



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:55 AM UTC

PDB ID : 2EJ2 / pdb_00002ej2
Title : Crystal Structure of T.th.HB8 Branched-Chain Amino Acid Aminotransferase
Complexed with N-(5'-Phosphopyridoxyl)-L-Glutamate
Authors : Goto, M.
Deposited on : 2007-03-14
Resolution : 2.00 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:

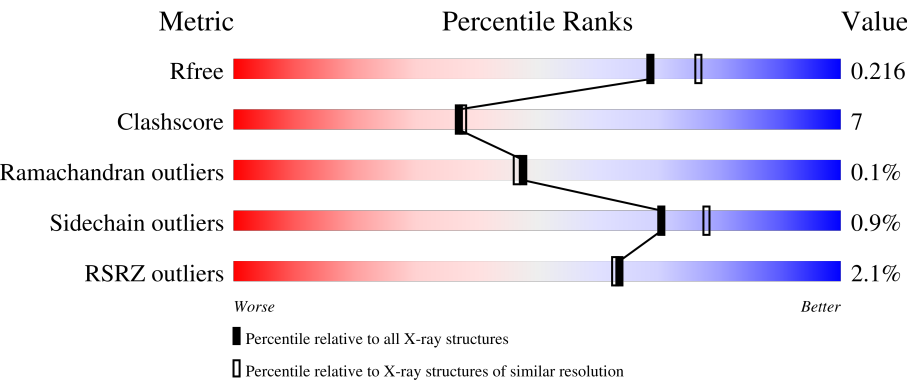
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	308	% 78%16%. 5%
1	B	308	3% 83%15%..
1	C	308	2% 81%14%.
1	D	308	2% 83%15%.
1	E	308	2% 80%17%..

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Mol	Chain	Length	Quality of chain
1	F	308	2% 78% 18% ••

2 Entry composition [i](#)

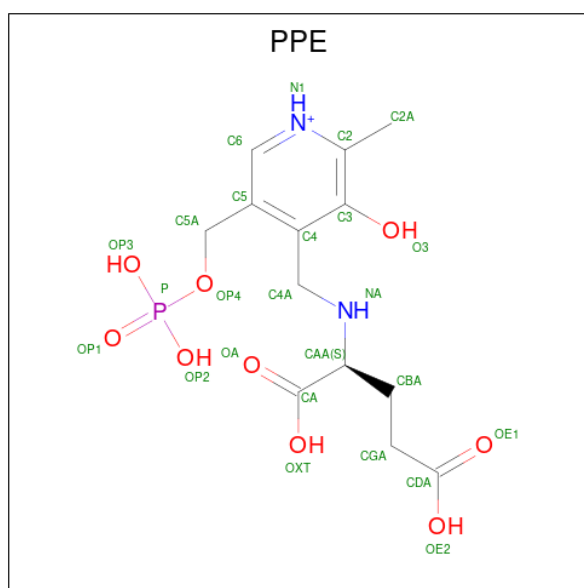
There are 4 unique types of molecules in this entry. The entry contains 15270 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Branched-chain amino acid aminotransferase.

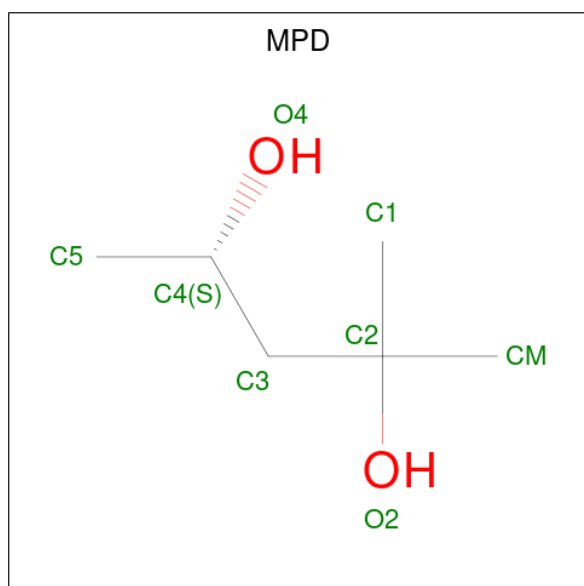
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2282	1460	397	415	10			
1	B	305	Total	C	N	O	S	0	0	0
			2369	1514	412	433	10			
1	C	297	Total	C	N	O	S	0	0	0
			2299	1470	399	420	10			
1	D	301	Total	C	N	O	S	0	0	0
			2326	1489	405	422	10			
1	E	298	Total	C	N	O	S	0	0	0
			2288	1464	396	418	10			
1	F	298	Total	C	N	O	S	0	0	0
			2304	1474	401	419	10			

- Molecule 2 is 4-[(1,3-DICARBOXY-PROPYLAMINO)-METHYL]-3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDINIUM (CCD ID: PPE) (formula: $C_{13}H_{20}N_2O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	C	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	D	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	E	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	F	1	Total	C	N	O	P	0	0
			25	13	2	9	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	208	Total	O	0	0
			208	208		
4	B	205	Total	O	0	0
			205	205		

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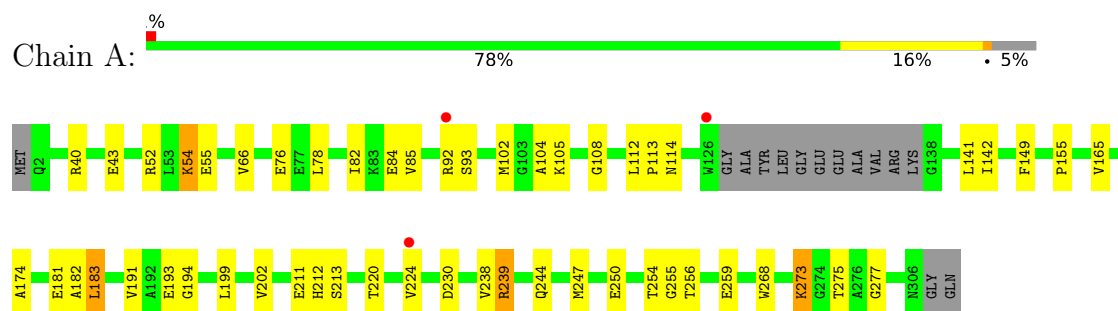
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	207	Total 207	O 207	0	0
4	D	213	Total 213	O 213	0	0
4	E	190	Total 190	O 190	0	0
4	F	213	Total 213	O 213	0	0

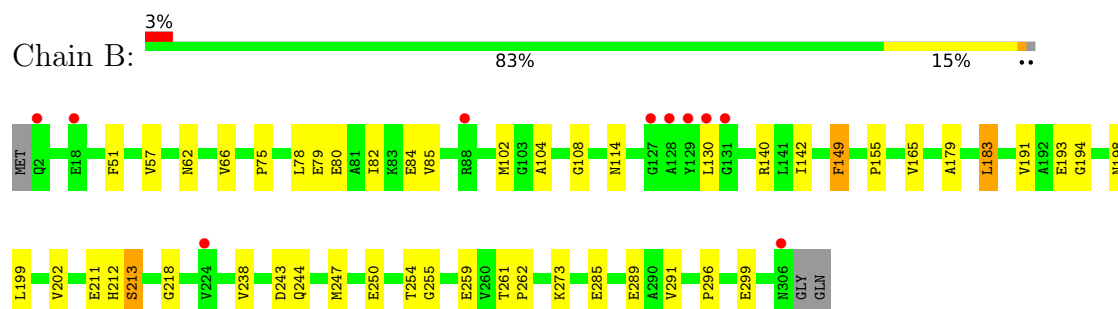
3 Residue-property plots [i](#)

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.

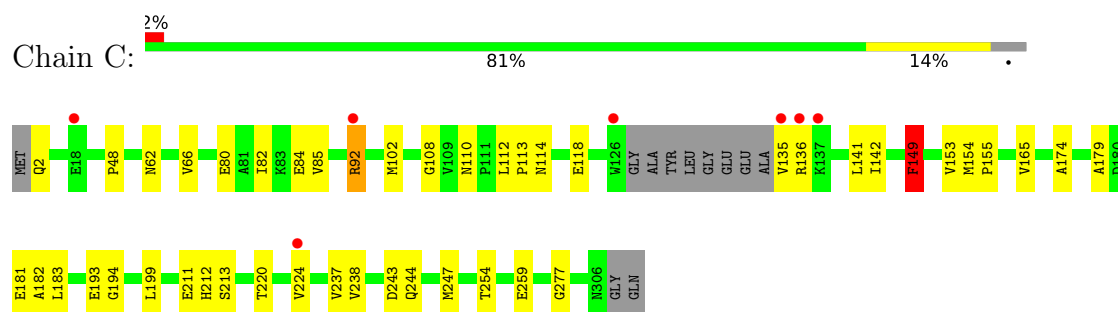
- Molecule 1: Branched-chain amino acid aminotransferase



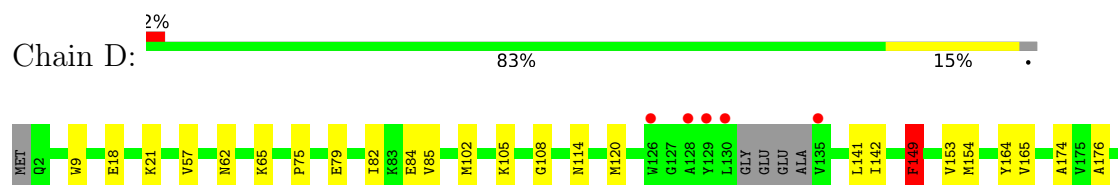
- Molecule 1: Branched-chain amino acid aminotransferase



- Molecule 1: Branched-chain amino acid aminotransferase

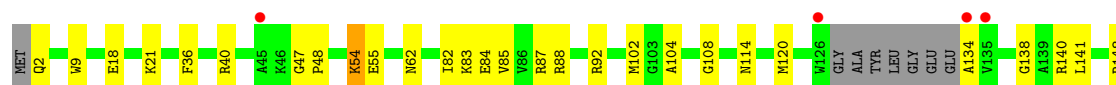
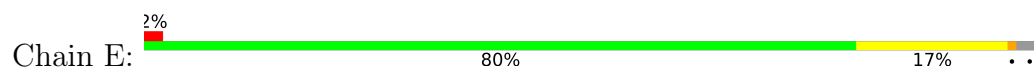


- Molecule 1: Branched-chain amino acid aminotransferase

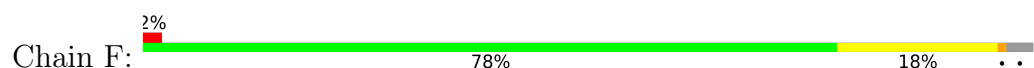




- Molecule 1: Branched-chain amino acid aminotransferase



- Molecule 1: Branched-chain amino acid aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.02Å 144.22Å 147.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.00 19.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.97-2.00) 96.8 (19.97-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.216 0.190 , 0.216	Depositor DCC
R_{free} test set	16164 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15270	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MPD, PPE

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	0.35	0/2334	0.88	6/3169 (0.2%)
1	B	0.35	0/2423	0.89	5/3289 (0.2%)
1	C	0.35	0/2351	0.90	8/3194 (0.3%)
1	D	0.36	0/2379	0.89	5/3232 (0.2%)
1	E	0.36	0/2340	0.90	9/3181 (0.3%)
1	F	0.35	0/2356	0.90	7/3200 (0.2%)
All	All	0.35	0/14183	0.89	40/19265 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	GLY	N-CA-C	-8.51	101.17	112.14
1	F	108	GLY	N-CA-C	-8.15	100.96	112.37
1	C	108	GLY	N-CA-C	-8.14	100.97	112.37
1	E	165	VAL	N-CA-C	-7.99	102.66	110.72
1	A	108	GLY	N-CA-C	-7.95	101.24	112.37
1	E	108	GLY	N-CA-C	-7.89	101.32	112.37
1	B	165	VAL	N-CA-C	-7.83	102.81	110.72
1	F	165	VAL	N-CA-C	-7.61	103.04	110.72
1	C	165	VAL	N-CA-C	-7.25	103.40	110.72
1	A	165	VAL	N-CA-C	-7.25	103.40	110.72
1	D	108	GLY	N-CA-C	-7.16	102.34	112.37
1	D	165	VAL	N-CA-C	-6.98	103.67	110.72
1	D	149	PHE	N-CA-C	6.59	118.97	109.48
1	B	244	GLN	N-CA-C	-6.45	104.34	111.82
1	E	149	PHE	N-CA-C	6.22	117.55	109.64
1	F	244	GLN	N-CA-C	-6.07	104.78	111.82
1	D	244	GLN	N-CA-C	-6.05	104.80	111.82
1	C	244	GLN	N-CA-C	-5.94	104.74	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	149	PHE	N-CA-C	5.93	117.17	109.64
1	B	149	PHE	N-CA-C	5.85	117.91	109.48
1	A	244	GLN	N-CA-C	-5.83	105.06	111.82
1	C	149	PHE	N-CA-C	5.69	117.67	109.48
1	E	239	ARG	N-CA-C	-5.65	100.50	109.76
1	A	149	PHE	N-CA-C	5.61	116.77	109.64
1	E	244	GLN	N-CA-C	-5.57	105.29	111.36
1	E	218	GLY	N-CA-C	5.43	117.72	111.36
1	F	31	TYR	N-CA-C	5.34	119.36	112.41
1	A	239	ARG	N-CA-C	-5.33	101.03	109.76
1	C	118	GLU	N-CA-C	-5.32	101.86	110.32
1	C	277	GLY	CA-C-N	5.28	124.91	119.05
1	C	277	GLY	C-N-CA	5.28	124.91	119.05
1	B	104	ALA	N-CA-C	5.28	118.53	112.57
1	F	104	ALA	N-CA-C	5.25	118.51	112.57
1	E	104	ALA	N-CA-C	5.17	118.41	112.57
1	C	92	ARG	N-CA-C	-5.17	103.64	111.34
1	D	164	TYR	N-CA-C	5.16	119.33	113.19
1	A	104	ALA	N-CA-C	5.11	118.38	112.97
1	E	47	GLY	CA-C-N	5.09	125.00	119.76
1	E	47	GLY	C-N-CA	5.09	125.00	119.76
1	F	164	TYR	N-CA-C	5.00	119.14	113.19

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	2282	0	2264	39	0
1	B	2369	0	2352	29	0
1	C	2299	0	2270	30	0
1	D	2326	0	2299	27	0
1	E	2288	0	2247	35	0
1	F	2304	0	2282	41	0
2	A	25	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	25	0	15	0	0
2	C	25	0	15	0	0
2	D	25	0	15	0	0
2	E	25	0	15	0	0
2	F	25	0	15	0	0
3	A	8	0	14	1	0
3	F	8	0	14	2	0
4	A	208	0	0	2	0
4	B	205	0	0	1	0
4	C	207	0	0	2	0
4	D	213	0	0	5	0
4	E	190	0	0	1	0
4	F	213	0	0	5	0
All	All	15270	0	13832	197	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 7.

All (197) 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:A:183:LEU:HD11	1:A:191:VAL:HG13	1.57	0.85
1:E:220:THR:O	1:E:224:VAL:HG23	1.84	0.77
1:A:52:ARG:HA	1:A:54:LYS:HE2	1.65	0.77
1:B:183:LEU:HD11	1:B:191:VAL:HG13	1.66	0.76
1:B:183:LEU:HD13	1:B:199:LEU:HD11	1.69	0.74
1:A:54:LYS:HD3	1:A:54:LYS:H	1.53	0.74
1:A:183:LEU:HD13	1:A:199:LEU:HD11	1.70	0.72
1:F:220:THR:O	1:F:224:VAL:HG23	1.92	0.69
1:A:220:THR:O	1:A:224:VAL:HG23	1.93	0.68
1:A:54:LYS:HD3	1:A:54:LYS:N	2.10	0.66
1:D:82:ILE:O	1:D:85:VAL:HG12	1.96	0.65
1:B:102:MET:HE3	1:B:114:ASN:HB2	1.79	0.65
1:D:84:GLU:HG2	4:D:2037:HOH:O	1.96	0.65
1:F:54:LYS:HD3	1:F:55:GLU:H	1.61	0.64
1:E:247:MET:HE3	1:F:62:ASN:HB3	1.80	0.64
1:E:141:LEU:HD22	1:E:181:GLU:HB3	1.78	0.64
1:A:82:ILE:O	1:A:85:VAL:HG12	1.97	0.64
1:F:54:LYS:NZ	1:F:55:GLU:HG2	2.12	0.64
1:E:82:ILE:O	1:E:85:VAL:HG12	1.98	0.63
1:C:102:MET:HE3	1:C:114:ASN:HB2	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:GLU:O	1:B:289:GLU:HG3	1.97	0.63
1:C:220:THR:O	1:C:224:VAL:HG23	1.99	0.63
1:C:193:GLU:HA	1:C:199:LEU:HD23	1.81	0.63
1:C:82:ILE:O	1:C:85:VAL:HG12	1.99	0.62
1:C:80:GLU:O	1:C:84:GLU:HG3	2.00	0.62
1:B:243:ASP:O	1:B:247:MET:HG2	2.00	0.62
1:A:52:ARG:CA	1:A:54:LYS:HE2	2.30	0.62
1:C:224:VAL:HG21	1:C:254:THR:HG21	1.82	0.61
1:D:57:VAL:HG21	1:D:79:GLU:HG2	1.83	0.61
1:F:82:ILE:O	1:F:85:VAL:HG12	2.01	0.61
1:E:54:LYS:N	1:E:54:LYS:HD3	2.17	0.60
1:F:52:ARG:HA	1:F:54:LYS:HE3	1.82	0.60
1:A:183:LEU:HD13	1:A:199:LEU:CD1	2.30	0.60
1:D:285:GLU:O	1:D:289:GLU:HG3	2.02	0.60
1:A:43:GLU:HG2	1:A:92:ARG:HB3	1.82	0.60
1:B:82:ILE:O	1:B:85:VAL:HG12	2.01	0.60
1:D:102:MET:HE3	1:D:114:ASN:HB2	1.84	0.59
1:B:80:GLU:O	1:B:84:GLU:HG3	2.01	0.59
1:B:183:LEU:HD13	1:B:199:LEU:CD1	2.33	0.59
1:F:54:LYS:HZ3	1:F:55:GLU:HG2	1.67	0.59
1:D:174:ALA:HB2	1:D:182:ALA:HB2	1.84	0.58
1:F:88:ARG:HH11	1:F:88:ARG:HG3	1.67	0.58
1:A:141:LEU:CD2	1:A:181:GLU:HB3	2.34	0.58
1:D:75:PRO:O	1:D:79:GLU:HG3	2.03	0.58
1:C:141:LEU:HD22	1:C:181:GLU:HB3	1.86	0.58
1:F:40:ARG:HG3	1:F:256:THR:CG2	2.34	0.57
1:A:43:GLU:HG3	1:A:93:SER:OG	2.06	0.56
1:E:54:LYS:HD3	1:E:54:LYS:H	1.69	0.56
3:F:2914:MPD:H53	4:F:2975:HOH:O	2.05	0.56
1:E:224:VAL:HG21	1:E:254:THR:HG21	1.86	0.56
1:A:54:LYS:HE3	1:A:55:GLU:HG2	1.88	0.55
1:E:102:MET:HE3	1:E:114:ASN:HB2	1.87	0.55
1:B:273:LYS:HG2	4:B:3964:HOH:O	2.07	0.55
1:B:57:VAL:HG21	1:B:79:GLU:HG2	1.89	0.54
1:C:141:LEU:CD2	1:C:181:GLU:HB3	2.37	0.54
1:D:220:THR:O	1:D:224:VAL:HG23	2.07	0.54
1:C:135:VAL:HG13	1:C:136:ARG:H	1.73	0.54
1:C:135:VAL:HG13	1:C:136:ARG:N	2.23	0.53
1:E:247:MET:HE3	1:F:62:ASN:CB	2.38	0.53
1:A:112:LEU:HB2	1:A:113:PRO:HD3	1.91	0.53
1:A:66:VAL:HG11	1:A:155:PRO:CB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:ALA:HB2	1:F:182:ALA:HB2	1.91	0.52
4:D:1924:HOH:O	1:F:247:MET:HE1	2.09	0.52
1:F:2:GLN:HG2	1:F:3:ILE:N	2.25	0.52
1:C:110:ASN:OD1	1:F:172:MET:HG2	2.10	0.52
1:D:211:GLU:HG3	1:D:238:VAL:C	2.34	0.52
1:A:102:MET:HE3	1:A:114:ASN:HB2	1.92	0.52
1:F:43:GLU:OE2	1:F:92:ARG:NE	2.33	0.51
1:C:174:ALA:HB2	1:C:182:ALA:HB2	1.92	0.51
1:C:211:GLU:HG3	1:C:238:VAL:C	2.35	0.51
1:F:40:ARG:HG3	1:F:256:THR:HG22	1.91	0.51
1:F:66:VAL:HG11	1:F:155:PRO:CB	2.41	0.51
1:A:193:GLU:HG3	1:A:194:GLY:O	2.11	0.51
1:A:54:LYS:HG2	1:A:55:GLU:N	2.26	0.51
1:A:40:ARG:HG3	1:A:256:THR:HG22	1.92	0.51
1:B:51:PHE:CD1	1:B:291:VAL:HG12	2.46	0.51
1:F:126:TRP:HH2	1:F:257:ALA:HB1	1.76	0.51
1:D:105:LYS:HE3	4:D:2029:HOH:O	2.10	0.50
1:A:76:GLU:H	1:A:76:GLU:CD	2.19	0.50
1:F:141:LEU:CD2	1:F:181:GLU:HB3	2.42	0.50
1:B:202:VAL:HB	1:B:250:GLU:HB2	1.92	0.50
1:D:141:LEU:CD2	1:D:181:GLU:HB3	2.42	0.49
1:E:181:GLU:HG3	1:E:182:ALA:N	2.27	0.49
1:C:48:PRO:HG3	1:C:92:ARG:HA	1.93	0.49
1:E:141:LEU:CD2	1:E:181:GLU:HB3	2.42	0.49
1:B:211:GLU:HG3	1:B:238:VAL:C	2.37	0.48
1:A:211:GLU:HG3	1:A:238:VAL:C	2.39	0.48
1:E:54:LYS:H	1:E:54:LYS:CD	2.26	0.48
1:F:254:THR:HA	1:F:259:GLU:O	2.14	0.48
1:F:183:LEU:C	1:F:183:LEU:HD23	2.39	0.48
1:E:54:LYS:NZ	1:E:55:GLU:HG2	2.29	0.48
1:B:130:LEU:HD12	1:B:130:LEU:N	2.28	0.48
1:C:183:LEU:C	1:C:183:LEU:HD23	2.39	0.48
1:F:224:VAL:HG21	1:F:254:THR:HG21	1.96	0.47
1:C:2:GLN:HG3	4:F:3032:HOH:O	2.14	0.47
1:C:224:VAL:HG21	1:C:254:THR:CG2	2.43	0.47
1:F:87:ARG:HG3	1:F:305:VAL:CG1	2.44	0.47
1:B:102:MET:HE3	1:B:114:ASN:CB	2.45	0.47
1:E:140:ARG:HH11	1:E:140:ARG:HG3	1.78	0.47
1:A:224:VAL:HG21	1:A:254:THR:HG21	1.96	0.47
1:A:84:GLU:HG2	4:A:3538:HOH:O	2.15	0.47
1:B:254:THR:HA	1:B:259:GLU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:GLU:CD	1:D:277:GLY:HA3	2.40	0.46
1:D:105:LYS:HG3	4:D:1993:HOH:O	2.15	0.46
1:C:254:THR:HA	1:C:259:GLU:O	2.15	0.46
1:D:183:LEU:C	1:D:183:LEU:HD23	2.41	0.46
1:A:254:THR:HA	1:A:259:GLU:O	2.17	0.45
1:D:226:ARG:HD3	1:D:301:TRP:CZ2	2.51	0.45
1:B:78:LEU:O	1:B:82:ILE:HG13	2.16	0.45
1:B:212:HIS:O	1:B:213:SER:C	2.59	0.45
1:F:273:LYS:HG2	4:F:3046:HOH:O	2.17	0.45
1:A:230:ASP:HB3	3:A:1415:MPD:H53	1.99	0.45
1:A:268:TRP:CD1	1:D:176:ALA:HB1	2.51	0.45
1:C:84:GLU:HG2	4:C:1555:HOH:O	2.16	0.45
1:D:102:MET:HE3	1:D:114:ASN:CB	2.47	0.45
1:F:226:ARG:HD3	1:F:301:TRP:CZ2	2.51	0.45
1:A:105:LYS:HE3	4:A:3550:HOH:O	2.17	0.44
1:D:153:VAL:HG12	1:D:154:MET:HG2	1.99	0.44
1:F:9:TRP:O	1:F:120:MET:HA	2.17	0.44
1:A:239:ARG:HG3	4:C:1497:HOH:O	2.16	0.44
1:C:112:LEU:HB2	1:C:113:PRO:HD3	2.00	0.44
1:D:18:GLU:O	1:D:21:LYS:HE2	2.17	0.44
1:E:153:VAL:HG12	1:E:154:MET:HG2	1.98	0.44
1:F:112:LEU:HB2	1:F:113:PRO:HD3	1.99	0.44
1:A:247:MET:HE3	1:B:62:ASN:HB3	1.98	0.44
1:C:62:ASN:HD22	1:C:62:ASN:HA	1.64	0.44
1:E:197:GLU:HB2	1:E:254:THR:O	2.17	0.44
1:F:84:GLU:OE1	1:F:88:ARG:NH1	2.51	0.44
1:A:52:ARG:CB	1:A:54:LYS:HE2	2.48	0.44
1:C:66:VAL:HG11	1:C:155:PRO:CB	2.48	0.44
1:E:212:HIS:O	1:E:213:SER:C	2.61	0.43
1:E:224:VAL:HG21	1:E:254:THR:CG2	2.48	0.43
1:E:18:GLU:O	1:E:21:LYS:HE2	2.18	0.43
1:E:48:PRO:HG3	1:E:92:ARG:HA	2.00	0.43
1:A:202:VAL:HB	1:A:250:GLU:HB2	2.00	0.43
1:D:149:PHE:CG	1:D:154:MET:HB2	2.54	0.43
1:B:62:ASN:HD22	1:B:62:ASN:HA	1.66	0.43
1:E:40:ARG:HG3	1:E:256:THR:HG22	1.99	0.43
1:C:211:GLU:HG2	1:C:237:VAL:HG12	2.01	0.43
1:C:153:VAL:HG12	1:C:154:MET:HG2	1.99	0.43
1:E:183:LEU:C	1:E:183:LEU:HD23	2.43	0.43
1:D:212:HIS:O	1:D:213:SER:C	2.60	0.43
1:F:54:LYS:CD	1:F:54:LYS:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LYS:HG3	1:A:275:THR:H	1.84	0.43
1:E:148:ARG:HD2	1:E:148:ARG:HA	1.89	0.43
1:E:134:ALA:O	1:E:138:GLY:N	2.51	0.42
1:F:190:TYR:CD2	1:F:239:ARG:HG2	2.55	0.42
1:F:230:ASP:HB3	3:F:2914:MPD:H51	2.01	0.42
1:A:250:GLU:CD	1:A:277:GLY:HA3	2.45	0.42
1:F:82:ILE:HG23	1:F:96:ILE:HG21	2.01	0.42
1:C:193:GLU:HG3	1:C:194:GLY:O	2.20	0.42
1:E:9:TRP:O	1:E:120:MET:HA	2.20	0.42
1:E:83:LYS:O	1:E:87:ARG:HG2	2.18	0.42
1:C:102:MET:HE3	1:C:114:ASN:CB	2.47	0.42
1:D:62:ASN:HD22	1:D:62:ASN:HA	1.64	0.42
1:F:125:GLU:HG2	4:F:2984:HOH:O	2.19	0.42
1:F:142:ILE:HG13	1:F:179:ALA:HB2	2.02	0.42
1:B:193:GLU:HG3	1:B:194:GLY:O	2.19	0.42
1:D:198:ASN:OD1	1:D:218:GLY:HA3	2.20	0.42
1:E:211:GLU:HG3	1:E:238:VAL:C	2.44	0.42
1:D:142:ILE:HG13	1:D:179:ALA:HB2	2.02	0.42
1:A:212:HIS:O	1:A:213:SER:C	2.62	0.42
1:D:9:TRP:O	1:D:120:MET:HA	2.20	0.42
1:A:142:ILE:HD11	1:A:268:TRP:CZ2	2.55	0.42
1:E:84:GLU:O	1:E:88:ARG:HG3	2.20	0.42
1:B:66:VAL:HG11	1:B:155:PRO:CB	2.50	0.42
1:E:254:THR:HA	1:E:259:GLU:O	2.20	0.42
1:F:198:ASN:C	1:F:199:LEU:HD22	2.45	0.42
1:D:65:LYS:NZ	4:D:2060:HOH:O	2.52	0.41
1:A:255:GLY:O	1:A:259:GLU:N	2.51	0.41
1:E:174:ALA:HB2	1:E:182:ALA:HB2	2.01	0.41
1:F:54:LYS:HD2	1:F:54:LYS:H	1.85	0.41
1:B:255:GLY:O	1:B:259:GLU:N	2.51	0.41
1:F:54:LYS:CD	1:F:54:LYS:H	2.34	0.41
1:F:141:LEU:HD22	1:F:181:GLU:HB3	2.01	0.41
1:C:149:PHE:CG	1:C:154:MET:HB2	2.56	0.41
1:E:2:GLN:N	4:E:2597:HOH:O	2.54	0.41
1:A:174:ALA:HB2	1:A:182:ALA:HB2	2.02	0.41
1:B:75:PRO:O	1:B:79:GLU:HG3	2.20	0.41
1:B:142:ILE:HG13	1:B:179:ALA:HB2	2.01	0.41
1:B:296:PRO:HA	1:B:299:GLU:HG2	2.01	0.41
1:D:254:THR:HA	1:D:259:GLU:O	2.19	0.41
1:E:36:PHE:CE1	1:E:159:LYS:HE2	2.56	0.41
1:E:62:ASN:HD22	1:E:62:ASN:HA	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:GLU:HB2	1:F:254:THR:O	2.21	0.41
1:B:140:ARG:HG3	1:B:140:ARG:HH11	1.86	0.41
1:C:212:HIS:O	1:C:213:SER:C	2.63	0.41
1:C:142:ILE:HG13	1:C:179:ALA:HB2	2.03	0.40
1:A:224:VAL:HG21	1:A:254:THR:CG2	2.50	0.40
1:B:261:THR:HA	1:B:262:PRO:HD3	1.96	0.40
1:A:40:ARG:HG3	1:A:256:THR:CG2	2.52	0.40
1:E:54:LYS:N	1:E:54:LYS:CD	2.83	0.40
1:E:285:GLU:OE1	1:E:289:GLU:OE2	2.39	0.40
1:B:198:ASN:OD1	1:B:218:GLY:HA3	2.21	0.40
1:C:243:ASP:O	1:C:247:MET:HG3	2.22	0.40
1:F:105:LYS:HE3	4:F:3024:HOH:O	2.20	0.40
1:F:250:GLU:CD	1:F:277:GLY:HA3	2.47	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	290/308 (94%)	281 (97%)	9 (3%)	0	100	100
1	B	303/308 (98%)	295 (97%)	7 (2%)	1 (0%)	36	35
1	C	293/308 (95%)	284 (97%)	9 (3%)	0	100	100
1	D	297/308 (96%)	289 (97%)	8 (3%)	0	100	100
1	E	294/308 (96%)	283 (96%)	11 (4%)	0	100	100
1	F	294/308 (96%)	286 (97%)	8 (3%)	0	100	100
All	All	1771/1848 (96%)	1718 (97%)	52 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	213	SER

5.3.2 Protein sidechains ⓘ

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	229/241 (95%)	225 (98%)	4 (2%)	53	60
1	B	237/241 (98%)	235 (99%)	2 (1%)	73	80
1	C	230/241 (95%)	229 (100%)	1 (0%)	84	89
1	D	231/241 (96%)	230 (100%)	1 (0%)	84	89
1	E	226/241 (94%)	224 (99%)	2 (1%)	70	78
1	F	230/241 (95%)	228 (99%)	2 (1%)	70	78
All	All	1383/1446 (96%)	1371 (99%)	12 (1%)	70	78

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	78	LEU
1	A	183	LEU
1	A	273	LYS
1	B	149	PHE
1	B	183	LEU
1	C	149	PHE
1	D	149	PHE
1	E	54	LYS
1	E	197	GLU
1	F	54	LYS
1	F	197	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN

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Mol	Chain	Res	Type
1	A	306	ASN
1	B	62	ASN
1	C	62	ASN
1	D	62	ASN
1	E	62	ASN
1	E	236	GLN
1	E	306	ASN
1	F	62	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PPE	F	2913	-	23,25,25	2.69	11 (47%)	24,35,35	2.48	10 (41%)
2	PPE	D	1913	-	23,25,25	2.55	8 (34%)	24,35,35	2.45	11 (45%)
2	PPE	B	3913	-	23,25,25	2.52	8 (34%)	24,35,35	2.40	9 (37%)
2	PPE	C	1413	-	23,25,25	2.68	8 (34%)	24,35,35	2.40	10 (41%)
3	MPD	A	1415	-	7,7,7	0.79	0	9,10,10	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PPE	A	3413	-	23,25,25	2.64	7 (30%)	24,35,35	2.42	10 (41%)
2	PPE	E	2413	-	23,25,25	2.75	9 (39%)	24,35,35	2.47	10 (41%)
3	MPD	F	2914	-	7,7,7	0.80	0	9,10,10	0.94	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
2	PPE	F	2913	-	-	3/17/20/20	0/1/1/1
2	PPE	D	1913	-	-	3/17/20/20	0/1/1/1
2	PPE	B	3913	-	-	3/17/20/20	0/1/1/1
2	PPE	C	1413	-	-	5/17/20/20	0/1/1/1
3	MPD	A	1415	-	-	3/5/5/5	-
2	PPE	A	3413	-	-	3/17/20/20	0/1/1/1
2	PPE	E	2413	-	-	4/17/20/20	0/1/1/1
3	MPD	F	2914	-	-	2/5/5/5	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1413	PPE	OP4-C5A	-6.56	1.36	1.43
2	A	3413	PPE	OP4-C5A	-6.31	1.37	1.43
2	E	2413	PPE	OP4-C5A	-5.74	1.37	1.43
2	D	1913	PPE	OP4-C5A	-5.73	1.37	1.43
2	F	2913	PPE	OP4-C5A	-5.69	1.37	1.43
2	B	3913	PPE	OP4-C5A	-5.62	1.37	1.43
2	E	2413	PPE	C4A-NA	5.47	1.52	1.46
2	F	2913	PPE	C4A-NA	5.37	1.52	1.46
2	E	2413	PPE	OA-CA	5.36	1.38	1.22
2	C	1413	PPE	OA-CA	5.18	1.37	1.22
2	F	2913	PPE	OA-CA	5.14	1.37	1.22
2	E	2413	PPE	C6-N1	5.13	1.41	1.32
2	A	3413	PPE	OA-CA	5.08	1.37	1.22
2	D	1913	PPE	OA-CA	5.05	1.37	1.22
2	B	3913	PPE	C6-N1	5.03	1.41	1.32
2	B	3913	PPE	OA-CA	4.97	1.36	1.22
2	A	3413	PPE	C6-N1	4.94	1.40	1.32
2	D	1913	PPE	C6-N1	4.82	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1413	PPE	C4A-NA	4.71	1.52	1.46
2	C	1413	PPE	C6-N1	4.67	1.40	1.32
2	F	2913	PPE	C6-N1	4.64	1.40	1.32
2	A	3413	PPE	C4A-NA	4.39	1.51	1.46
2	A	3413	PPE	C3-C2	4.28	1.48	1.38
2	B	3913	PPE	C3-C2	4.21	1.48	1.38
2	D	1913	PPE	C4A-NA	4.20	1.51	1.46
2	C	1413	PPE	C3-C2	4.16	1.48	1.38
2	D	1913	PPE	C3-C2	4.12	1.48	1.38
2	F	2913	PPE	C3-C2	4.10	1.48	1.38
2	E	2413	PPE	C3-C2	4.06	1.48	1.38
2	B	3913	PPE	C4A-NA	3.93	1.51	1.46
2	F	2913	PPE	CAA-NA	2.77	1.53	1.46
2	E	2413	PPE	CAA-NA	2.75	1.52	1.46
2	C	1413	PPE	CAA-NA	2.63	1.52	1.46
2	D	1913	PPE	C5A-C5	2.38	1.53	1.50
2	A	3413	PPE	CAA-NA	2.31	1.51	1.46
2	F	2913	PPE	CGA-CDA	2.21	1.55	1.50
2	D	1913	PPE	CAA-NA	2.21	1.51	1.46
2	C	1413	PPE	CGA-CDA	2.18	1.55	1.50
2	E	2413	PPE	CBA-CAA	2.17	1.58	1.53
2	E	2413	PPE	CGA-CDA	2.16	1.55	1.50
2	F	2913	PPE	P-OP1	-2.13	1.43	1.50
2	B	3913	PPE	C2A-C2	2.11	1.54	1.49
2	F	2913	PPE	C3-C4	-2.10	1.41	1.43
2	C	1413	PPE	C2A-C2	2.10	1.54	1.49
2	A	3413	PPE	C3-C4	-2.09	1.41	1.43
2	B	3913	PPE	P-OP1	-2.09	1.44	1.50
2	F	2913	PPE	CBA-CAA	2.06	1.58	1.53
2	B	3913	PPE	CAA-NA	2.05	1.51	1.46
2	D	1913	PPE	C2A-C2	2.05	1.53	1.49
2	F	2913	PPE	C5A-C5	2.01	1.52	1.50
2	E	2413	PPE	C2A-C2	2.00	1.53	1.49

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2913	PPE	O3-C3-C2	-5.63	112.73	118.29
2	E	2413	PPE	O3-C3-C2	-5.55	112.81	118.29
2	C	1413	PPE	O3-C3-C2	-5.47	112.89	118.29
2	D	1913	PPE	O3-C3-C2	-5.37	112.99	118.29
2	A	3413	PPE	O3-C3-C2	-5.29	113.06	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3913	PPE	O3-C3-C2	-5.17	113.18	118.29
2	A	3413	PPE	C2A-C2-C3	4.60	132.75	125.54
2	B	3913	PPE	C2A-C2-C3	4.58	132.72	125.54
2	F	2913	PPE	C2A-C2-C3	4.56	132.68	125.54
2	D	1913	PPE	C2A-C2-C3	4.52	132.62	125.54
2	C	1413	PPE	C2A-C2-C3	4.50	132.60	125.54
2	E	2413	PPE	C2A-C2-C3	4.45	132.51	125.54
2	B	3913	PPE	OA-CA-CAA	-3.95	109.51	122.26
2	F	2913	PPE	OA-CA-CAA	-3.91	109.63	122.26
2	B	3913	PPE	C3-C2-N1	-3.91	117.40	122.58
2	D	1913	PPE	OA-CA-CAA	-3.91	109.66	122.26
2	E	2413	PPE	OA-CA-CAA	-3.88	109.73	122.26
2	A	3413	PPE	OA-CA-CAA	-3.87	109.76	122.26
2	C	1413	PPE	OA-CA-CAA	-3.87	109.78	122.26
2	A	3413	PPE	C3-C2-N1	-3.82	117.52	122.58
2	E	2413	PPE	C3-C2-N1	-3.81	117.53	122.58
2	D	1913	PPE	C3-C2-N1	-3.80	117.55	122.58
2	C	1413	PPE	C3-C2-N1	-3.78	117.57	122.58
2	F	2913	PPE	C3-C2-N1	-3.74	117.63	122.58
2	E	2413	PPE	CGA-CBA-CAA	3.29	119.23	113.16
2	B	3913	PPE	OXT-CA-CAA	3.24	124.48	113.51
2	D	1913	PPE	OXT-CA-CAA	3.24	124.46	113.51
2	A	3413	PPE	OXT-CA-CAA	3.21	124.36	113.51
2	F	2913	PPE	OXT-CA-CAA	3.17	124.23	113.51
2	C	1413	PPE	OXT-CA-CAA	3.16	124.19	113.51
2	E	2413	PPE	OXT-CA-CAA	3.11	124.04	113.51
2	D	1913	PPE	O3-C3-C4	3.11	123.90	116.93
2	F	2913	PPE	O3-C3-C4	3.05	123.76	116.93
2	C	1413	PPE	O3-C3-C4	3.01	123.67	116.93
2	A	3413	PPE	O3-C3-C4	2.97	123.59	116.93
2	E	2413	PPE	O3-C3-C4	2.96	123.57	116.93
2	B	3913	PPE	O3-C3-C4	2.94	123.51	116.93
2	F	2913	PPE	CGA-CBA-CAA	2.59	117.94	113.16
2	D	1913	PPE	C4A-NA-CAA	-2.59	108.62	113.93
2	D	1913	PPE	OE2-CDA-OE1	2.49	129.74	123.33
2	F	2913	PPE	C4A-C4-C5	2.48	128.06	124.08
2	A	3413	PPE	OE2-CDA-OE1	2.43	129.59	123.33
2	B	3913	PPE	OE2-CDA-OE1	2.42	129.55	123.33
2	C	1413	PPE	C4A-C4-C5	2.41	127.95	124.08
2	E	2413	PPE	C4A-C4-C5	2.41	127.94	124.08
2	C	1413	PPE	OE2-CDA-OE1	2.35	129.38	123.33
2	E	2413	PPE	OE2-CDA-OE1	2.34	129.35	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2913	PPE	OE2-CDA-OE1	2.32	129.29	123.33
2	F	2913	PPE	OE1-CDA-CGA	-2.27	115.90	123.09
2	A	3413	PPE	CGA-CBA-CAA	2.24	117.30	113.16
2	B	3913	PPE	C4A-NA-CAA	-2.17	109.47	113.93
2	B	3913	PPE	OE1-CDA-CGA	-2.17	116.21	123.09
2	D	1913	PPE	CGA-CBA-CAA	2.13	117.09	113.16
2	C	1413	PPE	OE1-CDA-CGA	-2.11	116.41	123.09
2	E	2413	PPE	OE1-CDA-CGA	-2.08	116.51	123.09
2	D	1913	PPE	OE1-CDA-CGA	-2.07	116.53	123.09
2	A	3413	PPE	C4A-NA-CAA	-2.07	109.69	113.93
2	C	1413	PPE	C4-C4A-NA	-2.05	104.02	111.83
2	A	3413	PPE	OE1-CDA-CGA	-2.02	116.68	123.09
2	D	1913	PPE	OP4-P-OP1	2.02	111.89	106.44

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2913	PPE	CA-CAA-CBA-CGA
2	E	2413	PPE	NA-CAA-CBA-CGA
2	E	2413	PPE	CA-CAA-CBA-CGA
2	F	2913	PPE	NA-CAA-CBA-CGA
2	B	3913	PPE	CAA-CBA-CGA-CDA
2	D	1913	PPE	CAA-CBA-CGA-CDA
3	F	2914	MPD	O2-C2-C3-C4
2	C	1413	PPE	CA-CAA-CBA-CGA
2	A	3413	PPE	CAA-CBA-CGA-CDA
3	A	1415	MPD	C2-C3-C4-C5
3	F	2914	MPD	C2-C3-C4-C5
2	C	1413	PPE	CAA-CBA-CGA-CDA
2	F	2913	PPE	CAA-CBA-CGA-CDA
2	A	3413	PPE	OE1-CDA-CGA-CBA
2	A	3413	PPE	OE2-CDA-CGA-CBA
2	C	1413	PPE	NA-CAA-CBA-CGA
2	B	3913	PPE	OE1-CDA-CGA-CBA
2	E	2413	PPE	OE1-CDA-CGA-CBA
2	B	3913	PPE	OE2-CDA-CGA-CBA
2	D	1913	PPE	OE2-CDA-CGA-CBA
2	E	2413	PPE	OE2-CDA-CGA-CBA
2	D	1913	PPE	OE1-CDA-CGA-CBA
2	C	1413	PPE	OE1-CDA-CGA-CBA
3	A	1415	MPD	O2-C2-C3-C4

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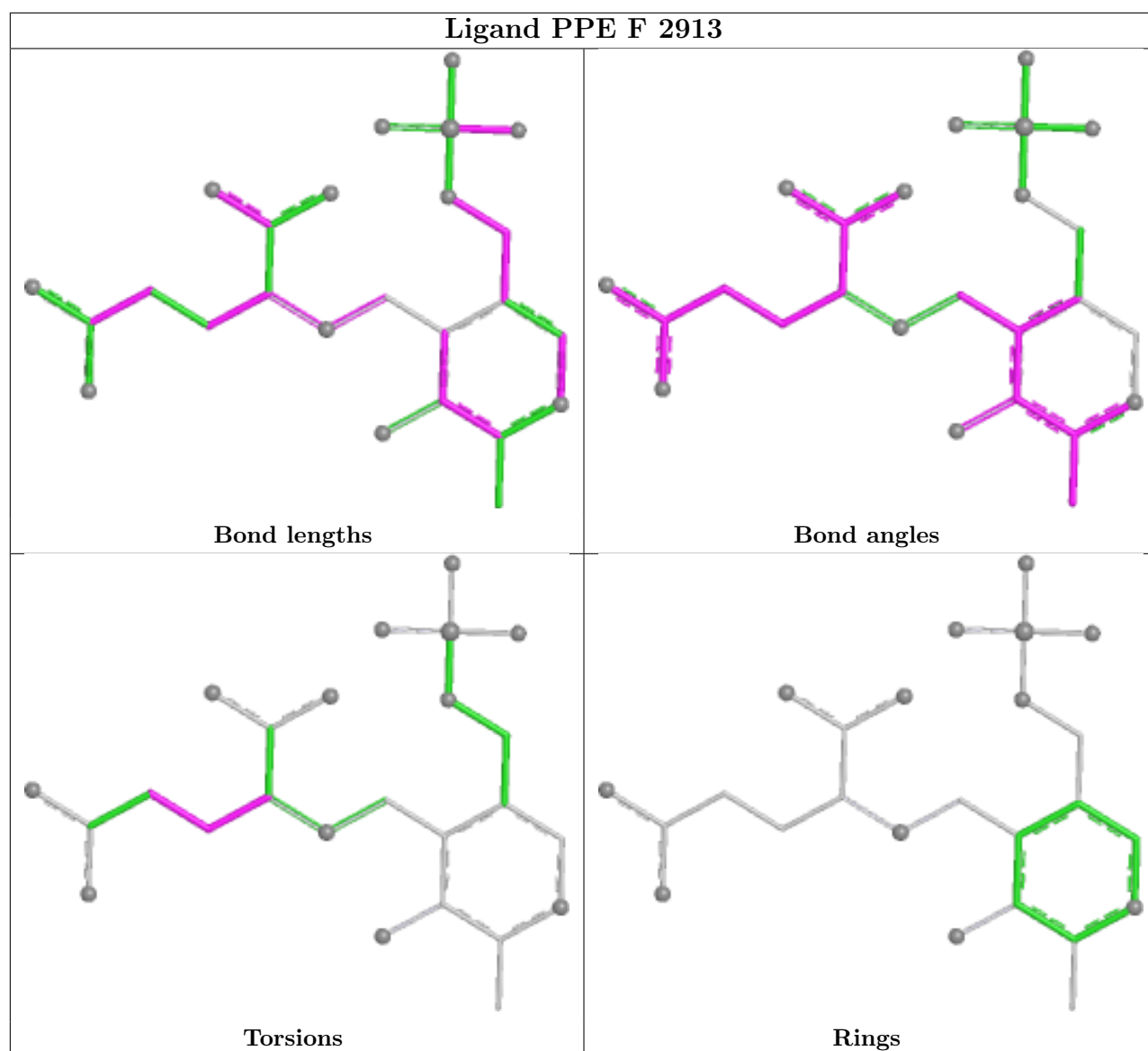
Mol	Chain	Res	Type	Atoms
3	A	1415	MPD	CM-C2-C3-C4
2	C	1413	PPE	OE2-CDA-CGA-CBA

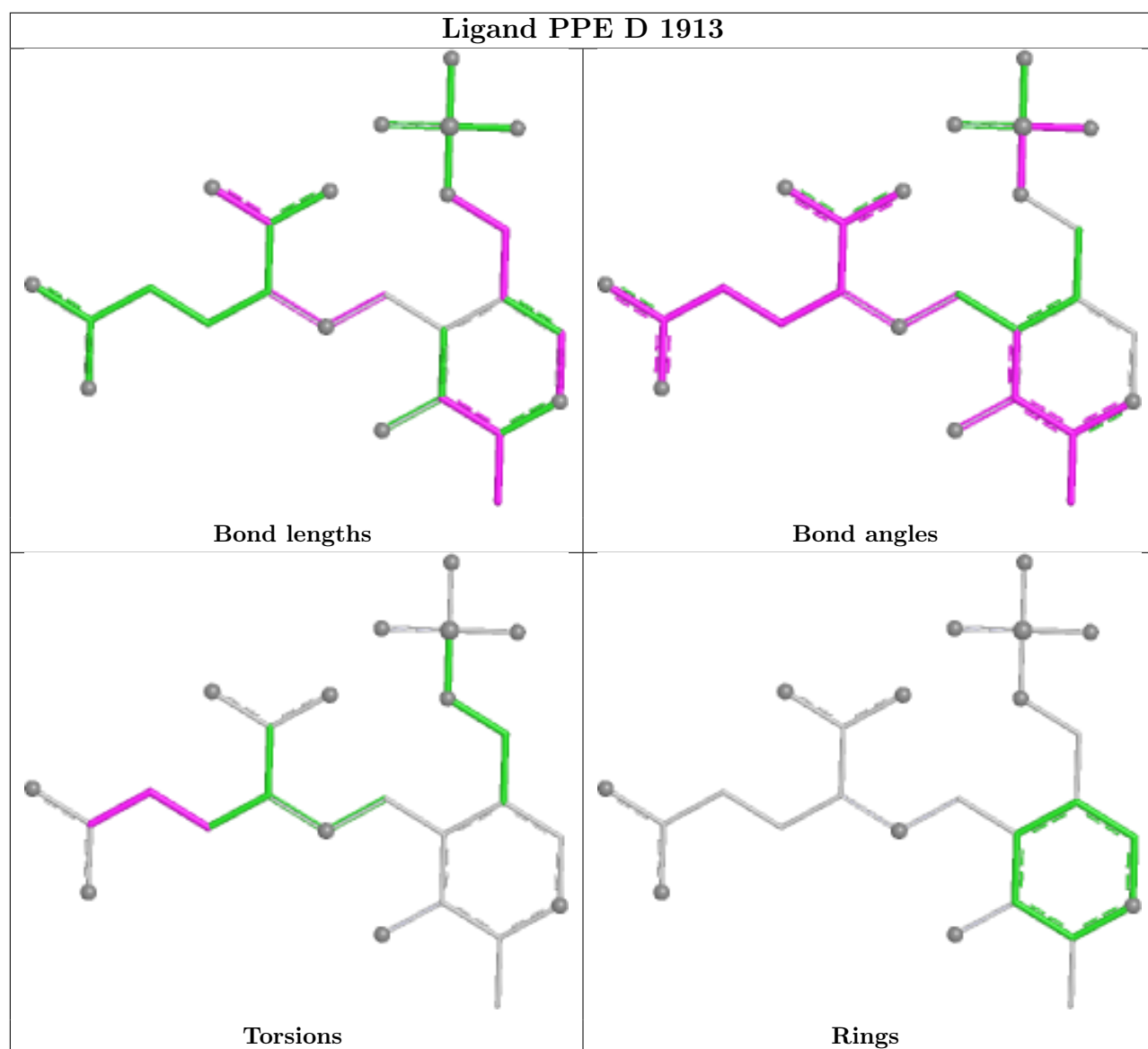
There are no ring outliers.

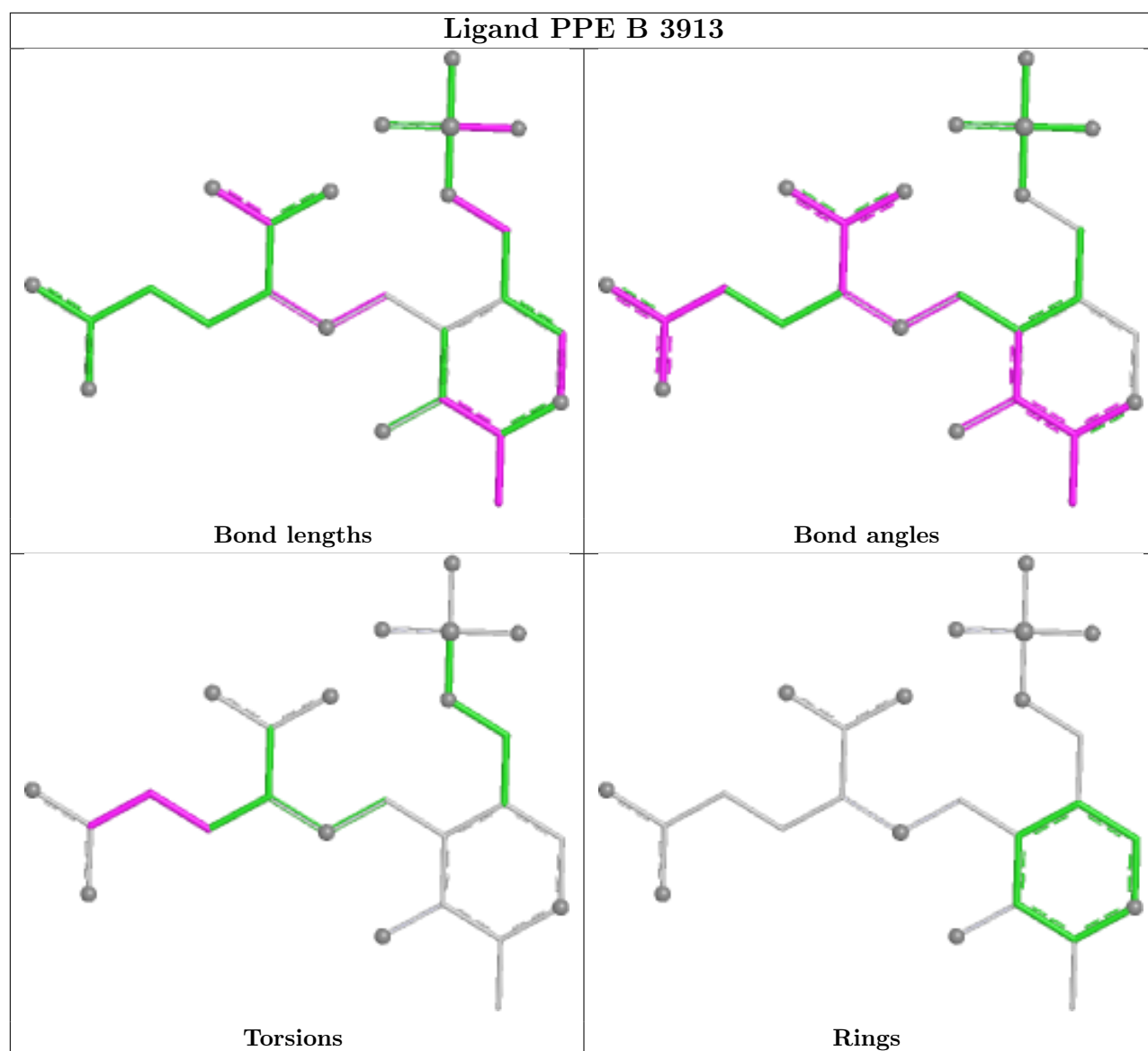
2 monomers are involved in 3 short contacts:

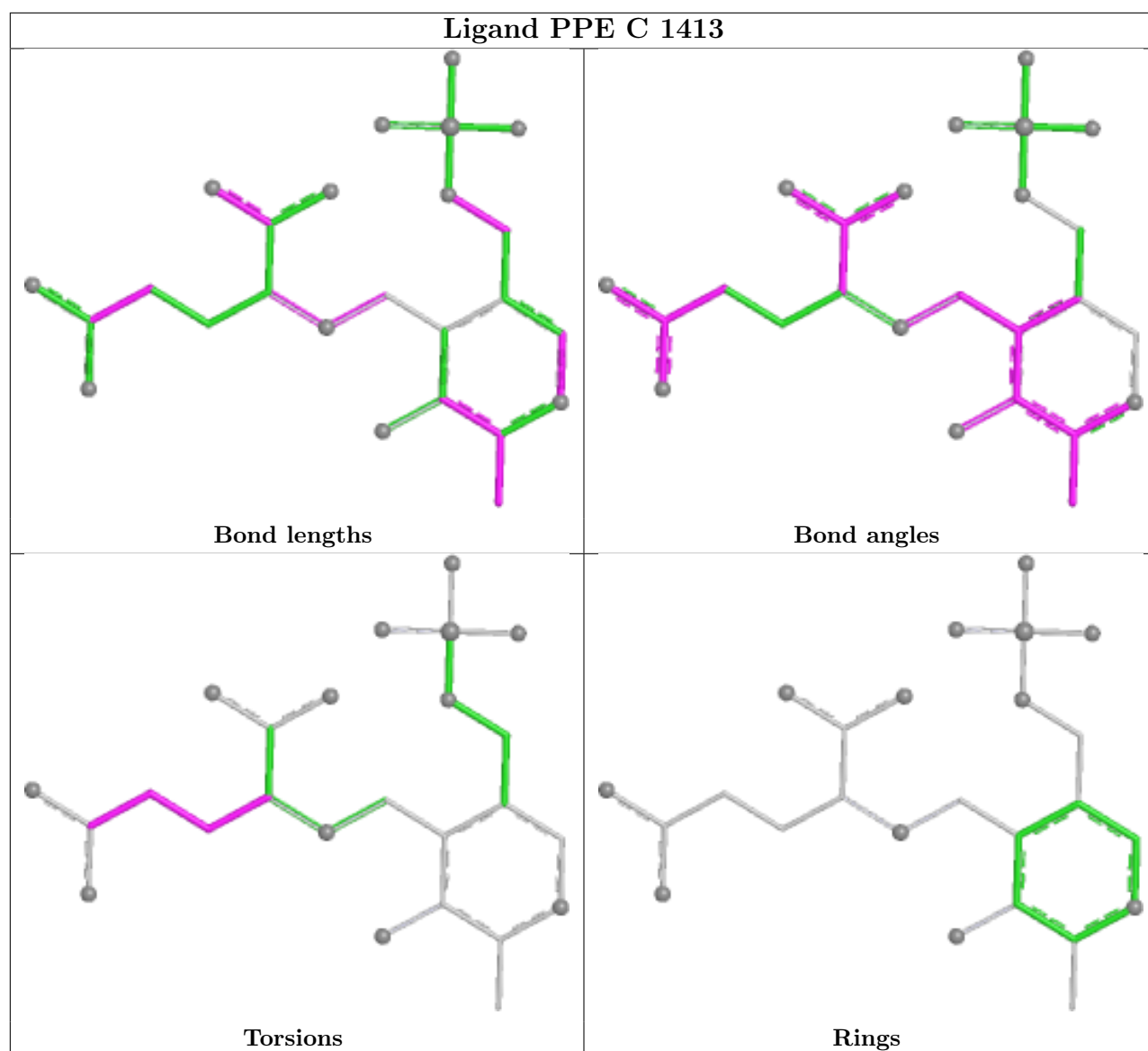
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1415	MPD	1	0
3	F	2914	MPD	2	0

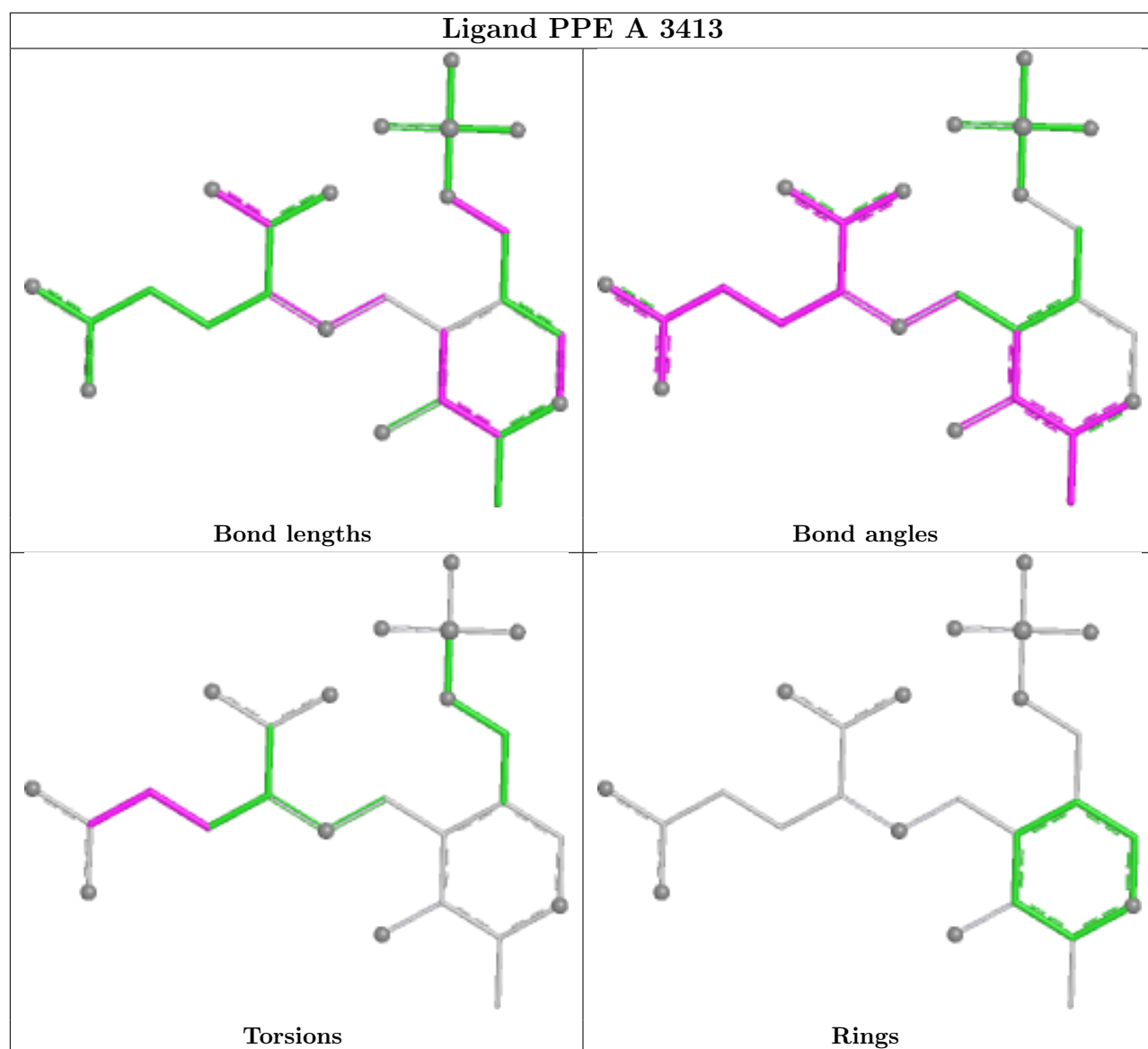
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

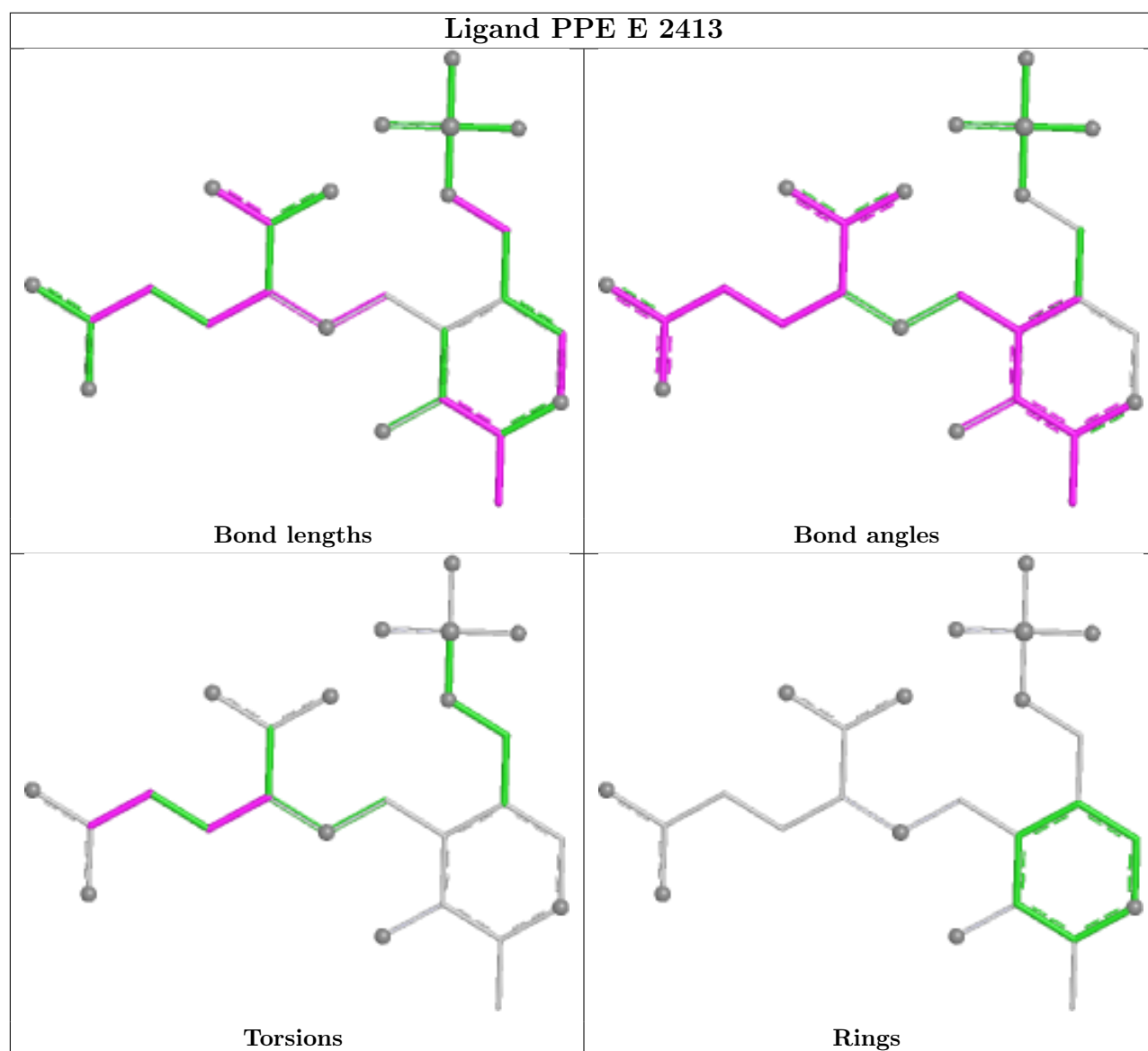












5.7 Other polymers [i](#)

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, 95th 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	294/308 (95%)	-0.22	3 (1%) 79 79	13, 20, 34, 47	0
1	B	305/308 (99%)	-0.13	10 (3%) 49 48	13, 21, 34, 47	0
1	C	297/308 (96%)	-0.15	7 (2%) 59 59	13, 20, 35, 55	0
1	D	301/308 (97%)	-0.20	6 (1%) 65 64	12, 21, 33, 57	0
1	E	298/308 (96%)	-0.16	6 (2%) 65 64	13, 21, 35, 47	0
1	F	298/308 (96%)	-0.20	6 (2%) 65 64	13, 20, 33, 52	0
All	All	1793/1848 (97%)	-0.18	38 (2%) 63 63	12, 20, 34, 57	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	VAL	6.3
1	D	130	LEU	5.2
1	B	127	GLY	4.8
1	C	136	ARG	3.9
1	B	128	ALA	3.9
1	C	224	VAL	3.7
1	F	224	VAL	3.6
1	D	129	TYR	3.6
1	E	135	VAL	3.5
1	B	224	VAL	3.3
1	D	224	VAL	3.3
1	F	134	ALA	3.3
1	F	126	TRP	3.2
1	C	126	TRP	3.2
1	A	224	VAL	3.1
1	D	126	TRP	3.1
1	B	131	GLY	3.1
1	E	224	VAL	3.0
1	D	128	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	130	LEU	2.8
1	C	18	GLU	2.7
1	A	126	TRP	2.7
1	F	135	VAL	2.7
1	B	129	TYR	2.5
1	E	134	ALA	2.5
1	F	305	VAL	2.5
1	E	306	ASN	2.4
1	E	126	TRP	2.3
1	A	92	ARG	2.3
1	B	306	ASN	2.2
1	C	92	ARG	2.2
1	C	137	LYS	2.2
1	B	18	GLU	2.2
1	E	45	ALA	2.2
1	D	135	VAL	2.2
1	F	306	ASN	2.1
1	B	88	ARG	2.0
1	B	2	GLN	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
3	MPD	F	2914	8/8	0.68	0.22	37,39,42,43	0
3	MPD	A	1415	8/8	0.71	0.20	43,44,45,46	0
2	PPE	B	3913	25/25	0.91	0.13	16,23,54,56	0
2	PPE	E	2413	25/25	0.93	0.10	16,21,49,50	0

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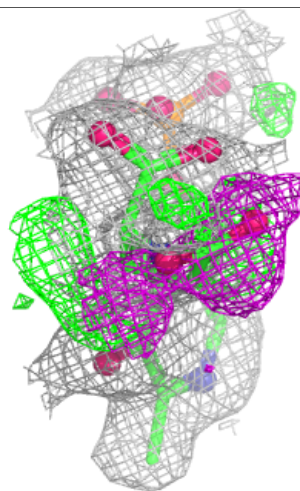
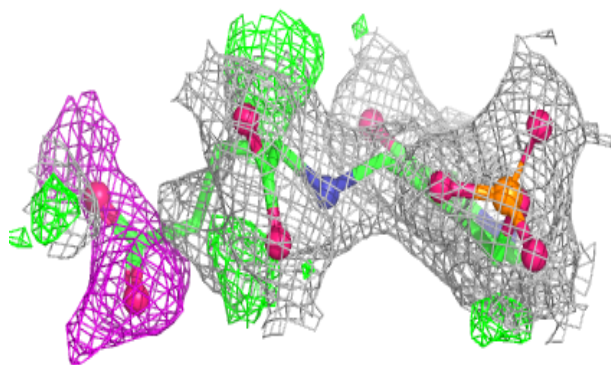
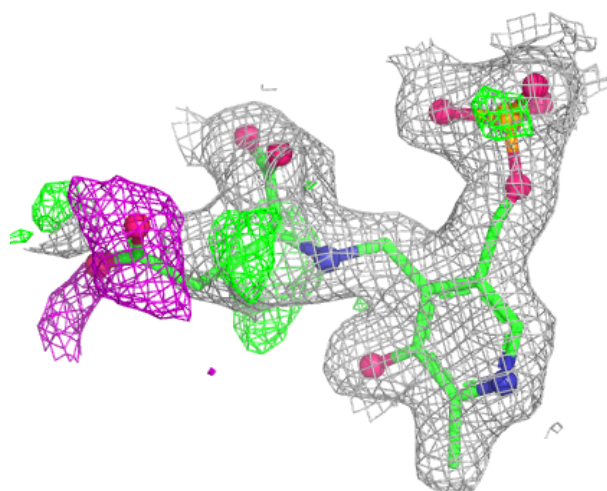
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PPE	F	2913	25/25	0.93	0.10	17,20,44,47	0
2	PPE	A	3413	25/25	0.93	0.11	17,20,48,49	0
2	PPE	C	1413	25/25	0.93	0.11	14,21,48,50	0
2	PPE	D	1913	25/25	0.94	0.10	15,21,49,51	0

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.

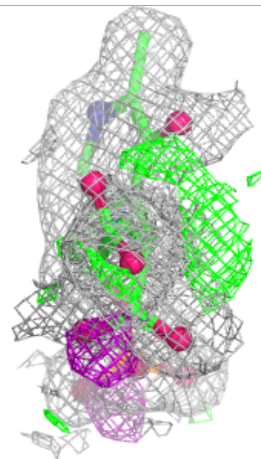
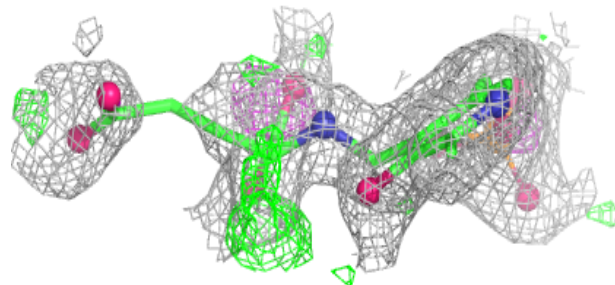
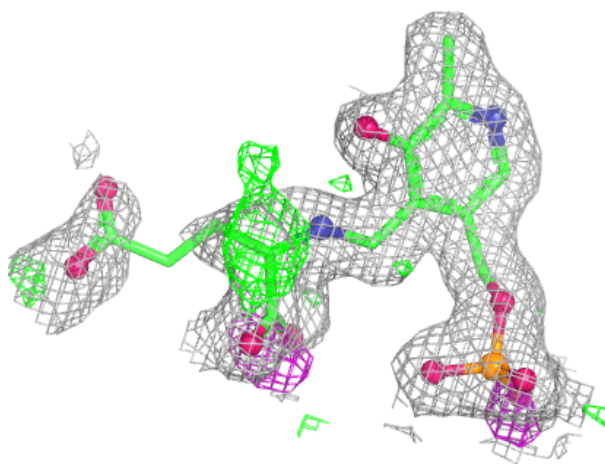
Electron density around PPE B 3913:

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



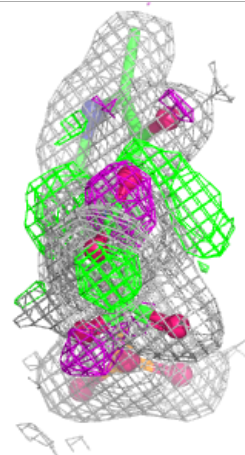
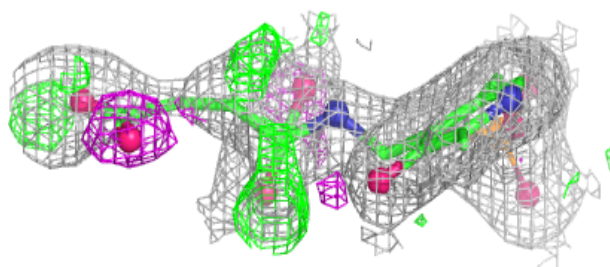
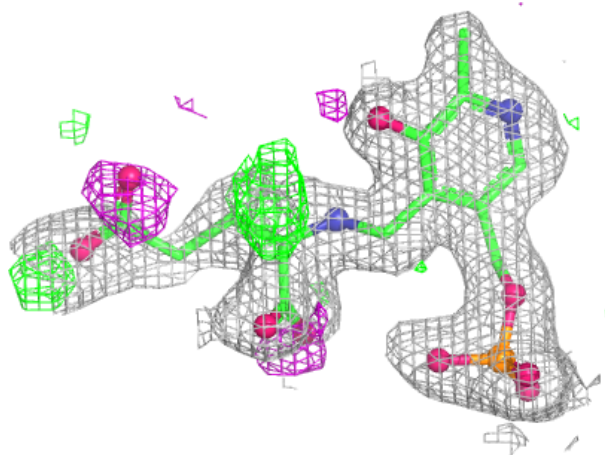
Electron density around PPE E 2413:

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



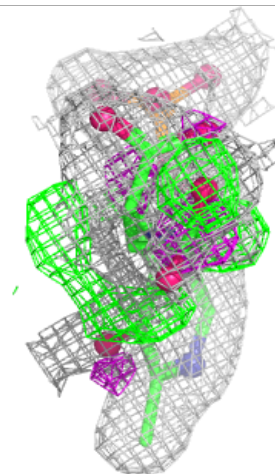
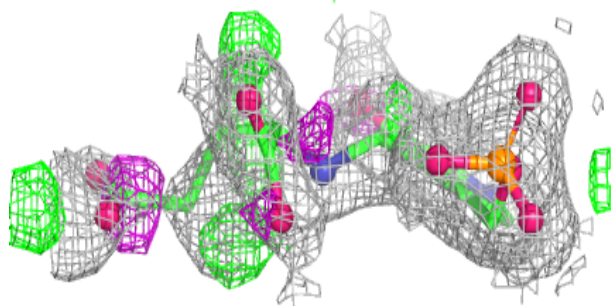
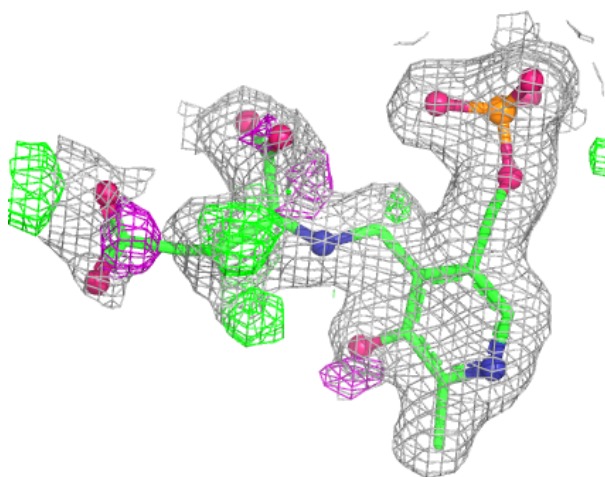
Electron density around PPE F 2913:

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



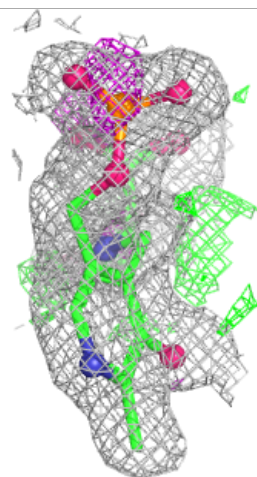
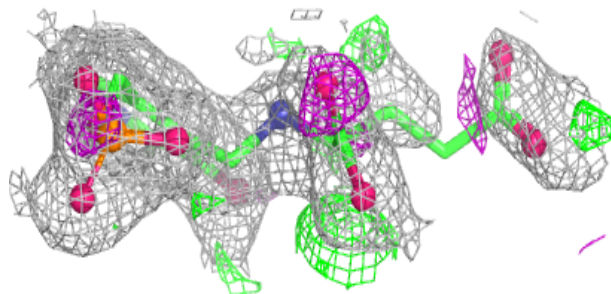
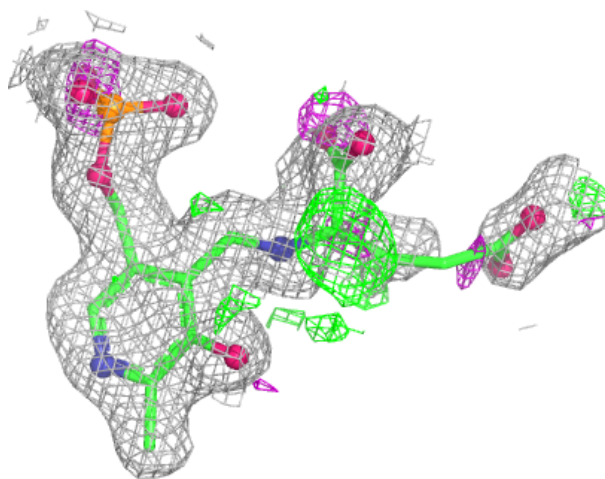
Electron density around PPE A 3413:

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



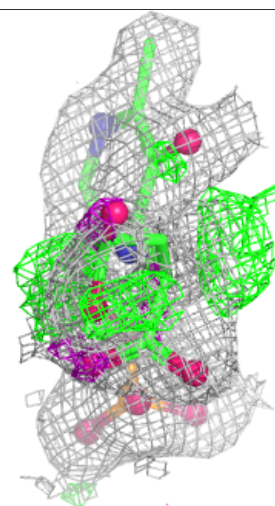
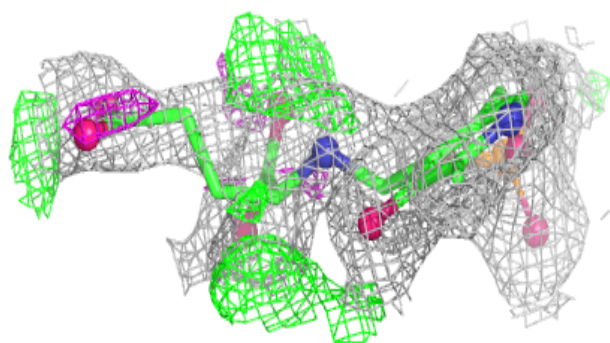
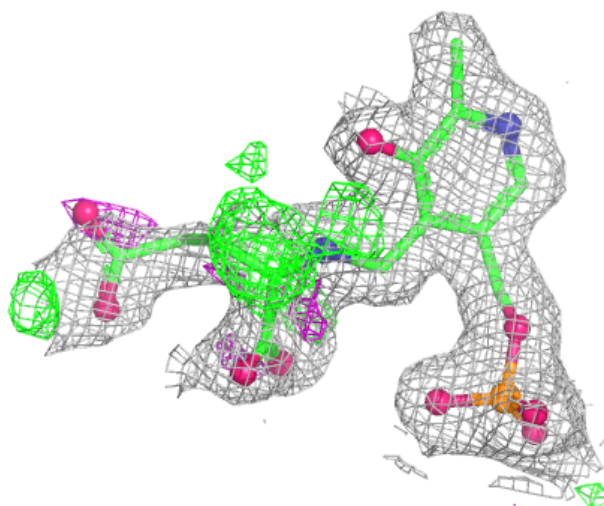
Electron density around PPE C 1413:

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



Electron density around PPE D 1913:

$2mF_o-DF_c$ (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.