Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2022 – 10:07 AM EDT

PDB ID	:	8D7F
Title	:	FlvF from Aspergillus flavus in complex with Bis-Tris
Authors	:	Tararina, M.A.; Christianson, D.W.
Deposited on	:	2022-06-07
Resolution	:	2.62 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 ⓘ 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 ⓘ) were used in the production of this report:

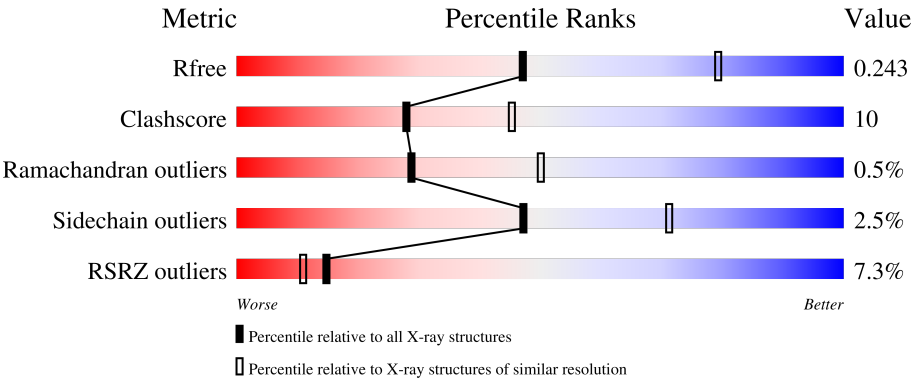
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	368	80% 17%
1	B	368	80% 17%
1	C	368	78% 15% 5%
1	D	368	75% 17% 6%
1	E	368	76% 15% 8%

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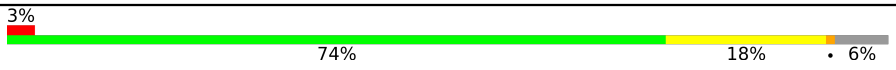
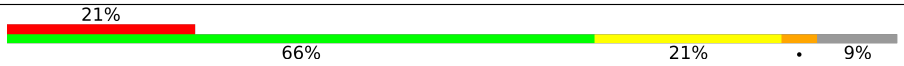
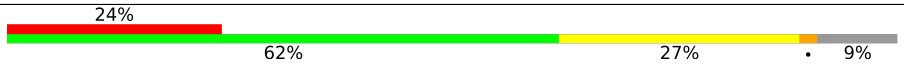
Mol	Chain	Length	Quality of chain
1	F	368	
1	G	368	
1	H	368	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22284 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 Terpene cyclase flvF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2939	1890	484	547	18			
1	B	361	Total	C	N	O	S	0	0	0
			2944	1895	485	547	17			
1	C	349	Total	C	N	O	S	0	1	0
			2806	1801	465	525	15			
1	D	345	Total	C	N	O	S	0	0	0
			2768	1778	456	519	15			
1	E	340	Total	C	N	O	S	0	0	0
			2756	1777	454	510	15			
1	F	345	Total	C	N	O	S	0	0	0
			2809	1809	465	520	15			
1	G	335	Total	C	N	O	S	0	0	0
			2580	1662	429	475	14			
1	H	334	Total	C	N	O	S	0	0	0
			2564	1654	428	468	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP B8NHE1
A	0	ASN	-	expression tag	UNP B8NHE1
A	1	ALA	-	expression tag	UNP B8NHE1
B	-1	SER	-	expression tag	UNP B8NHE1
B	0	ASN	-	expression tag	UNP B8NHE1
B	1	ALA	-	expression tag	UNP B8NHE1
C	-1	SER	-	expression tag	UNP B8NHE1
C	0	ASN	-	expression tag	UNP B8NHE1
C	1	ALA	-	expression tag	UNP B8NHE1
D	-1	SER	-	expression tag	UNP B8NHE1
D	0	ASN	-	expression tag	UNP B8NHE1
D	1	ALA	-	expression tag	UNP B8NHE1
E	-1	SER	-	expression tag	UNP B8NHE1

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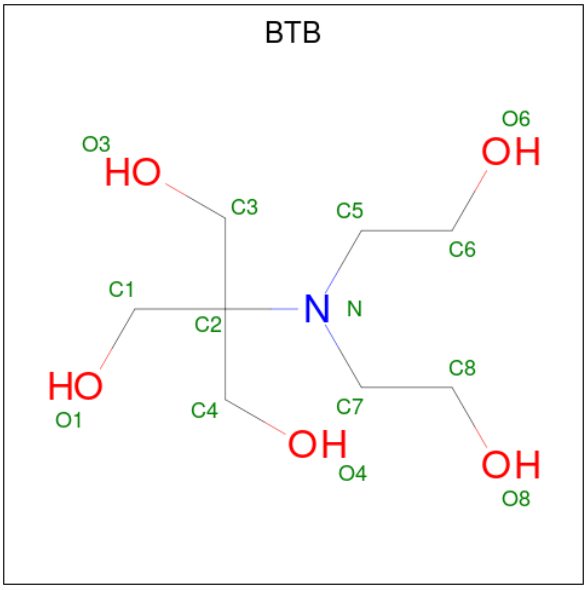
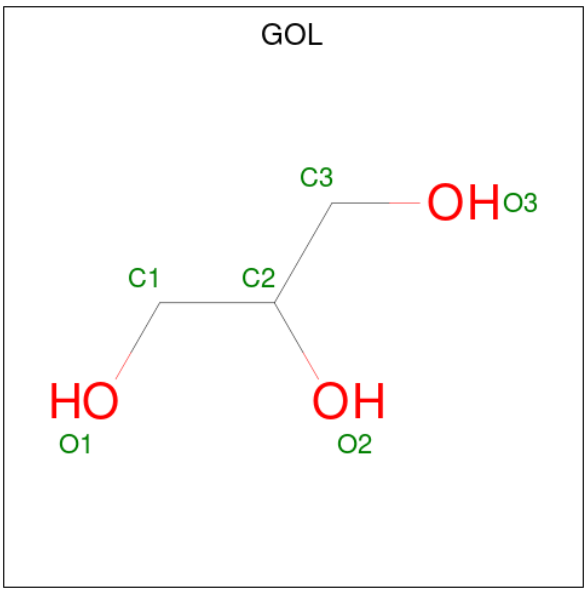
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ASN	-	expression tag	UNP B8NHE1
E	1	ALA	-	expression tag	UNP B8NHE1
F	-1	SER	-	expression tag	UNP B8NHE1
F	0	ASN	-	expression tag	UNP B8NHE1
F	1	ALA	-	expression tag	UNP B8NHE1
G	-1	SER	-	expression tag	UNP B8NHE1
G	0	ASN	-	expression tag	UNP B8NHE1
G	1	ALA	-	expression tag	UNP B8NHE1
H	-1	SER	-	expression tag	UNP B8NHE1
H	0	ASN	-	expression tag	UNP B8NHE1
H	1	ALA	-	expression tag	UNP B8NHE1

- Molecule 2 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



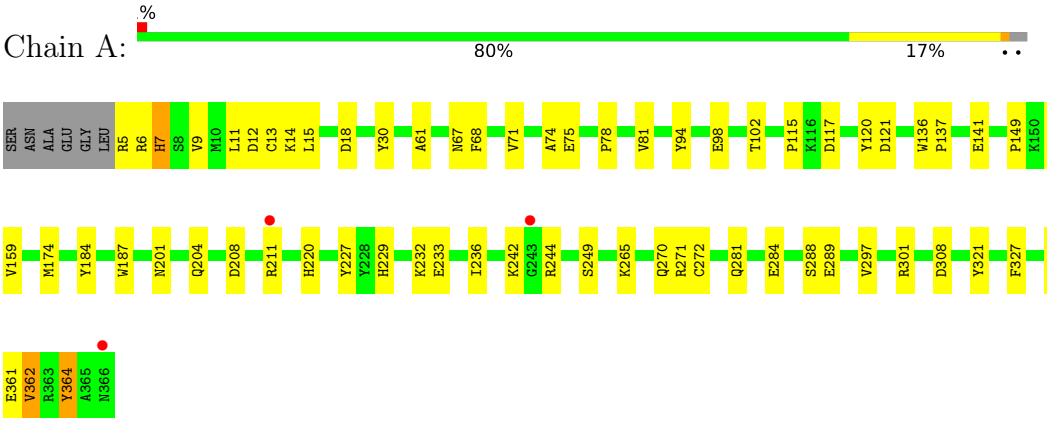
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0

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.

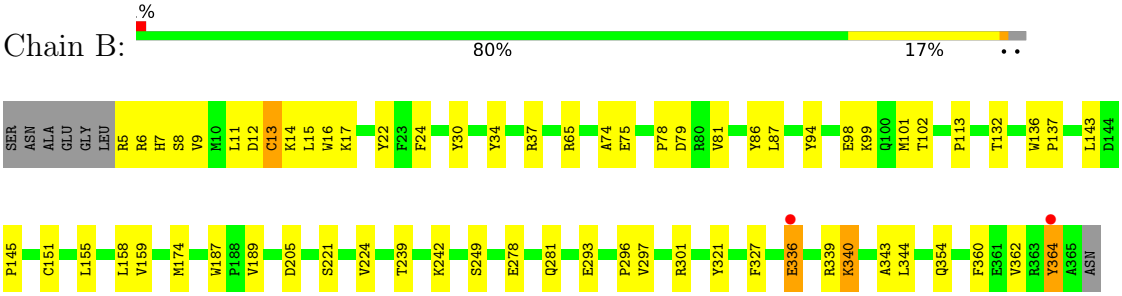
• Molecule 1: Terpene cyclase flvF

Chain A:



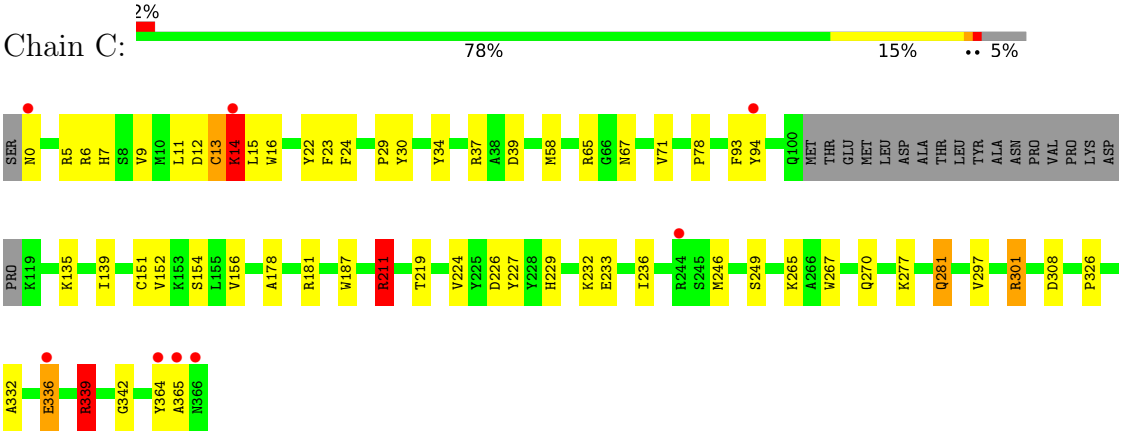
• Molecule 1: Terpene cyclase flvF

Chain B:



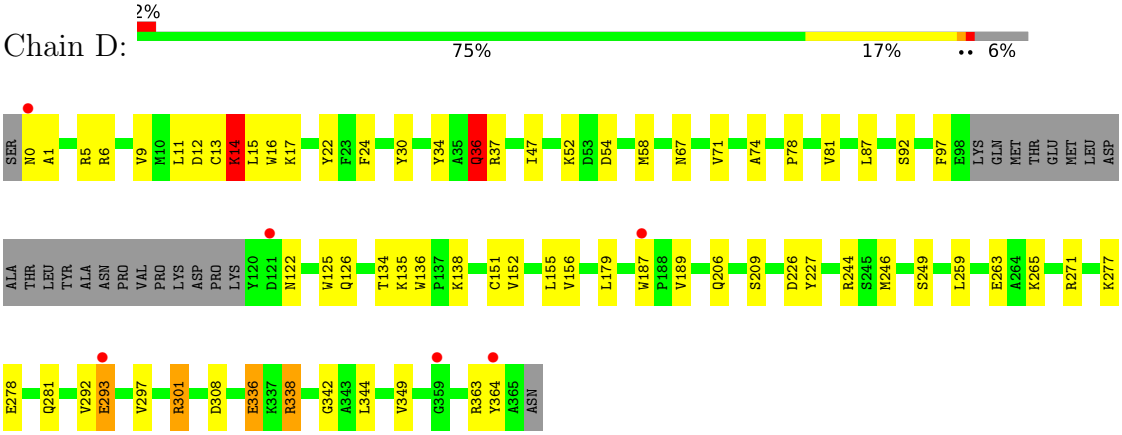
• Molecule 1: Terpene cyclase flvF

Chain C:



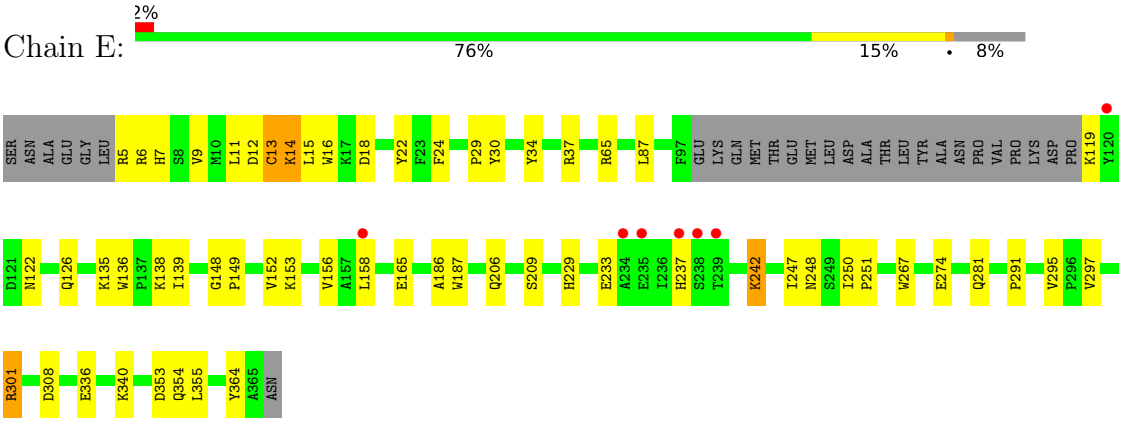
• Molecule 1: Terpene cyclase flvF

Chain D:



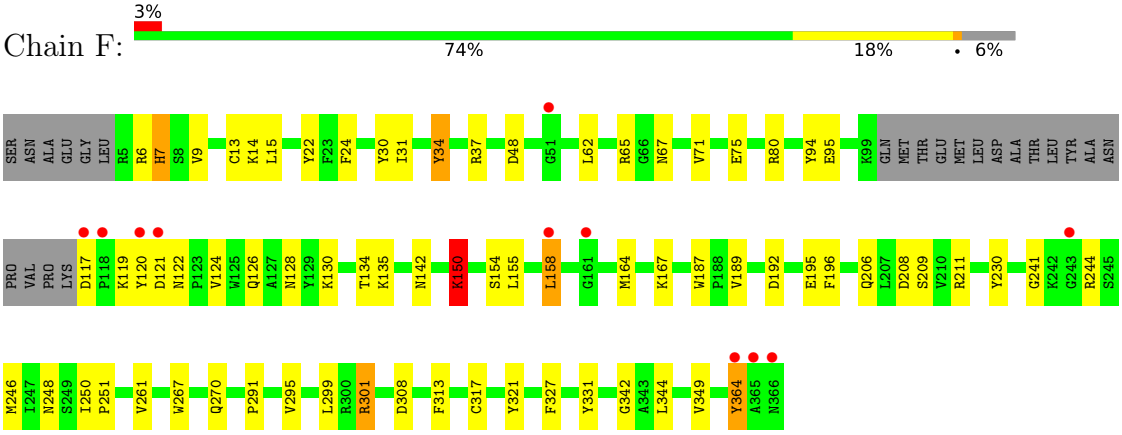
• Molecule 1: Terpene cyclase flvF

Chain E:



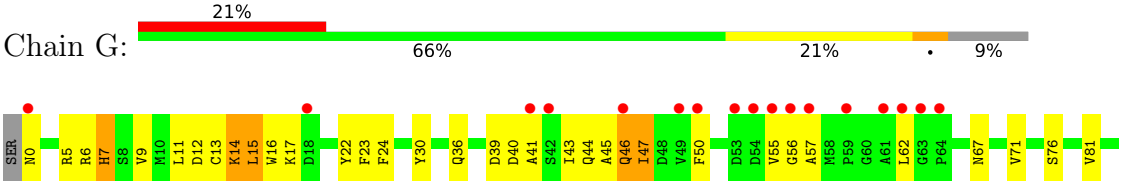
• Molecule 1: Terpene cyclase flvF

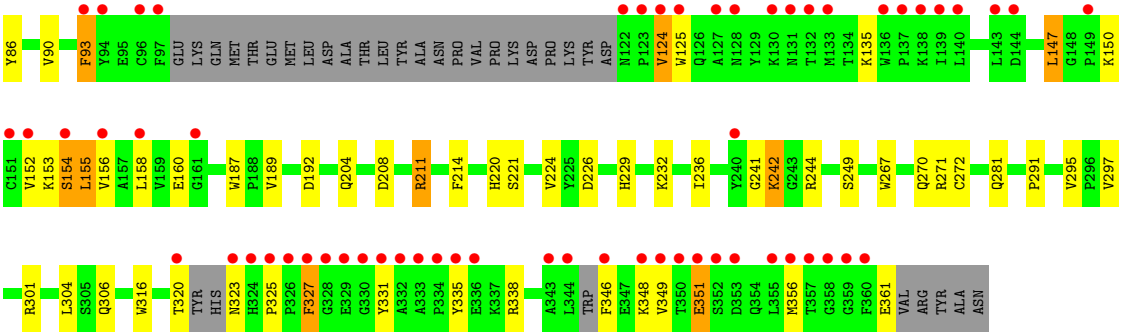
Chain F:



• Molecule 1: Terpene cyclase flvF

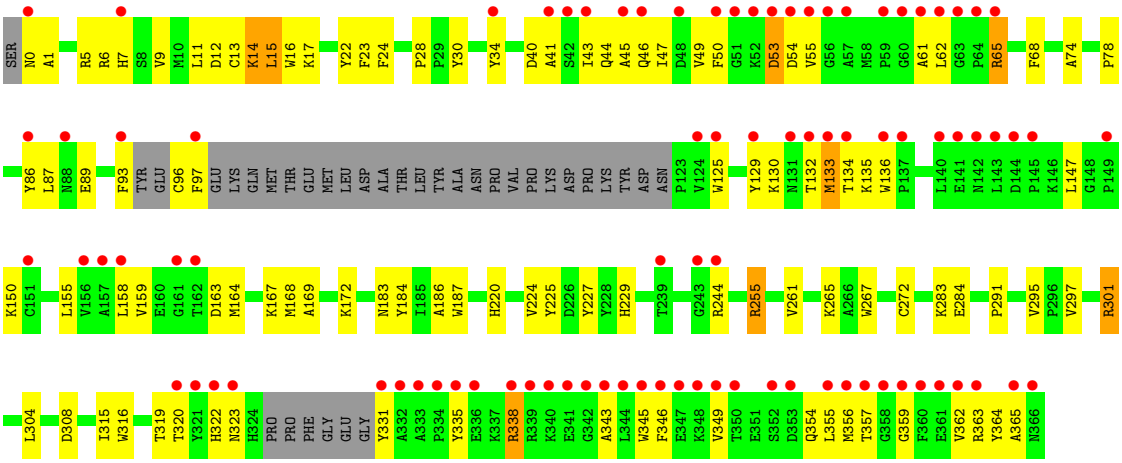
Chain G:





• Molecule 1: Terpene cyclase flvF

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.65Å 195.00Å 101.37Å 90.00° 106.19° 90.00°	Depositor
Resolution (Å)	97.35 – 2.62 97.35 – 2.62	Depositor EDS
% Data completeness (in resolution range)	98.8 (97.35-2.62) 98.7 (97.35-2.62)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.243 0.208 , 0.243	Depositor DCC
R_{free} test set	2000 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.2	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	0.92	EDS
Total number of atoms	22284	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BTB, GOL

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	0.36	1/3025 (0.0%)	0.54	2/4110 (0.0%)
1	B	0.41	2/3030 (0.1%)	0.59	6/4113 (0.1%)
1	C	0.42	2/2889 (0.1%)	0.85	14/3927 (0.4%)
1	D	0.40	1/2847 (0.0%)	0.65	5/3869 (0.1%)
1	E	0.36	0/2836	0.64	6/3849 (0.2%)
1	F	0.37	0/2891	0.58	3/3923 (0.1%)
1	G	0.45	1/2651 (0.0%)	0.70	9/3612 (0.2%)
1	H	0.34	0/2633	0.60	4/3588 (0.1%)
All	All	0.39	7/22802 (0.0%)	0.65	49/30991 (0.2%)

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	C	0	1
1	D	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	277	LYS	CD-CE	7.77	1.70	1.51
1	G	93	PHE	CB-CG	-6.97	1.39	1.51
1	A	284	GLU	CG-CD	6.87	1.62	1.51
1	D	293	GLU	CD-OE2	5.97	1.32	1.25
1	C	211	ARG	CZ-NH1	5.58	1.40	1.33
1	B	293	GLU	CB-CG	-5.34	1.42	1.52
1	B	336	GLU	CB-CG	-5.29	1.42	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	211	ARG	NE-CZ-NH2	-18.72	110.94	120.30
1	C	339	ARG	NE-CZ-NH2	-15.93	112.34	120.30
1	C	339	ARG	CD-NE-CZ	13.95	143.13	123.60
1	C	211	ARG	NE-CZ-NH1	13.54	127.07	120.30
1	C	277	LYS	CG-CD-CE	-11.43	77.61	111.90
1	C	14	LYS	CD-CE-NZ	-11.25	85.82	111.70
1	D	36	GLN	CA-CB-CG	-11.15	88.87	113.40
1	C	277	LYS	CB-CG-CD	10.89	139.91	111.60
1	B	336	GLU	CA-CB-CG	-10.48	90.34	113.40
1	E	353	ASP	CB-CG-OD2	-10.40	108.94	118.30
1	E	353	ASP	CB-CA-C	-9.82	90.75	110.40
1	D	293	GLU	CA-CB-CG	-9.65	92.18	113.40
1	G	211	ARG	CG-CD-NE	8.40	129.44	111.80
1	E	5	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	E	5	ARG	NE-CZ-NH2	7.92	124.26	120.30
1	G	351	GLU	N-CA-CB	-7.78	96.60	110.60
1	A	284	GLU	CG-CD-OE2	7.69	133.67	118.30
1	F	158	LEU	CB-CG-CD2	7.25	123.32	111.00
1	E	237	HIS	C-N-CA	-7.08	104.01	121.70
1	A	284	GLU	CG-CD-OE1	-7.02	104.26	118.30
1	G	211	ARG	CA-CB-CG	6.98	128.76	113.40
1	D	277	LYS	CB-CG-CD	-6.58	94.50	111.60
1	H	338	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	C	211	ARG	CD-NE-CZ	6.50	132.70	123.60
1	G	47	ILE	CG1-CB-CG2	6.28	125.21	111.40
1	B	293	GLU	CB-CG-CD	-6.21	97.44	114.20
1	F	150	LYS	CG-CD-CE	-6.18	93.37	111.90
1	C	211	ARG	CA-CB-CG	6.16	126.95	113.40
1	C	339	ARG	CB-CG-CD	-6.07	95.81	111.60
1	C	14	LYS	CA-CB-CG	6.01	126.63	113.40
1	B	339	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	D	54	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	C	277	LYS	CA-CB-CG	-5.97	100.27	113.40
1	D	336	GLU	CA-CB-CG	-5.96	100.28	113.40
1	G	46	GLN	CA-CB-CG	-5.86	100.51	113.40
1	B	340	LYS	CG-CD-CE	-5.85	94.36	111.90
1	G	160	GLU	CA-CB-CG	5.75	126.06	113.40
1	H	338	ARG	CG-CD-NE	-5.72	99.78	111.80
1	C	211	ARG	CB-CA-C	-5.58	99.24	110.40
1	B	79	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	G	147	LEU	CB-CG-CD2	5.33	120.05	111.00
1	F	150	LYS	CD-CE-NZ	5.21	123.68	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	211	ARG	CB-CA-C	5.16	120.72	110.40
1	C	336	GLU	N-CA-CB	-5.12	101.38	110.60
1	G	46	GLN	CB-CG-CD	-5.11	98.31	111.60
1	E	138	LYS	CD-CE-NZ	-5.07	100.05	111.70
1	H	15	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	87	LEU	CA-CB-CG	5.04	126.89	115.30
1	H	284	GLU	CA-CB-CG	-5.04	102.32	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	339	ARG	Sidechain
1	D	36	GLN	Sidechain

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	2939	0	2814	44	0
1	B	2944	0	2838	41	0
1	C	2806	0	2648	45	0
1	D	2768	0	2619	51	0
1	E	2756	0	2641	36	0
1	F	2809	0	2690	49	0
1	G	2580	0	2389	85	0
1	H	2564	0	2376	84	0
2	A	28	0	38	8	0
2	B	28	0	38	4	0
2	D	14	0	19	4	0
3	A	6	0	8	2	0
3	B	6	0	8	0	0
3	C	6	0	8	2	0
3	D	6	0	8	1	0
3	E	6	0	8	2	0
3	F	6	0	8	2	0
3	G	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	6	0	8	1	0
All	All	22284	0	21174	432	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 (432) 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:E:242:LYS:HD2	1:E:242:LYS:O	1.27	1.25
1:F:208:ASP:OD1	1:F:211:ARG:CZ	1.91	1.17
1:G:46:GLN:NE2	1:G:93:PHE:CZ	2.16	1.13
1:F:150:LYS:NZ	1:F:195:GLU:OE1	1.84	1.11
1:G:46:GLN:NE2	1:G:93:PHE:HZ	1.48	1.10
1:G:44:GLN:HG3	1:G:356:MET:HG2	1.35	1.04
1:B:15:LEU:HB3	1:B:65:ARG:HD3	1.50	0.93
1:G:325:PRO:HA	1:G:327:PHE:H	1.32	0.93
1:D:87:LEU:HD13	1:D:136:TRP:CZ3	2.07	0.90
1:E:242:LYS:O	1:E:242:LYS:CD	2.18	0.89
1:D:87:LEU:CD1	1:D:136:TRP:CZ3	2.56	0.88
1:G:204:GLN:OE1	1:G:211:ARG:NH2	2.08	0.87
1:A:13:CYS:O	1:A:15:LEU:N	2.07	0.87
1:D:13:CYS:O	1:D:15:LEU:N	2.08	0.86
1:B:158:LEU:HB3	2:B:401:BTB:H12	1.59	0.85
1:C:13:CYS:O	1:C:15:LEU:N	2.10	0.85
1:A:204:GLN:OE1	1:A:211:ARG:NH2	2.12	0.83
1:G:36:GLN:NE2	1:G:338:ARG:HD3	1.93	0.83
1:G:45:ALA:HB1	1:G:90:VAL:HG13	1.61	0.83
1:F:208:ASP:OD1	1:F:211:ARG:NH1	2.13	0.82
1:D:292:VAL:HG23	1:D:293:GLU:HG3	1.62	0.81
1:F:15:LEU:HB3	1:F:65:ARG:HD3	1.61	0.81
1:D:87:LEU:HD11	1:D:136:TRP:CH2	2.17	0.80
1:H:0:ASN:O	1:H:6:ARG:NH1	2.16	0.79
1:A:208:ASP:HA	1:A:211:ARG:HG3	1.65	0.78
1:D:0:ASN:O	1:D:6:ARG:NH1	2.17	0.78
1:H:343:ALA:HB1	1:H:362:VAL:HG21	1.65	0.78
1:E:15:LEU:HB3	1:E:65:ARG:HD3	1.65	0.77
1:C:11:LEU:HD23	1:C:12:ASP:O	1.83	0.77
1:C:34:TYR:HB3	1:C:37:ARG:HD3	1.67	0.77
1:G:46:GLN:CD	1:G:93:PHE:HZ	1.88	0.77
1:D:87:LEU:HD13	1:D:136:TRP:CE3	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:GLU:O	1:B:336:GLU:HG3	1.81	0.77
1:H:13:CYS:O	1:H:15:LEU:N	2.19	0.75
1:D:336:GLU:O	1:D:336:GLU:HG3	1.86	0.74
1:H:169:ALA:HA	1:H:255:ARG:HH12	1.53	0.73
1:D:87:LEU:CD1	1:D:136:TRP:CH2	2.71	0.73
1:H:135:LYS:NZ	1:H:354:GLN:O	2.20	0.73
1:G:62:LEU:HD22	1:G:331:TYR:CD1	2.24	0.73
1:F:208:ASP:OD1	1:F:211:ARG:NH2	2.23	0.72
1:D:36:GLN:HG3	1:D:36:GLN:O	1.89	0.71
2:A:402:BTB:HO4	2:A:402:BTB:HO1	1.36	0.71
1:C:332:ALA:O	1:C:336:GLU:HG3	1.91	0.71
1:F:208:ASP:HA	1:F:211:ARG:HG3	1.72	0.71
1:H:357:THR:HB	1:H:363:ARG:HB3	1.72	0.71
1:D:226:ASP:OD2	1:D:249:SER:OG	2.07	0.70
1:E:149:PRO:O	1:E:153:LYS:HG2	1.92	0.70
1:G:13:CYS:O	1:G:15:LEU:N	2.20	0.70
1:H:343:ALA:HB3	1:H:345:TRP:CZ2	2.26	0.70
1:G:124:VAL:HG13	1:G:125:TRP:H	1.57	0.70
1:G:5:ARG:O	1:G:301:ARG:NH2	2.25	0.69
1:D:36:GLN:NE2	1:D:338:ARG:HD2	2.07	0.69
1:A:281:GLN:NE2	1:G:281:GLN:OE1	2.26	0.68
1:E:229:HIS:ND1	1:E:233:GLU:HG3	2.08	0.68
1:B:6:ARG:HH11	1:B:9:VAL:HG11	1.59	0.68
1:E:122:ASN:O	1:E:126:GLN:HG3	1.94	0.68
1:F:13:CYS:SG	1:F:14:LYS:N	2.66	0.67
1:G:46:GLN:O	1:G:50:PHE:N	2.23	0.67
1:D:87:LEU:CD1	1:D:136:TRP:CE3	2.78	0.67
1:F:267:TRP:CD1	3:F:401:GOL:H32	2.31	0.66
1:C:9:VAL:HG21	1:C:30:TYR:HB3	1.75	0.66
1:F:164:MET:O	1:F:167:LYS:HB2	1.96	0.66
1:G:36:GLN:HE21	1:G:338:ARG:HD3	1.60	0.66
1:C:5:ARG:O	1:C:301:ARG:NH2	2.29	0.66
1:G:46:GLN:HA	1:G:46:GLN:OE1	1.96	0.66
1:G:11:LEU:HD23	1:G:12:ASP:O	1.95	0.65
2:A:402:BTB:O1	2:A:402:BTB:O4	2.10	0.65
1:C:135:LYS:HE3	1:C:139:ILE:HD11	1.78	0.65
1:H:65:ARG:HD3	1:H:319:THR:HG21	1.79	0.65
1:C:281[B]:GLN:OE1	1:E:281:GLN:NE2	2.29	0.64
1:H:6:ARG:NH2	1:H:308:ASP:OD1	2.30	0.64
1:F:117:ASP:HB3	1:F:120:TYR:HD2	1.63	0.64
1:E:11:LEU:HD23	1:E:12:ASP:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:TYR:HB3	1:D:37:ARG:HD3	1.81	0.63
1:D:5:ARG:O	1:D:301:ARG:NH2	2.31	0.63
1:G:241:GLY:O	1:G:242:LYS:HB2	1.99	0.62
1:A:159:VAL:HA	2:A:401:BTB:H42	1.80	0.62
1:C:9:VAL:CG2	1:C:30:TYR:HB3	2.29	0.62
1:F:158:LEU:HD11	1:F:189:VAL:HG21	1.81	0.62
1:F:130:LYS:O	1:F:134:THR:HG23	2.00	0.61
1:A:78:PRO:O	1:A:81:VAL:HG12	2.00	0.61
1:G:242:LYS:NZ	1:G:242:LYS:HB3	2.16	0.61
1:H:158:LEU:HD21	1:H:183:ASN:HB3	1.82	0.61
1:G:43:ILE:O	1:G:47:ILE:HG13	2.01	0.60
1:E:34:TYR:HB3	1:E:37:ARG:HD3	1.82	0.60
1:A:242:LYS:HD2	1:A:242:LYS:O	2.01	0.60
1:F:154:SER:OG	1:F:192:ASP:OD2	2.12	0.60
1:C:267:TRP:CD1	3:C:401:GOL:H32	2.36	0.60
1:F:9:VAL:HG21	1:F:30:TYR:HB3	1.84	0.60
1:B:159:VAL:HA	2:B:401:BTB:H31	1.84	0.60
1:E:6:ARG:HE	1:E:9:VAL:HG11	1.68	0.59
1:B:11:LEU:HD23	1:B:12:ASP:O	2.02	0.59
1:H:316:TRP:CZ2	1:H:320:THR:HG21	2.38	0.59
1:B:343:ALA:HB1	1:B:362:VAL:HG21	1.84	0.58
1:E:9:VAL:HG21	1:E:30:TYR:HB3	1.85	0.58
1:G:348:LYS:O	1:G:351:GLU:HB2	2.03	0.58
1:D:92:SER:HA	2:D:401:BTB:H82	1.86	0.58
1:A:115:PRO:HG3	1:A:244:ARG:HG3	1.85	0.58
1:E:9:VAL:CG2	1:E:30:TYR:HB3	2.34	0.58
1:H:89:GLU:OE2	1:H:331:TYR:OH	2.20	0.58
1:D:9:VAL:HG21	1:D:30:TYR:HB3	1.84	0.58
1:F:9:VAL:CG2	1:F:30:TYR:HB3	2.34	0.58
1:C:342:GLY:O	1:C:364:TYR:HB3	2.04	0.57
1:H:267:TRP:CD1	3:H:401:GOL:H31	2.39	0.57
1:H:11:LEU:HD12	1:H:12:ASP:N	2.19	0.57
1:F:135:LYS:HE3	1:F:349:VAL:HG22	1.87	0.57
1:D:11:LEU:HD23	1:D:12:ASP:O	2.04	0.57
1:B:98:GLU:O	1:B:102:THR:HG23	2.05	0.57
1:C:6:ARG:NH2	1:C:308:ASP:OD1	2.37	0.56
1:G:267:TRP:CD1	3:G:401:GOL:H31	2.40	0.56
1:A:5:ARG:O	1:A:301:ARG:NH2	2.38	0.56
1:A:6:ARG:NH2	1:A:308:ASP:OD1	2.38	0.56
1:F:34:TYR:HB3	1:F:37:ARG:HD3	1.86	0.56
1:G:62:LEU:HD22	1:G:331:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:ILE:HD11	1:H:345:TRP:NE1	2.21	0.56
1:D:36:GLN:O	1:D:36:GLN:CG	2.54	0.56
1:H:346:PHE:CZ	1:H:357:THR:HA	2.41	0.56
1:E:13:CYS:O	1:E:16:TRP:NE1	2.38	0.56
1:E:153:LYS:HA	1:E:156:VAL:HG22	1.85	0.56
1:H:62:LEU:O	1:H:320:THR:OG1	2.24	0.56
1:A:208:ASP:OD1	1:A:211:ARG:NE	2.36	0.56
1:D:9:VAL:CG2	1:D:30:TYR:HB3	2.36	0.56
1:G:62:LEU:HD22	1:G:331:TYR:HD1	1.72	0.55
1:B:9:VAL:CG2	1:B:30:TYR:HB3	2.37	0.55
1:E:135:LYS:HD3	1:E:139:ILE:HD11	1.88	0.55
1:G:55:VAL:HG11	1:G:335:TYR:HD2	1.71	0.55
1:F:155:LEU:HA	1:F:158:LEU:HD12	1.88	0.55
1:A:201:ASN:ND2	1:B:354:GLN:OE1	2.39	0.55
1:C:332:ALA:O	1:C:336:GLU:HB2	2.05	0.55
1:E:135:LYS:NZ	1:E:354:GLN:O	2.35	0.55
1:D:36:GLN:HE21	1:D:338:ARG:CD	2.18	0.55
1:G:9:VAL:CG2	1:G:30:TYR:HB3	2.36	0.55
1:H:9:VAL:CG2	1:H:30:TYR:HB3	2.37	0.55
1:E:18:ASP:OD2	1:G:0:ASN:N	2.35	0.55
1:G:325:PRO:HA	1:G:327:PHE:N	2.13	0.54
1:E:148:GLY:O	1:E:152:VAL:HG23	2.06	0.54
1:G:9:VAL:HG21	1:G:30:TYR:HB3	1.90	0.54
1:B:13:CYS:SG	1:B:14:LYS:N	2.79	0.54
1:G:50:PHE:CE2	1:G:57:ALA:HB3	2.42	0.54
1:D:271:ARG:HD3	3:D:402:GOL:H31	1.89	0.54
1:G:23:PHE:CD2	1:G:224:VAL:HG12	2.42	0.54
1:C:232:LYS:HE3	1:C:236:ILE:HD11	1.89	0.54
1:H:40:ASP:OD1	1:H:338:ARG:NH2	2.41	0.54
1:B:9:VAL:HG21	1:B:30:TYR:HB3	1.90	0.54
1:C:67:ASN:O	1:C:71:VAL:HG22	2.08	0.54
1:D:14:LYS:HG3	1:D:17:LYS:HB2	1.90	0.53
1:H:9:VAL:HG21	1:H:30:TYR:HB3	1.90	0.53
1:G:6:ARG:HH11	1:G:9:VAL:HG11	1.72	0.53
1:H:320:THR:HG23	1:H:322:HIS:H	1.74	0.53
1:D:16:TRP:CE3	1:D:17:LYS:HA	2.43	0.53
1:D:78:PRO:O	1:D:81:VAL:HG12	2.09	0.53
1:B:296:PRO:HG3	1:H:172:LYS:HD2	1.91	0.53
1:A:94:TYR:CE2	2:A:401:BTB:H82	2.43	0.53
1:D:134:THR:O	1:D:138:LYS:HD3	2.08	0.53
1:H:61:ALA:HB1	1:H:68:PHE:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:261:VAL:O	1:H:265:LYS:HG3	2.09	0.53
1:D:36:GLN:NE2	1:D:338:ARG:CD	2.70	0.53
1:A:18:ASP:CG	1:C:0:ASN:HA	2.29	0.52
1:B:239:THR:O	1:B:242:LYS:HE2	2.09	0.52
1:G:220:HIS:CD2	1:G:272:CYS:HB3	2.45	0.52
1:G:6:ARG:HG2	1:G:304:LEU:HD13	1.90	0.52
1:H:16:TRP:CH2	1:H:28:PRO:HB3	2.45	0.52
1:H:93:PHE:HB2	1:H:129:TYR:OH	2.09	0.52
1:B:155:LEU:HD13	1:B:189:VAL:HG21	1.92	0.52
1:H:16:TRP:CE3	1:H:17:LYS:HA	2.45	0.52
1:H:158:LEU:HD13	1:H:186:ALA:HA	1.91	0.52
1:H:55:VAL:HB	1:H:335:TYR:CE2	2.45	0.52
1:G:39:ASP:OD1	1:G:67:ASN:HB2	2.10	0.52
1:G:56:GLY:N	1:G:331:TYR:CD2	2.78	0.52
1:H:41:ALA:HB1	1:H:86:TYR:HB2	1.91	0.52
1:G:152:VAL:O	1:G:156:VAL:HG13	2.10	0.52
1:H:5:ARG:O	1:H:301:ARG:NH2	2.42	0.52
1:C:6:ARG:HE	1:C:9:VAL:HG11	1.75	0.51
1:F:48:ASP:O	1:F:128:ASN:HB3	2.10	0.51
1:B:34:TYR:HB3	1:B:37:ARG:HD3	1.91	0.51
1:D:278:GLU:O	1:D:281:GLN:HG3	2.10	0.51
1:E:291:PRO:O	1:E:295:VAL:HG23	2.11	0.51
1:A:289:GLU:HB2	1:G:271:ARG:CZ	2.40	0.51
1:D:1:ALA:HB2	1:D:6:ARG:HD2	1.93	0.51
1:F:208:ASP:HA	1:F:211:ARG:CG	2.39	0.51
1:G:16:TRP:CE3	1:G:17:LYS:HA	2.46	0.51
1:F:342:GLY:O	1:F:364:TYR:HB3	2.10	0.51
1:G:46:GLN:CD	1:G:93:PHE:CZ	2.73	0.51
1:G:208:ASP:HA	1:G:211:ARG:HD2	1.93	0.51
1:B:278:GLU:O	1:B:281:GLN:HG3	2.10	0.51
1:B:8:SER:HB3	1:B:34:TYR:HE2	1.76	0.51
1:A:174:MET:HE1	1:A:249:SER:HB2	1.93	0.51
1:F:230:TYR:CG	1:F:250:ILE:HD12	2.45	0.51
1:A:117:ASP:HB3	1:A:120:TYR:HD2	1.77	0.50
1:G:55:VAL:HG12	1:G:331:TYR:CD2	2.47	0.50
1:B:297:VAL:O	1:B:301:ARG:HG3	2.11	0.50
1:C:15:LEU:HB3	1:C:65:ARG:HD3	1.92	0.50
1:A:297:VAL:O	1:A:301:ARG:HG3	2.11	0.50
1:H:46:GLN:O	1:H:50:PHE:N	2.20	0.50
1:H:6:ARG:HG2	1:H:304:LEU:HD13	1.93	0.50
1:C:365:ALA:C	1:F:130:LYS:HD3	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:GLY:N	1:G:331:TYR:HD2	2.09	0.50
1:H:11:LEU:CD1	1:H:28:PRO:HB2	2.42	0.50
1:A:361:GLU:O	1:A:362:VAL:HG22	2.12	0.49
1:C:23:PHE:CD2	1:C:224:VAL:HG23	2.47	0.49
1:D:97:PHE:CD1	1:D:126:GLN:HG2	2.47	0.49
1:H:357:THR:HB	1:H:363:ARG:CB	2.39	0.49
1:A:11:LEU:HD23	1:A:12:ASP:O	2.12	0.49
1:H:343:ALA:CB	1:H:362:VAL:HG21	2.39	0.49
1:E:6:ARG:NH2	1:E:308:ASP:OD1	2.45	0.49
1:F:158:LEU:HD11	1:F:189:VAL:CG2	2.41	0.49
1:B:5:ARG:O	1:B:301:ARG:NH2	2.46	0.49
1:G:153:LYS:HA	1:G:156:VAL:HG22	1.94	0.49
1:A:270:GLN:HB3	3:A:403:GOL:O1	2.13	0.49
1:F:6:ARG:NH2	1:F:308:ASP:OD1	2.45	0.49
1:D:152:VAL:O	1:D:156:VAL:HG23	2.13	0.49
1:A:7:HIS:HB2	1:B:145:PRO:HG2	1.95	0.49
1:G:36:GLN:HE22	1:G:338:ARG:HD3	1.75	0.48
1:A:9:VAL:HG11	1:A:75:GLU:HG2	1.93	0.48
1:D:6:ARG:NH2	1:D:308:ASP:OD1	2.46	0.48
1:F:62:LEU:HB2	1:F:331:TYR:CZ	2.48	0.48
1:C:181:ARG:NH2	1:C:226:ASP:OD1	2.42	0.48
1:E:267:TRP:CE2	3:E:401:GOL:H12	2.47	0.48
1:G:41:ALA:HB1	1:G:86:TYR:HB2	1.95	0.48
1:B:22:TYR:CE2	1:B:24:PHE:HB2	2.48	0.48
1:B:94:TYR:HD1	1:B:101:MET:SD	2.36	0.48
1:H:0:ASN:OD1	1:H:283:LYS:NZ	2.46	0.48
1:D:6:ARG:HE	1:D:9:VAL:HG11	1.79	0.48
1:F:241:GLY:O	1:F:244:ARG:HB2	2.14	0.48
1:F:321:TYR:O	1:F:327:PHE:HA	2.14	0.48
1:H:355:LEU:HB3	1:H:356:MET:HG3	1.96	0.48
1:G:135:LYS:HD2	1:G:349:VAL:HG22	1.96	0.48
1:G:242:LYS:HB3	1:G:242:LYS:HZ2	1.79	0.48
1:A:98:GLU:O	1:A:102:THR:HG23	2.14	0.48
1:D:47:ILE:HG12	1:D:52:LYS:HA	1.95	0.48
1:D:344:LEU:HD22	1:D:364:TYR:HB2	1.95	0.48
1:G:23:PHE:HD2	1:G:224:VAL:HG12	1.79	0.48
1:A:136:TRP:CG	1:A:137:PRO:HD3	2.50	0.47
1:F:9:VAL:HG23	1:F:31:ILE:O	2.13	0.47
1:G:7:HIS:CD2	1:G:301:ARG:NH2	2.83	0.47
1:G:46:GLN:OE1	1:G:93:PHE:CZ	2.67	0.47
1:H:1:ALA:HB2	1:H:6:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:HIS:CD2	1:B:301:ARG:NH2	2.83	0.47
1:F:126:GLN:O	1:F:130:LYS:HG3	2.14	0.47
1:G:226:ASP:OD2	1:G:249:SER:OG	2.20	0.47
1:G:338:ARG:HA	1:G:338:ARG:HD2	1.69	0.47
1:B:16:TRP:CE3	1:B:17:LYS:HA	2.50	0.47
1:C:58:MET:HE2	1:C:93:PHE:HA	1.96	0.47
1:D:155:LEU:HD13	1:D:189:VAL:HG21	1.96	0.47
1:E:336:GLU:HG3	1:E:340:LYS:HE2	1.97	0.47
1:H:297:VAL:O	1:H:301:ARG:HG3	2.15	0.47
1:B:99:LYS:HE2	1:B:113:PRO:HB3	1.96	0.47
1:F:9:VAL:HG11	1:F:75:GLU:HG2	1.96	0.47
1:E:87:LEU:HD13	1:E:136:TRP:CZ3	2.50	0.47
1:G:291:PRO:O	1:G:295:VAL:HG23	2.15	0.47
1:H:43:ILE:HD11	1:H:345:TRP:CE2	2.49	0.47
1:H:130:LYS:O	1:H:134:THR:OG1	2.26	0.47
1:F:313:PHE:CZ	1:F:317:CYS:SG	3.08	0.46
1:G:270:GLN:HB3	3:G:401:GOL:O3	2.15	0.46
1:H:227:TYR:CE2	1:H:265:LYS:HB3	2.50	0.46
1:G:232:LYS:O	1:G:236:ILE:HG13	2.14	0.46
1:H:133:MET:HE3	1:H:136:TRP:HE1	1.79	0.46
1:C:229:HIS:CD2	1:C:233:GLU:HG3	2.50	0.46
1:G:346:PHE:HB3	1:G:351:GLU:OE1	2.15	0.46
1:C:13:CYS:SG	1:C:14:LYS:HB3	2.55	0.46
1:B:221:SER:HA	1:B:224:VAL:HG12	1.97	0.46
1:F:291:PRO:O	1:F:295:VAL:HG23	2.15	0.46
1:C:226:ASP:OD2	1:C:249:SER:OG	2.23	0.46
1:G:9:VAL:HG22	1:G:30:TYR:HD2	1.80	0.46
1:G:154:SER:O	1:G:189:VAL:HG22	2.14	0.46
1:H:45:ALA:HB2	1:H:86:TYR:CG	2.51	0.46
1:H:343:ALA:HA	1:H:365:ALA:HB3	1.96	0.46
1:B:78:PRO:O	1:B:81:VAL:HG12	2.15	0.46
1:B:344:LEU:HG	1:B:364:TYR:HB2	1.96	0.46
1:F:121:ASP:OD1	1:F:126:GLN:NE2	2.49	0.46
1:H:133:MET:CE	1:H:136:TRP:HE1	2.28	0.46
2:D:401:BTB:H71	2:D:401:BTB:H42	1.66	0.46
1:H:23:PHE:CD2	1:H:224:VAL:HG23	2.51	0.46
2:B:401:BTB:H52	2:B:401:BTB:H42	1.66	0.46
1:F:95:GLU:CD	1:F:95:GLU:H	2.20	0.46
1:F:250:ILE:HD13	1:F:261:VAL:HG23	1.98	0.45
1:C:15:LEU:O	1:C:65:ARG:NH1	2.47	0.45
1:D:342:GLY:O	1:D:364:TYR:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:VAL:O	1:G:301:ARG:HG3	2.16	0.45
1:D:122:ASN:HB3	1:D:125:TRP:HB2	1.98	0.45
1:E:274:GLU:OE2	3:E:401:GOL:O2	2.35	0.45
1:G:220:HIS:O	1:G:224:VAL:HG22	2.16	0.45
1:H:9:VAL:HG23	1:H:74:ALA:HB1	1.97	0.45
1:A:9:VAL:HG23	1:A:74:ALA:HB1	1.98	0.45
2:A:402:BTB:H31	2:A:402:BTB:H51	1.52	0.45
1:D:9:VAL:HG23	1:D:74:ALA:HB1	1.98	0.45
1:G:22:TYR:CE2	1:G:24:PHE:HB2	2.50	0.45
1:G:229:HIS:NE2	1:G:323:ASN:OD1	2.50	0.45
1:H:316:TRP:CE2	1:H:320:THR:HG21	2.51	0.45
1:G:43:ILE:HA	1:G:331:TYR:OH	2.16	0.45
1:B:99:LYS:O	1:B:102:THR:OG1	2.31	0.45
1:G:40:ASP:O	1:G:43:ILE:HG12	2.17	0.45
1:H:132:THR:HA	1:H:349:VAL:HG21	1.98	0.45
1:H:225:TYR:O	1:H:229:HIS:HB2	2.16	0.45
1:B:336:GLU:O	1:B:336:GLU:CG	2.49	0.45
1:G:76:SER:HB2	1:G:81:VAL:HB	1.98	0.45
1:H:362:VAL:O	1:H:362:VAL:HG13	2.16	0.45
1:A:9:VAL:CG2	1:A:30:TYR:HB3	2.48	0.44
1:A:61:ALA:HB1	1:A:68:PHE:HB3	1.99	0.44
1:E:250:ILE:HB	1:E:251:PRO:HD3	1.97	0.44
1:H:17:LYS:O	1:H:17:LYS:HD3	2.18	0.44
2:A:402:BTB:H72	2:A:402:BTB:H62	1.71	0.44
1:F:158:LEU:CD1	1:F:189:VAL:HG21	2.47	0.44
1:A:321:TYR:O	1:A:327:PHE:HA	2.17	0.44
2:D:401:BTB:H52	2:D:401:BTB:H32	1.61	0.44
1:H:34:TYR:CE2	1:H:78:PRO:HG3	2.53	0.44
1:H:87:LEU:HD11	1:H:136:TRP:CE3	2.51	0.44
1:C:178:ALA:HB1	1:C:219:THR:HG23	2.00	0.44
1:G:241:GLY:O	1:G:244:ARG:HG3	2.17	0.44
1:G:316:TRP:CZ2	1:G:320:THR:HG21	2.53	0.44
1:H:13:CYS:O	1:H:14:LYS:C	2.55	0.44
1:D:135:LYS:HD3	1:D:349:VAL:HG22	1.99	0.44
1:E:297:VAL:O	1:E:301:ARG:HG3	2.18	0.44
1:G:67:ASN:O	1:G:71:VAL:HG22	2.16	0.44
1:H:22:TYR:CZ	1:H:24:PHE:HB2	2.52	0.44
1:H:43:ILE:CD1	1:H:345:TRP:CE2	3.00	0.44
1:G:13:CYS:O	1:G:15:LEU:HG	2.18	0.44
1:A:227:TYR:CE2	1:A:265:LYS:HB3	2.52	0.44
1:G:150:LYS:HD3	1:G:192:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:ASP:OD1	1:G:211:ARG:CZ	2.66	0.44
1:H:316:TRP:CH2	1:H:320:THR:HG21	2.53	0.44
1:A:141:GLU:HG2	1:A:149:PRO:HG3	2.00	0.43
2:A:401:BTB:H32	2:A:401:BTB:H71	1.46	0.43
1:F:80:ARG:NH1	1:F:196:PHE:O	2.47	0.43
1:H:155:LEU:O	1:H:159:VAL:HG13	2.18	0.43
1:C:39:ASP:OD1	1:C:67:ASN:HB2	2.17	0.43
1:H:46:GLN:HA	1:H:49:VAL:CG2	2.48	0.43
1:C:227:TYR:CE2	1:C:265:LYS:HB3	2.54	0.43
1:G:316:TRP:CH2	1:G:320:THR:HG21	2.54	0.43
1:H:11:LEU:HD11	1:H:28:PRO:HB2	2.00	0.43
1:D:297:VAL:O	1:D:301:ARG:HG3	2.19	0.43
1:A:6:ARG:HE	1:A:9:VAL:HG11	1.84	0.43
1:A:208:ASP:HA	1:A:211:ARG:HE	1.83	0.43
1:C:22:TYR:CZ	1:C:24:PHE:HB2	2.53	0.43
1:C:211:ARG:HE	1:C:211:ARG:HB2	1.33	0.43
1:G:356:MET:HE2	1:G:361:GLU:O	2.18	0.43
1:C:232:LYS:O	1:C:236:ILE:HG13	2.19	0.43
1:C:297:VAL:O	1:C:301:ARG:HG3	2.18	0.43
1:C:332:ALA:O	1:C:336:GLU:CG	2.65	0.43
1:F:122:ASN:OD1	1:F:124:VAL:HG12	2.18	0.43
1:G:147:LEU:HD23	1:G:147:LEU:HA	1.89	0.43
1:A:67:ASN:O	1:A:71:VAL:HG22	2.18	0.43
1:A:220:HIS:CD2	1:A:272:CYS:HB3	2.53	0.43
1:B:86:TYR:OH	1:B:132:THR:HG23	2.19	0.43
1:B:174:MET:HE1	1:B:249:SER:HB2	2.01	0.43
1:H:6:ARG:HE	1:H:9:VAL:HG11	1.84	0.43
1:E:248:ASN:O	1:E:251:PRO:HD2	2.19	0.43
1:F:299:LEU:HD12	1:F:299:LEU:HA	1.87	0.42
1:H:53:ASP:OD1	1:H:53:ASP:N	2.52	0.42
1:C:229:HIS:CE1	1:C:232:LYS:HD3	2.54	0.42
1:G:211:ARG:HH11	1:G:211:ARG:HD3	1.64	0.42
1:G:221:SER:HA	1:G:224:VAL:HG22	2.01	0.42
1:H:50:PHE:HD2	1:H:54:ASP:O	2.02	0.42
1:C:152:VAL:O	1:C:156:VAL:HG23	2.19	0.42
1:C:339:ARG:HH11	1:C:339:ARG:HB3	1.84	0.42
1:H:164:MET:O	1:H:168:MET:N	2.52	0.42
1:A:184:TYR:CE2	2:A:401:BTB:H51	2.55	0.42
2:B:401:BTB:H42	2:B:401:BTB:O6	2.19	0.42
1:C:22:TYR:CE2	1:C:24:PHE:HB2	2.54	0.42
1:D:206:GLN:O	1:D:209:SER:OG	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164:MET:SD	1:H:184:TYR:HB2	2.58	0.42
1:D:9:VAL:CG2	1:D:74:ALA:HB1	2.50	0.42
1:D:22:TYR:CE2	1:D:24:PHE:HB2	2.54	0.42
2:D:401:BTB:O4	2:D:401:BTB:O1	2.35	0.42
1:H:220:HIS:CD2	1:H:272:CYS:HB3	2.55	0.42
1:A:153:LYS:HA	1:A:153:LYS:HD2	1.89	0.42
1:A:232:LYS:HZ2	1:A:236:ILE:HD11	1.84	0.42
1:F:344:LEU:HG	1:F:364:TYR:HB2	2.01	0.42
1:G:267:TRP:NE1	3:G:401:GOL:H31	2.35	0.42
1:H:47:ILE:HD11	1:H:335:TYR:HE1	1.83	0.42
1:F:206:GLN:O	1:F:209:SER:OG	2.29	0.42
1:G:214:PHE:CD2	1:G:306:GLN:HG3	2.54	0.42
1:A:242:LYS:C	1:A:244:ARG:H	2.22	0.42
1:B:9:VAL:HG12	1:B:75:GLU:OE2	2.20	0.42
1:B:143:LEU:HD12	1:B:360:PHE:CZ	2.55	0.42
1:C:13:CYS:C	1:C:15:LEU:H	2.14	0.42
1:C:229:HIS:HD2	1:C:233:GLU:OE2	2.03	0.42
1:D:259:LEU:HD22	1:D:263:GLU:HB3	2.01	0.42
1:E:13:CYS:SG	1:E:14:LYS:N	2.92	0.42
1:H:164:MET:O	1:H:168:MET:HG2	2.20	0.42
1:G:36:GLN:O	1:G:36:GLN:HG3	2.19	0.42
1:H:291:PRO:O	1:H:295:VAL:HG23	2.20	0.42
1:E:165:GLU:HB2	1:E:247:ILE:HD11	2.02	0.42
1:F:7:HIS:CD2	1:F:301:ARG:NH2	2.88	0.42
1:H:125:TRP:O	1:H:129:TYR:HB2	2.20	0.42
1:A:342:GLY:O	1:A:364:TYR:HB3	2.20	0.41
1:B:136:TRP:CG	1:B:137:PRO:HD3	2.55	0.41
1:B:205:ASP:OD2	1:H:167:LYS:NZ	2.52	0.41
1:D:67:ASN:O	1:D:71:VAL:HG22	2.20	0.41
1:F:270:GLN:HB3	3:F:401:GOL:O3	2.20	0.41
1:A:271:ARG:HD3	3:A:403:GOL:H31	2.01	0.41
1:E:16:TRP:CE2	1:E:29:PRO:HD2	2.56	0.41
1:H:147:LEU:O	1:H:150:LYS:HB2	2.20	0.41
1:E:22:TYR:CE2	1:E:24:PHE:HB2	2.56	0.41
1:G:44:GLN:HB3	1:G:86:TYR:CE2	2.54	0.41
1:H:22:TYR:CE2	1:H:24:PHE:HB2	2.56	0.41
1:E:14:LYS:HE2	1:G:14:LYS:CB	2.50	0.41
1:F:142:ASN:N	1:F:142:ASN:HD22	2.19	0.41
1:C:270:GLN:HB3	3:C:401:GOL:O3	2.21	0.41
1:A:242:LYS:C	1:A:244:ARG:N	2.72	0.41
1:F:67:ASN:O	1:F:71:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:CYS:HB3	1:H:97:PHE:HD1	1.84	0.41
1:C:37:ARG:CZ	1:C:78:PRO:HB2	2.50	0.41
1:E:206:GLN:O	1:E:209:SER:HB3	2.21	0.41
1:H:315:ILE:HD12	1:H:315:ILE:HA	1.89	0.41
1:B:6:ARG:HD3	1:B:9:VAL:HG13	2.03	0.41
1:B:9:VAL:HG23	1:B:74:ALA:HB1	2.03	0.41
1:B:17:LYS:HA	1:B:17:LYS:HD2	1.91	0.41
1:C:16:TRP:CE2	1:C:29:PRO:HD2	2.55	0.41
1:C:281[A]:GLN:NE2	1:E:281:GLN:HB3	2.36	0.41
1:D:87:LEU:HD12	1:D:136:TRP:CD2	2.56	0.41
1:D:138:LYS:HB2	1:D:138:LYS:HE2	1.83	0.41
1:D:179:LEU:HD23	1:D:179:LEU:HA	1.82	0.41
1:E:158:LEU:HD11	1:E:186:ALA:HA	2.03	0.41
1:F:22:TYR:CE2	1:F:24:PHE:HB2	2.56	0.41
1:F:208:ASP:HA	1:F:211:ARG:NE	2.36	0.41
1:G:155:LEU:HA	1:G:158:LEU:HB2	2.02	0.41
1:H:6:ARG:HB3	1:H:9:VAL:HG12	2.02	0.41
1:H:17:LYS:HD3	1:H:17:LYS:C	2.41	0.41
1:H:46:GLN:HE22	1:H:93:PHE:HE2	1.67	0.41
1:H:97:PHE:CD1	1:H:97:PHE:N	2.89	0.41
1:C:326:PRO:HG3	1:H:244:ARG:CB	2.51	0.40
1:D:58:MET:HE3	1:D:58:MET:HB2	1.94	0.40
1:F:248:ASN:O	1:F:251:PRO:HD2	2.21	0.40
1:B:321:TYR:O	1:B:327:PHE:HA	2.21	0.40
1:A:229:HIS:CD2	1:A:233:GLU:HG3	2.56	0.40
1:E:355:LEU:HD23	1:E:355:LEU:HA	1.95	0.40
1:G:55:VAL:HG11	1:G:335:TYR:CD2	2.55	0.40
1:G:220:HIS:NE2	1:G:272:CYS:HB3	2.36	0.40
1:A:6:ARG:HB3	1:A:9:VAL:CG1	2.51	0.40
1:D:227:TYR:CE2	1:D:265:LYS:HB3	2.56	0.40
1:H:44:GLN:NE2	1:H:346:PHE:H	2.20	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	360/368 (98%)	345 (96%)	13 (4%)	2 (1%)	25	45
1	B	359/368 (98%)	344 (96%)	14 (4%)	1 (0%)	41	62
1	C	346/368 (94%)	332 (96%)	13 (4%)	1 (0%)	41	62
1	D	341/368 (93%)	332 (97%)	8 (2%)	1 (0%)	41	62
1	E	336/368 (91%)	322 (96%)	13 (4%)	1 (0%)	41	62
1	F	341/368 (93%)	325 (95%)	16 (5%)	0	100	100
1	G	327/368 (89%)	307 (94%)	15 (5%)	5 (2%)	10	19
1	H	326/368 (89%)	310 (95%)	12 (4%)	4 (1%)	13	25
All	All	2736/2944 (93%)	2617 (96%)	104 (4%)	15 (0%)	29	50

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	362	VAL
1	C	14	LYS
1	D	14	LYS
1	G	14	LYS
1	G	155	LEU
1	H	14	LYS
1	B	13	CYS
1	E	13	CYS
1	G	124	VAL
1	H	359	GLY
1	H	364	TYR
1	G	242	LYS
1	G	327	PHE
1	H	323	ASN

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	310/318 (98%)	303 (98%)	7 (2%)	50 73
1	B	312/318 (98%)	308 (99%)	4 (1%)	69 85
1	C	290/318 (91%)	279 (96%)	11 (4%)	33 57
1	D	287/318 (90%)	278 (97%)	9 (3%)	40 65
1	E	289/318 (91%)	282 (98%)	7 (2%)	49 72
1	F	295/318 (93%)	286 (97%)	9 (3%)	40 65
1	G	253/318 (80%)	249 (98%)	4 (2%)	62 81
1	H	249/318 (78%)	241 (97%)	8 (3%)	39 63
All	All	2285/2544 (90%)	2226 (97%)	59 (3%)	47 70

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	121	ASP
1	A	151	CYS
1	A	187	TRP
1	A	288	SER
1	A	353	ASP
1	A	364	TYR
1	B	151	CYS
1	B	187	TRP
1	B	340	LYS
1	B	364	TYR
1	C	7	HIS
1	C	13	CYS
1	C	94	TYR
1	C	151	CYS
1	C	154	SER
1	C	187	TRP
1	C	211	ARG
1	C	246	MET
1	C	281[A]	GLN
1	C	281[B]	GLN
1	C	301	ARG
1	D	14	LYS
1	D	36	GLN
1	D	151	CYS
1	D	187	TRP
1	D	244	ARG

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Mol	Chain	Res	Type
1	D	246	MET
1	D	301	ARG
1	D	338	ARG
1	D	363	ARG
1	E	7	HIS
1	E	14	LYS
1	E	119	LYS
1	E	187	TRP
1	E	242	LYS
1	E	301	ARG
1	E	364	TYR
1	F	7	HIS
1	F	34	TYR
1	F	94	TYR
1	F	119	LYS
1	F	150	LYS
1	F	187	TRP
1	F	246	MET
1	F	301	ARG
1	F	364	TYR
1	G	7	HIS
1	G	15	LEU
1	G	154	SER
1	G	187	TRP
1	H	7	HIS
1	H	53	ASP
1	H	65	ARG
1	H	133	MET
1	H	163	ASP
1	H	187	TRP
1	H	255	ARG
1	H	301	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	201	ASN
1	A	281	GLN
1	B	193	ASN
1	B	270	GLN
1	D	36	GLN

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Mol	Chain	Res	Type
1	E	281	GLN
1	F	142	ASN
1	G	36	GLN
1	G	44	GLN
1	G	281	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	G	401	-	5,5,5	0.56	0	5,5,5	0.31	0
2	BTB	D	401	-	13,13,13	0.53	0	7,16,16	0.74	0
2	BTB	B	401	-	13,13,13	0.44	0	7,16,16	0.65	0
2	BTB	A	401	-	13,13,13	0.48	0	7,16,16	1.01	0
3	GOL	B	403	-	5,5,5	0.55	0	5,5,5	0.58	0
2	BTB	B	402	-	13,13,13	0.51	0	7,16,16	0.98	0
2	BTB	A	402	-	13,13,13	0.54	0	7,16,16	0.71	0
3	GOL	H	401	-	5,5,5	0.56	0	5,5,5	0.30	0
3	GOL	D	402	-	5,5,5	0.56	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	A	403	-	5,5,5	0.54	0	5,5,5	0.24	0
3	GOL	E	401	-	5,5,5	0.57	0	5,5,5	0.27	0
3	GOL	F	401	-	5,5,5	0.56	0	5,5,5	0.42	0
3	GOL	C	401	-	5,5,5	0.55	0	5,5,5	0.38	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	GOL	G	401	-	-	0/4/4/4	-
2	BTB	D	401	-	-	7/21/21/21	-
2	BTB	B	401	-	-	15/21/21/21	-
2	BTB	A	401	-	-	11/21/21/21	-
3	GOL	B	403	-	-	0/4/4/4	-
2	BTB	B	402	-	-	9/21/21/21	-
2	BTB	A	402	-	-	12/21/21/21	-
3	GOL	H	401	-	-	2/4/4/4	-
3	GOL	D	402	-	-	2/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	E	401	-	-	2/4/4/4	-
3	GOL	F	401	-	-	2/4/4/4	-
3	GOL	C	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	BTB	O1-C1-C2-C3
2	A	401	BTB	O1-C1-C2-C4
2	A	401	BTB	O1-C1-C2-N
2	A	401	BTB	C1-C2-N-C5
2	A	401	BTB	C1-C2-N-C7
2	A	401	BTB	C3-C2-N-C5
2	A	401	BTB	C3-C2-N-C7

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Mol	Chain	Res	Type	Atoms
2	A	401	BTB	C4-C2-N-C5
2	A	401	BTB	C4-C2-N-C7
2	A	401	BTB	N-C5-C6-O6
2	A	402	BTB	O1-C1-C2-C3
2	A	402	BTB	O1-C1-C2-C4
2	A	402	BTB	O1-C1-C2-N
2	A	402	BTB	C1-C2-C3-O3
2	A	402	BTB	C4-C2-C3-O3
2	A	402	BTB	N-C2-C3-O3
2	A	402	BTB	C1-C2-C4-O4
2	A	402	BTB	C3-C2-C4-O4
2	A	402	BTB	N-C2-C4-O4
2	B	401	BTB	O1-C1-C2-C3
2	B	401	BTB	O1-C1-C2-C4
2	B	401	BTB	O1-C1-C2-N
2	B	401	BTB	C1-C2-C4-O4
2	B	401	BTB	C3-C2-C4-O4
2	B	401	BTB	N-C2-C4-O4
2	B	401	BTB	C1-C2-N-C5
2	B	401	BTB	C1-C2-N-C7
2	B	401	BTB	C3-C2-N-C5
2	B	401	BTB	C3-C2-N-C7
2	B	401	BTB	C4-C2-N-C5
2	B	401	BTB	C4-C2-N-C7
2	B	402	BTB	O1-C1-C2-C3
2	B	402	BTB	O1-C1-C2-C4
2	B	402	BTB	O1-C1-C2-N
2	B	402	BTB	C1-C2-C4-O4
2	B	402	BTB	C3-C2-C4-O4
2	B	402	BTB	N-C2-C4-O4
2	D	401	BTB	O1-C1-C2-C3
2	D	401	BTB	O1-C1-C2-C4
2	D	401	BTB	O1-C1-C2-N
2	D	401	BTB	C1-C2-C3-O3
2	D	401	BTB	C4-C2-C3-O3
2	D	401	BTB	N-C2-C3-O3
3	A	403	GOL	C1-C2-C3-O3
3	C	401	GOL	C1-C2-C3-O3
3	D	402	GOL	C1-C2-C3-O3
3	E	401	GOL	C1-C2-C3-O3
3	F	401	GOL	C1-C2-C3-O3
3	H	401	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	402	BTB	N-C7-C8-O8
2	B	401	BTB	N-C5-C6-O6
2	B	401	BTB	N-C7-C8-O8
3	A	403	GOL	O2-C2-C3-O3
3	E	401	GOL	O2-C2-C3-O3
2	A	402	BTB	N-C5-C6-O6
2	B	402	BTB	N-C7-C8-O8
3	C	401	GOL	O2-C2-C3-O3
3	F	401	GOL	O2-C2-C3-O3
2	A	402	BTB	C6-C5-N-C7
3	D	402	GOL	O2-C2-C3-O3
3	H	401	GOL	O2-C2-C3-O3
2	D	401	BTB	N-C7-C8-O8
2	A	401	BTB	N-C7-C8-O8
2	B	401	BTB	C8-C7-N-C2
2	B	402	BTB	C1-C2-N-C5
2	B	402	BTB	C3-C2-N-C5

There are no ring outliers.

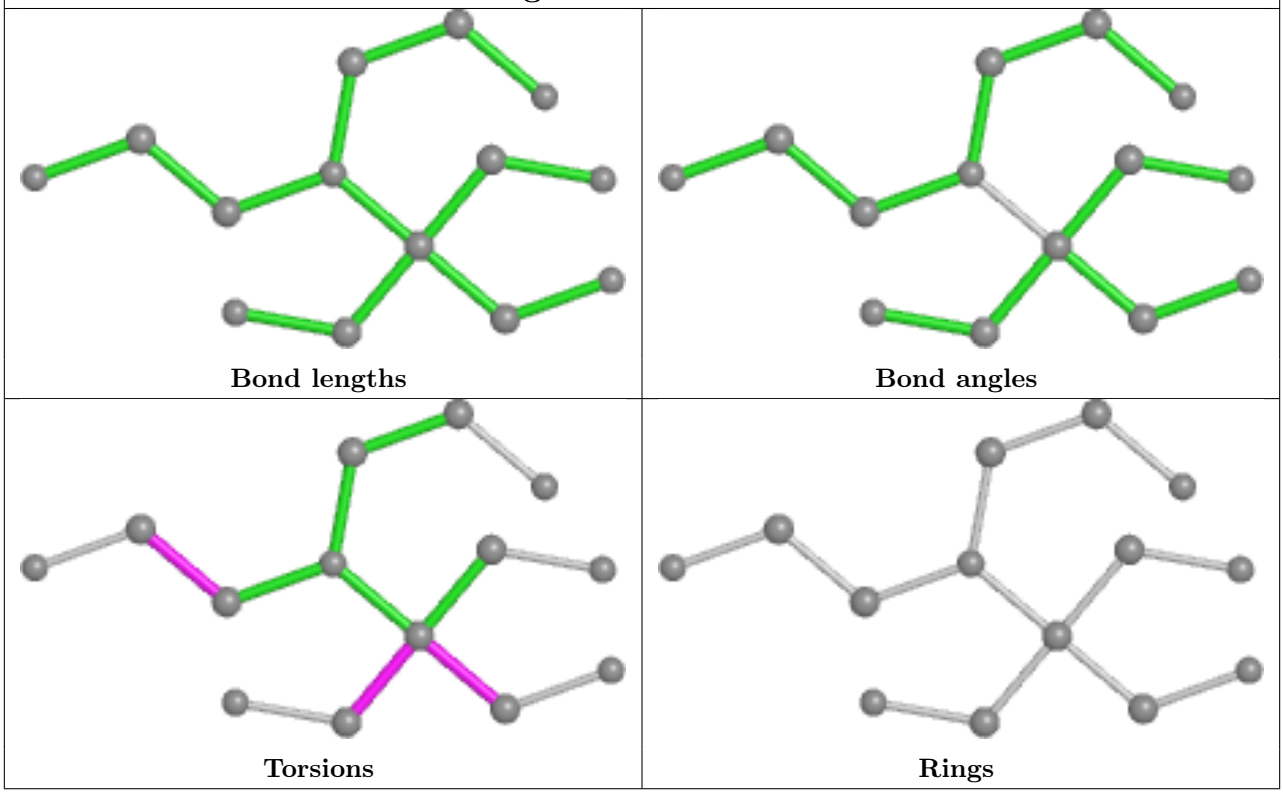
11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	GOL	3	0
2	D	401	BTB	4	0
2	B	401	BTB	4	0
2	A	401	BTB	4	0
2	A	402	BTB	4	0
3	H	401	GOL	1	0
3	D	402	GOL	1	0
3	A	403	GOL	2	0
3	E	401	GOL	2	0
3	F	401	GOL	2	0
3	C	401	GOL	2	0

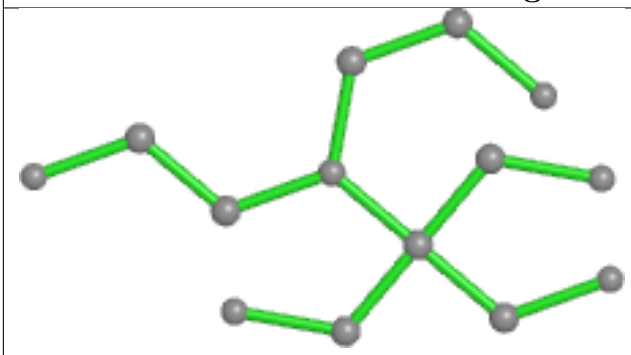
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

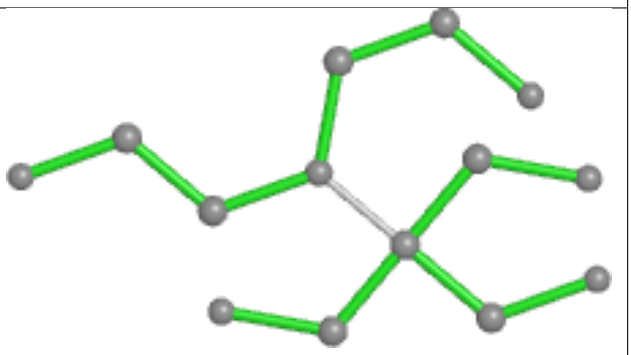
Ligand BTB D 401



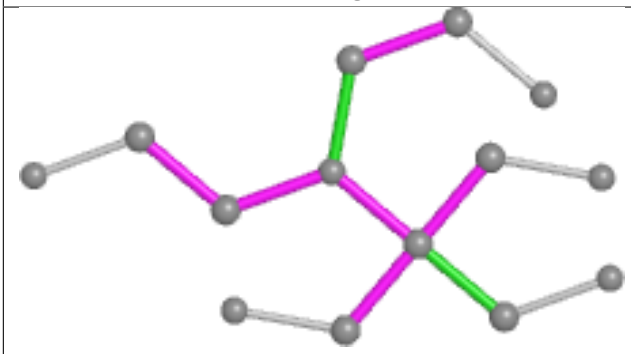
Ligand BTB B 401



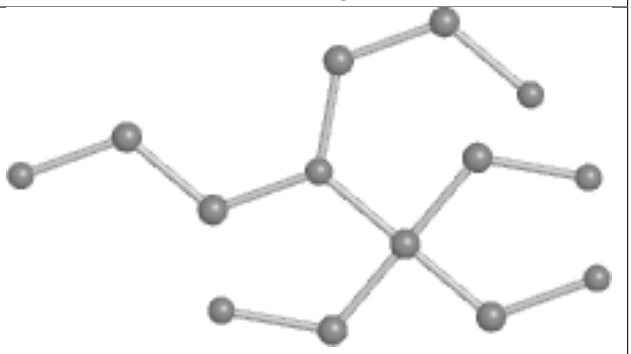
Bond lengths



Bond angles

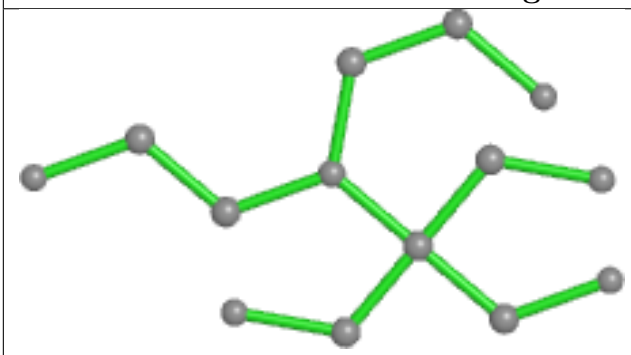


Torsions

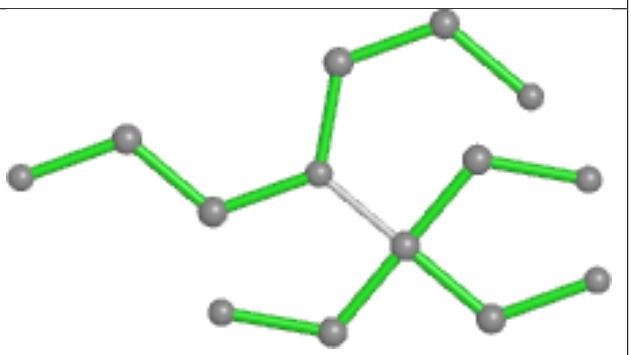


Rings

Ligand BTB A 401



Bond lengths



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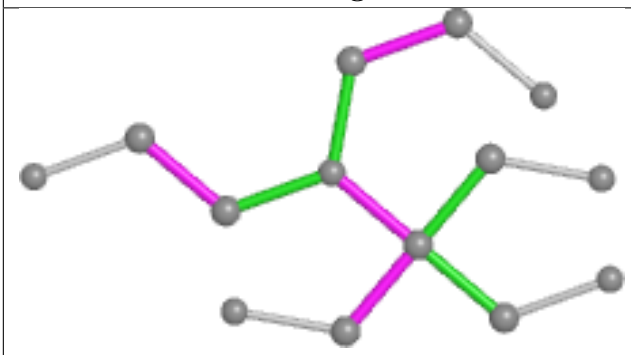

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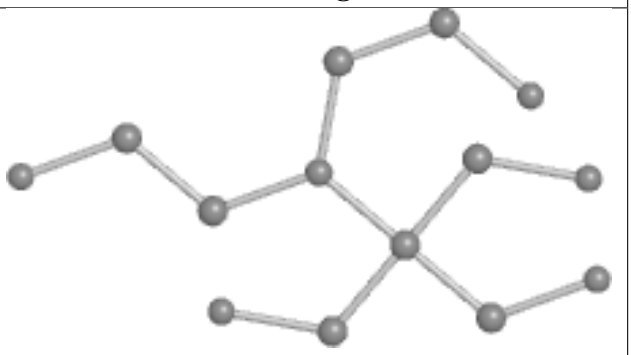
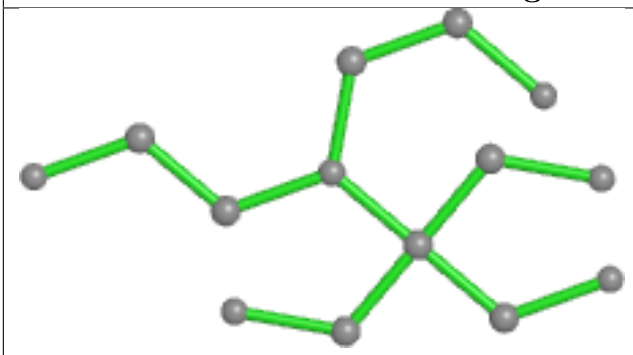
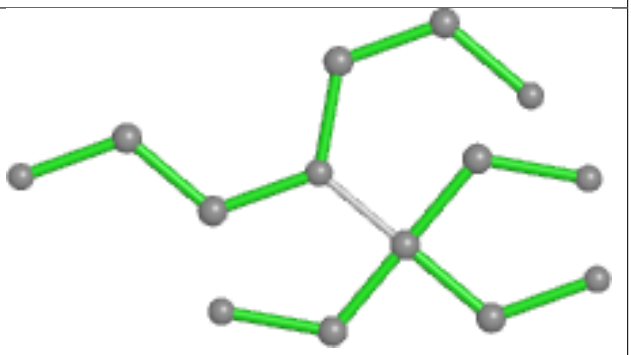


Rings

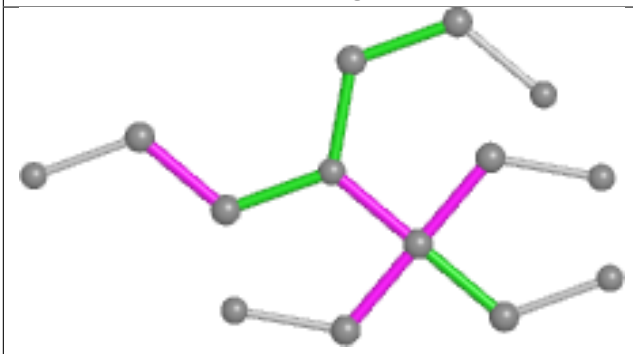
Ligand BTB B 402



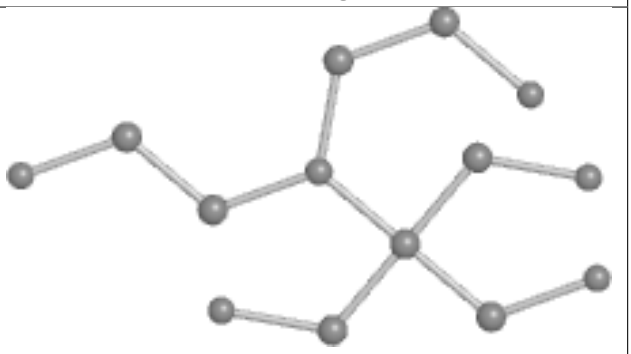
Bond lengths



Bond angles

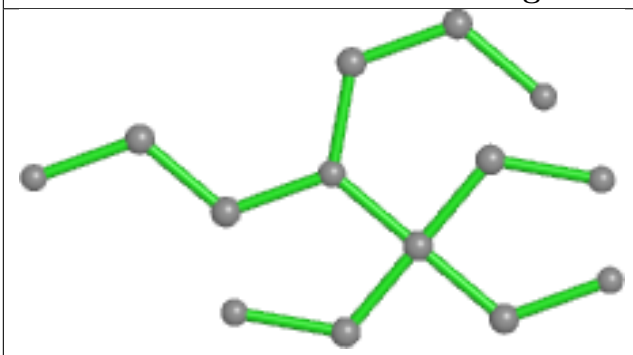


Torsions

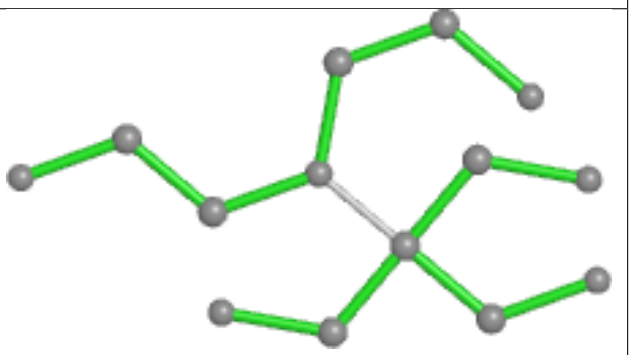


Rings

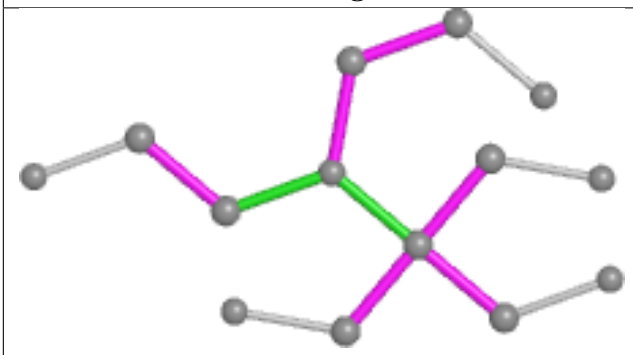
Ligand BTB A 402



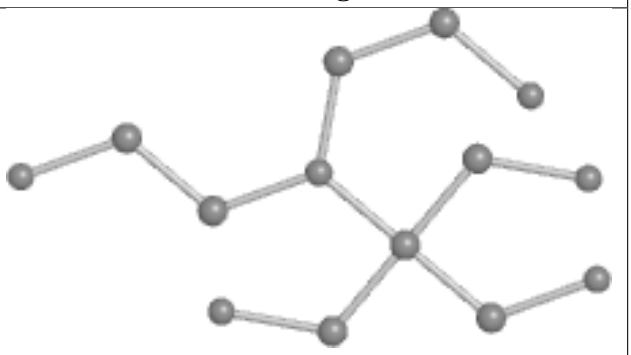
Bond lengths



Bond angles



Torsions



Rings

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

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	362/368 (98%)	0.11	3 (0%)	86	84	20, 36, 61, 106	0
1	B	361/368 (98%)	0.11	2 (0%)	89	88	21, 34, 63, 80	0
1	C	349/368 (94%)	0.23	8 (2%)	60	55	22, 40, 76, 104	0
1	D	345/368 (93%)	0.19	6 (1%)	70	66	21, 40, 71, 102	0
1	E	340/368 (92%)	0.22	7 (2%)	63	58	26, 41, 81, 111	0
1	F	345/368 (93%)	0.30	11 (3%)	47	41	23, 40, 87, 131	0
1	G	335/368 (91%)	1.12	76 (22%)	0	0	25, 57, 139, 162	0
1	H	334/368 (90%)	1.30	89 (26%)	0	0	26, 60, 142, 185	0
All	All	2771/2944 (94%)	0.44	202 (7%)	15	11	20, 42, 118, 185	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	345	TRP	10.1
1	G	358	GLY	9.5
1	G	326	PRO	7.7
1	H	335	TYR	7.5
1	H	362	VAL	7.4
1	G	353	ASP	7.4
1	H	57	ALA	7.2
1	F	366	ASN	6.9
1	H	360	PHE	6.9
1	H	50	PHE	6.8
1	H	358	GLY	6.7
1	G	335	TYR	6.6
1	H	63	GLY	6.6
1	G	154	SER	6.5
1	H	355	LEU	6.3
1	H	55	VAL	6.2

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Mol	Chain	Res	Type	RSRZ
1	G	343	ALA	5.7
1	H	125	TRP	5.6
1	G	350	THR	5.6
1	G	151	CYS	5.4
1	H	350	THR	5.4
1	H	137	PRO	5.2
1	H	132	THR	5.0
1	G	327	PHE	5.0
1	H	356	MET	4.8
1	H	156	VAL	4.8
1	H	61	ALA	4.8
1	G	64	PRO	4.8
1	H	158	LEU	4.6
1	G	122	ASN	4.5
1	H	343	ALA	4.5
1	G	55	VAL	4.5
1	H	157	ALA	4.4
1	F	158	LEU	4.4
1	H	359	GLY	4.3
1	H	361	GLU	4.3
1	H	64	PRO	4.3
1	G	139	ILE	4.3
1	H	334	PRO	4.2
1	G	331	TYR	4.2
1	H	352	SER	4.2
1	G	127	ALA	4.2
1	G	346	PHE	4.2
1	H	340	LYS	4.1
1	H	331	TYR	4.0
1	H	162	THR	4.0
1	G	352	SER	4.0
1	H	134	THR	3.9
1	H	53	ASP	3.9
1	H	365	ALA	3.9
1	F	120	TYR	3.9
1	H	60	GLY	3.9
1	G	124	VAL	3.9
1	G	356	MET	3.9
1	E	120	TYR	3.8
1	G	349	VAL	3.8
1	G	333	ALA	3.8
1	G	355	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	363	ARG	3.7
1	G	143	LEU	3.7
1	H	357	THR	3.7
1	H	129	TYR	3.7
1	H	144	ASP	3.7
1	G	329	GLU	3.7
1	H	59	PRO	3.7
1	G	325	PRO	3.7
1	G	136	TRP	3.7
1	H	347	GLU	3.6
1	H	333	ALA	3.6
1	H	151	CYS	3.6
1	G	334	PRO	3.6
1	H	338	ARG	3.5
1	H	339	ARG	3.5
1	F	118	PRO	3.5
1	H	320	THR	3.5
1	A	243	GLY	3.5
1	G	240	TYR	3.4
1	G	144	ASP	3.4
1	G	323	ASN	3.3
1	H	54	ASP	3.3
1	G	344	LEU	3.3
1	G	336	GLU	3.3
1	G	41	ALA	3.2
1	G	63	GLY	3.2
1	B	364	TYR	3.2
1	H	321	TYR	3.2
1	H	332	ALA	3.2
1	H	143	LEU	3.2
1	G	125	TRP	3.1
1	H	141	GLU	3.1
1	E	234	ALA	3.1
1	G	59	PRO	3.1
1	H	131	ASN	3.1
1	H	346	PHE	3.1
1	G	351	GLU	3.1
1	H	7	HIS	3.1
1	H	140	LEU	3.0
1	G	161	GLY	3.0
1	H	136	TRP	3.0
1	G	56	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	137	PRO	3.0
1	G	54	ASP	3.0
1	F	117	ASP	3.0
1	G	49	VAL	3.0
1	H	349	VAL	3.0
1	H	43	ILE	2.9
1	C	366	ASN	2.9
1	D	121	ASP	2.9
1	H	93	PHE	2.9
1	G	138	LYS	2.9
1	H	366	ASN	2.9
1	F	161	GLY	2.9
1	H	336	GLU	2.9
1	H	133	MET	2.9
1	G	94	TYR	2.9
1	H	323	ASN	2.8
1	H	244	ARG	2.8
1	G	348	LYS	2.8
1	F	243	GLY	2.8
1	H	41	ALA	2.8
1	G	156	VAL	2.7
1	H	344	LEU	2.7
1	C	364	TYR	2.7
1	G	50	PHE	2.7
1	H	42	SER	2.7
1	E	239	THR	2.7
1	H	124	VAL	2.7
1	G	332	ALA	2.7
1	G	128	ASN	2.7
1	G	330	GLY	2.7
1	H	142	ASN	2.6
1	H	353	ASP	2.6
1	H	51	GLY	2.6
1	G	152	VAL	2.6
1	G	158	LEU	2.6
1	H	243	GLY	2.5
1	H	322	HIS	2.5
1	G	324	HIS	2.5
1	E	158	LEU	2.5
1	C	244	ARG	2.5
1	C	365	ALA	2.5
1	H	86	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	61	ALA	2.5
1	G	140	LEU	2.5
1	H	239	THR	2.4
1	H	62	LEU	2.4
1	A	366	ASN	2.4
1	H	52	LYS	2.4
1	G	57	ALA	2.4
1	H	161	GLY	2.4
1	H	46	GLN	2.4
1	F	365	ALA	2.4
1	G	0	ASN	2.4
1	H	0	ASN	2.4
1	H	342	GLY	2.4
1	A	211	ARG	2.4
1	G	360	PHE	2.3
1	H	56	GLY	2.3
1	G	133	MET	2.3
1	H	341	GLU	2.3
1	G	132	THR	2.3
1	G	123	PRO	2.3
1	C	0	ASN	2.2
1	H	45	ALA	2.2
1	G	53	ASP	2.2
1	H	149	PRO	2.2
1	G	130	LYS	2.2
1	H	97	PHE	2.2
1	G	149	PRO	2.2
1	H	145	PRO	2.2
1	H	348	LYS	2.2
1	C	14	LYS	2.2
1	G	42	SER	2.2
1	F	51	GLY	2.2
1	F	364	TYR	2.2
1	G	97	PHE	2.2
1	E	235	GLU	2.2
1	G	131	ASN	2.2
1	G	18	ASP	2.2
1	H	88	ASN	2.1
1	E	237	HIS	2.1
1	F	121	ASP	2.1
1	H	48	ASP	2.1
1	G	357	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	293	GLU	2.1
1	D	0	ASN	2.1
1	D	359	GLY	2.1
1	H	34	TYR	2.1
1	D	187	TRP	2.1
1	G	93	PHE	2.1
1	B	336	GLU	2.1
1	G	62	LEU	2.1
1	G	328	GLY	2.1
1	G	359	GLY	2.1
1	C	336	GLU	2.0
1	H	65	ARG	2.0
1	D	364	TYR	2.0
1	C	94	TYR	2.0
1	E	238	SER	2.0
1	G	46	GLN	2.0
1	G	320	THR	2.0
1	G	96	CYS	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
2	BTB	A	401	14/14	0.61	0.35	67,72,78,86	0
2	BTB	B	401	14/14	0.72	0.29	56,63,70,72	0
2	BTB	D	401	14/14	0.82	0.23	54,62,81,81	0
2	BTB	B	402	14/14	0.84	0.27	53,62,69,73	0
3	GOL	B	403	6/6	0.87	0.41	35,37,43,47	0

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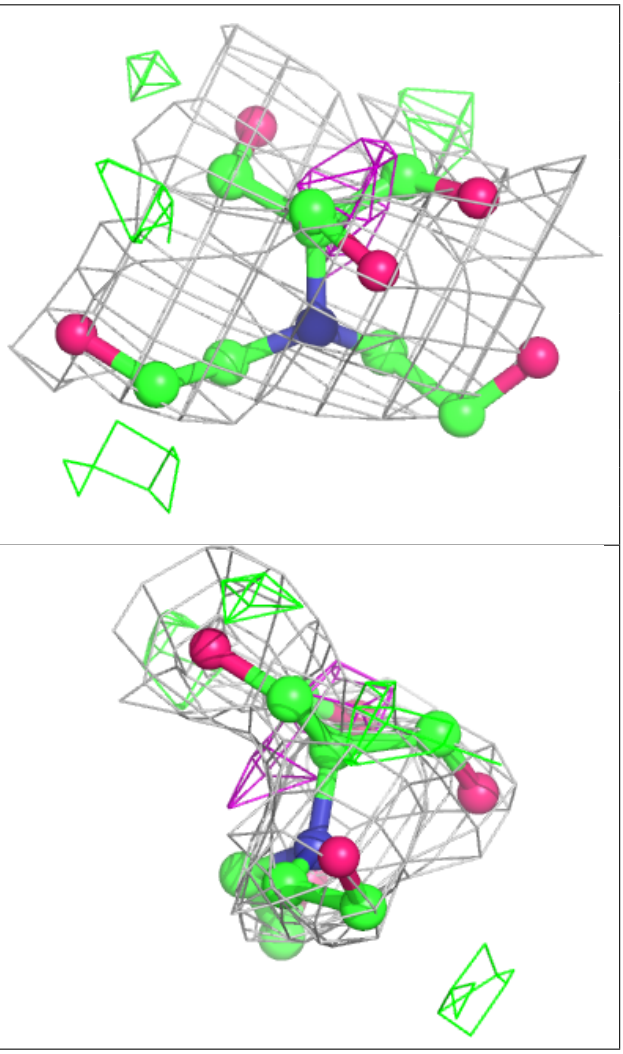
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	F	401	6/6	0.90	0.26	42,45,48,59	0
3	GOL	A	403	6/6	0.91	0.23	34,36,42,45	0
2	BTB	A	402	14/14	0.92	0.32	52,57,64,66	0
3	GOL	G	401	6/6	0.92	0.29	40,45,50,50	0
3	GOL	H	401	6/6	0.92	0.27	48,51,52,64	0
3	GOL	D	402	6/6	0.95	0.19	28,34,37,43	0
3	GOL	E	401	6/6	0.96	0.24	31,33,39,41	0
3	GOL	C	401	6/6	0.96	0.16	32,39,41,45	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.

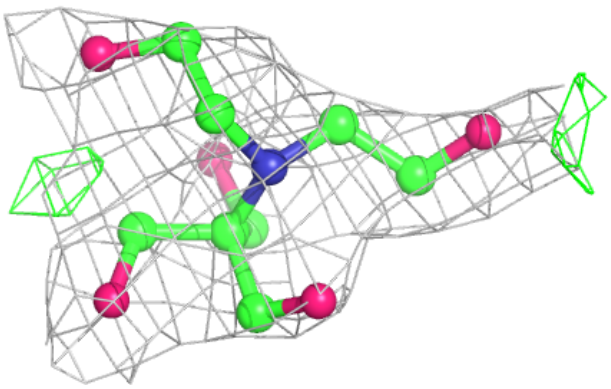
Electron density around BTB A 401:

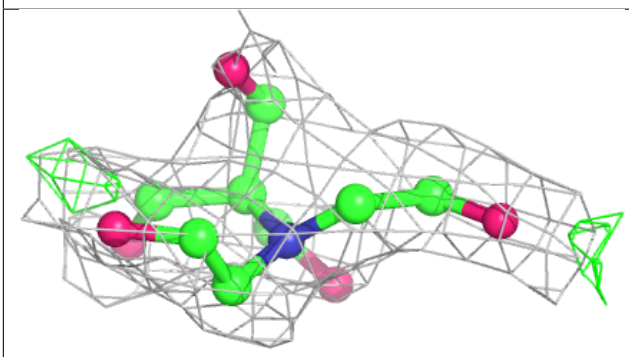
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

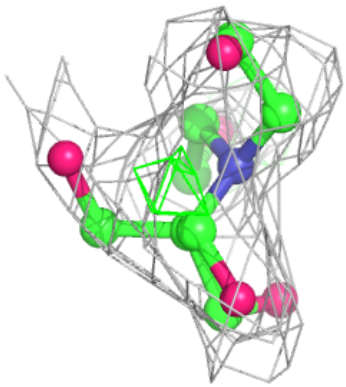


Electron density around BTB B 401:

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

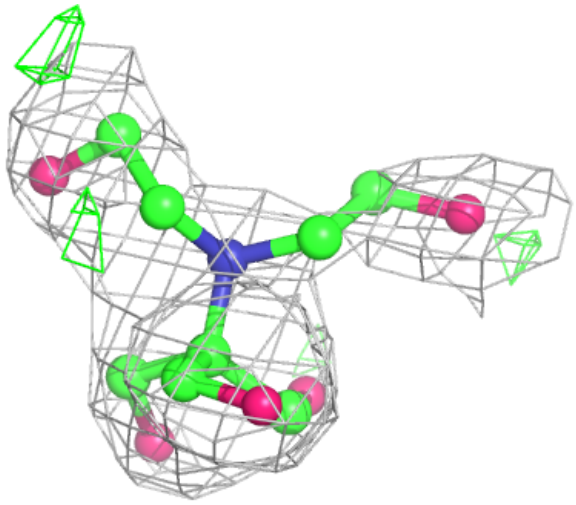


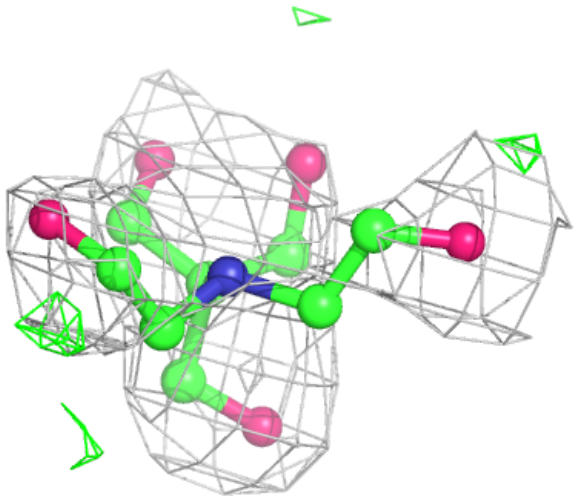


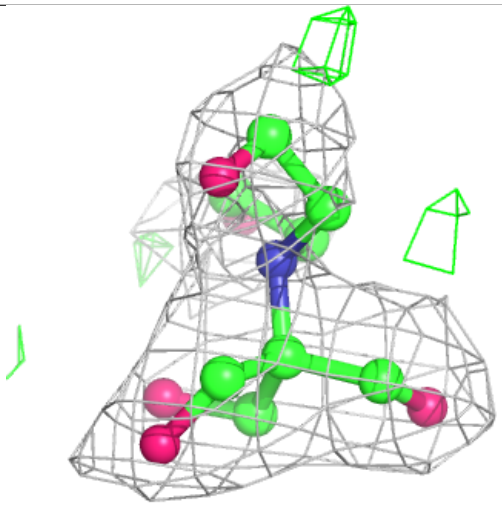


Electron density around BTB D 401:

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

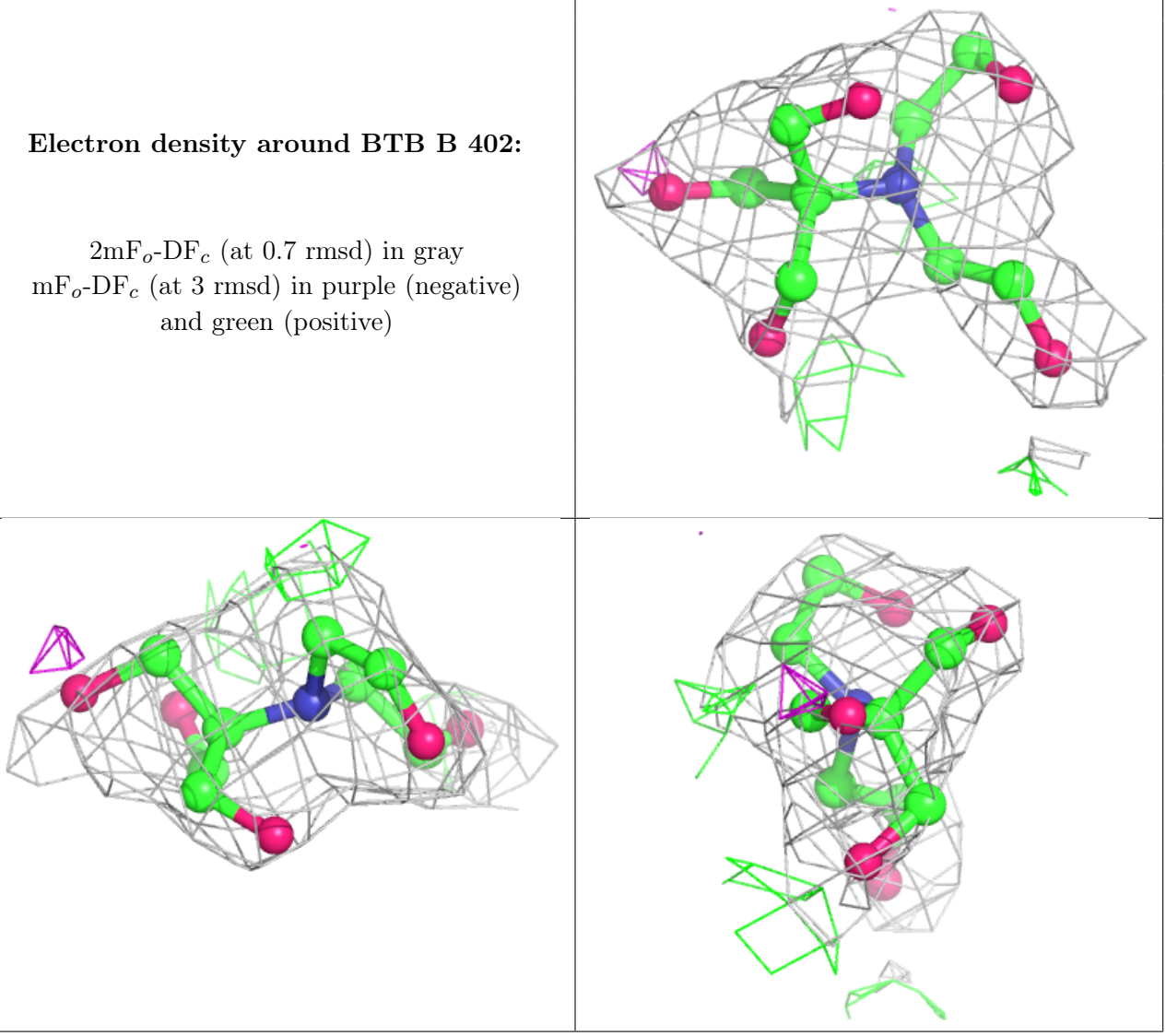






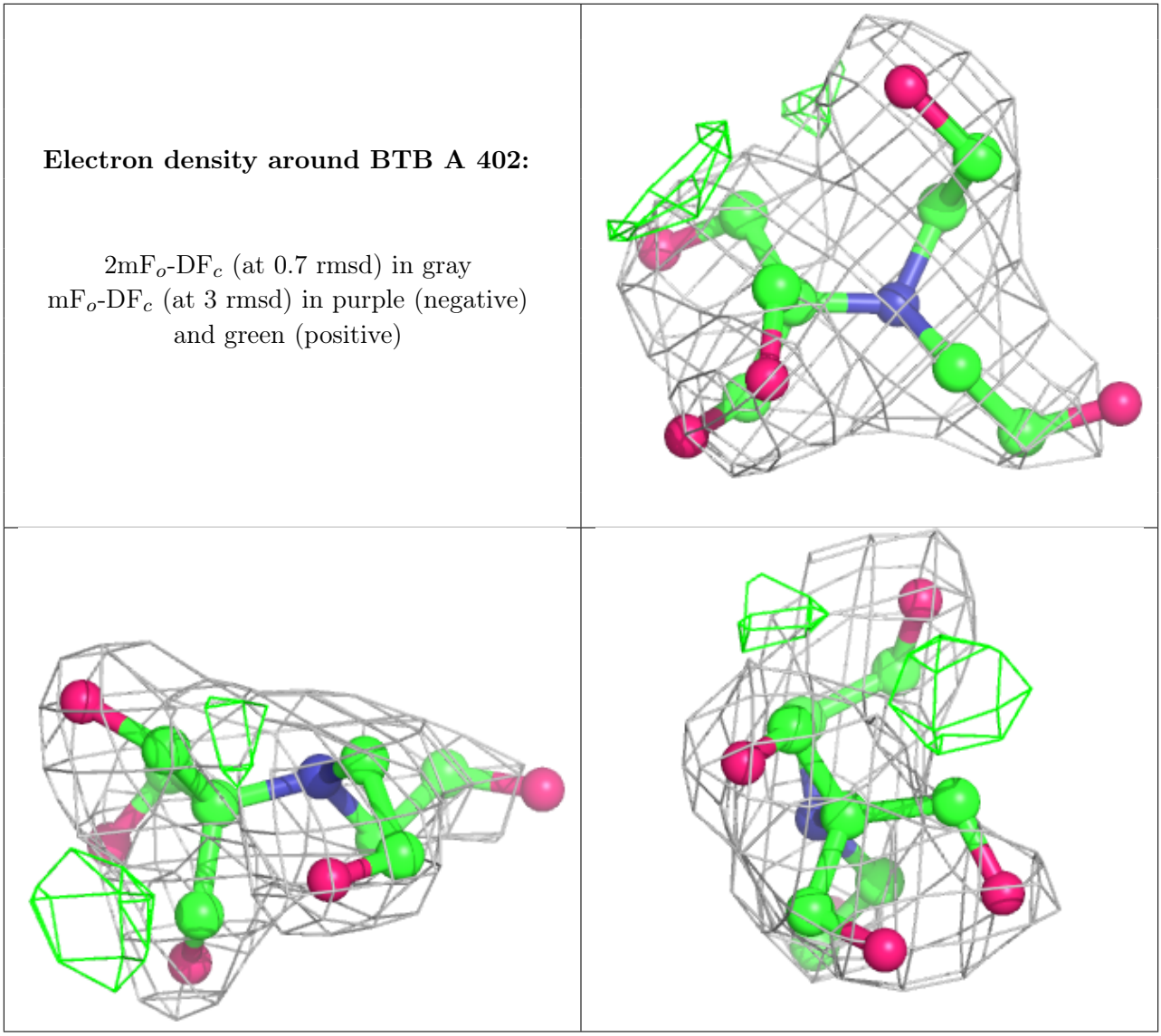
Electron density around BTB B 402:

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



Electron density around BTB A 402:

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



6.5 Other polymers

There are no such residues in this entry.