



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2024 – 03:23 PM EDT

PDB ID : 4D5E
Title : Crystal Structure of recombinant wildtype CDH
Authors : Loschonsky, S.; Wacker, T.; Waltzer, S.; Giovannini, P.P.; McLeish, M.J.;
Andrade, S.L.A.; Mueller, M.
Deposited on : 2014-11-03
Resolution : 1.43 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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

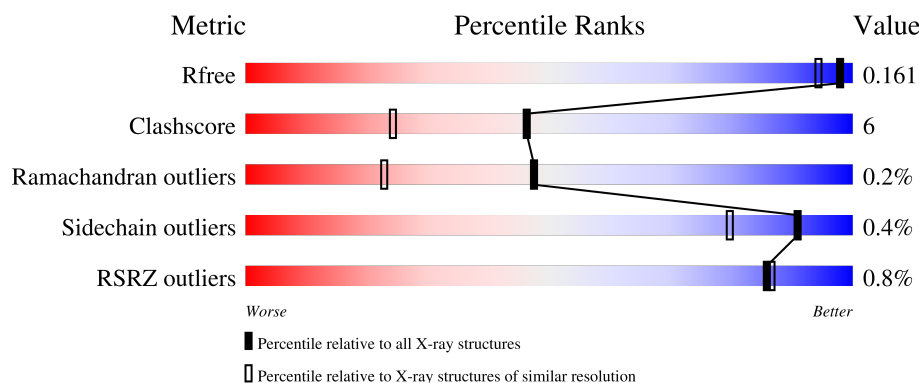
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.43 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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	589	 86% 11% ..
1	B	589	 87% 12% .

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
9	PG4	B	1596	-	-	X	-

2 Entry composition [i](#)

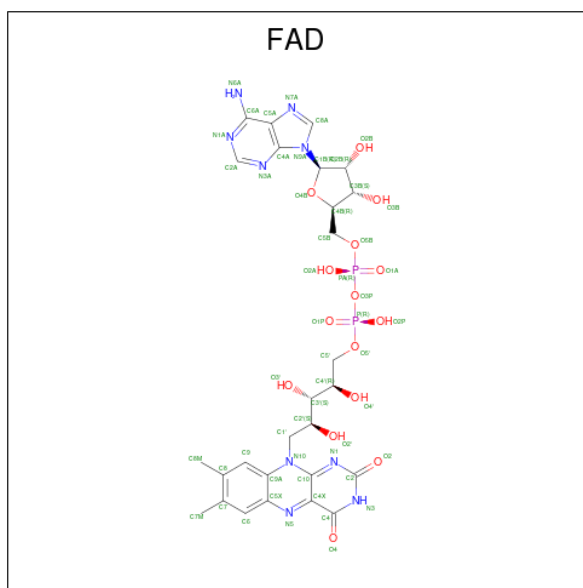
There are 12 unique types of molecules in this entry. The entry contains 10559 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

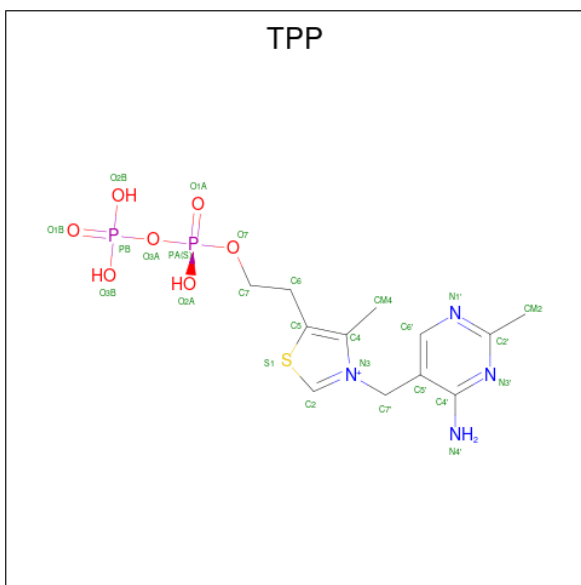
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	22	26	0
			4605	2917	812	851	25			
1	B	587	Total	C	N	O	S	41	21	0
			4598	2913	817	845	23			

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



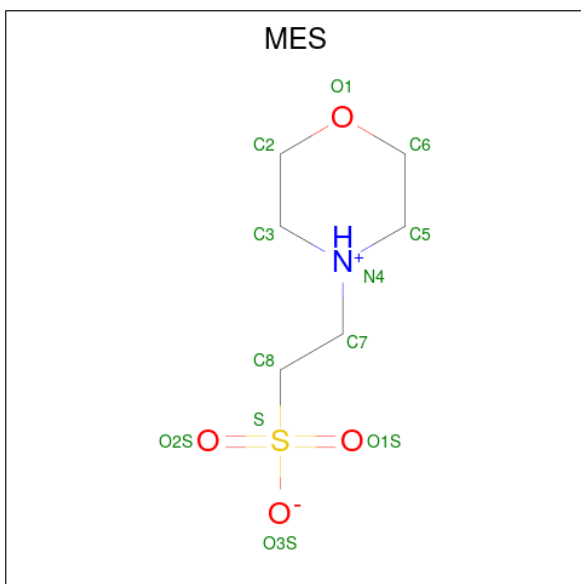
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

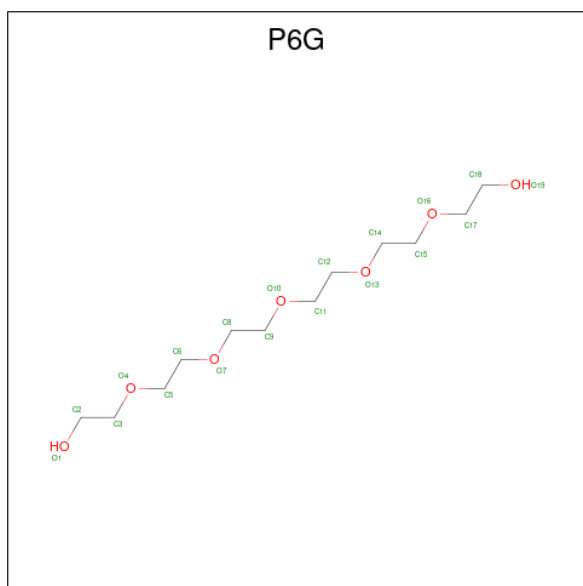
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

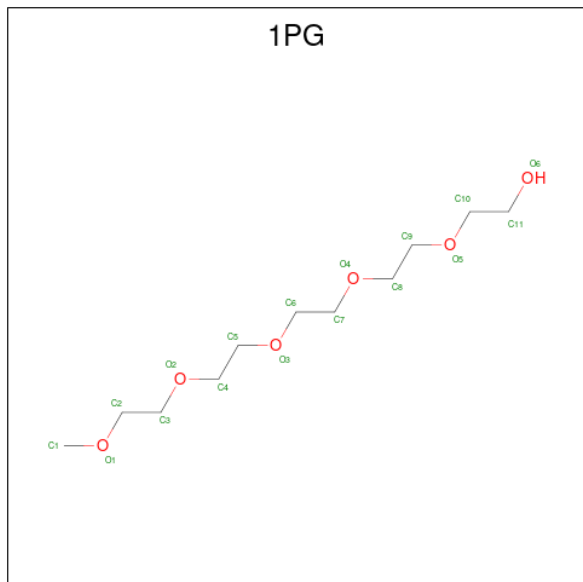
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	2	Total	Mg	0	0
			2	2		

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



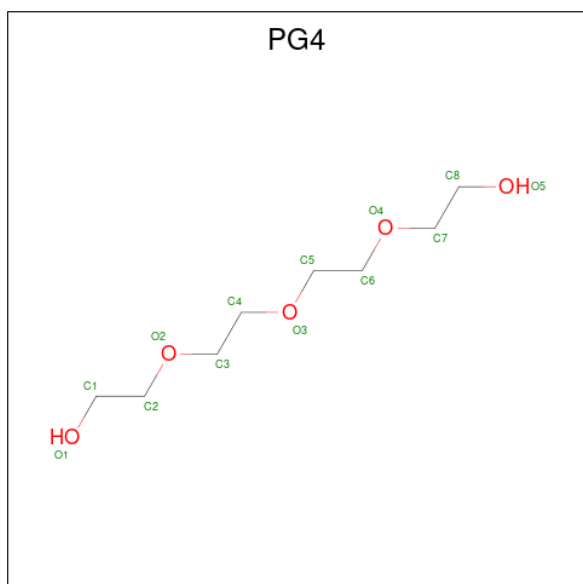
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			12	8	4		
7	A	1	Total	C	O	0	0
			17	11	6		

- Molecule 8 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (three-letter code: 1PG) (formula: C₁₁H₂₄O₆).



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

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



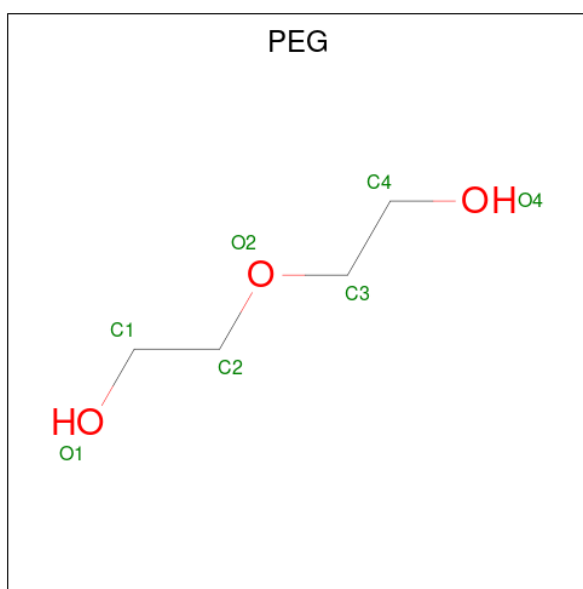
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			11	7	4		

Continued on next page...

Continued from previous page...

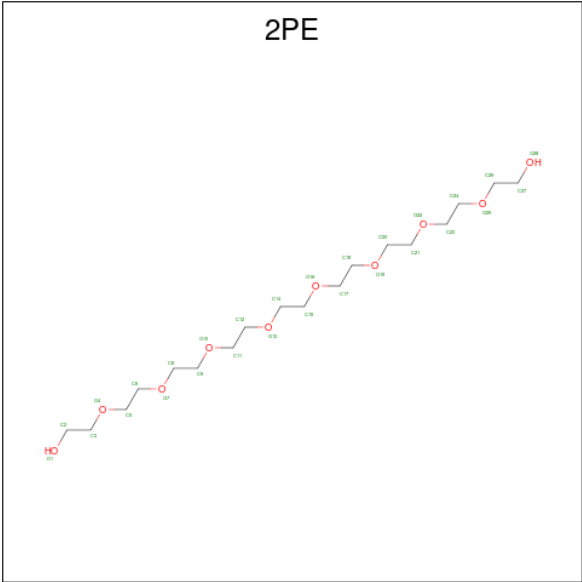
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	4	2		
9	A	1	Total	C	O	0	0
			13	8	5		
9	B	1	Total	C	O	0	0
			11	7	4		
9	B	1	Total	C	O	0	0
			6	4	2		
9	B	1	Total	C	O	0	0
			11	7	4		
9	B	1	Total	C	O	0	0
			8	5	3		
9	B	1	Total	C	O	0	0
			9	6	3		
9	B	1	Total	C	O	0	0
			8	6	2		

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



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

- Molecule 11 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			15	10	5		
11	B	1	Total	C	O	0	0
			19	12	7		
11	B	1	Total	C	O	0	0
			22	14	8		

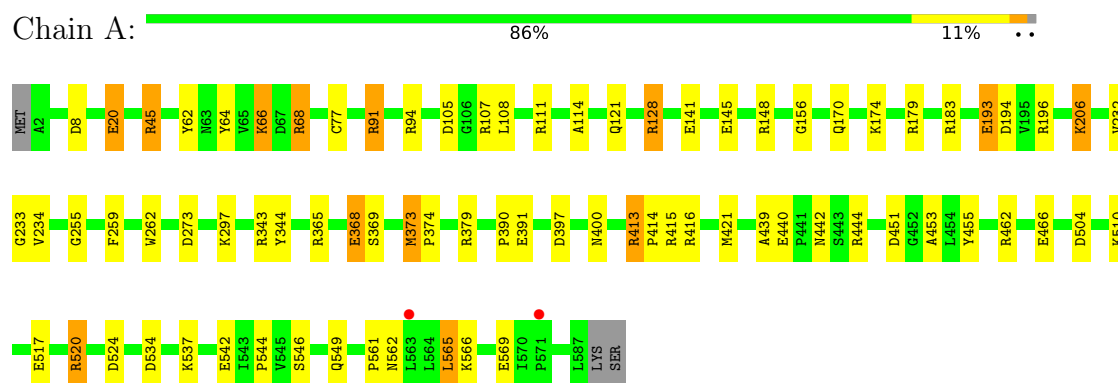
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	539	Total	O	0	0
			539	539		
12	B	431	Total	O	0	0
			431	431		

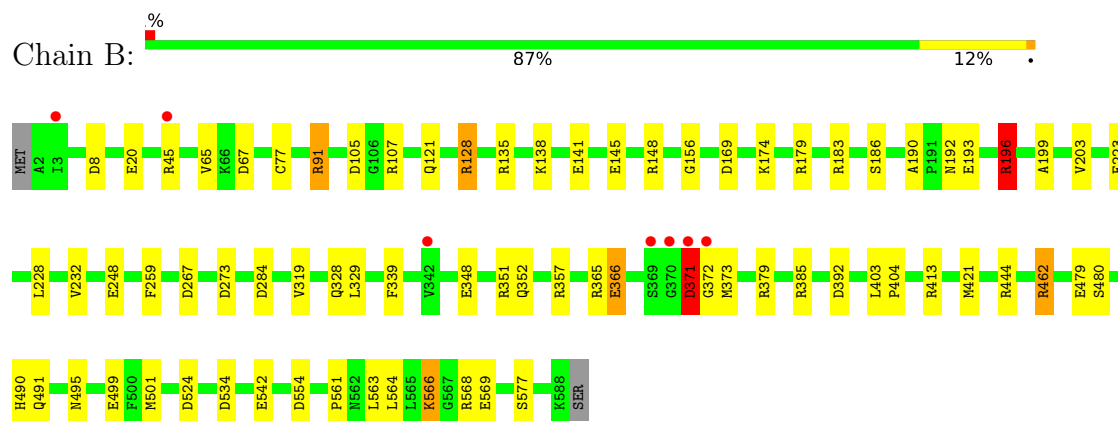
3 Residue-property plots

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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	123.19Å 123.19Å 143.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.68 – 1.43 46.68 – 1.43	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.68-1.43) 100.0 (46.68-1.43)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.122 , 0.147 0.138 , 0.161	Depositor DCC
R_{free} test set	10152 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10559	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: TPP, P6G, 1PG, MES, PG4, PEG, CL, MG, 2PE, FAD

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	2.55	30/4750 (0.6%)	2.17	54/6447 (0.8%)
1	B	2.30	22/4725 (0.5%)	1.79	49/6409 (0.8%)
All	All	2.43	52/9475 (0.5%)	1.99	103/12856 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	1	4
All	All	1	5

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20[A]	GLU	CD-OE2	-103.26	0.12	1.25
1	A	20[B]	GLU	CD-OE2	-103.26	0.12	1.25
1	B	348	GLU	CD-OE2	-68.21	0.50	1.25
1	B	196[A]	ARG	CZ-NH2	-55.03	0.61	1.33
1	B	196[B]	ARG	CZ-NH2	-55.03	0.61	1.33
1	B	348	GLU	CD-OE1	40.96	1.70	1.25
1	B	196[A]	ARG	CZ-NH1	40.65	1.85	1.33
1	B	196[B]	ARG	CZ-NH1	40.65	1.85	1.33
1	B	348	GLU	CG-CD	39.78	2.11	1.51
1	A	174	LYS	CD-CE	-33.22	0.68	1.51
1	B	366	GLU	CD-OE1	-24.93	0.98	1.25
1	A	569	GLU	CG-CD	-20.80	1.20	1.51
1	A	206	LYS	CE-NZ	19.82	1.98	1.49
1	B	223	GLU	CG-CD	18.58	1.79	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	LYS	CD-CE	-17.67	1.07	1.51
1	A	20[A]	GLU	CD-OE1	-12.63	1.11	1.25
1	A	20[B]	GLU	CD-OE1	-12.63	1.11	1.25
1	A	20[A]	GLU	CG-CD	11.46	1.69	1.51
1	A	20[B]	GLU	CG-CD	11.46	1.69	1.51
1	A	343	ARG	CD-NE	11.46	1.66	1.46
1	B	348	GLU	CB-CG	-11.28	1.30	1.52
1	A	440	GLU	CD-OE2	-8.84	1.16	1.25
1	A	193	GLU	CD-OE1	8.81	1.35	1.25
1	A	510	LYS	CD-CE	8.18	1.71	1.51
1	B	413	ARG	NE-CZ	8.15	1.43	1.33
1	A	413[A]	ARG	CD-NE	-7.82	1.33	1.46
1	A	413[B]	ARG	CD-NE	-7.82	1.33	1.46
1	B	141	GLU	CD-OE1	-7.67	1.17	1.25
1	B	371	ASP	C-O	7.43	1.37	1.23
1	A	141	GLU	CD-OE1	-6.94	1.18	1.25
1	A	141	GLU	CD-OE2	-6.54	1.18	1.25
1	B	145	GLU	CD-OE2	6.52	1.32	1.25
1	A	546[A]	SER	CB-OG	-6.35	1.33	1.42
1	A	546[B]	SER	CB-OG	-6.35	1.33	1.42
1	A	193	GLU	CG-CD	6.32	1.61	1.51
1	A	442	ASN	CB-CG	6.23	1.65	1.51
1	B	479	GLU	CD-OE2	6.22	1.32	1.25
1	B	479	GLU	CD-OE1	-6.09	1.19	1.25
1	A	64	TYR	CE1-CZ	-6.05	1.30	1.38
1	A	68	ARG	CZ-NH1	6.01	1.40	1.33
1	B	577	SER	CA-CB	-6.01	1.44	1.52
1	A	141	GLU	CG-CD	5.61	1.60	1.51
1	B	499	GLU	CG-CD	-5.60	1.43	1.51
1	A	391	GLU	CB-CG	-5.54	1.41	1.52
1	A	128[A]	ARG	CZ-NH1	-5.54	1.25	1.33
1	A	128[B]	ARG	CZ-NH1	-5.54	1.25	1.33
1	B	569	GLU	CD-OE2	-5.34	1.19	1.25
1	A	145	GLU	CD-OE2	5.30	1.31	1.25
1	B	566	LYS	C-N	-5.29	1.23	1.33
1	B	248	GLU	CD-OE2	5.25	1.31	1.25
1	B	193	GLU	CD-OE1	5.08	1.31	1.25
1	A	94	ARG	CG-CD	-5.01	1.39	1.51

All (103) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20[A]	GLU	OE1-CD-OE2	-100.02	3.27	123.30
1	A	20[B]	GLU	OE1-CD-OE2	-100.02	3.27	123.30
1	B	196[A]	ARG	NE-CZ-NH1	-63.72	88.44	120.30
1	B	196[B]	ARG	NE-CZ-NH1	-63.72	88.44	120.30
1	B	348	GLU	OE1-CD-OE2	28.48	157.48	123.30
1	B	371	ASP	O-C-N	-24.76	81.10	123.20
1	B	348	GLU	CG-CD-OE1	-21.08	76.14	118.30
1	A	174	LYS	CG-CD-CE	18.61	167.73	111.90
1	B	366	GLU	OE1-CD-OE2	-15.43	104.78	123.30
1	A	206	LYS	CD-CE-NZ	-13.65	80.30	111.70
1	B	193	GLU	OE1-CD-OE2	13.17	139.10	123.30
1	A	174	LYS	CD-CE-NZ	12.60	140.69	111.70
1	A	68	ARG	NE-CZ-NH2	-12.11	114.24	120.30
1	B	196[A]	ARG	NE-CZ-NH2	11.48	126.04	120.30
1	B	196[B]	ARG	NE-CZ-NH2	11.48	126.04	120.30
1	B	193	GLU	CG-CD-OE2	-11.20	95.90	118.30
1	B	196[A]	ARG	NH1-CZ-NH2	10.63	131.09	119.40
1	B	196[B]	ARG	NH1-CZ-NH2	10.63	131.09	119.40
1	B	366	GLU	CG-CD-OE1	10.35	138.99	118.30
1	A	91[A]	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	A	91[B]	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	B	174	LYS	CB-CG-CD	9.73	136.91	111.60
1	A	569	GLU	CB-CG-CD	9.15	138.90	114.20
1	B	107	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	91[A]	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	A	91[B]	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	A	45	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	B	223	GLU	CB-CG-CD	-8.32	91.74	114.20
1	B	357	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	105	ASP	CB-CG-OD2	-8.16	110.96	118.30
1	B	128[A]	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	B	128[B]	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	B	348	GLU	CA-CB-CG	8.03	131.07	113.40
1	B	128[A]	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	128[B]	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	135	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	B	554	ASP	CB-CG-OD1	7.84	125.35	118.30
1	A	111	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	B	105	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	A	68	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	A	524	ASP	CB-CG-OD2	-7.67	111.39	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	462	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	128[A]	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	A	128[B]	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	A	107	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	45	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	373[A]	MET	CG-SD-CE	7.41	112.06	100.20
1	A	373[B]	MET	CG-SD-CE	7.41	112.06	100.20
1	B	107	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	504	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	A	107	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	91[A]	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	91[B]	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	392	ASP	CB-CG-OD2	-7.11	111.91	118.30
1	B	444	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	343	ARG	CG-CD-NE	-7.04	97.02	111.80
1	B	138	LYS	CD-CE-NZ	-6.94	95.73	111.70
1	A	534	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	A	297	LYS	CG-CD-CE	6.83	132.39	111.90
1	A	148	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	108	LEU	CB-CG-CD1	6.77	122.51	111.00
1	B	371	ASP	CA-CB-CG	6.66	128.05	113.40
1	B	462	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	534	ASP	CB-CG-OD1	-6.43	112.51	118.30
1	A	66	LYS	CD-CE-NZ	6.43	126.48	111.70
1	B	105	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	67	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	B	444	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	462	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	520	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	B	183	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	A	196	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	416	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	A	451	ASP	CB-CG-OD1	6.13	123.81	118.30
1	B	273	ASP	CB-CG-OD1	6.05	123.74	118.30
1	B	554	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	A	194	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	179[A]	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	179[B]	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	62	TYR	CB-CG-CD1	5.80	124.48	121.00
1	A	444	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	344	TYR	CB-CG-CD2	5.73	124.44	121.00
1	B	169	ASP	CB-CG-OD1	5.63	123.37	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	B	524	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	A	128[A]	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	128[B]	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	193	GLU	CG-CD-OE1	5.50	129.31	118.30
1	A	415	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	273	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	517	GLU	OE1-CD-OE2	-5.44	116.77	123.30
1	B	385	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	8	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	91[A]	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	B	91[B]	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	A	413[A]	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	413[B]	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	351	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	373	MET	CG-SD-CE	5.25	108.59	100.20
1	A	94	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	267	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	A	368	GLU	CG-CD-OE1	5.12	128.53	118.30
1	A	562	ASN	C-N-CA	-5.06	109.05	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	371	ASP	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	GLY	Mainchain
1	B	196[A]	ARG	Sidechain
1	B	371	ASP	Mainchain
1	B	372	GLY	Peptide
1	B	480[B]	SER	Peptide

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	4605	0	4551	49	0
1	B	4598	0	4549	50	1
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	26	0	16	1	0
3	B	26	0	16	1	0
4	A	24	0	26	4	0
4	B	12	0	13	0	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	A	29	0	33	9	0
8	A	12	0	14	1	0
9	A	30	0	36	3	0
9	B	53	0	60	12	0
10	A	7	0	10	1	0
11	A	15	0	19	1	0
11	B	41	0	54	5	0
12	A	539	0	0	27	1
12	B	431	0	0	15	0
All	All	10559	0	9459	119	2

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 6.

All (119) 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:379[B]:ARG:HD3	12:B:2286:HOH:O	1.42	1.19
1:B:121[B]:GLN:NE2	12:B:2084:HOH:O	1.70	1.19
1:A:121[B]:GLN:OE1	12:A:2129:HOH:O	1.57	1.18
1:B:259[A]:PHE:CD2	1:B:561:PRO:HD3	1.89	1.06
7:A:1595:P6G:H91	12:A:2530:HOH:O	1.59	1.00
1:B:259[A]:PHE:CE2	1:B:561:PRO:HD3	1.95	0.99
7:A:1593:P6G:H92	12:A:2526:HOH:O	1.67	0.94
1:B:563[B]:LEU:H	1:B:563[B]:LEU:CD1	1.82	0.91
1:B:190:ALA:H	1:B:328:GLN:HE22	1.17	0.90
1:B:563[B]:LEU:H	1:B:563[B]:LEU:HD12	1.41	0.86
1:A:520:ARG:NH2	1:A:542[B]:GLU:OE2	2.10	0.85
1:B:568:ARG:HH22	9:B:1596:PG4:H21	1.40	0.85
1:A:232:VAL:HG12	1:A:234[A]:VAL:HG23	1.59	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413[B]:ARG:NH1	12:A:2395:HOH:O	2.09	0.82
1:A:259[B]:PHE:CD2	1:A:561:PRO:HD3	2.15	0.82
7:A:1593:P6G:H111	12:A:2528:HOH:O	1.81	0.80
1:A:413[A]:ARG:HD2	12:A:2394:HOH:O	1.81	0.79
1:A:121[B]:GLN:HE21	1:A:121[B]:GLN:H	1.29	0.79
3:A:1589:TPP:H2	5:B:1592:CL:CL	2.23	0.76
1:A:390[A]:PRO:O	1:A:413[A]:ARG:HD3	1.86	0.76
1:A:170:GLN:HG3	12:A:2182:HOH:O	1.85	0.76
1:A:259[B]:PHE:CE2	1:A:561:PRO:HD3	2.25	0.72
1:A:369[A]:SER:OG	12:A:2361:HOH:O	2.08	0.72
1:A:232:VAL:HG12	1:A:234[A]:VAL:CG2	2.21	0.71
4:A:1590[B]:MES:H32	12:A:2233:HOH:O	1.92	0.70
1:A:365:ARG:HD3	12:A:2360:HOH:O	1.91	0.70
7:A:1595:P6G:H142	12:A:2531:HOH:O	1.91	0.70
5:A:1591:CL:CL	3:B:1590:TPP:H2	2.29	0.70
1:B:319:VAL:HG21	11:B:1595:2PE:H151	1.75	0.68
1:A:20[B]:GLU:OE2	1:A:68:ARG:NH2	2.27	0.68
1:B:566:LYS:HD2	12:B:2408:HOH:O	1.94	0.68
7:A:1595:P6G:H61	12:A:2530:HOH:O	1.95	0.65
1:B:568:ARG:NH2	9:B:1596:PG4:H21	2.11	0.65
1:A:232:VAL:O	4:A:1590[B]:MES:H61	1.97	0.64
11:A:1598:2PE:H142	12:A:2532:HOH:O	1.95	0.64
1:B:501[B]:MET:O	1:B:501[B]:MET:HG3	1.96	0.64
1:B:566:LYS:CD	12:B:2408:HOH:O	2.46	0.63
1:B:568:ARG:HH22	9:B:1596:PG4:C2	2.11	0.63
1:B:561:PRO:O	1:B:563[B]:LEU:HD12	1.98	0.62
1:B:379[B]:ARG:NH2	12:B:2288:HOH:O	2.19	0.62
1:B:365[A]:ARG:NH1	12:B:2281:HOH:O	2.14	0.61
1:B:563[B]:LEU:HD22	1:B:564:LEU:HD23	1.83	0.61
7:A:1593:P6G:C3	12:A:2179:HOH:O	2.49	0.60
1:A:193:GLU:OE2	12:A:2220:HOH:O	2.16	0.59
1:B:568:ARG:NH1	9:B:1596:PG4:O1	2.37	0.58
7:A:1595:P6G:C6	12:A:2530:HOH:O	2.53	0.57
1:B:179:ARG:NH1	12:B:2138:HOH:O	2.38	0.56
9:B:1602:PG4:H22	12:B:2040:HOH:O	2.05	0.55
1:A:259[B]:PHE:CE2	1:A:561:PRO:HG3	2.42	0.55
1:A:206:LYS:CG	1:A:206:LYS:NZ	2.69	0.55
12:A:2184:HOH:O	9:B:1596:PG4:H12	2.07	0.54
1:A:413[B]:ARG:NH1	12:A:2396:HOH:O	2.37	0.54
9:B:1602:PG4:C2	12:B:2040:HOH:O	2.55	0.54
1:A:373[B]:MET:HA	1:A:374:PRO:C	2.28	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563[B]:LEU:HD22	1:B:564:LEU:CD2	2.38	0.54
1:A:413[A]:ARG:CG	12:A:2394:HOH:O	2.56	0.53
1:A:232:VAL:CG1	1:A:234[A]:VAL:HG23	2.37	0.53
1:A:91[B]:ARG:HH12	10:A:1597:PEG:H41	1.72	0.53
1:A:374:PRO:HG2	12:A:2525:HOH:O	2.08	0.53
1:B:490:HIS:HE1	12:B:2344:HOH:O	1.90	0.53
1:A:373[B]:MET:CE	1:A:544:PRO:HD2	2.38	0.53
1:B:568:ARG:CZ	9:B:1596:PG4:O1	2.59	0.51
7:A:1593:P6G:C3	12:A:2525:HOH:O	2.59	0.51
1:A:373[B]:MET:HE2	1:A:544:PRO:HD2	1.93	0.51
1:A:259[B]:PHE:CE2	1:A:561:PRO:CD	2.94	0.50
1:B:192:ASN:HD21	1:B:196[A]:ARG:HE	1.59	0.50
1:B:365[A]:ARG:HD3	12:B:2281:HOH:O	2.10	0.50
1:B:563[B]:LEU:H	1:B:563[B]:LEU:HD13	1.74	0.50
1:A:232:VAL:CG1	1:A:234[A]:VAL:CG2	2.89	0.49
1:B:563[B]:LEU:CD1	1:B:563[B]:LEU:N	2.58	0.49
1:B:259[A]:PHE:CE2	1:B:561:PRO:CD	2.83	0.48
1:B:352:GLN:HG3	12:B:2266:HOH:O	2.11	0.48
7:A:1593:P6G:H51	12:A:2526:HOH:O	2.12	0.48
1:A:121[B]:GLN:H	1:A:121[B]:GLN:NE2	2.05	0.48
1:B:91[A]:ARG:HE	1:B:128[A]:ARG:NH1	2.12	0.48
1:A:466:GLU:OE1	9:A:1599:PG4:H42	2.14	0.47
1:B:568:ARG:NH2	9:B:1596:PG4:C1	2.77	0.47
1:A:206:LYS:NZ	1:A:206:LYS:HG2	2.29	0.47
1:A:66:LYS:HE2	1:A:439:ALA:HB1	1.96	0.47
4:A:1590[B]:MES:H31	4:A:1590[B]:MES:H82	1.75	0.46
1:B:568:ARG:NH2	9:B:1596:PG4:O1	2.48	0.46
9:B:1596:PG4:H11	9:B:1596:PG4:H32	1.83	0.46
1:B:228:LEU:O	1:B:232:VAL:HG22	2.15	0.45
11:B:1595:2PE:H91	12:B:2124:HOH:O	2.16	0.45
1:A:121[B]:GLN:CD	12:A:2129:HOH:O	2.33	0.45
1:A:183:ARG:CZ	12:A:2169:HOH:O	2.65	0.45
1:A:455:TYR:CZ	1:B:462:ARG:HD3	2.51	0.45
9:A:1596:PG4:H51	12:A:2111:HOH:O	2.15	0.45
1:B:148:ARG:HA	9:B:1602:PG4:H32	1.97	0.45
1:A:565:LEU:C	1:A:565:LEU:HD12	2.37	0.45
1:B:186:SER:HB3	11:B:1595:2PE:H22	1.98	0.44
1:A:421:MET:O	2:A:1588:FAD:H9	2.17	0.44
1:B:403:LEU:HB3	1:B:404:PRO:HD3	1.99	0.44
1:A:368:GLU:O	1:A:379:ARG:HD3	2.18	0.44
1:A:413[B]:ARG:HB2	1:A:414:PRO:CD	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65[B]:VAL:HG12	12:B:2048:HOH:O	2.18	0.43
1:A:45:ARG:NE	12:A:2027:HOH:O	2.51	0.43
1:B:421:MET:O	2:B:1589:FAD:H9	2.18	0.43
1:B:91[A]:ARG:O	1:B:128[A]:ARG:NH2	2.51	0.43
1:B:203[B]:VAL:HG21	1:B:339:PHE:HA	2.01	0.43
1:A:128[A]:ARG:HD2	1:A:156:GLY:HA3	1.99	0.43
1:A:466:GLU:OE1	9:A:1599:PG4:C4	2.67	0.42
4:A:1590[A]:MES:H32	4:A:1590[A]:MES:H81	1.47	0.42
1:B:563[B]:LEU:HD12	1:B:563[B]:LEU:N	2.22	0.42
11:B:1595:2PE:H52	11:B:1595:2PE:H81	1.82	0.42
1:B:495:ASN:H	1:B:495:ASN:ND2	2.18	0.42
1:A:397:ASP:CG	1:A:453:ALA:HB1	2.40	0.41
1:A:114:ALA:HA	1:B:284:ASP:HB2	2.02	0.41
1:B:128[A]:ARG:HD2	1:B:156:GLY:HA3	2.02	0.41
1:B:199:ALA:HB2	1:B:329[A]:LEU:CD1	2.51	0.41
11:B:1597:2PE:O10	12:B:2327:HOH:O	2.22	0.41
1:A:255:GLY:HA3	1:A:262:TRP:CE3	2.55	0.41
1:B:91[A]:ARG:CD	1:B:128[A]:ARG:HG2	2.51	0.41
1:B:491:GLN:HG3	1:B:564:LEU:HD13	2.03	0.40
1:A:466:GLU:HG3	1:B:501[B]:MET:HG2	2.03	0.40
1:B:20:GLU:O	1:B:45:ARG:HD3	2.20	0.40
1:A:400:ASN:HB3	1:A:549:GLN:O	2.22	0.40
1:A:183:ARG:CD	12:A:2171:HOH:O	2.70	0.40
1:A:537:LYS:NZ	8:A:1594:1PG:C9	2.84	0.40

All (2) 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)
12:A:2528:HOH:O	12:A:2534:HOH:O[3_445]	2.06	0.14
1:B:366:GLU:OE2	1:B:366:GLU:OE2[8_444]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	610/589 (104%)	599 (98%)	10 (2%)	1 (0%)	47	23
1	B	606/589 (103%)	595 (98%)	10 (2%)	1 (0%)	47	23
All	All	1216/1178 (103%)	1194 (98%)	20 (2%)	2 (0%)	47	23

All (2) Ramachandran outliers are listed below:

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

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	475/453 (105%)	473 (100%)	2 (0%)	91	80
1	B	472/453 (104%)	469 (99%)	3 (1%)	86	68
All	All	947/906 (104%)	942 (100%)	5 (0%)	91	74

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	565	LEU
1	A	566	LYS
1	B	371	ASP
1	B	542[A]	GLU
1	B	542[B]	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	116	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	170	GLN
1	A	412	GLN
1	A	442	ASN
1	B	116	GLN
1	B	153	HIS
1	B	328	GLN
1	B	490	HIS
1	B	495	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 28 ligands modelled in this entry, 5 are monoatomic - leaving 23 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
4	MES	A	1590[B]	-	12,12,12	2.16	2 (16%)	14,16,16	2.97	7 (50%)
9	PG4	B	1598	-	5,5,12	0.65	0	4,4,11	0.61	0
7	P6G	A	1595	-	16,16,18	1.29	2 (12%)	15,15,17	2.11	2 (13%)
9	PG4	B	1599	-	10,10,12	0.51	0	9,9,11	0.56	0
9	PG4	B	1601	-	8,8,12	0.51	0	7,7,11	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PG4	A	1596	-	10,10,12	1.28	1 (10%)	9,9,11	1.27	1 (11%)
9	PG4	A	1600	-	12,12,12	0.73	0	11,11,11	0.88	0
9	PG4	B	1602	-	7,7,12	1.18	0	6,6,11	0.66	0
9	PG4	B	1600	-	7,7,12	1.04	0	6,6,11	0.41	0
3	TPP	B	1590	6	22,27,27	2.08	3 (13%)	29,40,40	1.69	6 (20%)
11	2PE	A	1598	-	14,14,27	0.75	0	13,13,26	1.34	1 (7%)
9	PG4	B	1596	-	10,10,12	1.99	4 (40%)	9,9,11	2.54	3 (33%)
10	PEG	A	1597	-	6,6,6	0.28	0	5,5,5	1.02	0
11	2PE	B	1597	-	21,21,27	0.73	0	20,20,26	1.21	1 (5%)
4	MES	A	1590[A]	-	12,12,12	3.32	2 (16%)	14,16,16	4.08	7 (50%)
9	PG4	A	1599	-	5,5,12	0.60	0	4,4,11	0.67	0
8	1PG	A	1594	-	11,11,16	0.63	0	10,10,15	0.99	0
2	FAD	A	1588	-	53,58,58	1.01	4 (7%)	68,89,89	1.07	2 (2%)
11	2PE	B	1595	-	18,18,27	1.18	2 (11%)	17,17,26	1.13	2 (11%)
3	TPP	A	1589	6	22,27,27	1.52	3 (13%)	29,40,40	1.59	4 (13%)
4	MES	B	1591	-	12,12,12	1.72	2 (16%)	14,16,16	1.76	3 (21%)
7	P6G	A	1593	-	11,11,18	0.94	0	10,10,17	1.74	3 (30%)
2	FAD	B	1589	-	53,58,58	1.20	6 (11%)	68,89,89	1.37	12 (17%)

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
4	MES	A	1590[B]	-	-	6/6/14/14	0/1/1/1
9	PG4	B	1598	-	-	1/3/3/10	-
7	P6G	A	1595	-	-	10/14/14/16	-
9	PG4	B	1599	-	-	2/8/8/10	-
9	PG4	B	1601	-	-	2/6/6/10	-
9	PG4	A	1596	-	-	3/8/8/10	-
9	PG4	A	1600	-	-	1/10/10/10	-
9	PG4	B	1602	-	-	3/5/5/10	-
9	PG4	B	1600	-	-	0/5/5/10	-
3	TPP	B	1590	6	-	0/16/17/17	0/2/2/2
11	2PE	A	1598	-	-	6/12/12/25	-
9	PG4	B	1596	-	-	3/8/8/10	-
10	PEG	A	1597	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	2PE	B	1597	-	-	14/19/19/25	-
4	MES	A	1590[A]	-	-	4/6/14/14	0/1/1/1
9	PG4	A	1599	-	-	1/3/3/10	-
8	1PG	A	1594	-	-	1/9/9/14	-
2	FAD	A	1588	-	-	3/30/50/50	0/6/6/6
11	2PE	B	1595	-	-	8/16/16/25	-
3	TPP	A	1589	6	-	0/16/17/17	0/2/2/2
4	MES	B	1591	-	-	0/6/14/14	0/1/1/1
7	P6G	A	1593	-	-	4/9/9/16	-
2	FAD	B	1589	-	-	3/30/50/50	0/6/6/6

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1590[A]	MES	C8-S	-10.67	1.62	1.77
3	B	1590	TPP	C4-N3	-8.39	1.32	1.39
4	A	1590[B]	MES	C8-S	-6.40	1.68	1.77
3	A	1589	TPP	C6-C5	-4.45	1.49	1.50
9	B	1596	PG4	O2-C2	3.63	1.57	1.42
7	A	1595	P6G	O13-C14	3.59	1.57	1.42
2	B	1589	FAD	C2A-N3A	3.55	1.37	1.32
4	B	1591	MES	C8-S	-3.42	1.72	1.77
11	B	1595	2PE	O10-C11	3.35	1.56	1.42
2	B	1589	FAD	C4-N3	-3.31	1.32	1.38
4	A	1590[A]	MES	O2S-S	3.28	1.54	1.45
9	B	1596	PG4	O3-C4	3.20	1.55	1.42
4	B	1591	MES	O1S-S	3.18	1.54	1.45
2	B	1589	FAD	C5'-C4'	-3.09	1.47	1.51
7	A	1595	P6G	O13-C12	3.02	1.55	1.42
4	A	1590[B]	MES	C7-N4	2.67	1.53	1.47
2	A	1588	FAD	C9-C8	2.56	1.43	1.39
3	A	1589	TPP	C2'-N1'	2.53	1.38	1.34
3	B	1590	TPP	C7'-N3	2.53	1.53	1.48
3	A	1589	TPP	C5'-C4'	2.36	1.47	1.42
2	A	1588	FAD	C2A-N3A	2.35	1.35	1.32
2	A	1588	FAD	O4B-C1B	2.31	1.44	1.41
2	A	1588	FAD	C4X-N5	2.29	1.35	1.30
11	B	1595	2PE	O10-C9	-2.29	1.32	1.42
2	B	1589	FAD	O4B-C1B	2.25	1.44	1.41
2	B	1589	FAD	C7M-C7	-2.20	1.46	1.51
9	B	1596	PG4	O4-C6	2.19	1.53	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1596	PG4	O1-C1	-2.16	1.30	1.42
9	B	1596	PG4	O2-C3	2.14	1.51	1.42
2	B	1589	FAD	C10-N10	2.12	1.42	1.37
3	B	1590	TPP	C6-C5	2.05	1.51	1.50

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1590[A]	MES	O1S-S-C8	10.20	119.20	106.92
4	A	1590[B]	MES	O1S-S-C8	6.90	115.22	106.92
4	A	1590[A]	MES	C2-C3-N4	6.29	119.64	110.10
4	A	1590[A]	MES	O2S-S-C8	5.56	113.61	106.92
7	A	1595	P6G	O13-C12-C11	5.49	135.15	110.39
4	A	1590[B]	MES	O2S-S-C8	5.42	113.44	106.92
7	A	1595	P6G	O13-C14-C15	5.28	134.21	110.39
9	B	1596	PG4	C3-O2-C2	-5.23	90.63	113.29
4	A	1590[A]	MES	O3S-S-O1S	-4.49	100.30	111.27
2	A	1588	FAD	C4A-C5A-N7A	4.38	113.96	109.40
3	A	1589	TPP	C6-C5-C4	4.33	130.91	127.43
9	B	1596	PG4	C5-O3-C4	-4.23	94.97	113.29
4	A	1590[A]	MES	O3S-S-C8	-4.18	99.01	105.77
4	B	1591	MES	O3S-S-C8	4.11	112.41	105.77
3	B	1590	TPP	C7'-N3-C2	-4.02	118.09	125.35
3	B	1590	TPP	C6-C5-C4	4.01	130.65	127.43
4	A	1590[B]	MES	C2-C3-N4	-3.41	104.94	110.10
4	A	1590[B]	MES	C7-N4-C5	3.03	118.97	111.23
2	B	1589	FAD	C2A-N1A-C6A	3.03	123.93	118.75
11	B	1597	2PE	C17-O16-C15	3.02	126.35	113.29
2	B	1589	FAD	O4-C4-C4X	-2.99	118.67	126.60
4	A	1590[B]	MES	O1-C2-C3	-2.96	105.27	111.80
4	B	1591	MES	O3S-S-O2S	-2.91	104.16	111.27
2	B	1589	FAD	C6-C5X-C9A	2.91	123.06	118.94
7	A	1593	P6G	C3-O4-C5	-2.88	95.03	112.96
2	A	1588	FAD	N3A-C2A-N1A	-2.88	124.18	128.68
11	A	1598	2PE	C14-O13-C12	2.86	123.13	112.90
3	A	1589	TPP	C7'-N3-C2	-2.84	120.23	125.35
4	A	1590[B]	MES	O3S-S-O2S	-2.74	104.57	111.27
2	B	1589	FAD	C8M-C8-C9	-2.69	114.52	119.49
2	B	1589	FAD	C5A-C6A-N1A	-2.63	114.38	120.35
7	A	1593	P6G	O10-C11-C12	2.52	121.78	110.39
3	A	1589	TPP	N1'-C2'-N3'	-2.51	121.22	125.54
4	A	1590[A]	MES	C6-O1-C2	2.50	118.25	109.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1590	TPP	C6'-N1'-C2'	2.45	120.14	115.96
2	B	1589	FAD	C9-C8-C7	2.45	123.17	119.67
2	B	1589	FAD	O2-C2-N1	-2.44	117.78	121.83
3	A	1589	TPP	CM2-C2'-N1'	2.39	119.77	117.14
7	A	1593	P6G	O10-C9-C8	2.33	120.89	110.39
3	B	1590	TPP	N4'-C4'-N3'	-2.32	113.75	117.03
11	B	1595	2PE	O10-C9-C8	-2.32	99.95	110.39
2	B	1589	FAD	C5A-C6A-N6A	2.29	123.83	120.35
2	B	1589	FAD	C4-C4X-N5	2.28	121.48	118.23
3	B	1590	TPP	N1'-C2'-N3'	-2.27	121.64	125.54
11	B	1595	2PE	C8-O7-C6	-2.26	103.49	113.29
2	B	1589	FAD	N3A-C2A-N1A	-2.24	125.17	128.68
2	B	1589	FAD	C6-C7-C8	-2.11	116.64	119.67
2	B	1589	FAD	C9A-C5X-N5	-2.10	120.15	122.43
9	B	1596	PG4	O2-C3-C4	2.08	119.78	110.39
3	B	1590	TPP	C5'-C4'-N3'	2.04	124.45	121.24
4	A	1590[B]	MES	O2S-S-O1S	-2.04	106.89	113.95
4	B	1591	MES	O1-C2-C3	-2.02	107.34	111.80
4	A	1590[A]	MES	O1-C2-C3	2.00	116.20	111.80
9	A	1596	PG4	O2-C2-C1	-2.00	101.28	110.07

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1588	FAD	PA-O3P-P-O5'
4	A	1590[A]	MES	C8-C7-N4-C3
4	A	1590[A]	MES	C7-C8-S-O2S
4	A	1590[B]	MES	C8-C7-N4-C3
4	A	1590[B]	MES	C7-C8-S-O1S
11	B	1597	2PE	C14-C15-O16-C17
7	A	1595	P6G	C14-C15-O16-C17
9	B	1602	PG4	C3-C4-O3-C5
11	A	1598	2PE	C2-C3-O4-C5
11	B	1597	2PE	O4-C5-C6-O7
11	B	1595	2PE	O7-C8-C9-O10
9	B	1596	PG4	O3-C5-C6-O4
9	B	1599	PG4	O2-C3-C4-O3
11	B	1597	2PE	C6-C5-O4-C3
7	A	1593	P6G	O4-C5-C6-O7
9	A	1599	PG4	O2-C3-C4-O3
4	A	1590[B]	MES	C7-C8-S-O3S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	1600	PG4	O1-C1-C2-O2
11	A	1598	2PE	O1-C2-C3-O4
11	B	1595	2PE	O1-C2-C3-O4
9	A	1596	PG4	O3-C5-C6-O4
9	B	1602	PG4	C1-C2-O2-C3
11	B	1595	2PE	O13-C14-C15-O16
7	A	1593	P6G	O10-C11-C12-O13
11	B	1597	2PE	C2-C3-O4-C5
11	B	1597	2PE	O16-C17-C18-O19
11	B	1595	2PE	O16-C17-C18-O19
4	A	1590[A]	MES	C7-C8-S-O3S
9	A	1596	PG4	O1-C1-C2-O2
7	A	1595	P6G	O16-C17-C18-O19
11	B	1597	2PE	O1-C2-C3-O4
11	B	1597	2PE	O7-C8-C9-O10
9	B	1601	PG4	C6-C5-O3-C4
9	B	1602	PG4	O2-C3-C4-O3
2	B	1589	FAD	PA-O3P-P-O5'
8	A	1594	1PG	O3-C6-C7-O4
7	A	1595	P6G	C15-C14-O13-C12
11	B	1597	2PE	C9-C8-O7-C6
7	A	1595	P6G	C6-C5-O4-C3
9	B	1599	PG4	C6-C5-O3-C4
11	B	1597	2PE	C11-C12-O13-C14
7	A	1595	P6G	C11-C12-O13-C14
11	B	1597	2PE	O10-C11-C12-O13
11	A	1598	2PE	C11-C12-O13-C14
11	B	1597	2PE	C15-C14-O13-C12
4	A	1590[A]	MES	C7-C8-S-O1S
4	A	1590[B]	MES	C7-C8-S-O2S
11	A	1598	2PE	C12-C11-O10-C9
7	A	1595	P6G	C5-C6-O7-C8
11	B	1597	2PE	C5-C6-O7-C8
7	A	1595	P6G	O10-C11-C12-O13
7	A	1595	P6G	C9-C8-O7-C6
11	B	1595	2PE	C6-C5-O4-C3
11	B	1595	2PE	C14-C15-O16-C17
11	A	1598	2PE	C6-C5-O4-C3
2	B	1589	FAD	C4B-C5B-O5B-PA
11	B	1597	2PE	C21-C20-O19-C18
9	B	1598	PG4	O1-C1-C2-O2
4	A	1590[B]	MES	C8-C7-N4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1588	FAD	O4B-C4B-C5B-O5B
7	A	1593	P6G	C9-C8-O7-C6
2	B	1589	FAD	O4B-C4B-C5B-O5B
11	B	1597	2PE	C18-C17-O16-C15
9	B	1596	PG4	C3-C4-O3-C5
11	A	1598	2PE	O4-C5-C6-O7
2	A	1588	FAD	C4B-C5B-O5B-PA
9	B	1601	PG4	C4-C3-O2-C2
11	B	1595	2PE	C15-C14-O13-C12
7	A	1593	P6G	O7-C8-C9-O10
11	B	1595	2PE	O4-C5-C6-O7
7	A	1595	P6G	O13-C14-C15-O16
4	A	1590[B]	MES	N4-C7-C8-S
9	A	1596	PG4	O2-C3-C4-O3
9	B	1596	PG4	O2-C3-C4-O3
7	A	1595	P6G	O7-C8-C9-O10

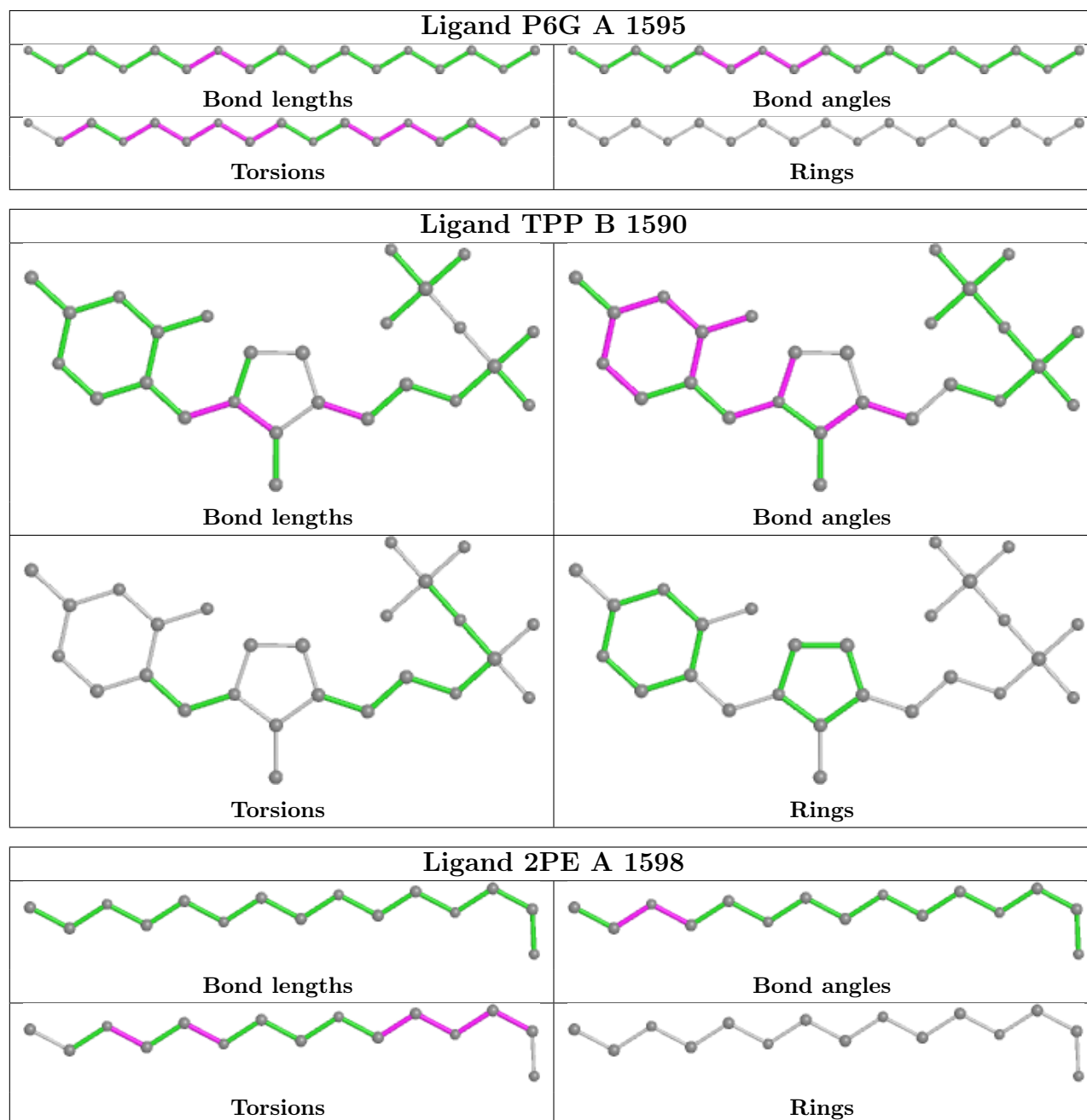
There are no ring outliers.

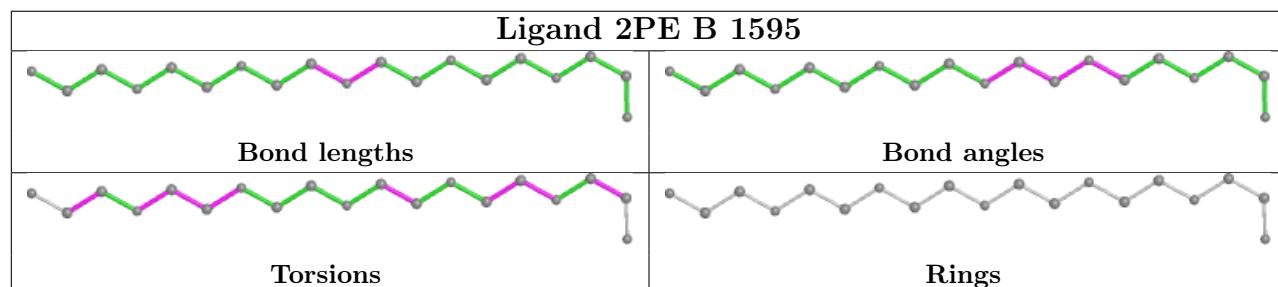
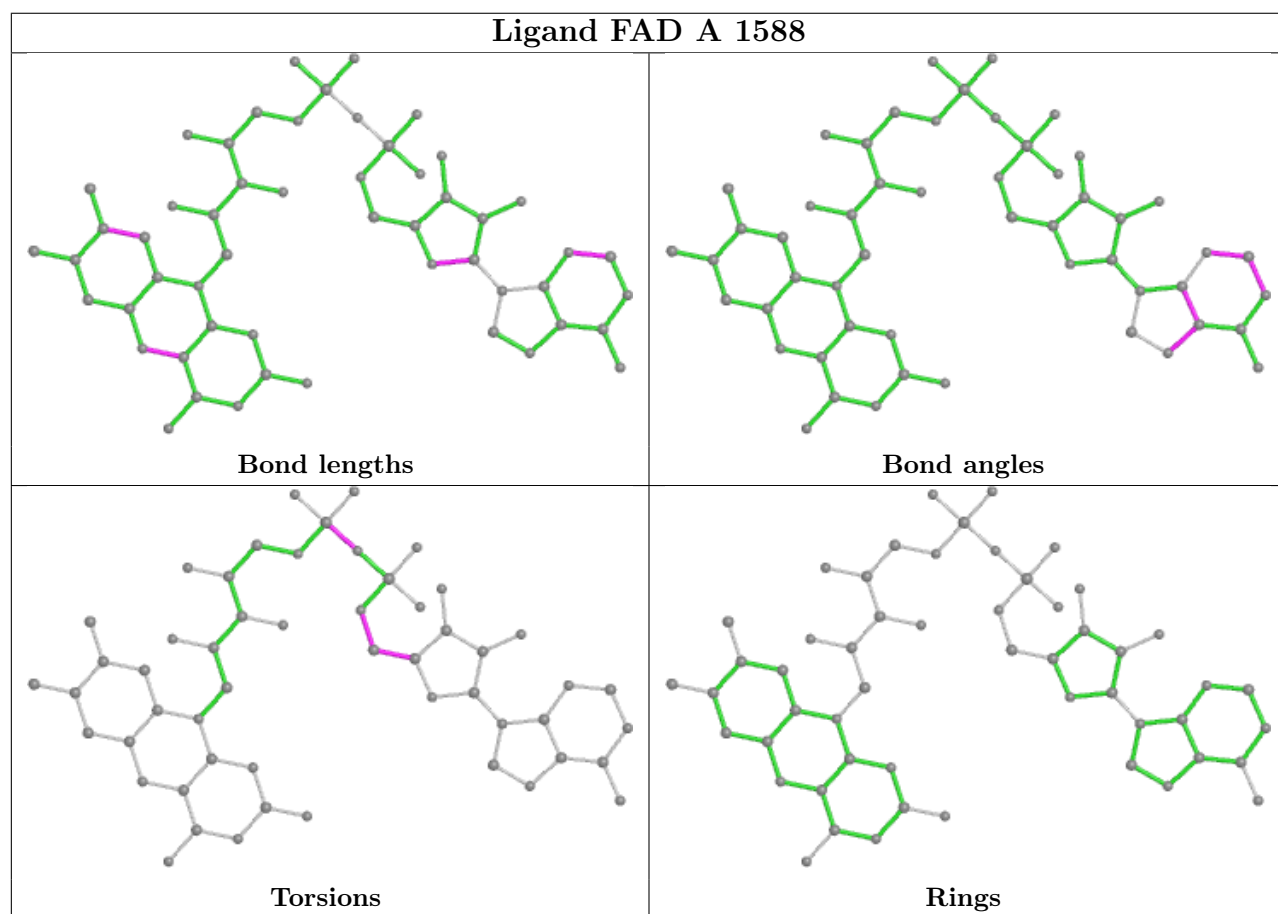
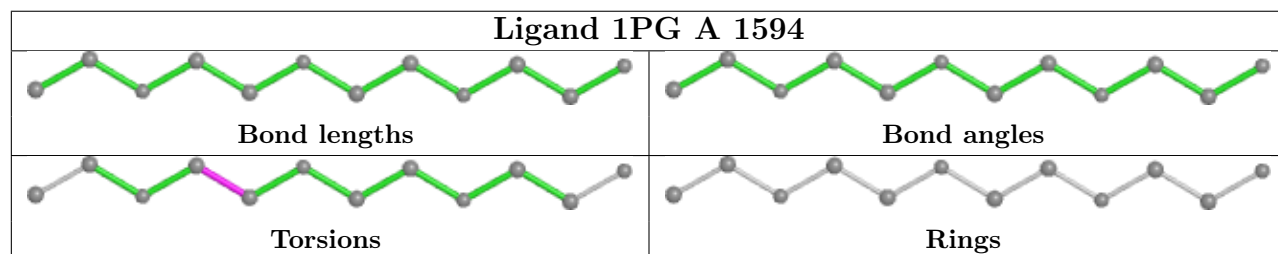
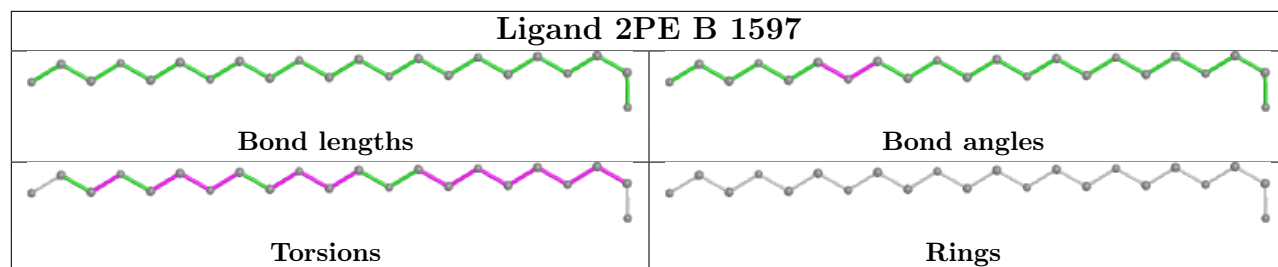
17 monomers are involved in 40 short contacts:

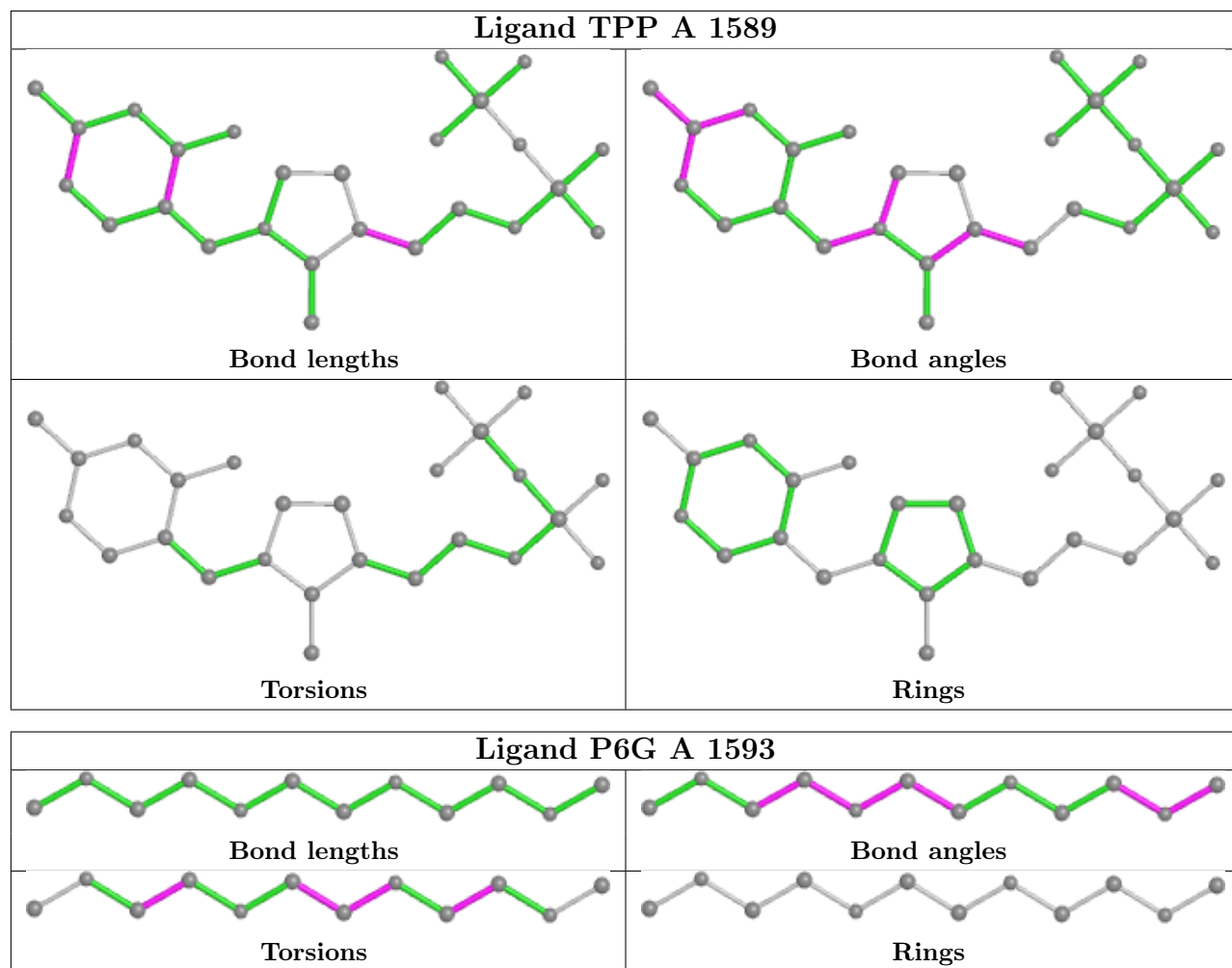
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1590[B]	MES	3	0
7	A	1595	P6G	4	0
9	A	1596	PG4	1	0
9	B	1602	PG4	3	0
3	B	1590	TPP	1	0
11	A	1598	2PE	1	0
9	B	1596	PG4	9	0
10	A	1597	PEG	1	0
11	B	1597	2PE	1	0
4	A	1590[A]	MES	1	0
9	A	1599	PG4	2	0
8	A	1594	1PG	1	0
2	A	1588	FAD	1	0
11	B	1595	2PE	4	0
3	A	1589	TPP	1	0
7	A	1593	P6G	5	0
2	B	1589	FAD	1	0

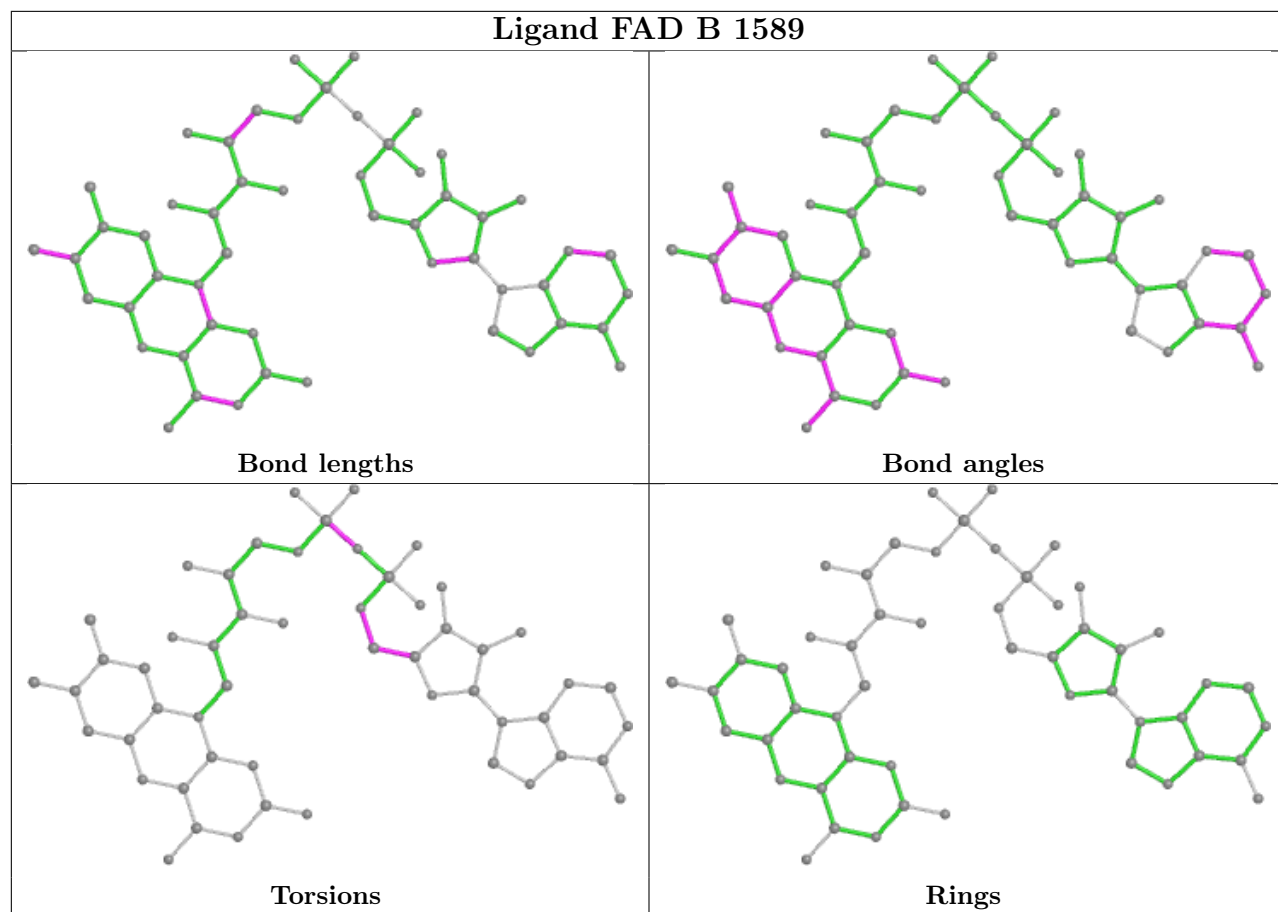
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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 [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%)	-0.52	2 (0%)	94 95	7, 11, 22, 47	13 (2%)
1	B	587/589 (99%)	-0.51	7 (1%)	79 79	7, 12, 26, 57	19 (3%)
All	All	1173/1178 (99%)	-0.52	9 (0%)	86 86	7, 11, 24, 57	32 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ILE	4.9
1	A	563[A]	LEU	3.5
1	B	371	ASP	3.1
1	B	45	ARG	3.0
1	B	369	SER	3.0
1	B	370	GLY	2.8
1	A	571	PRO	2.7
1	B	372	GLY	2.4
1	B	342	VAL	2.4

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,

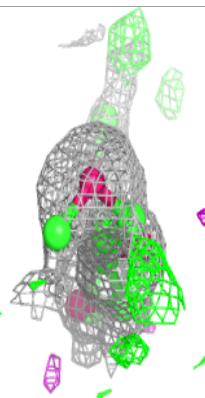
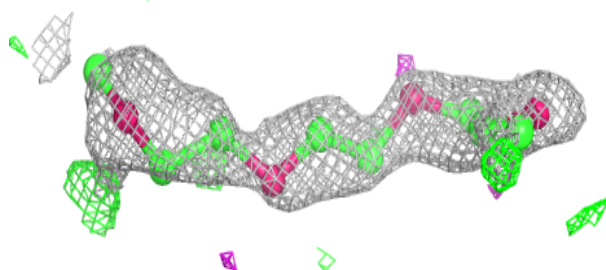
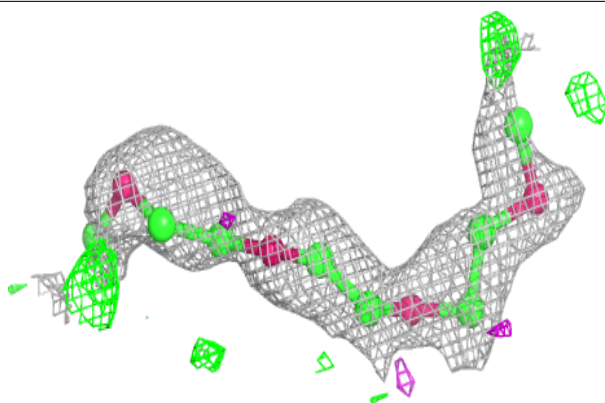
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	PG4	A	1599	6/13	0.68	0.17	36,40,41,45	0
4	MES	A	1590[B]	12/12	0.75	0.30	24,29,38,40	12
7	P6G	A	1593	12/19	0.75	0.16	36,46,53,57	0
4	MES	A	1590[A]	12/12	0.75	0.30	23,27,35,38	12
11	2PE	B	1597	22/28	0.76	0.23	38,51,71,77	0
9	PG4	B	1598	6/13	0.79	0.18	35,41,48,50	0
9	PG4	B	1596	11/13	0.83	0.16	20,24,41,53	0
9	PG4	B	1602	8/13	0.86	0.13	24,33,44,44	0
9	PG4	B	1599	11/13	0.86	0.14	49,52,61,65	0
11	2PE	B	1595	19/28	0.88	0.14	21,35,44,45	19
7	P6G	A	1595	17/19	0.89	0.10	19,29,41,46	0
9	PG4	B	1600	8/13	0.90	0.08	21,23,26,26	0
9	PG4	A	1596	11/13	0.90	0.12	19,26,39,44	0
8	1PG	A	1594	12/17	0.90	0.17	30,32,37,37	0
9	PG4	A	1600	13/13	0.90	0.11	22,26,34,41	0
9	PG4	B	1601	9/13	0.91	0.10	34,38,47,49	0
11	2PE	A	1598	15/28	0.91	0.12	21,29,42,43	0
10	PEG	A	1597	7/7	0.94	0.08	34,39,42,51	0
6	MG	B	1593	1/1	0.95	0.08	38,38,38,38	0
4	MES	B	1591	12/12	0.96	0.18	18,23,28,31	0
2	FAD	A	1588	53/53	0.99	0.05	6,8,9,10	0
2	FAD	B	1589	53/53	0.99	0.05	6,8,10,10	0
3	TPP	A	1589	26/26	0.99	0.06	6,7,9,11	0
3	TPP	B	1590	26/26	0.99	0.05	7,8,9,12	0
5	CL	B	1592	1/1	1.00	0.04	12,12,12,12	0
6	MG	A	1592	1/1	1.00	0.08	5,5,5,5	0
5	CL	A	1591	1/1	1.00	0.02	14,14,14,14	0
6	MG	B	1594	1/1	1.00	0.07	7,7,7,7	0

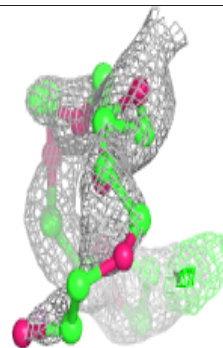
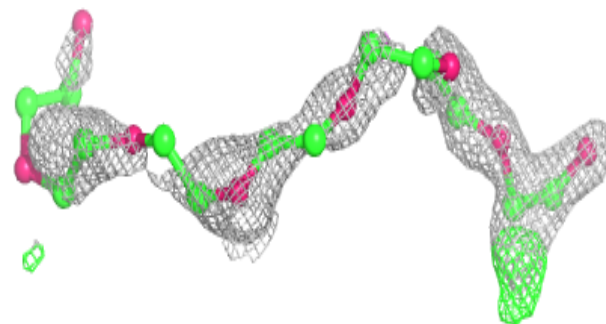
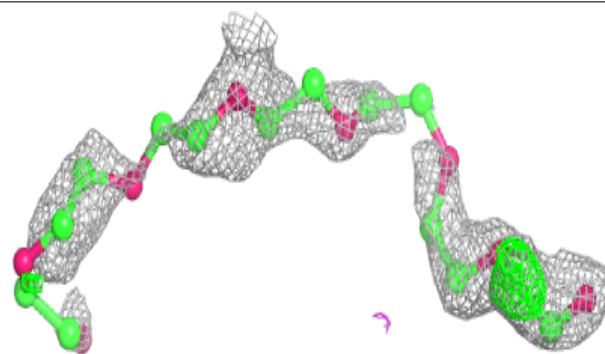
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G A 1593:

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

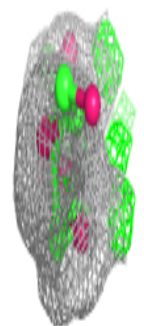
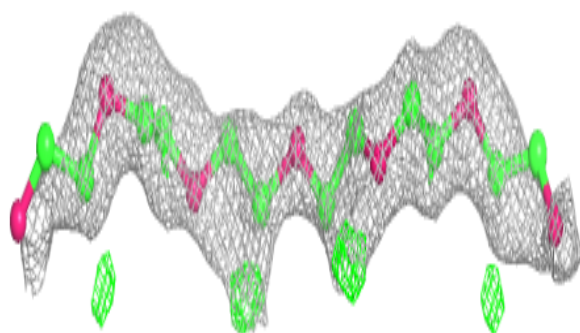
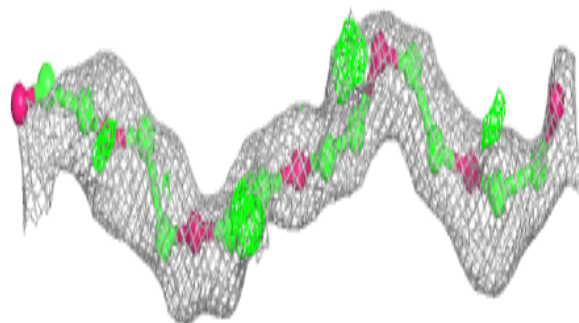
**Electron density around 2PE B 1597:**

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

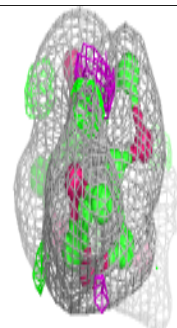
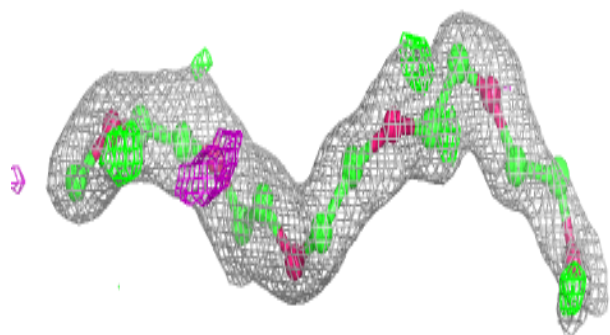
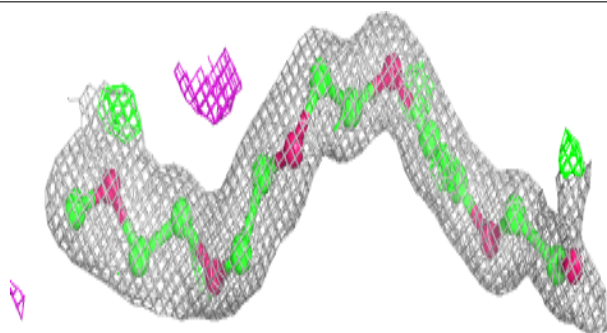


Electron density around 2PE B 1595:

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

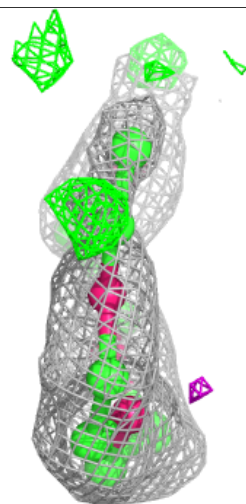
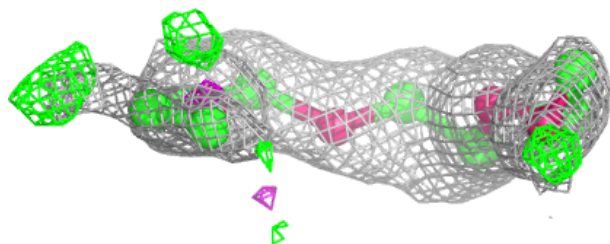
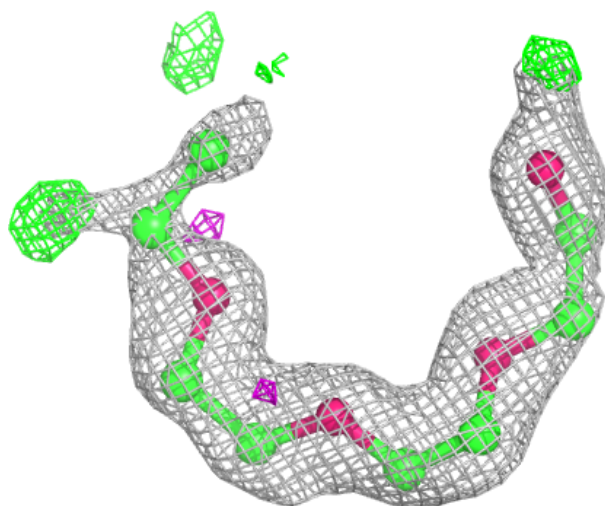
**Electron density around P6G A 1595:**

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



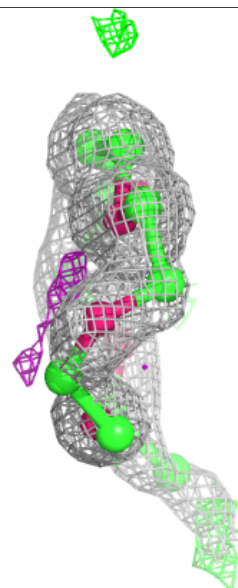
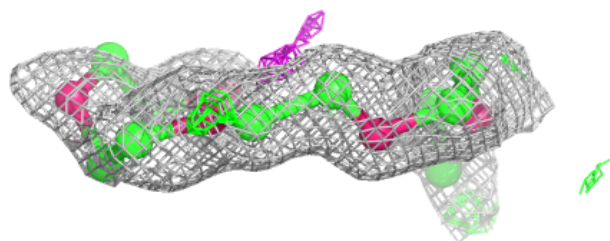
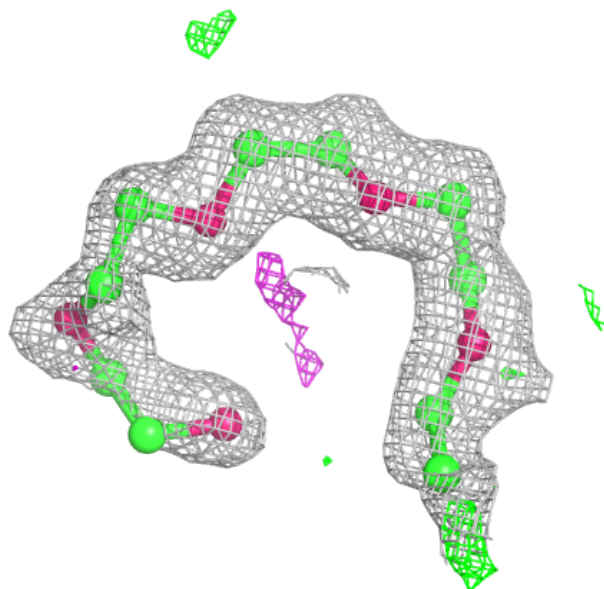
Electron density around 1PG A 1594:

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



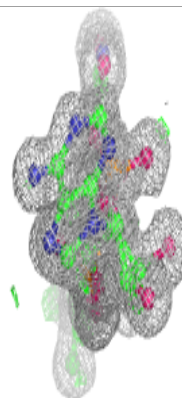
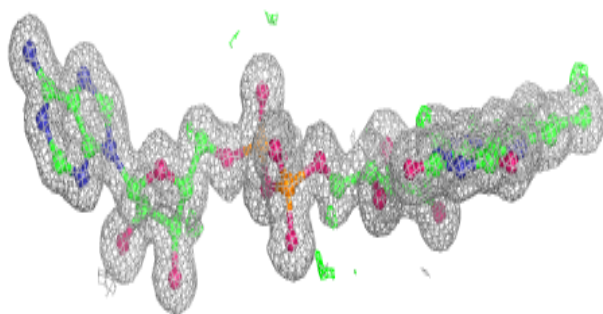
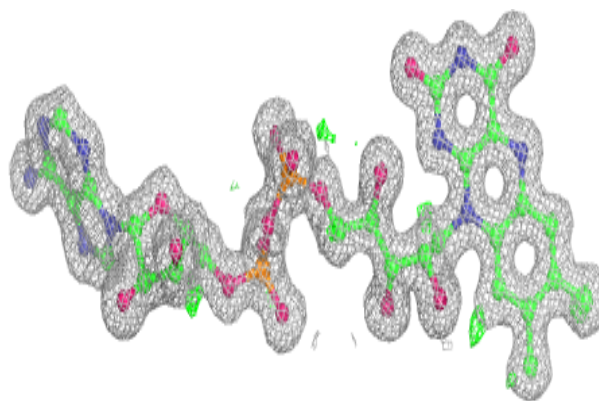
Electron density around 2PE A 1598:

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

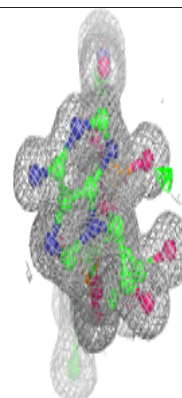
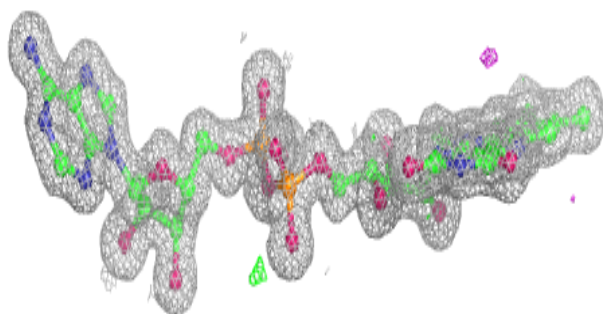
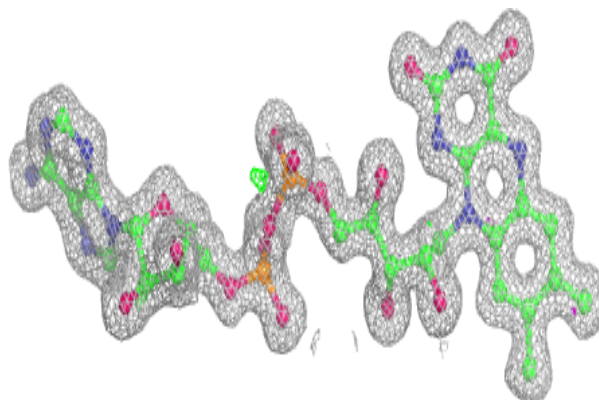


Electron density around FAD A 1588:

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

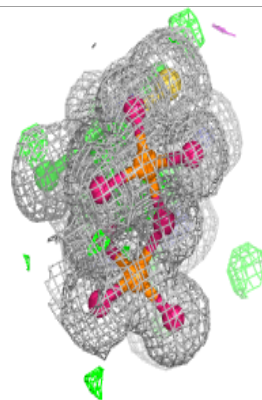
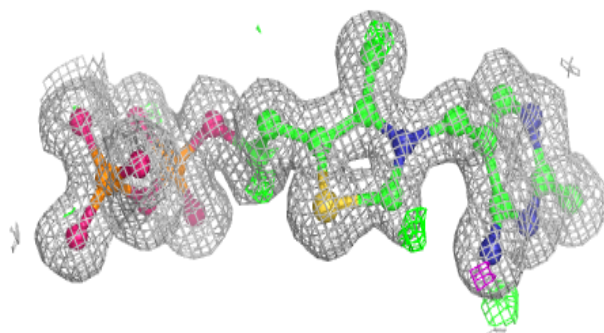
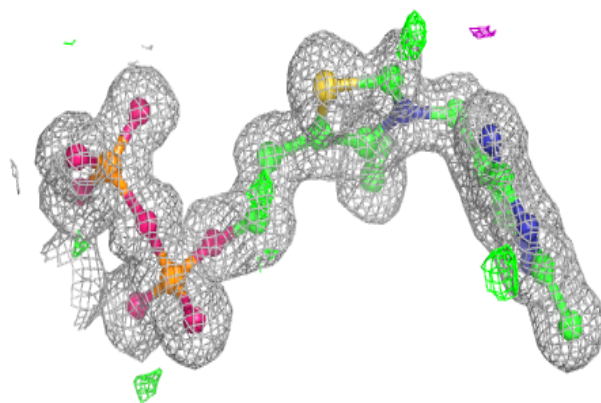
**Electron density around FAD B 1589:**

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

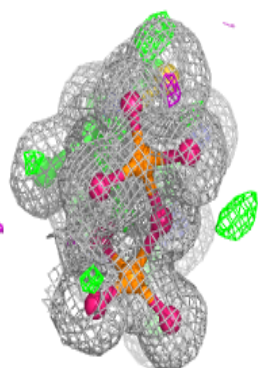
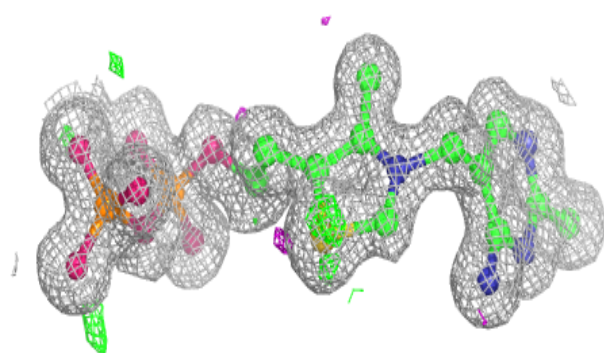
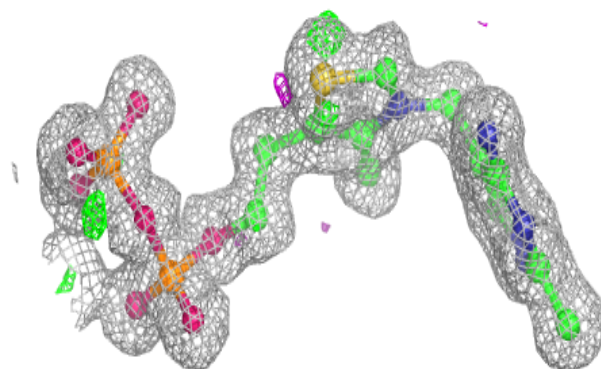


Electron density around TPP A 1589:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.