Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 02:33 am GMT

PDB ID	:	4UOV
Title	:	The structure of a tetrameric alpha-carbonic anhydrase from Thermovibrio ammonificans reveals a core formed around intermolecular disulfides, which contribute to its thermostability.
Authors	:	James, P.; Isupov, M.; Sayer, C.; Berg, S.; Lioliou, M.; Kotlar, H.; Littlechild, J.
Deposited on	:	2014-06-10
Resolution	:	1.85 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 (1)) were used in the production of this report:

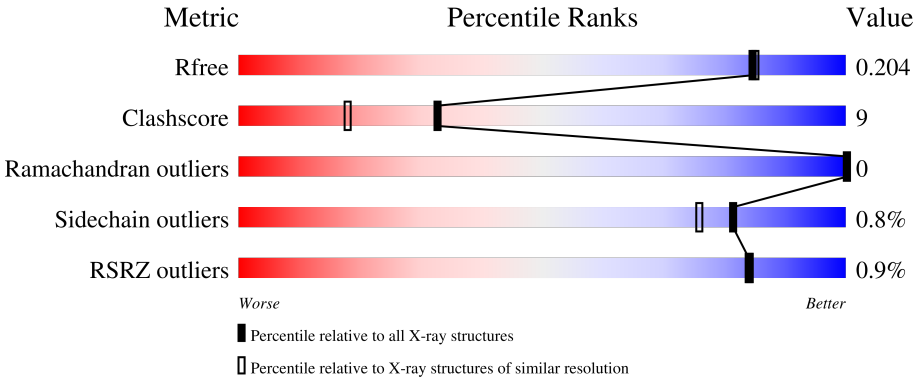
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	247	.% 84% 7% 9%
1	B	247	81% 10% 9%
1	C	247	.% 82% 9% 9%
1	D	247	2% 86% 5% 9%
1	E	247	.% 82% 9% 9%

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Mol	Chain	Length	Quality of chain
1	F	247	81% 10% 9%

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
11	PG5	B	312	-	-	X	-
5	B3P	C	301	-	X	-	X
5	B3P	D	301	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 14247 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.

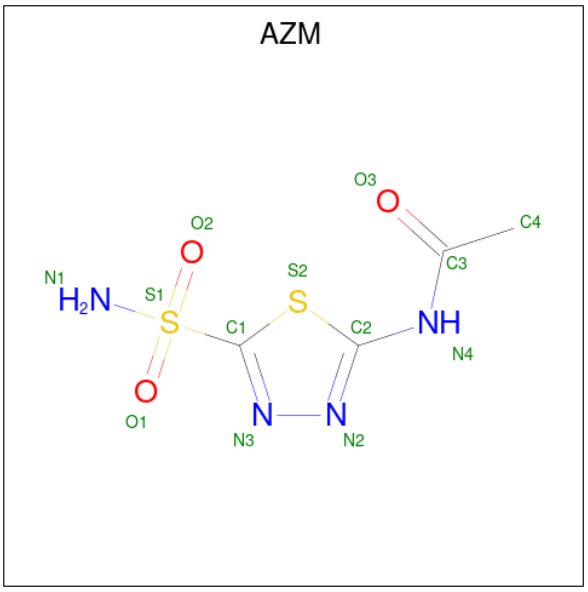
- Molecule 1 is a protein called CARBONATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	34	0
			1994	1296	342	343	13			
1	B	225	Total	C	N	O	S	0	33	0
			1997	1299	343	344	11			
1	C	225	Total	C	N	O	S	0	30	0
			1979	1286	342	339	12			
1	D	225	Total	C	N	O	S	0	31	0
			1991	1293	346	341	11			
1	E	225	Total	C	N	O	S	0	27	0
			1961	1273	337	339	12			
1	F	225	Total	C	N	O	S	0	26	0
			1962	1272	342	337	11			

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

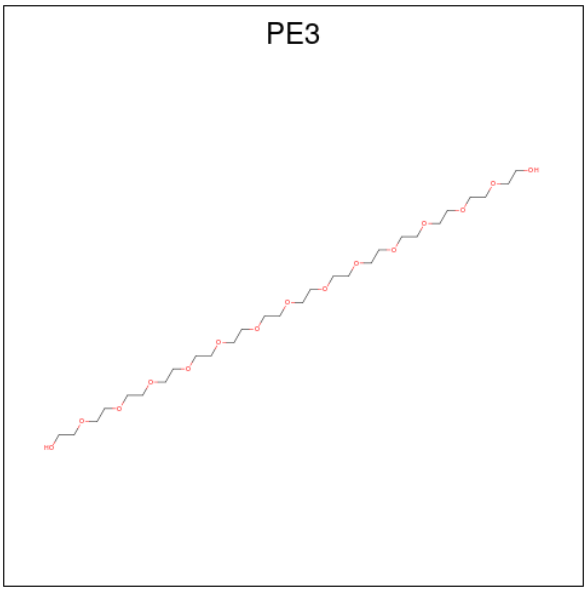
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 5-ACETAMIDO-1,3,4-THIADIAZOLE-2-SULFONAMIDE (three-letter code: AZM) (formula: $C_4H_6N_4O_3S_2$).



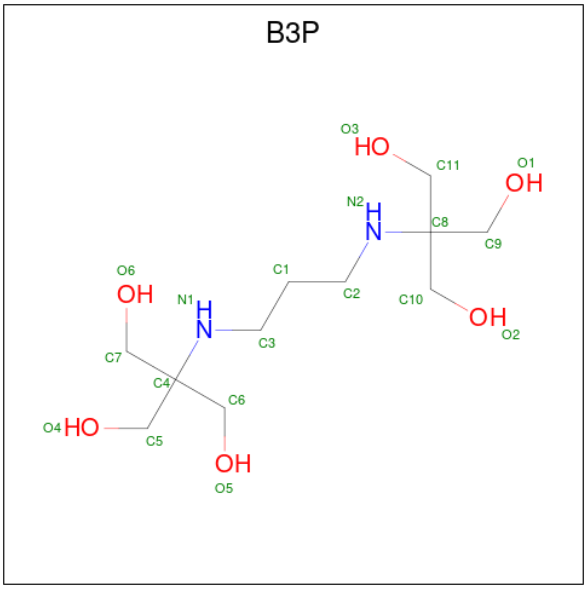
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			13	4	4	3	2		
3	B	1	Total	C	N	O	S	0	0
			13	4	4	3	2		
3	C	1	Total	C	N	O	S	0	0
			13	4	4	3	2		
3	D	1	Total	C	N	O	S	0	0
			13	4	4	3	2		
3	E	1	Total	C	N	O	S	0	0
			13	4	4	3	2		
3	F	1	Total	C	N	O	S	0	0
			13	4	4	3	2		

- Molecule 4 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1 ,41-DIOL (three-letter code: PE3) (formula: $C_{28}H_{58}O_{15}$).



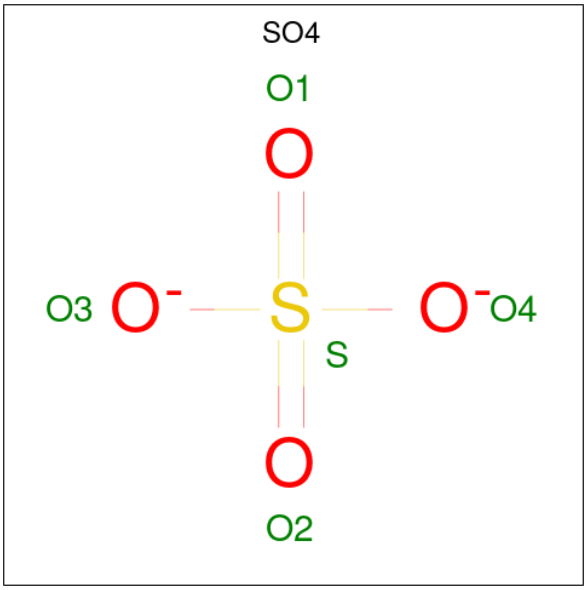
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 21 14 7	0	0
4	B	1	Total C O 21 14 7	0	0
4	F	1	Total C O 21 14 7	0	0

- Molecule 5 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 24 14 2 8	0	1
5	C	1	Total C N O 19 11 2 6	0	0
5	D	1	Total C N O 19 11 2 6	0	0
5	E	1	Total C N O 22 11 2 9	0	1
5	F	1	Total C N O 21 11 2 8	0	1

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

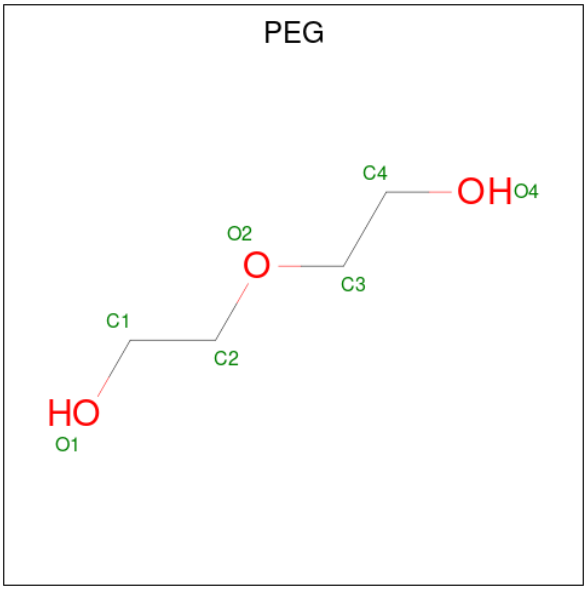


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	F	1	Total O S 5 4 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total Cl 3 3	0	0
7	B	3	Total Cl 3 3	0	0
7	C	3	Total Cl 3 3	0	0
7	D	2	Total Cl 2 2	0	0
7	E	2	Total Cl 2 2	0	0
7	F	2	Total Cl 2 2	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0
8	C	1	Total C O 7 4 3	0	0
8	E	1	Total C O 7 4 3	0	0
8	E	1	Total C O 7 4 3	0	0

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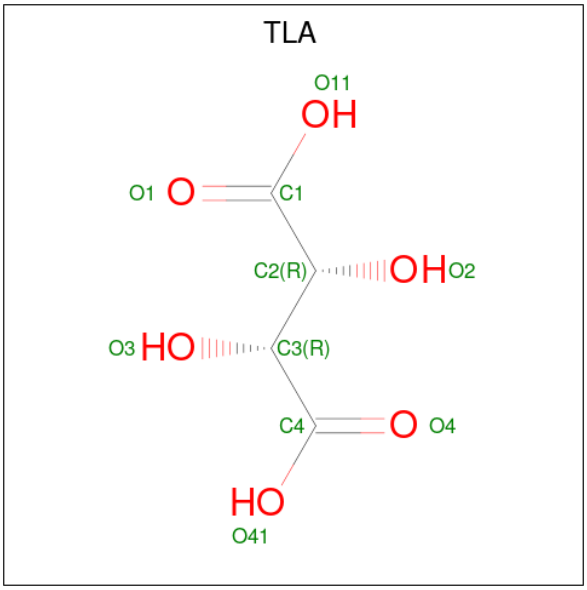
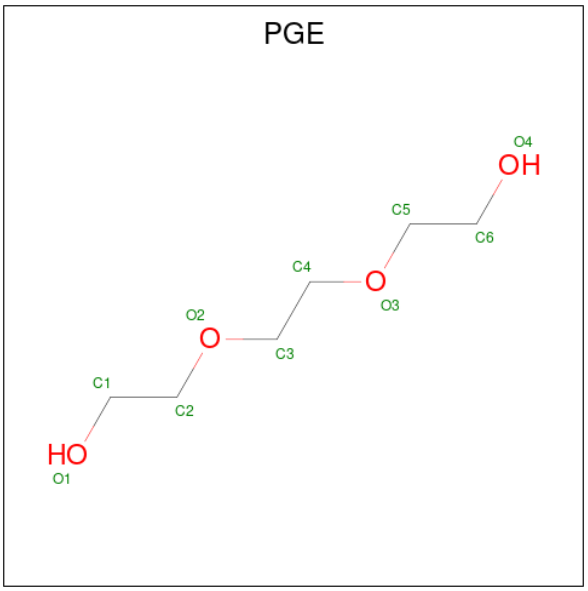
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	1	Total C O 7 4 3	0	0
8	F	1	Total C O 7 4 3	0	0

- Molecule 9 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



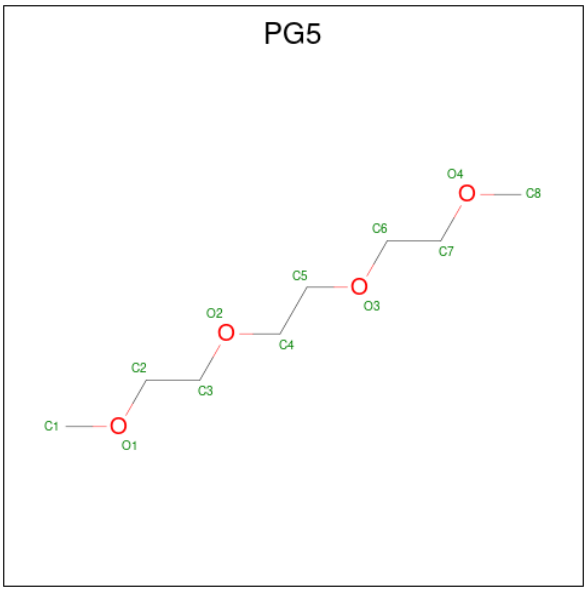
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 10 4 6	0	0
9	B	1	Total C O 10 4 6	0	0
9	F	1	Total C O 10 4 6	0	0

- Molecule 10 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 10 6 4	0	0
10	C	1	Total C O 10 6 4	0	0
10	D	1	Total C O 10 6 4	0	0
10	E	1	Total C O 10 6 4	0	0
10	F	1	Total C O 10 6 4	0	0

- Molecule 11 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY]-ETHANE (three-letter code: PG5) (formula: $C_8H_{18}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C O 12 8 4	0	0

- Molecule 12 is water.

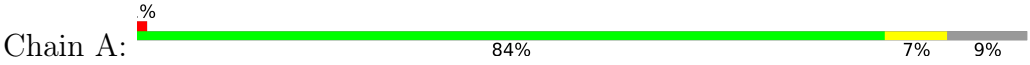
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	360	Total O 360 360	0	0
12	B	363	Total O 363 363	0	0
12	C	291	Total O 291 291	0	0
12	D	242	Total O 242 242	0	0
12	E	339	Total O 339 339	0	0
12	F	323	Total O 323 323	0	0

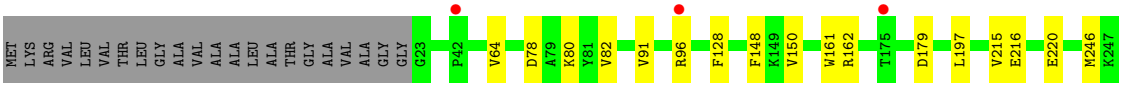
3 Residue-property plots (i)

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: CARBONATE DEHYDRATASE

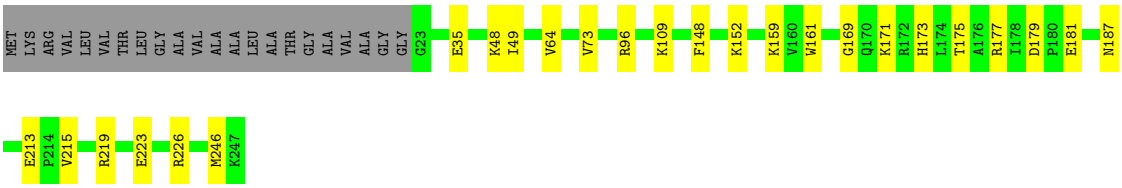
Chain A:





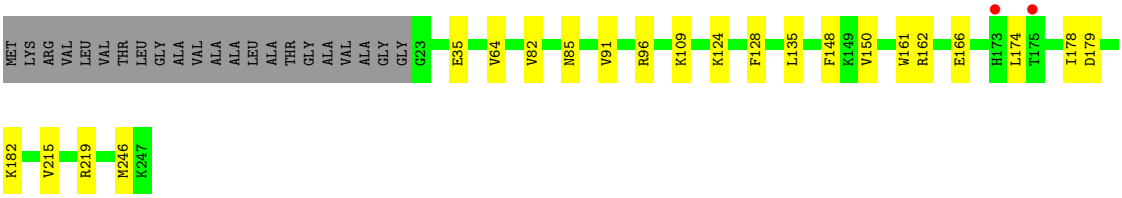
• Molecule 1: CARBONATE DEHYDRATASE

Chain B:



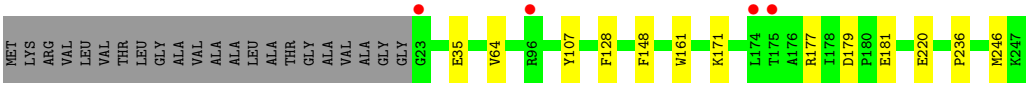
• Molecule 1: CARBONATE DEHYDRATASE

Chain C:



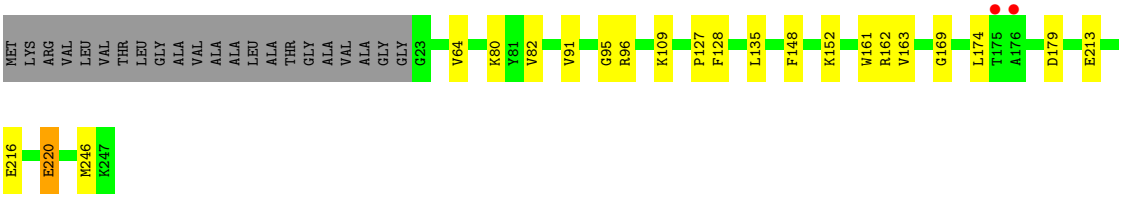
• Molecule 1: CARBONATE DEHYDRATASE

Chain D:



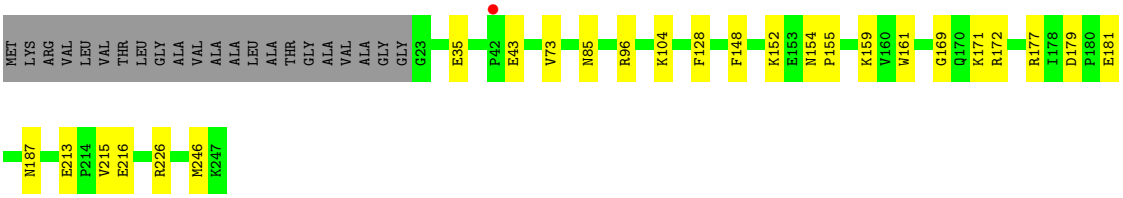
• Molecule 1: CARBONATE DEHYDRATASE

Chain E:



• Molecule 1: CARBONATE DEHYDRATASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.75Å 283.02Å 52.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.01 – 1.85 42.01 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.01-1.85) 99.5 (42.01-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.172 , 0.204 0.172 , 0.204	Depositor DCC
R_{free} test set	10399 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14247	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, TLA, B3P, PE3, ZN, CL, PGE, PEG, AZM, PG5

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	0.42	0/2152	0.54	0/2904
1	B	0.44	0/2153	0.56	0/2904
1	C	0.41	0/2126	0.53	0/2867
1	D	0.41	0/2141	0.54	0/2886
1	E	0.44	0/2097	0.55	0/2829
1	F	0.46	0/2096	0.56	0/2825
All	All	0.43	0/12765	0.55	0/17215

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	1994	0	2071	26	0
1	B	1997	0	2070	76	1
1	C	1979	0	2048	30	0
1	D	1991	0	2064	28	0
1	E	1961	0	2024	38	0
1	F	1962	0	2022	39	1
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	A	13	0	6	0	0
3	B	13	0	5	0	0
3	C	13	0	6	1	0
3	D	13	0	6	0	0
3	E	13	0	6	0	0
3	F	13	0	6	0	0
4	A	21	0	24	0	0
4	B	21	0	24	0	0
4	F	21	0	24	0	0
5	A	24	0	20	0	0
5	C	19	0	26	3	0
5	D	19	0	26	0	0
5	E	22	0	18	0	0
5	F	21	0	12	0	0
6	A	5	0	0	1	0
6	B	5	0	0	0	0
6	C	5	0	0	1	0
6	D	5	0	0	0	0
6	E	5	0	0	0	0
6	F	5	0	0	0	0
7	A	3	0	0	1	0
7	B	3	0	0	1	0
7	C	3	0	0	1	0
7	D	2	0	0	1	0
7	E	2	0	0	1	0
7	F	2	0	0	1	0
8	A	7	0	10	1	0
8	B	14	0	20	2	0
8	C	7	0	10	1	0
8	E	14	0	20	3	0
8	F	14	0	20	4	0
9	A	10	0	4	0	0
9	B	10	0	4	0	0
9	F	10	0	4	0	0
10	B	10	0	14	5	0
10	C	10	0	14	0	0
10	D	10	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	E	10	0	14	1	0
10	F	10	0	14	0	0
11	B	12	0	18	31	0
12	A	360	0	0	13	0
12	B	363	0	0	16	0
12	C	291	0	0	8	0
12	D	242	0	0	15	0
12	E	339	0	0	18	0
12	F	323	0	0	11	0
All	All	14247	0	12688	218	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (218) 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:246[B]:MET:CE	1:D:64[B]:VAL:HG11	1.55	1.35
1:A:64[B]:VAL:HG11	1:C:246[B]:MET:CE	1.57	1.32
1:B:171[B]:LYS:NZ	11:B:312:PG5:H12	1.46	1.26
1:E:220[B]:GLU:CD	12:E:2279:HOH:O	1.73	1.24
1:B:173[B]:HIS:NE2	11:B:312:PG5:O1	1.71	1.23
1:B:173[B]:HIS:CE1	11:B:312:PG5:O1	1.94	1.20
1:A:64[B]:VAL:CG1	1:C:246[B]:MET:HE1	1.70	1.20
1:E:220[B]:GLU:OE1	12:E:2279:HOH:O	1.56	1.20
1:E:96[B]:ARG:CZ	12:E:2115:HOH:O	1.90	1.19
1:B:171[B]:LYS:CE	11:B:312:PG5:H12	1.72	1.18
1:B:173[B]:HIS:NE2	11:B:312:PG5:C1	2.06	1.17
1:B:171[B]:LYS:HE3	11:B:312:PG5:C2	1.73	1.17
1:B:109[B]:LYS:HE2	10:B:305:PGE:H42	1.25	1.13
1:E:64[B]:VAL:HG11	1:F:246[B]:MET:CE	1.78	1.13
1:B:173[B]:HIS:CD2	12:B:2134:HOH:O	1.99	1.13
1:C:162[B]:ARG:HG2	1:C:162[B]:ARG:HH11	1.09	1.13
1:B:171[B]:LYS:HE3	11:B:312:PG5:H22	1.12	1.11
1:A:220[A]:GLU:OE2	12:A:2309:HOH:O	1.67	1.11
1:A:246[B]:MET:HE1	1:C:64[B]:VAL:CG1	1.81	1.11
1:B:171[B]:LYS:CE	11:B:312:PG5:C1	2.30	1.10
1:B:171[B]:LYS:CE	11:B:312:PG5:H22	1.82	1.10
1:A:246[B]:MET:CE	1:C:64[B]:VAL:HG11	1.82	1.09
1:B:171[B]:LYS:NZ	11:B:312:PG5:C1	2.16	1.07
1:D:179[B]:ASP:OD2	12:D:2181:HOH:O	1.70	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177[B]:ARG:HH11	1:B:177[B]:ARG:HG2	0.94	1.06
8:A:305:PEG:O1	12:A:2186:HOH:O	1.69	1.06
1:F:226[B]:ARG:HH11	1:F:226[B]:ARG:HG2	0.90	1.05
1:B:96[B]:ARG:NH2	12:B:2130:HOH:O	1.84	1.05
1:D:220[B]:GLU:CG	12:D:2211:HOH:O	2.02	1.05
1:B:171[B]:LYS:HE3	11:B:312:PG5:C1	1.84	1.04
1:B:173[B]:HIS:NE2	11:B:312:PG5:H11	1.72	1.04
1:B:246[B]:MET:CE	1:D:64[B]:VAL:CG1	2.35	1.04
1:B:177[B]:ARG:HD2	12:B:2126:HOH:O	1.58	1.03
1:F:177[B]:ARG:HG2	1:F:177[B]:ARG:HH11	0.93	1.03
1:A:64[B]:VAL:CG1	1:C:246[B]:MET:CE	2.32	1.01
1:E:152[B]:LYS:HE3	12:E:2212:HOH:O	0.83	1.00
1:E:64[B]:VAL:CG1	1:F:246[B]:MET:HE3	1.89	1.00
1:C:179[B]:ASP:OD2	12:C:2223:HOH:O	1.82	0.98
1:B:177[B]:ARG:HH11	1:B:177[B]:ARG:CG	1.75	0.97
6:A:302:SO4:O4	12:A:2192:HOH:O	1.83	0.97
1:E:179[B]:ASP:OD2	12:E:2241:HOH:O	1.81	0.97
1:B:246[B]:MET:HE1	1:D:64[B]:VAL:HG11	0.99	0.97
1:C:179[B]:ASP:HB2	12:C:2222:HOH:O	1.63	0.97
1:E:64[B]:VAL:CG1	1:F:246[B]:MET:CE	2.44	0.95
1:F:226[B]:ARG:HG2	1:F:226[B]:ARG:NH1	1.70	0.95
1:B:177[B]:ARG:HG2	1:B:177[B]:ARG:NH1	1.75	0.95
1:D:181[A]:GLU:OE1	12:D:2072:HOH:O	1.83	0.94
1:B:171[B]:LYS:HG3	11:B:312:PG5:H22	1.47	0.94
1:B:246[B]:MET:HE1	1:D:64[B]:VAL:CG1	1.93	0.94
1:A:246[B]:MET:HE1	1:C:64[B]:VAL:HG11	1.41	0.94
1:D:35[A]:GLU:OE1	12:D:2012:HOH:O	1.84	0.93
1:F:177[B]:ARG:HG2	1:F:177[B]:ARG:NH1	1.66	0.93
1:C:162[B]:ARG:HG2	1:C:162[B]:ARG:NH1	1.81	0.92
1:F:177[B]:ARG:HH11	1:F:177[B]:ARG:CG	1.82	0.92
1:E:64[B]:VAL:HG11	1:F:246[B]:MET:HE1	1.51	0.92
1:B:246[B]:MET:HE3	1:D:64[B]:VAL:CG1	1.99	0.91
1:F:226[B]:ARG:HH11	1:F:226[B]:ARG:CG	1.83	0.91
1:B:96[B]:ARG:NE	12:B:2130:HOH:O	1.99	0.91
1:B:171[B]:LYS:HE3	11:B:312:PG5:H12	1.43	0.90
1:E:213[B]:GLU:OE1	12:E:2276:HOH:O	1.90	0.88
1:E:80[B]:LYS:NZ	12:E:2118:HOH:O	1.71	0.87
1:B:173[B]:HIS:CD2	11:B:312:PG5:O1	2.27	0.87
1:B:171[B]:LYS:HZ1	11:B:312:PG5:H12	1.05	0.87
1:E:64[B]:VAL:HG13	1:F:246[B]:MET:HE3	1.57	0.84
1:E:96[B]:ARG:NH2	12:E:2115:HOH:O	2.00	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220[B]:GLU:HG2	12:D:2211:HOH:O	1.71	0.83
1:F:43[A]:GLU:CG	12:F:2033:HOH:O	2.27	0.83
1:D:171[B]:LYS:CE	12:D:2177:HOH:O	2.27	0.83
1:A:162[A]:ARG:NE	12:A:2246:HOH:O	1.96	0.83
1:B:213[B]:GLU:CD	12:B:2297:HOH:O	2.16	0.82
1:B:171[B]:LYS:CG	11:B:312:PG5:H22	2.07	0.82
1:A:179[B]:ASP:OD2	12:A:2262:HOH:O	1.97	0.82
7:D:304:CL:CL	12:D:2090:HOH:O	2.34	0.82
1:E:220[A]:GLU:OE1	12:E:2222:HOH:O	1.98	0.82
1:E:220[B]:GLU:OE2	12:E:2279:HOH:O	1.85	0.82
1:F:171[A]:LYS:NZ	12:F:2121:HOH:O	2.13	0.81
1:B:171[B]:LYS:HG3	11:B:312:PG5:C2	2.09	0.81
1:D:177[B]:ARG:HA	1:D:177[B]:ARG:HH11	1.46	0.79
1:A:246[B]:MET:HE1	1:C:64[B]:VAL:HG13	1.63	0.79
1:A:64[B]:VAL:HG11	1:C:246[B]:MET:HE1	0.82	0.78
1:B:171[B]:LYS:HZ1	11:B:312:PG5:C1	1.85	0.78
1:F:35[B]:GLU:HG2	12:F:2019:HOH:O	1.83	0.78
1:A:246[B]:MET:HE2	1:C:64[B]:VAL:HG11	1.67	0.77
7:C:304:CL:CL	12:C:2123:HOH:O	2.39	0.77
1:B:177[B]:ARG:NH2	1:B:179[B]:ASP:OD2	2.17	0.77
1:B:96[B]:ARG:CZ	12:B:2130:HOH:O	2.19	0.75
7:A:304:CL:CL	12:A:2143:HOH:O	2.41	0.75
1:B:173[B]:HIS:HD2	12:B:2134:HOH:O	1.49	0.75
1:B:171[B]:LYS:CD	11:B:312:PG5:H22	2.16	0.75
1:B:109[B]:LYS:CE	10:B:305:PGE:H42	2.13	0.72
1:A:64[B]:VAL:CG1	1:C:246[B]:MET:HE3	2.18	0.72
7:F:304:CL:CL	12:F:2125:HOH:O	2.45	0.72
1:B:213[B]:GLU:HG2	12:B:2276:HOH:O	1.90	0.71
1:D:35[B]:GLU:HG2	12:D:2012:HOH:O	1.91	0.71
1:B:246[B]:MET:HE3	1:D:64[B]:VAL:HG13	1.73	0.71
1:F:215[B]:VAL:HG11	12:F:2223:HOH:O	1.91	0.70
1:C:124[B]:LYS:HE3	6:C:302:SO4:O2	1.90	0.70
1:E:246[B]:MET:HE1	1:F:246[B]:MET:HG2	1.71	0.70
1:C:35[B]:GLU:OE2	12:C:2025:HOH:O	0.70	0.70
1:C:162[B]:ARG:HH11	1:C:162[B]:ARG:CG	1.95	0.70
1:B:177[B]:ARG:CD	12:B:2126:HOH:O	2.28	0.69
1:B:109[B]:LYS:HZ1	10:B:305:PGE:H2	1.56	0.69
7:B:304:CL:CL	12:B:2146:HOH:O	2.47	0.69
1:B:171[B]:LYS:CE	11:B:312:PG5:H13	2.22	0.68
1:A:246[B]:MET:CE	1:C:64[B]:VAL:CG1	2.51	0.67
1:D:35[B]:GLU:OE1	12:D:2016:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171[B]:LYS:HE3	12:D:2177:HOH:O	1.93	0.66
1:B:215[B]:VAL:HG11	12:B:2241:HOH:O	1.95	0.66
1:B:177[B]:ARG:HH22	1:B:179[B]:ASP:CG	2.00	0.65
1:A:197:LEU:HD12	12:A:2294:HOH:O	1.96	0.65
1:D:35[B]:GLU:OE1	1:D:35[B]:GLU:HA	1.96	0.65
1:D:177[B]:ARG:HA	1:D:177[B]:ARG:NH1	2.12	0.65
7:E:304:CL:CL	12:E:2125:HOH:O	2.50	0.65
1:E:152[B]:LYS:CE	12:E:2212:HOH:O	1.65	0.64
1:B:173[B]:HIS:CD2	11:B:312:PG5:C1	2.81	0.64
1:A:64[B]:VAL:HG13	1:C:246[B]:MET:HE3	1.81	0.62
1:F:159:LYS:HA	8:F:310:PEG:H31	1.83	0.60
1:B:173[B]:HIS:CE1	11:B:312:PG5:H32	2.36	0.60
8:F:310:PEG:H22	12:F:2120:HOH:O	2.03	0.59
1:A:215[B]:VAL:HG11	12:A:2236:HOH:O	2.00	0.59
1:E:246[B]:MET:CE	1:F:246[B]:MET:HG2	2.32	0.59
1:D:171[B]:LYS:CD	12:D:2177:HOH:O	2.50	0.59
1:B:48[A]:LYS:HG3	1:B:49:ILE:HG23	1.84	0.59
1:D:107:TYR:CD2	10:D:305:PGE:H52	2.38	0.58
1:E:64[B]:VAL:HG11	1:F:246[B]:MET:HE3	1.56	0.58
5:C:301:B3P:H31	12:C:2269:HOH:O	2.03	0.58
1:D:171[B]:LYS:HD2	12:D:2177:HOH:O	2.02	0.57
1:E:96[B]:ARG:NH1	12:E:2115:HOH:O	2.18	0.57
1:D:220[B]:GLU:HG3	12:D:2211:HOH:O	1.84	0.57
1:F:177[B]:ARG:NH1	1:F:177[B]:ARG:CG	2.49	0.57
1:E:82[B]:VAL:HG22	1:E:91:VAL:HG22	1.87	0.56
1:F:226[B]:ARG:NH1	1:F:226[B]:ARG:CG	2.53	0.56
1:C:96[B]:ARG:NH2	12:C:2116:HOH:O	2.39	0.56
1:B:223[B]:GLU:HA	1:B:223[B]:GLU:OE1	2.06	0.56
1:E:64[B]:VAL:CG1	1:F:246[B]:MET:HE1	2.23	0.56
1:B:109[B]:LYS:NZ	10:B:305:PGE:H52	2.20	0.55
1:A:78:ASP:HB2	1:A:96[A]:ARG:HH21	1.72	0.55
1:B:177[B]:ARG:CG	1:B:177[B]:ARG:NH1	2.47	0.54
1:B:213[B]:GLU:CG	12:B:2297:HOH:O	2.55	0.54
1:B:169:GLY:HA2	8:B:314:PEG:H32	1.89	0.53
1:A:82[A]:VAL:HG22	1:A:91:VAL:HG22	1.90	0.53
1:B:171[B]:LYS:HZ2	11:B:312:PG5:C1	2.17	0.53
1:B:177[B]:ARG:HG3	12:B:2126:HOH:O	2.08	0.53
1:B:219:ARG:O	1:B:223[B]:GLU:HG2	2.08	0.53
1:E:152[A]:LYS:NZ	12:E:2210:HOH:O	2.40	0.52
1:B:64[B]:VAL:HG11	1:D:246[B]:MET:HE1	1.91	0.52
1:E:127:PRO:HA	8:E:313:PEG:H22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82[A]:VAL:HG22	1:C:91:VAL:HG22	1.92	0.52
1:C:109[B]:LYS:HE3	1:C:135[B]:LEU:HD12	1.92	0.51
1:E:95:GLY:HA3	10:E:305:PGE:H5	1.92	0.51
1:B:177[B]:ARG:CG	12:B:2126:HOH:O	2.59	0.51
1:E:246[B]:MET:HE3	1:F:246[B]:MET:CE	2.41	0.50
1:F:43[A]:GLU:HG3	12:F:2033:HOH:O	2.02	0.50
1:A:179[B]:ASP:CG	12:A:2262:HOH:O	2.47	0.50
1:D:220[B]:GLU:OE2	12:D:2211:HOH:O	2.20	0.50
1:F:73:VAL:HG11	1:F:181[B]:GLU:HG3	1.94	0.50
1:C:128:PHE:HB3	1:C:148:PHE:HB2	1.93	0.50
1:F:169:GLY:HA2	8:F:314:PEG:H21	1.93	0.49
1:B:213[B]:GLU:HG2	12:B:2297:HOH:O	2.11	0.49
1:B:173[B]:HIS:CE1	11:B:312:PG5:C2	2.94	0.49
1:E:152[A]:LYS:HG2	1:E:216:GLU:OE1	2.13	0.49
1:E:169:GLY:HA2	8:E:314:PEG:H21	1.95	0.48
1:B:109[B]:LYS:HE2	10:B:305:PGE:C4	2.19	0.48
1:F:128:PHE:HB3	1:F:148:PHE:HB2	1.95	0.47
1:B:187:ASN:HB3	1:B:213[B]:GLU:HG3	1.96	0.46
1:B:177[B]:ARG:NH2	1:B:179[B]:ASP:CG	2.62	0.46
1:A:215[B]:VAL:HG12	1:A:216:GLU:N	2.31	0.46
1:B:171[B]:LYS:HD2	11:B:312:PG5:H13	1.97	0.46
1:C:219:ARG:NH1	12:C:2250:HOH:O	2.41	0.46
1:D:35[B]:GLU:OE1	1:D:35[B]:GLU:CA	2.61	0.46
1:F:96[B]:ARG:HH11	1:F:96[B]:ARG:HG3	1.80	0.46
1:B:64[A]:VAL:HG11	1:D:246[A]:MET:SD	2.56	0.45
12:A:2322:HOH:O	8:E:313:PEG:H41	2.16	0.45
1:B:171[B]:LYS:CD	11:B:312:PG5:H13	2.47	0.45
1:F:187:ASN:HB3	1:F:213[B]:GLU:HG3	1.99	0.45
1:C:166:GLU:O	5:C:301:B3P:O3	2.25	0.45
1:B:35[B]:GLU:HA	1:B:35[B]:GLU:OE1	2.16	0.44
1:A:162[A]:ARG:CZ	12:A:2246:HOH:O	2.50	0.44
1:F:177[B]:ARG:HH22	1:F:179:ASP:HB2	1.83	0.44
1:A:162[A]:ARG:NH2	12:A:2246:HOH:O	2.48	0.44
1:E:80[A]:LYS:NZ	12:E:2117:HOH:O	2.50	0.44
1:E:246[B]:MET:HE3	1:F:246[B]:MET:HE2	1.98	0.44
1:E:152[B]:LYS:CG	12:E:2212:HOH:O	2.61	0.43
1:F:85:ASN:HA	8:F:314:PEG:H22	2.01	0.43
1:C:148:PHE:CD2	1:C:215[A]:VAL:HG23	2.54	0.43
1:B:226[B]:ARG:NH2	12:B:2302:HOH:O	2.51	0.43
1:F:43[A]:GLU:HG2	12:F:2033:HOH:O	2.05	0.43
1:F:215[B]:VAL:HG12	1:F:216:GLU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171[B]:LYS:NZ	12:D:2177:HOH:O	2.40	0.43
3:C:299:AZM:S2	3:C:299:AZM:O3	2.77	0.42
1:F:154:ASN:HA	1:F:155:PRO:HD3	1.91	0.42
1:A:150[B]:VAL:HG22	12:A:2223:HOH:O	2.18	0.42
1:F:43[A]:GLU:CD	12:F:2033:HOH:O	2.53	0.42
1:B:173[B]:HIS:CG	11:B:312:PG5:O1	2.72	0.42
1:B:152[B]:LYS:HE2	1:B:152[B]:LYS:HB3	1.82	0.42
1:B:171[B]:LYS:HE3	11:B:312:PG5:O1	2.07	0.42
1:B:159:LYS:HA	8:B:310:PEG:H22	2.01	0.42
1:B:171[B]:LYS:NZ	11:B:312:PG5:H13	2.20	0.42
1:E:64[B]:VAL:HG13	1:F:246[B]:MET:CE	2.32	0.42
1:C:174:LEU:HD22	1:C:178:ILE:HD11	2.01	0.41
1:A:78:ASP:O	1:A:80[B]:LYS:HE3	2.20	0.41
1:B:173[B]:HIS:CD2	11:B:312:PG5:H11	2.48	0.41
1:C:179[A]:ASP:HB2	1:C:182:LYS:HD2	2.02	0.41
1:E:82[B]:VAL:CG2	1:E:174:LEU:HD21	2.50	0.41
1:E:109:LYS:HE3	1:E:135[B]:LEU:HD12	2.02	0.41
1:E:162[B]:ARG:HG3	1:E:163:VAL:HG13	2.03	0.41
1:D:128:PHE:HB3	1:D:148:PHE:HB2	2.02	0.41
1:B:73:VAL:HG11	1:B:181[B]:GLU:HG3	2.03	0.41
1:A:128:PHE:HB3	1:A:148:PHE:HB2	2.02	0.41
1:C:150[B]:VAL:HG22	12:C:2197:HOH:O	2.20	0.41
5:C:301:B3P:H21	5:C:301:B3P:H112	1.70	0.41
1:E:152[B]:LYS:CD	12:E:2212:HOH:O	2.35	0.41
1:F:104[B]:LYS:NZ	12:F:2157:HOH:O	2.52	0.41
1:B:148:PHE:CD2	1:B:215[A]:VAL:HG23	2.56	0.40
1:F:104[A]:LYS:HE3	12:F:2157:HOH:O	2.21	0.40
1:E:128:PHE:HB3	1:E:148:PHE:HB2	2.03	0.40
1:C:85:ASN:HA	8:C:314:PEG:H22	2.03	0.40
1:E:162[A]:ARG:NH2	12:E:2220:HOH:O	2.54	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:THR:OG1	1:F:172[B]:ARG:NH2[3_444]	2.14	0.06

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	257/247 (104%)	253 (98%)	4 (2%)	0	100	100
1	B	256/247 (104%)	252 (98%)	4 (2%)	0	100	100
1	C	253/247 (102%)	249 (98%)	4 (2%)	0	100	100
1	D	254/247 (103%)	250 (98%)	4 (2%)	0	100	100
1	E	250/247 (101%)	245 (98%)	5 (2%)	0	100	100
1	F	249/247 (101%)	245 (98%)	4 (2%)	0	100	100
All	All	1519/1482 (102%)	1494 (98%)	25 (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	230/208 (111%)	229 (100%)	1 (0%)	91	89
1	B	229/208 (110%)	228 (100%)	1 (0%)	91	89
1	C	226/208 (109%)	225 (100%)	1 (0%)	91	89
1	D	227/208 (109%)	225 (99%)	2 (1%)	78	72
1	E	223/208 (107%)	220 (99%)	3 (1%)	69	58
1	F	222/208 (107%)	219 (99%)	3 (1%)	67	55
All	All	1357/1248 (109%)	1346 (99%)	11 (1%)	81	76

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	TRP
1	B	161	TRP
1	C	161	TRP
1	D	161	TRP
1	D	236	PRO
1	E	161	TRP
1	E	220[A]	GLU
1	E	220[B]	GLU
1	F	152[A]	LYS
1	F	152[B]	LYS
1	F	161	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	140	ASN

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 61 ligands modelled in this entry, 21 are monoatomic - leaving 40 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	$\#\|Z\| > 2$
8	PEG	E	313	-	6,6,6	0.46	0	5,5,5	0.53	0
10	PGE	E	305	-	9,9,9	0.44	0	8,8,8	0.28	0
5	B3P	F	301[B]	-	18,18,18	0.42	0	21,23,23	1.82	3 (14%)
6	SO4	C	302	-	4,4,4	0.33	0	6,6,6	0.22	0
8	PEG	E	314	-	6,6,6	0.41	0	5,5,5	0.39	0
5	B3P	A	301[A]	-	18,18,18	0.52	0	21,23,23	1.97	2 (9%)
8	PEG	F	314	-	6,6,6	0.41	0	5,5,5	0.37	0
4	PE3	A	300	-	20,20,42	0.52	0	19,19,41	0.30	0
4	PE3	B	300	-	20,20,42	0.53	0	19,19,41	0.22	0
3	AZM	F	299	2	8,13,13	0.44	0	9,19,19	2.76	4 (44%)
6	SO4	A	302	-	4,4,4	0.28	0	6,6,6	0.07	0
8	PEG	A	305	-	6,6,6	0.40	0	5,5,5	0.37	0
9	TLA	B	306	-	9,9,9	1.10	0	12,12,12	1.11	2 (16%)
6	SO4	B	302	-	4,4,4	0.26	0	6,6,6	0.08	0
5	B3P	F	301[A]	-	18,18,18	0.42	0	21,23,23	1.82	3 (14%)
6	SO4	E	302	-	4,4,4	0.25	0	6,6,6	0.06	0
10	PGE	D	305	-	9,9,9	0.44	0	8,8,8	0.22	0
10	PGE	F	309	-	9,9,9	0.44	0	8,8,8	0.30	0
4	PE3	F	300	-	20,20,42	0.48	0	19,19,41	0.23	0
5	B3P	E	301[B]	-	18,18,18	0.52	0	21,23,23	1.80	2 (9%)
5	B3P	C	301	-	18,18,18	0.65	0	21,23,23	5.54	13 (61%)
3	AZM	E	299	2	8,13,13	0.24	0	9,19,19	1.84	2 (22%)
9	TLA	A	306	-	9,9,9	1.10	0	12,12,12	0.89	0
8	PEG	B	310	-	6,6,6	0.49	0	5,5,5	0.21	0
10	PGE	B	305	-	9,9,9	0.47	0	8,8,8	0.34	0
3	AZM	A	299	2	8,13,13	0.35	0	9,19,19	2.16	2 (22%)
11	PG5	B	312	-	11,11,11	0.49	0	10,10,10	0.30	0
6	SO4	F	302	-	4,4,4	0.31	0	6,6,6	0.06	0
8	PEG	B	314	-	6,6,6	0.45	0	5,5,5	0.37	0
5	B3P	E	301[A]	-	18,18,18	0.51	0	21,23,23	1.80	2 (9%)
6	SO4	D	302	-	4,4,4	0.34	0	6,6,6	0.07	0
8	PEG	F	310	-	6,6,6	0.55	0	5,5,5	0.36	0
9	TLA	F	306	-	9,9,9	1.13	0	12,12,12	0.96	0
10	PGE	C	305	-	9,9,9	0.45	0	8,8,8	0.27	0
3	AZM	D	299	2	8,13,13	0.29	0	9,19,19	1.90	2 (22%)
3	AZM	B	299	2	8,13,13	0.32	0	9,19,19	2.44	3 (33%)
5	B3P	A	301[B]	-	18,18,18	0.56	0	21,23,23	1.84	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	AZM	C	299	2	8,13,13	0.28	0	9,19,19	2.41	4 (44%)
8	PEG	C	314	-	6,6,6	0.46	0	5,5,5	0.32	0
5	B3P	D	301	-	18,18,18	0.45	0	21,23,23	2.14	2 (9%)

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
8	PEG	E	313	-	-	4/4/4/4	-
10	PGE	E	305	-	-	5/7/7/7	-
5	B3P	F	301[B]	-	-	2/28/28/28	-
8	PEG	E	314	-	-	1/4/4/4	-
5	B3P	A	301[A]	-	-	16/28/28/28	-
8	PEG	F	314	-	-	2/4/4/4	-
4	PE3	A	300	-	-	3/18/18/40	-
4	PE3	B	300	-	-	3/18/18/40	-
3	AZM	F	299	2	-	0/2/10/10	0/1/1/1
8	PEG	A	305	-	-	4/4/4/4	-
9	TLA	B	306	-	-	2/12/12/12	-
5	B3P	F	301[A]	-	-	1/28/28/28	-
10	PGE	F	309	-	-	4/7/7/7	-
10	PGE	D	305	-	-	3/7/7/7	-
4	PE3	F	300	-	-	1/18/18/40	-
5	B3P	E	301[B]	-	-	9/28/28/28	-
5	B3P	C	301	-	-	17/28/28/28	-
3	AZM	E	299	2	-	0/2/10/10	0/1/1/1
9	TLA	A	306	-	-	0/12/12/12	-
8	PEG	B	310	-	-	2/4/4/4	-
10	PGE	B	305	-	-	5/7/7/7	-
3	AZM	A	299	2	-	0/2/10/10	0/1/1/1
11	PG5	B	312	-	-	7/9/9/9	-
8	PEG	B	314	-	-	2/4/4/4	-
5	B3P	E	301[A]	-	-	5/28/28/28	-
8	PEG	F	310	-	-	2/4/4/4	-
9	TLA	F	306	-	-	0/12/12/12	-
10	PGE	C	305	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AZM	D	299	2	-	0/2/10/10	0/1/1/1
3	AZM	B	299	2	-	2/2/10/10	0/1/1/1
5	B3P	A	301[B]	-	-	18/28/28/28	-
3	AZM	C	299	2	-	2/2/10/10	0/1/1/1
8	PEG	C	314	-	-	2/4/4/4	-
5	B3P	D	301	-	-	7/28/28/28	-

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	301	B3P	C10-C8-C9	-11.56	85.60	110.04
5	C	301	B3P	C6-C4-C5	-10.84	87.11	110.04
5	C	301	B3P	C7-C4-C5	-9.77	89.39	110.04
5	C	301	B3P	C9-C8-N2	-7.48	86.52	109.03
5	C	301	B3P	C5-C4-N1	-7.35	86.92	109.03
5	C	301	B3P	C11-C8-C9	-7.13	94.97	110.04
5	D	301	B3P	C3-N1-C4	6.59	125.42	116.08
3	F	299	AZM	O1-S1-C1	-6.48	100.98	108.59
5	A	301[A]	B3P	C2-N2-C8	6.46	125.24	116.08
5	A	301[B]	B3P	C2-N2-C8	6.46	125.24	116.08
5	D	301	B3P	C2-N2-C8	6.19	124.86	116.08
5	F	301[A]	B3P	C3-N1-C4	6.08	124.71	116.08
5	F	301[B]	B3P	C3-N1-C4	6.08	124.71	116.08
5	A	301[A]	B3P	C3-N1-C4	5.66	124.10	116.08
5	E	301[A]	B3P	C3-N1-C4	5.60	124.02	116.08
5	E	301[B]	B3P	C3-N1-C4	5.60	124.02	116.08
5	E	301[A]	B3P	C2-N2-C8	5.56	123.96	116.08
5	E	301[B]	B3P	C2-N2-C8	5.56	123.96	116.08
5	C	301	B3P	C3-N1-C4	5.40	123.74	116.08
3	C	299	AZM	O1-S1-C1	-5.38	102.27	108.59
3	B	299	AZM	O1-S1-C1	-5.09	102.61	108.59
5	C	301	B3P	C10-C8-N2	4.98	123.99	109.03
3	A	299	AZM	O1-S1-C1	-4.82	102.93	108.59
5	C	301	B3P	C11-C8-C10	4.60	119.77	110.04
5	F	301[A]	B3P	C2-N2-C8	4.58	122.58	116.08
5	F	301[B]	B3P	C2-N2-C8	4.58	122.58	116.08
5	C	301	B3P	C7-C4-N1	4.56	122.75	109.03
5	A	301[B]	B3P	C3-N1-C4	4.48	122.44	116.08
3	D	299	AZM	O1-S1-C1	-4.32	103.52	108.59
5	C	301	B3P	C7-C4-C6	4.25	119.04	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	299	AZM	O1-S1-C1	-4.25	103.60	108.59
3	B	299	AZM	O1-S1-N1	3.29	112.24	107.36
3	F	299	AZM	O1-S1-N1	3.11	111.98	107.36
3	B	299	AZM	C1-S1-N1	-3.08	102.57	108.25
5	C	301	B3P	C6-C4-N1	2.91	117.78	109.03
3	C	299	AZM	C1-S1-N1	-2.67	103.32	108.25
3	F	299	AZM	O2-S1-N1	2.55	111.14	107.36
3	A	299	AZM	O2-S1-N1	2.54	111.12	107.36
5	F	301[A]	B3P	C7-C4-C5	-2.42	104.92	110.04
5	F	301[B]	B3P	C7-C4-C5	-2.42	104.92	110.04
5	C	301	B3P	C11-C8-N2	2.36	116.12	109.03
9	B	306	TLA	O11-C1-C2	2.18	119.16	113.27
9	B	306	TLA	O41-C4-C3	2.16	119.11	113.27
3	F	299	AZM	O2-S1-C1	-2.12	106.10	108.59
3	C	299	AZM	O2-S1-O1	2.11	122.22	118.76
3	E	299	AZM	O1-S1-N1	2.08	110.45	107.36
3	D	299	AZM	O2-S1-N1	2.06	110.42	107.36
3	C	299	AZM	O3-C3-N4	-2.00	120.41	123.04

There are no chirality outliers.

All (135) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	299	AZM	C4-C3-N4-C2
3	B	299	AZM	O3-C3-N4-C2
5	A	301[A]	B3P	C5-C4-N1-C3
5	A	301[A]	B3P	C6-C4-N1-C3
5	A	301[A]	B3P	C7-C4-N1-C3
5	A	301[A]	B3P	C9-C8-N2-C2
5	A	301[A]	B3P	C10-C8-N2-C2
5	A	301[A]	B3P	C11-C8-N2-C2
5	A	301[A]	B3P	N2-C8-C9-O1
5	A	301[A]	B3P	C10-C8-C9-O1
5	A	301[A]	B3P	C11-C8-C9-O1
5	A	301[B]	B3P	C5-C4-N1-C3
5	A	301[B]	B3P	C6-C4-N1-C3
5	A	301[B]	B3P	C9-C8-N2-C2
5	A	301[B]	B3P	C10-C8-N2-C2
5	A	301[B]	B3P	C11-C8-N2-C2
5	A	301[B]	B3P	N2-C8-C9-O1
5	A	301[B]	B3P	C10-C8-C9-O1
5	A	301[B]	B3P	C11-C8-C9-O1

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Mol	Chain	Res	Type	Atoms
5	C	301	B3P	C5-C4-N1-C3
5	C	301	B3P	C6-C4-N1-C3
5	C	301	B3P	C7-C4-N1-C3
5	C	301	B3P	C7-C4-C6-O5
5	C	301	B3P	C6-C4-C7-O6
5	C	301	B3P	C9-C8-N2-C2
5	C	301	B3P	C11-C8-N2-C2
5	C	301	B3P	O2-C10-C8-C9
5	C	301	B3P	O3-C11-C8-N2
5	D	301	B3P	C9-C8-N2-C2
5	D	301	B3P	C11-C8-N2-C2
5	E	301[A]	B3P	C5-C4-N1-C3
5	E	301[A]	B3P	C6-C4-N1-C3
5	E	301[A]	B3P	C7-C4-N1-C3
5	E	301[B]	B3P	C5-C4-N1-C3
5	E	301[B]	B3P	C6-C4-N1-C3
5	E	301[B]	B3P	C7-C4-N1-C3
5	E	301[B]	B3P	O2-C10-C8-N2
5	E	301[B]	B3P	O2-C10-C8-C9
5	E	301[B]	B3P	O2-C10-C8-C11
10	B	305	PGE	O2-C3-C4-O3
11	B	312	PG5	O2-C4-C5-O3
11	B	312	PG5	O1-C2-C3-O2
5	C	301	B3P	C3-C1-C2-N2
4	F	300	PE3	O22-C23-C24-O25
4	A	300	PE3	O37-C38-C39-O40
4	A	300	PE3	O22-C23-C24-O25
5	A	301[A]	B3P	O2-C10-C8-C9
5	A	301[A]	B3P	O3-C11-C8-C9
5	A	301[B]	B3P	O2-C10-C8-C9
5	A	301[B]	B3P	O3-C11-C8-C9
5	C	301	B3P	O3-C11-C8-C9
8	A	305	PEG	O1-C1-C2-O2
8	E	313	PEG	O1-C1-C2-O2
8	E	313	PEG	C4-C3-O2-C2
8	B	310	PEG	O1-C1-C2-O2
10	F	309	PGE	O1-C1-C2-O2
8	F	310	PEG	O2-C3-C4-O4
10	C	305	PGE	O3-C5-C6-O4
10	E	305	PGE	O3-C5-C6-O4
5	A	301[A]	B3P	O3-C11-C8-N2
5	A	301[B]	B3P	O3-C11-C8-N2

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Mol	Chain	Res	Type	Atoms
5	C	301	B3P	N1-C4-C7-O6
5	C	301	B3P	O2-C10-C8-N2
10	B	305	PGE	O3-C5-C6-O4
5	A	301[A]	B3P	C2-C1-C3-N1
5	A	301[B]	B3P	C2-C1-C3-N1
5	F	301[A]	B3P	C1-C2-N2-C8
5	F	301[B]	B3P	C1-C2-N2-C8
10	F	309	PGE	O2-C3-C4-O3
3	C	299	AZM	C4-C3-N4-C2
5	A	301[B]	B3P	C7-C4-N1-C3
5	D	301	B3P	C6-C4-N1-C3
5	D	301	B3P	C7-C4-N1-C3
5	D	301	B3P	C10-C8-N2-C2
8	C	314	PEG	O2-C3-C4-O4
8	E	313	PEG	O2-C3-C4-O4
8	F	314	PEG	O2-C3-C4-O4
9	B	306	TLA	C2-C3-C4-O4
4	B	300	PE3	O37-C38-C39-O40
11	B	312	PG5	C3-C2-O1-C1
3	C	299	AZM	O3-C3-N4-C2
5	A	301[A]	B3P	O2-C10-C8-N2
5	A	301[B]	B3P	O2-C10-C8-N2
5	C	301	B3P	O2-C10-C8-C11
9	B	306	TLA	C2-C3-C4-O41
4	B	300	PE3	C24-C23-O22-C21
5	D	301	B3P	C3-C1-C2-N2
5	C	301	B3P	C1-C3-N1-C4
10	C	305	PGE	O1-C1-C2-O2
10	D	305	PGE	O3-C5-C6-O4
10	C	305	PGE	C4-C3-O2-C2
10	D	305	PGE	C1-C2-O2-C3
10	F	309	PGE	C4-C3-O2-C2
10	B	305	PGE	C6-C5-O3-C4
10	E	305	PGE	C1-C2-O2-C3
8	B	314	PEG	C1-C2-O2-C3
5	A	301[A]	B3P	O3-C11-C8-C10
5	A	301[B]	B3P	O3-C11-C8-C10
8	A	305	PEG	O2-C3-C4-O4
10	E	305	PGE	O1-C1-C2-O2
11	B	312	PG5	C2-C3-O2-C4
11	B	312	PG5	C5-C4-O2-C3
5	C	301	B3P	C1-C2-N2-C8

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Mol	Chain	Res	Type	Atoms
11	B	312	PG5	C4-C5-O3-C6
10	E	305	PGE	O2-C3-C4-O3
5	F	301[B]	B3P	O3-C11-C8-C9
5	E	301[A]	B3P	C2-C1-C3-N1
5	E	301[B]	B3P	C2-C1-C3-N1
8	F	310	PEG	C1-C2-O2-C3
8	A	305	PEG	C4-C3-O2-C2
5	E	301[B]	B3P	C5-C4-C6-O5
4	A	300	PE3	C26-C27-O28-C29
8	C	314	PEG	C4-C3-O2-C2
8	A	305	PEG	C1-C2-O2-C3
10	D	305	PGE	C6-C5-O3-C4
4	B	300	PE3	C27-C26-O25-C24
5	C	301	B3P	C2-C1-C3-N1
8	E	314	PEG	O1-C1-C2-O2
5	A	301[B]	B3P	C5-C4-C7-O6
5	A	301[B]	B3P	C6-C4-C7-O6
5	D	301	B3P	C5-C4-N1-C3
11	B	312	PG5	C6-C7-O4-C8
8	F	314	PEG	C4-C3-O2-C2
5	A	301[A]	B3P	O2-C10-C8-C11
5	A	301[B]	B3P	O2-C10-C8-C11
10	C	305	PGE	C1-C2-O2-C3
8	B	310	PEG	C1-C2-O2-C3
8	E	313	PEG	C1-C2-O2-C3
10	E	305	PGE	C4-C3-O2-C2
10	B	305	PGE	C3-C4-O3-C5
8	B	314	PEG	O1-C1-C2-O2
10	B	305	PGE	O1-C1-C2-O2
5	E	301[A]	B3P	C11-C8-N2-C2
5	E	301[B]	B3P	C11-C8-N2-C2
10	F	309	PGE	C1-C2-O2-C3

There are no ring outliers.

16 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	313	PEG	2	0
10	E	305	PGE	1	0
6	C	302	SO4	1	0
8	E	314	PEG	1	0
8	F	314	PEG	2	0

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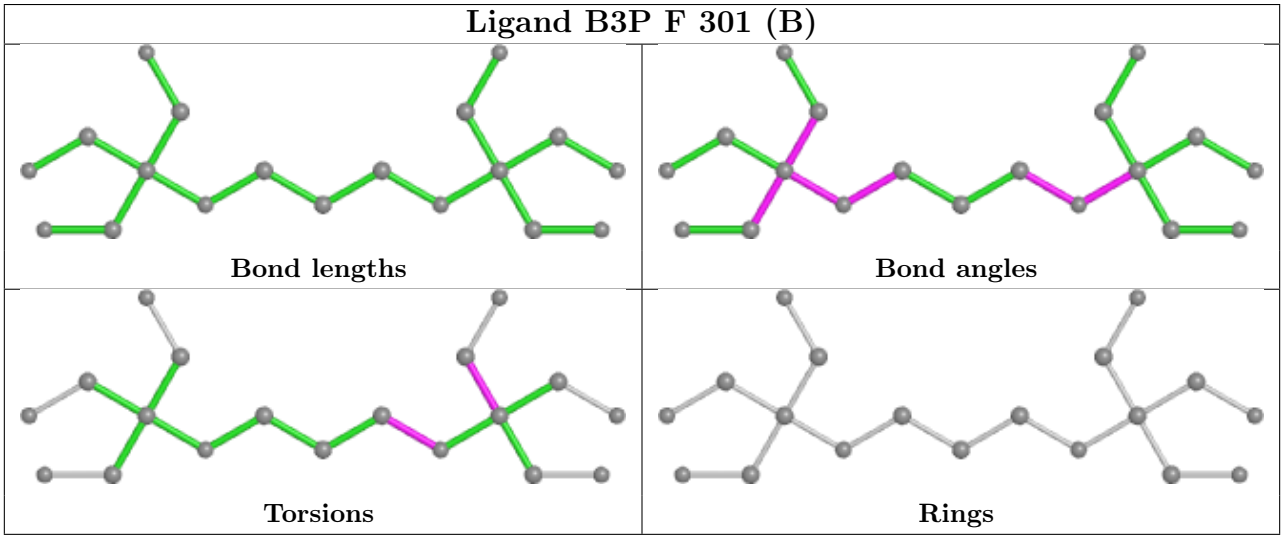
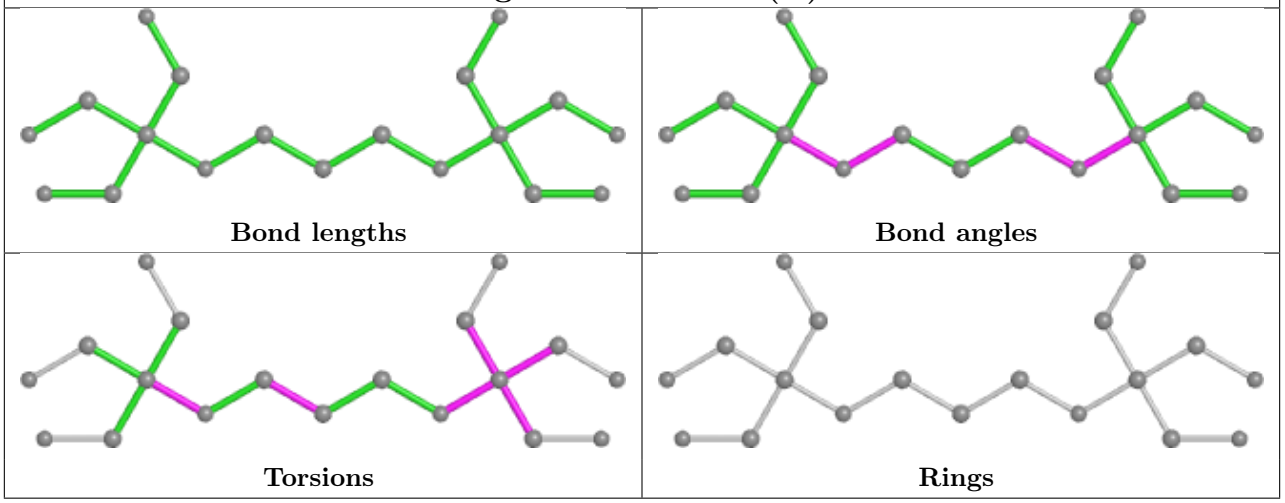
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	302	SO4	1	0
8	A	305	PEG	1	0
10	D	305	PGE	1	0
5	C	301	B3P	3	0
8	B	310	PEG	1	0
10	B	305	PGE	5	0
11	B	312	PG5	31	0
8	B	314	PEG	1	0
8	F	310	PEG	2	0
3	C	299	AZM	1	0
8	C	314	PEG	1	0

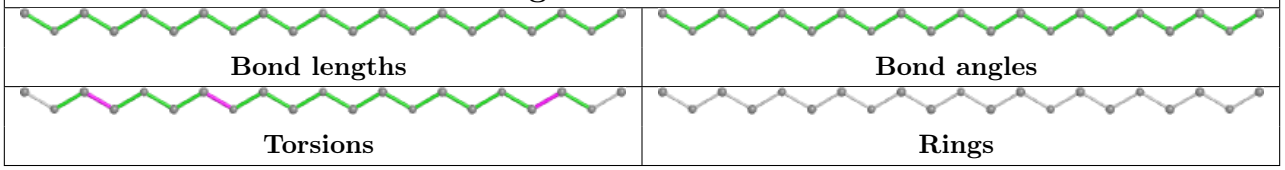
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



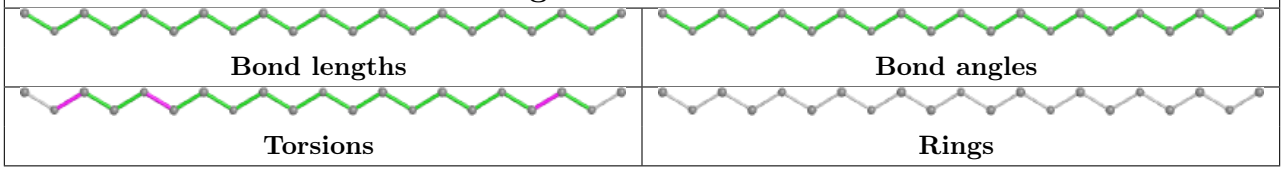
Ligand B3P A 301 (A)



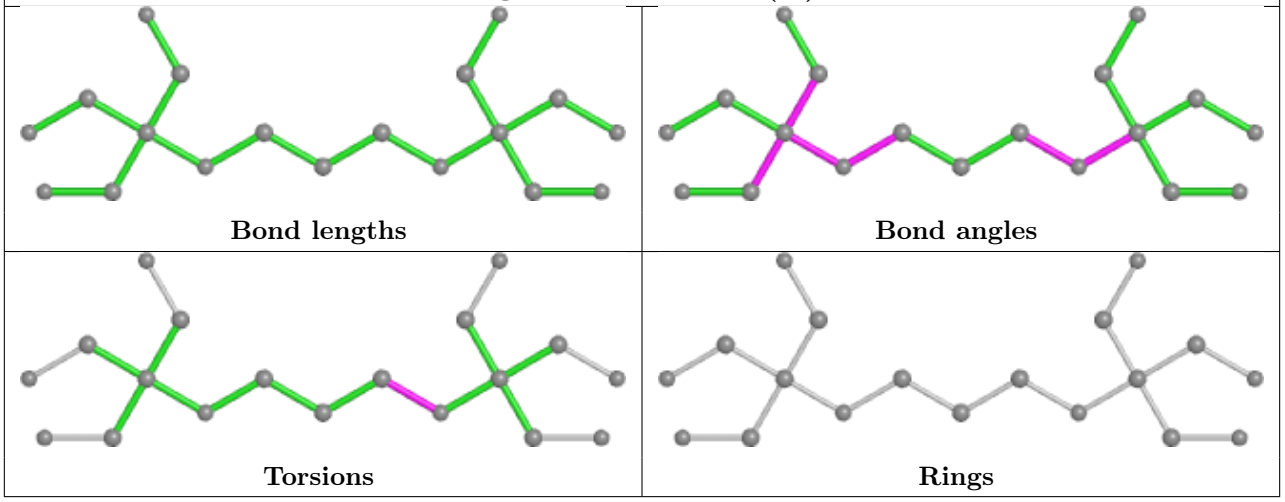
Ligand PE3 A 300



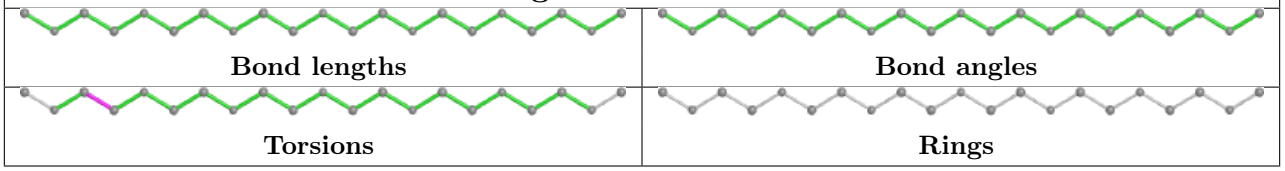
Ligand PE3 B 300



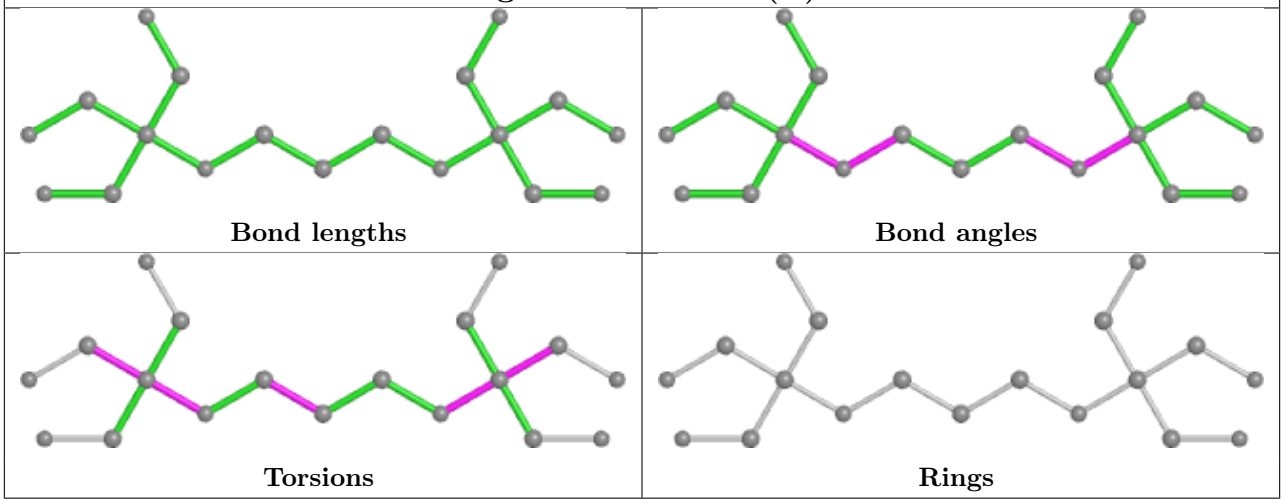
Ligand B3P F 301 (A)



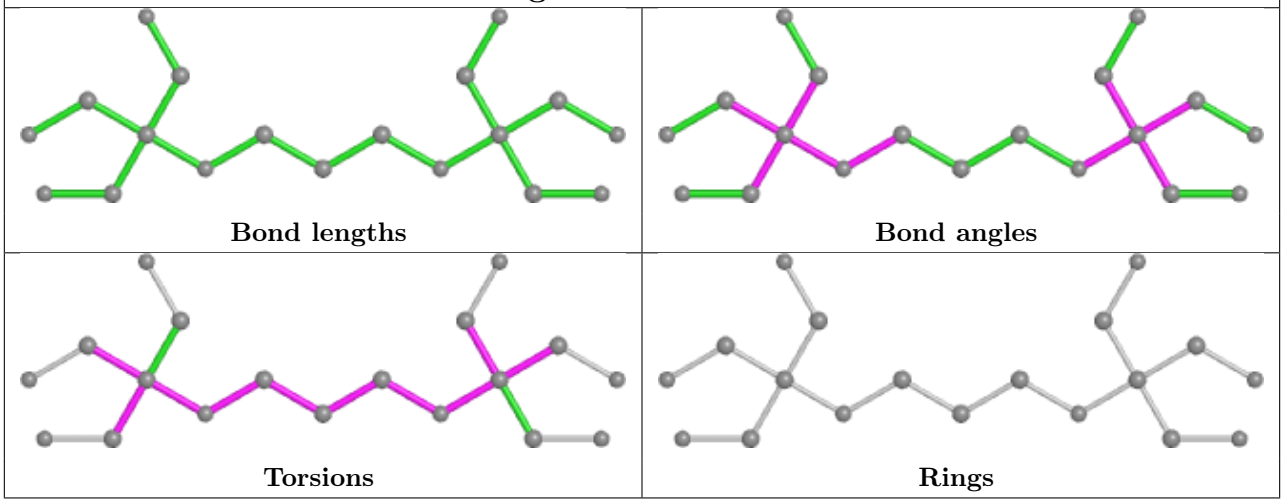
Ligand PE3 F 300



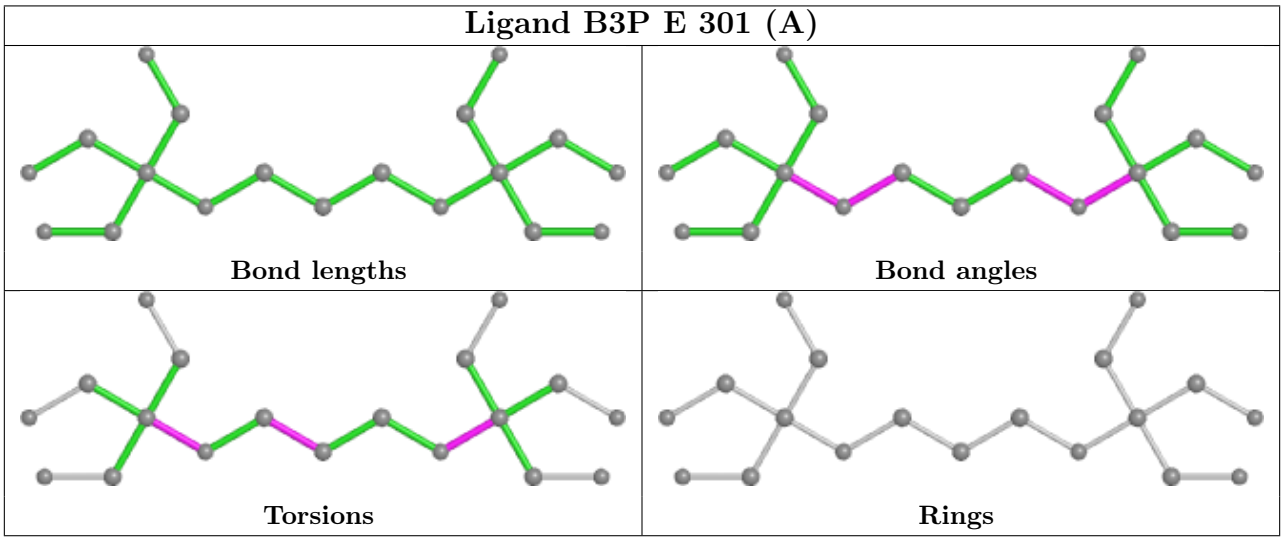
Ligand B3P E 301 (B)

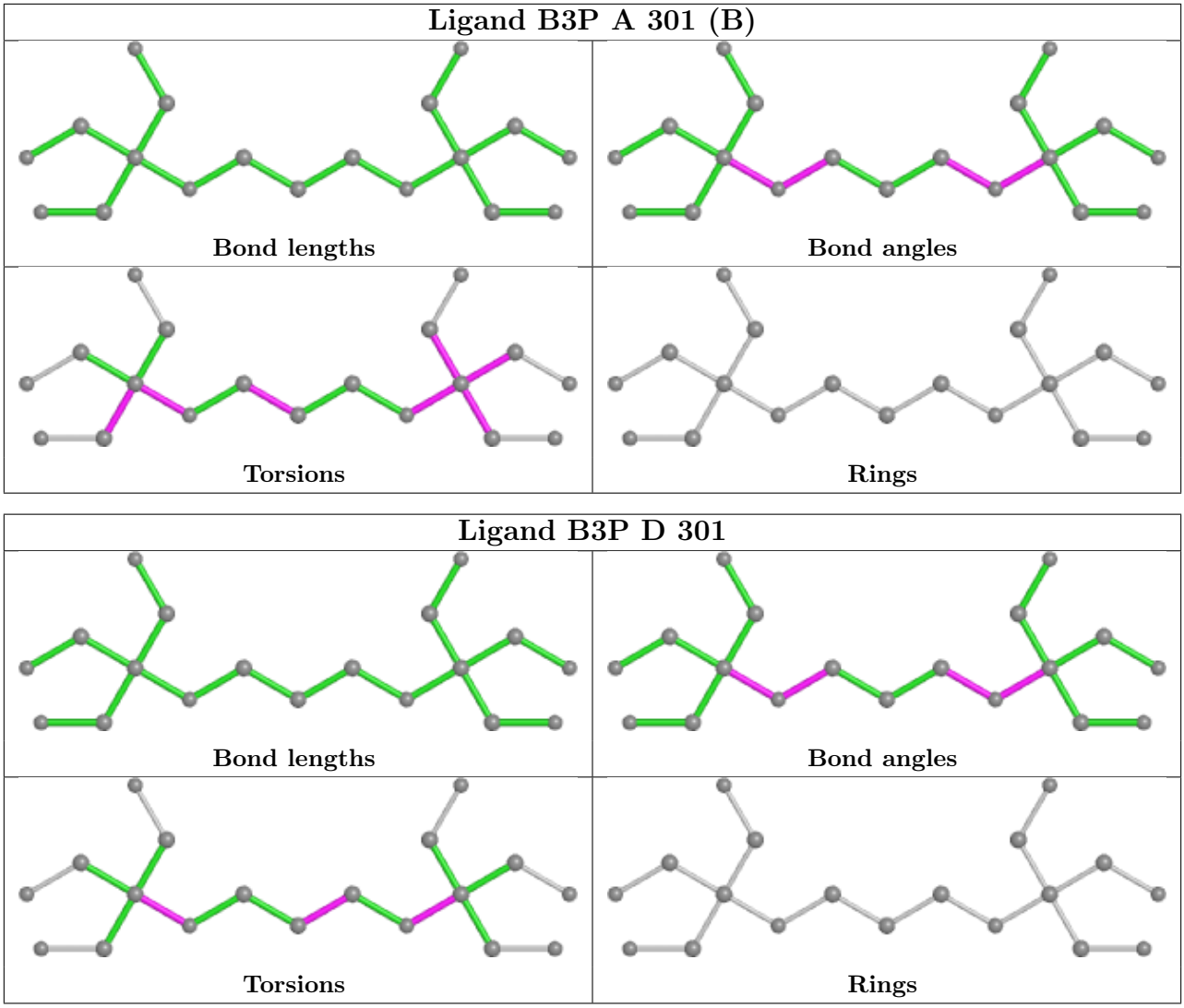


Ligand B3P C 301



Ligand B3P E 301 (A)





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	225/247 (91%)	-0.17	3 (1%) 77 78	14, 24, 42, 65	0
1	B	225/247 (91%)	-0.27	0 100 100	13, 22, 39, 61	0
1	C	225/247 (91%)	-0.20	2 (0%) 84 84	14, 26, 45, 71	0
1	D	225/247 (91%)	-0.14	4 (1%) 68 68	14, 26, 43, 67	0
1	E	225/247 (91%)	-0.23	2 (0%) 84 84	13, 24, 43, 58	0
1	F	225/247 (91%)	-0.36	1 (0%) 92 92	12, 21, 36, 61	0
All	All	1350/1482 (91%)	-0.23	12 (0%) 84 84	12, 24, 43, 71	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	175	THR	3.9
1	C	175	THR	3.2
1	C	173[A]	HIS	3.1
1	D	23	GLY	2.9
1	A	175	THR	2.5
1	E	175	THR	2.4
1	D	174	LEU	2.4
1	A	96[A]	ARG	2.2
1	D	96[A]	ARG	2.2
1	A	42	PRO	2.2
1	E	176	ALA	2.1
1	F	42	PRO	2.1

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

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
5	B3P	C	301	19/19	0.66	0.43	38,46,53,54	19
5	B3P	D	301	19/19	0.70	0.42	32,40,52,54	19
8	PEG	F	310	7/7	0.75	0.29	30,32,44,45	7
10	PGE	D	305	10/10	0.75	0.24	36,49,55,64	10
7	CL	D	307	1/1	0.76	0.13	48,48,48,48	1
10	PGE	F	309	10/10	0.77	0.18	34,38,42,42	10
10	PGE	B	305	10/10	0.78	0.17	34,43,54,59	10
8	PEG	B	310	7/7	0.79	0.26	24,29,32,38	7
10	PGE	E	305	10/10	0.81	0.17	33,42,47,51	10
8	PEG	C	314	7/7	0.85	0.18	46,61,79,85	0
9	TLA	B	306	10/10	0.85	0.22	20,25,27,30	10
11	PG5	B	312	12/12	0.85	0.21	33,40,44,47	12
5	B3P	E	301[A]	19/19	0.86	0.22	26,30,46,49	19
8	PEG	E	314	7/7	0.86	0.20	26,37,47,50	7
5	B3P	E	301[B]	19/19	0.86	0.22	23,34,46,49	19
8	PEG	A	305	7/7	0.87	0.17	33,35,43,52	7
10	PGE	C	305	10/10	0.87	0.21	43,47,56,56	10
8	PEG	B	314	7/7	0.87	0.19	36,53,64,68	0
5	B3P	A	301[A]	19/19	0.88	0.23	22,32,48,48	19
5	B3P	A	301[B]	19/19	0.88	0.23	25,33,48,48	19
8	PEG	E	313	7/7	0.89	0.17	39,41,45,50	7
8	PEG	F	314	7/7	0.89	0.18	25,30,41,43	7
4	PE3	A	300	21/43	0.89	0.17	35,41,63,66	0
7	CL	A	307	1/1	0.90	0.12	37,37,37,37	1
9	TLA	F	306	10/10	0.90	0.16	20,24,25,25	10
4	PE3	B	300	21/43	0.90	0.20	38,43,64,68	0
9	TLA	A	306	10/10	0.90	0.15	20,25,27,28	10
7	CL	C	307	1/1	0.91	0.10	33,33,33,33	1
5	B3P	F	301[B]	19/19	0.91	0.12	27,33,47,52	2
7	CL	E	307	1/1	0.91	0.11	37,37,37,37	1
5	B3P	F	301[A]	19/19	0.91	0.12	26,33,47,52	2
7	CL	C	303	1/1	0.91	0.17	37,37,37,37	1

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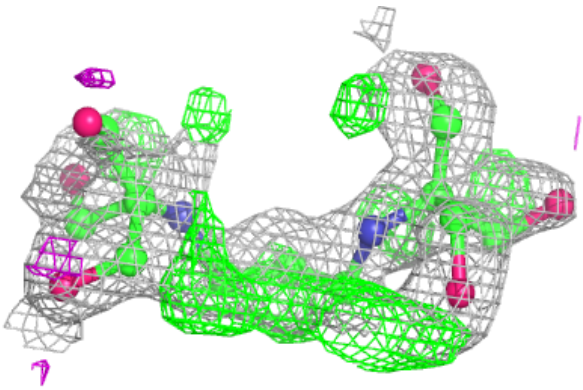
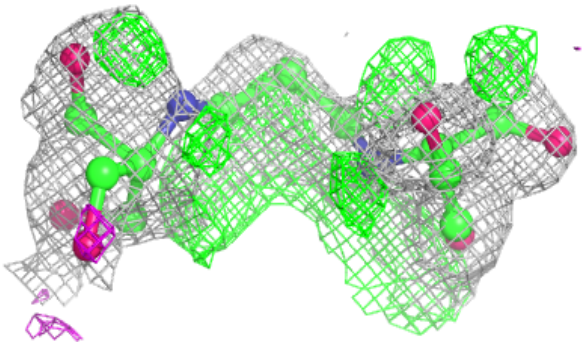
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PE3	F	300	21/43	0.92	0.15	33,40,62,67	0
7	CL	A	303	1/1	0.92	0.10	34,34,34,34	1
7	CL	F	308	1/1	0.94	0.11	25,25,25,25	1
6	SO4	A	302	5/5	0.95	0.17	37,41,46,51	5
6	SO4	D	302	5/5	0.95	0.13	71,73,74,79	0
6	SO4	F	302	5/5	0.96	0.14	50,51,52,57	5
7	CL	B	303	1/1	0.96	0.09	29,29,29,29	0
6	SO4	C	302	5/5	0.96	0.11	44,50,52,53	5
6	SO4	E	302	5/5	0.97	0.11	37,41,42,47	5
7	CL	B	304	1/1	0.97	0.11	31,31,31,31	1
6	SO4	B	302	5/5	0.97	0.12	43,46,49,52	5
3	AZM	F	299	13/13	0.98	0.10	17,25,44,45	0
3	AZM	B	299	13/13	0.98	0.10	17,29,54,56	0
7	CL	F	304	1/1	0.98	0.07	32,32,32,32	0
7	CL	B	308	1/1	0.98	0.08	30,30,30,30	1
3	AZM	D	299	13/13	0.98	0.07	18,29,36,36	0
3	AZM	E	299	13/13	0.98	0.07	18,27,37,41	0
7	CL	D	304	1/1	0.98	0.05	34,34,34,34	0
2	ZN	B	298	1/1	0.99	0.07	17,17,17,17	0
3	AZM	C	299	13/13	0.99	0.08	17,27,36,41	0
7	CL	A	304	1/1	0.99	0.16	24,24,24,24	1
7	CL	E	304	1/1	0.99	0.05	34,34,34,34	0
3	AZM	A	299	13/13	0.99	0.10	21,28,42,43	0
7	CL	C	304	1/1	0.99	0.07	34,34,34,34	0
2	ZN	A	298	1/1	1.00	0.07	19,19,19,19	0
2	ZN	C	298	1/1	1.00	0.07	20,20,20,20	0
2	ZN	D	298	1/1	1.00	0.07	20,20,20,20	0
2	ZN	E	298	1/1	1.00	0.08	18,18,18,18	0
2	ZN	F	298	1/1	1.00	0.07	17,17,17,17	0

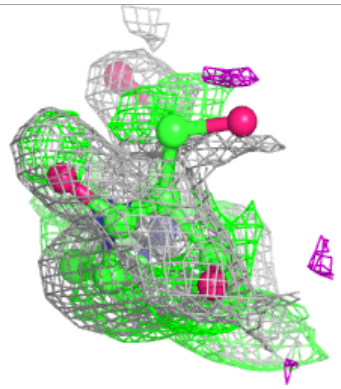
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P C 301:

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

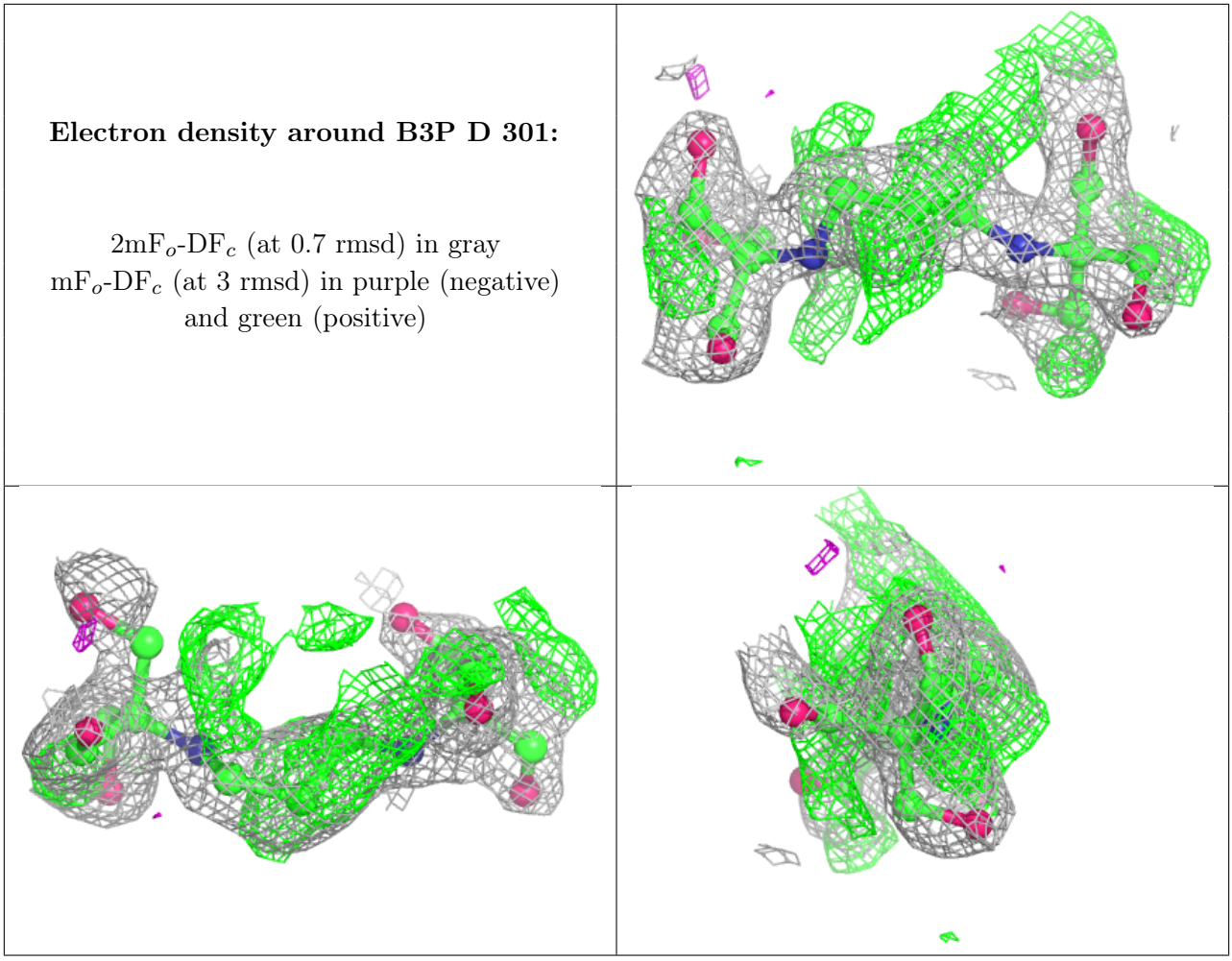






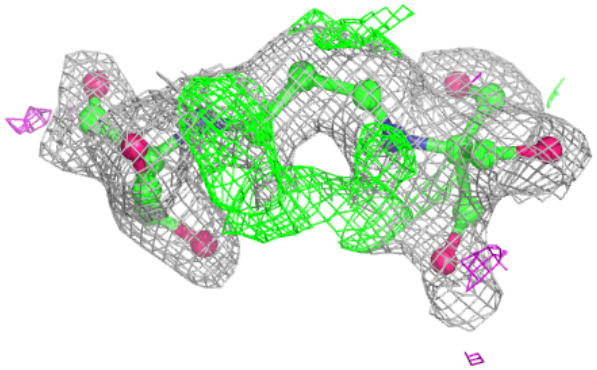
Electron density around B3P D 301:

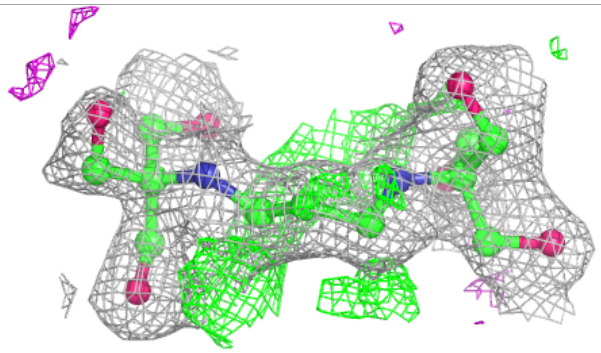
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

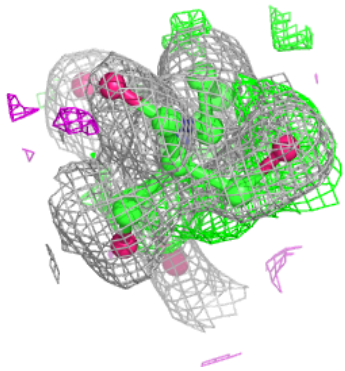


Electron density around B3P E 301 (A):

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

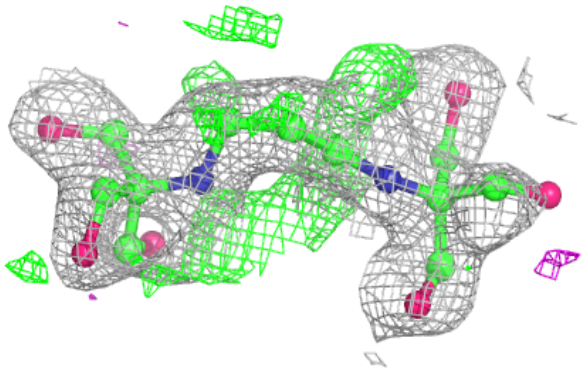


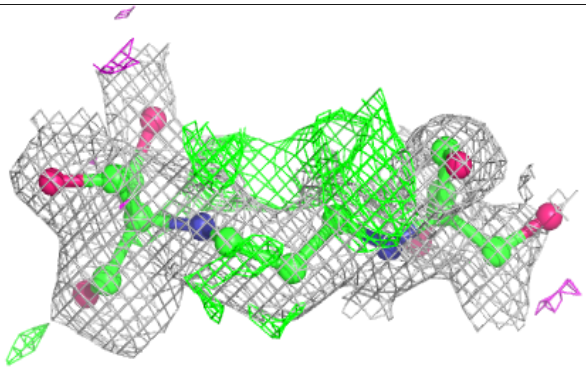


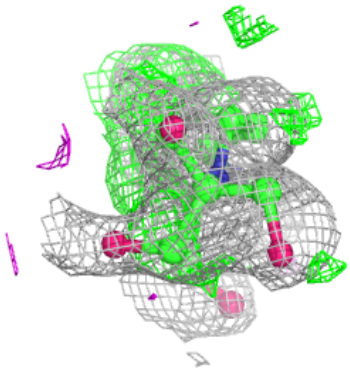


Electron density around B3P E 301 (B):

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

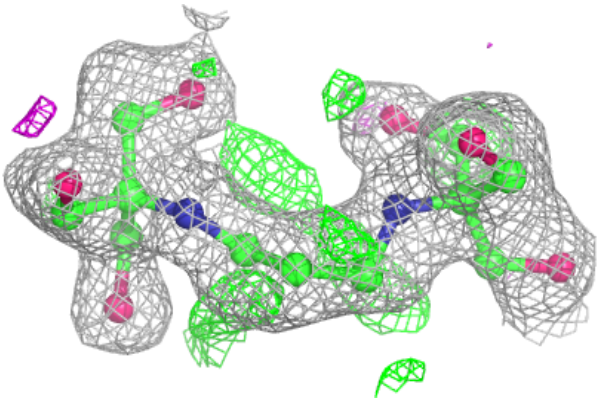


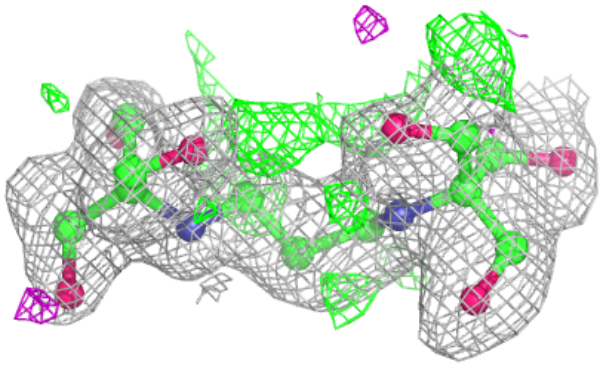


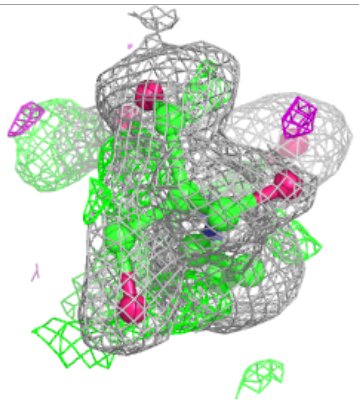


Electron density around B3P A 301 (A):

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

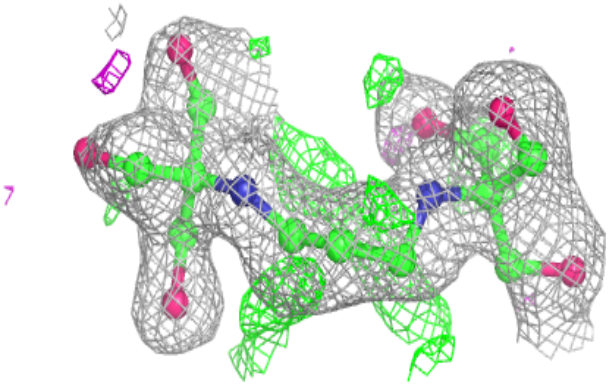


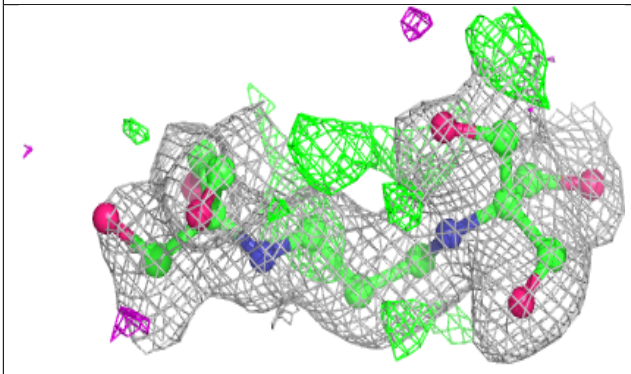


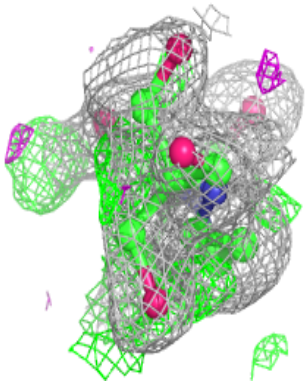


Electron density around B3P A 301 (B):

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

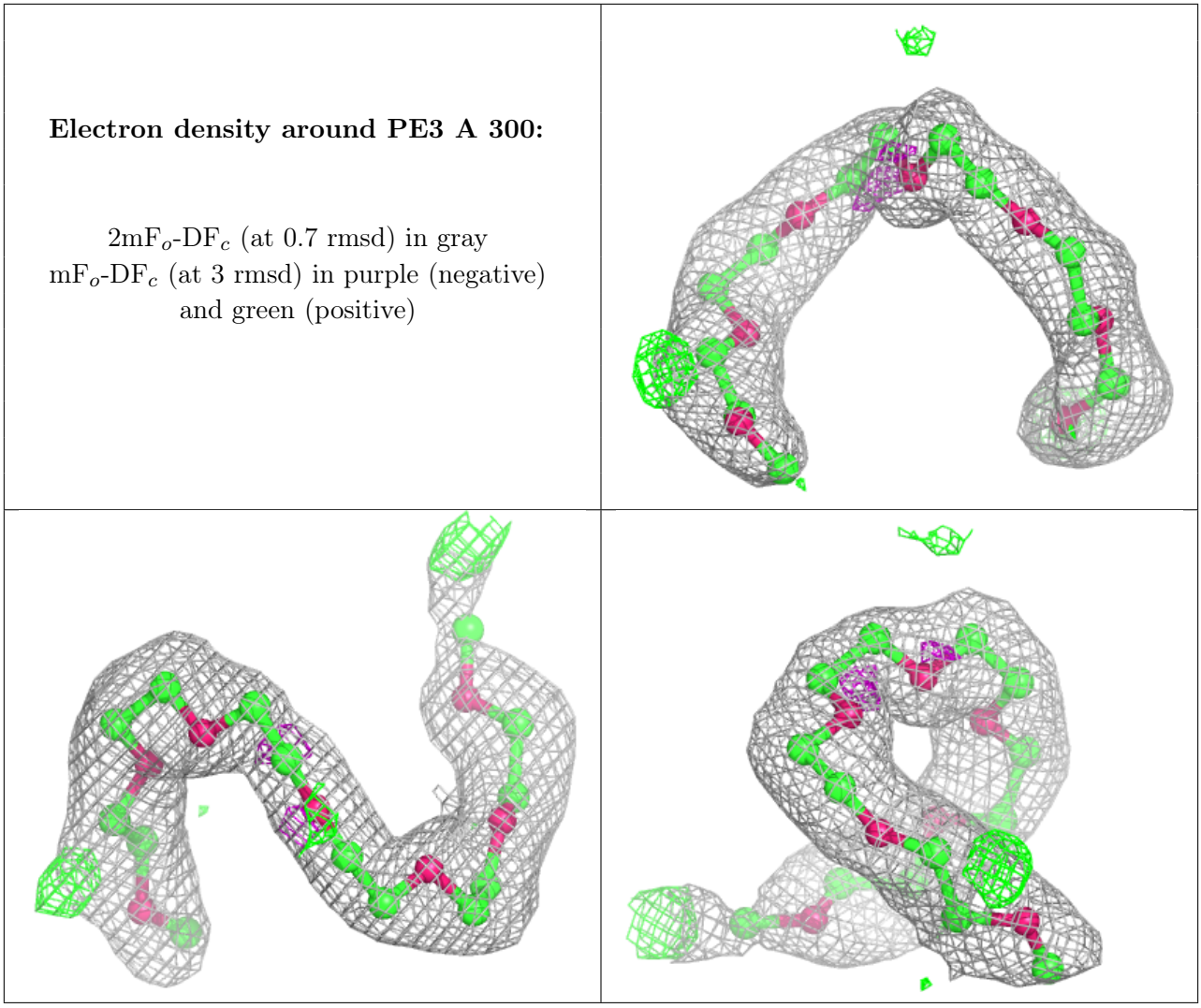






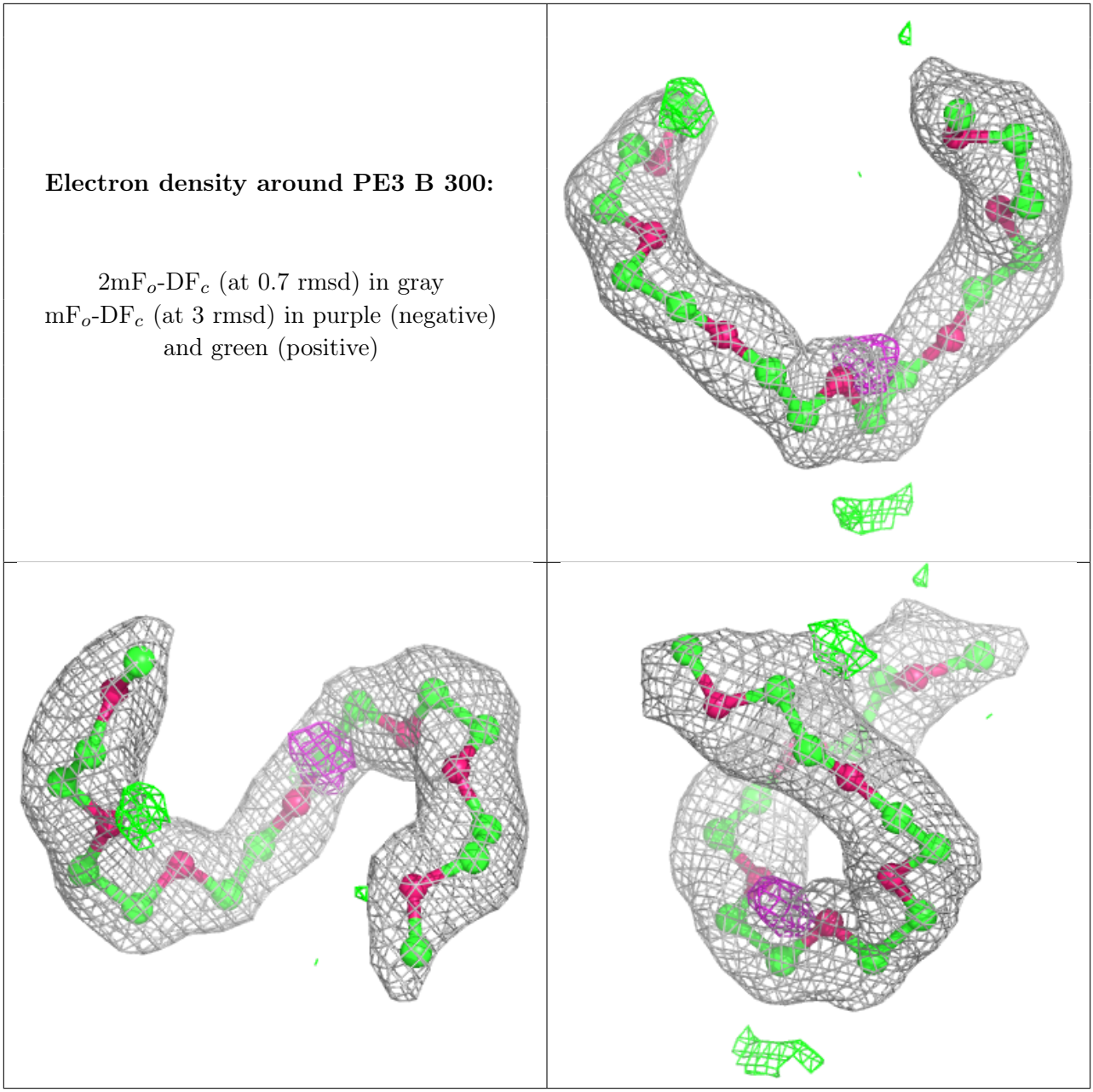
Electron density around PE3 A 300:

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



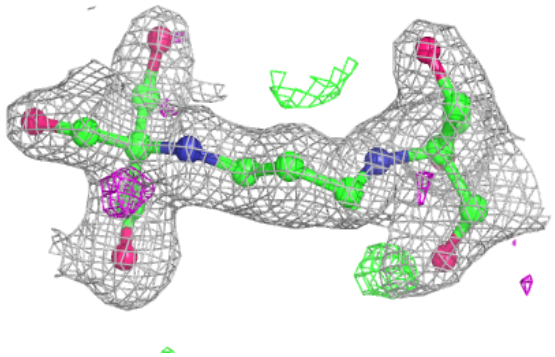
Electron density around PE3 B 300:

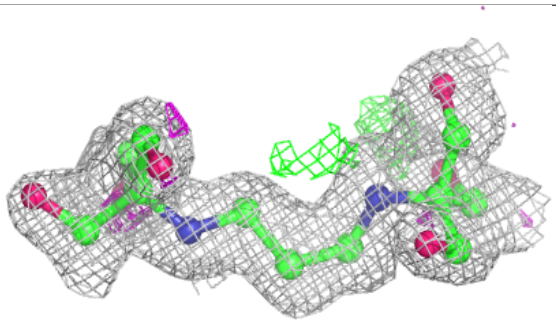
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

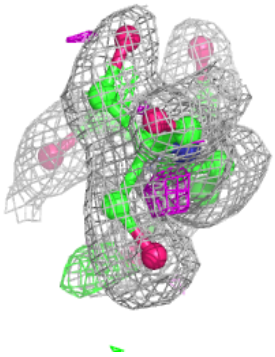


Electron density around B3P F 301 (B):

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

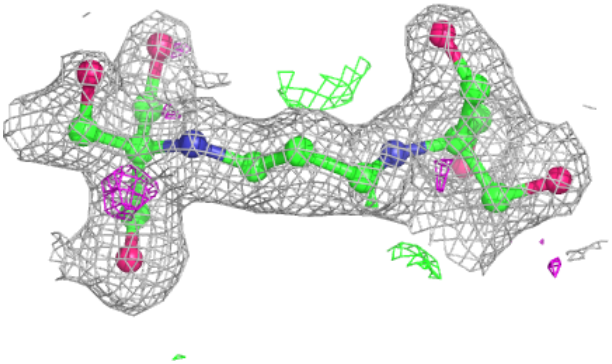


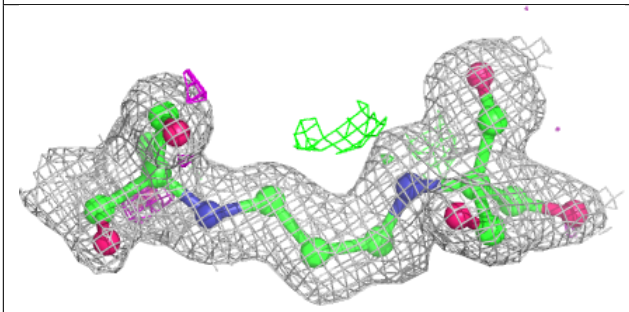


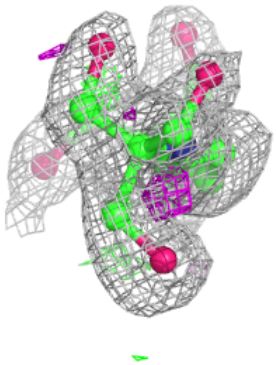


Electron density around B3P F 301 (A):

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

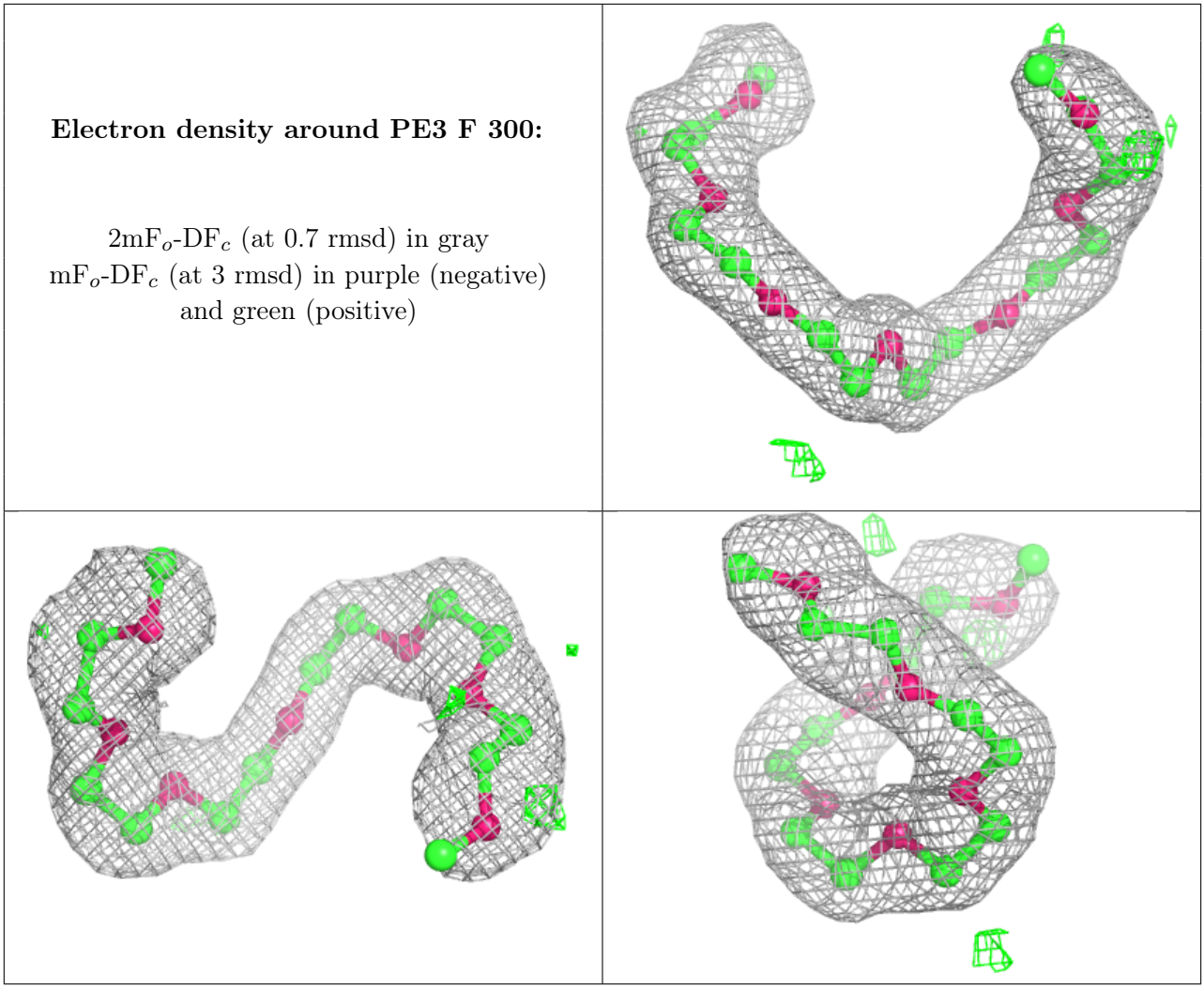






Electron density around PE3 F 300:

$2mF_o$-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.