Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 11:40 pm GMT

PDB ID	:	6TWM
Title	:	Product bound structure of the Ectoine utilization protein EutE (DoeB) from Ruegeria pomeroyi
Authors	:	Mais, C.-N.; Altegoer, F.; Bange, G.
Deposited on	:	2020-01-13
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

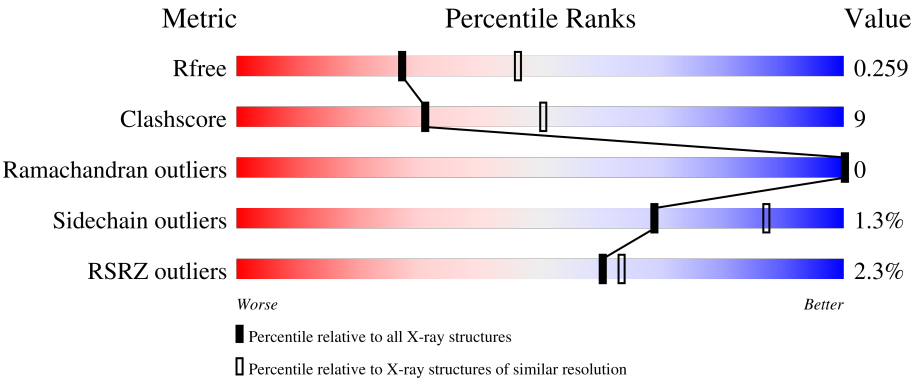
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	337	79% 17%
1	B	337	% 78% 18%
1	C	337	% 79% 18%
1	D	337	2% 75% 20%
1	E	337	% 79% 17%

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Mol	Chain	Length	Quality of chain
1	F	337	82% 15%
1	G	337	4% 72% 23%
1	H	337	% 79% 18%
1	I	337	4% 79% 17%
1	J	337	4% 75% 22%
1	K	337	2% 82% 15%
1	L	337	6% 67% 28%

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
3	DAB	B	402	-	-	X	-
4	ACT	C	402	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 30865 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 N-acetyl-L-2,4-diaminobutyric acid deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2442	1544	422	464	12			
1	B	326	Total	C	N	O	S	0	0	0
			2442	1544	422	464	12			
1	C	325	Total	C	N	O	S	0	0	0
			2434	1538	421	463	12			
1	D	328	Total	C	N	O	S	0	0	0
			2461	1555	427	467	12			
1	E	327	Total	C	N	O	S	0	0	0
			2451	1549	424	466	12			
1	F	327	Total	C	N	O	S	0	0	0
			2446	1546	423	465	12			
1	G	327	Total	C	N	O	S	0	0	0
			2451	1549	424	466	12			
1	H	327	Total	C	N	O	S	0	0	0
			2451	1549	424	466	12			
1	I	326	Total	C	N	O	S	0	0	0
			2442	1544	422	464	12			
1	J	326	Total	C	N	O	S	0	0	0
			2443	1543	423	465	12			
1	K	327	Total	C	N	O	S	0	0	0
			2451	1549	424	466	12			
1	L	324	Total	C	N	O	S	0	0	0
			2426	1532	421	461	12			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q5LUB5
A	-5	GLY	-	expression tag	UNP Q5LUB5
A	-4	HIS	-	expression tag	UNP Q5LUB5
A	-3	HIS	-	expression tag	UNP Q5LUB5
A	-2	HIS	-	expression tag	UNP Q5LUB5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP Q5LUB5
A	0	HIS	-	expression tag	UNP Q5LUB5
A	1	HIS	-	expression tag	UNP Q5LUB5
B	-6	MET	-	initiating methionine	UNP Q5LUB5
B	-5	GLY	-	expression tag	UNP Q5LUB5
B	-4	HIS	-	expression tag	UNP Q5LUB5
B	-3	HIS	-	expression tag	UNP Q5LUB5
B	-2	HIS	-	expression tag	UNP Q5LUB5
B	-1	HIS	-	expression tag	UNP Q5LUB5
B	0	HIS	-	expression tag	UNP Q5LUB5
B	1	HIS	-	expression tag	UNP Q5LUB5
C	-6	MET	-	initiating methionine	UNP Q5LUB5
C	-5	GLY	-	expression tag	UNP Q5LUB5
C	-4	HIS	-	expression tag	UNP Q5LUB5
C	-3	HIS	-	expression tag	UNP Q5LUB5
C	-2	HIS	-	expression tag	UNP Q5LUB5
C	-1	HIS	-	expression tag	UNP Q5LUB5
C	0	HIS	-	expression tag	UNP Q5LUB5
C	1	HIS	-	expression tag	UNP Q5LUB5
D	-6	MET	-	initiating methionine	UNP Q5LUB5
D	-5	GLY	-	expression tag	UNP Q5LUB5
D	-4	HIS	-	expression tag	UNP Q5LUB5
D	-3	HIS	-	expression tag	UNP Q5LUB5
D	-2	HIS	-	expression tag	UNP Q5LUB5
D	-1	HIS	-	expression tag	UNP Q5LUB5
D	0	HIS	-	expression tag	UNP Q5LUB5
D	1	HIS	-	expression tag	UNP Q5LUB5
E	-6	MET	-	initiating methionine	UNP Q5LUB5
E	-5	GLY	-	expression tag	UNP Q5LUB5
E	-4	HIS	-	expression tag	UNP Q5LUB5
E	-3	HIS	-	expression tag	UNP Q5LUB5
E	-2	HIS	-	expression tag	UNP Q5LUB5
E	-1	HIS	-	expression tag	UNP Q5LUB5
E	0	HIS	-	expression tag	UNP Q5LUB5
E	1	HIS	-	expression tag	UNP Q5LUB5
F	-6	MET	-	initiating methionine	UNP Q5LUB5
F	-5	GLY	-	expression tag	UNP Q5LUB5
F	-4	HIS	-	expression tag	UNP Q5LUB5
F	-3	HIS	-	expression tag	UNP Q5LUB5
F	-2	HIS	-	expression tag	UNP Q5LUB5
F	-1	HIS	-	expression tag	UNP Q5LUB5
F	0	HIS	-	expression tag	UNP Q5LUB5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	HIS	-	expression tag	UNP Q5LUB5
G	-6	MET	-	initiating methionine	UNP Q5LUB5
G	-5	GLY	-	expression tag	UNP Q5LUB5
G	-4	HIS	-	expression tag	UNP Q5LUB5
G	-3	HIS	-	expression tag	UNP Q5LUB5
G	-2	HIS	-	expression tag	UNP Q5LUB5
G	-1	HIS	-	expression tag	UNP Q5LUB5
G	0	HIS	-	expression tag	UNP Q5LUB5
G	1	HIS	-	expression tag	UNP Q5LUB5
H	-6	MET	-	initiating methionine	UNP Q5LUB5
H	-5	GLY	-	expression tag	UNP Q5LUB5
H	-4	HIS	-	expression tag	UNP Q5LUB5
H	-3	HIS	-	expression tag	UNP Q5LUB5
H	-2	HIS	-	expression tag	UNP Q5LUB5
H	-1	HIS	-	expression tag	UNP Q5LUB5
H	0	HIS	-	expression tag	UNP Q5LUB5
H	1	HIS	-	expression tag	UNP Q5LUB5
I	-6	MET	-	initiating methionine	UNP Q5LUB5
I	-5	GLY	-	expression tag	UNP Q5LUB5
I	-4	HIS	-	expression tag	UNP Q5LUB5
I	-3	HIS	-	expression tag	UNP Q5LUB5
I	-2	HIS	-	expression tag	UNP Q5LUB5
I	-1	HIS	-	expression tag	UNP Q5LUB5
I	0	HIS	-	expression tag	UNP Q5LUB5
I	1	HIS	-	expression tag	UNP Q5LUB5
J	-6	MET	-	initiating methionine	UNP Q5LUB5
J	-5	GLY	-	expression tag	UNP Q5LUB5
J	-4	HIS	-	expression tag	UNP Q5LUB5
J	-3	HIS	-	expression tag	UNP Q5LUB5
J	-2	HIS	-	expression tag	UNP Q5LUB5
J	-1	HIS	-	expression tag	UNP Q5LUB5
J	0	HIS	-	expression tag	UNP Q5LUB5
J	1	HIS	-	expression tag	UNP Q5LUB5
K	-6	MET	-	initiating methionine	UNP Q5LUB5
K	-5	GLY	-	expression tag	UNP Q5LUB5
K	-4	HIS	-	expression tag	UNP Q5LUB5
K	-3	HIS	-	expression tag	UNP Q5LUB5
K	-2	HIS	-	expression tag	UNP Q5LUB5
K	-1	HIS	-	expression tag	UNP Q5LUB5
K	0	HIS	-	expression tag	UNP Q5LUB5
K	1	HIS	-	expression tag	UNP Q5LUB5
L	-6	MET	-	initiating methionine	UNP Q5LUB5

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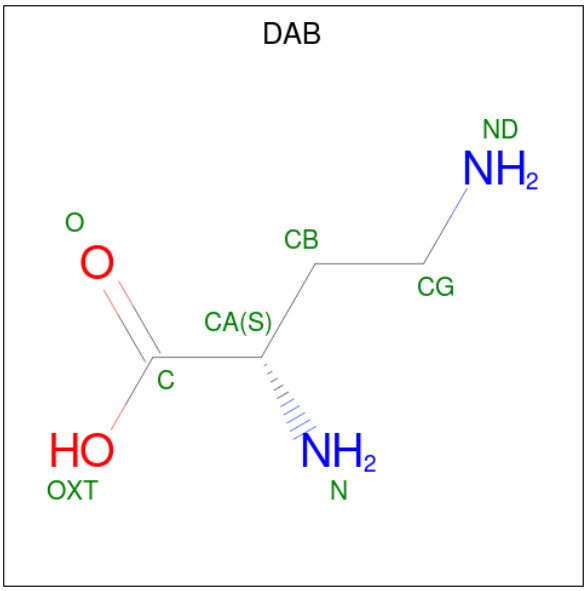
Chain	Residue	Modelled	Actual	Comment	Reference
L	-5	GLY	-	expression tag	UNP Q5LUB5
L	-4	HIS	-	expression tag	UNP Q5LUB5
L	-3	HIS	-	expression tag	UNP Q5LUB5
L	-2	HIS	-	expression tag	UNP Q5LUB5
L	-1	HIS	-	expression tag	UNP Q5LUB5
L	0	HIS	-	expression tag	UNP Q5LUB5
L	1	HIS	-	expression tag	UNP Q5LUB5

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

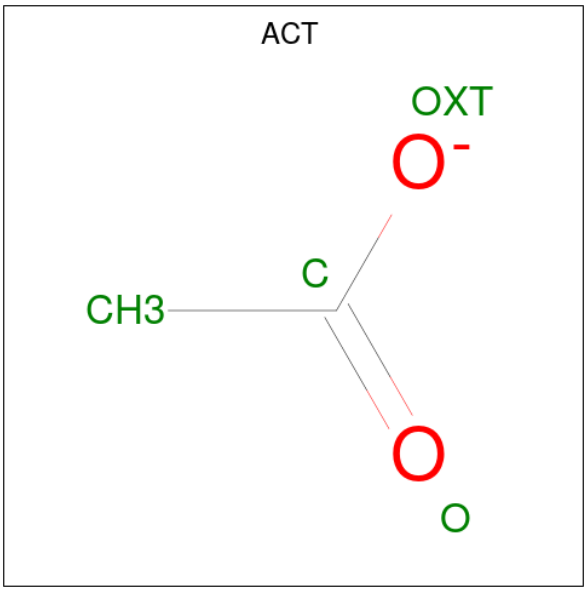
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0

- Molecule 3 is 2,4-DIAMINOBUTYRIC ACID (three-letter code: DAB) (formula: $C_4H_{10}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 8 4 2 2	0	0
3	B	1	Total C N O 8 4 2 2	0	0
3	D	1	Total C N O 8 4 2 2	0	0
3	E	1	Total C N O 8 4 2 2	0	0
3	F	1	Total C N O 8 4 2 2	0	0
3	J	1	Total C N O 8 4 2 2	0	0
3	K	1	Total C N O 8 4 2 2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	144	Total O 144 144	0	0
5	B	130	Total O 130 130	0	0
5	C	130	Total O 130 130	0	0
5	D	111	Total O 111 111	0	0
5	E	117	Total O 117 117	0	0
5	F	131	Total O 131 131	0	0
5	G	121	Total O 121 121	0	0
5	H	112	Total O 112 112	0	0
5	I	108	Total O 108 108	0	0

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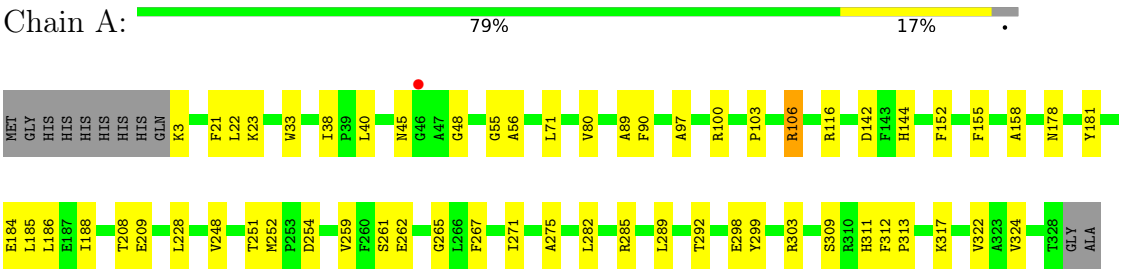
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	118	Total O 118 118	0	0
5	K	118	Total O 118 118	0	0
5	L	107	Total O 107 107	0	0

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.

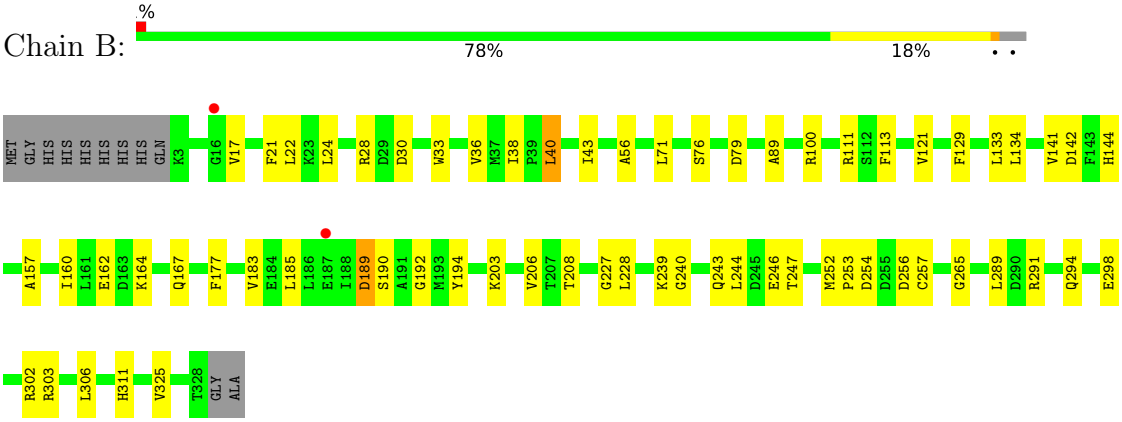
• Molecule 1: N-acetyl-L-2,4-diaminobutyric acid deacetylase

Chain A:



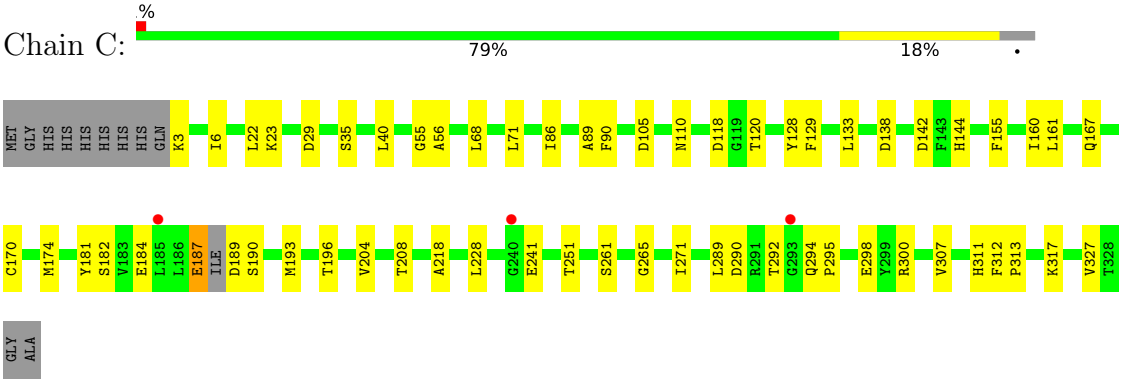
• Molecule 1: N-acetyl-L-2,4-diaminobutyric acid deacetylase

Chain B:



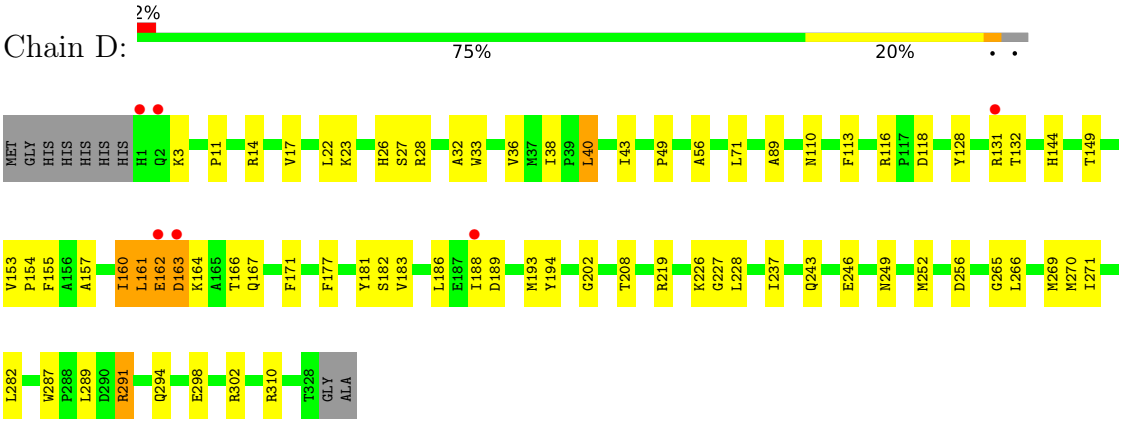
• Molecule 1: N-acetyl-L-2,4-diaminobutyric acid deacetylase

Chain C:



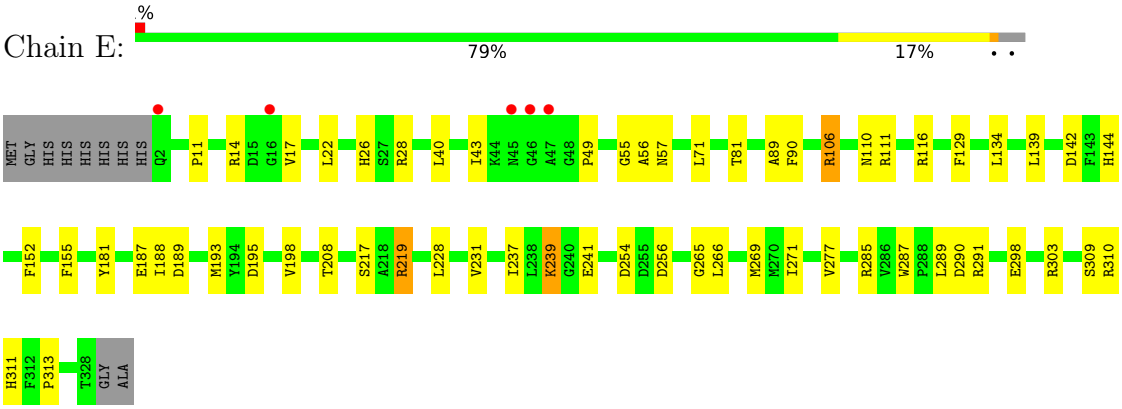
• Molecule 1: N-acetyl-L-2,4-diaminobutyric acid deacetylase

Chain D:



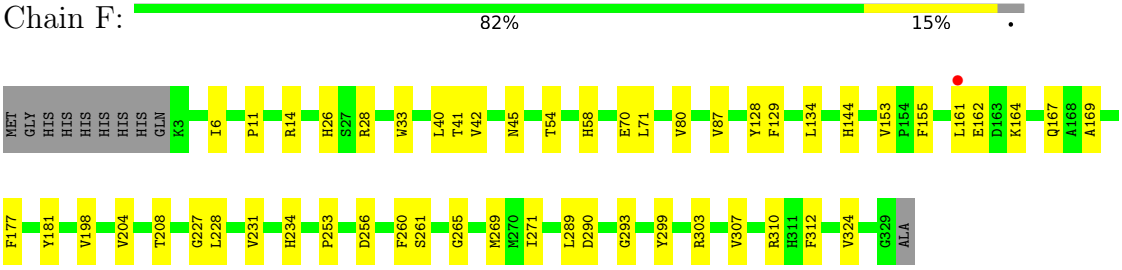
• Molecule 1: N-acetyl-L-2,4-diaminobutyric acid deacetylase

Chain E:



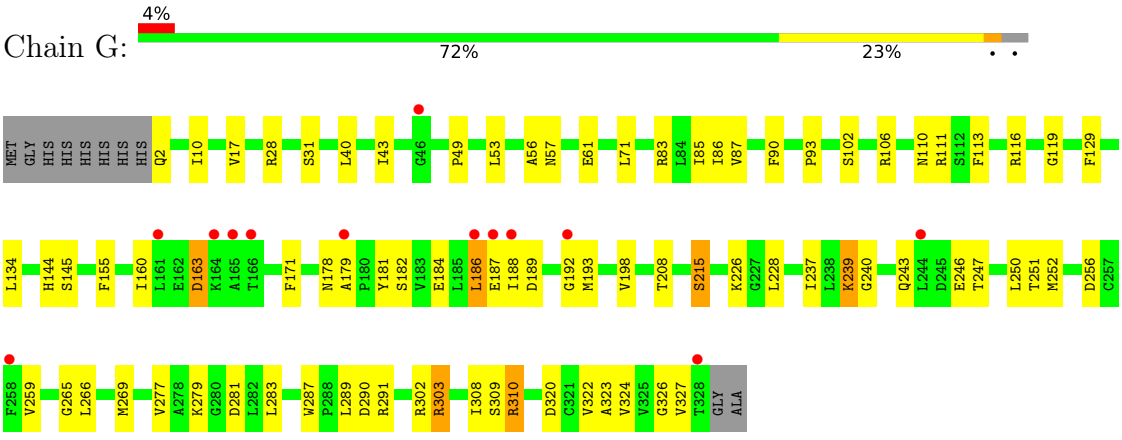
• Molecule 1: N-acetyl-L-2,4-diaminobutyric acid deacetylase

Chain F:



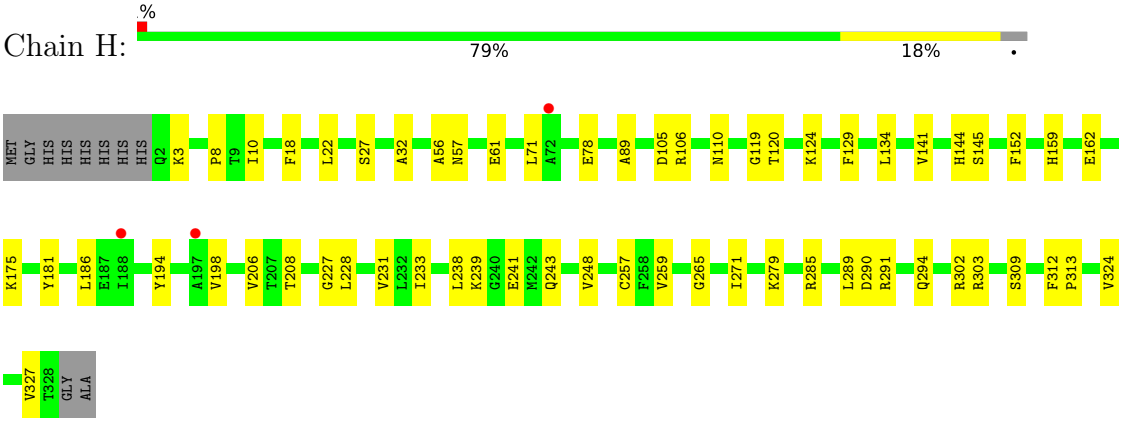
• Molecule 1: N-acetyl-L-2,4-diaminobutyric acid deacetylase

Chain G:



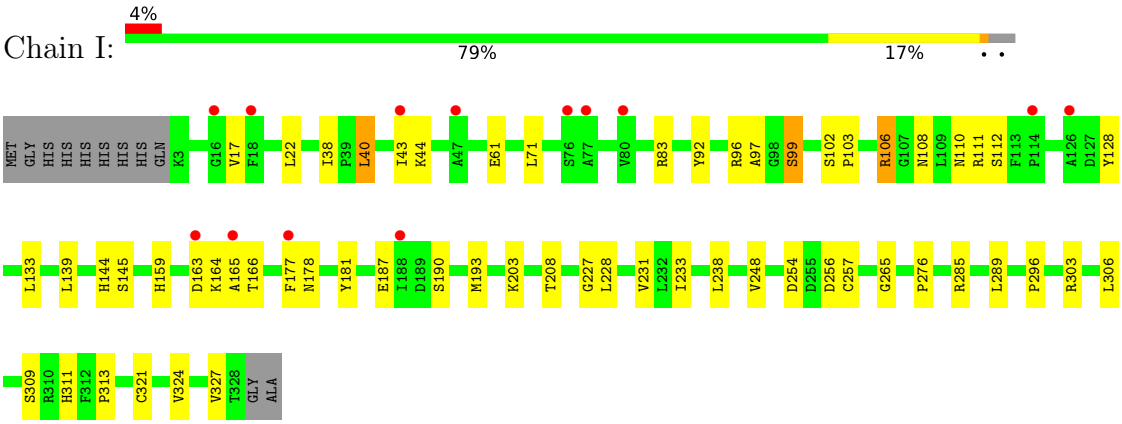
• Molecule 1: N-acetyl-L-2,4-diaminobutyric acid deacetylase

Chain H:



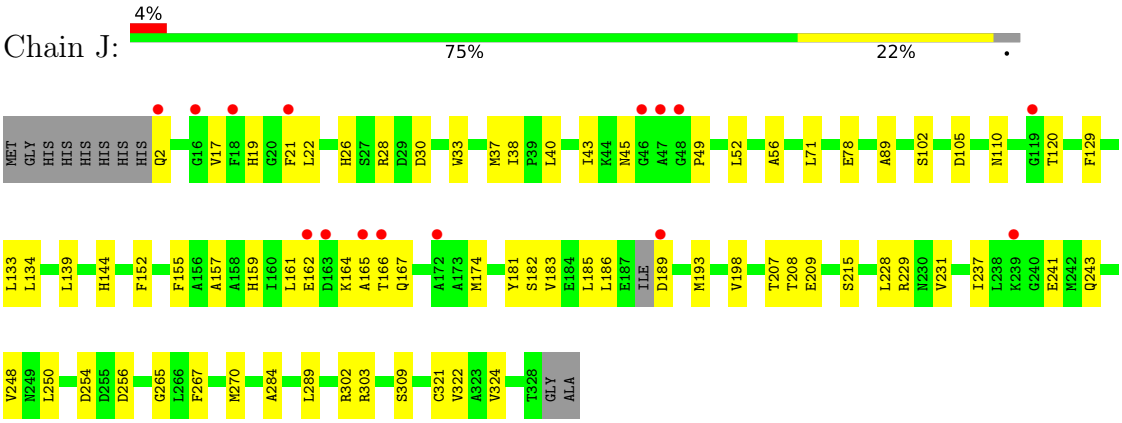
• Molecule 1: N-acetyl-L-2,4-diaminobutyric acid deacetylase

Chain I:



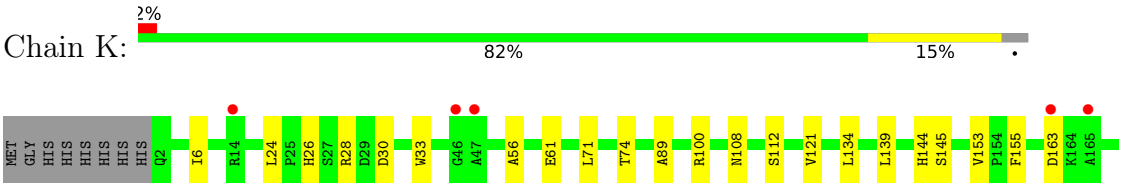
• Molecule 1: N-acetyl-L-2,4-diaminobutyric acid deacetylase

Chain J:



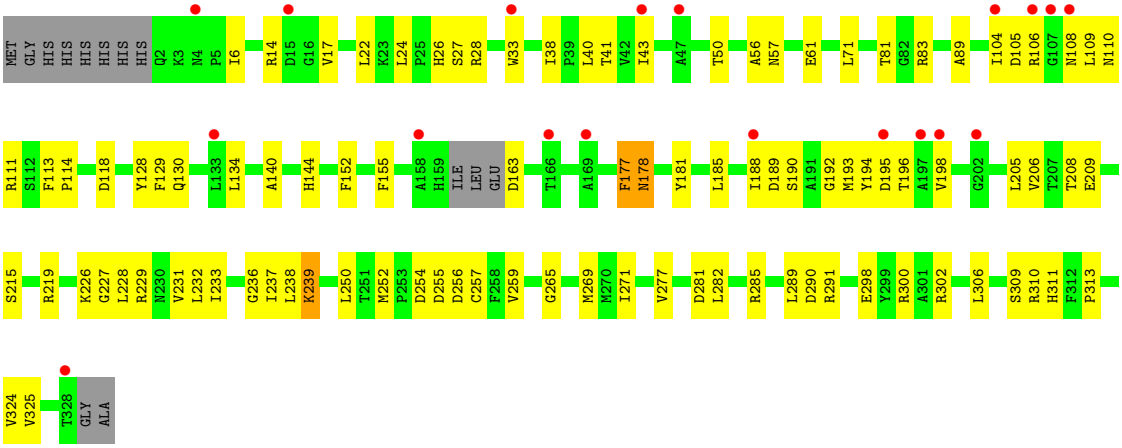
• Molecule 1: N-acetyl-L-2,4-diaminobutyric acid deacetylase

Chain K:



• Molecule 1: N-acetyl-L-2,4-diaminobutyric acid deacetylase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.67Å 145.95Å 164.12Å 90.00° 92.30° 90.00°	Depositor
Resolution (Å)	46.64 – 2.50 46.64 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.64-2.50) 98.4 (46.64-2.26)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.209 , 0.262 0.207 , 0.259	Depositor DCC
R_{free} test set	1568 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	30865	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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 24.38 % 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 3.8815e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ACT, DAB

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	0.27	0/2495	0.50	0/3390
1	B	0.28	0/2495	0.50	0/3390
1	C	0.28	0/2487	0.51	0/3379
1	D	0.34	2/2515 (0.1%)	0.58	2/3417 (0.1%)
1	E	0.29	0/2504	0.51	1/3402 (0.0%)
1	F	0.27	0/2499	0.49	0/3395
1	G	0.28	0/2504	0.53	0/3402
1	H	0.27	0/2504	0.51	0/3402
1	I	0.32	1/2495 (0.0%)	0.56	2/3390 (0.1%)
1	J	0.28	0/2495	0.51	0/3388
1	K	0.29	0/2504	0.51	0/3402
1	L	0.27	0/2478	0.51	0/3365
All	All	0.29	3/29975 (0.0%)	0.52	5/40722 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	3
1	G	0	1
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	131	ARG	NE-CZ	6.52	1.41	1.33
1	D	131	ARG	CZ-NH1	-6.22	1.25	1.33
1	I	99	SER	CA-CB	-5.03	1.45	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	131	ARG	NE-CZ-NH2	10.43	125.51	120.30
1	I	106	ARG	NE-CZ-NH1	10.21	125.40	120.30
1	D	161	LEU	CA-CB-CG	7.62	132.84	115.30
1	E	219	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	I	106	ARG	NH1-CZ-NH2	-5.38	113.48	119.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	ILE	Peptide
1	C	187	GLU	Peptide
1	D	160	ILE	Peptide
1	D	161	LEU	Peptide
1	D	162	GLU	Peptide
1	G	188	ILE	Peptide
1	J	162	GLU	Peptide
1	K	163	ASP	Peptide
1	L	239	LYS	Peptide

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	2442	0	2423	40	0
1	B	2442	0	2423	43	2
1	C	2434	0	2412	38	1
1	D	2461	0	2441	53	0
1	E	2451	0	2431	40	0
1	F	2446	0	2426	38	0
1	G	2451	0	2431	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2451	0	2431	35	0
1	I	2442	0	2423	41	1
1	J	2443	0	2419	50	0
1	K	2451	0	2431	34	0
1	L	2426	0	2402	76	3
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	L	1	0	0	0	0
3	A	8	0	8	1	0
3	B	8	0	9	2	2
3	D	8	0	9	0	0
3	E	8	0	9	1	1
3	F	8	0	9	0	0
3	J	8	0	9	1	0
3	K	8	0	9	2	0
4	C	4	0	3	0	0
4	G	4	0	3	0	0
4	H	4	0	3	0	0
5	A	144	0	0	6	0
5	B	130	0	0	4	0
5	C	130	0	0	8	0
5	D	111	0	0	4	0
5	E	117	0	0	3	0
5	F	131	0	0	2	0
5	G	121	0	0	10	0
5	H	112	0	0	4	0
5	I	108	0	0	5	0
5	J	118	0	0	7	0
5	K	118	0	0	0	0
5	L	107	0	0	9	0
All	All	30865	0	29164	532	5

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 9.

All (532) 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:22:LEU:HG	1:B:40:LEU:HD22	1.28	1.06
1:I:22:LEU:HG	1:I:40:LEU:HD22	1.34	1.05
1:I:103:PRO:HA	1:I:106:ARG:HH21	1.23	1.03
1:D:22:LEU:HG	1:D:40:LEU:HD22	1.40	1.00
1:G:303:ARG:NH1	1:G:303:ARG:HB3	1.80	0.97
1:G:303:ARG:HB3	1:G:303:ARG:HH11	1.28	0.97
1:G:256:ASP:HB2	1:G:303:ARG:HD2	1.55	0.87
1:J:229:ARG:NH2	5:J:502:HOH:O	2.06	0.87
1:G:269:MET:HE3	1:G:310:ARG:HB2	1.55	0.87
1:G:303:ARG:HH11	1:G:303:ARG:CB	1.89	0.85
1:L:109:LEU:HD22	1:L:111:ARG:H	1.40	0.84
1:H:271:ILE:HD12	1:H:271:ILE:O	1.78	0.83
1:I:99:SER:CB	5:I:501:HOH:O	2.26	0.81
1:L:111:ARG:NH1	5:L:501:HOH:O	2.13	0.81
1:G:239:LYS:HD2	1:G:240:GLY:H	1.45	0.81
1:C:68:LEU:HD12	1:C:86:ILE:HG23	1.64	0.80
1:D:269:MET:HE3	1:D:310:ARG:HB2	1.67	0.76
1:J:302:ARG:NH1	5:J:504:HOH:O	2.17	0.76
1:K:254:ASP:OD2	1:K:303:ARG:NH2	2.18	0.76
1:D:162:GLU:HG3	1:D:167:GLN:OE1	1.85	0.76
1:B:239:LYS:HD2	1:B:240:GLY:H	1.51	0.75
1:L:109:LEU:HD22	1:L:111:ARG:HB2	1.67	0.75
1:A:185:LEU:O	5:A:501:HOH:O	2.05	0.74
1:L:111:ARG:HG3	1:L:193:MET:HA	1.67	0.74
1:B:265:GLY:HA2	1:B:289:LEU:HG	1.68	0.74
1:A:324:VAL:HG21	1:K:33:TRP:HZ3	1.54	0.73
1:G:279:LYS:HG2	1:G:303:ARG:HA	1.69	0.73
1:H:159:HIS:HD2	1:H:186:LEU:HA	1.52	0.73
1:F:269:MET:HE3	1:F:310:ARG:HB2	1.69	0.72
1:H:279:LYS:NZ	5:H:501:HOH:O	2.10	0.71
1:L:256:ASP:OD1	1:L:302:ARG:NH1	2.23	0.71
1:F:155:PHE:HB3	1:F:181:TYR:HB2	1.71	0.70
1:J:254:ASP:HB2	1:J:303:ARG:HH12	1.56	0.70
1:C:23:LYS:NZ	5:C:506:HOH:O	2.22	0.70
1:H:271:ILE:HD12	1:H:271:ILE:C	2.12	0.70
1:L:219:ARG:NH2	5:L:504:HOH:O	2.25	0.70
1:J:22:LEU:HG	1:J:40:LEU:HD22	1.74	0.70
1:B:162:GLU:OE2	5:B:501:HOH:O	2.10	0.69
1:E:106:ARG:NH1	5:E:503:HOH:O	2.25	0.69
3:A:402:DAB:HA	1:K:33:TRP:HE1	1.58	0.69
1:L:50:THR:HG22	1:L:83:ARG:HB3	1.74	0.69
1:D:294:GLN:OE1	5:D:501:HOH:O	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:PHE:N	5:G:504:HOH:O	2.24	0.69
1:J:241:GLU:N	5:J:502:HOH:O	2.16	0.68
1:I:99:SER:OG	5:I:501:HOH:O	2.09	0.68
1:A:3:LYS:N	5:A:505:HOH:O	2.27	0.68
1:A:265:GLY:HA2	1:A:289:LEU:HG	1.75	0.68
1:L:193:MET:HB3	1:L:195:ASP:OD1	1.93	0.68
1:H:105:ASP:OD2	1:H:120:THR:HB	1.94	0.68
1:K:265:GLY:HA2	1:K:289:LEU:HG	1.76	0.68
1:A:262:GLU:O	1:D:291:ARG:NH1	2.25	0.68
1:C:265:GLY:HA2	1:C:289:LEU:HG	1.75	0.67
1:D:155:PHE:HB3	1:D:181:TYR:HB2	1.76	0.67
1:F:271:ILE:HD13	1:F:307:VAL:HG21	1.76	0.67
1:E:254:ASP:OD2	5:E:501:HOH:O	2.11	0.67
1:D:162:GLU:OE2	1:D:167:GLN:OE1	2.12	0.67
1:C:155:PHE:HB3	1:C:181:TYR:HB2	1.77	0.66
1:E:269:MET:HE3	1:E:310:ARG:HB2	1.76	0.66
1:J:161:LEU:H	1:J:167:GLN:NE2	1.93	0.66
1:G:290:ASP:OD1	5:G:501:HOH:O	2.13	0.66
1:D:265:GLY:HA2	1:D:289:LEU:HG	1.77	0.65
1:K:285:ARG:NH1	1:K:298:GLU:OE2	2.29	0.65
1:D:3:LYS:NZ	5:D:507:HOH:O	2.28	0.65
1:I:265:GLY:HA2	1:I:289:LEU:HG	1.79	0.65
1:J:52:LEU:HD23	1:J:134:LEU:HD12	1.77	0.65
1:H:265:GLY:HA2	1:H:289:LEU:HG	1.79	0.64
1:B:22:LEU:HG	1:B:40:LEU:CD2	2.17	0.64
1:L:109:LEU:HD22	1:L:111:ARG:N	2.12	0.64
1:C:187:GLU:N	1:C:187:GLU:OE1	2.31	0.64
1:E:26:HIS:CD2	1:E:28:ARG:HD3	2.33	0.63
1:K:254:ASP:HB3	1:K:256:ASP:H	1.62	0.63
1:K:177:PHE:CD1	1:K:227:GLY:HA3	2.34	0.62
1:I:17:VAL:HG13	1:I:43:ILE:HG12	1.82	0.62
1:G:56:ALA:N	5:G:504:HOH:O	2.32	0.62
1:L:155:PHE:HB3	1:L:181:TYR:HB2	1.82	0.62
1:L:265:GLY:HA2	1:L:289:LEU:HG	1.82	0.62
1:B:160:ILE:HA	1:B:167:GLN:HE21	1.63	0.62
1:D:177:PHE:CD1	1:D:227:GLY:HA3	2.34	0.62
1:I:103:PRO:HA	1:I:106:ARG:NH2	2.07	0.62
1:D:71:LEU:HD22	1:D:228:LEU:HD21	1.81	0.62
1:E:71:LEU:HD22	1:E:228:LEU:HD21	1.80	0.62
1:G:49:PRO:HG2	1:G:237:ILE:HG12	1.81	0.62
1:D:23:LYS:NZ	5:D:509:HOH:O	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:PHE:CD1	1:F:227:GLY:HA3	2.34	0.61
1:D:166:THR:HG21	1:D:202:GLY:HA2	1.82	0.61
1:C:71:LEU:HD22	1:C:228:LEU:HD21	1.82	0.61
1:B:177:PHE:CD1	1:B:227:GLY:HA3	2.36	0.61
1:D:160:ILE:O	1:D:162:GLU:HG3	2.00	0.61
1:G:160:ILE:HG12	1:G:186:LEU:HB2	1.82	0.61
1:I:177:PHE:CD1	1:I:227:GLY:HA3	2.36	0.61
1:C:271:ILE:HD11	1:C:307:VAL:HG21	1.83	0.61
1:E:56:ALA:HB3	1:E:89:ALA:HA	1.82	0.61
1:I:17:VAL:HG22	1:I:43:ILE:HG23	1.82	0.61
1:C:174:MET:SD	1:C:182:SER:HB3	2.41	0.61
1:G:116:ARG:NH2	5:G:510:HOH:O	2.34	0.60
1:J:265:GLY:HA2	1:J:289:LEU:HG	1.83	0.60
1:I:163:ASP:OD1	5:I:502:HOH:O	2.16	0.60
1:G:71:LEU:HD22	1:G:228:LEU:HD21	1.81	0.60
1:L:227:GLY:O	1:L:231:VAL:HG22	2.01	0.60
1:B:17:VAL:HG22	1:B:43:ILE:HG12	1.82	0.60
1:D:56:ALA:HB3	1:D:89:ALA:HA	1.82	0.60
1:C:3:LYS:NZ	5:C:518:HOH:O	2.34	0.60
1:L:232:LEU:HB3	1:L:238:LEU:HD12	1.82	0.60
1:C:218:ALA:O	5:C:501:HOH:O	2.17	0.59
1:D:26:HIS:CD2	1:D:28:ARG:HD3	2.37	0.59
1:L:81:THR:OG1	1:L:236:GLY:O	2.20	0.59
1:J:164:LYS:HB3	1:J:166:THR:H	1.67	0.59
1:F:153:VAL:HG23	1:F:155:PHE:HD2	1.66	0.59
1:A:282:LEU:HD21	1:A:285:ARG:HD3	1.84	0.59
1:L:177:PHE:CD1	1:L:227:GLY:HA3	2.36	0.59
1:L:269:MET:HE3	1:L:310:ARG:HB2	1.83	0.59
1:L:105:ASP:OD1	1:L:108:ASN:HB2	2.02	0.59
1:G:243:GLN:NE2	5:G:512:HOH:O	2.35	0.58
1:A:254:ASP:OD2	1:A:303:ARG:NH2	2.37	0.58
1:E:271:ILE:HD13	1:E:277:VAL:HG12	1.84	0.58
1:A:100:ARG:NH1	5:A:508:HOH:O	2.34	0.58
1:J:157:ALA:HB1	1:J:185:LEU:HD13	1.85	0.58
1:E:187:GLU:OE2	3:E:402:DAB:ND	2.36	0.58
1:G:279:LYS:HE3	1:G:303:ARG:HA	1.84	0.58
1:K:56:ALA:HB3	1:K:89:ALA:HA	1.86	0.57
1:J:26:HIS:CD2	1:J:28:ARG:HD3	2.40	0.57
1:H:291:ARG:HD3	1:H:294:GLN:HG3	1.87	0.57
1:L:109:LEU:HD21	1:L:111:ARG:HD3	1.85	0.57
1:D:164:LYS:HG3	1:D:166:THR:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:LEU:HD22	1:F:228:LEU:HD21	1.86	0.57
1:G:110:ASN:O	1:G:111:ARG:HD3	2.04	0.57
1:D:154:PRO:HG3	1:D:219:ARG:HH12	1.70	0.57
1:I:103:PRO:CA	1:I:106:ARG:HH21	2.09	0.57
1:L:190:SER:HG	1:L:196:THR:HG1	1.52	0.57
1:A:285:ARG:HG2	1:A:298:GLU:HG2	1.86	0.56
1:H:61:GLU:HB3	1:H:145:SER:HB2	1.87	0.56
1:L:56:ALA:HB3	1:L:89:ALA:HA	1.86	0.56
1:H:141:VAL:HG22	1:H:206:VAL:HB	1.87	0.56
1:B:28:ARG:HG3	1:B:30:ASP:HB2	1.86	0.56
1:G:302:ARG:NH2	5:G:516:HOH:O	2.38	0.56
1:H:71:LEU:HD22	1:H:228:LEU:HD21	1.88	0.56
1:F:33:TRP:HZ3	1:K:324:VAL:HG21	1.71	0.56
1:I:108:ASN:HD21	1:I:111:ARG:HH11	1.54	0.56
1:A:56:ALA:HB3	1:A:89:ALA:HA	1.87	0.56
1:J:243:GLN:NE2	5:J:501:HOH:O	1.83	0.55
1:K:269:MET:HE3	1:K:310:ARG:HB2	1.86	0.55
1:D:162:GLU:OE1	1:E:241:GLU:OE2	2.23	0.55
1:E:129:PHE:O	1:E:134:LEU:HB2	2.06	0.55
1:K:100:ARG:HH12	3:K:401:DAB:HD1	1.53	0.55
1:E:22:LEU:HG	1:E:40:LEU:HD22	1.89	0.55
1:J:2:GLN:NE2	5:J:516:HOH:O	2.38	0.55
1:F:26:HIS:CD2	1:F:28:ARG:HD3	2.42	0.55
1:L:189:ASP:HA	5:L:502:HOH:O	2.05	0.55
1:L:309:SER:HB3	1:L:324:VAL:HG12	1.89	0.55
1:K:155:PHE:HB3	1:K:181:TYR:HB2	1.89	0.55
1:L:188:ILE:O	5:L:502:HOH:O	2.18	0.55
1:B:142:ASP:OD2	1:B:144:HIS:NE2	2.36	0.55
1:L:109:LEU:CD2	1:L:111:ARG:H	2.15	0.55
1:H:110:ASN:N	5:H:505:HOH:O	2.30	0.55
1:D:49:PRO:HG2	1:D:237:ILE:HG13	1.88	0.55
1:D:22:LEU:HG	1:D:40:LEU:CD2	2.26	0.55
1:E:217:SER:HB2	1:E:219:ARG:HH21	1.72	0.55
1:F:11:PRO:HG3	1:F:14:ARG:NH2	2.22	0.55
1:K:71:LEU:HD22	1:K:228:LEU:HD21	1.89	0.54
1:D:17:VAL:HG13	1:D:43:ILE:HG12	1.88	0.54
1:L:269:MET:HG3	1:L:271:ILE:O	2.07	0.54
1:B:56:ALA:HB3	1:B:89:ALA:HA	1.89	0.54
1:J:302:ARG:NH2	5:J:518:HOH:O	2.40	0.54
1:G:61:GLU:HB3	1:G:145:SER:HB2	1.90	0.54
1:L:144:HIS:HB2	1:L:208:THR:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:183:VAL:HG22	1:J:250:LEU:HB2	1.90	0.54
1:C:294:GLN:HG2	1:C:295:PRO:HD2	1.90	0.53
1:K:61:GLU:HB3	1:K:145:SER:HB2	1.89	0.53
1:C:298:GLU:OE1	1:C:300:ARG:NH2	2.41	0.53
1:G:10:ILE:HD11	1:G:40:LEU:HD23	1.90	0.53
1:D:282:LEU:HD11	1:D:298:GLU:HB3	1.91	0.53
1:I:311:HIS:HB2	1:I:321:CYS:O	2.09	0.53
1:L:152:PHE:CD1	1:L:309:SER:HB2	2.43	0.53
1:B:177:PHE:CE1	1:B:227:GLY:HA3	2.44	0.53
1:C:292:THR:HB	1:L:41:THR:OG1	2.09	0.53
1:E:17:VAL:HG22	1:E:43:ILE:HG12	1.91	0.53
1:G:303:ARG:NH1	1:G:303:ARG:CB	2.57	0.53
1:J:28:ARG:NE	1:J:30:ASP:OD1	2.41	0.53
1:I:112:SER:OG	5:I:503:HOH:O	2.19	0.53
1:L:71:LEU:HD22	1:L:228:LEU:HD21	1.90	0.53
1:I:102:SER:O	1:I:106:ARG:NH2	2.42	0.53
1:E:254:ASP:HB3	1:E:256:ASP:H	1.74	0.53
1:A:33:TRP:CZ3	1:F:324:VAL:HG21	2.45	0.52
1:F:129:PHE:O	1:F:134:LEU:HB2	2.09	0.52
1:E:155:PHE:HB3	1:E:181:TYR:HB2	1.92	0.52
1:G:239:LYS:HD2	1:G:240:GLY:N	2.19	0.52
1:G:277:VAL:HG23	1:G:281:ASP:HB2	1.90	0.52
1:B:160:ILE:HA	1:B:167:GLN:NE2	2.24	0.52
1:L:311:HIS:CE1	1:L:313:PRO:HD2	2.44	0.52
1:F:256:ASP:HB3	1:F:303:ARG:HG3	1.92	0.52
1:F:271:ILE:CD1	1:F:307:VAL:HG21	2.39	0.52
1:L:291:ARG:NH1	5:L:505:HOH:O	2.28	0.52
1:K:134:LEU:HD11	1:K:198:VAL:HG22	1.91	0.52
1:C:317:LYS:NZ	5:C:521:HOH:O	2.38	0.52
1:D:188:ILE:HG13	1:D:189:ASP:N	2.25	0.52
1:B:100:ARG:HH22	3:B:402:DAB:H	1.57	0.51
1:C:187:GLU:HG2	1:C:190:SER:N	2.25	0.51
1:H:152:PHE:CD1	1:H:309:SER:HB2	2.46	0.51
1:B:111:ARG:NH1	1:B:189:ASP:O	2.42	0.51
1:C:22:LEU:HG	1:C:40:LEU:HD22	1.92	0.51
1:F:265:GLY:HA2	1:F:289:LEU:HG	1.93	0.51
1:J:22:LEU:HB2	1:J:38:ILE:HB	1.93	0.51
1:C:170:CYS:HA	1:C:204:VAL:HG23	1.92	0.51
1:G:134:LEU:HD11	1:G:198:VAL:HG22	1.93	0.51
1:J:186:LEU:O	5:J:505:HOH:O	2.19	0.51
1:C:138:ASP:OD1	5:C:502:HOH:O	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:SER:HA	1:F:299:TYR:CE2	2.45	0.51
1:H:271:ILE:C	1:H:271:ILE:CD1	2.78	0.50
1:J:49:PRO:HG2	1:J:237:ILE:HG13	1.92	0.50
1:H:8:PRO:HB3	1:H:22:LEU:HD23	1.93	0.50
1:F:11:PRO:HG3	1:F:14:ARG:HH21	1.76	0.50
1:L:233:ILE:HA	1:L:238:LEU:O	2.12	0.50
1:A:48:GLY:O	5:A:503:HOH:O	2.19	0.50
1:B:71:LEU:HD22	1:B:228:LEU:HD21	1.93	0.50
1:B:257:CYS:HB3	1:B:325:VAL:O	2.11	0.50
1:L:285:ARG:NH1	1:L:298:GLU:OE2	2.44	0.50
1:B:291:ARG:HH21	1:B:294:GLN:CD	2.15	0.50
1:L:114:PRO:HA	1:L:130:GLN:HE21	1.76	0.50
1:C:187:GLU:OE1	5:C:503:HOH:O	2.20	0.50
1:G:155:PHE:HB3	1:G:181:TYR:HB2	1.94	0.50
1:I:311:HIS:CE1	1:I:313:PRO:HD2	2.46	0.50
1:A:267:PHE:HE1	1:A:322:VAL:HG13	1.77	0.50
1:E:217:SER:HB2	1:E:219:ARG:NH2	2.26	0.50
1:F:40:LEU:CD2	1:F:42:VAL:HG23	2.42	0.50
1:G:163:ASP:OD1	1:G:163:ASP:N	2.45	0.50
1:J:56:ALA:HB3	1:J:89:ALA:HA	1.94	0.50
1:D:270:MET:O	1:D:271:ILE:HD13	2.12	0.49
1:F:40:LEU:HD23	1:F:41:THR:N	2.26	0.49
1:J:159:HIS:HB2	1:J:161:LEU:HD21	1.94	0.49
1:C:56:ALA:HB3	1:C:89:ALA:HA	1.93	0.49
1:G:251:THR:OG1	5:G:502:HOH:O	2.19	0.49
1:I:97:ALA:HB2	1:I:103:PRO:HG3	1.94	0.49
1:I:164:LYS:HE3	1:I:166:THR:HG23	1.92	0.49
1:D:27:SER:OG	1:D:32:ALA:O	2.25	0.49
1:I:108:ASN:ND2	1:I:111:ARG:HH11	2.10	0.49
1:L:229:ARG:NE	5:L:516:HOH:O	2.44	0.49
1:A:21:PHE:HA	1:A:40:LEU:HD23	1.93	0.49
1:F:293:GLY:HA3	1:J:19:HIS:CE1	2.48	0.49
1:G:93:PRO:HB2	1:G:102:SER:HB2	1.95	0.49
1:I:309:SER:HB3	1:I:324:VAL:HB	1.95	0.49
1:B:157:ALA:HA	1:B:183:VAL:O	2.13	0.49
1:D:186:LEU:HB2	1:D:252:MET:O	2.12	0.49
1:J:152:PHE:CD1	1:J:309:SER:HB2	2.47	0.49
1:K:139:LEU:HD21	1:K:231:VAL:HG12	1.95	0.49
1:K:198:VAL:HG13	1:K:203:LYS:HB2	1.94	0.49
1:G:17:VAL:HG13	1:G:43:ILE:HG12	1.95	0.48
1:G:279:LYS:CG	1:G:303:ARG:HA	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:LEU:HD13	1:G:323:ALA:HB3	1.94	0.48
1:H:227:GLY:O	1:H:231:VAL:HG13	2.12	0.48
1:C:292:THR:OG1	5:C:504:HOH:O	2.20	0.48
1:J:267:PHE:HE1	1:J:322:VAL:HG13	1.77	0.48
1:B:134:LEU:O	1:B:203:LYS:NZ	2.46	0.48
1:L:26:HIS:CE1	1:L:28:ARG:HD3	2.48	0.48
1:G:110:ASN:O	1:G:193:MET:HA	2.13	0.48
1:J:71:LEU:HD22	1:J:228:LEU:HD21	1.95	0.48
1:A:71:LEU:HD22	1:A:228:LEU:HD21	1.95	0.48
1:D:188:ILE:HG13	1:D:189:ASP:H	1.78	0.48
1:G:2:GLN:NE2	5:G:521:HOH:O	2.45	0.48
1:G:160:ILE:HG13	1:G:160:ILE:O	2.13	0.48
1:J:189:ASP:N	1:J:189:ASP:OD1	2.47	0.48
1:D:116:ARG:HH21	1:D:118:ASP:CG	2.17	0.48
1:H:144:HIS:HB2	1:H:208:THR:O	2.14	0.48
1:A:312:PHE:O	1:G:215:SER:HB2	2.13	0.48
1:D:266:LEU:HB3	1:D:287:TRP:HB2	1.96	0.48
1:K:250:LEU:HD21	1:K:306:LEU:HD12	1.95	0.48
1:A:317:LYS:HE3	1:K:30:ASP:HB3	1.95	0.47
1:E:110:ASN:O	1:E:193:MET:HA	2.14	0.47
1:F:33:TRP:HE1	3:K:401:DAB:HG3	1.79	0.47
1:I:92:TYR:OH	1:I:96:ARG:NH1	2.44	0.47
1:L:14:ARG:HD3	5:L:595:HOH:O	2.14	0.47
1:L:104:ILE:C	1:L:106:ARG:H	2.15	0.47
1:L:250:LEU:HD21	1:L:306:LEU:HD12	1.96	0.47
1:L:282:LEU:HA	1:L:300:ARG:HG2	1.96	0.47
1:C:190:SER:HB3	1:C:196:THR:OG1	2.13	0.47
1:E:152:PHE:CD1	1:E:309:SER:HB2	2.49	0.47
1:I:128:TYR:CE2	1:I:133:LEU:HD11	2.48	0.47
1:L:185:LEU:HD23	1:L:252:MET:HE3	1.96	0.47
1:D:256:ASP:OD1	1:D:302:ARG:NH2	2.47	0.47
1:F:161:LEU:HB2	1:F:167:GLN:HB2	1.96	0.47
1:G:83:ARG:HD2	1:G:85:ILE:HD11	1.96	0.47
1:B:246:GLU:HG2	1:B:247:THR:N	2.30	0.47
1:D:162:GLU:CG	1:D:167:GLN:OE1	2.61	0.47
1:D:149:THR:HG21	1:G:31:SER:HA	1.96	0.47
1:E:144:HIS:HB2	1:E:208:THR:O	2.14	0.47
1:I:144:HIS:HB2	1:I:208:THR:O	2.14	0.47
1:L:290:ASP:OD1	1:L:291:ARG:HD2	2.14	0.47
1:G:256:ASP:HB2	1:G:303:ARG:CD	2.38	0.47
1:A:22:LEU:HG	1:A:40:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:ASN:HB3	1:G:144:HIS:CE1	2.50	0.47
1:J:254:ASP:HB2	1:J:303:ARG:NH1	2.28	0.47
1:L:195:ASP:OD1	1:L:195:ASP:N	2.42	0.47
1:G:178:ASN:ND2	1:G:247:THR:OG1	2.48	0.47
1:G:187:GLU:OE1	1:G:187:GLU:N	2.41	0.47
1:F:40:LEU:HD21	1:F:42:VAL:HG23	1.97	0.47
1:I:71:LEU:HD22	1:I:228:LEU:HD21	1.96	0.47
1:K:270:MET:HE3	1:K:285:ARG:HE	1.80	0.47
1:D:164:LYS:HG3	1:D:166:THR:HG23	1.97	0.46
1:E:11:PRO:HB2	1:E:14:ARG:HG3	1.97	0.46
1:J:139:LEU:HD21	1:J:231:VAL:HG12	1.97	0.46
1:K:26:HIS:CD2	1:K:28:ARG:HD3	2.49	0.46
1:B:113:PHE:O	1:B:192:GLY:HA2	2.15	0.46
1:L:178:ASN:HB3	1:L:226:LYS:NZ	2.31	0.46
1:E:139:LEU:HD21	1:E:231:VAL:HG12	1.98	0.46
1:H:159:HIS:CD2	1:H:186:LEU:HA	2.42	0.46
1:L:109:LEU:HD22	1:L:111:ARG:CB	2.41	0.46
1:E:55:GLY:O	1:E:90:PHE:N	2.47	0.46
1:F:45:ASN:HB3	1:F:80:VAL:O	2.15	0.46
1:F:177:PHE:CE1	1:F:227:GLY:HA3	2.50	0.46
1:G:250:LEU:HD12	1:G:326:GLY:C	2.35	0.46
1:H:10:ILE:HD12	1:H:18:PHE:HB2	1.98	0.46
1:H:57:ASN:ND2	1:H:110:ASN:OD1	2.48	0.46
1:H:285:ARG:NH1	5:H:513:HOH:O	2.41	0.46
1:J:144:HIS:HB2	1:J:208:THR:O	2.15	0.46
1:L:109:LEU:CD2	1:L:111:ARG:HD3	2.45	0.46
1:L:129:PHE:O	1:L:134:LEU:HB2	2.15	0.46
1:L:236:GLY:HA2	1:L:239:LYS:HE3	1.98	0.46
1:D:11:PRO:HG3	1:D:14:ARG:HE	1.80	0.46
1:F:253:PRO:HG2	1:F:303:ARG:NH2	2.30	0.46
1:G:324:VAL:HG21	1:J:33:TRP:HZ3	1.81	0.46
1:B:100:ARG:NH2	3:B:402:DAB:H	2.14	0.46
1:E:188:ILE:H	1:E:188:ILE:HD12	1.80	0.46
1:E:265:GLY:HA2	1:E:289:LEU:HG	1.97	0.46
1:G:113:PHE:O	1:G:192:GLY:HA2	2.16	0.46
1:A:311:HIS:CE1	1:A:313:PRO:HD2	2.51	0.46
1:B:253:PRO:HB3	1:D:246:GLU:HG2	1.98	0.46
1:E:134:LEU:HD21	1:E:198:VAL:HG22	1.98	0.46
1:G:111:ARG:NH1	1:G:189:ASP:O	2.48	0.46
1:G:129:PHE:O	1:G:134:LEU:HB2	2.16	0.46
1:L:81:THR:O	1:L:237:ILE:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASP:OD2	1:A:144:HIS:NE2	2.48	0.46
1:A:155:PHE:CE2	1:A:209:GLU:HB2	2.51	0.46
1:C:144:HIS:HB2	1:C:208:THR:O	2.16	0.46
1:I:61:GLU:HB3	1:I:145:SER:HB2	1.97	0.46
1:J:181:TYR:CD1	1:J:248:VAL:HB	2.51	0.46
1:C:311:HIS:CE1	1:C:313:PRO:HD2	2.51	0.45
1:I:254:ASP:HB3	1:I:256:ASP:H	1.80	0.45
1:K:303:ARG:HD3	1:K:327:VAL:HG11	1.99	0.45
1:A:55:GLY:O	1:A:90:PHE:N	2.46	0.45
1:A:158:ALA:O	1:A:184:GLU:HA	2.16	0.45
1:D:113:PHE:CE2	1:D:194:TYR:HD1	2.34	0.45
1:I:257:CYS:SG	1:I:303:ARG:HD2	2.55	0.45
1:K:259:VAL:O	1:K:322:VAL:N	2.48	0.45
1:B:113:PHE:CE2	1:B:194:TYR:HD1	2.34	0.45
1:K:6:ILE:HG12	1:K:24:LEU:HB2	1.98	0.45
1:G:265:GLY:HA2	1:G:289:LEU:HG	1.99	0.45
1:I:181:TYR:CD1	1:I:248:VAL:HB	2.50	0.45
1:I:238:LEU:O	5:I:504:HOH:O	2.20	0.45
1:J:21:PHE:CD2	1:J:37:MET:HB3	2.52	0.45
1:E:237:ILE:O	1:E:239:LYS:NZ	2.50	0.45
1:L:177:PHE:CE1	1:L:227:GLY:HA3	2.51	0.45
1:D:33:TRP:HZ3	1:J:324:VAL:HG21	1.81	0.45
1:E:142:ASP:OD2	1:E:144:HIS:NE2	2.49	0.45
1:G:309:SER:HB3	1:G:324:VAL:HB	1.98	0.45
1:I:285:ARG:HB3	1:I:296:PRO:HB2	1.99	0.45
1:B:239:LYS:HD2	1:B:240:GLY:N	2.24	0.45
1:C:251:THR:OG1	1:C:327:VAL:HB	2.15	0.45
1:G:144:HIS:HB2	1:G:208:THR:O	2.17	0.45
1:L:57:ASN:OD1	1:L:110:ASN:HB3	2.17	0.45
1:B:164:LYS:HD2	1:B:167:GLN:OE1	2.17	0.45
1:C:142:ASP:OD2	1:C:144:HIS:NE2	2.48	0.45
1:C:241:GLU:O	5:C:505:HOH:O	2.21	0.45
1:F:312:PHE:O	1:J:215:SER:HB2	2.17	0.45
1:C:160:ILE:HD11	1:C:184:GLU:OE1	2.17	0.45
1:G:182:SER:OG	1:G:247:THR:HG21	2.16	0.45
1:J:17:VAL:HG13	1:J:43:ILE:HG12	1.98	0.45
1:L:155:PHE:CZ	1:L:209:GLU:HB2	2.51	0.45
1:F:134:LEU:HD11	1:F:198:VAL:HG22	1.98	0.45
1:K:285:ARG:HD3	1:K:296:PRO:HG2	1.99	0.45
1:D:167:GLN:NE2	1:D:171:PHE:CZ	2.80	0.44
1:E:285:ARG:HG2	1:E:298:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:74:THR:HG22	1:K:74:THR:O	2.17	0.44
1:D:177:PHE:CE1	1:D:227:GLY:HA3	2.52	0.44
1:B:144:HIS:HB2	1:B:208:THR:O	2.17	0.44
1:D:33:TRP:HE3	1:J:321:CYS:HG	1.66	0.44
1:H:233:ILE:HA	1:H:238:LEU:O	2.17	0.44
1:J:256:ASP:O	1:J:302:ARG:HB2	2.16	0.44
1:J:270:MET:HG2	1:J:284:ALA:HA	1.99	0.44
1:C:105:ASP:OD2	1:C:120:THR:HB	2.17	0.44
1:I:22:LEU:HG	1:I:40:LEU:CD2	2.25	0.44
1:I:276:PRO:HA	1:I:306:LEU:HD23	1.98	0.44
1:A:23:LYS:HE3	1:F:260:PHE:CD1	2.52	0.44
1:C:290:ASP:OD1	1:C:290:ASP:N	2.49	0.44
1:F:164:LYS:HA	1:F:167:GLN:HB3	1.99	0.44
1:G:160:ILE:CG1	1:G:186:LEU:HB2	2.45	0.44
1:A:45:ASN:HB3	1:A:80:VAL:O	2.17	0.44
1:K:144:HIS:HB2	1:K:208:THR:O	2.18	0.44
1:A:184:GLU:HG2	1:A:251:THR:HG22	2.00	0.43
1:B:311:HIS:ND1	5:B:510:HOH:O	2.35	0.43
1:D:182:SER:HB2	1:D:249:ASN:OD1	2.18	0.43
1:I:110:ASN:O	1:I:193:MET:HA	2.18	0.43
1:J:129:PHE:HA	1:J:133:LEU:HB2	2.00	0.43
1:L:109:LEU:HD23	1:L:110:ASN:N	2.32	0.43
1:L:134:LEU:HD21	1:L:198:VAL:HG22	1.99	0.43
1:D:144:HIS:HB2	1:D:208:THR:O	2.18	0.43
1:E:269:MET:CE	1:E:310:ARG:HB2	2.47	0.43
1:F:144:HIS:HB2	1:F:208:THR:O	2.17	0.43
1:G:259:VAL:O	1:G:322:VAL:N	2.51	0.43
1:L:163:ASP:OD1	1:L:163:ASP:N	2.51	0.43
1:E:311:HIS:CE1	1:E:313:PRO:HD2	2.54	0.43
1:A:144:HIS:HB2	1:A:208:THR:O	2.18	0.43
1:H:56:ALA:HB3	1:H:89:ALA:HA	2.01	0.43
1:H:162:GLU:H	1:H:162:GLU:CD	2.21	0.43
1:C:6:ILE:HD12	1:C:128:TYR:HB2	2.00	0.43
1:D:164:LYS:HD2	1:D:164:LYS:HA	1.65	0.43
1:D:243:GLN:O	5:D:502:HOH:O	2.21	0.43
1:H:181:TYR:CD1	1:H:248:VAL:HB	2.54	0.43
1:L:22:LEU:HB2	1:L:38:ILE:HB	2.00	0.43
1:A:155:PHE:CZ	1:A:209:GLU:HB2	2.54	0.43
1:C:129:PHE:HA	1:C:133:LEU:HB2	2.00	0.43
1:E:290:ASP:OD1	1:E:291:ARG:NH1	2.52	0.43
1:A:282:LEU:HD11	1:A:285:ARG:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:VAL:HG12	1:D:38:ILE:HG13	2.01	0.43
1:H:129:PHE:O	1:H:134:LEU:HB2	2.19	0.43
1:J:105:ASP:OD2	1:J:120:THR:HB	2.19	0.43
1:K:177:PHE:CE1	1:K:227:GLY:HA3	2.54	0.43
1:I:303:ARG:HD3	1:I:327:VAL:CG2	2.48	0.43
1:K:303:ARG:HD3	1:K:327:VAL:CG1	2.49	0.43
1:D:128:TYR:O	1:D:132:THR:HB	2.19	0.43
1:H:27:SER:OG	1:H:32:ALA:O	2.31	0.43
1:L:254:ASP:OD1	1:L:255:ASP:N	2.51	0.43
1:B:22:LEU:HB2	1:B:38:ILE:HB	2.00	0.43
1:E:81:THR:CB	1:E:239:LYS:HZ1	2.32	0.42
1:J:174:MET:SD	1:J:182:SER:HB3	2.58	0.42
1:E:57:ASN:HB3	1:E:144:HIS:CE1	2.54	0.42
1:F:162:GLU:O	1:F:162:GLU:HG2	2.18	0.42
1:I:22:LEU:HB2	1:I:38:ILE:HB	2.01	0.42
1:H:134:LEU:HD11	1:H:198:VAL:HG22	2.00	0.42
1:H:303:ARG:HD3	1:H:327:VAL:HG22	2.01	0.42
1:H:119:GLY:O	1:H:124:LYS:NZ	2.39	0.42
1:K:108:ASN:O	1:K:112:SER:OG	2.33	0.42
1:B:298:GLU:O	5:B:502:HOH:O	2.21	0.42
1:C:187:GLU:HG2	1:C:189:ASP:N	2.35	0.42
1:D:162:GLU:HB3	1:D:163:ASP:H	1.46	0.42
1:A:152:PHE:CE1	1:A:309:SER:HB2	2.55	0.42
1:L:118:ASP:OD1	1:L:118:ASP:N	2.53	0.42
1:A:97:ALA:HB2	1:A:103:PRO:HG3	2.02	0.42
1:E:256:ASP:HB3	1:E:303:ARG:HG3	2.02	0.42
1:F:54:THR:HG22	1:F:87:VAL:HB	2.02	0.42
1:I:44:LYS:HD2	1:I:83:ARG:HD3	2.02	0.42
1:J:267:PHE:CE1	1:J:322:VAL:HG13	2.55	0.42
1:B:121:VAL:HG23	5:B:584:HOH:O	2.19	0.42
1:E:254:ASP:OD2	1:E:303:ARG:NH1	2.53	0.42
1:J:155:PHE:CE2	1:J:209:GLU:HB2	2.55	0.42
1:J:164:LYS:HE3	1:J:165:ALA:H	1.84	0.42
1:A:186:LEU:HB2	1:A:252:MET:O	2.20	0.42
1:A:261:SER:HA	1:A:299:TYR:CE1	2.55	0.42
1:B:306:LEU:O	1:B:325:VAL:HA	2.20	0.42
1:I:159:HIS:ND1	1:I:187:GLU:HB3	2.34	0.42
1:L:61:GLU:OE1	5:L:503:HOH:O	2.21	0.42
1:L:152:PHE:CE1	1:L:309:SER:HB2	2.55	0.42
1:J:134:LEU:HD21	1:J:198:VAL:HG22	2.02	0.42
1:A:106:ARG:NH1	5:A:517:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:O	1:A:322:VAL:N	2.53	0.41
1:G:116:ARG:HH21	1:G:119:GLY:HA2	1.85	0.41
1:G:179:ALA:O	1:G:247:THR:HG23	2.20	0.41
1:J:110:ASN:O	1:J:193:MET:HA	2.19	0.41
1:L:205:LEU:HG	1:L:206:VAL:N	2.34	0.41
1:L:259:VAL:HA	5:L:580:HOH:O	2.20	0.41
1:E:303:ARG:NH2	5:E:522:HOH:O	2.53	0.41
1:G:266:LEU:HB3	1:G:287:TRP:HB2	2.02	0.41
1:H:194:TYR:O	1:H:198:VAL:HG23	2.20	0.41
1:K:153:VAL:HB	1:K:181:TYR:CE1	2.55	0.41
1:E:49:PRO:HG2	1:E:237:ILE:HG13	2.02	0.41
1:E:266:LEU:HB3	1:E:287:TRP:HB2	2.01	0.41
1:G:252:MET:SD	1:G:308:ILE:HD11	2.60	0.41
1:H:243:GLN:HG2	5:H:529:HOH:O	2.20	0.41
1:H:259:VAL:HG22	1:H:302:ARG:HG3	2.02	0.41
1:I:164:LYS:HG3	1:I:165:ALA:N	2.34	0.41
1:L:17:VAL:HA	1:L:43:ILE:HD13	2.01	0.41
1:L:113:PHE:CE2	1:L:194:TYR:HD1	2.38	0.41
1:A:152:PHE:CD1	1:A:309:SER:HB2	2.55	0.41
1:F:169:ALA:HB1	1:F:204:VAL:HG22	2.01	0.41
1:G:303:ARG:HH12	1:G:327:VAL:HG22	1.85	0.41
1:B:141:VAL:HG22	1:B:206:VAL:CG2	2.50	0.41
1:B:141:VAL:HA	1:B:206:VAL:HG23	2.02	0.41
1:F:58:HIS:ND1	5:F:502:HOH:O	2.22	0.41
1:F:290:ASP:HB2	5:G:523:HOH:O	2.21	0.41
1:G:320:ASP:OD1	1:G:320:ASP:N	2.54	0.41
1:L:22:LEU:HG	1:L:40:LEU:HD22	2.03	0.41
1:B:129:PHE:HA	1:B:133:LEU:HB2	2.02	0.41
1:G:40:LEU:HD12	1:G:87:VAL:HG22	2.01	0.41
1:G:53:LEU:HD12	1:G:86:ILE:HG12	2.03	0.41
1:G:246:GLU:HG3	5:G:608:HOH:O	2.19	0.41
1:L:111:ARG:NH1	1:L:194:TYR:H	2.18	0.41
1:L:113:PHE:O	1:L:192:GLY:HA2	2.20	0.41
1:A:292:THR:OG1	5:A:502:HOH:O	2.15	0.41
1:B:185:LEU:HD23	1:B:252:MET:SD	2.60	0.41
1:L:277:VAL:HG23	1:L:281:ASP:HB2	2.01	0.41
1:A:271:ILE:HG22	1:A:275:ALA:HB3	2.02	0.41
1:B:24:LEU:HB3	1:B:36:VAL:HB	2.03	0.41
1:C:110:ASN:O	1:C:193:MET:HA	2.20	0.41
1:C:161:LEU:HB2	1:C:167:GLN:HB2	2.03	0.41
1:F:6:ILE:HD12	1:F:128:TYR:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:VAL:HA	1:F:234:HIS:HB3	2.01	0.41
1:K:290:ASP:C	1:K:291:ARG:HG3	2.41	0.41
1:L:6:ILE:HG12	1:L:24:LEU:HB2	2.01	0.41
1:B:243:GLN:O	1:B:244:LEU:HD23	2.19	0.41
1:B:254:ASP:OD1	1:B:303:ARG:NH2	2.53	0.41
1:B:256:ASP:O	1:B:302:ARG:HB2	2.21	0.41
1:E:106:ARG:HE	1:E:106:ARG:HB2	1.71	0.41
1:G:171:PHE:CZ	1:G:184:GLU:HG2	2.56	0.41
1:K:24:LEU:HD21	1:K:121:VAL:HG13	2.03	0.41
1:L:105:ASP:CG	1:L:108:ASN:HB2	2.41	0.41
1:B:21:PHE:HE1	1:H:290:ASP:O	2.03	0.41
1:C:118:ASP:OD1	1:C:118:ASP:N	2.53	0.41
1:D:110:ASN:O	1:D:193:MET:HA	2.20	0.41
1:D:226:LYS:HG3	1:D:243:GLN:HB2	2.02	0.41
1:E:111:ARG:NH1	1:E:189:ASP:O	2.51	0.41
1:H:257:CYS:O	1:H:324:VAL:HA	2.21	0.41
1:D:157:ALA:HA	1:D:183:VAL:O	2.21	0.40
1:J:45:ASN:ND2	1:J:78:GLU:HA	2.36	0.40
1:L:104:ILE:C	1:L:106:ARG:N	2.75	0.40
1:L:178:ASN:HB3	1:L:226:LYS:HZ1	1.84	0.40
1:A:22:LEU:HB2	1:A:38:ILE:HB	2.02	0.40
1:C:55:GLY:O	1:C:90:PHE:N	2.48	0.40
1:D:160:ILE:O	1:D:167:GLN:OE1	2.39	0.40
1:I:139:LEU:HD21	1:I:231:VAL:HG12	2.03	0.40
1:A:181:TYR:CD2	1:A:248:VAL:HB	2.55	0.40
1:B:76:SER:OG	1:B:79:ASP:N	2.49	0.40
1:C:312:PHE:O	1:L:215:SER:HB2	2.22	0.40
1:D:153:VAL:HG23	1:D:155:PHE:HD2	1.86	0.40
1:K:311:HIS:CE1	1:K:313:PRO:HD2	2.56	0.40
1:L:6:ILE:HD12	1:L:128:TYR:HB2	2.04	0.40
1:L:257:CYS:HB3	1:L:325:VAL:O	2.20	0.40
1:I:177:PHE:CE1	1:I:227:GLY:HA3	2.55	0.40
1:I:233:ILE:HA	1:I:238:LEU:O	2.22	0.40
1:J:155:PHE:HB3	1:J:181:TYR:HB2	2.02	0.40
1:L:140:ALA:HB3	1:L:198:VAL:HG11	2.02	0.40
1:F:70:GLU:OE2	5:F:501:HOH:O	2.22	0.40
1:H:312:PHE:HB3	1:H:313:PRO:HD3	2.02	0.40
1:J:152:PHE:HE2	3:J:402:DAB:HG3	1.86	0.40
1:J:157:ALA:HB3	1:J:207:THR:HG23	2.03	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:TRP:CZ2	3:B:402:DAB:ND[1_545]	1.66	0.54
1:B:100:ARG:NH1	1:L:27:SER:OG[1_565]	2.08	0.12
1:L:33:TRP:NE1	3:B:402:DAB:ND[1_545]	2.10	0.10
1:B:33:TRP:CE2	3:E:402:DAB:CG[2_555]	2.15	0.05
1:C:29:ASP:OD2	1:I:106:ARG:NH1[2_645]	2.15	0.05

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	324/337 (96%)	318 (98%)	6 (2%)	0	100	100
1	B	324/337 (96%)	318 (98%)	6 (2%)	0	100	100
1	C	323/337 (96%)	315 (98%)	8 (2%)	0	100	100
1	D	326/337 (97%)	314 (96%)	12 (4%)	0	100	100
1	E	325/337 (96%)	322 (99%)	3 (1%)	0	100	100
1	F	325/337 (96%)	319 (98%)	6 (2%)	0	100	100
1	G	325/337 (96%)	316 (97%)	9 (3%)	0	100	100
1	H	325/337 (96%)	319 (98%)	6 (2%)	0	100	100
1	I	324/337 (96%)	320 (99%)	4 (1%)	0	100	100
1	J	322/337 (96%)	318 (99%)	4 (1%)	0	100	100
1	K	325/337 (96%)	320 (98%)	5 (2%)	0	100	100
1	L	320/337 (95%)	308 (96%)	12 (4%)	0	100	100
All	All	3888/4044 (96%)	3807 (98%)	81 (2%)	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	257/265 (97%)	254 (99%)	3 (1%)	71	88
1	B	257/265 (97%)	254 (99%)	3 (1%)	71	88
1	C	256/265 (97%)	254 (99%)	2 (1%)	81	93
1	D	259/265 (98%)	256 (99%)	3 (1%)	71	88
1	E	258/265 (97%)	254 (98%)	4 (2%)	62	84
1	F	257/265 (97%)	257 (100%)	0	100	100
1	G	258/265 (97%)	248 (96%)	10 (4%)	32	57
1	H	258/265 (97%)	252 (98%)	6 (2%)	50	76
1	I	257/265 (97%)	253 (98%)	4 (2%)	62	84
1	J	257/265 (97%)	256 (100%)	1 (0%)	91	97
1	K	258/265 (97%)	257 (100%)	1 (0%)	91	97
1	L	255/265 (96%)	253 (99%)	2 (1%)	81	93
All	All	3087/3180 (97%)	3048 (99%)	39 (1%)	69	87

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ARG
1	A	116	ARG
1	A	178	ASN
1	B	40	LEU
1	B	189	ASP
1	B	190	SER
1	C	35	SER
1	C	261	SER
1	D	40	LEU
1	D	163	ASP
1	D	291	ARG
1	E	106	ARG
1	E	116	ARG
1	E	195	ASP
1	E	239	LYS
1	G	28	ARG
1	G	106	ARG
1	G	163	ASP

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Mol	Chain	Res	Type
1	G	186	LEU
1	G	215	SER
1	G	226	LYS
1	G	239	LYS
1	G	291	ARG
1	G	303	ARG
1	G	310	ARG
1	H	3	LYS
1	H	78	GLU
1	H	106	ARG
1	H	175	LYS
1	H	239	LYS
1	H	241	GLU
1	I	40	LEU
1	I	178	ASN
1	I	190	SER
1	I	203	LYS
1	J	102	SER
1	K	178	ASN
1	L	177	PHE
1	L	178	ASN

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

Mol	Chain	Res	Type
1	I	45	ASN
1	I	108	ASN
1	I	159	HIS
1	J	167	GLN
1	L	130	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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DAB	J	402	2	6,7,7	0.79	0	6,8,8	1.01	0
3	DAB	D	402	2	6,7,7	0.85	0	6,8,8	0.89	0
4	ACT	C	402	2	3,3,3	1.21	0	3,3,3	1.55	0
4	ACT	G	402	-	3,3,3	1.31	0	3,3,3	1.36	0
4	ACT	H	402	2	3,3,3	1.29	0	3,3,3	1.49	0
3	DAB	A	402	1,2	6,7,7	0.84	0	6,8,8	0.85	0
3	DAB	K	401	-	6,7,7	0.81	0	6,8,8	0.90	0
3	DAB	B	402	1,2	6,7,7	0.84	0	6,8,8	1.23	1 (16%)
3	DAB	E	402	1,2	6,7,7	0.81	0	6,8,8	0.98	0
3	DAB	F	401	-	6,7,7	0.83	0	6,8,8	0.86	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	DAB	J	402	2	-	4/7/7/7	-
3	DAB	D	402	2	-	3/7/7/7	-
3	DAB	A	402	1,2	-	2/7/7/7	-
3	DAB	K	401	-	-	5/7/7/7	-
3	DAB	B	402	1,2	-	3/7/7/7	-
3	DAB	E	402	1,2	-	0/7/7/7	-
3	DAB	F	401	-	-	1/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	DAB	CB-CA-C	-2.23	105.00	110.30

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	402	DAB	CA-CB-CG-ND
3	J	402	DAB	O-C-CA-N
3	J	402	DAB	CA-CB-CG-ND
3	K	401	DAB	O-C-CA-N
3	K	401	DAB	CA-CB-CG-ND
3	J	402	DAB	OXT-C-CA-N
3	K	401	DAB	OXT-C-CA-N
3	B	402	DAB	OXT-C-CA-N
3	A	402	DAB	OXT-C-CA-N
3	A	402	DAB	O-C-CA-N
3	B	402	DAB	O-C-CA-N
3	K	401	DAB	OXT-C-CA-CB
3	B	402	DAB	C-CA-CB-CG
3	K	401	DAB	O-C-CA-CB
3	D	402	DAB	O-C-CA-CB
3	D	402	DAB	OXT-C-CA-CB
3	J	402	DAB	OXT-C-CA-CB
3	F	401	DAB	N-CA-CB-CG

There are no ring outliers.

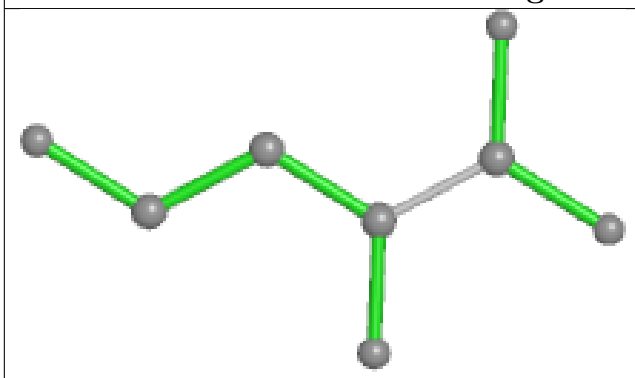
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	402	DAB	1	0
3	A	402	DAB	1	0
3	K	401	DAB	2	0
3	B	402	DAB	2	2
3	E	402	DAB	1	1

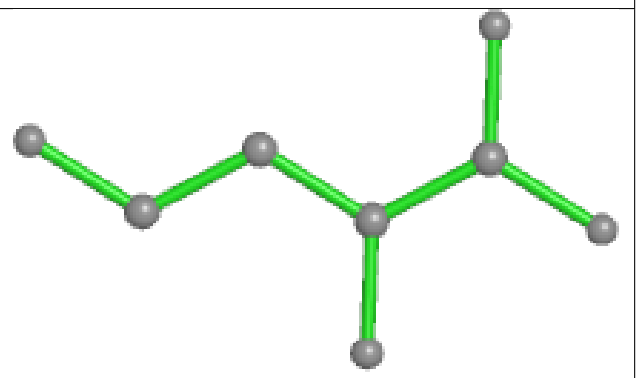
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

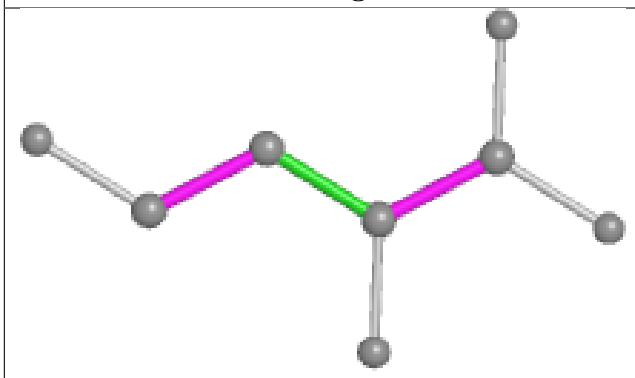
Ligand DAB J 402



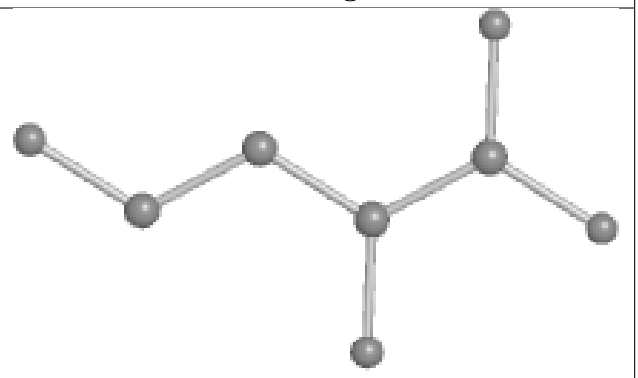
Bond lengths



Bond angles

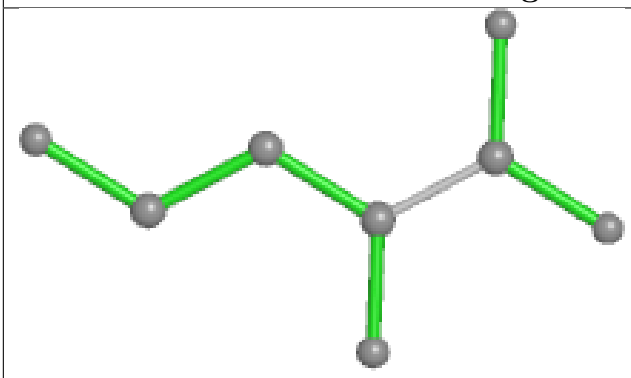


Torsions

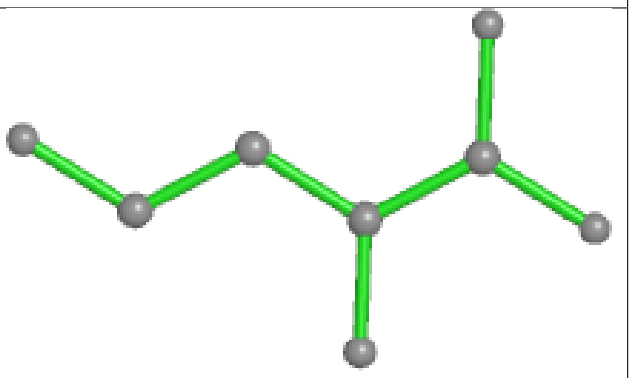


Rings

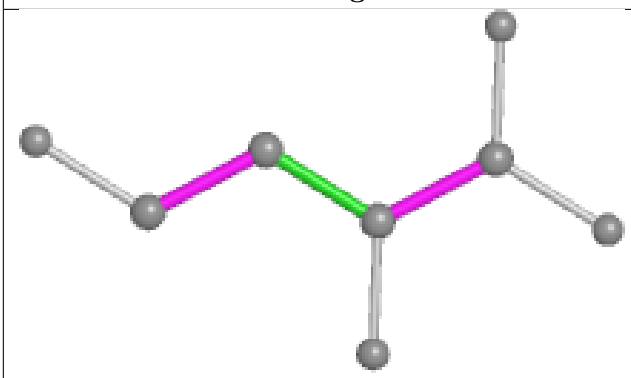
Ligand DAB D 402



Bond lengths



Bond angles



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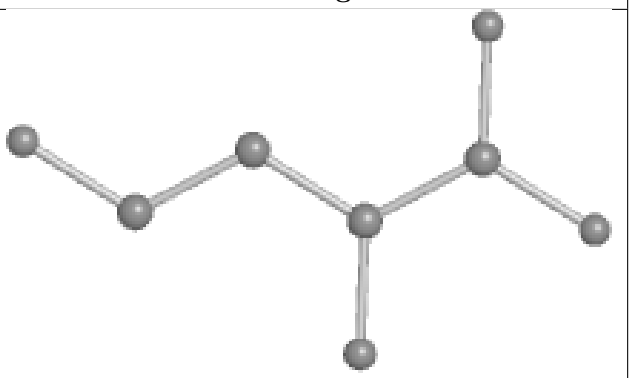
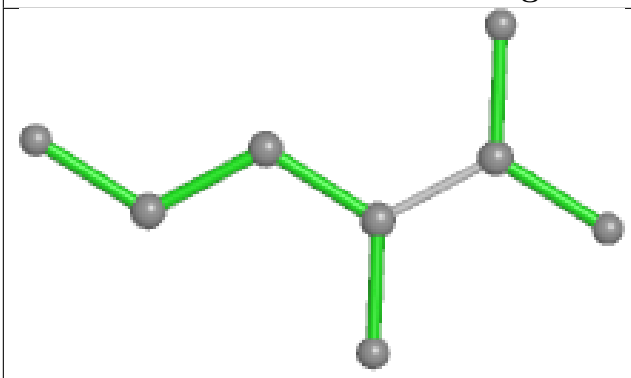
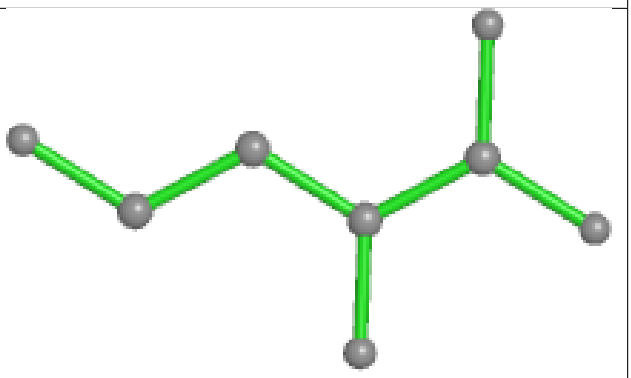


Rings

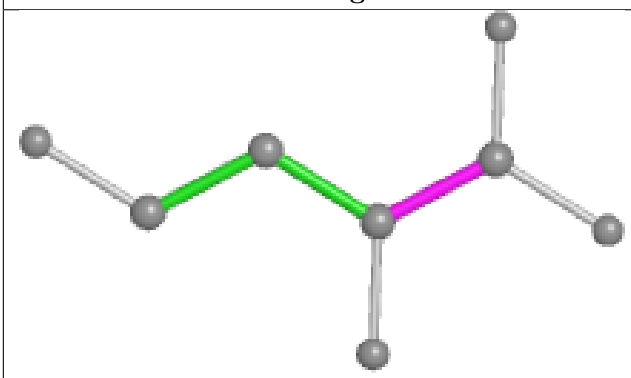
Ligand DAB A 402



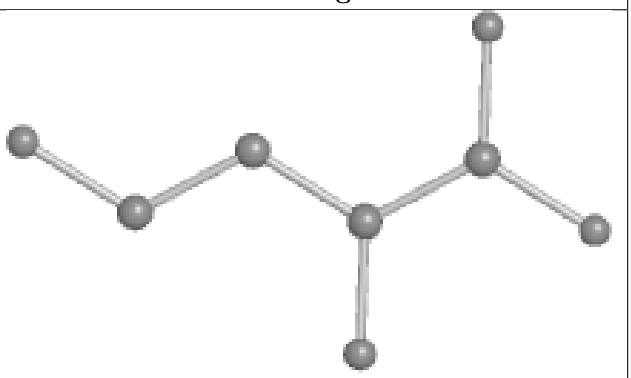
Bond lengths



Bond angles

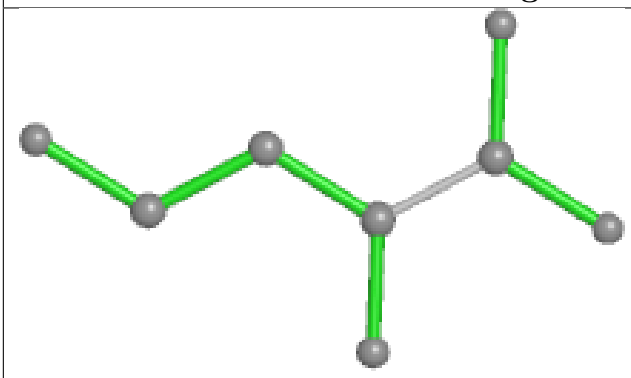


Torsions

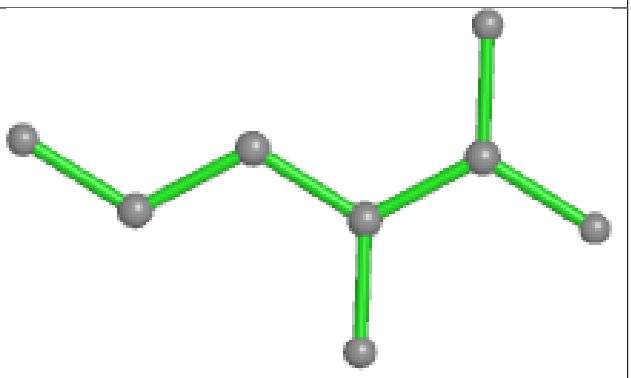


Rings

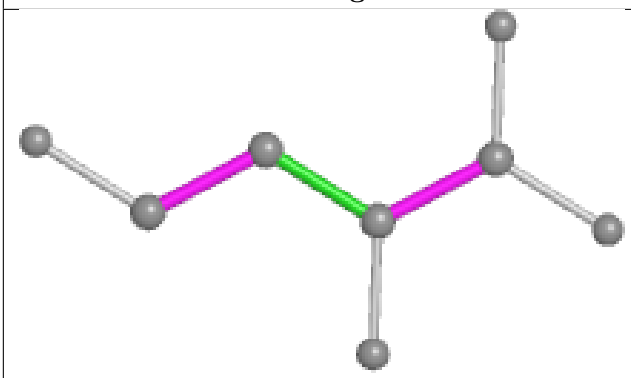
Ligand DAB K 401



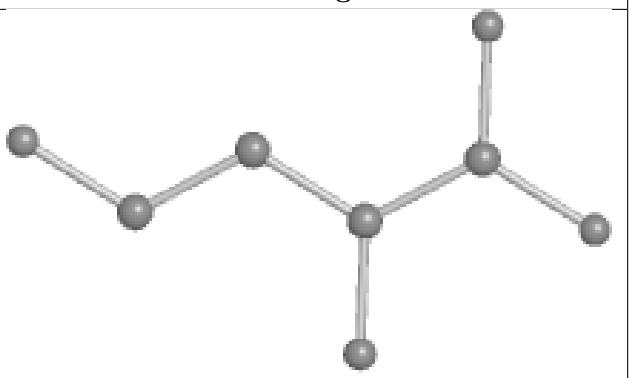
Bond lengths



Bond angles

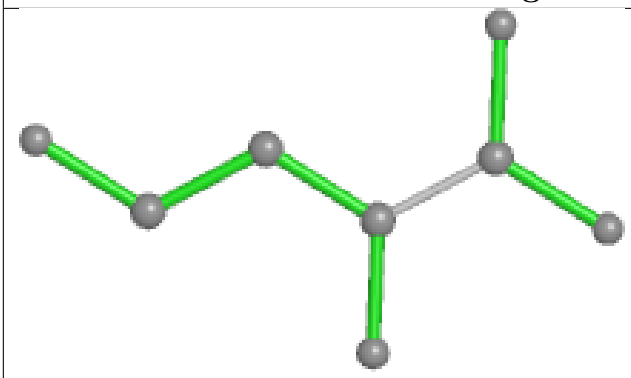


Torsions

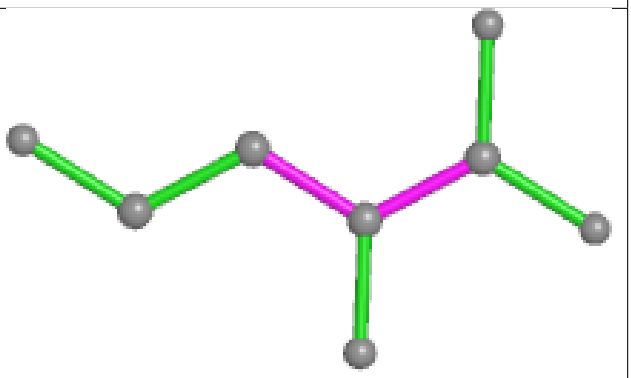


Rings

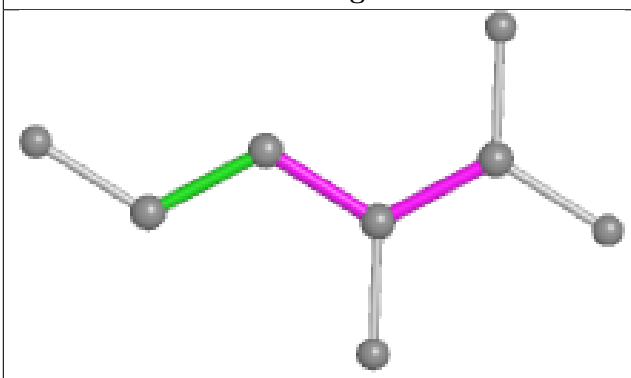
Ligand DAB B 402



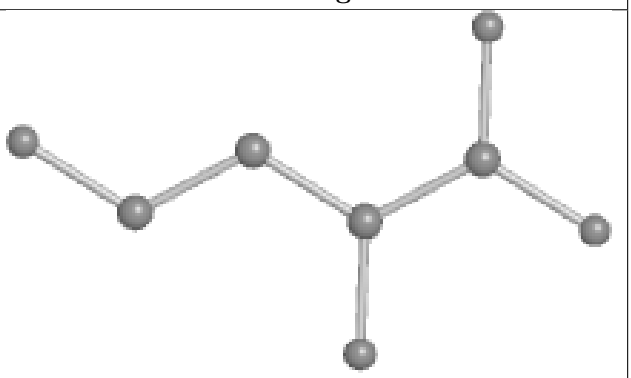
Bond lengths



Bond angles

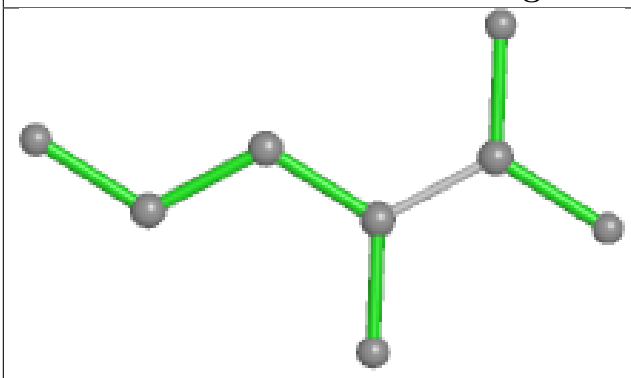


Torsions

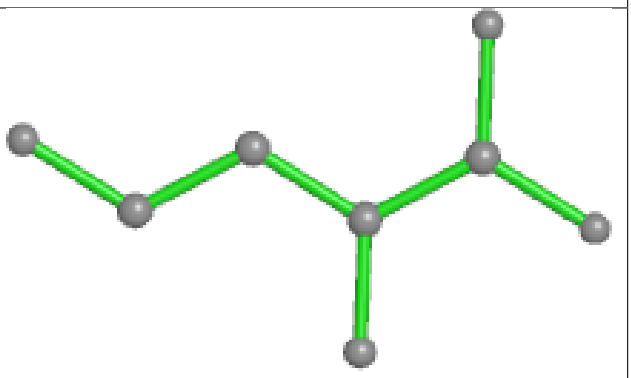


Rings

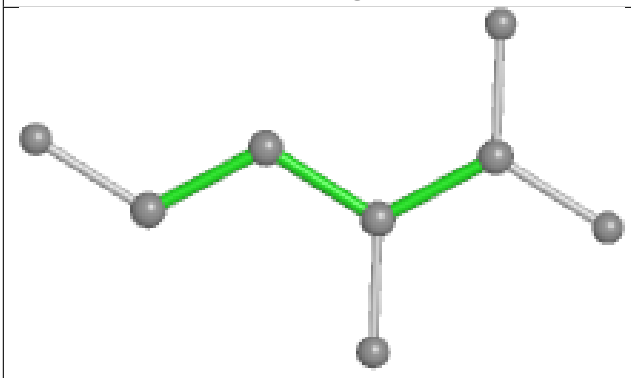
Ligand DAB E 402



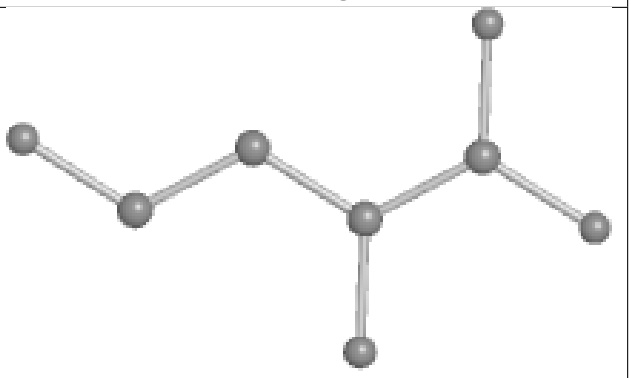
Bond lengths



Bond angles

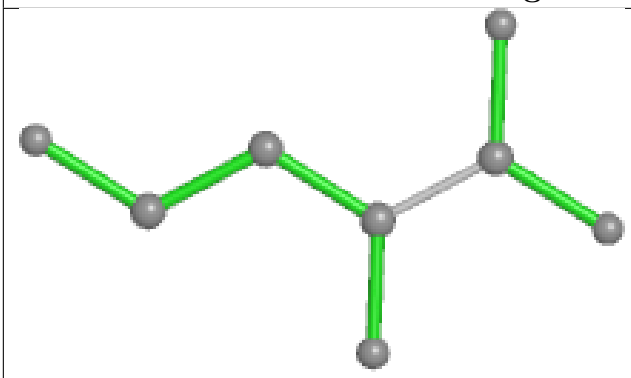


Torsions

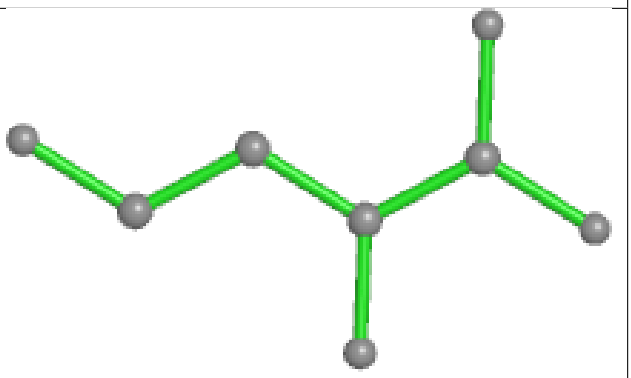


Rings

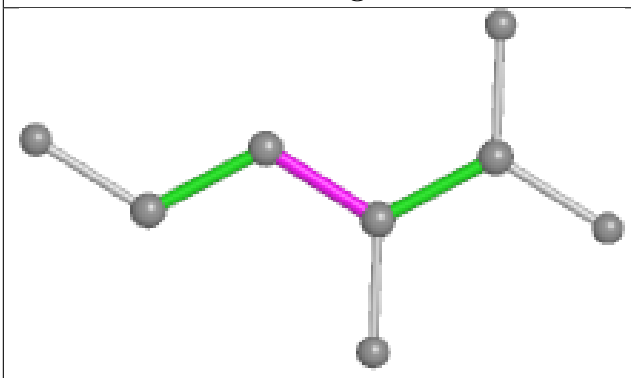
Ligand DAB F 401



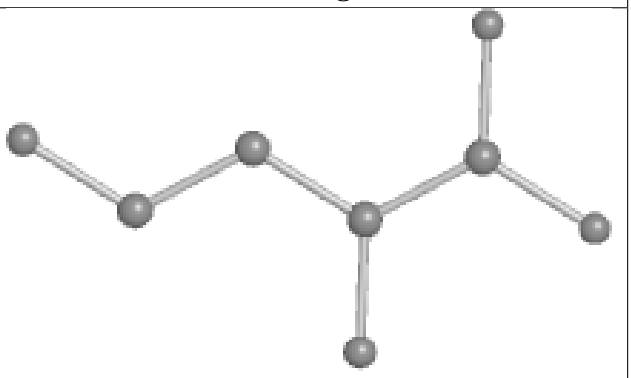
Bond lengths



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	326/337 (96%)	-0.20	1 (0%)	94	94	28, 41, 72, 125	0
1	B	326/337 (96%)	-0.10	2 (0%)	89	90	27, 44, 74, 139	0
1	C	325/337 (96%)	-0.12	3 (0%)	84	86	24, 44, 73, 115	0
1	D	328/337 (97%)	-0.13	6 (1%)	68	71	25, 43, 76, 132	0
1	E	327/337 (97%)	-0.11	5 (1%)	73	75	28, 43, 68, 95	0
1	F	327/337 (97%)	-0.14	1 (0%)	94	94	26, 44, 66, 92	0
1	G	327/337 (97%)	0.12	13 (3%)	38	41	30, 48, 83, 117	0
1	H	327/337 (97%)	0.01	3 (0%)	84	86	31, 48, 84, 125	0
1	I	326/337 (96%)	0.20	13 (3%)	38	41	29, 51, 88, 139	0
1	J	326/337 (96%)	0.07	15 (4%)	32	34	29, 47, 83, 138	0
1	K	327/337 (97%)	0.02	8 (2%)	59	62	31, 48, 76, 130	0
1	L	324/337 (96%)	0.34	19 (5%)	22	23	34, 60, 92, 130	0
All	All	3916/4044 (96%)	-0.00	89 (2%)	60	63	24, 46, 80, 139	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	47	ALA	6.7
1	L	108	ASN	6.6
1	J	163	ASP	6.3
1	G	165	ALA	6.3
1	D	163	ASP	6.3
1	K	163	ASP	6.2
1	K	188	ILE	5.5
1	E	46	GLY	5.3
1	L	106	ARG	5.1
1	I	77	ALA	4.7
1	L	188	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	131	ARG	4.1
1	D	162	GLU	4.1
1	I	47	ALA	3.9
1	J	16	GLY	3.7
1	J	46	GLY	3.5
1	K	46	GLY	3.5
1	L	202	GLY	3.5
1	L	107	GLY	3.5
1	I	188	ILE	3.4
1	I	165	ALA	3.3
1	C	240	GLY	3.3
1	G	186	LEU	3.3
1	E	47	ALA	3.3
1	G	188	ILE	3.3
1	I	43	ILE	3.3
1	I	126	ALA	3.2
1	L	169	ALA	3.1
1	J	2	GLN	3.1
1	G	258	PHE	3.1
1	L	4	ASN	3.1
1	D	188	ILE	3.1
1	E	2	GLN	3.1
1	K	165	ALA	3.1
1	L	47	ALA	3.1
1	J	162	GLU	3.0
1	I	163	ASP	3.0
1	G	187	GLU	3.0
1	G	46	GLY	3.0
1	C	185	LEU	2.9
1	H	188	ILE	2.9
1	G	166	THR	2.9
1	L	166	THR	2.8
1	I	76	SER	2.8
1	G	161	LEU	2.8
1	J	166	THR	2.7
1	I	80	VAL	2.7
1	L	197	ALA	2.7
1	L	33	TRP	2.7
1	D	2	GLN	2.6
1	J	165	ALA	2.6
1	C	293	GLY	2.6
1	E	16	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	18	PHE	2.5
1	L	133	LEU	2.5
1	L	198	VAL	2.5
1	I	114	PRO	2.5
1	L	15	ASP	2.5
1	I	18	PHE	2.4
1	J	48	GLY	2.4
1	G	179	ALA	2.4
1	H	197	ALA	2.4
1	G	328	THR	2.4
1	L	43	ILE	2.4
1	J	21	PHE	2.4
1	K	14	ARG	2.4
1	L	195	ASP	2.3
1	F	161	LEU	2.3
1	J	172	ALA	2.3
1	G	192	GLY	2.3
1	A	46	GLY	2.3
1	J	239	LYS	2.3
1	J	119	GLY	2.3
1	G	244	LEU	2.3
1	E	45	ASN	2.2
1	B	16	GLY	2.2
1	J	189	ASP	2.2
1	K	280	GLY	2.2
1	L	158	ALA	2.2
1	I	177	PHE	2.2
1	D	1	HIS	2.2
1	G	164	LYS	2.1
1	H	72	ALA	2.1
1	B	187	GLU	2.1
1	L	328	THR	2.1
1	K	271	ILE	2.1
1	I	16	GLY	2.1
1	K	47	ALA	2.0
1	L	104	ILE	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)

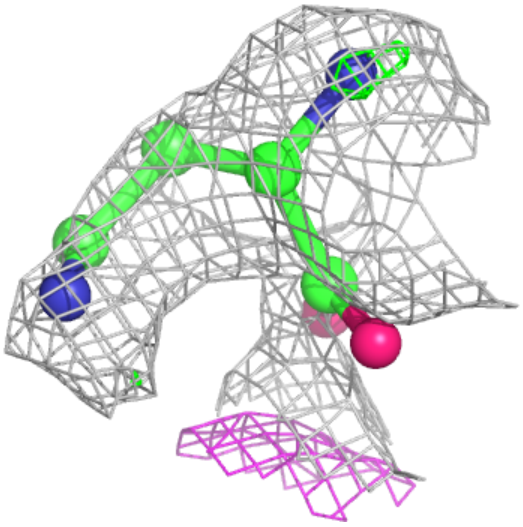
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

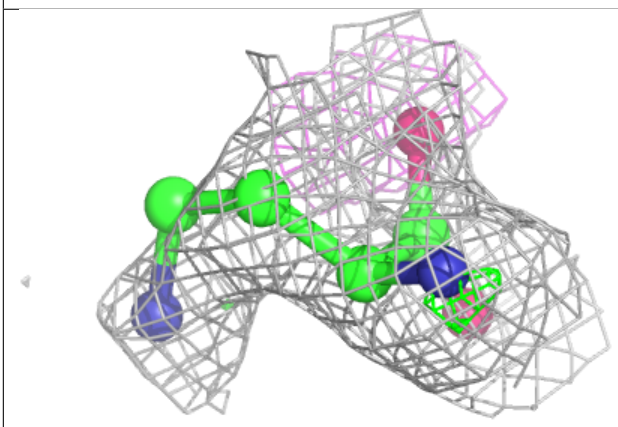
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DAB	J	402	8/8	0.45	0.31	85,87,89,90	0
3	DAB	E	402	8/8	0.46	0.34	59,77,89,95	0
3	DAB	K	401	8/8	0.46	0.36	90,91,93,93	0
2	ZN	D	401	1/1	0.61	0.17	134,134,134,134	0
3	DAB	A	402	8/8	0.68	0.22	100,101,105,105	0
3	DAB	B	402	8/8	0.70	0.24	59,76,78,81	0
4	ACT	G	402	4/4	0.70	0.24	82,83,83,83	0
2	ZN	H	401	1/1	0.74	0.27	132,132,132,132	0
2	ZN	C	401	1/1	0.77	0.13	114,114,114,114	0
4	ACT	C	402	4/4	0.79	0.44	110,110,111,112	0
3	DAB	F	401	8/8	0.80	0.24	61,62,63,64	0
3	DAB	D	402	8/8	0.81	0.29	84,85,86,86	0
2	ZN	G	401	1/1	0.82	0.42	83,83,83,83	0
4	ACT	H	402	4/4	0.83	0.17	75,75,76,76	0
2	ZN	L	401	1/1	0.85	0.17	133,133,133,133	0
2	ZN	E	401	1/1	0.91	0.21	101,101,101,101	0
2	ZN	J	401	1/1	0.92	0.19	72,72,72,72	0
2	ZN	B	401	1/1	0.93	0.13	84,84,84,84	0
2	ZN	A	401	1/1	0.96	0.06	101,101,101,101	0
2	ZN	I	401	1/1	0.97	0.08	95,95,95,95	0

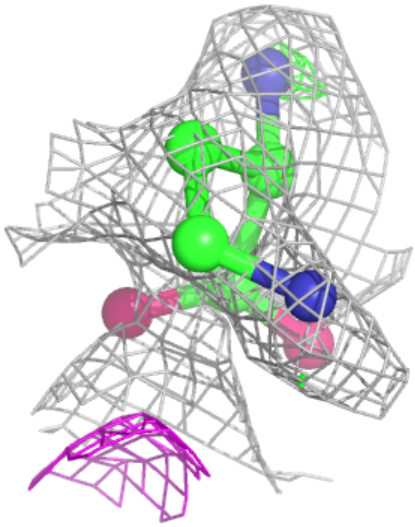
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DAB J 402:

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

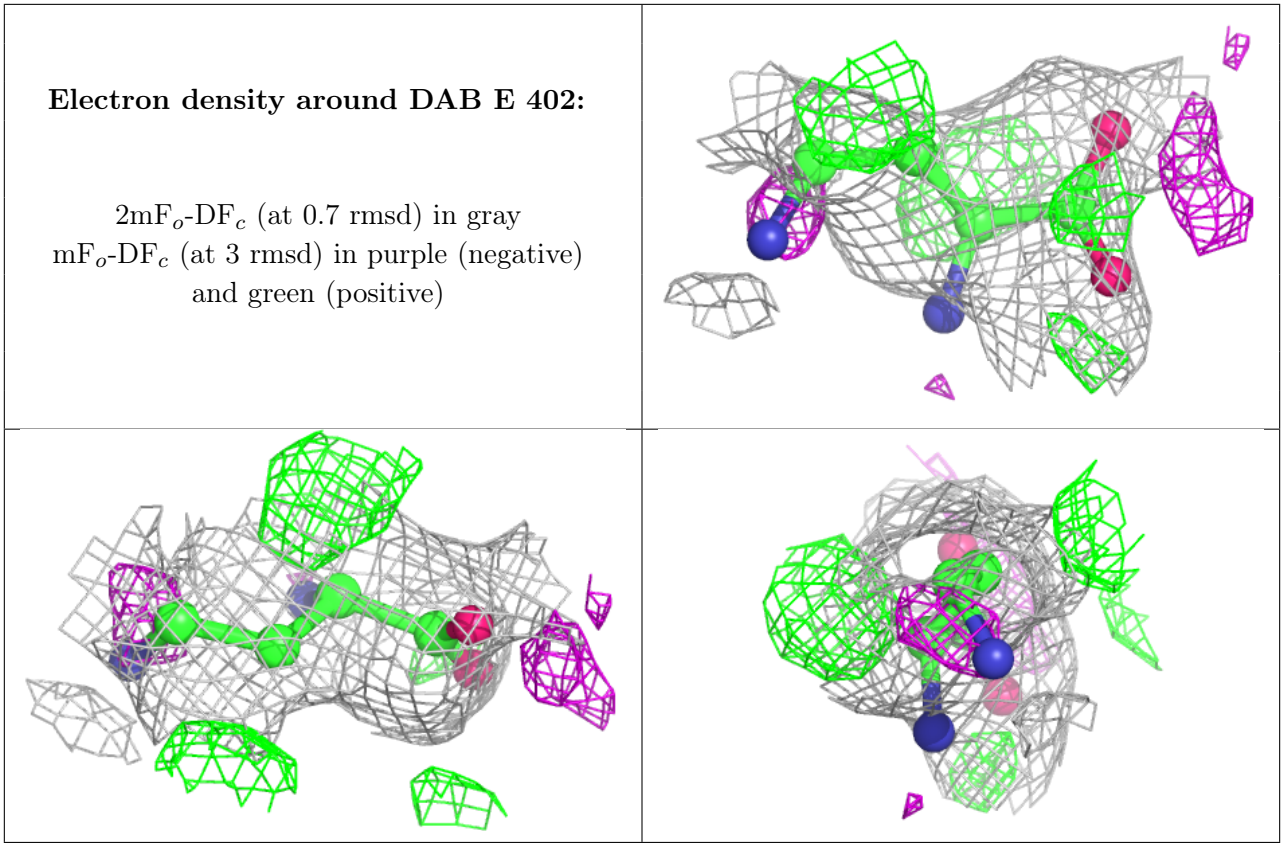






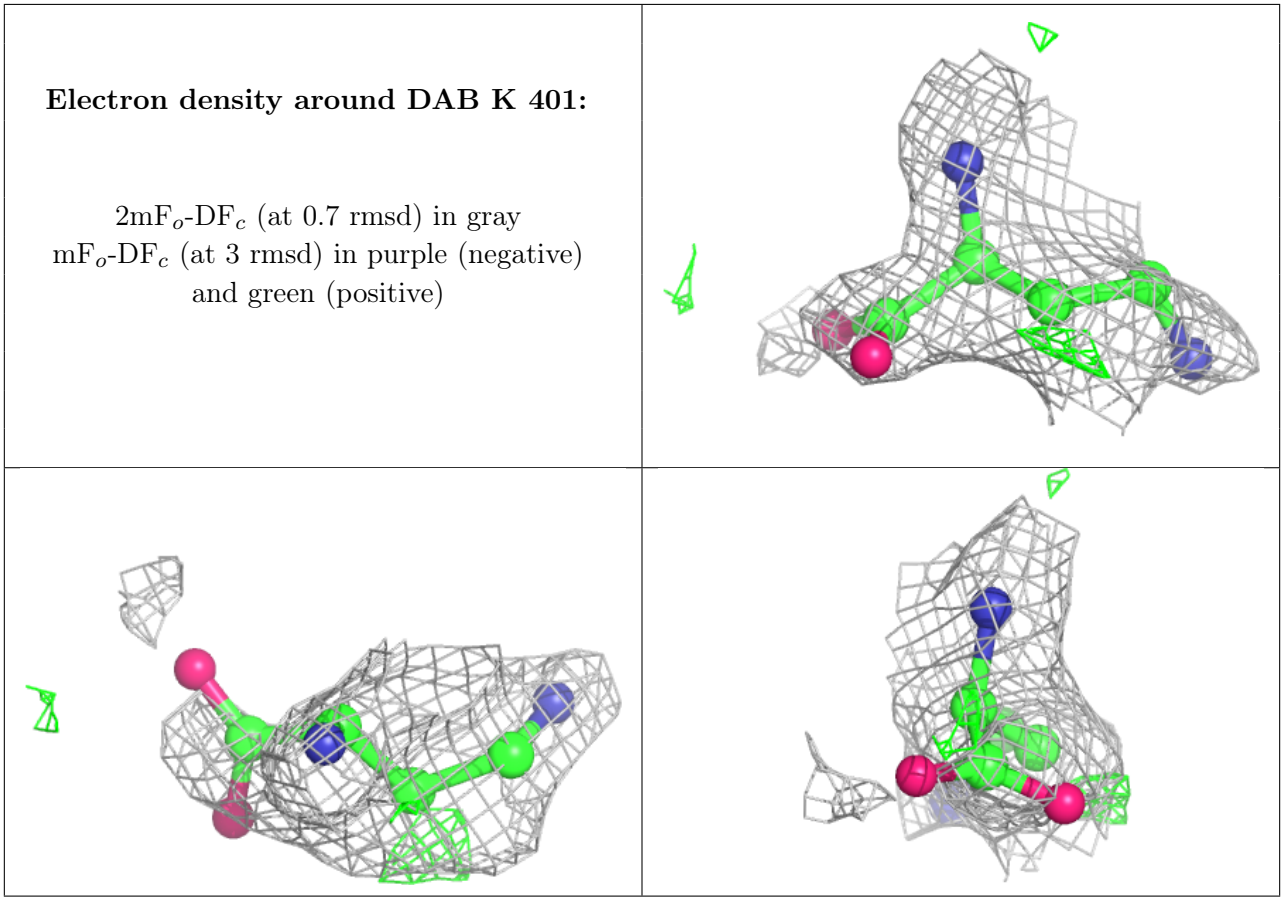
Electron density around DAB E 402:

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



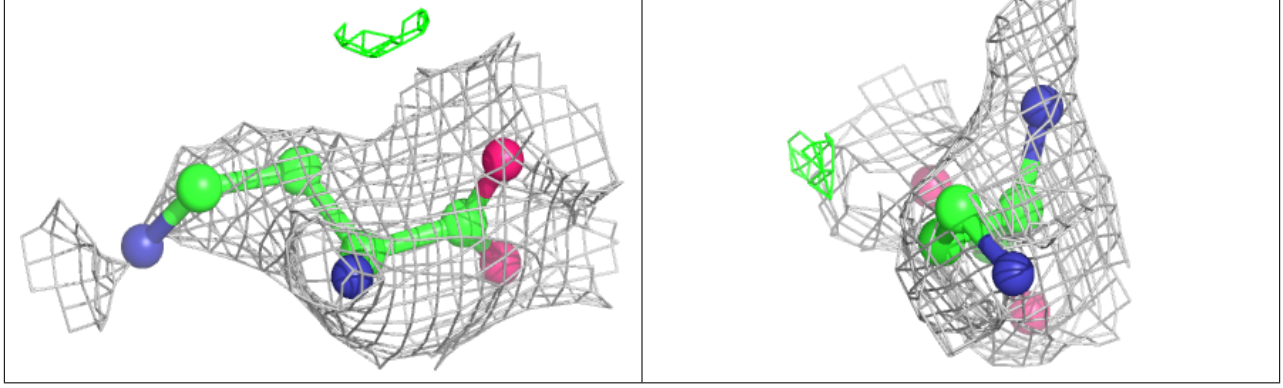
Electron density around DAB K 401:

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



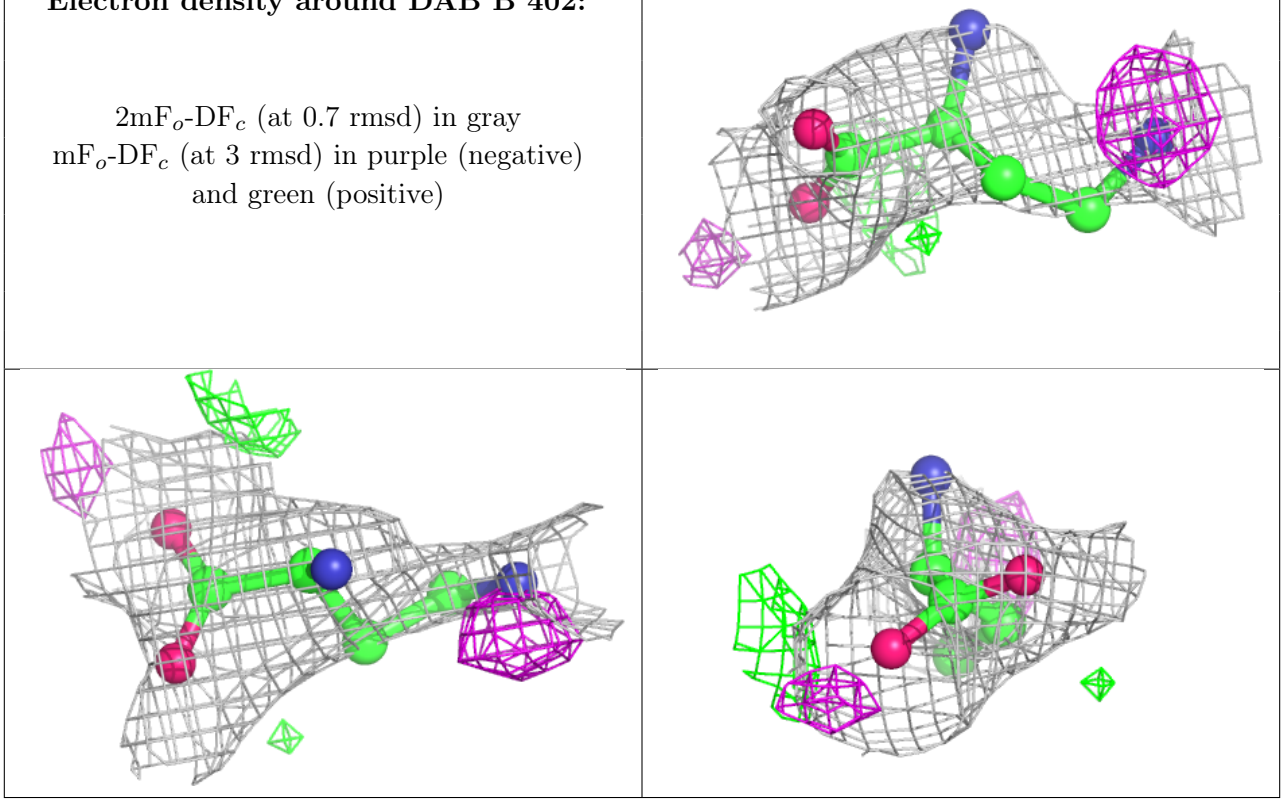
Electron density around DAB A 402:

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



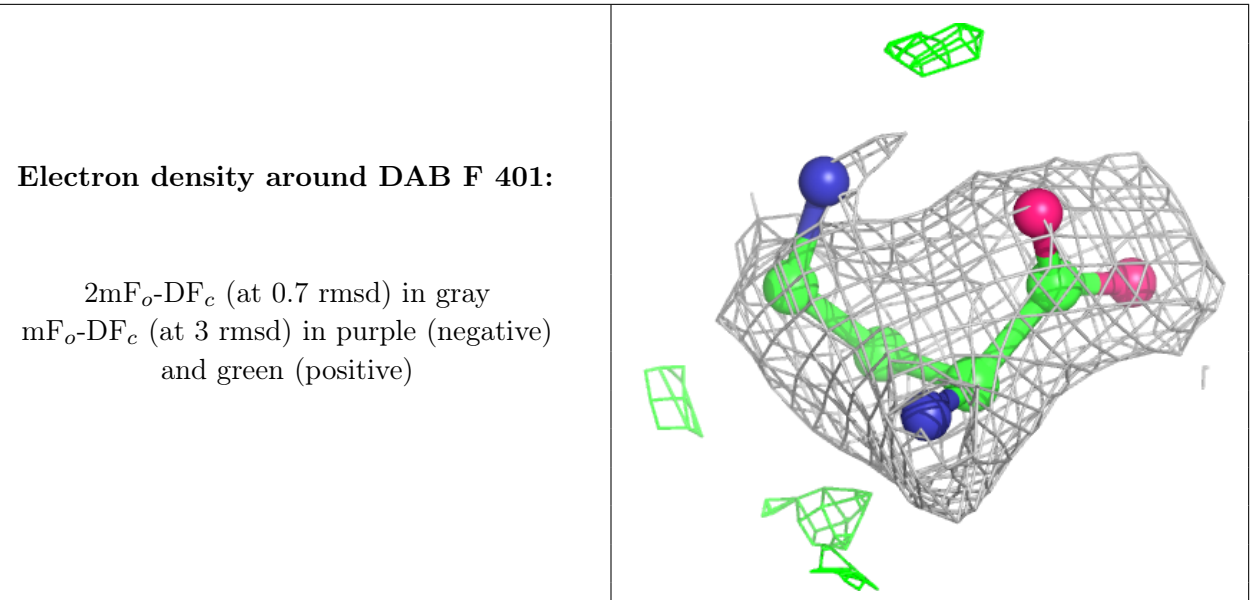
Electron density around DAB B 402:

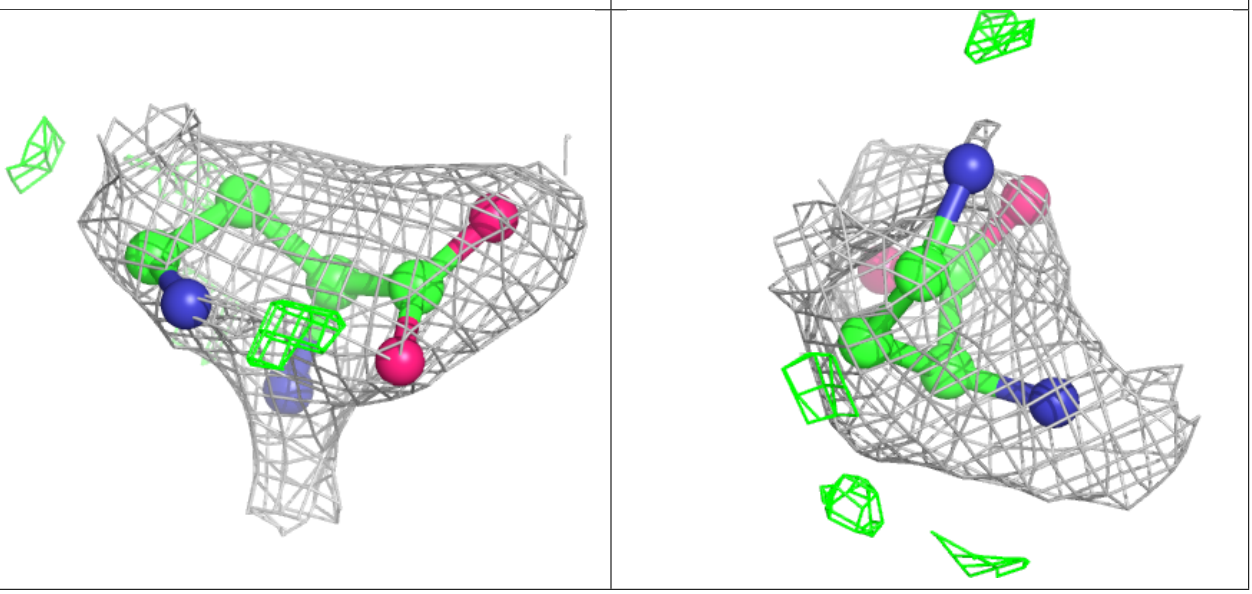
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DAB F 401:

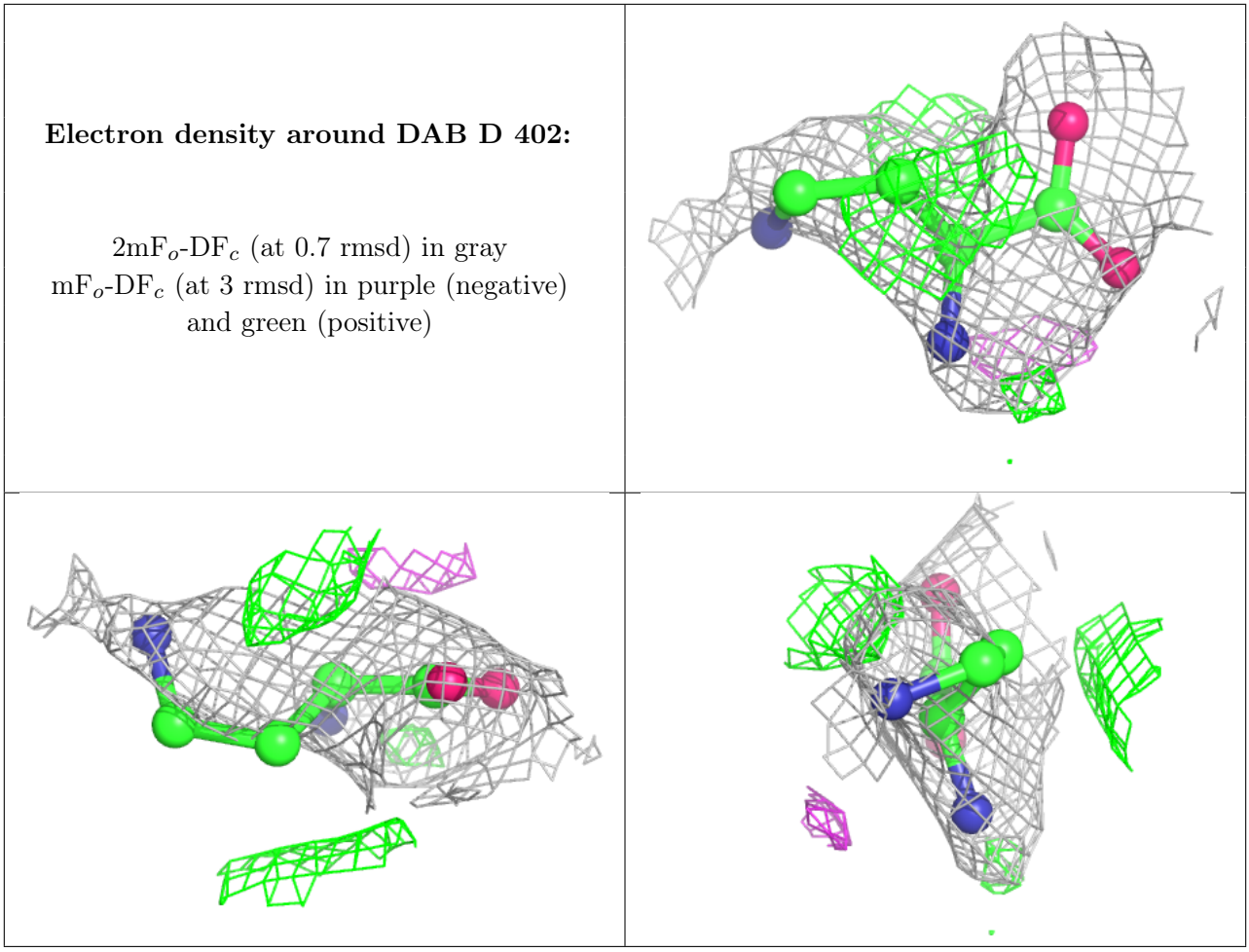
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around DAB D 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.