Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 01:33 am BST

PDB ID	:	4D5G
Title	:	Structure of recombinant CDH-H28AN484A
Authors	:	Loschonsky, S.; Wacker, T.; Waltzer, S.; Giovannini, P.P.; McLeish, M.J.; Andrade, S.L.A.; Mueller, M.
Deposited on	:	2014-11-04
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 (i) 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 (i)) were used in the production of this report:

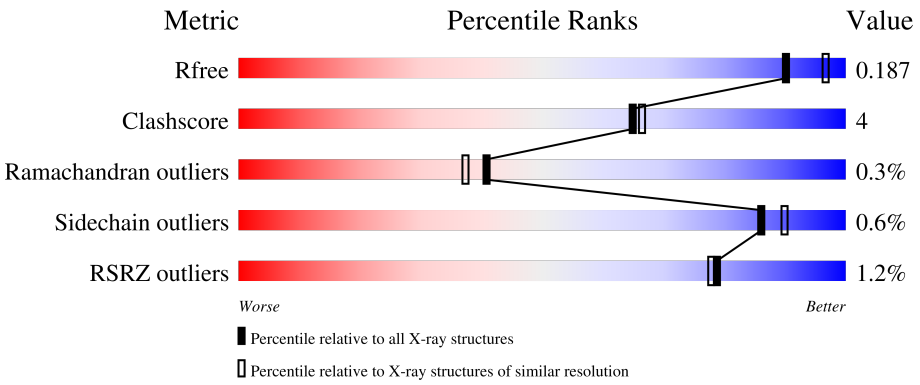
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	589	.% 88% 11% ••
1	B	589	2% 90% 9% •

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9962 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.

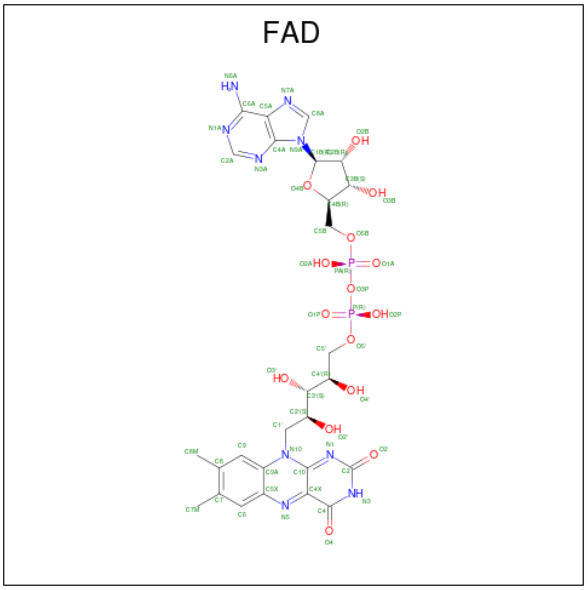
- Molecule 1 is a protein called CYCLOHEXANE-1,2-DIONE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	586	4521	2872	797	830	22	41	17	0
1	B	587	4516	2870	796	828	22	55	15	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ALA	HIS	engineered mutation	UNP P0CH62
B	28	ALA	HIS	engineered mutation	UNP P0CH62

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

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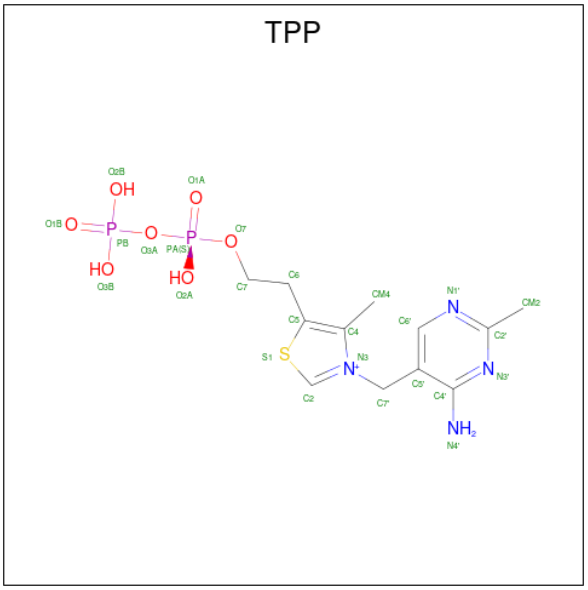
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	53	27	9	15	2	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).

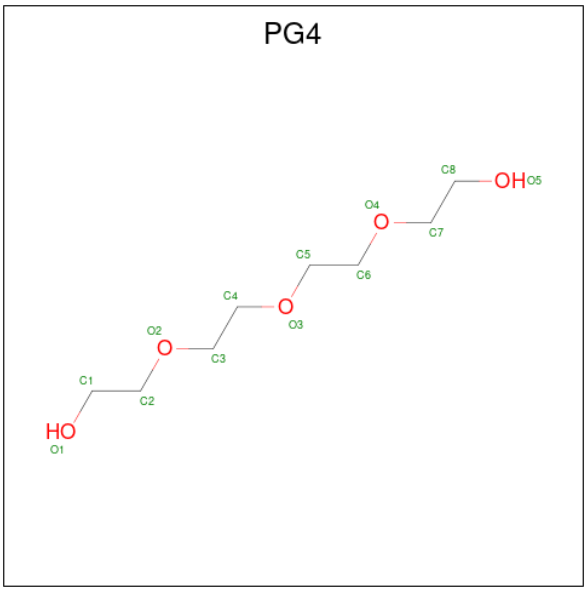


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	26	12	4	7	2	1	0	0
			Total	C	N	O	P	S		
3	B	1	26	12	4	7	2	1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

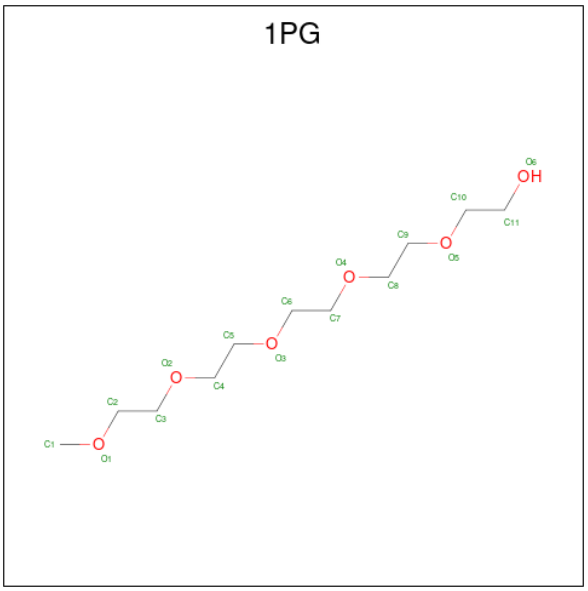
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	2	2	2	0	0
			Total	Mg		
4	B	1	1	1	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



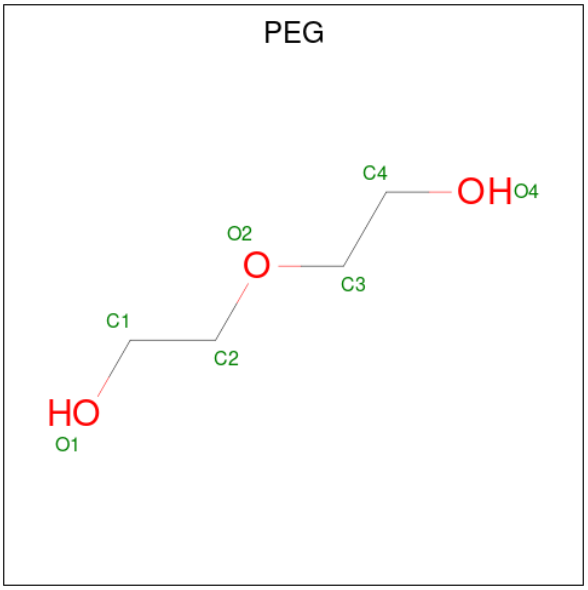
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 11	C 7	O 4	0	0
5	A	1	Total 13	C 8	O 5	0	0
5	A	1	Total 8	C 5	O 3	0	0
5	A	1	Total 11	C 7	O 4	0	0
5	A	1	Total 13	C 8	O 5	0	0
5	A	1	Total 9	C 6	O 3	0	0
5	B	1	Total 10	C 6	O 4	0	0
5	B	1	Total 6	C 4	O 2	0	0
5	B	1	Total 11	C 7	O 4	0	0

- Molecule 6 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (three-letter code: 1PG) (formula: $C_{11}H_{24}O_6$).



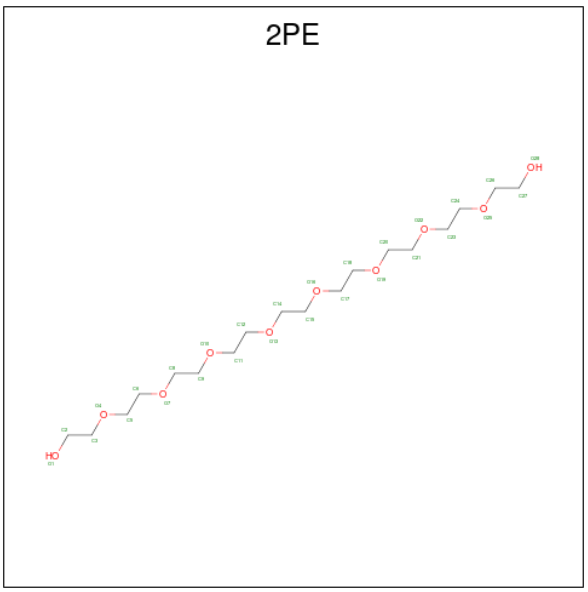
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	12	8	4	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 8 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	B	1	21	14	7	0	0
			Total	C	O		
8	B	1	22	14	8	0	0

- Molecule 9 is water.

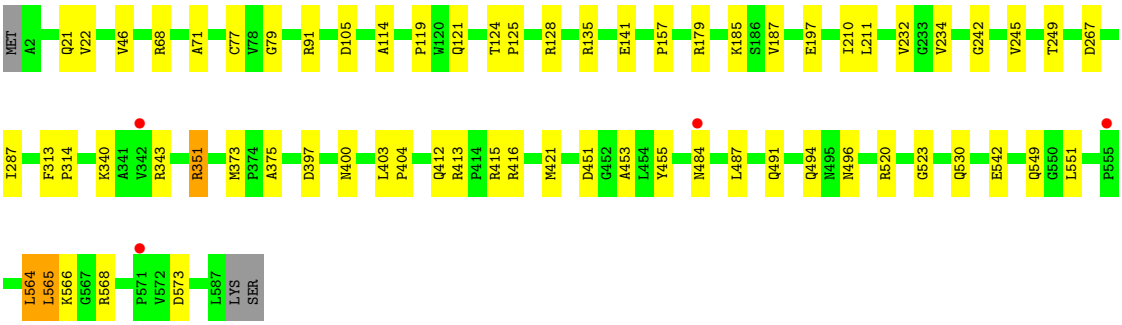
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	359	359	359	0	0
			Total	O		
9	B	237	237	237	0	0

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.

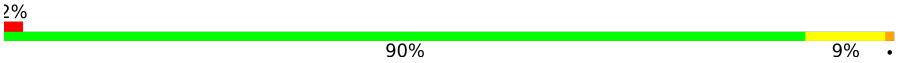
• Molecule 1: CYCLOHEXANE-1,2-DIONE HYDROLASE

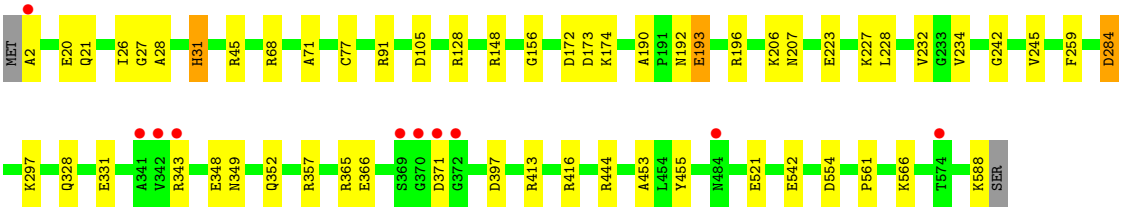
Chain A:



• Molecule 1: CYCLOHEXANE-1,2-DIONE HYDROLASE

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	122.83Å 122.83Å 143.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.63 – 2.00 46.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.63-2.00) 99.5 (46.59-2.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.134 , 0.179 0.148 , 0.187	Depositor DCC
R_{free} test set	3716 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 67.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9962	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, FAD, 1PG, TPP, PEG, 2PE, MG

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	1.06	8/4680 (0.2%)	2.05	22/6352 (0.3%)
1	B	1.61	15/4667 (0.3%)	1.44	25/6333 (0.4%)
All	All	1.36	23/9347 (0.2%)	1.77	47/12685 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68[A]	ARG	CZ-NH2	-42.49	0.77	1.33
1	B	68[B]	ARG	CZ-NH2	-42.49	0.77	1.33
1	B	68[A]	ARG	NE-CZ	-33.40	0.89	1.33
1	B	68[B]	ARG	NE-CZ	-33.40	0.89	1.33
1	B	331	GLU	CG-CD	-32.08	1.03	1.51
1	A	565	LEU	C-N	-23.31	0.80	1.34
1	B	223	GLU	CG-CD	16.49	1.76	1.51
1	B	297	LYS	CB-CG	-15.85	1.09	1.52
1	A	351	ARG	CG-CD	-15.31	1.13	1.51
1	B	68[A]	ARG	CZ-NH1	12.97	1.50	1.33
1	B	68[B]	ARG	CZ-NH1	12.97	1.50	1.33
1	B	588	LYS	CA-CB	-12.48	1.26	1.53
1	A	343	ARG	CG-CD	11.37	1.80	1.51
1	A	568	ARG	CG-CD	-11.36	1.23	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	LYS	CE-NZ	-8.29	1.28	1.49
1	B	174	LYS	CB-CG	-8.26	1.30	1.52
1	A	351	ARG	NE-CZ	8.07	1.43	1.33
1	A	487	LEU	CG-CD2	-7.38	1.24	1.51
1	B	566	LYS	CA-CB	-6.95	1.38	1.53
1	A	197	GLU	CD-OE2	-6.83	1.18	1.25
1	B	343	ARG	CB-CG	-6.76	1.34	1.52
1	A	141	GLU	CD-OE2	-6.26	1.18	1.25
1	B	521	GLU	CG-CD	-5.66	1.43	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	351	ARG	NE-CZ-NH1	-138.21	51.20	120.30
1	B	68[A]	ARG	NE-CZ-NH1	-43.10	98.75	120.30
1	B	68[B]	ARG	NE-CZ-NH1	-43.10	98.75	120.30
1	A	351	ARG	NE-CZ-NH2	-31.79	104.40	120.30
1	B	68[A]	ARG	NH1-CZ-NH2	28.76	151.04	119.40
1	B	68[B]	ARG	NH1-CZ-NH2	28.76	151.04	119.40
1	A	565	LEU	O-C-N	-20.80	89.43	122.70
1	B	68[A]	ARG	NE-CZ-NH2	-20.21	110.20	120.30
1	B	68[B]	ARG	NE-CZ-NH2	-20.21	110.20	120.30
1	B	68[A]	ARG	CD-NE-CZ	20.11	151.76	123.60
1	B	68[B]	ARG	CD-NE-CZ	20.11	151.76	123.60
1	A	351	ARG	CB-CG-CD	14.17	148.45	111.60
1	B	297	LYS	CA-CB-CG	13.82	143.80	113.40
1	A	487	LEU	CB-CG-CD2	12.79	132.75	111.00
1	B	193	GLU	OE1-CD-OE2	-11.54	109.45	123.30
1	A	565	LEU	CA-C-N	11.51	142.53	117.20
1	A	197	GLU	OE1-CD-OE2	-9.62	111.75	123.30
1	B	331	GLU	CB-CG-CD	9.48	139.81	114.20
1	A	565	LEU	C-N-CA	8.05	141.84	121.70
1	A	340	LYS	CA-CB-CG	7.80	130.56	113.40
1	B	91[A]	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	B	91[B]	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	A	573	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	564	LEU	CB-CG-CD2	6.83	122.62	111.00
1	A	351	ARG	CG-CD-NE	6.71	125.89	111.80
1	A	105	ASP	CB-CG-OD1	6.68	124.31	118.30
1	B	105	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	416	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	416	ARG	NE-CZ-NH1	6.47	123.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	105	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	B	357	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	267	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	343	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	284	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	193	GLU	CG-CD-OE2	-5.64	107.02	118.30
1	A	415	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	68	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	223	GLU	CB-CG-CD	-5.60	99.07	114.20
1	A	451	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	105	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	554	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	413	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	343	ARG	CB-CG-CD	-5.20	98.07	111.60
1	A	68	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	444	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	568	ARG	CG-CD-NE	5.07	122.44	111.80
1	B	20	GLU	CB-CA-C	-5.05	100.29	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	ARG	Sidechain
1	A	565	LEU	Peptide,Mainchain
1	B	193	GLU	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4521	0	4499	44	0
1	B	4516	0	4496	29	1
2	A	53	0	31	1	0
2	B	53	0	31	0	0
3	A	26	0	16	0	0
3	B	26	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	65	0	82	4	0
5	B	27	0	30	1	0
6	A	12	0	15	0	0
7	A	14	0	20	5	0
7	B	7	0	10	0	0
8	B	43	0	53	3	0
9	A	359	0	0	6	0
9	B	237	0	0	7	0
All	All	9962	0	9299	75	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 4.

All (75) 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:91[A]:ARG:HH22	7:A:1596:PEG:H42	1.20	1.02
1:B:28:ALA:O	1:B:31[B]:HIS:ND1	2.02	0.91
1:B:28:ALA:O	1:B:31[B]:HIS:CE1	2.24	0.91
1:A:91[A]:ARG:NH2	7:A:1596:PEG:H42	1.85	0.90
1:A:484:ASN:ND2	9:A:2298:HOH:O	2.08	0.87
1:B:190:ALA:H	1:B:328:GLN:HE22	1.29	0.80
1:A:121[B]:GLN:HE21	1:A:121[B]:GLN:H	1.31	0.77
1:A:491[A]:GLN:NE2	1:A:564:LEU:HA	1.99	0.77
1:A:484:ASN:OD1	1:B:26:ILE:HG13	1.84	0.77
1:B:259[B]:PHE:CE2	1:B:561:PRO:HD3	2.26	0.70
1:B:259[B]:PHE:CD2	1:B:561:PRO:HD3	2.28	0.69
1:B:192:ASN:HD21	1:B:196:ARG:HE	1.40	0.67
1:A:530:GLN:OE1	9:A:2326:HOH:O	2.11	0.67
1:B:352:GLN:OE1	9:B:2145:HOH:O	2.13	0.66
1:B:207:ASN:HD21	1:B:352:GLN:HE22	1.44	0.65
1:A:373:MET:HE1	1:A:375:ALA:HB2	1.79	0.63
1:A:179[B]:ARG:NH1	9:A:2133:HOH:O	2.33	0.61
1:B:542[A]:GLU:OE2	9:B:2192:HOH:O	2.16	0.60
1:A:413:ARG:HD2	9:A:2266:HOH:O	2.02	0.59
1:A:121[B]:GLN:H	1:A:121[B]:GLN:NE2	1.98	0.58
1:B:352:GLN:HG3	9:B:2145:HOH:O	2.03	0.58
1:A:494:GLN:HE22	7:A:1597:PEG:H22	1.69	0.58
5:A:1595:PG4:C8	9:B:2225:HOH:O	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:GLN:NE2	7:A:1597:PEG:H22	2.21	0.56
1:A:491[A]:GLN:HE21	1:A:564:LEU:HA	1.69	0.56
1:B:148:ARG:HA	5:B:1594:PG4:H41	1.88	0.55
1:B:128[A]:ARG:HD2	1:B:156:GLY:HA3	1.88	0.55
1:A:484:ASN:HD21	1:B:27:GLY:HA2	1.71	0.54
1:A:91[B]:ARG:HH22	7:A:1596:PEG:H42	1.71	0.54
1:A:551:LEU:C	1:A:551:LEU:HD23	2.29	0.53
1:A:520:ARG:NH2	1:A:542[B]:GLU:OE2	2.41	0.53
1:A:400:ASN:HB3	1:A:549:GLN:O	2.09	0.53
8:B:1592:2PE:C11	9:B:2236:HOH:O	2.56	0.52
1:A:114:ALA:HA	1:B:284:ASP:HB2	1.92	0.52
1:B:192:ASN:HD21	1:B:196:ARG:NE	2.08	0.51
1:A:185:LYS:HB3	1:A:187:VAL:HG22	1.92	0.50
1:A:403:LEU:HB3	1:A:404:PRO:HD3	1.92	0.50
1:B:242:GLY:O	1:B:245:VAL:HG22	2.11	0.50
1:A:373:MET:HE2	1:A:523:GLY:HA2	1.93	0.50
1:B:2:ALA:HA	1:B:173:ASP:OD1	2.11	0.50
1:B:21:GLN:NE2	1:B:45:ARG:O	2.44	0.49
1:B:128[A]:ARG:HG2	1:B:128[A]:ARG:HH11	1.78	0.49
1:B:397:ASP:CG	1:B:453:ALA:HB1	2.34	0.48
8:B:1592:2PE:H111	9:B:2236:HOH:O	2.15	0.47
1:A:135:ARG:HG2	5:A:1595:PG4:C5	2.45	0.46
1:A:421:MET:O	2:A:1588:FAD:H9	2.16	0.46
1:A:397:ASP:CG	1:A:453:ALA:HB1	2.36	0.46
1:B:232:VAL:HG23	1:B:234:VAL:HG23	1.98	0.45
1:A:128[A]:ARG:HG3	1:A:157:PRO:HD2	1.99	0.45
1:A:79:GLY:HA2	3:B:1590:TPP:HM22	1.99	0.45
1:A:119:PRO:HA	1:A:121[B]:GLN:HE22	1.83	0.44
1:A:211:LEU:C	1:A:211:LEU:HD23	2.38	0.44
1:A:249:THR:OG1	1:A:412[A]:GLN:NE2	2.46	0.44
1:A:373:MET:CE	1:A:375:ALA:HB2	2.46	0.44
1:B:228:LEU:O	1:B:232:VAL:HG22	2.17	0.44
1:A:242:GLY:O	1:A:245:VAL:HG22	2.18	0.44
8:B:1593:2PE:H122	8:B:1593:2PE:H152	1.73	0.43
1:B:128[A]:ARG:HG2	1:B:128[A]:ARG:NH1	2.33	0.43
1:A:313:PHE:HA	1:A:314:PRO:HD3	1.81	0.43
1:A:211:LEU:HD11	1:A:287:ILE:HG13	2.01	0.42
1:A:21:GLN:O	1:A:71:ALA:HA	2.19	0.42
5:A:1595:PG4:H72	9:A:2104:HOH:O	2.20	0.42
1:A:232:VAL:HG12	1:A:234[A]:VAL:HG23	2.02	0.42
1:B:348:GLU:N	9:B:2142:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HB	1:A:46:VAL:HG22	2.01	0.42
1:A:496:ASN:ND2	9:A:2302:HOH:O	2.46	0.41
1:B:192:ASN:ND2	1:B:196:ARG:HE	2.11	0.41
1:B:206:LYS:O	1:B:349:ASN:ND2	2.39	0.41
1:A:124:THR:N	1:A:125:PRO:CD	2.83	0.41
1:A:551:LEU:HD23	1:A:551:LEU:O	2.21	0.41
1:A:135:ARG:HG2	5:A:1595:PG4:H51	2.03	0.41
1:B:21:GLN:O	1:B:71:ALA:HA	2.21	0.41
1:B:2:ALA:HB1	1:B:172:ASP:OD1	2.21	0.40
1:A:210:ILE:HD12	1:A:234[B]:VAL:HG13	2.03	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:366:GLU:OE2	1:B:366:GLU:OE2[8_444]	1.97	0.23

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	601/589 (102%)	585 (97%)	15 (2%)	1 (0%)	47	44
1	B	600/589 (102%)	586 (98%)	12 (2%)	2 (0%)	41	37
All	All	1201/1178 (102%)	1171 (98%)	27 (2%)	3 (0%)	41	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	371	ASP
1	A	77	CYS
1	B	77	CYS

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	466/452 (103%)	464 (100%)	2 (0%)	91 93
1	B	465/452 (103%)	461 (99%)	4 (1%)	78 83
All	All	931/904 (103%)	925 (99%)	6 (1%)	86 90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	455	TYR
1	A	566	LYS
1	B	31[A]	HIS
1	B	31[B]	HIS
1	B	365	ARG
1	B	455	TYR

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

Mol	Chain	Res	Type
1	A	116	GLN
1	A	153	HIS
1	A	442	ASN
1	A	494	GLN
1	A	530	GLN
1	B	21	GLN
1	B	116	GLN
1	B	153	HIS
1	B	192	ASN
1	B	328	GLN
1	B	352	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 3 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PG4	B	1594	-	9,9,12	0.93	0	8,8,11	0.96	0
2	FAD	A	1588	-	53,58,58	1.31	4 (7%)	68,89,89	1.28	10 (14%)
8	2PE	B	1592	-	20,20,27	0.61	0	19,19,26	0.46	0
5	PG4	B	1595	-	5,5,12	0.49	0	4,4,11	0.31	0
3	TPP	B	1590	-	22,27,27	1.77	3 (13%)	29,40,40	2.04	8 (27%)
2	FAD	B	1589	-	53,58,58	1.38	9 (16%)	68,89,89	1.23	8 (11%)
5	PG4	A	1593	-	12,12,12	0.46	0	11,11,11	0.46	0
3	TPP	A	1589	-	22,27,27	1.94	4 (18%)	29,40,40	2.55	10 (34%)
7	PEG	A	1596	-	6,6,6	0.41	0	5,5,5	0.29	0
5	PG4	A	1594	-	7,7,12	0.72	0	6,6,11	0.73	0
5	PG4	A	1598	-	12,12,12	0.61	0	11,11,11	0.36	0
5	PG4	B	1597	-	10,10,12	0.55	0	9,9,11	0.88	0
7	PEG	A	1597	-	6,6,6	0.52	0	5,5,5	0.56	0
7	PEG	B	1596	-	6,6,6	0.42	0	5,5,5	0.66	0
5	PG4	A	1591	-	10,10,12	0.93	0	9,9,11	0.82	0
5	PG4	A	1595	-	10,10,12	0.54	0	9,9,11	0.73	0
5	PG4	A	1599	-	8,8,12	0.52	0	7,7,11	0.75	0
8	2PE	B	1593	-	21,21,27	0.56	0	20,20,26	0.53	0
6	1PG	A	1592	-	11,11,16	0.65	0	10,10,15	1.02	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	B	1594	-	-	4/7/7/10	-
2	FAD	A	1588	-	-	3/30/50/50	0/6/6/6
8	2PE	B	1592	-	-	7/18/18/25	-
5	PG4	B	1595	-	-	3/3/3/10	-
3	TPP	B	1590	-	-	1/16/17/17	0/2/2/2
2	FAD	B	1589	-	-	3/30/50/50	0/6/6/6
5	PG4	A	1593	-	-	6/10/10/10	-
3	TPP	A	1589	-	-	1/16/17/17	0/2/2/2
7	PEG	A	1596	-	-	2/4/4/4	-
5	PG4	A	1594	-	-	4/5/5/10	-
5	PG4	A	1598	-	-	2/10/10/10	-
5	PG4	B	1597	-	-	3/8/8/10	-
7	PEG	A	1597	-	-	1/4/4/4	-
7	PEG	B	1596	-	-	3/4/4/4	-
5	PG4	A	1591	-	-	3/8/8/10	-
5	PG4	A	1595	-	-	5/8/8/10	-
5	PG4	A	1599	-	-	0/6/6/10	-
8	2PE	B	1593	-	-	10/19/19/25	-
6	1PG	A	1592	-	-	5/9/9/14	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1589	TPP	C6-C5	-5.95	1.48	1.50
3	B	1590	TPP	C4-N3	-5.33	1.35	1.39
2	A	1588	FAD	C9A-C5X	4.89	1.49	1.41
2	B	1589	FAD	C9A-C5X	4.71	1.49	1.41
3	A	1589	TPP	C5'-C4'	4.36	1.50	1.42
3	B	1590	TPP	C5'-C4'	3.66	1.49	1.42
3	A	1589	TPP	C4-N3	-3.59	1.36	1.39
3	B	1590	TPP	C6-C5	3.51	1.52	1.50
2	A	1588	FAD	C8-C7	2.79	1.47	1.40
2	B	1589	FAD	C8-C7	2.68	1.47	1.40
2	B	1589	FAD	C2A-N3A	2.68	1.36	1.32
2	A	1588	FAD	C4-N3	-2.53	1.34	1.38
3	A	1589	TPP	C2'-N1'	2.51	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1589	FAD	C4-N3	-2.42	1.34	1.38
2	B	1589	FAD	C9A-N10	-2.37	1.37	1.41
2	B	1589	FAD	O2-C2	2.31	1.28	1.24
2	B	1589	FAD	C6-C5X	-2.23	1.36	1.40
2	B	1589	FAD	C4A-N3A	2.11	1.38	1.35
2	A	1588	FAD	C10-N10	2.09	1.41	1.37
2	B	1589	FAD	C5X-N5	-2.09	1.35	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1589	TPP	CM2-C2'-N1'	7.75	125.67	117.14
3	A	1589	TPP	C6-C5-C4	7.48	133.44	127.43
3	B	1590	TPP	CM4-C4-N3	4.86	128.72	122.53
3	B	1590	TPP	C6-C5-C4	4.21	130.81	127.43
2	A	1588	FAD	N3A-C2A-N1A	-3.72	122.87	128.68
3	B	1590	TPP	C6'-N1'-C2'	3.61	122.10	115.96
3	B	1590	TPP	CM4-C4-C5	-3.34	120.29	127.60
3	B	1590	TPP	O3B-PB-O2B	3.28	120.16	107.64
2	A	1588	FAD	O2-C2-N1	-3.25	116.44	121.83
2	B	1589	FAD	C1B-N9A-C4A	-3.24	120.96	126.64
3	A	1589	TPP	C6'-N1'-C2'	3.12	121.26	115.96
3	A	1589	TPP	N1'-C2'-N3'	-3.07	120.25	125.54
2	B	1589	FAD	C1'-N10-C9A	2.98	125.48	120.51
2	B	1589	FAD	N3A-C2A-N1A	-2.90	124.15	128.68
3	A	1589	TPP	C2'-N3'-C4'	2.88	122.57	118.08
2	B	1589	FAD	O4'-C4'-C3'	2.85	116.02	109.10
6	A	1592	1PG	C5-O3-C6	2.73	122.67	112.90
3	B	1590	TPP	N1'-C2'-N3'	-2.68	120.93	125.54
2	A	1588	FAD	C4X-C10-N10	2.63	120.33	116.48
3	A	1589	TPP	C5'-C4'-N4'	2.61	125.88	122.19
2	A	1588	FAD	N3-C2-N1	2.59	124.47	119.38
3	A	1589	TPP	C5-C4-N3	2.54	112.65	107.57
3	B	1590	TPP	CM2-C2'-N1'	2.53	119.92	117.14
2	B	1589	FAD	C4X-C10-N10	2.53	120.17	116.48
2	B	1589	FAD	C4-C4X-N5	2.47	121.74	118.23
3	A	1589	TPP	CM4-C4-C5	-2.32	122.53	127.60
2	A	1588	FAD	O2P-P-O1P	2.27	123.48	112.24
2	A	1588	FAD	C4-C4X-N5	2.24	121.42	118.23
2	A	1588	FAD	C1'-N10-C9A	2.21	124.20	120.51
3	A	1589	TPP	O3B-PB-O2B	2.20	116.05	107.64
2	A	1588	FAD	C4-N3-C2	-2.18	121.61	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1589	TPP	CM2-C2'-N3'	-2.14	113.81	117.15
2	A	1588	FAD	O4-C4-C4X	-2.09	121.06	126.60
2	B	1589	FAD	O4-C4-C4X	-2.08	121.07	126.60
2	A	1588	FAD	C2A-N1A-C6A	2.08	122.31	118.75
2	B	1589	FAD	O4'-C4'-C5'	-2.04	105.34	109.92
3	B	1590	TPP	C7'-N3-C2	-2.01	121.72	125.35

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1593	2PE	C15-C14-O13-C12
5	A	1594	PG4	C1-C2-O2-C3
7	A	1596	PEG	O1-C1-C2-O2
8	B	1593	2PE	O13-C14-C15-O16
8	B	1592	2PE	O7-C8-C9-O10
8	B	1592	2PE	C12-C11-O10-C9
8	B	1593	2PE	O7-C8-C9-O10
5	A	1595	PG4	O2-C3-C4-O3
5	B	1594	PG4	O3-C5-C6-O4
5	A	1593	PG4	O4-C7-C8-O5
6	A	1592	1PG	C4-C5-O3-C6
5	A	1594	PG4	O2-C3-C4-O3
5	A	1591	PG4	O2-C3-C4-O3
5	A	1595	PG4	O4-C7-C8-O5
5	B	1597	PG4	O1-C1-C2-O2
7	A	1596	PEG	O2-C3-C4-O4
7	A	1597	PEG	O2-C3-C4-O4
8	B	1593	2PE	O19-C20-C21-O22
5	B	1597	PG4	O3-C5-C6-O4
5	B	1595	PG4	O2-C3-C4-O3
5	A	1594	PG4	C3-C4-O3-C5
6	A	1592	1PG	O4-C8-C9-O5
5	A	1598	PG4	O2-C3-C4-O3
5	B	1595	PG4	C3-C4-O3-C5
5	B	1595	PG4	C4-C3-O2-C2
8	B	1593	2PE	O10-C11-C12-O13
8	B	1592	2PE	O16-C17-C18-O19
2	A	1588	FAD	PA-O3P-P-O5'
2	B	1589	FAD	PA-O3P-P-O5'
5	A	1595	PG4	C6-C5-O3-C4
5	A	1595	PG4	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
5	A	1593	PG4	C5-C6-O4-C7
3	B	1590	TPP	PA-O3A-PB-O3B
5	A	1593	PG4	C4-C3-O2-C2
5	B	1594	PG4	C6-C5-O3-C4
5	A	1593	PG4	C1-C2-O2-C3
7	B	1596	PEG	O2-C3-C4-O4
5	A	1598	PG4	C8-C7-O4-C6
5	A	1591	PG4	C1-C2-O2-C3
7	B	1596	PEG	C4-C3-O2-C2
7	B	1596	PEG	C1-C2-O2-C3
6	A	1592	1PG	O3-C6-C7-O4
6	A	1592	1PG	C11-C10-O5-C9
8	B	1593	2PE	C2-C3-O4-C5
2	A	1588	FAD	C4B-C5B-O5B-PA
8	B	1593	2PE	C17-C18-O19-C20
8	B	1592	2PE	O10-C11-C12-O13
5	A	1593	PG4	O3-C5-C6-O4
8	B	1593	2PE	O1-C2-C3-O4
2	B	1589	FAD	C4B-C5B-O5B-PA
2	A	1588	FAD	O4B-C4B-C5B-O5B
8	B	1593	2PE	C21-C20-O19-C18
8	B	1592	2PE	C17-C18-O19-C20
5	A	1595	PG4	O3-C5-C6-O4
5	A	1594	PG4	O1-C1-C2-O2
8	B	1592	2PE	C18-C17-O16-C15
3	A	1589	TPP	C5-C6-C7-O7
5	B	1597	PG4	C4-C3-O2-C2
5	A	1593	PG4	O1-C1-C2-O2
2	B	1589	FAD	O4B-C4B-C5B-O5B
8	B	1592	2PE	O4-C5-C6-O7
5	B	1594	PG4	O2-C3-C4-O3
6	A	1592	1PG	C8-C9-O5-C10
5	A	1591	PG4	O1-C1-C2-O2
8	B	1593	2PE	C6-C5-O4-C3
5	B	1594	PG4	C1-C2-O2-C3

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1594	PG4	1	0
2	A	1588	FAD	1	0

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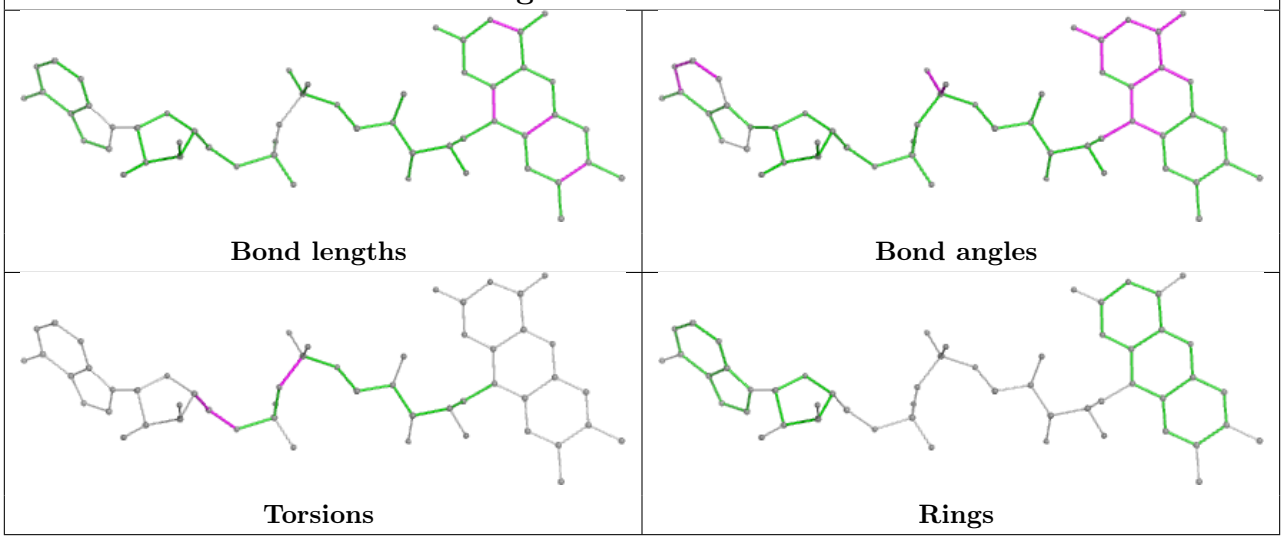
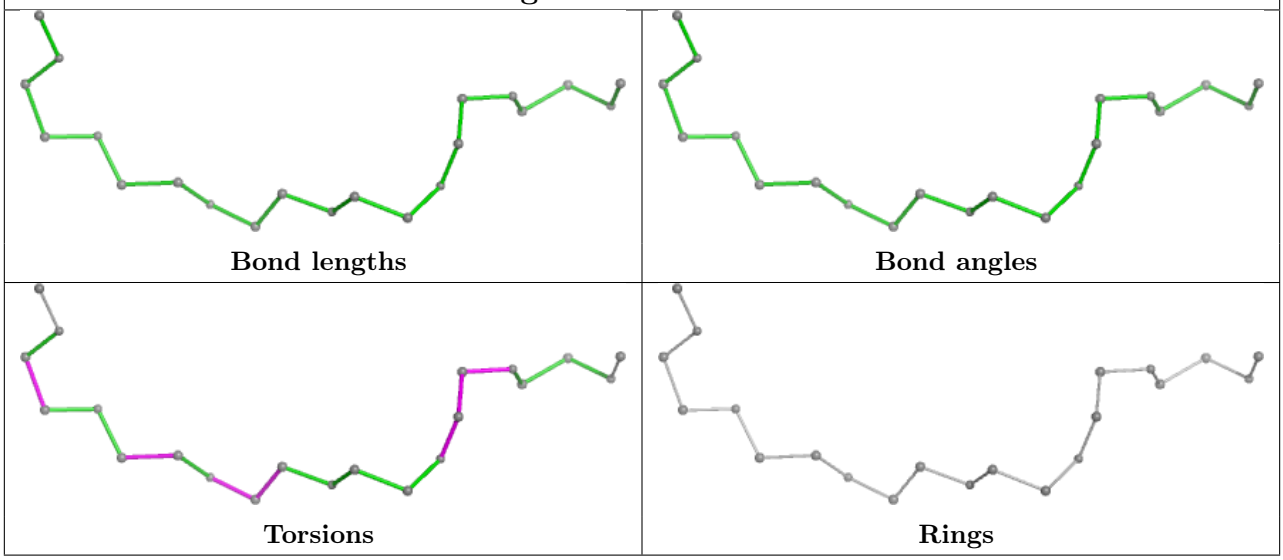
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1592	2PE	2	0
3	B	1590	TPP	1	0
7	A	1596	PEG	3	0
7	A	1597	PEG	2	0
5	A	1595	PG4	4	0
8	B	1593	2PE	1	0

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.

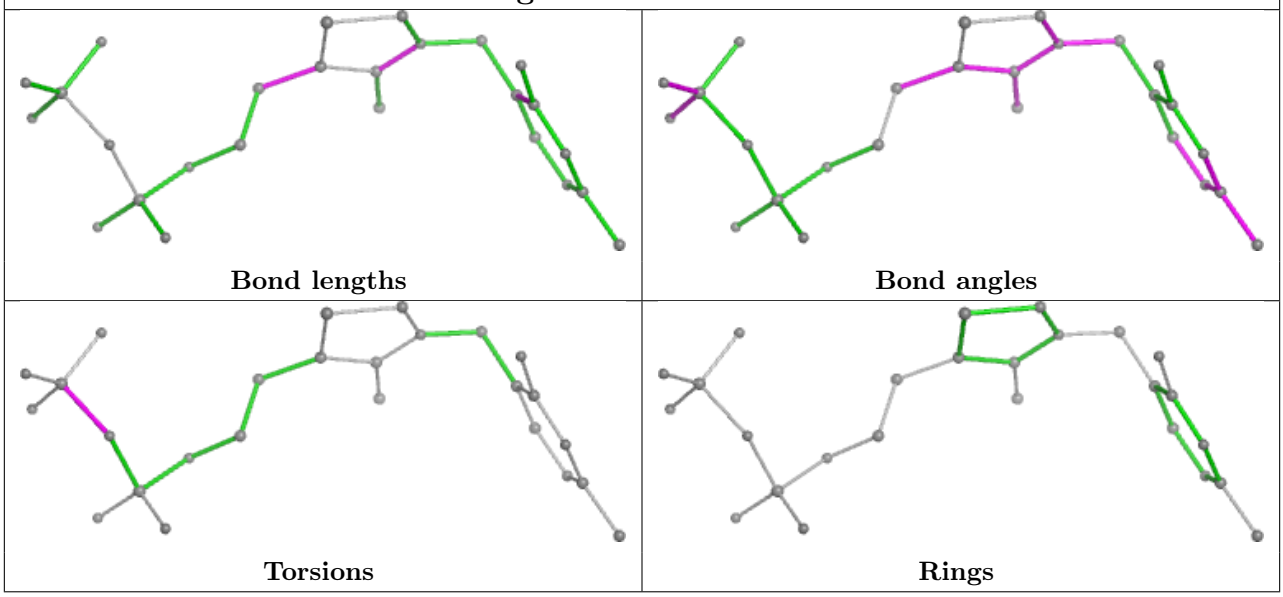
Ligand FAD A 1588



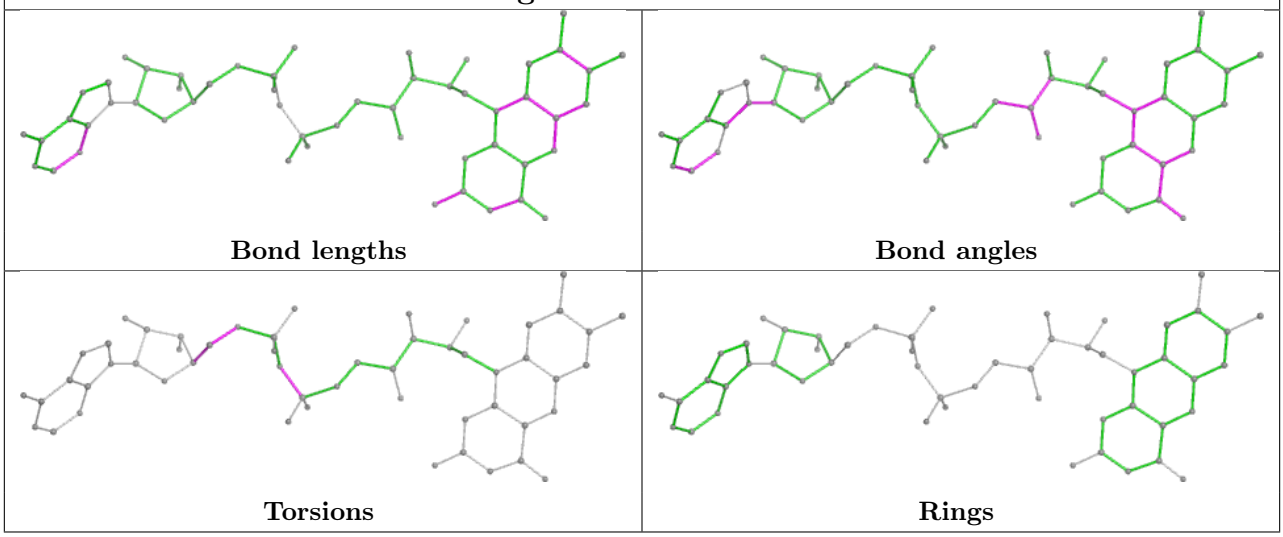
Ligand 2PE B 1592



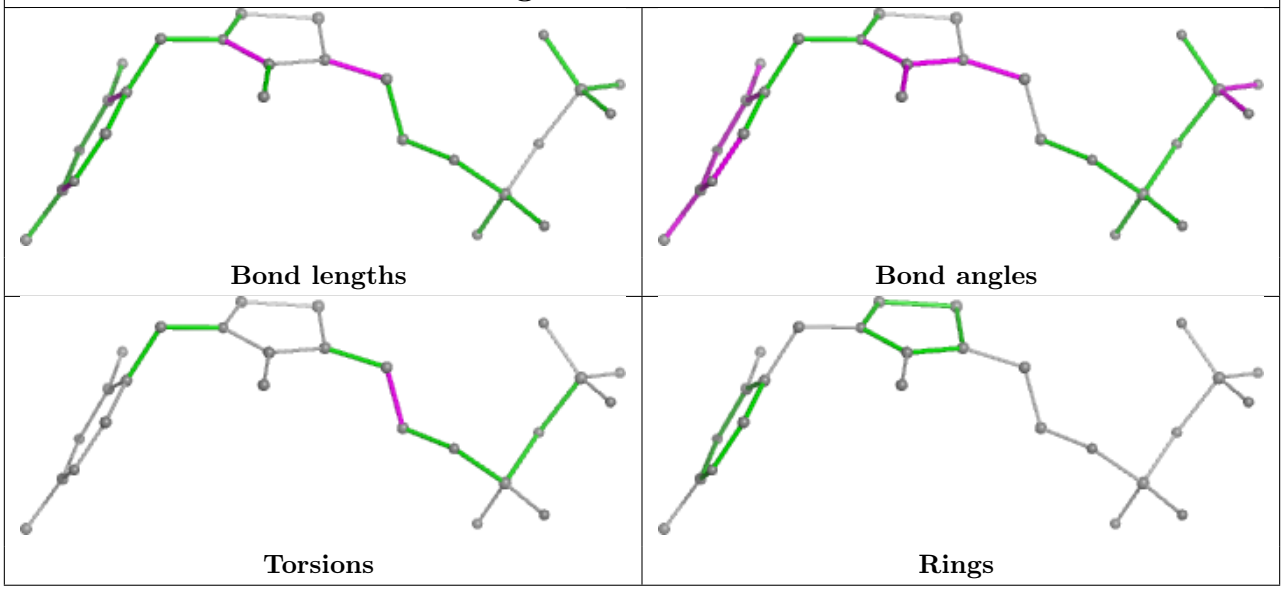
Ligand TPP B 1590



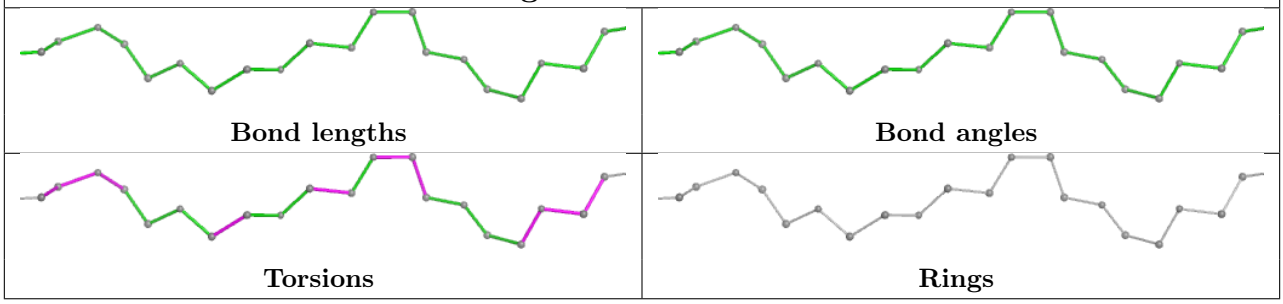
Ligand FAD B 1589



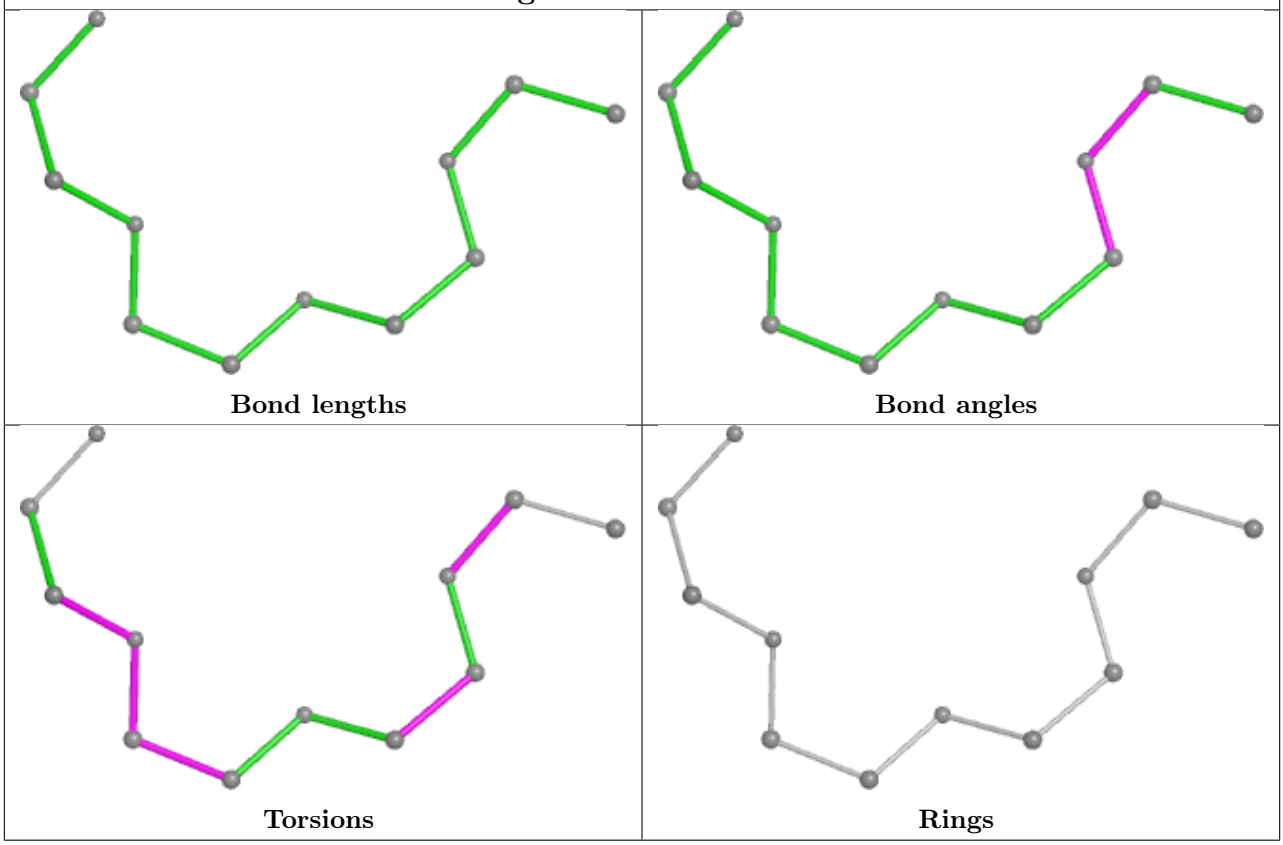
Ligand TPP A 1589



Ligand 2PE B 1593



Ligand 1PG A 1592



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	565:LEU	C	566:LYS	N	0.80

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	586/589 (99%)	-0.63	4 (0%)	87	87	11, 17, 35, 59	13 (2%)
1	B	587/589 (99%)	-0.63	10 (1%)	70	68	11, 18, 38, 61	16 (2%)
All	All	1173/1178 (99%)	-0.63	14 (1%)	79	78	11, 17, 37, 61	29 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	ASN	4.5
1	B	372	GLY	3.4
1	B	484	ASN	3.2
1	B	574	THR	3.1
1	B	342	VAL	3.1
1	B	2	ALA	3.0
1	B	343	ARG	2.9
1	B	369	SER	2.9
1	B	341	ALA	2.8
1	B	370	GLY	2.7
1	A	571	PRO	2.4
1	B	371	ASP	2.4
1	A	342	VAL	2.4
1	A	555	PRO	2.3

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

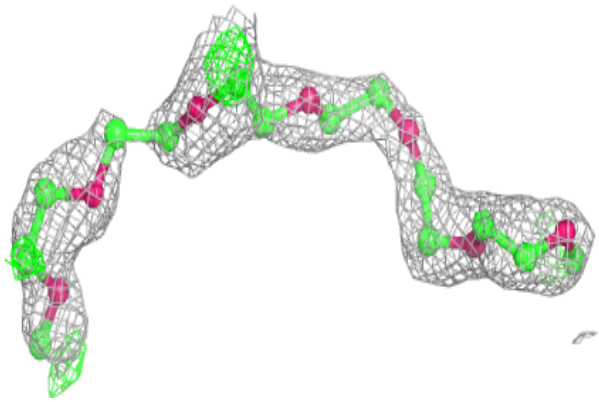
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

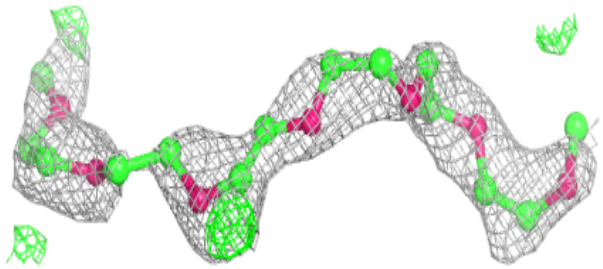
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PEG	A	1597	7/7	0.78	0.18	43,46,53,53	0
5	PG4	A	1595	11/13	0.80	0.19	1,37,54,57	0
7	PEG	A	1596	7/7	0.81	0.53	25,26,28,30	7
5	PG4	A	1591	11/13	0.81	0.14	31,37,44,44	0
5	PG4	A	1593	13/13	0.82	0.23	53,56,59,60	0
5	PG4	B	1594	10/13	0.83	0.14	31,41,44,46	0
7	PEG	B	1596	7/7	0.83	0.10	53,57,61,61	0
8	2PE	B	1592	21/28	0.83	0.21	44,52,57,60	0
6	1PG	A	1592	12/17	0.84	0.23	34,39,51,52	0
8	2PE	B	1593	22/28	0.84	0.20	33,40,56,62	22
5	PG4	B	1597	11/13	0.86	0.16	27,29,37,39	0
5	PG4	A	1594	8/13	0.87	0.15	43,45,54,56	0
5	PG4	A	1598	13/13	0.87	0.17	31,33,44,49	0
5	PG4	B	1595	6/13	0.91	0.13	38,40,43,44	0
5	PG4	A	1599	9/13	0.94	0.09	24,25,29,30	0
2	FAD	A	1588	53/53	0.98	0.06	9,12,14,16	0
2	FAD	B	1589	53/53	0.98	0.08	11,13,16,17	0
4	MG	A	1600	1/1	0.98	0.08	32,32,32,32	0
3	TPP	B	1590	26/26	0.99	0.06	11,14,16,20	0
3	TPP	A	1589	26/26	0.99	0.10	12,13,15,17	0
4	MG	B	1591	1/1	0.99	0.07	9,9,9,9	0
4	MG	A	1590	1/1	1.00	0.12	9,9,9,9	0

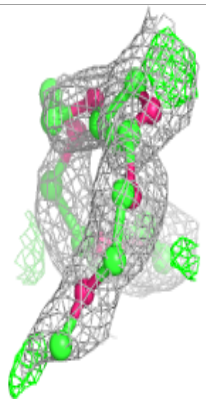
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2PE B 1592:

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

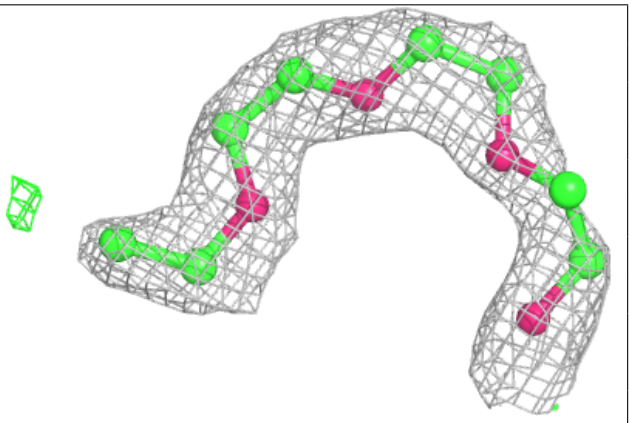


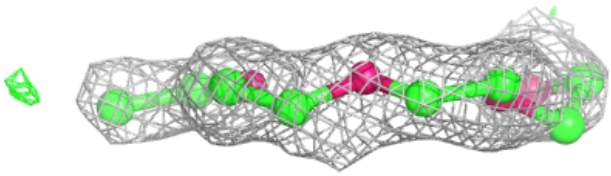


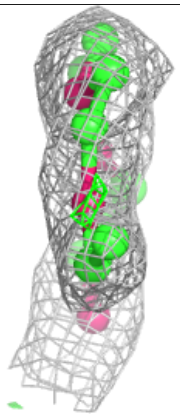


Electron density around 1PG A 1592:

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

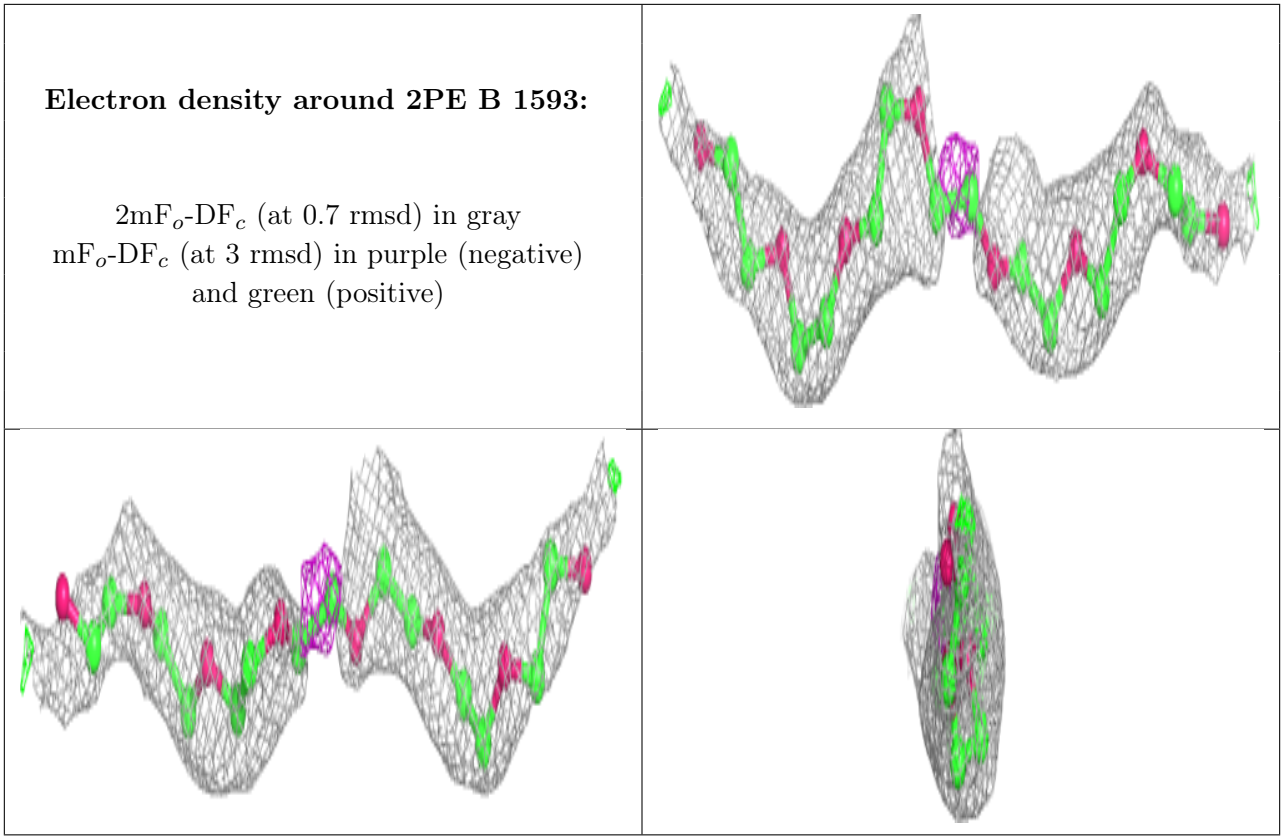






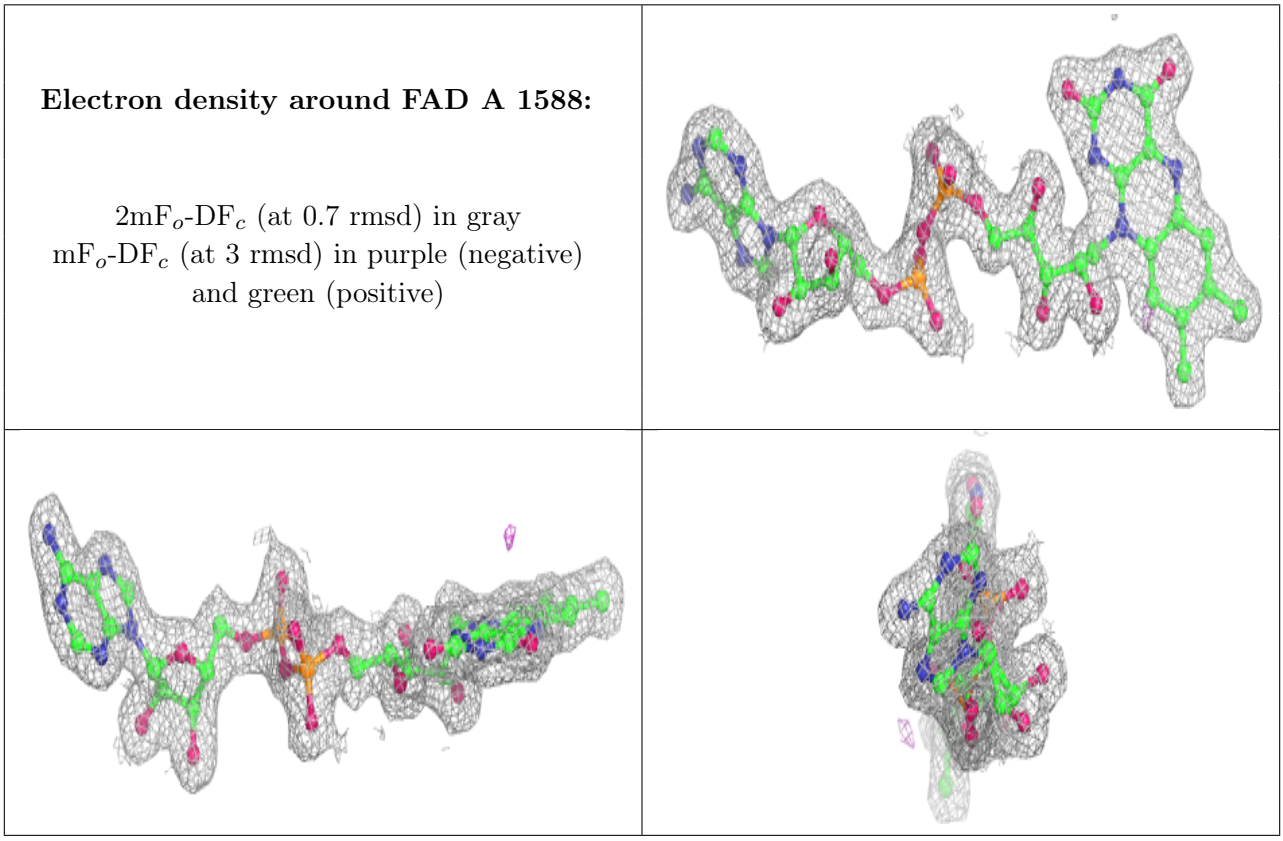
Electron density around 2PE B 1593:

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



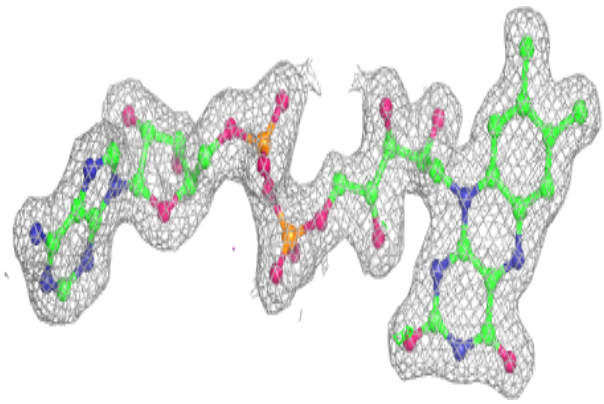
Electron density around FAD A 1588:

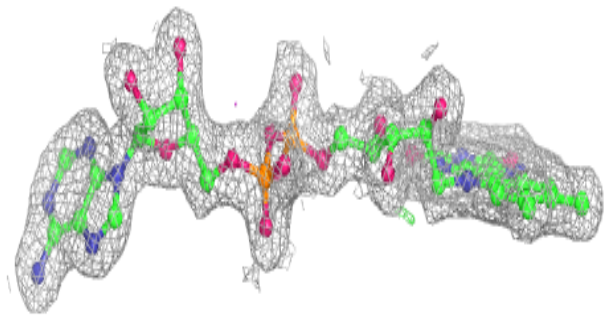
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

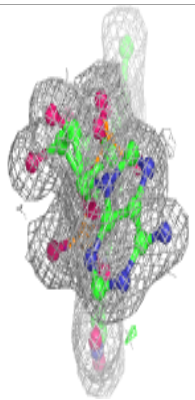


Electron density around FAD B 1589:

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

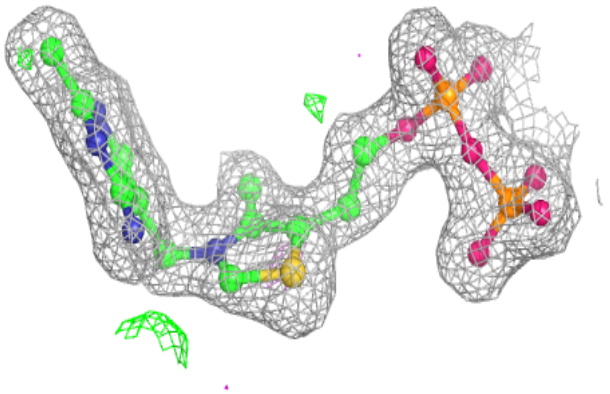


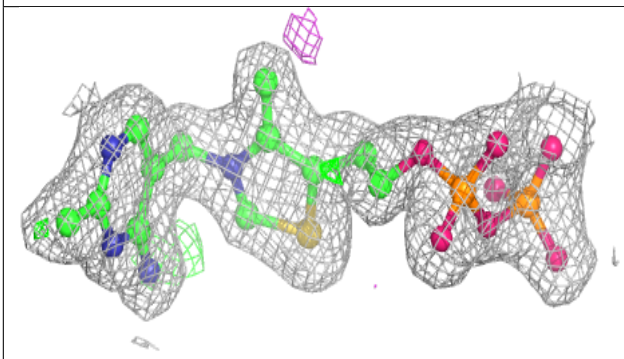


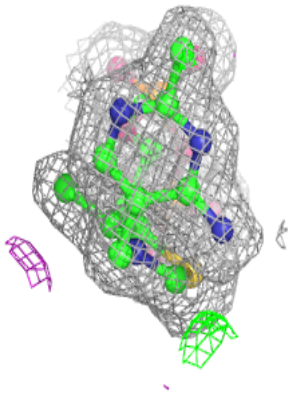


Electron density around TPP B 1590:

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







Electron density around TPP A 1589:

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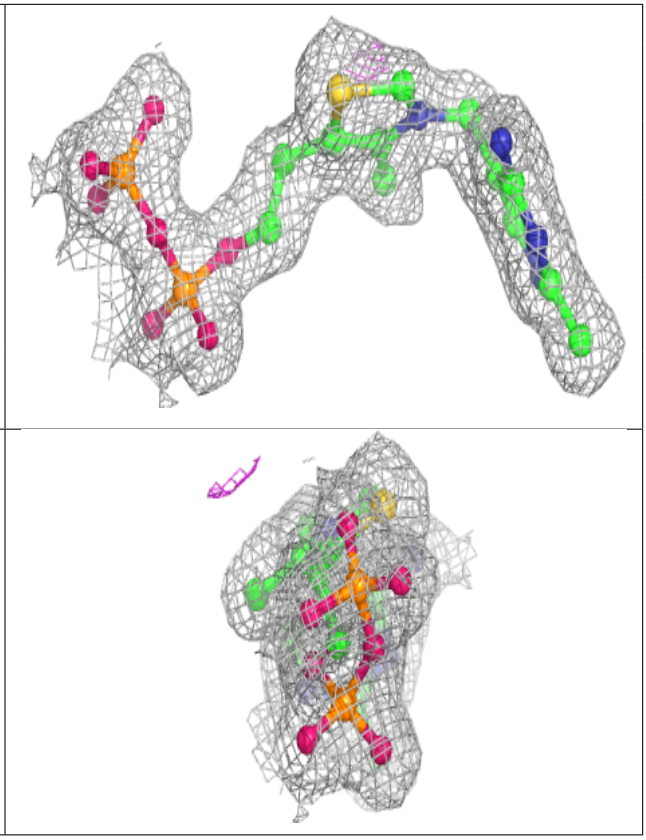
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.