Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2023 – 03:34 AM EDT

PDB ID	:	8U9B
Title	:	Crystal Structure of Betaine aldehyde dehydrogenase (BetB) from Klebsiella aerogenes (Apo, P21 Form)
Authors	:	Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2023-09-18
Resolution	:	1.90 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:

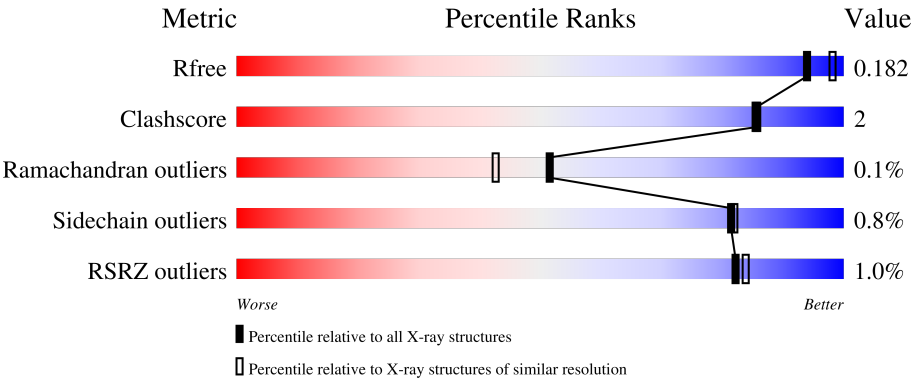
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	499	94% 5%
1	B	499	96%
1	C	499	95%
1	D	499	93% 5%

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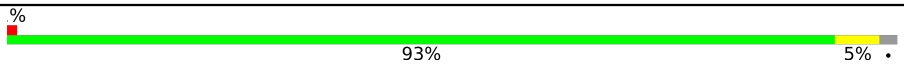
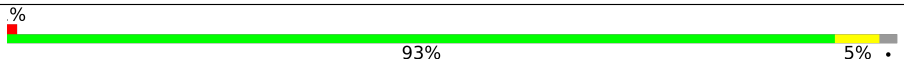
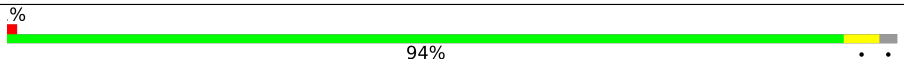
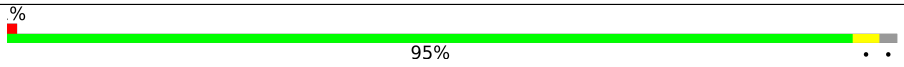
Mol	Chain	Length	Quality of chain
1	E	499	
1	F	499	
1	G	499	
1	H	499	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MLI	E	508	-	-	-	X
8	EPE	E	509	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 33696 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 Betaine aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	6	0
			3773	2381	656	718	18			
1	B	493	Total	C	N	O	S	0	7	0
			3761	2375	654	714	18			
1	C	493	Total	C	N	O	S	0	7	0
			3772	2382	657	716	17			
1	D	489	Total	C	N	O	S	0	6	0
			3733	2358	643	715	17			
1	E	488	Total	C	N	O	S	0	6	0
			3710	2343	636	714	17			
1	F	489	Total	C	N	O	S	0	7	0
			3733	2357	644	715	17			
1	G	488	Total	C	N	O	S	0	4	0
			3708	2343	638	710	17			
1	H	488	Total	C	N	O	S	0	4	0
			3701	2338	639	707	17			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP A0A447LC14
A	-7	ALA	-	expression tag	UNP A0A447LC14
A	-6	HIS	-	expression tag	UNP A0A447LC14
A	-5	HIS	-	expression tag	UNP A0A447LC14
A	-4	HIS	-	expression tag	UNP A0A447LC14
A	-3	HIS	-	expression tag	UNP A0A447LC14
A	-2	HIS	-	expression tag	UNP A0A447LC14
A	-1	HIS	-	expression tag	UNP A0A447LC14
A	0	HIS	-	expression tag	UNP A0A447LC14
A	62	ALA	VAL	engineered mutation	UNP A0A447LC14
A	485	PRO	GLN	engineered mutation	UNP A0A447LC14
B	-8	MET	-	expression tag	UNP A0A447LC14
B	-7	ALA	-	expression tag	UNP A0A447LC14

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP A0A447LC14
B	-5	HIS	-	expression tag	UNP A0A447LC14
B	-4	HIS	-	expression tag	UNP A0A447LC14
B	-3	HIS	-	expression tag	UNP A0A447LC14
B	-2	HIS	-	expression tag	UNP A0A447LC14
B	-1	HIS	-	expression tag	UNP A0A447LC14
B	0	HIS	-	expression tag	UNP A0A447LC14
B	62	ALA	VAL	engineered mutation	UNP A0A447LC14
B	485	PRO	GLN	engineered mutation	UNP A0A447LC14
C	-8	MET	-	expression tag	UNP A0A447LC14
C	-7	ALA	-	expression tag	UNP A0A447LC14
C	-6	HIS	-	expression tag	UNP A0A447LC14
C	-5	HIS	-	expression tag	UNP A0A447LC14
C	-4	HIS	-	expression tag	UNP A0A447LC14
C	-3	HIS	-	expression tag	UNP A0A447LC14
C	-2	HIS	-	expression tag	UNP A0A447LC14
C	-1	HIS	-	expression tag	UNP A0A447LC14
C	0	HIS	-	expression tag	UNP A0A447LC14
C	62	ALA	VAL	engineered mutation	UNP A0A447LC14
C	485	PRO	GLN	engineered mutation	UNP A0A447LC14
D	-8	MET	-	expression tag	UNP A0A447LC14
D	-7	ALA	-	expression tag	UNP A0A447LC14
D	-6	HIS	-	expression tag	UNP A0A447LC14
D	-5	HIS	-	expression tag	UNP A0A447LC14
D	-4	HIS	-	expression tag	UNP A0A447LC14
D	-3	HIS	-	expression tag	UNP A0A447LC14
D	-2	HIS	-	expression tag	UNP A0A447LC14
D	-1	HIS	-	expression tag	UNP A0A447LC14
D	0	HIS	-	expression tag	UNP A0A447LC14
D	62	ALA	VAL	engineered mutation	UNP A0A447LC14
D	485	PRO	GLN	engineered mutation	UNP A0A447LC14
E	-8	MET	-	expression tag	UNP A0A447LC14
E	-7	ALA	-	expression tag	UNP A0A447LC14
E	-6	HIS	-	expression tag	UNP A0A447LC14
E	-5	HIS	-	expression tag	UNP A0A447LC14
E	-4	HIS	-	expression tag	UNP A0A447LC14
E	-3	HIS	-	expression tag	UNP A0A447LC14
E	-2	HIS	-	expression tag	UNP A0A447LC14
E	-1	HIS	-	expression tag	UNP A0A447LC14
E	0	HIS	-	expression tag	UNP A0A447LC14
E	62	ALA	VAL	engineered mutation	UNP A0A447LC14
E	485	PRO	GLN	engineered mutation	UNP A0A447LC14

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-8	MET	-	expression tag	UNP A0A447LC14
F	-7	ALA	-	expression tag	UNP A0A447LC14
F	-6	HIS	-	expression tag	UNP A0A447LC14
F	-5	HIS	-	expression tag	UNP A0A447LC14
F	-4	HIS	-	expression tag	UNP A0A447LC14
F	-3	HIS	-	expression tag	UNP A0A447LC14
F	-2	HIS	-	expression tag	UNP A0A447LC14
F	-1	HIS	-	expression tag	UNP A0A447LC14
F	0	HIS	-	expression tag	UNP A0A447LC14
F	62	ALA	VAL	engineered mutation	UNP A0A447LC14
F	485	PRO	GLN	engineered mutation	UNP A0A447LC14
G	-8	MET	-	expression tag	UNP A0A447LC14
G	-7	ALA	-	expression tag	UNP A0A447LC14
G	-6	HIS	-	expression tag	UNP A0A447LC14
G	-5	HIS	-	expression tag	UNP A0A447LC14
G	-4	HIS	-	expression tag	UNP A0A447LC14
G	-3	HIS	-	expression tag	UNP A0A447LC14
G	-2	HIS	-	expression tag	UNP A0A447LC14
G	-1	HIS	-	expression tag	UNP A0A447LC14
G	0	HIS	-	expression tag	UNP A0A447LC14
G	62	ALA	VAL	engineered mutation	UNP A0A447LC14
G	485	PRO	GLN	engineered mutation	UNP A0A447LC14
H	-8	MET	-	expression tag	UNP A0A447LC14
H	-7	ALA	-	expression tag	UNP A0A447LC14
H	-6	HIS	-	expression tag	UNP A0A447LC14
H	-5	HIS	-	expression tag	UNP A0A447LC14
H	-4	HIS	-	expression tag	UNP A0A447LC14
H	-3	HIS	-	expression tag	UNP A0A447LC14
H	-2	HIS	-	expression tag	UNP A0A447LC14
H	-1	HIS	-	expression tag	UNP A0A447LC14
H	0	HIS	-	expression tag	UNP A0A447LC14
H	62	ALA	VAL	engineered mutation	UNP A0A447LC14
H	485	PRO	GLN	engineered mutation	UNP A0A447LC14

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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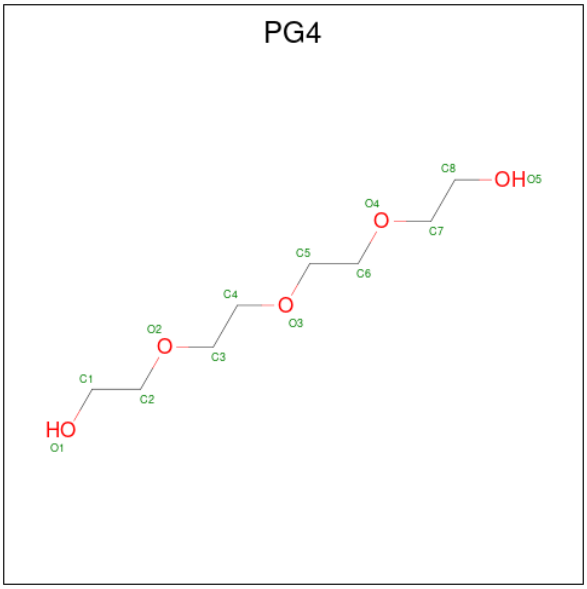
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0
2	G	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 13 8 5	0	0
3	D	1	Total C O 13 8 5	0	0
3	E	1	Total C O 13 8 5	0	0
3	F	1	Total C O 13 8 5	0	0

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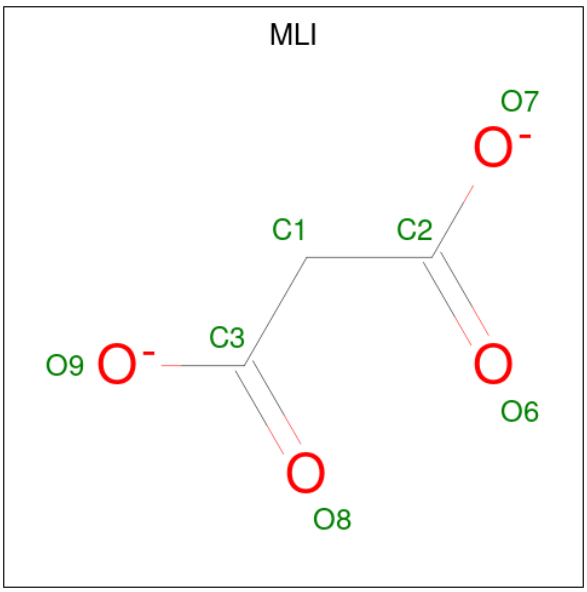
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 13 8 5	0	0
3	H	1	Total C O 13 8 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

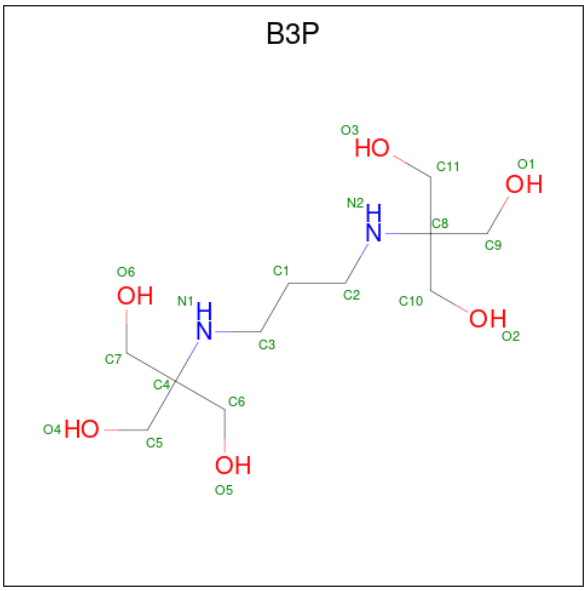
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	G	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



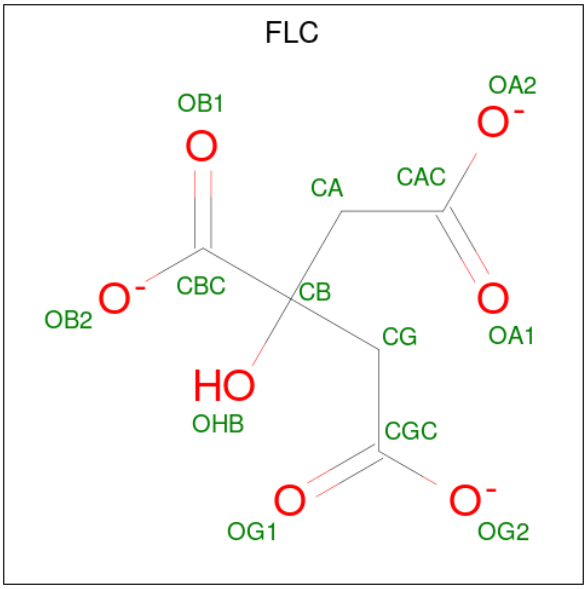
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 3 4	0	0
5	B	1	Total C O 7 3 4	0	0
5	C	1	Total C O 7 3 4	0	0
5	D	1	Total C O 7 3 4	0	0
5	D	1	Total C O 7 3 4	0	0
5	E	1	Total C O 7 3 4	0	0
5	E	1	Total C O 7 3 4	0	0
5	E	1	Total C O 7 3 4	0	0
5	F	1	Total C O 7 3 4	0	0
5	F	1	Total C O 7 3 4	0	0
5	F	1	Total C O 7 3 4	0	0
5	G	1	Total C O 7 3 4	0	0
5	G	1	Total C O 7 3 4	0	0
5	H	1	Total C O 7 3 4	0	0

- Molecule 6 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



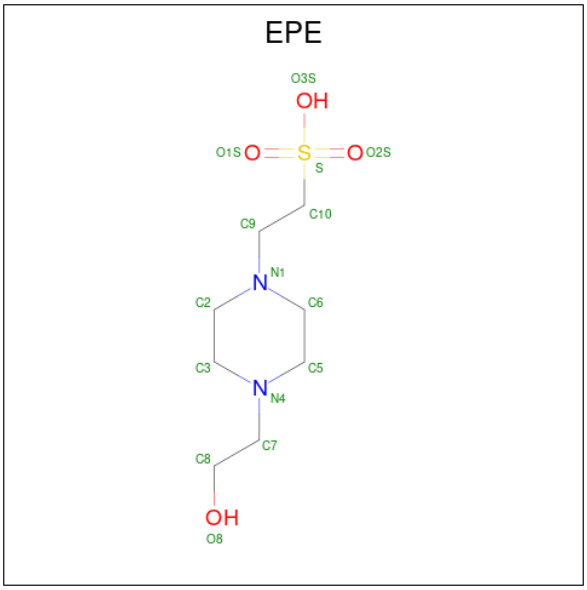
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 10 6 1 3	0	0
6	C	1	Total C N O 10 6 1 3	0	0
6	E	1	Total C N O 12 7 2 3	0	0
6	E	1	Total C N O 9 5 1 3	0	0
6	F	1	Total C N O 12 7 2 3	0	0

- Molecule 7 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 13 6 7	0	0

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	439	Total O 439 439	0	0
9	B	419	Total O 419 419	0	0
9	C	460	Total O 460 460	0	0
9	D	447	Total O 447 447	0	0
9	E	426	Total O 426 426	0	0
9	F	496	Total O 496 496	0	0
9	G	419	Total O 419 419	0	0

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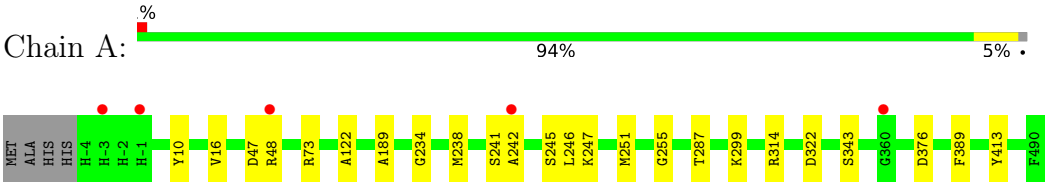
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	400	Total	O	0	0
			400	400		

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.

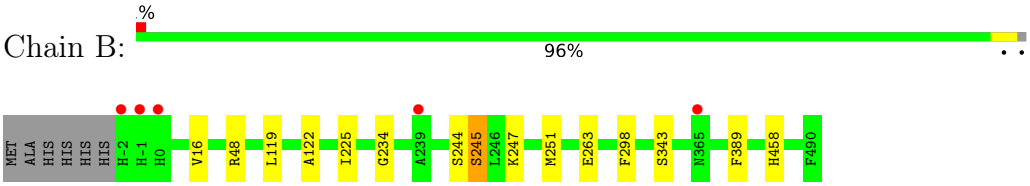
• Molecule 1: Betaine aldehyde dehydrogenase

Chain A:



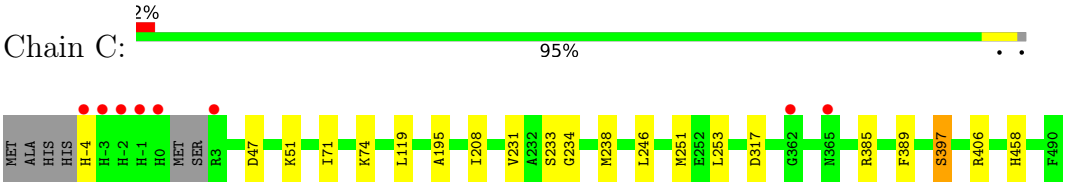
• Molecule 1: Betaine aldehyde dehydrogenase

Chain B:



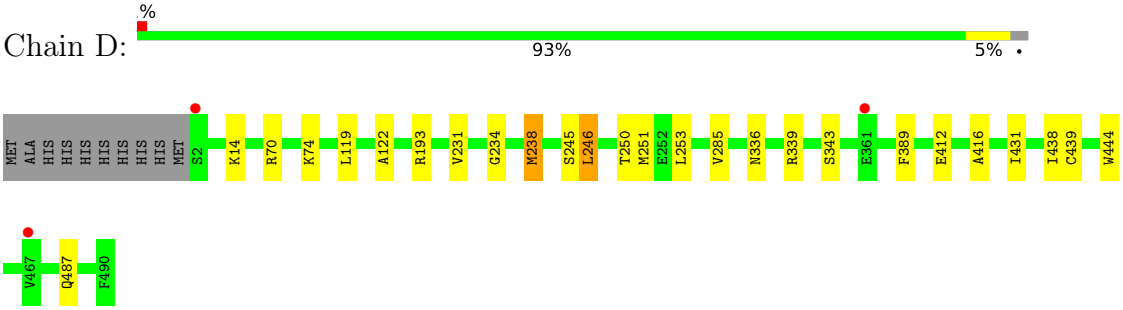
• Molecule 1: Betaine aldehyde dehydrogenase

Chain C:



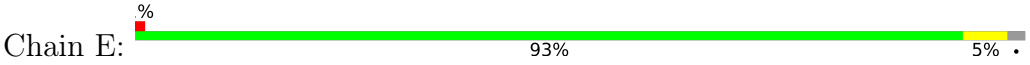
• Molecule 1: Betaine aldehyde dehydrogenase

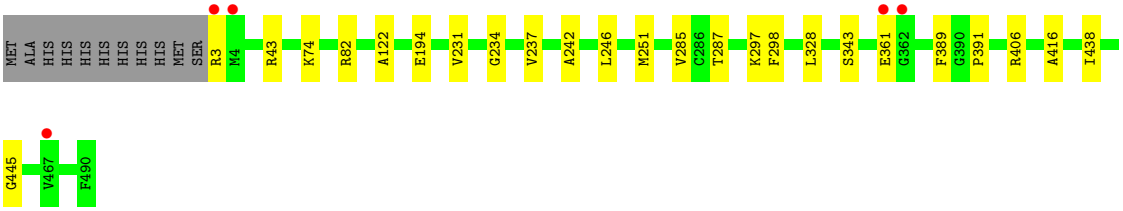
Chain D:



• Molecule 1: Betaine aldehyde dehydrogenase

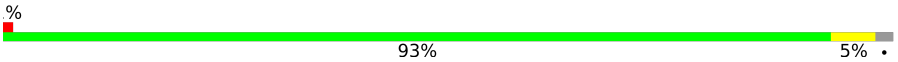
Chain E:

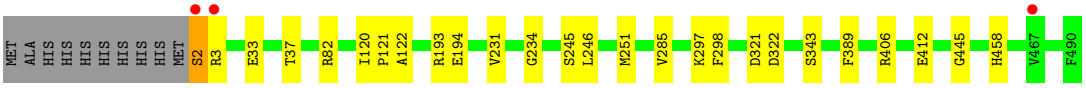




• Molecule 1: Betaine aldehyde dehydrogenase

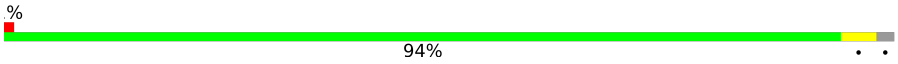
Chain F:

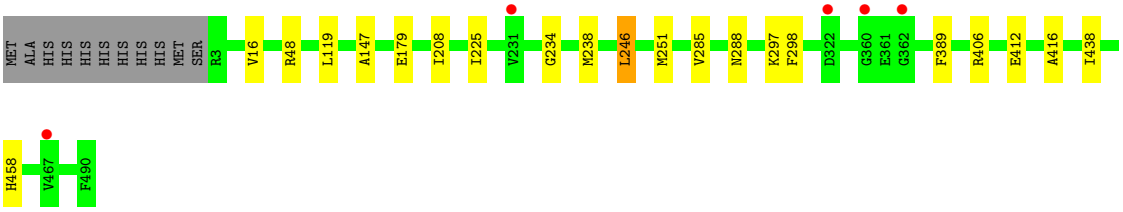




• Molecule 1: Betaine aldehyde dehydrogenase

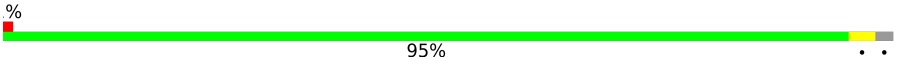
Chain G:

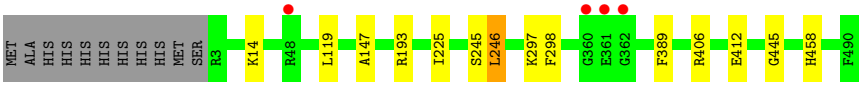




• Molecule 1: Betaine aldehyde dehydrogenase

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	101.27Å 161.24Å 158.71Å 90.00° 101.11° 90.00°	Depositor
Resolution (Å)	27.39 – 1.90 47.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (27.39-1.90) 100.0 (47.95-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5057: ???)	Depositor
R, R_{free}	0.147 , 0.175 0.158 , 0.182	Depositor DCC
R_{free} test set	19514 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33696	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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 45.23 % 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 1.3621e-04. 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: B3P, NA, MLI, FLC, PG4, EPE, CL

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	0.38	0/3867	0.60	0/5245
1	B	0.38	0/3856	0.61	0/5228
1	C	0.39	0/3867	0.62	0/5241
1	D	0.38	0/3822	0.62	0/5180
1	E	0.37	0/3799	0.60	0/5154
1	F	0.39	0/3825	0.63	0/5186
1	G	0.38	0/3791	0.60	0/5141
1	H	0.38	0/3785	0.61	0/5134
All	All	0.38	0/30612	0.61	0/41509

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3773	0	3740	17	0
1	B	3761	0	3746	13	0
1	C	3772	0	3754	18	0
1	D	3733	0	3729	30	0
1	E	3710	0	3683	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3733	0	3720	23	0
1	G	3708	0	3691	15	0
1	H	3701	0	3675	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	13	0	18	1	0
3	B	13	0	18	0	0
3	C	13	0	18	0	0
3	D	13	0	18	4	0
3	E	13	0	18	5	0
3	F	13	0	18	5	0
3	G	13	0	18	3	0
3	H	13	0	18	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	1	0
4	D	1	0	0	0	0
4	E	1	0	0	1	0
4	F	1	0	0	1	0
4	G	1	0	0	0	0
4	H	1	0	0	1	0
5	A	7	0	2	0	0
5	B	7	0	2	0	0
5	C	7	0	2	0	0
5	D	14	0	4	1	0
5	E	21	0	6	0	0
5	F	21	0	6	0	0
5	G	14	0	4	0	0
5	H	7	0	2	0	0
6	B	10	0	12	1	0
6	C	10	0	12	1	0
6	E	21	0	26	1	0
6	F	12	0	16	0	0
7	C	13	0	5	0	0
8	E	15	0	18	1	0
9	A	439	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	419	0	0	1	0
9	C	460	0	0	4	0
9	D	447	0	0	6	0
9	E	426	0	0	4	0
9	F	496	0	0	3	0
9	G	419	0	0	3	0
9	H	400	0	0	3	0
All	All	33696	0	29999	134	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 2.

All (134) 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:F:412:GLU:OE1	1:F:458:HIS:CE1	2.31	0.83
1:E:285:VAL:HG11	3:E:502:PG4:H11	1.71	0.72
1:D:74:LYS:HE2	9:D:791:HOH:O	1.89	0.72
1:F:193:ARG:NH1	9:F:601:HOH:O	2.23	0.71
1:F:285:VAL:HG11	3:F:502:PG4:C1	2.23	0.69
1:C:251:MET:HE2	1:F:246:LEU:HD11	1.73	0.69
1:F:285:VAL:HG11	3:F:502:PG4:H11	1.73	0.69
1:A:16:VAL:HG21	1:A:48:ARG:NH2	2.10	0.65
1:D:251:MET:HE2	1:E:246:LEU:HD11	1.79	0.65
1:D:246:LEU:HD11	1:E:251:MET:HE2	1.79	0.65
6:B:504:B3P:C1	9:B:809:HOH:O	2.46	0.63
1:F:231:VAL:HG13	9:F:838:HOH:O	1.98	0.63
6:E:504:B3P:N2	9:E:604:HOH:O	2.31	0.62
1:F:412:GLU:OE1	1:F:458:HIS:ND1	2.32	0.62
1:G:412:GLU:OE1	1:G:458:HIS:CE1	2.54	0.61
1:C:246:LEU:HD11	1:F:251:MET:HE2	1.82	0.61
1:B:16:VAL:HG21	1:B:48:ARG:NH1	2.16	0.61
1:D:487:GLN:NE2	9:D:602:HOH:O	2.33	0.61
1:A:16:VAL:HG21	1:A:48:ARG:HH22	1.66	0.60
1:D:444:TRP:CD1	3:D:502:PG4:H12	2.37	0.59
1:F:3[B]:ARG:NH2	1:F:37:THR:OG1	2.36	0.59
1:D:285:VAL:HG11	3:D:502:PG4:C2	2.34	0.58
1:D:285:VAL:HG11	3:D:502:PG4:H22	1.86	0.57
1:G:297:LYS:HE3	1:G:298:PHE:CE2	2.39	0.57
1:G:406:ARG:NH2	9:G:603:HOH:O	2.36	0.57
6:C:504:B3P:C1	9:C:921:HOH:O	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:502:PG4:H21	9:F:694:HOH:O	2.05	0.56
1:E:287:THR:HG1	3:E:502:PG4:C1	2.19	0.56
1:B:234:GLY:HA3	1:B:251:MET:HE3	1.87	0.56
1:C:231:VAL:HG13	9:C:798:HOH:O	2.05	0.55
1:E:74:LYS:HD3	9:E:629:HOH:O	2.06	0.55
1:F:234:GLY:HA3	1:F:251:MET:HE3	1.89	0.55
1:F:412:GLU:CD	1:F:458:HIS:CE1	2.82	0.53
1:D:238:MET:HG2	1:E:242:ALA:CB	2.38	0.52
1:B:122:ALA:HB2	1:D:119:LEU:HD21	1.92	0.51
1:D:251:MET:CE	1:E:246:LEU:HD11	2.41	0.51
1:A:234:GLY:HA3	1:A:251:MET:HE3	1.93	0.51
1:B:251:MET:HE2	1:H:246:LEU:HD11	1.92	0.51
1:E:445:GLY:CA	3:E:502:PG4:H21	2.41	0.51
1:A:242:ALA:CB	1:G:238:MET:HB3	2.41	0.50
1:B:16:VAL:HG21	1:B:48:ARG:HH12	1.77	0.50
1:D:234:GLY:HA3	1:D:251:MET:HE3	1.93	0.50
1:A:287:THR:HG1	3:A:502:PG4:C1	2.24	0.50
1:A:299:LYS:NZ	1:A:376:ASP:OD1	2.36	0.50
1:D:14:LYS:HE2	9:D:607:HOH:O	2.12	0.50
1:E:122:ALA:HB2	1:H:119:LEU:HD21	1.93	0.50
1:F:285:VAL:HG11	3:F:502:PG4:H12	1.93	0.49
1:C:74:LYS:HE2	1:C:195:ALA:O	2.11	0.49
1:D:246:LEU:HD11	1:E:251:MET:CE	2.41	0.49
1:F:297:LYS:HE3	1:F:298:PHE:CE2	2.47	0.49
1:C:406:ARG:NE	4:C:503:CL:CL	2.66	0.49
1:E:406:ARG:NE	4:E:503:CL:CL	2.74	0.49
1:F:2:SER:N	1:F:33:GLU:OE2	2.46	0.49
1:G:285:VAL:HG11	3:G:502:PG4:H12	1.95	0.49
1:F:445:GLY:HA3	3:F:502:PG4:H41	1.94	0.48
1:B:225:ILE:HG12	1:B:247:LYS:HD3	1.94	0.48
1:B:244:SER:OG	1:B:245:SER:N	2.46	0.48
1:C:208:ILE:HG22	9:C:867:HOH:O	2.13	0.48
1:H:412:GLU:OE1	1:H:458:HIS:CD2	2.66	0.48
1:F:234:GLY:CA	1:F:251:MET:HE3	2.44	0.48
1:C:234:GLY:O	1:C:251:MET:HE1	2.13	0.48
1:D:234:GLY:CA	1:D:251:MET:HE3	2.44	0.48
1:E:231:VAL:HG13	9:E:848:HOH:O	2.12	0.47
1:A:122:ALA:HB2	1:C:119:LEU:HD21	1.96	0.47
1:A:242:ALA:HB1	1:G:238:MET:HB3	1.96	0.47
1:B:458:HIS:NE2	1:H:245:SER:HB2	2.30	0.46
1:D:193:ARG:NH1	9:D:604:HOH:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:ARG:NH2	1:E:194:GLU:OE2	2.49	0.46
1:D:238:MET:HG2	1:E:242:ALA:HB2	1.98	0.46
1:D:444:TRP:HD1	3:D:502:PG4:H12	1.81	0.46
1:G:234:GLY:HA3	1:G:251:MET:HE3	1.98	0.46
1:A:314:ARG:NE	1:A:322:ASP:O	2.42	0.46
1:H:147:ALA:HB3	1:H:225:ILE:HD13	1.98	0.46
1:F:321:ASP:OD1	1:F:322:ASP:N	2.49	0.45
1:D:231:VAL:HA	1:D:253:LEU:HD13	1.98	0.45
1:B:234:GLY:CA	1:B:251:MET:HE3	2.47	0.45
1:H:245:SER:O	1:H:246:LEU:C	2.55	0.45
1:D:412:GLU:HB2	5:D:505:MLI:O9	2.16	0.45
1:E:297:LYS:HE3	1:E:298:PHE:CE2	2.52	0.45
1:F:122:ALA:HB2	1:G:119:LEU:HD21	1.97	0.45
1:G:48:ARG:NH1	9:G:612:HOH:O	2.50	0.45
1:H:406:ARG:NE	4:H:503:CL:CL	2.79	0.45
1:A:251:MET:HE2	1:G:246:LEU:HD11	1.99	0.44
1:E:234:GLY:HA3	1:E:251:MET:HE3	1.98	0.44
1:H:445:GLY:HA3	3:H:502:PG4:H41	1.99	0.44
1:C:234:GLY:HA3	1:C:251:MET:HE3	1.99	0.44
1:E:74:LYS:CD	9:E:629:HOH:O	2.64	0.43
1:D:245:SER:O	1:D:246:LEU:C	2.56	0.43
1:G:288:ASN:OD1	3:G:502:PG4:C1	2.67	0.43
1:E:445:GLY:HA2	3:E:502:PG4:H21	1.99	0.43
1:B:263:GLU:O	1:B:298:PHE:CE2	2.72	0.43
1:D:231:VAL:HG13	9:D:862:HOH:O	2.18	0.43
1:G:179:GLU:OE2	1:G:208:ILE:HG23	2.17	0.43
1:H:14:LYS:NZ	9:H:613:HOH:O	2.52	0.43
1:C:-4:HIS:ND1	1:C:317:ASP:OD2	2.50	0.43
1:C:246:LEU:HD11	1:F:251:MET:CE	2.48	0.43
1:E:234:GLY:CA	1:E:251:MET:HE3	2.49	0.43
1:G:16:VAL:HG21	1:G:48:ARG:NH2	2.35	0.42
1:D:238:MET:HG2	1:E:242:ALA:HB1	2.02	0.42
1:B:122:ALA:HB2	1:D:119:LEU:CD2	2.48	0.42
1:D:431:ILE:HD12	1:D:439:CYS:HB3	2.02	0.42
3:G:502:PG4:H42	9:G:630:HOH:O	2.19	0.42
1:F:82:ARG:NH2	1:F:194:GLU:OE2	2.53	0.42
1:A:16:VAL:HG21	1:A:48:ARG:CZ	2.50	0.42
1:D:231:VAL:HG23	9:D:689:HOH:O	2.20	0.42
1:E:287:THR:OG1	3:E:502:PG4:C1	2.68	0.42
1:C:231:VAL:HA	1:C:253:LEU:HD13	2.01	0.42
1:A:10:TYR:CD1	1:A:189:ALA:HB1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:406:ARG:NE	4:F:503:CL:CL	2.76	0.41
1:C:397:SER:OG	9:C:601:HOH:O	2.22	0.41
1:F:120:ILE:HB	1:F:121:PRO:HD3	2.03	0.41
1:D:70:ARG:O	1:D:74:LYS:HG2	2.19	0.41
1:D:250:THR:C	1:D:251:MET:HG2	2.40	0.41
1:E:416:ALA:HA	1:E:438:ILE:O	2.21	0.41
1:A:245:SER:O	1:A:247:LYS:HG3	2.20	0.41
1:C:458:HIS:NE2	1:F:245:SER:HB2	2.36	0.41
1:B:16:VAL:HG21	1:B:48:ARG:CZ	2.51	0.41
1:C:71:ILE:HA	1:C:74:LYS:HD3	2.03	0.41
1:E:328:LEU:HD21	1:E:391:PRO:HD3	2.03	0.41
1:H:297:LYS:HE3	1:H:298:PHE:CZ	2.56	0.41
1:G:147:ALA:HB3	1:G:225:ILE:HD13	2.02	0.41
1:C:234:GLY:CA	1:C:251:MET:HE3	2.51	0.40
1:E:237:VAL:HG22	8:E:509:EPE:H52	2.03	0.40
1:A:73[B]:ARG:HG2	9:A:629:HOH:O	2.21	0.40
1:A:241:SER:O	1:A:245:SER:O	2.38	0.40
1:G:416:ALA:HA	1:G:438:ILE:O	2.22	0.40
1:B:119:LEU:HD21	1:D:122:ALA:HB2	2.03	0.40
1:D:416:ALA:HA	1:D:438:ILE:O	2.20	0.40
1:A:122:ALA:HB2	1:C:119:LEU:CD2	2.51	0.40
1:A:255:GLY:HA2	1:A:413:TYR:CD1	2.56	0.40
1:H:193:ARG:NH1	9:H:622:HOH:O	2.55	0.40
3:H:502:PG4:H22	9:H:702:HOH:O	2.21	0.40
1:C:47[B]:ASP:OD2	1:C:51:LYS:HE2	2.21	0.40
1:D:336:ASN:OD1	1:D:339:ARG:NH2	2.55	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	499/499 (100%)	486 (97%)	12 (2%)	1 (0%)	47 38
1	B	498/499 (100%)	486 (98%)	12 (2%)	0	100 100
1	C	496/499 (99%)	484 (98%)	12 (2%)	0	100 100
1	D	493/499 (99%)	480 (97%)	12 (2%)	1 (0%)	47 38
1	E	492/499 (99%)	482 (98%)	10 (2%)	0	100 100
1	F	494/499 (99%)	483 (98%)	11 (2%)	0	100 100
1	G	490/499 (98%)	476 (97%)	13 (3%)	1 (0%)	47 38
1	H	490/499 (98%)	477 (97%)	12 (2%)	1 (0%)	47 38
All	All	3952/3992 (99%)	3854 (98%)	94 (2%)	4 (0%)	51 42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	246	LEU
1	H	246	LEU
1	A	246	LEU
1	G	246	LEU

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	393/394 (100%)	389 (99%)	4 (1%)	76 76
1	B	392/394 (100%)	389 (99%)	3 (1%)	81 82
1	C	393/394 (100%)	388 (99%)	5 (1%)	69 68
1	D	391/394 (99%)	388 (99%)	3 (1%)	81 82
1	E	387/394 (98%)	382 (99%)	5 (1%)	69 68
1	F	390/394 (99%)	387 (99%)	3 (1%)	81 82
1	G	386/394 (98%)	385 (100%)	1 (0%)	92 93
1	H	384/394 (98%)	383 (100%)	1 (0%)	92 93
All	All	3116/3152 (99%)	3091 (99%)	25 (1%)	81 82

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	238	MET
1	A	343	SER
1	A	389	PHE
1	B	245	SER
1	B	343	SER
1	B	389	PHE
1	C	233	SER
1	C	238	MET
1	C	385	ARG
1	C	389	PHE
1	C	397	SER
1	D	238	MET
1	D	343	SER
1	D	389	PHE
1	E	3	ARG
1	E	43	ARG
1	E	343	SER
1	E	361	GLU
1	E	389	PHE
1	F	2	SER
1	F	343	SER
1	F	389	PHE
1	G	389	PHE
1	H	389	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (i)

Of 45 ligands modelled in this entry, 16 are monoatomic - leaving 29 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	$\#\|Z\| > 2$
5	MLI	D	504	-	6,6,6	1.59	1 (16%)	7,7,7	1.24	1 (14%)
5	MLI	G	504	-	6,6,6	1.71	1 (16%)	7,7,7	0.88	0
3	PG4	C	502	-	12,12,12	0.34	0	11,11,11	0.56	0
5	MLI	A	504	-	6,6,6	1.86	1 (16%)	7,7,7	0.85	0
6	B3P	C	504	-	9,9,18	0.82	0	11,11,23	1.33	1 (9%)
5	MLI	E	506	-	6,6,6	1.82	1 (16%)	7,7,7	0.69	0
5	MLI	E	508	-	6,6,6	1.62	1 (16%)	7,7,7	1.04	0
3	PG4	E	502	-	12,12,12	0.40	0	11,11,11	0.48	0
5	MLI	F	505	-	6,6,6	1.70	2 (33%)	7,7,7	1.37	1 (14%)
5	MLI	H	504	-	6,6,6	1.71	1 (16%)	7,7,7	1.27	0
3	PG4	G	502	-	12,12,12	0.31	0	11,11,11	0.39	0
8	EPE	E	509	-	15,15,15	0.92	1 (6%)	18,20,20	1.35	3 (16%)
5	MLI	F	507	-	6,6,6	1.66	1 (16%)	7,7,7	1.26	1 (14%)
3	PG4	F	502	-	12,12,12	0.29	0	11,11,11	0.34	0
7	FLC	C	506	-	12,12,12	1.21	0	17,17,17	1.77	3 (17%)
5	MLI	F	506	-	6,6,6	1.92	1 (16%)	7,7,7	0.94	0
5	MLI	C	505	-	6,6,6	1.71	1 (16%)	7,7,7	0.81	0
3	PG4	A	502	-	12,12,12	0.38	0	11,11,11	0.59	0
5	MLI	B	505	-	6,6,6	1.69	1 (16%)	7,7,7	1.31	1 (14%)
6	B3P	E	505	-	8,8,18	0.99	1 (12%)	9,10,23	1.04	0
5	MLI	D	505	-	6,6,6	1.84	1 (16%)	7,7,7	0.88	0
3	PG4	H	502	-	12,12,12	0.30	0	11,11,11	0.38	0
5	MLI	G	505	-	6,6,6	1.52	1 (16%)	7,7,7	1.26	0
3	PG4	B	502	-	12,12,12	0.41	0	11,11,11	0.59	0
5	MLI	E	507	-	6,6,6	1.71	1 (16%)	7,7,7	1.29	1 (14%)
6	B3P	F	504	-	11,11,18	0.82	0	12,13,23	1.59	3 (25%)
6	B3P	B	504	-	9,9,18	0.81	0	11,11,23	1.39	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PG4	D	502	-	12,12,12	0.46	0	11,11,11	0.76	0
6	B3P	E	504	-	11,11,18	0.99	1 (9%)	12,13,23	0.98	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
5	MLI	D	504	-	-	3/4/4/4	-
5	MLI	G	504	-	-	2/4/4/4	-
3	PG4	C	502	-	-	5/10/10/10	-
5	MLI	A	504	-	-	0/4/4/4	-
6	B3P	C	504	-	-	6/13/13/28	-
5	MLI	E	506	-	-	0/4/4/4	-
5	MLI	E	508	-	-	1/4/4/4	-
3	PG4	E	502	-	-	4/10/10/10	-
5	MLI	F	505	-	-	0/4/4/4	-
5	MLI	H	504	-	-	0/4/4/4	-
3	PG4	G	502	-	-	4/10/10/10	-
8	EPE	E	509	-	-	2/9/19/19	0/1/1/1
5	MLI	F	507	-	-	0/4/4/4	-
3	PG4	F	502	-	-	8/10/10/10	-
7	FLC	C	506	-	-	0/16/16/16	-
5	MLI	F	506	-	-	2/4/4/4	-
5	MLI	C	505	-	-	2/4/4/4	-
3	PG4	A	502	-	-	2/10/10/10	-
5	MLI	B	505	-	-	0/4/4/4	-
6	B3P	E	505	-	-	1/9/12/28	-
5	MLI	D	505	-	-	2/4/4/4	-
3	PG4	H	502	-	-	5/10/10/10	-
5	MLI	G	505	-	-	2/4/4/4	-
3	PG4	B	502	-	-	4/10/10/10	-
5	MLI	E	507	-	-	3/4/4/4	-
6	B3P	F	504	-	-	7/15/15/28	-
6	B3P	B	504	-	-	4/13/13/28	-
3	PG4	D	502	-	-	3/10/10/10	-
6	B3P	E	504	-	-	8/15/15/28	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	506	MLI	C1-C3	3.28	1.56	1.51
5	D	505	MLI	C1-C3	3.07	1.55	1.51
5	E	507	MLI	C1-C3	2.93	1.55	1.51
5	A	504	MLI	C1-C3	2.92	1.55	1.51
5	H	504	MLI	C1-C3	2.89	1.55	1.51
5	B	505	MLI	C1-C3	2.81	1.55	1.51
5	E	506	MLI	C1-C3	2.80	1.55	1.51
5	F	505	MLI	C1-C3	2.72	1.55	1.51
5	F	507	MLI	C1-C3	2.70	1.55	1.51
5	C	505	MLI	C1-C3	2.66	1.55	1.51
5	E	508	MLI	C1-C3	2.64	1.55	1.51
5	G	504	MLI	C1-C3	2.62	1.55	1.51
6	E	505	B3P	C11-C8	2.56	1.56	1.53
5	G	505	MLI	C1-C3	2.52	1.54	1.51
5	D	504	MLI	C1-C3	2.50	1.54	1.51
8	E	509	EPE	C10-S	2.44	1.81	1.77
6	E	504	B3P	C7-C4	2.40	1.56	1.53
5	F	505	MLI	C1-C2	2.15	1.54	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	506	FLC	OB1-CBC-CB	-5.14	114.98	122.25
6	F	504	B3P	C11-C8-C10	-3.27	103.12	110.04
6	F	504	B3P	C2-N2-C8	3.26	120.70	116.08
7	C	506	FLC	OB2-CBC-CB	3.21	118.62	113.05
8	E	509	EPE	C6-N1-C2	2.62	114.73	108.83
5	F	505	MLI	O8-C3-C1	-2.57	114.56	122.08
6	B	504	B3P	C3-N1-C4	2.54	120.08	116.23
6	B	504	B3P	C7-C4-C6	-2.42	104.93	110.04
6	C	504	B3P	C3-N1-C4	2.39	119.86	116.23
8	E	509	EPE	O1S-S-C10	-2.38	104.05	106.92
6	F	504	B3P	C11-C8-N2	2.23	115.73	109.03
5	E	507	MLI	O8-C3-C1	-2.20	115.66	122.08
7	C	506	FLC	OG1-CGC-CG	-2.17	116.59	122.94
5	F	507	MLI	O8-C3-C1	-2.14	115.84	122.08
5	B	505	MLI	O8-C3-C1	-2.13	115.85	122.08
5	D	504	MLI	O8-C3-C1	-2.11	115.92	122.08
8	E	509	EPE	C5-C6-N1	2.01	114.78	110.64

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	504	B3P	N1-C4-C5-O4
6	B	504	B3P	C6-C4-C5-O4
6	B	504	B3P	C7-C4-C5-O4
6	C	504	B3P	C5-C4-N1-C3
6	C	504	B3P	C6-C4-N1-C3
6	C	504	B3P	C7-C4-N1-C3
6	C	504	B3P	C7-C4-C5-O4
6	E	504	B3P	C5-C4-N1-C3
6	E	504	B3P	C6-C4-N1-C3
6	E	504	B3P	C6-C4-C7-O6
6	F	504	B3P	C9-C8-N2-C2
6	F	504	B3P	C10-C8-N2-C2
6	F	504	B3P	C11-C8-N2-C2
6	F	504	B3P	N2-C8-C9-O1
6	F	504	B3P	C10-C8-C9-O1
6	F	504	B3P	C11-C8-C9-O1
8	E	509	EPE	C10-C9-N1-C6
6	E	504	B3P	C2-C1-C3-N1
3	G	502	PG4	O2-C3-C4-O3
6	F	504	B3P	C3-C1-C2-N2
3	H	502	PG4	O2-C3-C4-O3
3	E	502	PG4	O1-C1-C2-O2
3	F	502	PG4	O4-C7-C8-O5
3	H	502	PG4	O1-C1-C2-O2
3	H	502	PG4	C6-C5-O3-C4
3	E	502	PG4	O4-C7-C8-O5
3	F	502	PG4	O1-C1-C2-O2
3	G	502	PG4	O1-C1-C2-O2
6	E	505	B3P	O3-C11-C8-C10
3	B	502	PG4	O3-C5-C6-O4
5	G	505	MLI	C3-C1-C2-O7
6	E	504	B3P	C7-C4-N1-C3
3	B	502	PG4	O4-C7-C8-O5
3	D	502	PG4	O1-C1-C2-O2
6	C	504	B3P	C6-C4-C5-O4
5	D	504	MLI	C2-C1-C3-O9
5	E	507	MLI	C2-C1-C3-O9
5	G	505	MLI	C3-C1-C2-O6
3	F	502	PG4	O3-C5-C6-O4
3	E	502	PG4	C3-C4-O3-C5
3	F	502	PG4	O2-C3-C4-O3
3	C	502	PG4	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
3	C	502	PG4	O4-C7-C8-O5
3	A	502	PG4	C8-C7-O4-C6
5	D	504	MLI	C2-C1-C3-O8
5	E	507	MLI	C2-C1-C3-O8
5	G	504	MLI	C3-C1-C2-O6
3	H	502	PG4	C5-C6-O4-C7
3	G	502	PG4	C1-C2-O2-C3
3	D	502	PG4	C1-C2-O2-C3
3	B	502	PG4	C3-C4-O3-C5
3	C	502	PG4	C5-C6-O4-C7
3	F	502	PG4	C3-C4-O3-C5
6	E	504	B3P	C5-C4-C7-O6
3	C	502	PG4	C8-C7-O4-C6
6	B	504	B3P	C5-C4-C6-O5
3	A	502	PG4	C3-C4-O3-C5
5	C	505	MLI	C2-C1-C3-O8
5	D	505	MLI	C2-C1-C3-O9
3	D	502	PG4	O4-C7-C8-O5
3	E	502	PG4	C1-C2-O2-C3
3	G	502	PG4	C8-C7-O4-C6
5	G	504	MLI	C3-C1-C2-O7
5	C	505	MLI	C2-C1-C3-O9
6	E	504	B3P	C3-C1-C2-N2
3	F	502	PG4	C6-C5-O3-C4
3	F	502	PG4	C5-C6-O4-C7
5	D	505	MLI	C2-C1-C3-O8
3	B	502	PG4	C8-C7-O4-C6
5	F	506	MLI	C3-C1-C2-O6
8	E	509	EPE	N4-C7-C8-O8
3	H	502	PG4	O3-C5-C6-O4
6	C	504	B3P	N1-C4-C5-O4
6	E	504	B3P	N1-C4-C7-O6
5	D	504	MLI	C3-C1-C2-O7
5	E	508	MLI	C2-C1-C3-O8
3	C	502	PG4	C1-C2-O2-C3
3	F	502	PG4	C8-C7-O4-C6
5	F	506	MLI	C3-C1-C2-O7
5	E	507	MLI	C3-C1-C2-O6

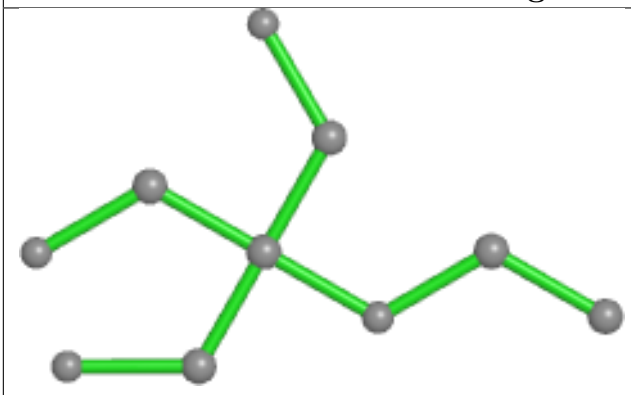
There are no ring outliers.

11 monomers are involved in 25 short contacts:

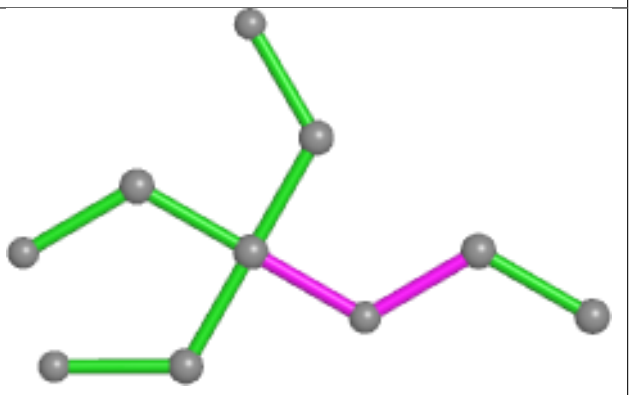
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	504	B3P	1	0
3	E	502	PG4	5	0
3	G	502	PG4	3	0
8	E	509	EPE	1	0
3	F	502	PG4	5	0
3	A	502	PG4	1	0
5	D	505	MLI	1	0
3	H	502	PG4	2	0
6	B	504	B3P	1	0
3	D	502	PG4	4	0
6	E	504	B3P	1	0

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

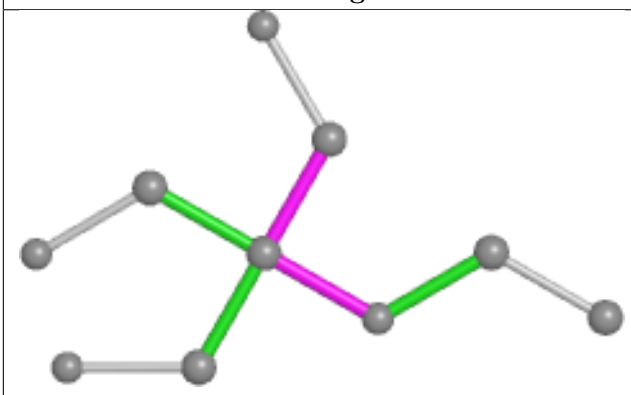
Ligand B3P C 504



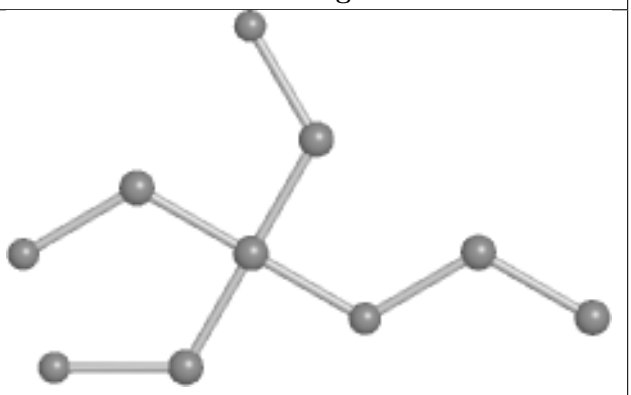
Bond lengths



Bond angles

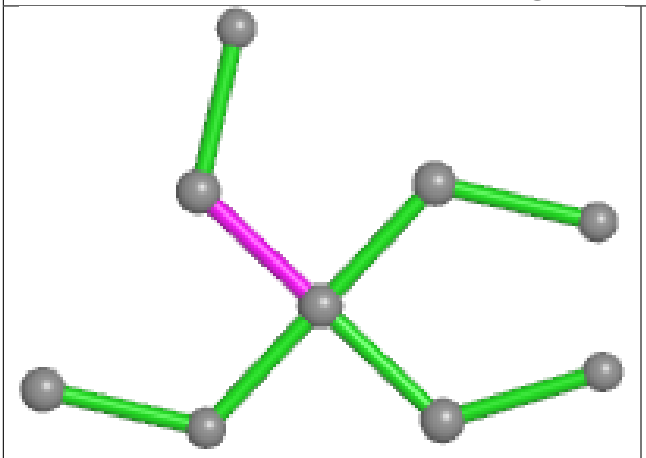


Torsions

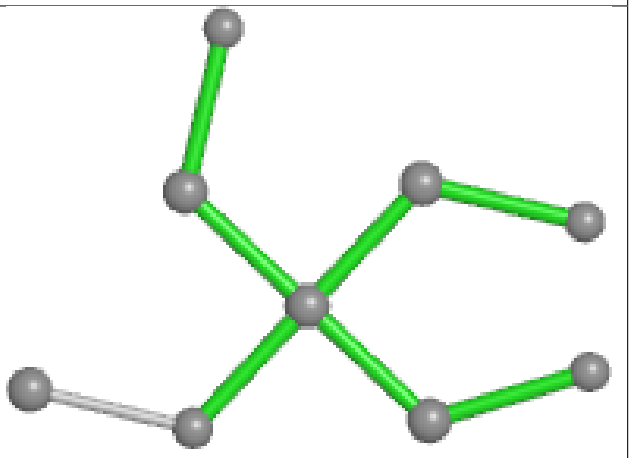


Rings

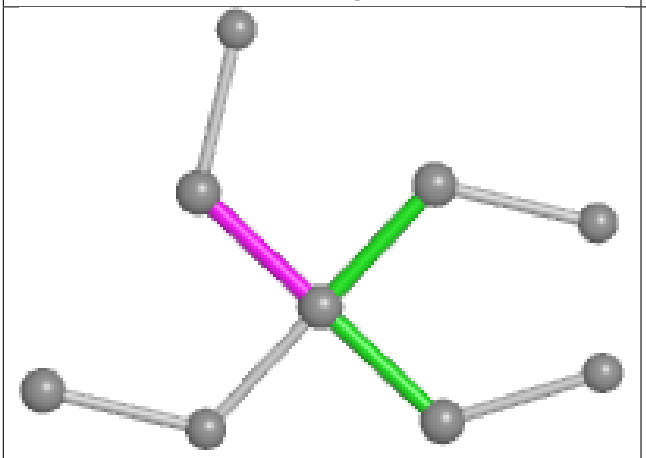
Ligand B3P E 505



Bond lengths



Bond angles



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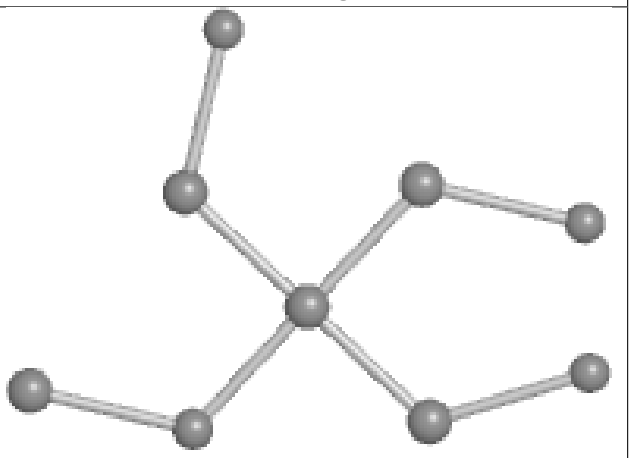
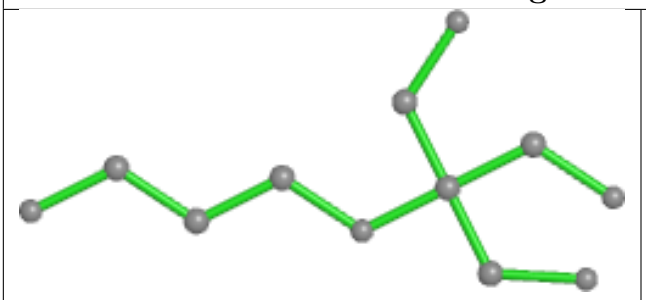
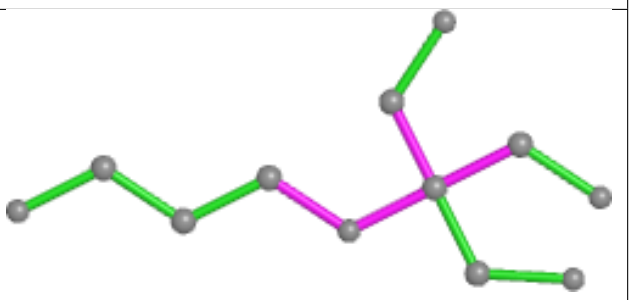


Rings

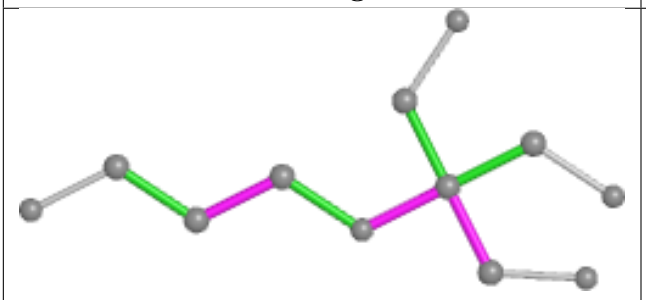
Ligand B3P F 504



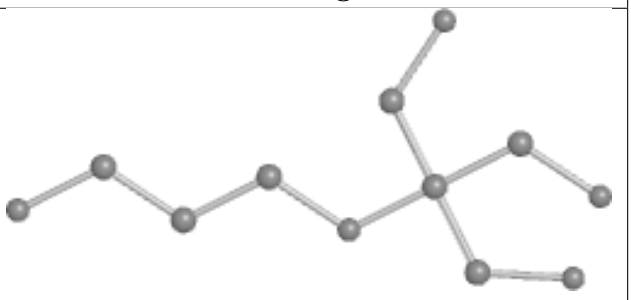
Bond lengths



Bond angles

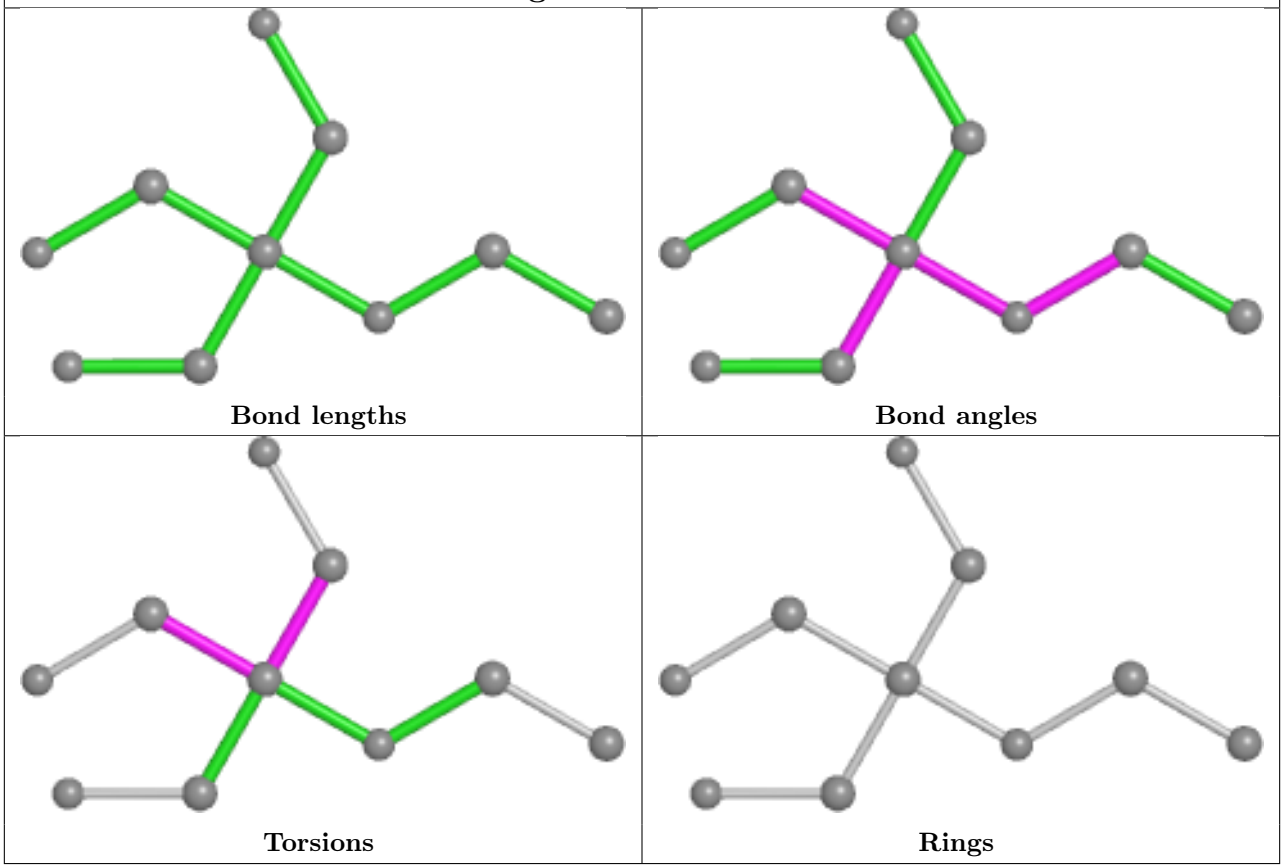


Torsions

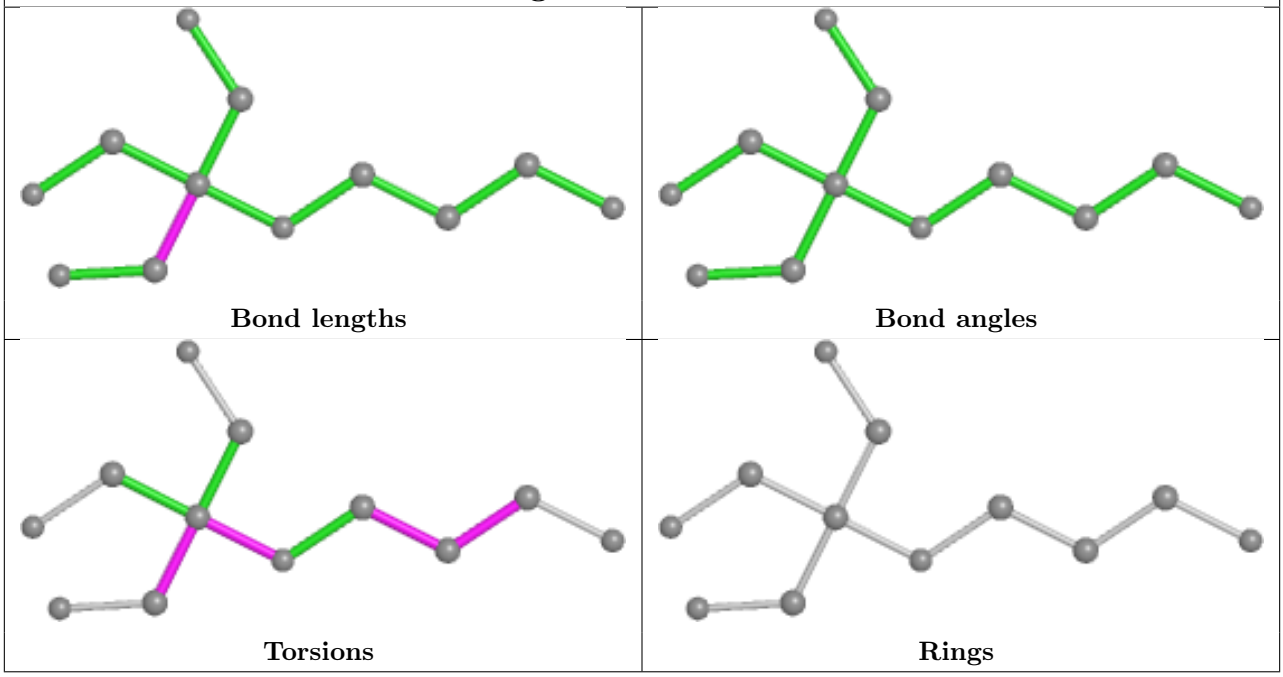


Rings

Ligand B3P B 504



Ligand B3P E 504



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	495/499 (99%)	-0.33	5 (1%)	82 84	17, 26, 50, 90	0
1	B	493/499 (98%)	-0.36	5 (1%)	82 84	18, 26, 50, 94	0
1	C	493/499 (98%)	-0.44	8 (1%)	72 74	17, 25, 47, 71	0
1	D	489/499 (97%)	-0.41	3 (0%)	89 90	17, 26, 47, 79	0
1	E	488/499 (97%)	-0.40	5 (1%)	82 84	17, 26, 48, 82	0
1	F	489/499 (97%)	-0.47	3 (0%)	89 90	17, 23, 44, 70	0
1	G	488/499 (97%)	-0.35	5 (1%)	82 84	17, 27, 53, 85	0
1	H	488/499 (97%)	-0.31	4 (0%)	86 87	17, 27, 52, 78	0
All	All	3923/3992 (98%)	-0.38	38 (0%)	82 84	17, 26, 49, 94	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-3	HIS	5.2
1	C	-2	HIS	5.0
1	C	-3	HIS	4.6
1	G	360	GLY	4.0
1	D	2	SER	4.0
1	B	-2	HIS	3.8
1	C	0	HIS	3.7
1	A	-1	HIS	3.7
1	C	-4	HIS	3.5
1	H	362	GLY	3.4
1	B	0	HIS	3.3
1	H	360	GLY	3.1
1	E	3	ARG	3.1
1	C	362	GLY	3.0
1	B	239	ALA	3.0
1	A	360	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	-1	HIS	2.9
1	H	48	ARG	2.7
1	E	467[A]	VAL	2.7
1	D	467[A]	VAL	2.6
1	E	361	GLU	2.6
1	H	361	GLU	2.5
1	E	4	MET	2.5
1	F	467[A]	VAL	2.4
1	B	-1	HIS	2.4
1	A	48	ARG	2.4
1	C	3	ARG	2.4
1	F	3[A]	ARG	2.3
1	B	365	ASN	2.2
1	C	365	ASN	2.2
1	G	362	GLY	2.2
1	E	362	GLY	2.1
1	G	231	VAL	2.1
1	G	467[A]	VAL	2.1
1	A	242	ALA	2.1
1	G	322	ASP	2.1
1	F	2	SER	2.0
1	D	361	GLU	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
8	EPE	E	509	15/15	0.60	0.49	47,62,75,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MLI	E	507	7/7	0.66	0.18	54,61,74,75	0
5	MLI	F	506	7/7	0.69	0.26	53,63,70,79	0
4	CL	D	503	1/1	0.69	0.14	70,70,70,70	0
4	CL	A	503	1/1	0.72	0.07	64,64,64,64	0
5	MLI	G	504	7/7	0.75	0.20	56,61,77,78	0
5	MLI	E	508	7/7	0.75	0.41	55,61,67,80	0
5	MLI	G	505	7/7	0.76	0.39	53,58,64,65	0
5	MLI	D	505	7/7	0.76	0.27	52,56,66,83	0
5	MLI	F	505	7/7	0.77	0.25	46,56,65,67	0
5	MLI	F	507	7/7	0.81	0.36	50,56,62,65	0
5	MLI	B	505	7/7	0.82	0.21	48,58,71,71	0
5	MLI	E	506	7/7	0.82	0.27	42,55,67,70	0
5	MLI	H	504	7/7	0.83	0.19	50,62,68,68	0
5	MLI	C	505	7/7	0.84	0.23	38,49,64,65	0
5	MLI	D	504	7/7	0.85	0.23	38,56,68,71	0
4	CL	H	503	1/1	0.85	0.17	67,67,67,67	0
6	B3P	E	505	9/19	0.85	0.18	33,41,47,49	0
5	MLI	A	504	7/7	0.85	0.21	50,57,62,68	0
7	FLC	C	506	13/13	0.86	0.29	45,49,60,65	0
3	PG4	D	502	13/13	0.87	0.15	24,34,45,56	0
4	CL	G	503	1/1	0.87	0.19	65,65,65,65	0
6	B3P	E	504	12/19	0.88	0.12	28,38,43,45	0
3	PG4	C	502	13/13	0.88	0.17	21,38,59,61	0
3	PG4	G	502	13/13	0.89	0.17	16,37,61,64	0
4	CL	E	503	1/1	0.89	0.08	60,60,60,60	0
6	B3P	F	504	12/19	0.89	0.13	30,39,46,51	0
3	PG4	A	502	13/13	0.89	0.15	19,35,61,61	0
6	B3P	B	504	10/19	0.89	0.15	29,40,44,48	0
6	B3P	C	504	10/19	0.90	0.14	27,40,46,47	0
4	CL	C	503	1/1	0.90	0.10	56,56,56,56	0
3	PG4	H	502	13/13	0.90	0.15	21,38,52,68	0
4	CL	B	503	1/1	0.91	0.11	69,69,69,69	0
3	PG4	F	502	13/13	0.91	0.15	13,37,48,57	0
3	PG4	E	502	13/13	0.91	0.15	18,35,45,57	0
4	CL	F	503	1/1	0.92	0.16	62,62,62,62	0
3	PG4	B	502	13/13	0.93	0.12	20,35,50,62	0
2	NA	A	501	1/1	0.96	0.06	29,29,29,29	0
2	NA	E	501	1/1	0.97	0.06	34,34,34,34	0
2	NA	D	501	1/1	0.97	0.06	27,27,27,27	0
2	NA	F	501	1/1	0.98	0.04	23,23,23,23	0
2	NA	B	501	1/1	0.99	0.05	27,27,27,27	0
2	NA	H	501	1/1	0.99	0.06	28,28,28,28	0

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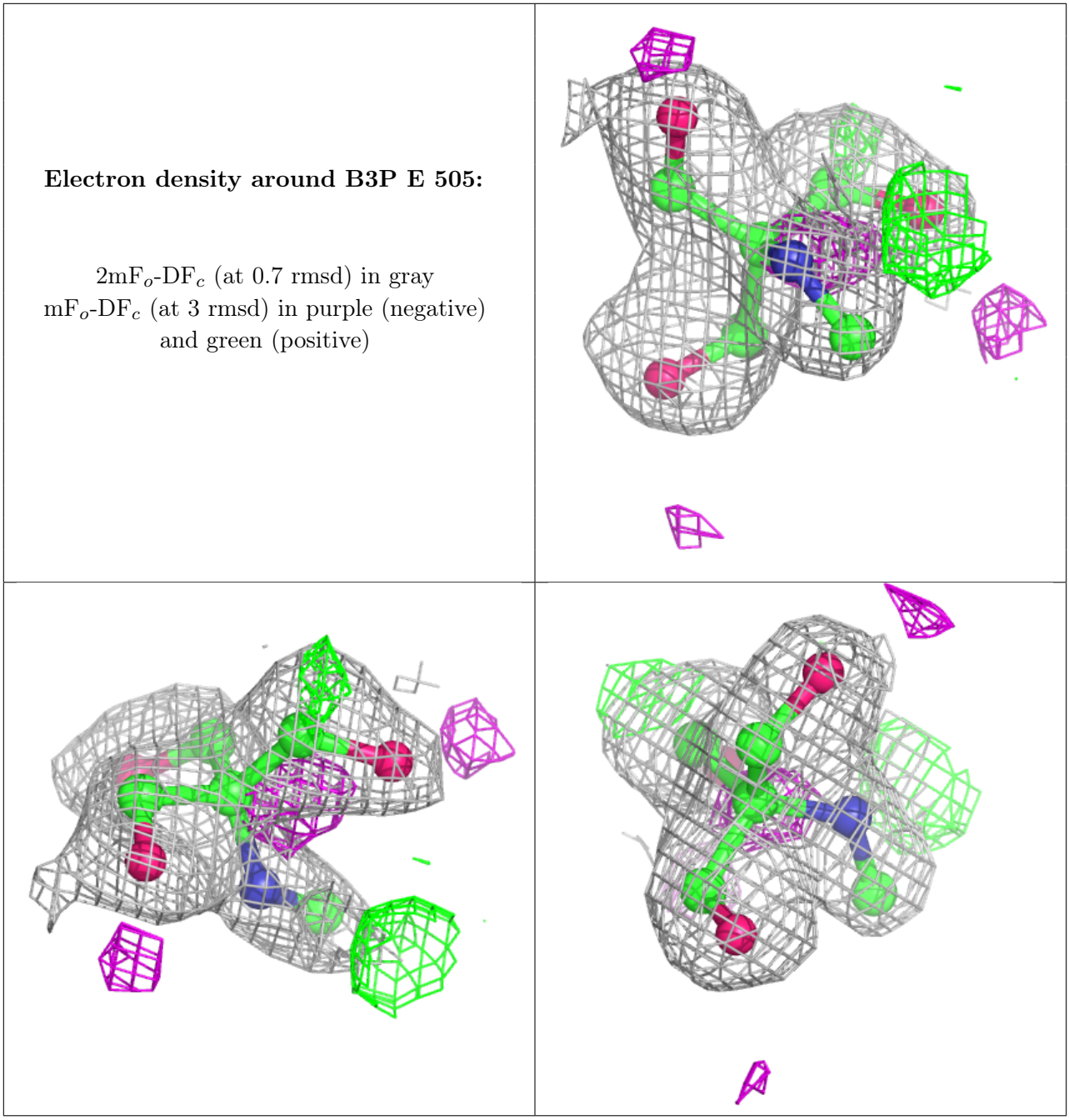
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	C	501	1/1	0.99	0.04	27,27,27,27	0
2	NA	G	501	1/1	1.00	0.05	26,26,26,26	0

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.

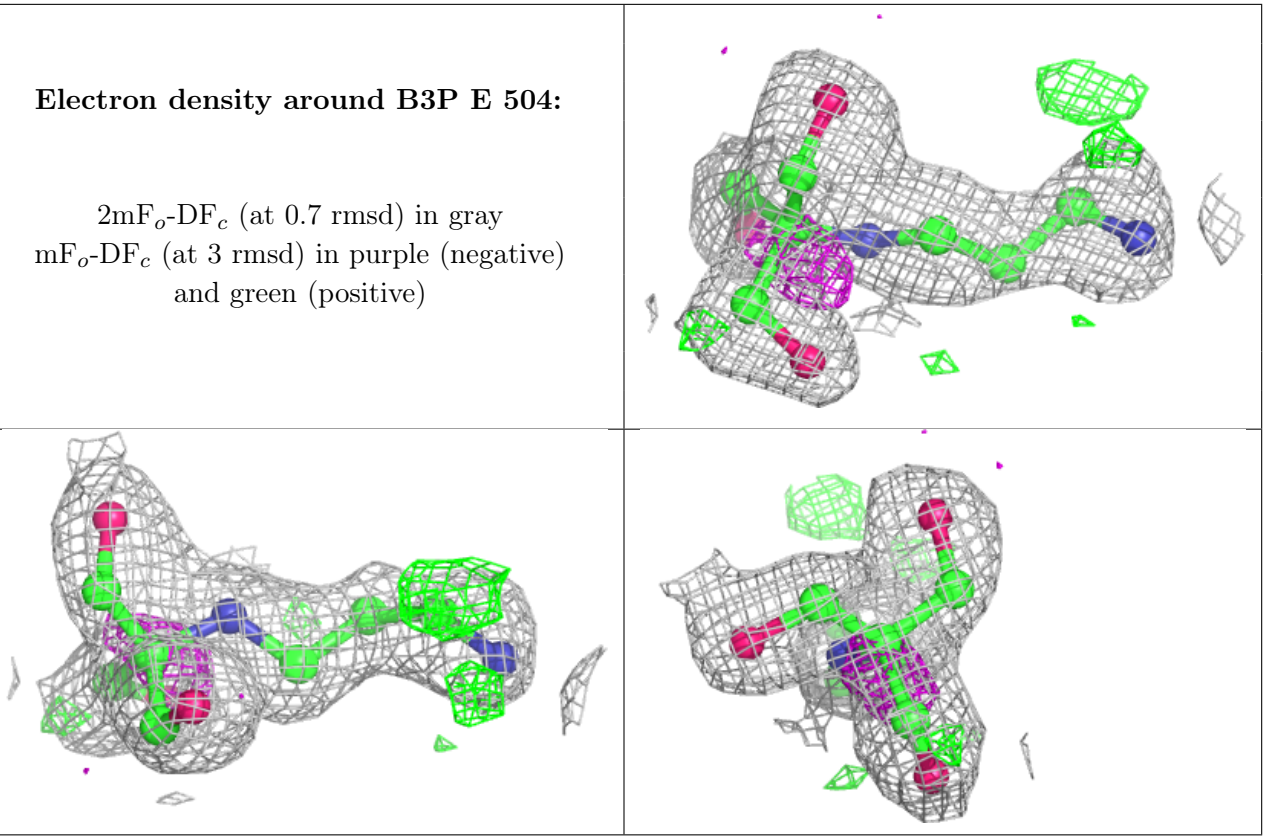
Electron density around B3P E 505:

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



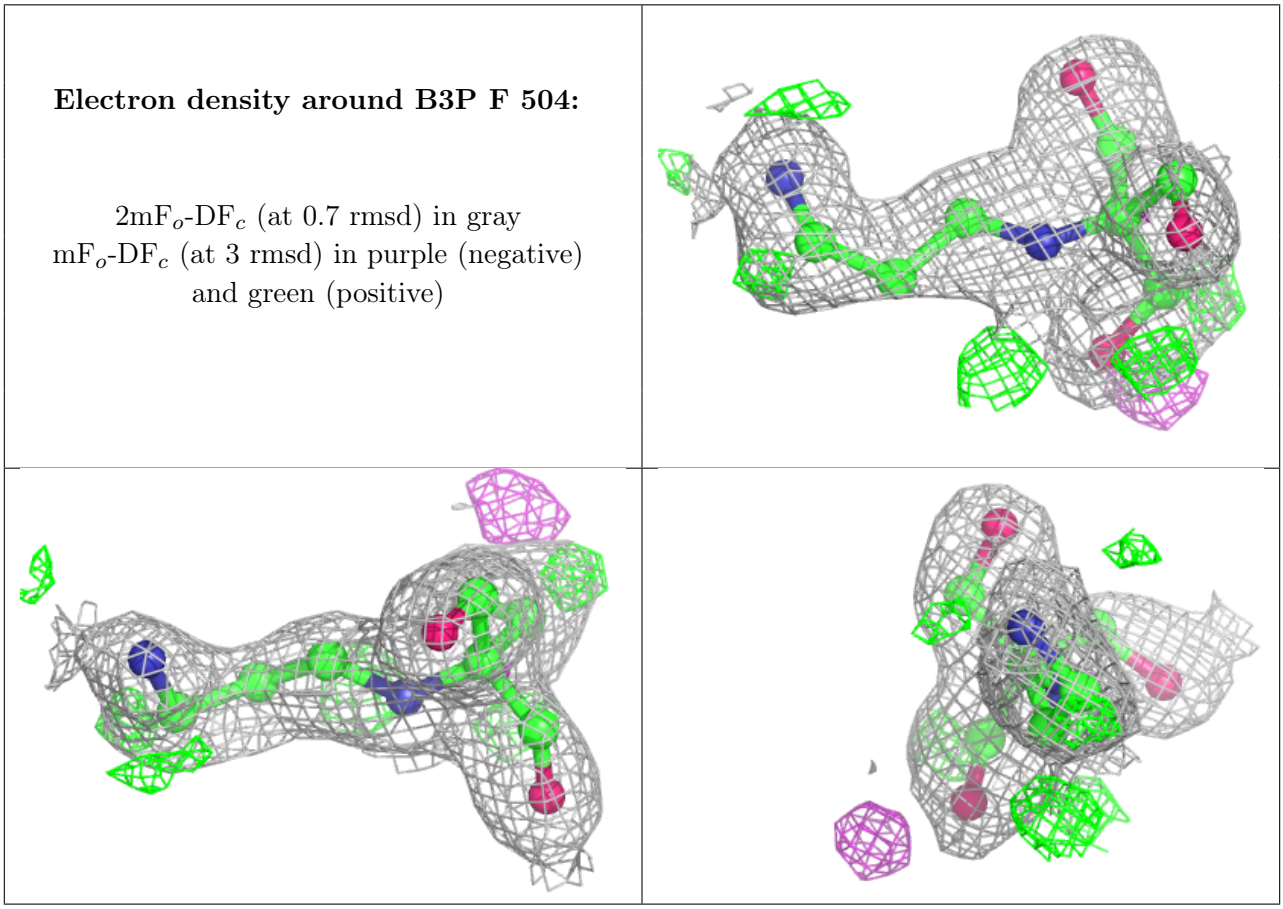
Electron density around B3P E 504:

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



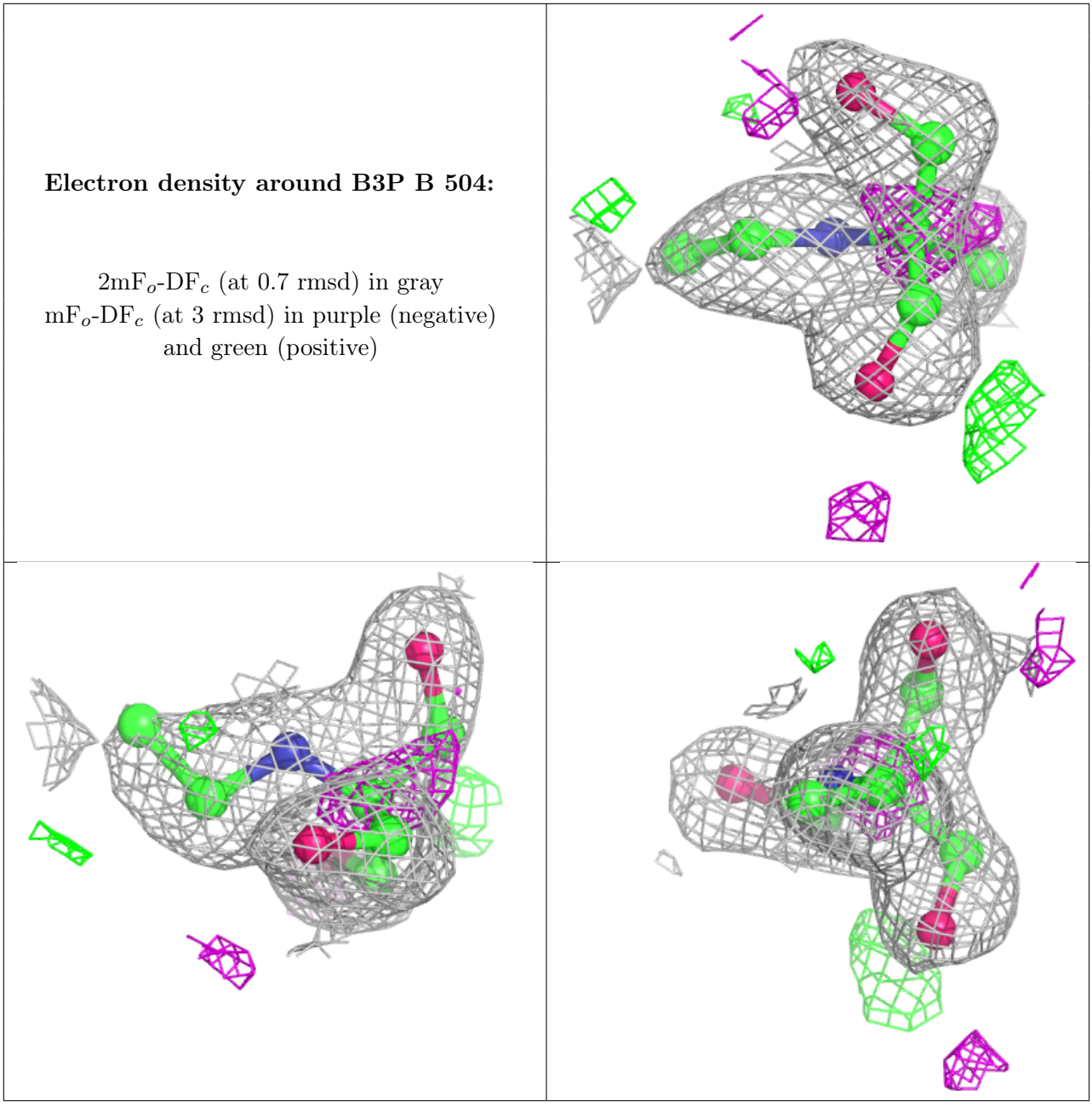
Electron density around B3P F 504:

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



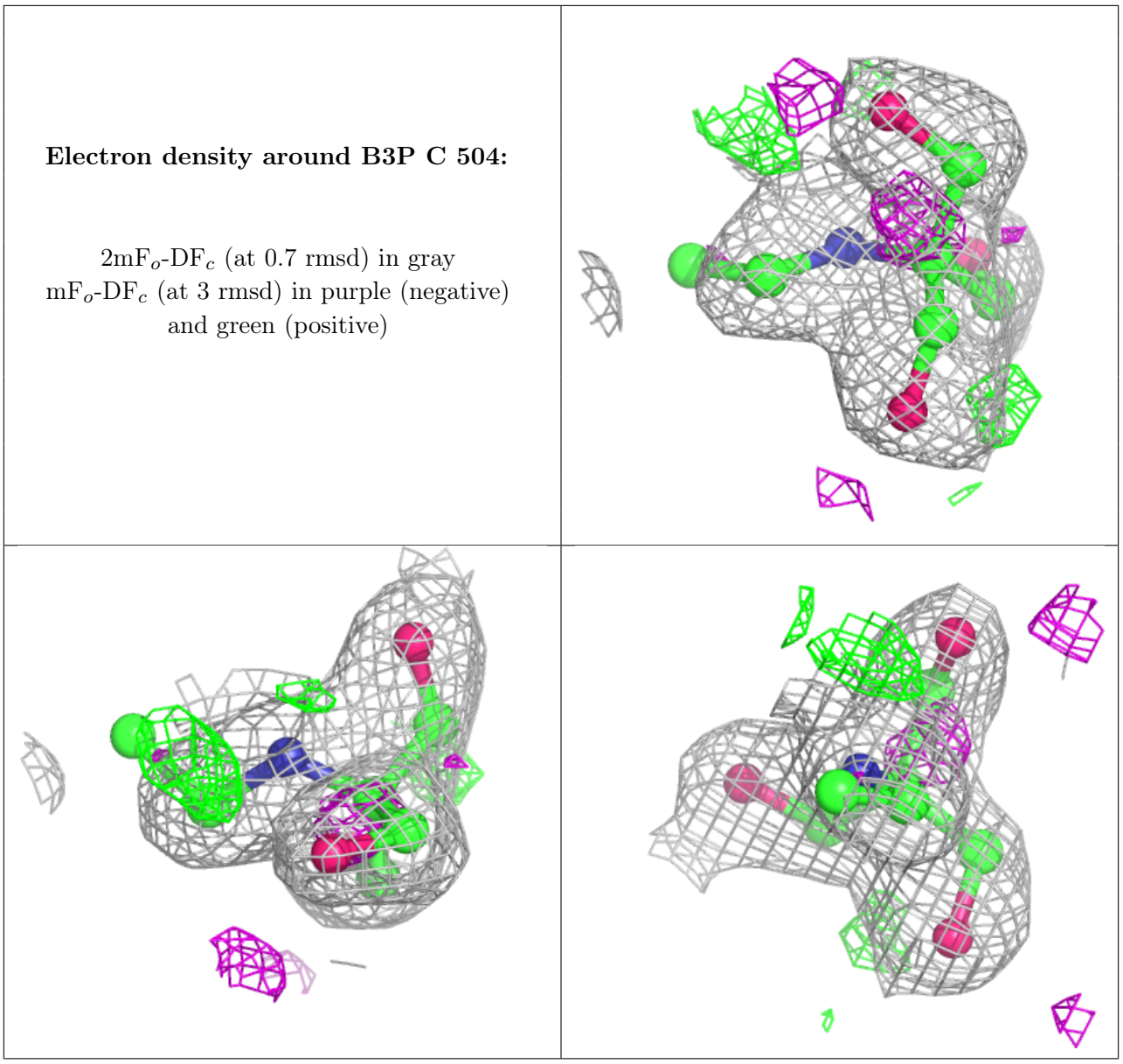
Electron density around B3P B 504:

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



Electron density around B3P C 504:

$2mF_o$-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.