115.30
1	D	158	LEU	CA-CB-CG	-6.18	101.08	115.30
1	B	375	GLU	CB-CG-CD	5.92	130.18	114.20
1	A	45	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	A	135	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	158	LEU	CA-CB-CG	-5.57	102.49	115.30
1	C	158	LEU	CA-CB-CG	-5.37	102.95	115.30
1	D	278	LEU	CA-CB-CG	5.20	127.27	115.30
1	A	353	LYS	CB-CG-CD	5.06	124.75	111.60
1	A	45	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	B	158	LEU	CA-CB-CG	-5.03	103.72	115.30
1	B	288	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2931	0	2890	48	0
1	B	2910	0	2878	65	0
1	C	2937	0	2918	57	0
1	D	2887	0	2848	79	0
2	A	16	0	6	0	0
2	B	16	0	6	1	0
2	C	16	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	16	0	6	0	0
3	A	14	0	9	0	0
3	B	14	0	9	0	0
3	C	14	0	9	1	0
3	D	14	0	9	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	4	0
6	A	6	0	8	4	0
6	B	6	0	8	6	0
6	D	6	0	8	1	0
7	A	149	0	0	6	0
7	B	140	0	0	4	0
7	C	140	0	0	3	0
7	D	132	0	0	7	0
All	All	12384	0	11630	231	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 10.

All (231) 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:B:301:LYS:HG3	5:B:1106:EDO:H22	1.24	1.16
1:D:292:ILE:HD11	7:D:1164:HOH:O	1.46	1.15
1:D:241:ILE:HG23	1:D:277:MET:CE	1.77	1.15
1:A:126:ASP:OD1	7:A:1161:HOH:O	1.65	1.13
1:D:241:ILE:HG23	1:D:277:MET:HE1	1.43	1.00
1:D:241:ILE:HG23	1:D:277:MET:HE3	1.50	0.91
1:B:240:VAL:HG22	1:B:284:GLN:HG2	1.50	0.90
1:C:164:TYR:HB2	1:D:185[B]:ARG:HD3	1.52	0.89
1:C:164:TYR:CB	1:D:185[B]:ARG:HD3	2.05	0.87
1:B:244:THR:O	1:B:248:SER:HB2	1.76	0.85
1:D:240:VAL:HG22	1:D:284:GLN:HG2	1.58	0.83
1:A:143:LEU:HD13	6:A:1106:GOL:H32	1.61	0.83
1:B:296:SER:HB3	6:B:1105:GOL:H32	1.62	0.80
1:A:36:PHE:CE2	1:A:40[B]:MET:SD	2.75	0.80
1:C:304:SER:HA	1:C:307[B]:GLN:OE1	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185[A]:ARG:HH11	1:C:185[A]:ARG:HB2	1.46	0.79
1:D:233[B]:PHE:HE2	1:D:320:GLU:OE2	1.67	0.76
1:D:241:ILE:CG2	1:D:277:MET:HE3	2.14	0.76
1:D:244:THR:O	1:D:248:SER:HB2	1.85	0.74
1:A:134:MET:HG2	7:A:1232:HOH:O	1.87	0.74
1:D:281:GLU:O	1:D:285:ILE:HG13	1.88	0.73
1:D:144:LEU:HB2	1:D:147:VAL:HG13	1.69	0.73
1:D:306:ILE:HD12	6:D:1105:GOL:H11	1.69	0.73
1:B:43:LYS:HE2	1:B:106:GLU:HG3	1.70	0.72
1:D:246:TYR:CE1	1:D:277:MET:HE1	2.25	0.72
1:A:58:GLU:HB2	1:A:61:ILE:HD12	1.72	0.71
1:B:233[B]:PHE:HE2	1:B:320:GLU:OE1	1.73	0.70
1:A:332:LYS:O	1:A:336:LYS:HE2	1.92	0.70
1:A:168:GLU:OE2	1:B:185[A]:ARG:NH1	2.26	0.69
1:B:389:LEU:O	7:B:1192:HOH:O	2.10	0.69
1:D:82:ASN:O	1:D:86:ILE:HG12	1.93	0.69
1:B:185[A]:ARG:NH2	1:B:186:ASP:OD1	2.26	0.68
1:B:340:ALA:O	1:B:344:VAL:HG23	1.94	0.68
1:A:164:TYR:OH	1:A:185[A]:ARG:HG3	1.93	0.67
1:C:96:LYS:HE2	1:C:96:LYS:HA	1.77	0.66
1:D:241:ILE:CG2	1:D:277:MET:CE	2.64	0.65
1:B:296:SER:HB3	6:B:1105:GOL:C3	2.28	0.64
1:D:246:TYR:CE1	1:D:277:MET:CE	2.80	0.64
1:A:164:TYR:CB	1:B:185[B]:ARG:HD3	2.28	0.64
1:A:143:LEU:CD1	6:A:1106:GOL:H32	2.26	0.63
1:B:245:ALA:HB2	1:B:280:GLY:HA3	1.81	0.62
1:B:250:PHE:O	1:B:254:VAL:HG23	1.99	0.62
1:B:89:ILE:HG23	1:B:105[A]:TRP:CZ3	2.34	0.62
1:C:257:MET:HE1	1:C:268:ILE:HG23	1.82	0.61
1:D:285:ILE:HD12	1:D:361:TYR:CZ	2.34	0.61
1:C:185[B]:ARG:NH2	1:C:186:ASP:OD1	2.34	0.61
1:A:241:ILE:HG23	1:A:277:MET:SD	2.42	0.60
1:B:301:LYS:HG3	5:B:1106:EDO:C2	2.17	0.60
1:C:164:TYR:HB3	1:D:185[B]:ARG:HD3	1.83	0.59
1:D:185[A]:ARG:NH2	7:D:1199:HOH:O	2.36	0.59
1:A:244:THR:O	1:A:248:SER:HB2	2.03	0.59
1:A:219[B]:ASN:HD22	1:A:219[B]:ASN:H	1.51	0.59
1:A:164:TYR:HB2	1:B:185[B]:ARG:HD3	1.83	0.59
1:C:89:ILE:HD12	1:C:112:ALA:HB2	1.84	0.58
1:B:101:ASN:O	1:B:105[B]:TRP:CE3	2.56	0.58
1:B:233[B]:PHE:HE1	1:B:313:TRP:CD1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:LYS:HE2	1:D:106:GLU:HG3	1.84	0.57
1:C:163:ILE:O	1:C:167:ILE:HG13	2.04	0.57
1:D:223:GLN:HE21	1:D:223:GLN:HA	1.70	0.56
1:C:185[A]:ARG:HH11	1:C:185[A]:ARG:CB	2.18	0.56
1:B:303:GLY:N	6:B:1105:GOL:H12	2.21	0.56
7:A:1170:HOH:O	1:B:129:MET:CE	2.53	0.55
1:D:320:GLU:HG2	1:D:321:LEU:HD13	1.87	0.55
1:A:96:LYS:HE2	1:A:96:LYS:HA	1.88	0.55
1:A:236:TYR:HB2	1:A:316:ILE:CD1	2.37	0.55
1:A:343:LYS:HE3	1:C:346:ASP:OD1	2.05	0.55
1:A:226:ILE:HD11	1:A:331:VAL:HG22	1.87	0.55
1:B:338:ASN:HD21	1:D:133:GLU:CD	2.10	0.55
2:B:397:ZOL:O16	5:B:1106:EDO:H11	2.07	0.55
1:C:285:ILE:HG12	1:C:313:TRP:CD1	2.42	0.54
1:D:41:TYR:HB2	1:D:113:TRP:CZ2	2.42	0.54
1:D:233[A]:PHE:CE2	1:D:237:LYS:HE2	2.43	0.54
1:B:342:VAL:HG23	1:D:339:LEU:HD13	1.88	0.54
1:D:152:ALA:O	1:D:156:VAL:HG23	2.08	0.54
1:C:127:ASP:OD2	1:C:135:ARG:HD2	2.08	0.53
1:A:150[B]:LYS:HG2	1:A:151:ASN:N	2.24	0.53
1:B:233[B]:PHE:CE1	1:B:313:TRP:CD1	2.96	0.53
1:A:245:ALA:HB2	1:A:280:GLY:HA3	1.91	0.53
1:D:69:TYR:CD1	1:D:158:LEU:HD22	2.44	0.53
1:D:149:THR:O	1:D:153:VAL:HG23	2.09	0.53
1:A:36:PHE:CZ	1:A:40[B]:MET:SD	3.01	0.53
1:C:40:MET:HE3	1:C:43:LYS:HG2	1.91	0.52
1:C:307[B]:GLN:H	1:C:307[B]:GLN:CD	2.13	0.52
1:C:395:GLY:O	1:C:396:VAL:CB	2.58	0.52
1:D:324[B]:GLU:HG3	1:D:325:PRO:HD3	1.90	0.52
1:D:140:CYS:HB2	1:D:143:LEU:HD22	1.92	0.52
1:A:119:GLN:NE2	1:A:123:LEU:HD21	2.25	0.51
1:B:233[B]:PHE:CE2	1:B:320:GLU:OE1	2.60	0.51
1:C:40:MET:CE	1:C:43:LYS:HG2	2.39	0.51
1:C:189[A]:LEU:HD13	1:D:161:ASN:HB3	1.91	0.51
1:A:236:TYR:CZ	1:A:240:VAL:HG11	2.46	0.51
1:A:327:LYS:O	1:A:331:VAL:HG23	2.11	0.51
1:B:303:GLY:HA2	5:B:1106:EDO:H21	1.91	0.51
1:B:249:PHE:O	1:B:253:ILE:HG13	2.10	0.51
1:C:370:LEU:HD13	1:C:389:LEU:HD23	1.93	0.51
1:D:240:VAL:CG1	1:D:281:GLU:HA	2.41	0.50
1:D:281:GLU:OE2	7:D:1267:HOH:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:TYR:HB3	1:B:185[B]:ARG:HD3	1.92	0.50
7:A:1170:HOH:O	1:B:129:MET:HE1	2.11	0.50
1:B:236:TYR:O	1:B:240:VAL:HB	2.12	0.50
1:C:236:TYR:CZ	1:C:240:VAL:HG11	2.47	0.50
1:C:46:ASP:O	1:C:50:SER:HB2	2.11	0.50
1:C:100:ILE:N	7:C:1209:HOH:O	2.45	0.50
1:C:370:LEU:HD13	1:C:389:LEU:CD2	2.41	0.50
1:A:125:ALA:O	1:A:129:MET:HG3	2.12	0.49
1:C:244:THR:O	1:C:248:SER:HB2	2.12	0.49
1:D:278:LEU:HB3	1:D:369:ILE:HG12	1.94	0.49
1:A:205:LYS:HG3	7:B:1225:HOH:O	2.13	0.49
1:B:303:GLY:H	6:B:1105:GOL:H12	1.76	0.49
1:C:36:PHE:O	1:C:40:MET:HG2	2.12	0.49
1:C:391:ILE:HD12	1:C:391:ILE:C	2.32	0.49
1:D:111:LEU:O	1:D:115:ILE:HG13	2.13	0.49
1:D:233[B]:PHE:CE2	1:D:320:GLU:OE2	2.57	0.49
1:A:205:LYS:HG2	1:A:213:ILE:HG13	1.95	0.49
1:B:91:ILE:HD12	1:B:384:VAL:HG11	1.94	0.49
1:B:91:ILE:O	1:B:95:VAL:HG23	2.13	0.49
1:D:245:ALA:HB2	1:D:280:GLY:HA3	1.94	0.49
1:D:235:VAL:O	1:D:238:ASN:HB2	2.13	0.49
1:B:395:GLY:O	1:B:396:VAL:HG22	2.13	0.48
1:D:236:TYR:HB2	1:D:316:ILE:CD1	2.43	0.48
1:D:240:VAL:HG22	1:D:284:GLN:CG	2.37	0.48
6:A:1106:GOL:H31	1:B:218:ILE:HD13	1.95	0.48
1:B:373:ILE:O	1:B:376:LEU:HB2	2.13	0.48
1:D:142:TYR:CZ	1:D:143:LEU:HD13	2.48	0.48
1:B:339:LEU:O	1:B:343:LYS:HB2	2.12	0.48
1:B:303:GLY:H	6:B:1105:GOL:H31	1.77	0.48
1:C:41:TYR:HB2	1:C:113:TRP:CZ2	2.48	0.48
1:C:131:LYS:NZ	7:C:1140:HOH:O	2.37	0.48
1:C:135:ARG:NH2	2:C:397:ZOL:O15	2.30	0.47
1:A:119:GLN:NE2	1:A:123:LEU:CD2	2.77	0.47
1:A:89:ILE:HD11	1:A:109:ALA:HA	1.95	0.47
1:A:195:GLN:NE2	7:A:1161:HOH:O	2.42	0.47
1:A:41:TYR:HB2	1:A:113:TRP:CZ2	2.49	0.47
1:B:41:TYR:HB2	1:B:113:TRP:CZ2	2.50	0.47
1:A:72:LEU:O	1:A:76:ASN:HB2	2.14	0.47
1:B:240:VAL:HG22	1:B:284:GLN:CG	2.35	0.47
1:C:165:LYS:NZ	1:D:185[A]:ARG:HH11	2.11	0.47
1:A:133:GLU:CD	1:C:338:ASN:HD21	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1170:HOH:O	1:B:129:MET:HE3	2.15	0.47
1:D:69:TYR:CE1	1:D:158:LEU:HD22	2.49	0.47
6:A:1106:GOL:H31	1:B:218:ILE:CD1	2.43	0.47
1:C:185[A]:ARG:HD2	1:D:161:ASN:OD1	2.14	0.46
1:D:115:ILE:HD13	1:D:251:LEU:HG	1.96	0.46
1:B:163:ILE:O	1:B:167:ILE:HG13	2.15	0.46
1:B:137:ASN:ND2	7:B:1173:HOH:O	2.28	0.46
1:A:185[A]:ARG:HG2	1:B:161:ASN:OD1	2.16	0.46
1:C:89:ILE:HD11	1:C:109:ALA:HA	1.97	0.46
1:C:338:ASN:O	1:C:342:VAL:HG13	2.16	0.46
1:D:205:LYS:HG3	1:D:206:TYR:CD2	2.51	0.46
1:A:244:THR:OG1	1:A:284:GLN:OE1	2.24	0.46
1:B:236:TYR:CZ	1:B:240:VAL:HG21	2.51	0.46
1:B:312:THR:HB	1:B:314:PRO:HD2	1.97	0.46
1:C:73:PHE:O	1:C:77:CYS:HB2	2.16	0.46
1:A:199:THR:HG22	1:A:200:ASN:ND2	2.31	0.45
1:D:83:ASN:HB2	7:D:1218:HOH:O	2.15	0.45
1:C:127:ASP:OD2	1:C:135:ARG:CD	2.65	0.45
1:A:98:ARG:O	1:A:100:ILE:N	2.50	0.45
1:D:61:ILE:O	1:D:65:ILE:HG12	2.17	0.45
1:B:205:LYS:HG3	1:B:206:TYR:CD2	2.51	0.45
1:B:339:LEU:HD21	1:D:342:VAL:HG11	1.99	0.45
1:D:226:ILE:HD11	1:D:331:VAL:HG22	1.99	0.45
1:C:40:MET:O	1:C:43:LYS:HB3	2.16	0.45
1:D:312:THR:HB	1:D:314:PRO:HD2	1.98	0.45
1:D:190:LYS:O	1:D:242:HIS:HB3	2.17	0.44
1:D:204:ASP:OD2	1:D:222:GLU:HG2	2.17	0.44
1:D:131:LYS:NZ	7:D:1156:HOH:O	2.48	0.44
1:C:282:TYR:OH	1:C:362:GLU:OE2	2.26	0.44
1:B:81:LYS:HE3	7:B:1262:HOH:O	2.16	0.44
1:B:89:ILE:HD11	1:B:109:ALA:HA	1.99	0.44
1:C:292:ILE:HG23	1:C:293:PHE:CE2	2.52	0.44
1:C:306:ILE:HB	1:C:307[B]:GLN:NE2	2.33	0.44
1:D:142:TYR:CE1	1:D:143:LEU:HD13	2.53	0.44
1:B:387:TYR:O	1:B:391:ILE:HG13	2.18	0.43
1:D:222:GLU:O	1:D:224:PRO:HD3	2.18	0.43
1:D:241:ILE:HD11	7:D:1267:HOH:O	2.18	0.43
1:B:152:ALA:O	1:B:156:VAL:HG23	2.18	0.43
1:B:296:SER:CB	6:B:1105:GOL:H32	2.40	0.43
1:C:185[B]:ARG:HH21	1:C:186:ASP:CG	2.21	0.43
1:C:135:ARG:HB3	7:C:1114:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:GLU:N	1:C:325:PRO:HD2	2.33	0.43
1:D:236:TYR:CZ	1:D:240:VAL:HG21	2.53	0.43
1:B:369:ILE:O	1:B:373:ILE:HG13	2.18	0.43
1:C:115:ILE:HD13	1:C:251:LEU:HG	2.00	0.43
1:C:228:ILE:HA	1:C:231:ILE:HD12	2.01	0.43
1:D:101:ASN:OD1	1:D:101:ASN:C	2.57	0.43
1:A:168:GLU:O	1:A:172:ARG:HG2	2.19	0.43
3:C:1101:IPE:H41	3:C:1101:IPE:H11	1.71	0.43
1:D:190:LYS:HD3	1:D:246:TYR:CE1	2.54	0.43
1:D:233[A]:PHE:CD2	1:D:237:LYS:HE3	2.54	0.43
1:C:220:VAL:O	1:D:145:LYS:HG3	2.19	0.43
1:C:250:PHE:O	1:C:254:VAL:HG23	2.18	0.43
1:D:191:THR:HA	1:D:242:HIS:O	2.19	0.43
1:B:91:ILE:HG22	1:B:256:GLY:HA3	2.01	0.42
1:B:72:LEU:HD11	1:B:155:ASP:HB3	2.02	0.42
1:D:168:GLU:O	1:D:172:ARG:HG2	2.20	0.42
1:B:326:ASP:O	1:B:330:ILE:HG13	2.20	0.42
1:A:84:ARG:HB3	1:A:115:ILE:HG21	2.01	0.42
1:B:36:PHE:HZ	1:B:105[A]:TRP:HB3	1.85	0.42
1:D:119:GLN:NE2	1:D:123:LEU:HD11	2.35	0.42
1:D:233[A]:PHE:CE2	1:D:237:LYS:CE	3.03	0.42
1:D:133:GLU:OE2	7:D:1268:HOH:O	2.21	0.41
1:C:270:LYS:HD2	1:C:270:LYS:HA	1.82	0.41
1:D:322:CYS:HA	1:D:352:TYR:CE1	2.55	0.41
1:D:391:ILE:O	1:D:395:GLY:N	2.47	0.41
1:A:164:TYR:HH	1:A:185[A]:ARG:HG3	1.84	0.41
1:A:193:ILE:HG13	1:B:55:TYR:CE2	2.55	0.41
1:A:395:GLY:O	1:A:396:VAL:CB	2.67	0.41
1:D:291:ASP:OD2	1:D:303:GLY:HA2	2.21	0.41
1:A:286:HIS:O	1:A:289:TYR:HB3	2.21	0.41
1:C:69:TYR:O	1:C:73:PHE:HD2	2.04	0.41
1:B:273:GLU:O	1:B:277:MET:HG2	2.21	0.41
1:B:235:VAL:O	1:B:238:ASN:HB2	2.20	0.41
1:D:67:LYS:HB2	1:D:67:LYS:HE3	1.64	0.41
1:D:188:THR:HG22	1:D:192:ILE:HD11	2.01	0.41
1:A:185[A]:ARG:HD2	1:B:164:TYR:HB2	2.02	0.41
1:A:204:ASP:OD2	1:A:222:GLU:HG3	2.21	0.41
1:B:137:ASN:ND2	1:B:300:GLY:HA2	2.35	0.41
1:C:43:LYS:NZ	1:C:106:GLU:OE2	2.47	0.41
1:D:145:LYS:HA	1:D:145:LYS:HD2	1.80	0.41
1:A:119:GLN:CD	1:A:123:LEU:HD22	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:HIS:CE1	1:D:57:LEU:HD13	2.56	0.40
1:D:285:ILE:HD12	1:D:361:TYR:OH	2.21	0.40
1:D:308:ASN:HB3	1:D:310:LYS:HE2	2.03	0.40
1:C:322:CYS:HA	1:C:352:TYR:CE2	2.56	0.40
1:C:100:ILE:HA	1:C:104:GLU:OE1	2.21	0.40
1:B:36:PHE:CZ	1:B:105[A]:TRP:HB3	2.57	0.40
1:C:122:PHE:HZ	1:C:188:THR:HG23	1.86	0.40
1:C:313:TRP:HB3	1:C:314:PRO:HD3	2.04	0.40
1:D:236:TYR:HB2	1:D:316:ILE:HD11	2.02	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	356/396 (90%)	349 (98%)	7 (2%)	0	100	100
1	B	348/396 (88%)	338 (97%)	10 (3%)	0	100	100
1	C	357/396 (90%)	347 (97%)	10 (3%)	0	100	100
1	D	345/396 (87%)	333 (96%)	12 (4%)	0	100	100
All	All	1406/1584 (89%)	1367 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	314/357 (88%)	301 (96%)	13 (4%)	30	43
1	B	312/357 (87%)	296 (95%)	16 (5%)	24	33
1	C	316/357 (88%)	297 (94%)	19 (6%)	19	26
1	D	309/357 (87%)	295 (96%)	14 (4%)	27	39
All	All	1251/1428 (88%)	1189 (95%)	62 (5%)	25	34

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	103	SER
1	A	111	LEU
1	A	115	ILE
1	A	123	LEU
1	A	134	MET
1	A	144	LEU
1	A	158	LEU
1	A	319	PHE
1	A	339	LEU
1	A	360	SER
1	A	363	LYS
1	A	370	LEU
1	B	36	PHE
1	B	50	SER
1	B	91	ILE
1	B	103	SER
1	B	111	LEU
1	B	138	LYS
1	B	165	LYS
1	B	189	LEU
1	B	193	ILE
1	B	198	ASP
1	B	241	ILE
1	B	278	LEU
1	B	319	PHE
1	B	356	LYS
1	B	371	SER
1	B	376	LEU
1	C	49	LEU
1	C	65	ILE
1	C	89	ILE
1	C	96	LYS

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Mol	Chain	Res	Type
1	C	111	LEU
1	C	158	LEU
1	C	175	SER
1	C	181	ILE
1	C	185[A]	ARG
1	C	185[B]	ARG
1	C	189[A]	LEU
1	C	189[B]	LEU
1	C	268	ILE
1	C	271	LYS
1	C	319	PHE
1	C	339	LEU
1	C	347	SER
1	C	359	GLU
1	C	370	LEU
1	D	49	LEU
1	D	57	LEU
1	D	143	LEU
1	D	144	LEU
1	D	147	VAL
1	D	211	ARG
1	D	213	ILE
1	D	223	GLN
1	D	240	VAL
1	D	278	LEU
1	D	296	SER
1	D	319	PHE
1	D	321	LEU
1	D	379	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	337	ASN
1	B	338	ASN
1	B	351	GLN
1	C	82	ASN
1	C	97	ASN
1	D	82	ASN
1	D	223	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
2	ZOL	C	397	4	14,16,16	2.65	8 (57%)	20,26,26	1.95	8 (40%)
6	GOL	B	1105	-	5,5,5	0.44	0	5,5,5	0.81	0
3	IPE	D	1101	-	11,13,13	2.17	2 (18%)	15,19,19	1.17	2 (13%)
2	ZOL	B	397	4	14,16,16	3.16	7 (50%)	20,26,26	2.13	8 (40%)
3	IPE	A	1101	-	11,13,13	2.30	2 (18%)	15,19,19	1.08	0
2	ZOL	D	397	4	14,16,16	3.02	8 (57%)	20,26,26	1.99	5 (25%)
5	EDO	B	1106	-	3,3,3	0.94	0	2,2,2	0.68	0
6	GOL	A	1106	-	5,5,5	0.41	0	5,5,5	0.42	0
2	ZOL	A	397	4	14,16,16	3.34	10 (71%)	20,26,26	1.69	4 (20%)
6	GOL	D	1105	-	5,5,5	0.45	0	5,5,5	0.37	0
3	IPE	B	1101	-	11,13,13	2.15	2 (18%)	15,19,19	1.38	4 (26%)
5	EDO	A	1105	-	3,3,3	0.58	0	2,2,2	0.14	0
3	IPE	C	1101	-	11,13,13	2.26	2 (18%)	15,19,19	1.85	4 (26%)

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
2	ZOL	C	397	4	-	2/23/23/23	0/1/1/1
6	GOL	B	1105	-	-	4/4/4/4	-
3	IPE	D	1101	-	-	3/13/13/13	-
2	ZOL	B	397	4	-	2/23/23/23	0/1/1/1
3	IPE	A	1101	-	-	2/13/13/13	-
2	ZOL	D	397	4	-	3/23/23/23	0/1/1/1
5	EDO	B	1106	-	-	1/1/1/1	-
6	GOL	A	1106	-	-	2/4/4/4	-
2	ZOL	A	397	4	-	2/23/23/23	0/1/1/1
6	GOL	D	1105	-	-	2/4/4/4	-
3	IPE	B	1101	-	-	0/13/13/13	-
5	EDO	A	1105	-	-	0/1/1/1	-
3	IPE	C	1101	-	-	4/13/13/13	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	397	ZOL	P9-O12	7.22	1.61	1.50
2	A	397	ZOL	P9-O12	6.33	1.60	1.50
3	A	1101	IPE	C4-C3	6.32	1.51	1.33
3	C	1101	IPE	C4-C3	6.07	1.50	1.33
2	D	397	ZOL	P14-O15	5.82	1.59	1.50
3	D	1101	IPE	C4-C3	5.80	1.49	1.33
3	B	1101	IPE	C4-C3	5.56	1.48	1.33
2	C	397	ZOL	P9-O12	5.37	1.58	1.50
2	D	397	ZOL	P9-O12	5.07	1.58	1.50
2	B	397	ZOL	P14-O15	4.68	1.57	1.50
2	D	397	ZOL	P9-O11	4.35	1.62	1.54
2	B	397	ZOL	P14-O16	4.23	1.62	1.54
2	A	397	ZOL	P9-O10	-4.18	1.47	1.54
2	C	397	ZOL	P14-O17	-4.18	1.47	1.54
2	A	397	ZOL	P14-O16	4.16	1.62	1.54
2	A	397	ZOL	P9-O11	4.08	1.62	1.54
2	A	397	ZOL	P14-O17	-4.06	1.47	1.54
2	A	397	ZOL	P14-O15	4.06	1.56	1.50
3	B	1101	IPE	C5-C3	-4.04	1.32	1.48
2	C	397	ZOL	P14-C8	3.95	1.88	1.85
3	D	1101	IPE	C5-C3	-3.85	1.33	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	397	ZOL	P14-O16	3.82	1.61	1.54
3	C	1101	IPE	C5-C3	-3.74	1.33	1.48
3	A	1101	IPE	C5-C3	-3.74	1.33	1.48
2	B	397	ZOL	O13-C8	-3.72	1.40	1.44
2	D	397	ZOL	P14-O17	-3.49	1.48	1.54
2	A	397	ZOL	O13-C8	-3.27	1.40	1.44
2	B	397	ZOL	P14-C8	-3.19	1.82	1.85
2	B	397	ZOL	P9-O10	-3.05	1.49	1.54
2	A	397	ZOL	P14-C8	2.99	1.87	1.85
2	C	397	ZOL	P14-O15	2.99	1.55	1.50
2	B	397	ZOL	P14-O17	-2.87	1.49	1.54
2	D	397	ZOL	P9-C8	2.84	1.87	1.85
2	C	397	ZOL	O13-C8	-2.67	1.41	1.44
2	C	397	ZOL	P9-O10	-2.57	1.50	1.54
2	A	397	ZOL	P9-C8	-2.35	1.83	1.85
2	C	397	ZOL	P14-O16	2.30	1.59	1.54
2	A	397	ZOL	C19-N15	-2.25	1.33	1.37
2	C	397	ZOL	C19-N15	-2.21	1.33	1.37
2	D	397	ZOL	P14-C8	2.19	1.86	1.85
2	D	397	ZOL	P9-O10	-2.15	1.50	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	397	ZOL	O16-P14-O15	-4.78	102.32	113.06
2	B	397	ZOL	O10-P9-C8	4.29	115.78	106.17
2	D	397	ZOL	O11-P9-O12	-4.02	104.03	113.06
2	A	397	ZOL	O17-P14-C8	3.88	114.86	106.17
2	B	397	ZOL	O17-P14-C8	3.62	114.30	106.17
2	C	397	ZOL	P9-C8-P14	-3.61	106.35	112.81
2	B	397	ZOL	P9-C8-P14	-3.56	106.43	112.81
3	C	1101	IPE	PA-O1-C1	3.45	138.55	121.59
3	C	1101	IPE	O2A-PA-O1	3.40	123.53	107.75
2	A	397	ZOL	O10-P9-C8	3.14	113.20	106.17
2	C	397	ZOL	O10-P9-C8	2.96	112.80	106.17
3	C	1101	IPE	O1-PA-O1A	-2.94	97.59	109.07
2	D	397	ZOL	O16-P14-O17	2.90	116.17	107.99
2	C	397	ZOL	O17-P14-C8	2.86	112.58	106.17
2	B	397	ZOL	O12-P9-C8	-2.84	102.44	109.86
2	A	397	ZOL	O17-P14-O15	2.82	119.39	113.06
2	C	397	ZOL	O11-P9-O12	-2.67	107.07	113.06
2	B	397	ZOL	C19-N15-C16	2.60	110.77	108.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1101	IPE	C5-C3-C2	2.58	123.33	115.24
2	C	397	ZOL	O10-P9-O12	-2.57	107.29	113.06
2	C	397	ZOL	O16-P14-C8	-2.45	100.66	106.17
2	B	397	ZOL	O16-P14-O17	2.45	114.92	107.99
3	C	1101	IPE	O3B-PB-O1B	2.43	116.94	107.64
2	D	397	ZOL	O11-P9-O10	2.38	114.70	107.99
2	A	397	ZOL	O15-P14-C8	-2.34	103.74	109.86
3	B	1101	IPE	O3B-PB-O2B	2.32	119.76	110.68
2	C	397	ZOL	O11-P9-O10	2.22	114.26	107.99
2	D	397	ZOL	P9-C8-P14	-2.21	108.86	112.81
2	C	397	ZOL	C19-N15-C16	2.21	110.38	108.21
2	B	397	ZOL	O16-P14-C8	-2.19	101.26	106.17
3	D	1101	IPE	O2A-PA-O1A	2.18	123.04	112.24
3	B	1101	IPE	O2A-PA-O1A	2.13	122.75	112.24
3	D	1101	IPE	O3B-PB-O1B	2.09	115.64	107.64
2	B	397	ZOL	O15-P14-C8	-2.05	104.50	109.86
3	B	1101	IPE	C5-C3-C4	-2.02	117.53	121.98

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	397	ZOL	C8-C7-N15-C16
2	A	397	ZOL	C8-C7-N15-C19
2	B	397	ZOL	C8-C7-N15-C16
2	B	397	ZOL	C8-C7-N15-C19
2	C	397	ZOL	C8-C7-N15-C16
2	C	397	ZOL	C8-C7-N15-C19
2	D	397	ZOL	C8-C7-N15-C16
2	D	397	ZOL	C8-C7-N15-C19
3	A	1101	IPE	PA-O3A-PB-O1B
3	C	1101	IPE	O1-C1-C2-C3
3	D	1101	IPE	O1-C1-C2-C3
3	D	1101	IPE	PA-O3A-PB-O1B
6	B	1105	GOL	C1-C2-C3-O3
6	D	1105	GOL	C1-C2-C3-O3
6	A	1106	GOL	O1-C1-C2-O2
6	A	1106	GOL	O1-C1-C2-C3
6	B	1105	GOL	O1-C1-C2-C3
6	B	1105	GOL	O2-C2-C3-O3
6	D	1105	GOL	O2-C2-C3-O3
5	B	1106	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	B	1105	GOL	O1-C1-C2-O2
3	C	1101	IPE	PA-O3A-PB-O2B
3	D	1101	IPE	C1-C2-C3-C5
3	C	1101	IPE	C1-O1-PA-O3A
3	A	1101	IPE	C1-C2-C3-C5
3	C	1101	IPE	C1-C2-C3-C5
2	D	397	ZOL	C7-C8-P14-O15

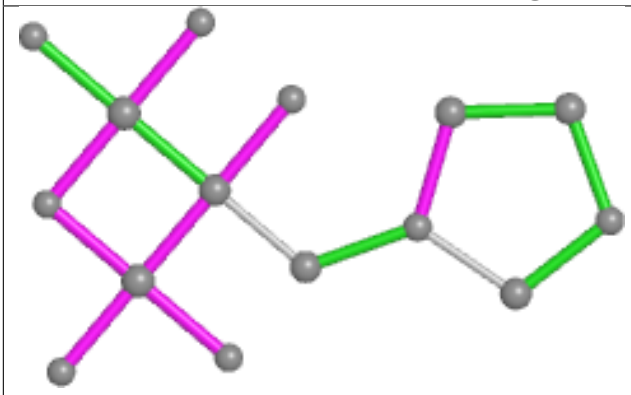
There are no ring outliers.

7 monomers are involved in 17 short contacts:

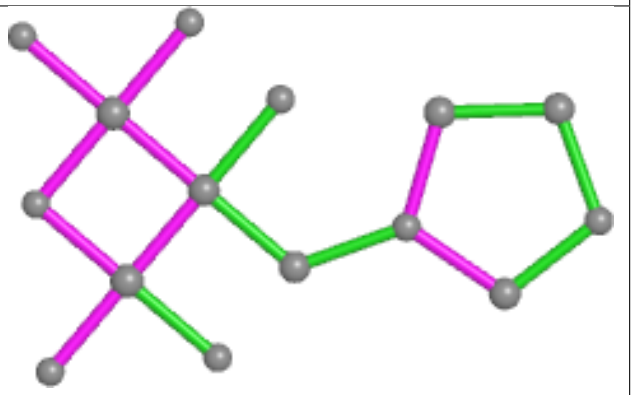
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	397	ZOL	1	0
6	B	1105	GOL	6	0
2	B	397	ZOL	1	0
5	B	1106	EDO	4	0
6	A	1106	GOL	4	0
6	D	1105	GOL	1	0
3	C	1101	IPE	1	0

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 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.

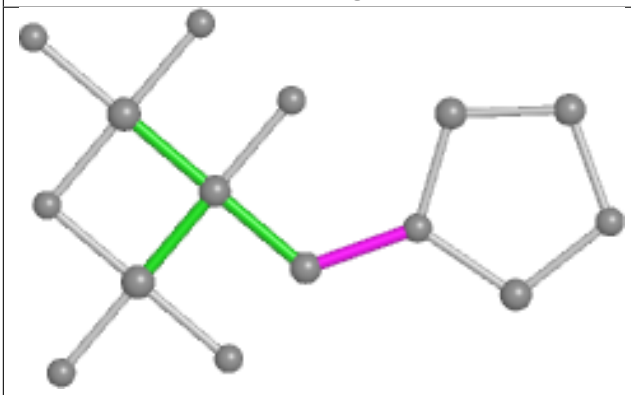
Ligand ZOL C 397



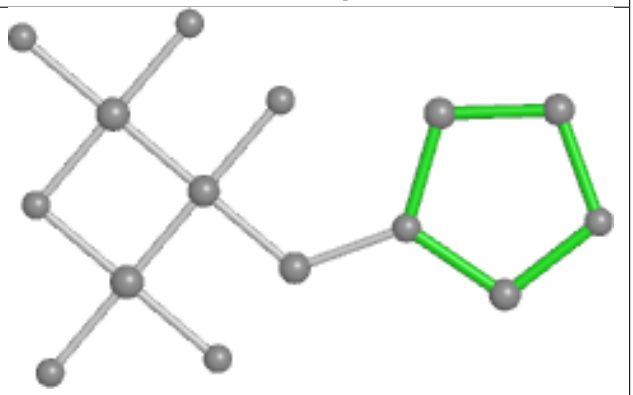
Bond lengths



Bond angles

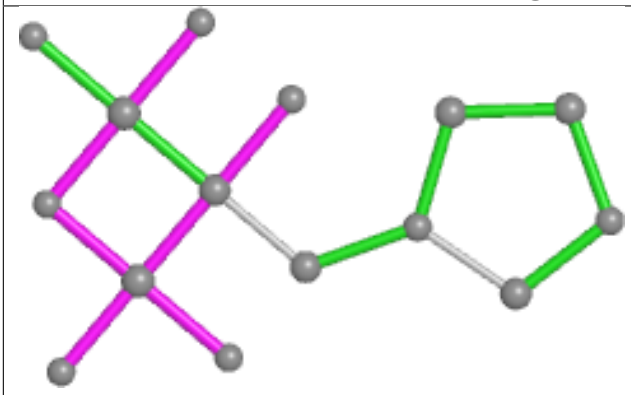


Torsions

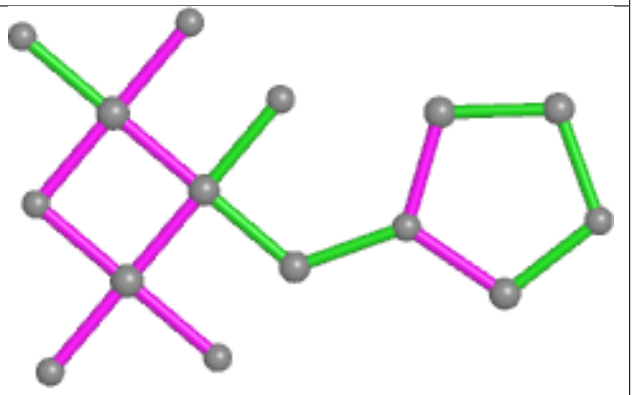


Rings

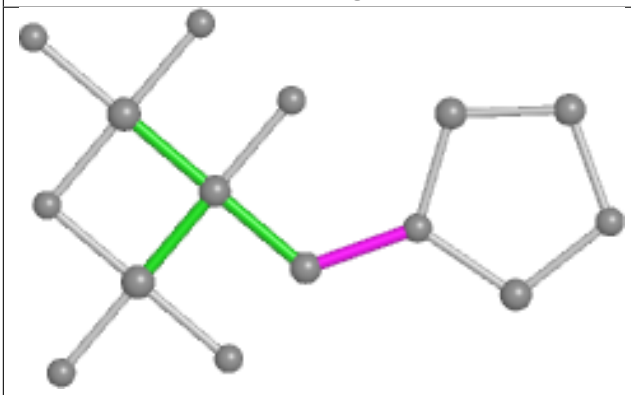
Ligand ZOL B 397



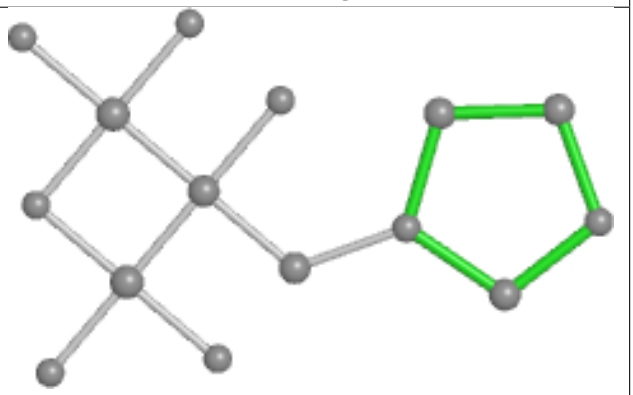
Bond lengths



Bond angles

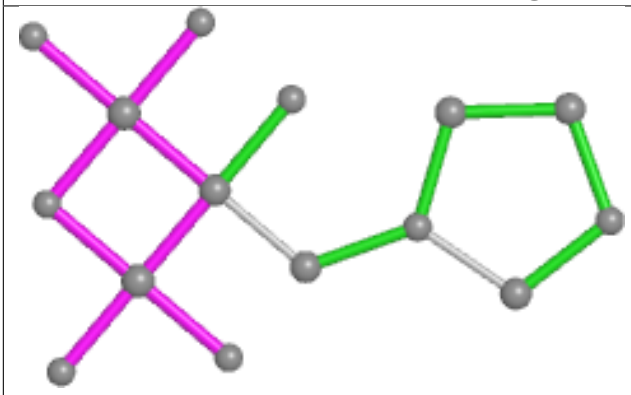


Torsions

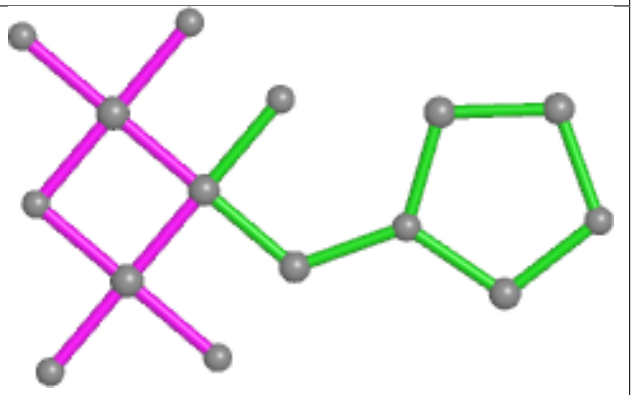


Rings

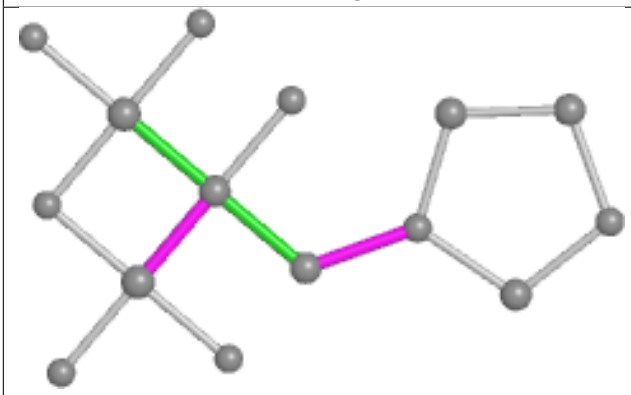
Ligand ZOL D 397



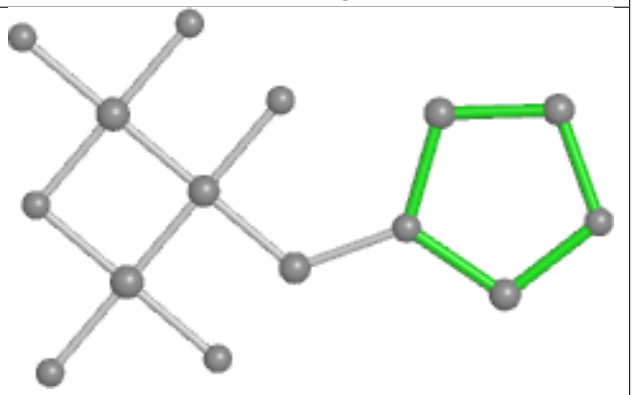
Bond lengths



Bond angles

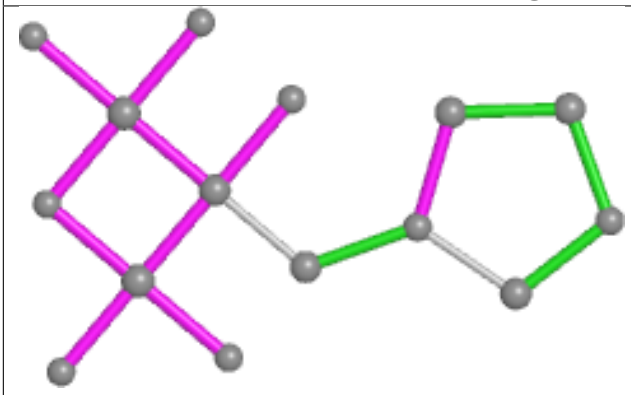


Torsions

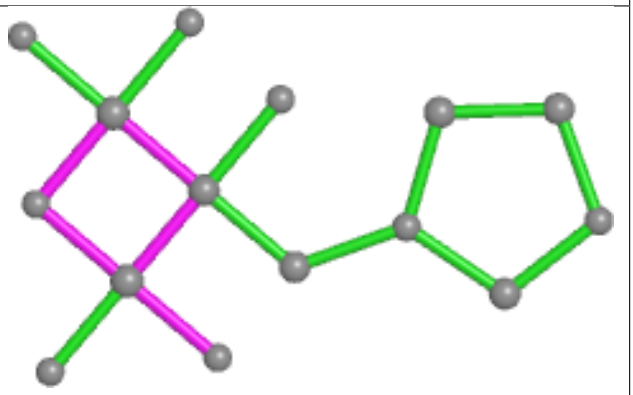


Rings

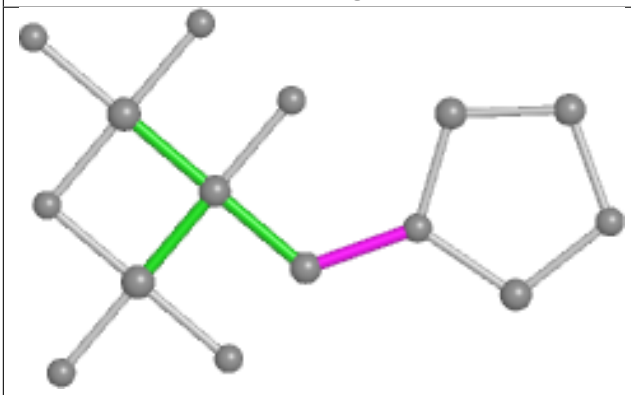
Ligand ZOL A 397



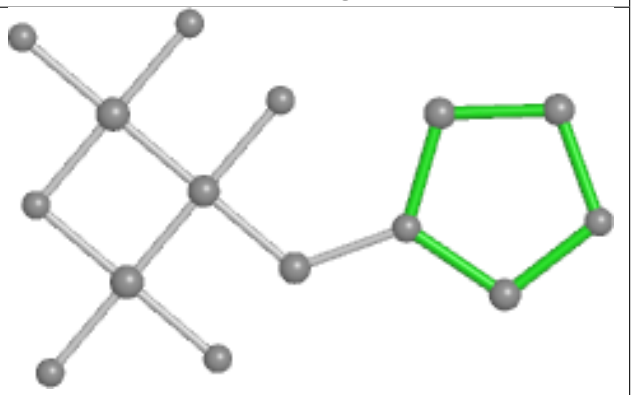
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	358/396 (90%)	0.64	34 (9%) 8 11	16, 24, 32, 49	18 (5%)
1	B	353/396 (89%)	0.63	28 (7%) 12 17	18, 24, 31, 48	15 (4%)
1	C	357/396 (90%)	0.67	34 (9%) 8 11	17, 24, 32, 46	12 (3%)
1	D	351/396 (88%)	0.65	38 (10%) 5 8	17, 24, 32, 52	7 (1%)
All	All	1419/1584 (89%)	0.65	134 (9%) 8 11	16, 24, 32, 52	52 (3%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	ALA	7.5
1	B	36	PHE	6.9
1	C	207	SER	6.3
1	B	396	VAL	5.6
1	A	207	SER	5.6
1	B	377	HIS	5.5
1	B	105[A]	TRP	5.5
1	C	35	ALA	5.5
1	C	111	LEU	4.9
1	D	223	GLN	4.6
1	A	98	ARG	4.4
1	C	354	ILE	4.4
1	D	37	PHE	4.4
1	A	311	LEU	4.3
1	D	297	THR	4.3
1	A	312	THR	4.3
1	A	111	LEU	4.2
1	D	88	VAL	4.2
1	B	253	ILE	4.1
1	D	101	ASN	4.0
1	A	315	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	87	LEU	4.0
1	B	88	VAL	4.0
1	C	352	TYR	3.9
1	A	101	ASN	3.9
1	B	101	ASN	3.8
1	C	355	ARG	3.6
1	D	374	ASN	3.6
1	C	312	THR	3.5
1	C	206	TYR	3.5
1	D	233[A]	PHE	3.4
1	D	266	ASN	3.4
1	B	210	HIS	3.4
1	C	36	PHE	3.4
1	A	34	LEU	3.4
1	D	315	LEU	3.4
1	D	102	SER	3.3
1	D	337	ASN	3.3
1	C	97	ASN	3.3
1	D	312	THR	3.2
1	D	267	LEU	3.2
1	C	359	GLU	3.1
1	D	261	GLY	3.1
1	D	311	LEU	3.1
1	A	72	LEU	3.1
1	C	229	ASN	3.0
1	A	355	ARG	3.0
1	A	206	TYR	3.0
1	C	102	SER	3.0
1	B	328	ILE	2.9
1	B	297	THR	2.8
1	D	72	LEU	2.8
1	D	87	LEU	2.8
1	D	253	ILE	2.8
1	A	36	PHE	2.8
1	D	117	ILE	2.8
1	A	97	ASN	2.8
1	D	105	TRP	2.8
1	C	37	PHE	2.7
1	B	103	SER	2.7
1	C	253	ILE	2.7
1	B	96	LYS	2.7
1	B	233[A]	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	337	ASN	2.7
1	B	91	ILE	2.7
1	A	360	SER	2.6
1	C	314	PRO	2.6
1	B	383	TYR	2.6
1	D	207	SER	2.6
1	A	265	ASP	2.6
1	B	385	LEU	2.6
1	B	111	LEU	2.6
1	C	396	VAL	2.6
1	C	306	ILE	2.6
1	C	267	LEU	2.6
1	D	212	GLU	2.6
1	B	207	SER	2.5
1	A	263	ALA	2.5
1	A	100	ILE	2.5
1	C	101	ASN	2.5
1	A	325	PRO	2.5
1	D	314	PRO	2.5
1	D	379	GLU	2.5
1	B	39	ASN	2.5
1	A	377	HIS	2.5
1	D	363	LYS	2.5
1	D	211	ARG	2.4
1	C	265	ASP	2.4
1	D	239	ILE	2.4
1	A	68	TYR	2.4
1	D	94	TYR	2.4
1	B	239	ILE	2.3
1	B	354	ILE	2.3
1	D	96	LYS	2.3
1	B	252	PRO	2.3
1	D	252	PRO	2.3
1	D	355	ARG	2.3
1	A	297	THR	2.3
1	B	249	PHE	2.3
1	B	379	GLU	2.3
1	C	375	GLU	2.3
1	A	110	CYS	2.3
1	A	363	LYS	2.2
1	A	295	ASP	2.2
1	C	360	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	228	ILE	2.2
1	C	228	ILE	2.2
1	D	210	HIS	2.2
1	C	311	LEU	2.2
1	C	173	ASN	2.2
1	D	345	ILE	2.2
1	D	255	CYS	2.2
1	A	229	ASN	2.1
1	C	297	THR	2.1
1	C	96	LYS	2.1
1	C	363	LYS	2.1
1	D	364	ALA	2.1
1	A	102	SER	2.1
1	C	39	ASN	2.1
1	D	111	LEU	2.1
1	C	322	CYS	2.1
1	A	167	ILE	2.1
1	B	376	LEU	2.1
1	B	229	ASN	2.1
1	C	264	VAL	2.1
1	A	314	PRO	2.1
1	D	229	ASN	2.1
1	B	296	SER	2.1
1	A	197	LEU	2.0
1	A	285	ILE	2.0
1	C	324	GLU	2.0
1	D	68	TYR	2.0
1	A	262	ILE	2.0
1	A	264	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

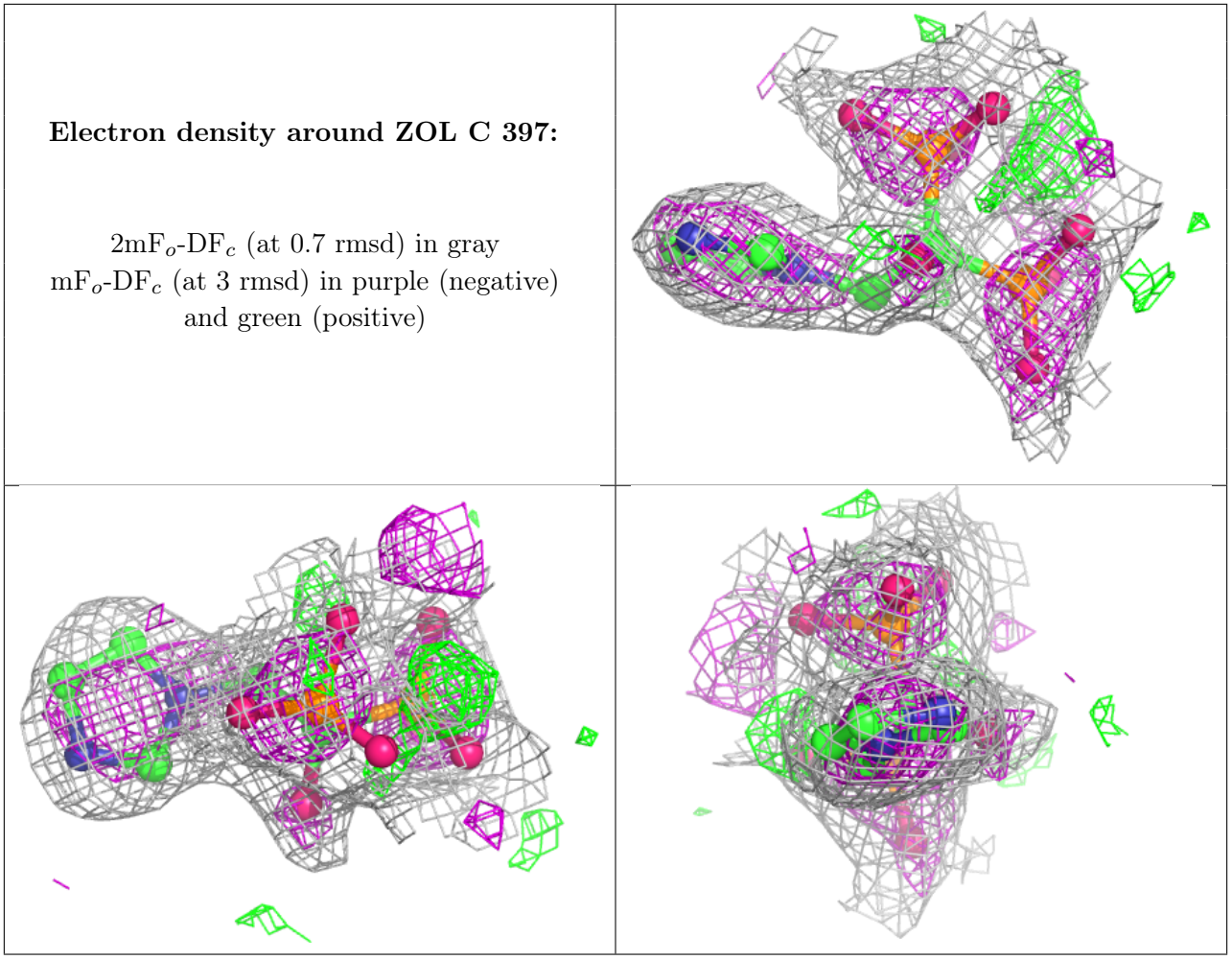
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	GOL	A	1106	6/6	0.63	0.46	50,52,53,53	0
5	EDO	B	1106	4/4	0.72	0.51	25,25,25,26	0
5	EDO	A	1105	4/4	0.75	0.32	47,50,51,51	0
6	GOL	D	1105	6/6	0.80	0.49	36,41,42,43	0
6	GOL	B	1105	6/6	0.83	0.39	32,36,37,38	0
4	MG	A	1103	1/1	0.90	0.05	18,18,18,18	0
4	MG	C	1104	1/1	0.94	0.05	16,16,16,16	0
3	IPE	C	1101	14/14	0.95	0.15	2,15,19,20	3
4	MG	B	1102	1/1	0.95	0.06	12,12,12,12	0
4	MG	C	1102	1/1	0.95	0.11	10,10,10,10	0
4	MG	A	1102	1/1	0.96	0.13	9,9,9,9	0
4	MG	B	1103	1/1	0.96	0.03	10,10,10,10	0
2	ZOL	C	397	16/16	0.96	0.11	10,13,18,19	0
4	MG	A	1104	1/1	0.96	0.05	12,12,12,12	0
4	MG	D	1104	1/1	0.96	0.08	8,8,8,8	0
2	ZOL	B	397	16/16	0.97	0.12	11,14,17,19	0
2	ZOL	A	397	16/16	0.97	0.10	11,15,19,20	0
4	MG	D	1102	1/1	0.97	0.05	9,9,9,9	0
4	MG	D	1103	1/1	0.97	0.03	12,12,12,12	0
4	MG	B	1104	1/1	0.97	0.06	6,6,6,6	0
2	ZOL	D	397	16/16	0.98	0.10	7,12,17,17	0
3	IPE	A	1101	14/14	0.98	0.11	14,16,18,19	0
4	MG	C	1103	1/1	0.98	0.06	17,17,17,17	0
3	IPE	B	1101	14/14	0.98	0.11	12,14,16,17	0
3	IPE	D	1101	14/14	0.99	0.09	9,16,20,21	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.

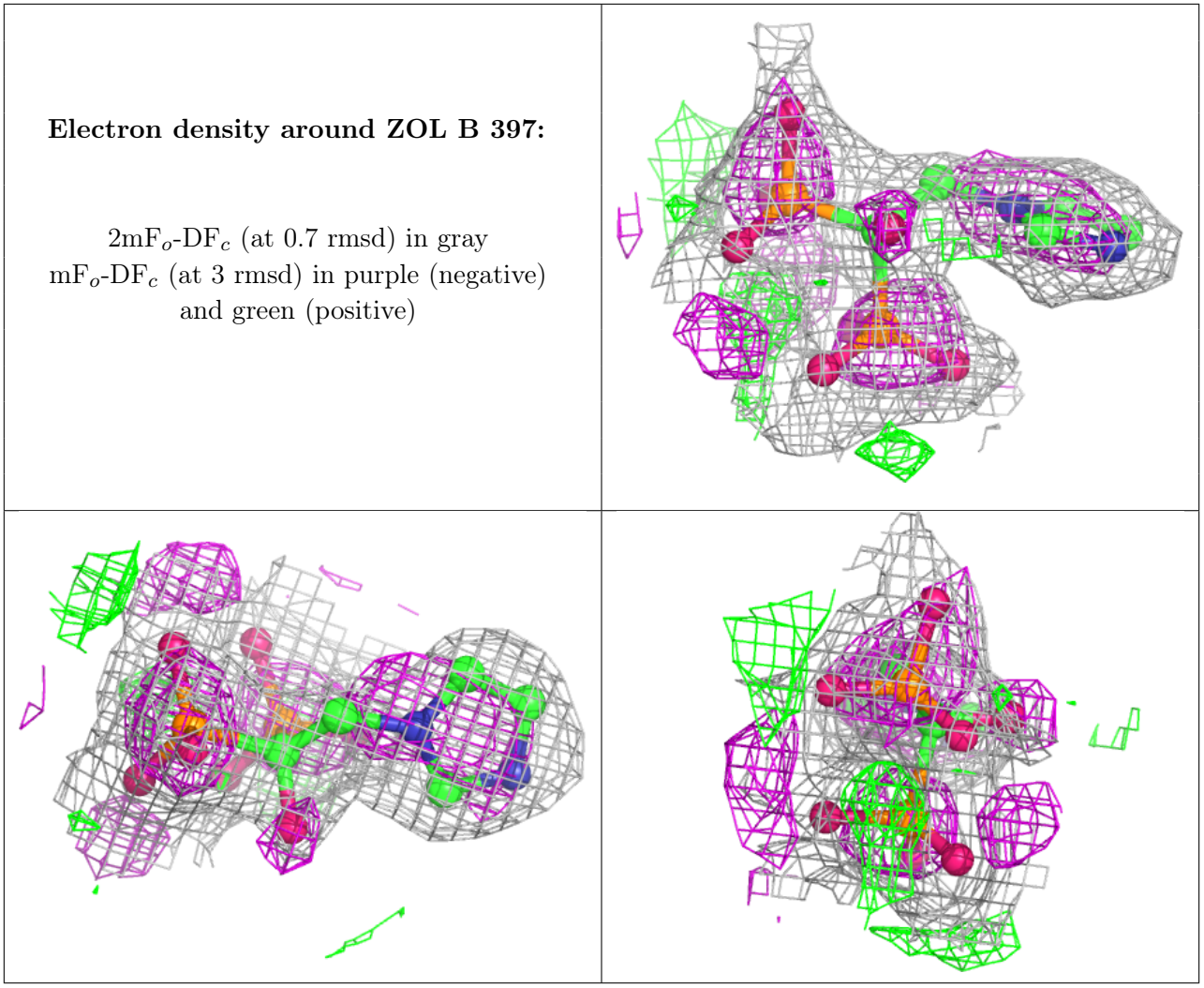
Electron density around ZOL C 397:

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



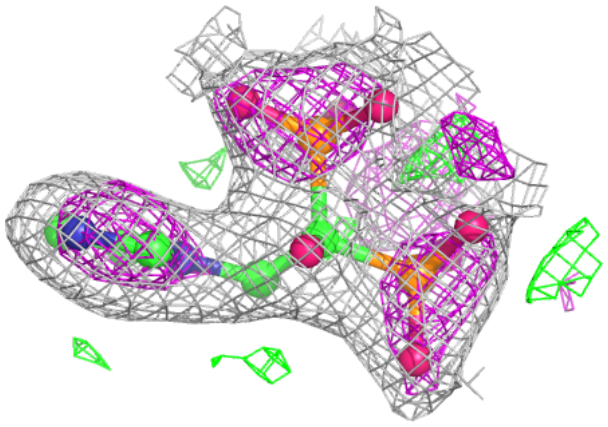
Electron density around ZOL B 397:

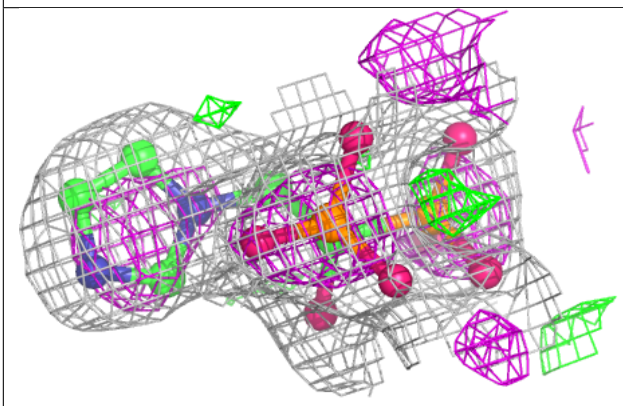
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

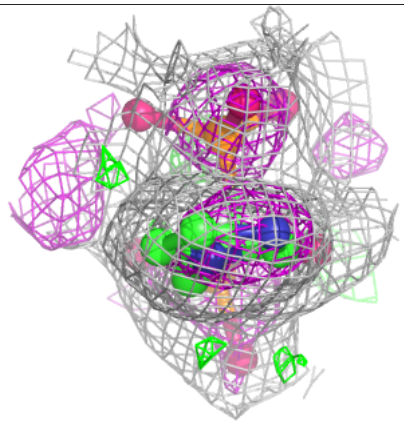


Electron density around ZOL A 397:

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

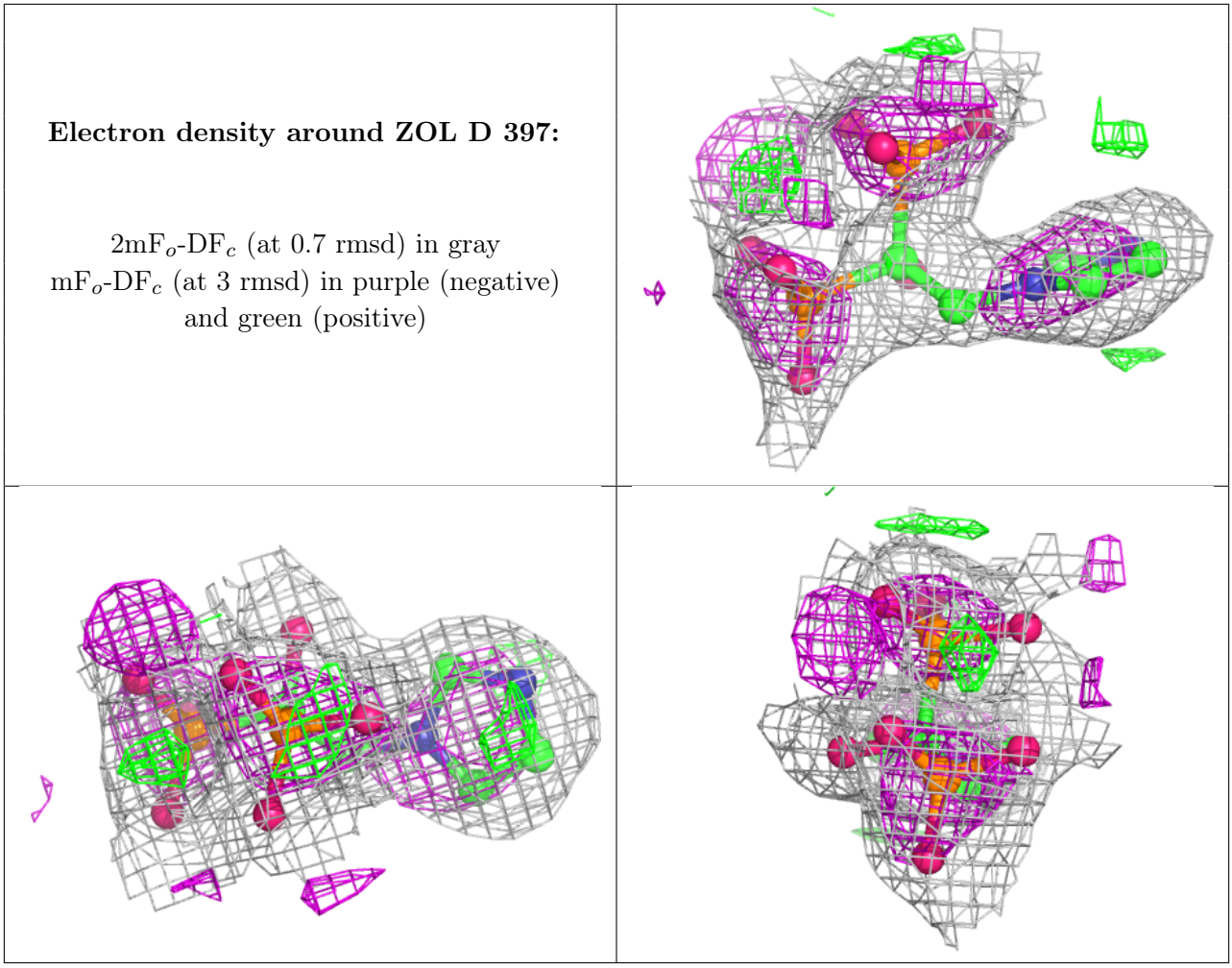






Electron density around ZOL D 397:

$2mF_o$-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.