Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 12:15 AM EDT

PDB ID	:	7KAW
Title	:	Crystal structure of OhyA-PEG400-FAD complex from Staphylococcus aureus
Authors	:	Radka, C.D.; Rock, C.O.
Deposited on	:	2020-10-01
Resolution	:	2.10 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:

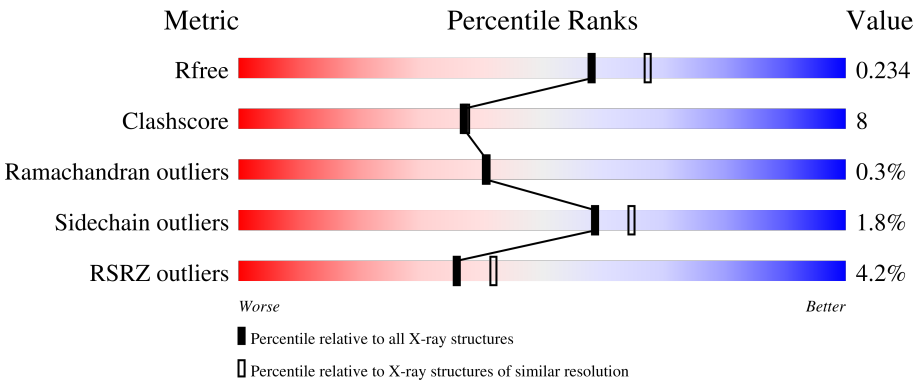
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	611	5% 81% 14% • 5%
1	B	611	4% 76% 18% • 5%
1	C	611	3% 85% 12% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16111 atoms, of which 16 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 Oleate hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	593	4771	3038	788	923	22	0	0	0
1	B	582	4700	2997	776	906	21	0	0	0
1	A	582	4696	2994	775	906	21	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP A0A0D6GJV1
C	-18	GLY	-	expression tag	UNP A0A0D6GJV1
C	-17	SER	-	expression tag	UNP A0A0D6GJV1
C	-16	SER	-	expression tag	UNP A0A0D6GJV1
C	-15	HIS	-	expression tag	UNP A0A0D6GJV1
C	-14	HIS	-	expression tag	UNP A0A0D6GJV1
C	-13	HIS	-	expression tag	UNP A0A0D6GJV1
C	-12	HIS	-	expression tag	UNP A0A0D6GJV1
C	-11	HIS	-	expression tag	UNP A0A0D6GJV1
C	-10	HIS	-	expression tag	UNP A0A0D6GJV1
C	-9	SER	-	expression tag	UNP A0A0D6GJV1
C	-8	SER	-	expression tag	UNP A0A0D6GJV1
C	-7	GLY	-	expression tag	UNP A0A0D6GJV1
C	-6	LEU	-	expression tag	UNP A0A0D6GJV1
C	-5	VAL	-	expression tag	UNP A0A0D6GJV1
C	-4	PRO	-	expression tag	UNP A0A0D6GJV1
C	-3	ARG	-	expression tag	UNP A0A0D6GJV1
C	-2	GLY	-	expression tag	UNP A0A0D6GJV1
C	-1	SER	-	expression tag	UNP A0A0D6GJV1
C	0	HIS	-	expression tag	UNP A0A0D6GJV1
B	-19	MET	-	initiating methionine	UNP A0A0D6GJV1
B	-18	GLY	-	expression tag	UNP A0A0D6GJV1
B	-17	SER	-	expression tag	UNP A0A0D6GJV1

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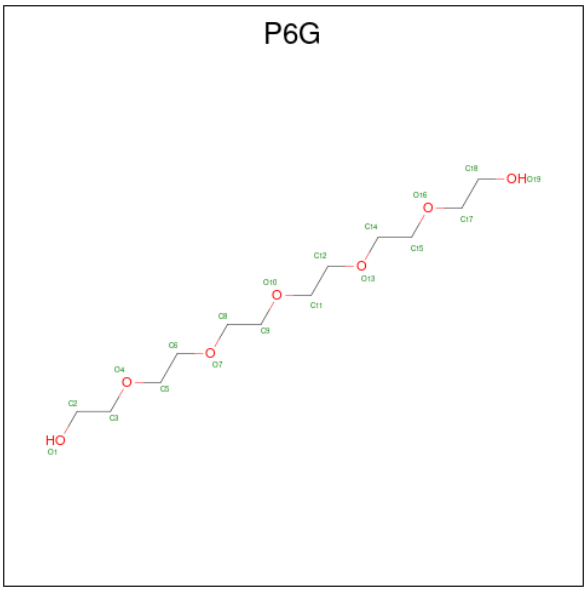
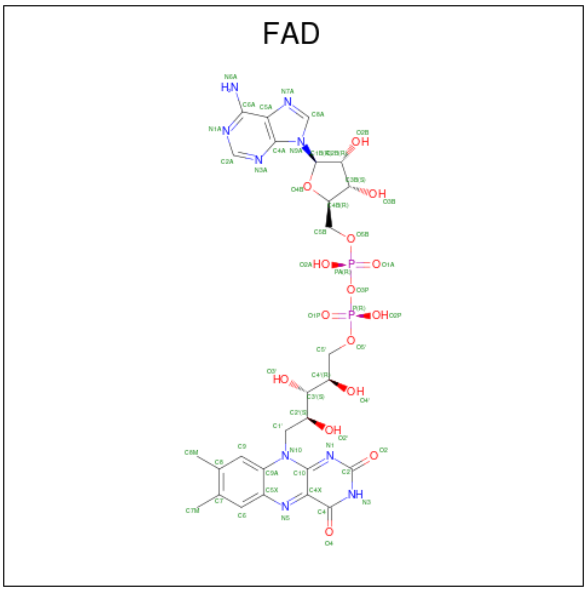
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP A0A0D6GJV1
B	-15	HIS	-	expression tag	UNP A0A0D6GJV1
B	-14	HIS	-	expression tag	UNP A0A0D6GJV1
B	-13	HIS	-	expression tag	UNP A0A0D6GJV1
B	-12	HIS	-	expression tag	UNP A0A0D6GJV1
B	-11	HIS	-	expression tag	UNP A0A0D6GJV1
B	-10	HIS	-	expression tag	UNP A0A0D6GJV1
B	-9	SER	-	expression tag	UNP A0A0D6GJV1
B	-8	SER	-	expression tag	UNP A0A0D6GJV1
B	-7	GLY	-	expression tag	UNP A0A0D6GJV1
B	-6	LEU	-	expression tag	UNP A0A0D6GJV1
B	-5	VAL	-	expression tag	UNP A0A0D6GJV1
B	-4	PRO	-	expression tag	UNP A0A0D6GJV1
B	-3	ARG	-	expression tag	UNP A0A0D6GJV1
B	-2	GLY	-	expression tag	UNP A0A0D6GJV1
B	-1	SER	-	expression tag	UNP A0A0D6GJV1
B	0	HIS	-	expression tag	UNP A0A0D6GJV1
A	-19	MET	-	initiating methionine	UNP A0A0D6GJV1
A	-18	GLY	-	expression tag	UNP A0A0D6GJV1
A	-17	SER	-	expression tag	UNP A0A0D6GJV1
A	-16	SER	-	expression tag	UNP A0A0D6GJV1
A	-15	HIS	-	expression tag	UNP A0A0D6GJV1
A	-14	HIS	-	expression tag	UNP A0A0D6GJV1
A	-13	HIS	-	expression tag	UNP A0A0D6GJV1
A	-12	HIS	-	expression tag	UNP A0A0D6GJV1
A	-11	HIS	-	expression tag	UNP A0A0D6GJV1
A	-10	HIS	-	expression tag	UNP A0A0D6GJV1
A	-9	SER	-	expression tag	UNP A0A0D6GJV1
A	-8	SER	-	expression tag	UNP A0A0D6GJV1
A	-7	GLY	-	expression tag	UNP A0A0D6GJV1
A	-6	LEU	-	expression tag	UNP A0A0D6GJV1
A	-5	VAL	-	expression tag	UNP A0A0D6GJV1
A	-4	PRO	-	expression tag	UNP A0A0D6GJV1
A	-3	ARG	-	expression tag	UNP A0A0D6GJV1
A	-2	GLY	-	expression tag	UNP A0A0D6GJV1
A	-1	SER	-	expression tag	UNP A0A0D6GJV1
A	0	HIS	-	expression tag	UNP A0A0D6GJV1

- Molecule 2 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$) (labeled as "Ligand of Interest" by depositor).



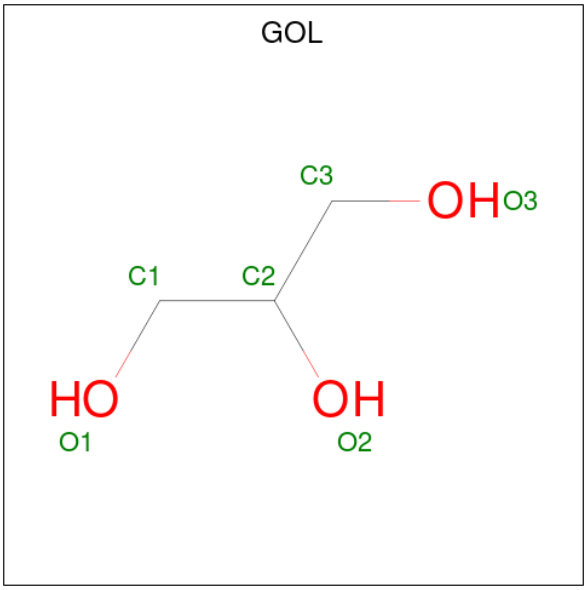
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	C	1	19	12	7	0	0
			Total	C	O		
2	B	1	19	12	7	0	0
			Total	C	O		
2	A	1	19	12	7	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	C	1	6	3	3		0	0
			Total	C	O			
4	B	1	6	3	3		0	0
			Total	C	H	O		
4	A	1	14	3	8	3	0	0
			Total	C	H	O		
4	A	1	14	3	8	3	0	0

- Molecule 5 is water.

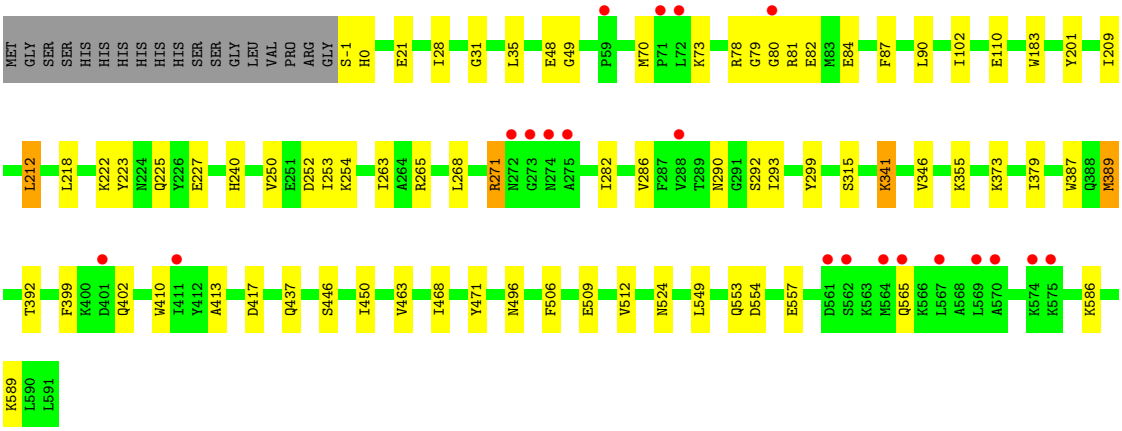
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	580	580	580	0	0
			Total	O		
5	B	604	604	604	0	0
			Total	O		
5	A	557	557	557	0	0

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.

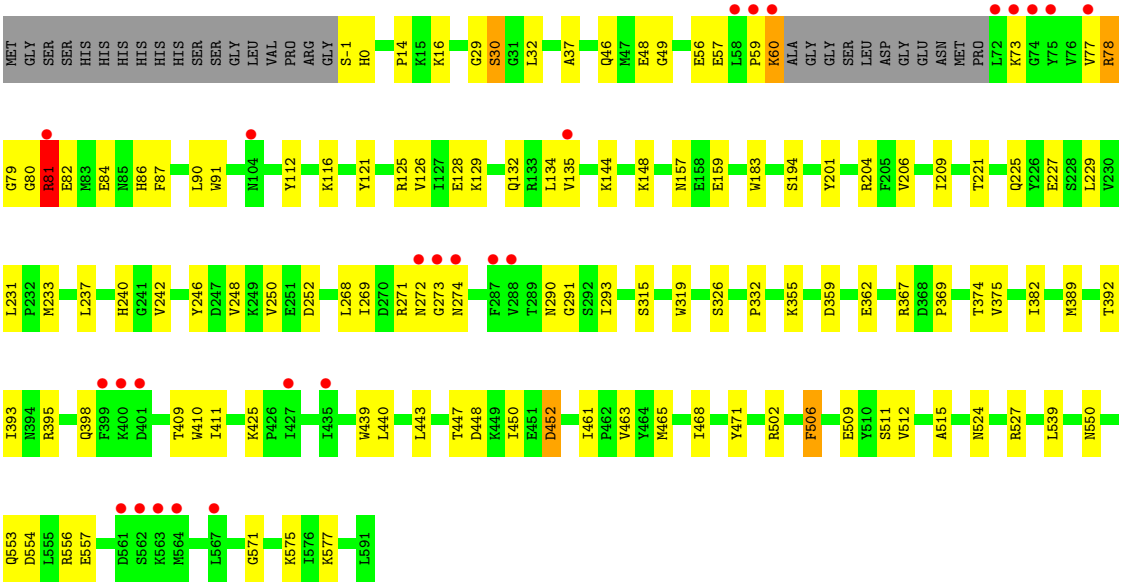
• Molecule 1: Oleate hydratase

Chain C:



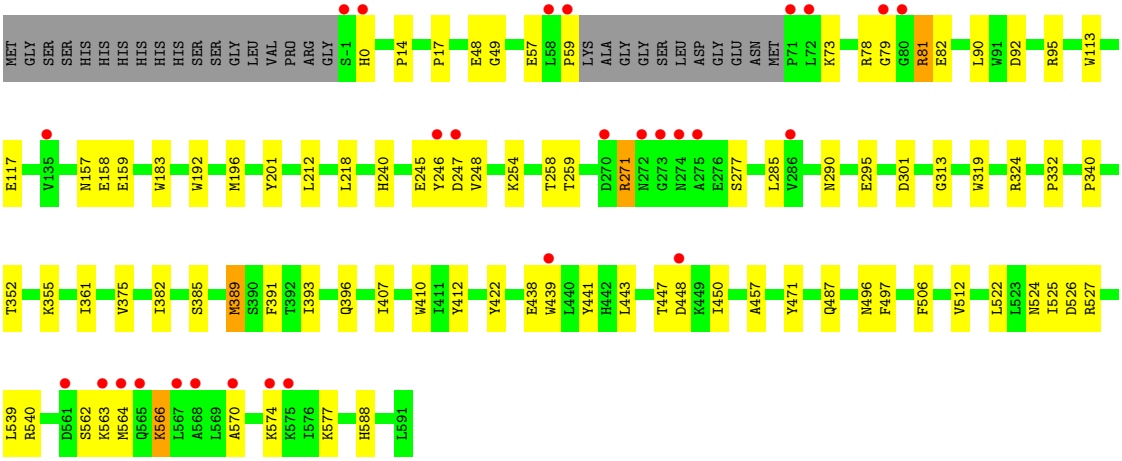
• Molecule 1: Oleate hydratase

Chain B:



• Molecule 1: Oleate hydratase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	188.08Å 112.92Å 119.06Å 90.00° 116.97° 90.00°	Depositor
Resolution (Å)	23.00 – 2.10 23.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (23.00-2.10) 98.7 (23.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.11Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.189 , 0.232 0.197 , 0.234	Depositor DCC
R_{free} test set	2004 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16111	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: GOL, FAD, P6G

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.42	0/4804	0.54	0/6511
1	B	0.39	0/4808	0.55	0/6515
1	C	0.42	0/4881	0.54	0/6615
All	All	0.41	0/14493	0.54	0/19641

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	4696	0	4569	60	0
1	B	4700	0	4580	104	0
1	C	4771	0	4643	58	0
2	A	19	0	26	1	0
2	B	19	0	26	4	0
2	C	19	0	26	3	0
3	B	53	0	31	18	0
3	C	53	0	31	7	0
4	A	12	16	16	5	0
4	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	6	0	8	0	0
5	A	557	0	0	3	0
5	B	604	0	0	17	0
5	C	580	0	0	9	0
All	All	16095	16	13964	222	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (222) 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:56:GLU:OE1	3:B:602:FAD:H1B	1.60	1.01
1:A:59:PRO:HA	1:A:246:TYR:HB3	1.44	0.99
1:C:79:GLY:HA3	3:C:602:FAD:HM72	1.46	0.97
1:A:352:THR:HA	4:A:602:GOL:H31	1.51	0.92
1:A:295:GLU:OE1	4:A:603:GOL:H11	1.70	0.91
1:B:80:GLY:O	1:B:81:ARG:NH2	2.06	0.89
1:B:315:SER:HB2	3:B:602:FAD:H2A	1.56	0.88
1:A:457:ALA:O	4:A:602:GOL:H32	1.75	0.87
1:B:56:GLU:HA	3:B:602:FAD:H8A	1.59	0.84
1:A:113:TRP:O	1:A:117:GLU:HG3	1.81	0.80
1:B:248:VAL:HG22	1:B:271:ARG:HG2	1.66	0.76
1:B:315:SER:HB2	3:B:602:FAD:C2A	2.18	0.73
1:B:80:GLY:HA2	3:B:602:FAD:C4X	2.20	0.71
1:A:82:GLU:HG2	1:A:218:LEU:HD13	1.72	0.70
1:B:132:GLN:NE2	5:B:708:HOH:O	2.25	0.69
1:B:315:SER:CB	3:B:602:FAD:H2A	2.23	0.69
1:B:78:ARG:CZ	1:B:81:ARG:HH12	2.07	0.68
1:B:116:LYS:NZ	1:A:526:ASP:OD1	2.24	0.68
1:A:245:GLU:OE1	1:A:271:ARG:NH2	2.27	0.67
1:B:81:ARG:HB2	1:B:221:THR:H	1.60	0.67
1:B:506:PHE:CG	2:B:601:P6G:H82	2.30	0.67
1:C:254:LYS:HG2	1:C:268:LEU:HD21	1.76	0.67
1:B:121:TYR:O	1:B:367:ARG:NH2	2.26	0.67
1:A:0:HIS:ND1	1:A:524:ASN:OD1	2.28	0.67
1:C:271:ARG:NH2	5:C:709:HOH:O	2.29	0.66
1:B:554:ASP:HB2	1:B:557:GLU:HG3	1.77	0.65
1:C:70:MET:HG2	1:C:73:LYS:HD2	1.79	0.65
1:A:248:VAL:HG22	1:A:271:ARG:HG3	1.77	0.64
1:B:382:ILE:HD12	1:B:389:MET:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:LYS:HA	1:A:566:LYS:HE2	1.81	0.62
1:B:78:ARG:NH1	1:B:81:ARG:HH12	1.97	0.62
1:B:57:GLU:H	3:B:602:FAD:C8A	2.12	0.62
1:B:362:GLU:HB2	1:B:369:PRO:HD3	1.82	0.61
1:C:79:GLY:CA	3:C:602:FAD:HM72	2.27	0.60
1:A:259:THR:O	1:A:487:GLN:NE2	2.30	0.60
1:B:468:ILE:CD1	3:B:602:FAD:HM83	2.32	0.60
1:B:78:ARG:HH12	1:B:392:THR:HG21	1.66	0.59
1:B:57:GLU:H	3:B:602:FAD:H8A	1.66	0.59
1:B:79:GLY:O	1:B:225:GLN:OE1	2.21	0.59
1:C:82:GLU:HB3	1:C:218:LEU:HD22	1.86	0.57
1:B:246:TYR:O	1:B:248:VAL:HG23	2.05	0.57
1:B:293:ILE:CD1	3:B:602:FAD:HM81	2.34	0.57
1:B:32:LEU:HD23	1:B:511:SER:HB2	1.87	0.57
1:B:539:LEU:HD21	1:A:539:LEU:HD21	1.85	0.57
1:C:49:GLY:HA3	1:C:240:HIS:O	2.06	0.56
1:B:440:LEU:HD23	1:B:443:LEU:HD12	1.88	0.56
1:A:82:GLU:HB2	2:A:601:P6G:H61	1.87	0.56
1:C:315:SER:HB2	3:C:602:FAD:N7A	2.21	0.56
1:C:-1:SER:OG	1:C:0:HIS:N	2.37	0.55
1:B:389:MET:HE2	1:B:411:ILE:CG2	2.36	0.55
1:A:295:GLU:OE1	4:A:603:GOL:C1	2.49	0.55
1:A:570:ALA:O	1:A:574:LYS:HG3	2.06	0.54
1:A:352:THR:HA	4:A:602:GOL:C3	2.32	0.54
1:B:80:GLY:HA2	3:B:602:FAD:C4	2.37	0.54
1:B:389:MET:HE1	1:B:411:ILE:HG21	1.90	0.54
1:A:396:GLN:HG3	1:A:407:ILE:HG22	1.90	0.54
1:B:-1:SER:N	5:B:711:HOH:O	2.28	0.54
1:B:56:GLU:CD	3:B:602:FAD:H1B	2.27	0.54
1:B:293:ILE:HD11	3:B:602:FAD:HM81	1.90	0.53
1:A:183:TRP:CZ2	1:A:201:TYR:HB3	2.44	0.53
3:B:602:FAD:H3B	5:B:778:HOH:O	2.06	0.53
1:B:389:MET:CE	1:B:411:ILE:CG2	2.87	0.53
1:C:373:LYS:HE3	5:B:921:HOH:O	2.07	0.53
1:A:324:ARG:NH1	5:A:732:HOH:O	2.42	0.53
1:C:553:GLN:HB3	1:C:557:GLU:HB2	1.90	0.52
1:B:159:GLU:H	1:B:159:GLU:CD	2.12	0.52
1:B:506:PHE:CZ	2:B:601:P6G:H62	2.44	0.52
1:A:254:LYS:NZ	5:A:704:HOH:O	2.23	0.52
1:B:293:ILE:HD13	1:B:471:TYR:CE2	2.44	0.52
1:B:84:GLU:OE2	1:B:86:HIS:C	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:LYS:NZ	1:C:417:ASP:OD2	2.44	0.51
1:A:17:PRO:HG3	1:A:525:ILE:HG12	1.93	0.51
1:B:29:GLY:HA2	3:B:602:FAD:C8A	2.41	0.51
1:A:59:PRO:HB3	1:A:247:ASP:OD1	2.10	0.51
1:C:28:ILE:HD12	1:C:250:VAL:HG21	1.93	0.50
1:B:237:LEU:HD22	1:B:242:VAL:HG21	1.93	0.50
1:B:395:ARG:O	1:B:398:GLN:NE2	2.35	0.50
1:C:293:ILE:HD13	1:C:471:TYR:CE2	2.46	0.50
1:A:447:THR:HA	1:A:450:ILE:HD12	1.94	0.50
1:C:80:GLY:HA2	5:C:883:HOH:O	2.10	0.50
1:B:129:LYS:HB3	5:B:708:HOH:O	2.12	0.50
1:B:32:LEU:HD12	1:B:233:MET:HE1	1.94	0.49
1:C:253:ILE:HD13	1:C:286:VAL:HG11	1.93	0.49
1:A:159:GLU:CD	1:A:159:GLU:H	2.16	0.49
1:B:367:ARG:HD2	1:B:374:THR:O	2.12	0.49
1:A:361:ILE:HG21	1:A:393:ILE:HD13	1.93	0.49
1:C:84:GLU:HB3	2:C:601:P6G:H142	1.94	0.49
1:B:14:PRO:HD3	1:B:527:ARG:HD2	1.95	0.49
1:A:389:MET:HE1	1:A:438:GLU:HG3	1.95	0.48
1:C:81:ARG:HA	3:C:602:FAD:C4	2.43	0.48
1:B:78:ARG:HD2	1:B:81:ARG:HH12	1.78	0.48
1:A:82:GLU:H	1:A:82:GLU:CD	2.16	0.48
1:C:468:ILE:CD1	3:C:602:FAD:HM83	2.44	0.48
1:C:589:LYS:NZ	5:C:725:HOH:O	2.45	0.48
1:B:82:GLU:HB2	3:B:602:FAD:O4	2.14	0.48
1:B:78:ARG:CZ	1:B:81:ARG:NH1	2.75	0.48
1:B:78:ARG:HD3	1:B:410:TRP:CD2	2.48	0.48
1:A:81:ARG:HA	1:A:81:ARG:NE	2.28	0.48
1:B:183:TRP:CZ2	1:B:201:TYR:HB3	2.49	0.48
1:B:468:ILE:HD11	3:B:602:FAD:HM83	1.96	0.48
1:C:341:LYS:CE	1:C:417:ASP:OD2	2.62	0.47
1:B:78:ARG:NE	1:B:81:ARG:HH22	2.12	0.47
1:B:452:ASP:OD1	1:B:452:ASP:N	2.48	0.47
1:C:263:ILE:HD13	1:C:282:ILE:HD12	1.97	0.47
1:B:225:GLN:HG3	1:B:229:LEU:HD12	1.97	0.47
1:B:506:PHE:CD1	2:B:601:P6G:H82	2.50	0.47
1:A:562:SER:C	1:A:564:MET:H	2.18	0.47
1:B:78:ARG:HG3	3:B:602:FAD:H6	1.96	0.46
1:B:206:VAL:O	1:B:209:ILE:HG12	2.15	0.46
1:B:59:PRO:HA	1:B:246:TYR:HB3	1.96	0.46
1:B:463:VAL:HG12	1:B:465:MET:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ASN:ND2	5:B:717:HOH:O	2.31	0.46
1:C:90:LEU:HA	1:C:512:VAL:HG11	1.98	0.46
1:A:82:GLU:HG2	1:A:218:LEU:CD1	2.43	0.46
1:C:81:ARG:HB2	1:C:225:GLN:NE2	2.31	0.46
1:C:252:ASP:HB3	1:C:268:LEU:HD23	1.97	0.46
2:C:601:P6G:H52	2:C:601:P6G:H81	1.78	0.46
1:B:60:LYS:HD2	1:B:60:LYS:N	2.30	0.46
1:C:212:LEU:HD12	2:C:601:P6G:O19	2.16	0.46
1:B:157:ASN:HB3	1:B:159:GLU:OE1	2.16	0.46
1:A:471:TYR:CE1	1:A:496:ASN:HB2	2.51	0.46
1:B:355:LYS:HD3	1:B:359:ASP:OD2	2.16	0.46
1:A:295:GLU:CD	1:A:313:GLY:HA3	2.35	0.46
1:B:30:SER:HB2	1:B:56:GLU:OE1	2.16	0.45
1:B:37:ALA:HB2	1:B:515:ALA:HB1	1.98	0.45
1:B:425:LYS:NZ	5:B:737:HOH:O	2.48	0.45
1:C:79:GLY:HA2	1:C:410:TRP:CE2	2.50	0.45
1:B:90:LEU:HA	1:B:512:VAL:HG11	1.97	0.45
1:B:135:VAL:HG13	5:B:757:HOH:O	2.15	0.45
1:B:144:LYS:NZ	5:B:705:HOH:O	2.22	0.45
1:B:319:TRP:CD2	1:B:332:PRO:HB3	2.52	0.45
1:A:92:ASP:O	1:A:95:ARG:HG3	2.17	0.45
1:C:222:LYS:HD3	1:C:223:TYR:CE2	2.52	0.45
1:B:227:GLU:HA	1:B:231:LEU:HD12	1.99	0.45
1:C:0:HIS:ND1	1:C:524:ASN:OD1	2.37	0.45
1:B:290:ASN:HA	5:B:812:HOH:O	2.17	0.45
1:B:60:LYS:CD	1:B:60:LYS:H	2.28	0.45
1:B:78:ARG:NH1	1:B:81:ARG:NH1	2.62	0.45
1:B:16:LYS:HG3	1:B:46:GLN:HB2	2.00	0.44
1:C:227:GLU:HB3	5:C:892:HOH:O	2.17	0.44
1:B:87:PHE:CG	1:B:509:GLU:HB2	2.51	0.44
1:A:79:GLY:HA2	1:A:81:ARG:HH22	1.82	0.44
1:C:209:ILE:CD1	1:C:549:LEU:HG	2.47	0.44
1:B:447:THR:HA	1:B:450:ILE:HD12	1.99	0.44
1:B:272:ASN:O	1:B:274:ASN:N	2.51	0.44
1:A:49:GLY:HA3	1:A:240:HIS:O	2.18	0.44
1:C:265:ARG:NH2	5:C:716:HOH:O	2.37	0.44
1:C:21:GLU:CD	1:C:21:GLU:H	2.22	0.43
1:B:134:LEU:HD12	5:B:757:HOH:O	2.17	0.43
1:A:258:THR:O	5:A:701:HOH:O	2.21	0.43
1:B:0:HIS:HB3	1:B:524:ASN:ND2	2.33	0.43
1:B:112:TYR:CZ	1:B:116:LYS:HE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASN:HB3	1:A:159:GLU:OE1	2.17	0.43
1:A:192:TRP:NE1	1:A:340:PRO:HG2	2.33	0.43
1:A:375:VAL:HB	1:A:393:ILE:O	2.18	0.43
1:B:125:ARG:HG3	1:B:126:VAL:HG23	2.01	0.43
1:B:550:ASN:O	1:B:553:GLN:HG3	2.18	0.43
1:A:319:TRP:CD2	1:A:332:PRO:HB3	2.52	0.43
1:C:315:SER:HB2	3:C:602:FAD:C8A	2.48	0.43
1:B:60:LYS:HD2	1:B:60:LYS:H	1.84	0.43
1:A:540:ARG:HB3	1:A:588:HIS:CE1	2.54	0.43
1:C:82:GLU:H	1:C:82:GLU:HG3	1.65	0.43
1:C:87:PHE:CG	1:C:509:GLU:HB2	2.54	0.43
1:B:49:GLY:HA3	1:B:240:HIS:O	2.19	0.43
1:C:292:SER:HA	5:C:728:HOH:O	2.19	0.42
1:C:341:LYS:HD2	1:C:417:ASP:OD2	2.19	0.42
1:B:82:GLU:OE2	2:B:601:P6G:O1	2.31	0.42
1:B:448:ASP:O	5:B:702:HOH:O	2.21	0.42
1:C:341:LYS:CD	1:C:417:ASP:OD2	2.67	0.42
1:B:553:GLN:HB3	1:B:557:GLU:HB2	2.01	0.42
1:A:391:PHE:HA	1:A:410:TRP:O	2.18	0.42
1:C:31:GLY:O	1:C:35:LEU:HG	2.20	0.42
1:C:102:ILE:HD12	1:C:110:GLU:HB2	2.02	0.42
1:C:399:PHE:HB2	1:C:402:GLN:HB2	2.00	0.42
1:B:439:TRP:CZ2	1:B:443:LEU:HD11	2.55	0.42
1:A:57:GLU:O	1:A:247:ASP:HA	2.18	0.42
1:C:183:TRP:HZ2	1:C:201:TYR:HB3	1.84	0.42
1:C:468:ILE:HD11	3:C:602:FAD:HM83	2.02	0.42
1:B:48:GLU:OE2	5:B:703:HOH:O	2.22	0.42
1:A:562:SER:C	1:A:564:MET:N	2.72	0.42
1:B:252:ASP:HB3	1:B:268:LEU:HD12	2.01	0.42
1:C:554:ASP:OD1	1:C:557:GLU:HG3	2.20	0.42
1:C:379:ILE:HA	1:C:392:THR:HB	2.02	0.42
1:C:389:MET:HE2	1:C:389:MET:HB2	1.78	0.42
1:B:91:TRP:HA	1:B:91:TRP:CE3	2.54	0.42
1:C:437:GLN:HG2	1:C:450:ILE:HG22	2.02	0.41
1:A:90:LEU:HA	1:A:512:VAL:HG11	2.02	0.41
1:A:73:LYS:HD2	1:A:301:ASP:OD2	2.20	0.41
1:C:471:TYR:CE1	1:C:496:ASN:HB2	2.55	0.41
1:A:566:LYS:HE2	1:A:566:LYS:HB2	1.73	0.41
1:C:299:TYR:CD2	1:C:463:VAL:HG22	2.55	0.41
1:A:59:PRO:O	1:A:246:TYR:CD1	2.74	0.41
1:A:285:LEU:HD22	1:A:522:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:LYS:HE3	1:A:563:LYS:HB3	1.78	0.41
1:C:252:ASP:OD2	5:C:701:HOH:O	2.21	0.41
1:C:565:GLN:HG3	5:C:1065:HOH:O	2.20	0.41
1:A:382:ILE:CG2	1:A:385:SER:HB3	2.50	0.41
1:C:346:VAL:HA	1:C:463:VAL:O	2.21	0.41
1:B:291:GLY:O	5:B:704:HOH:O	2.22	0.41
1:B:409:THR:HG21	1:B:439:TRP:CZ2	2.56	0.41
1:A:14:PRO:HD3	1:A:527:ARG:HD2	2.02	0.41
1:C:387:TRP:HB3	1:C:413:ALA:HB1	2.03	0.41
1:B:128:GLU:OE2	5:B:706:HOH:O	2.22	0.41
1:B:375:VAL:HB	1:B:393:ILE:O	2.21	0.41
1:A:158:GLU:HG3	1:A:196:MET:HG3	2.02	0.41
1:A:439:TRP:CZ2	1:A:443:LEU:HD11	2.56	0.41
1:A:563:LYS:HA	1:A:566:LYS:CE	2.50	0.41
1:C:290:ASN:HA	5:C:852:HOH:O	2.20	0.41
1:C:355:LYS:HD3	1:C:355:LYS:HA	1.85	0.41
1:A:290:ASN:O	1:A:497:PHE:HB2	2.21	0.41
1:A:422:TYR:HB2	1:A:441:TYR:CG	2.56	0.41
1:C:80:GLY:O	1:C:81:ARG:HD3	2.20	0.40
1:B:78:ARG:CD	1:B:81:ARG:HH12	2.34	0.40
1:B:204:ARG:HA	5:B:844:HOH:O	2.21	0.40
1:B:554:ASP:HB3	1:B:556:ARG:H	1.86	0.40
1:B:571:GLY:O	1:B:575:LYS:HD2	2.22	0.40
1:B:148:LYS:NZ	5:B:753:HOH:O	2.55	0.40
1:A:448:ASP:OD1	1:A:448:ASP:N	2.54	0.40
1:C:586:LYS:HE3	1:C:586:LYS:HB3	1.79	0.40
1:B:73:LYS:HG3	1:B:461:ILE:HD12	2.04	0.40
1:B:250:VAL:HG22	1:B:269:ILE:HG22	2.03	0.40
1:A:183:TRP:HZ2	1:A:201:TYR:HB3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	578/611 (95%)	557 (96%)	20 (4%)	1 (0%)	47	49
1	B	578/611 (95%)	553 (96%)	21 (4%)	4 (1%)	22	18
1	C	591/611 (97%)	572 (97%)	19 (3%)	0	100	100
All	All	1747/1833 (95%)	1682 (96%)	60 (3%)	5 (0%)	41	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	502	ARG
1	B	78	ARG
1	B	81	ARG
1	B	273	GLY
1	A	81	ARG

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	518/544 (95%)	507 (98%)	11 (2%)	53	59
1	B	519/544 (95%)	510 (98%)	9 (2%)	60	67
1	C	526/544 (97%)	518 (98%)	8 (2%)	65	71
All	All	1563/1632 (96%)	1535 (98%)	28 (2%)	59	65

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	48	GLU
1	C	78	ARG
1	C	212	LEU
1	C	271	ARG
1	C	341	LYS
1	C	389	MET
1	C	446	SER
1	C	506	PHE

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Mol	Chain	Res	Type
1	B	30	SER
1	B	60	LYS
1	B	77	VAL
1	B	81	ARG
1	B	194	SER
1	B	326	SER
1	B	452	ASP
1	B	506	PHE
1	B	577	LYS
1	A	48	GLU
1	A	78	ARG
1	A	212	LEU
1	A	271	ARG
1	A	277	SER
1	A	355	LYS
1	A	389	MET
1	A	412	TYR
1	A	506	PHE
1	A	566	LYS
1	A	577	LYS

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

Mol	Chain	Res	Type
1	B	272	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)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	B	603	-	5,5,5	1.00	0	5,5,5	1.22	0
4	GOL	A	603	-	5,5,5	0.15	0	5,5,5	0.47	0
4	GOL	C	603	-	5,5,5	1.11	0	5,5,5	0.81	0
3	FAD	B	602	-	53,58,58	1.28	5 (9%)	68,89,89	1.34	10 (14%)
3	FAD	C	602	-	53,58,58	1.70	11 (20%)	68,89,89	1.37	12 (17%)
2	P6G	B	601	-	18,18,18	0.54	0	17,17,17	0.42	0
2	P6G	C	601	-	18,18,18	0.50	0	17,17,17	0.31	0
2	P6G	A	601	-	18,18,18	0.53	0	17,17,17	0.29	0
4	GOL	A	602	-	5,5,5	0.69	0	5,5,5	1.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	603	-	-	2/4/4/4	-
4	GOL	A	603	-	-	1/4/4/4	-
4	GOL	C	603	-	-	1/4/4/4	-
3	FAD	B	602	-	-	6/30/50/50	0/6/6/6
3	FAD	C	602	-	-	3/30/50/50	0/6/6/6
2	P6G	B	601	-	-	5/16/16/16	-
2	P6G	C	601	-	-	8/16/16/16	-
2	P6G	A	601	-	-	5/16/16/16	-
4	GOL	A	602	-	-	4/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	FAD	C9A-C5X	5.03	1.49	1.41
3	C	602	FAD	C4-N3	-4.87	1.29	1.38
3	C	602	FAD	C1'-C2'	-4.26	1.46	1.52
3	C	602	FAD	C9A-C5X	3.99	1.47	1.41
3	B	602	FAD	C8-C7	3.31	1.49	1.40
3	C	602	FAD	C2-N3	-3.15	1.31	1.39
3	C	602	FAD	C5X-N5	-2.79	1.34	1.39
3	C	602	FAD	P-O1P	-2.74	1.41	1.50
3	B	602	FAD	C4X-N5	2.53	1.35	1.30
3	B	602	FAD	C5A-C4A	2.48	1.47	1.40
3	C	602	FAD	C8-C7	2.43	1.47	1.40
3	B	602	FAD	C4-N3	-2.43	1.34	1.38
3	C	602	FAD	P-O2P	-2.28	1.44	1.55
3	C	602	FAD	PA-O2A	-2.09	1.45	1.55
3	C	602	FAD	O4B-C4B	-2.08	1.40	1.45
3	C	602	FAD	PA-O1A	-2.07	1.43	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	FAD	P-O3P-PA	-3.56	120.62	132.83
3	B	602	FAD	C3B-C2B-C1B	3.39	106.08	100.98
3	C	602	FAD	C4-C4X-N5	3.33	122.97	118.23
3	B	602	FAD	N3A-C2A-N1A	-3.16	123.73	128.68
3	C	602	FAD	O2'-C2'-C3'	2.98	116.35	109.10
3	C	602	FAD	N3A-C2A-N1A	-2.96	124.06	128.68
3	C	602	FAD	O3B-C3B-C4B	-2.81	102.93	111.05
3	B	602	FAD	C4-C4X-N5	2.71	122.09	118.23
3	B	602	FAD	C4A-C5A-N7A	-2.71	106.58	109.40
3	B	602	FAD	C4X-C10-N1	-2.62	118.65	124.73
3	C	602	FAD	C4X-C10-N1	-2.48	118.97	124.73
3	C	602	FAD	O3'-C3'-C4'	-2.44	102.91	108.81
3	C	602	FAD	C10-N1-C2	2.42	121.74	116.90
3	B	602	FAD	C10-N1-C2	2.23	121.37	116.90
3	C	602	FAD	C4X-C4-N3	2.23	118.84	113.19
3	B	602	FAD	O4-C4-C4X	-2.20	120.76	126.60
3	C	602	FAD	C1'-C2'-C3'	-2.17	103.73	109.79
3	C	602	FAD	O4-C4-C4X	-2.14	120.93	126.60
3	C	602	FAD	C4X-C10-N10	2.13	119.59	116.48
3	B	602	FAD	C4X-C4-N3	2.08	118.48	113.19
3	B	602	FAD	C4X-C10-N10	2.03	119.45	116.48
3	C	602	FAD	O2'-C2'-C1'	-2.03	104.90	109.80

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	FAD	C5B-O5B-PA-O3P
3	B	602	FAD	C3B-C4B-C5B-O5B
4	A	602	GOL	O1-C1-C2-C3
2	B	601	P6G	O13-C14-C15-O16
2	A	601	P6G	O4-C5-C6-O7
3	B	602	FAD	O4B-C4B-C5B-O5B
4	B	603	GOL	O1-C1-C2-C3
2	C	601	P6G	O7-C8-C9-O10
4	A	602	GOL	O1-C1-C2-O2
3	B	602	FAD	C4B-C5B-O5B-PA
2	B	601	P6G	O16-C17-C18-O19
2	A	601	P6G	O13-C14-C15-O16
2	C	601	P6G	C5-C6-O7-C8
3	C	602	FAD	PA-O3P-P-O5'
2	B	601	P6G	O10-C11-C12-O13
2	B	601	P6G	C14-C15-O16-C17
2	C	601	P6G	O1-C2-C3-O4
3	C	602	FAD	O4B-C4B-C5B-O5B
3	B	602	FAD	C5B-O5B-PA-O1A
2	A	601	P6G	C6-C5-O4-C3
3	C	602	FAD	N10-C1'-C2'-O2'
2	C	601	P6G	C12-C11-O10-C9
4	C	603	GOL	C1-C2-C3-O3
4	A	602	GOL	C1-C2-C3-O3
4	A	603	GOL	C1-C2-C3-O3
4	B	603	GOL	O1-C1-C2-O2
2	C	601	P6G	O10-C11-C12-O13
2	B	601	P6G	O1-C2-C3-O4
2	C	601	P6G	C15-C14-O13-C12
4	A	602	GOL	O2-C2-C3-O3
2	C	601	P6G	O4-C5-C6-O7
2	C	601	P6G	O13-C14-C15-O16
2	A	601	P6G	C18-C17-O16-C15
3	B	602	FAD	N10-C1'-C2'-O2'
2	A	601	P6G	O7-C8-C9-O10

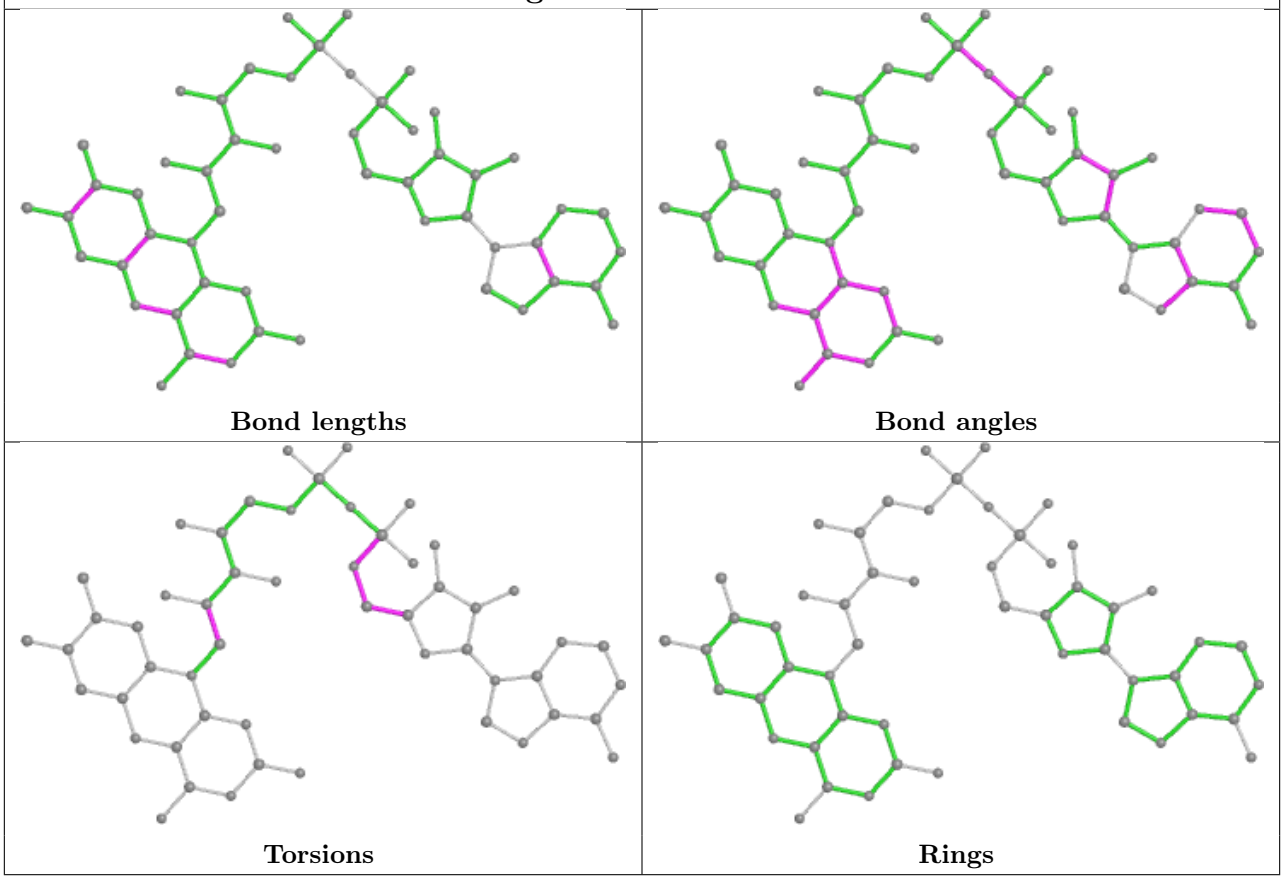
There are no ring outliers.

7 monomers are involved in 38 short contacts:

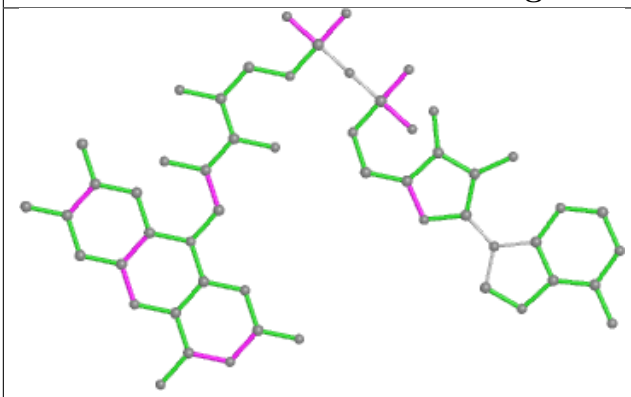
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	GOL	2	0
3	B	602	FAD	18	0
3	C	602	FAD	7	0
2	B	601	P6G	4	0
2	C	601	P6G	3	0
2	A	601	P6G	1	0
4	A	602	GOL	3	0

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.

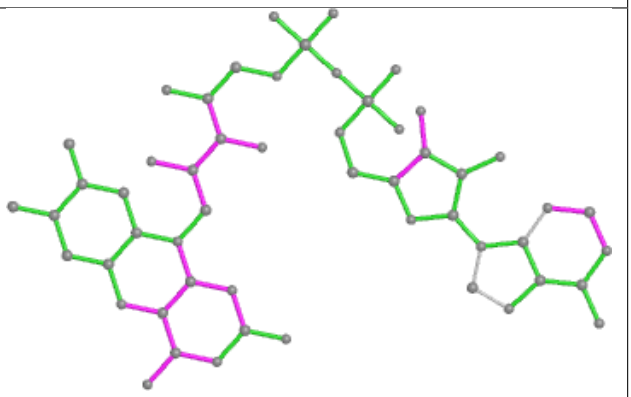
Ligand FAD B 602



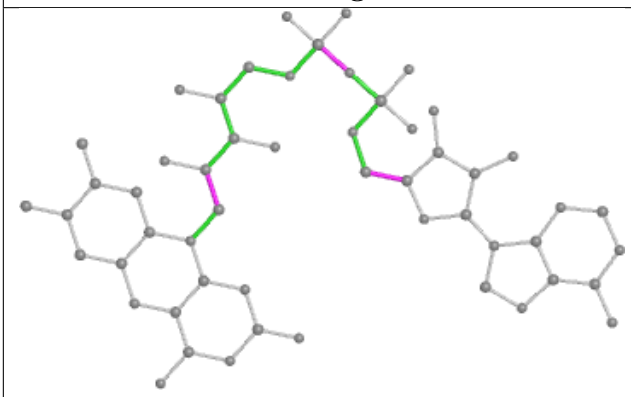
Ligand FAD C 602



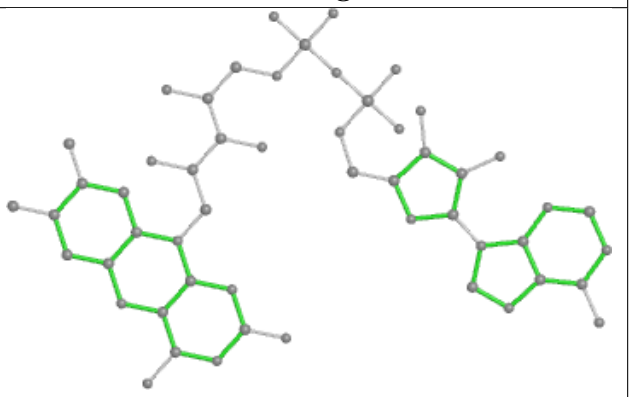
Bond lengths



Bond angles

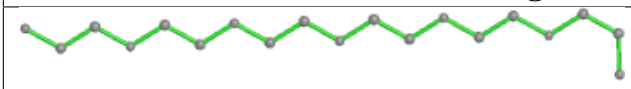


Torsions

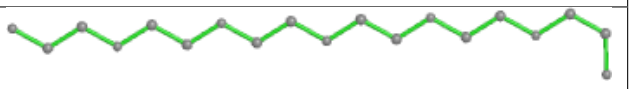


Rings

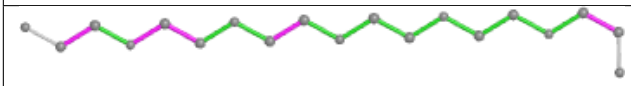
Ligand P6G B 601



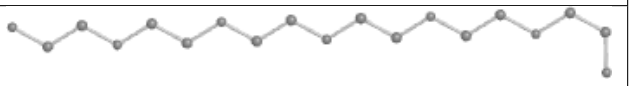
Bond lengths



Bond angles

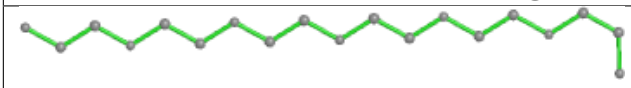


Torsions

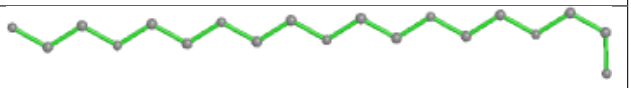


Rings

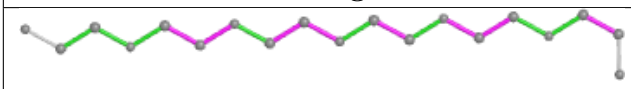
Ligand P6G C 601



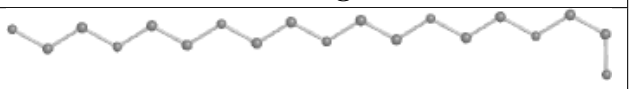
Bond lengths



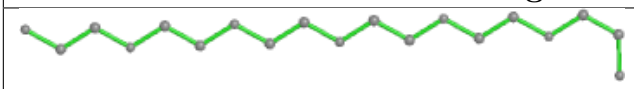
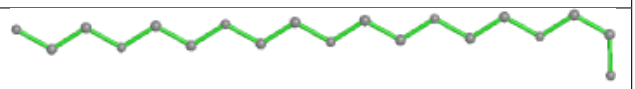
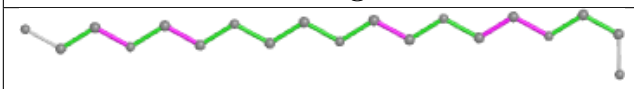
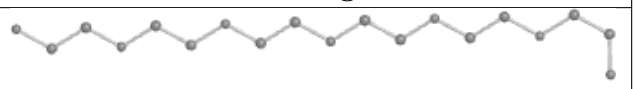
Bond angles



Torsions



Rings

Ligand P6G A 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	582/611 (95%)	-0.01	28 (4%)	30	36	23, 32, 54, 79	4 (0%)
1	B	582/611 (95%)	0.10	26 (4%)	33	38	22, 35, 56, 79	4 (0%)
1	C	593/611 (97%)	0.03	20 (3%)	45	51	21, 32, 54, 76	4 (0%)
All	All	1757/1833 (95%)	0.04	74 (4%)	36	42	21, 33, 55, 79	12 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	GLY	7.6
1	B	59	PRO	7.1
1	A	59	PRO	6.8
1	C	564	MET	6.2
1	B	58	LEU	5.6
1	C	72	LEU	5.3
1	B	60	LYS	5.2
1	B	72	LEU	5.0
1	B	567	LEU	4.8
1	B	564	MET	4.7
1	A	567	LEU	4.6
1	A	246	TYR	4.6
1	B	273	GLY	4.4
1	A	273	GLY	4.1
1	A	-1	SER	4.1
1	B	73	LYS	3.9
1	A	71	PRO	3.9
1	A	272	ASN	3.9
1	B	272	ASN	3.8
1	C	272	ASN	3.7
1	B	74	GLY	3.7
1	C	567	LEU	3.7
1	A	58	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	563	LYS	3.5
1	A	247	ASP	3.5
1	C	274	ASN	3.4
1	B	401	ASP	3.4
1	C	562	SER	3.3
1	C	59	PRO	3.3
1	C	71	PRO	3.3
1	C	565	GLN	3.2
1	A	564	MET	3.2
1	C	561	ASP	3.1
1	B	563	LYS	3.1
1	C	80	GLY	3.1
1	A	448	ASP	3.1
1	B	274	ASN	3.0
1	C	275	ALA	3.0
1	B	561	ASP	3.0
1	B	81	ARG	3.0
1	C	570	ALA	2.9
1	A	565	GLN	2.9
1	A	561	ASP	2.9
1	B	399	PHE	2.9
1	A	274	ASN	2.9
1	B	435	ILE	2.8
1	A	570	ALA	2.7
1	C	401	ASP	2.7
1	B	75	TYR	2.7
1	A	275	ALA	2.6
1	B	562	SER	2.6
1	A	80	GLY	2.6
1	C	273	GLY	2.6
1	A	439	TRP	2.6
1	B	104	ASN	2.6
1	A	286	VAL	2.5
1	A	574	LYS	2.5
1	B	135	VAL	2.4
1	B	400	LYS	2.4
1	A	568	ALA	2.3
1	B	427	ILE	2.3
1	C	575	LYS	2.3
1	A	0	HIS	2.3
1	C	574	LYS	2.2
1	C	288	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	270	ASP	2.2
1	A	135	VAL	2.2
1	B	77	VAL	2.2
1	A	72	LEU	2.2
1	B	288	VAL	2.2
1	B	287	PHE	2.1
1	C	411	ILE	2.0
1	C	569	LEU	2.0
1	A	575	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

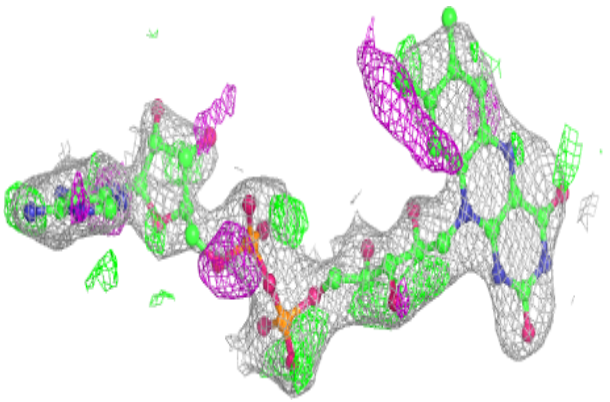
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

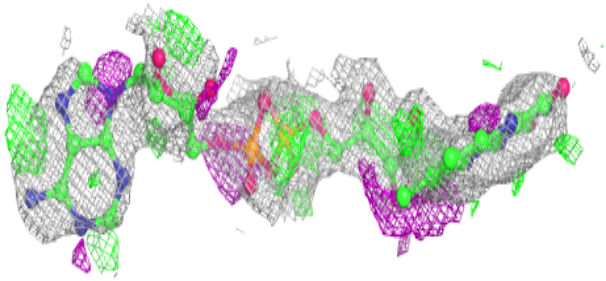
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FAD	B	602	53/53	0.78	0.26	29,42,49,54	53
4	GOL	A	603	6/6	0.81	0.43	20,20,20,20	0
4	GOL	A	602	6/6	0.86	0.45	20,20,20,20	0
2	P6G	C	601	19/19	0.87	0.16	28,37,44,45	0
4	GOL	C	603	6/6	0.90	0.11	23,28,29,36	0
4	GOL	B	603	6/6	0.93	0.13	36,42,45,45	0
3	FAD	C	602	53/53	0.94	0.11	24,33,37,41	53
2	P6G	A	601	19/19	0.94	0.12	32,38,45,46	0
2	P6G	B	601	19/19	0.95	0.09	32,38,44,47	0

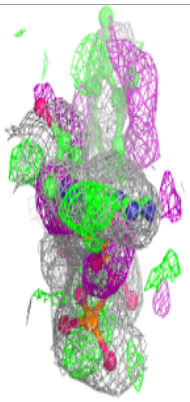
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 602:

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

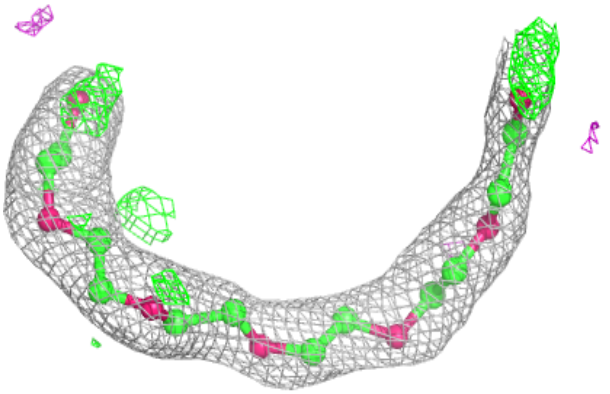


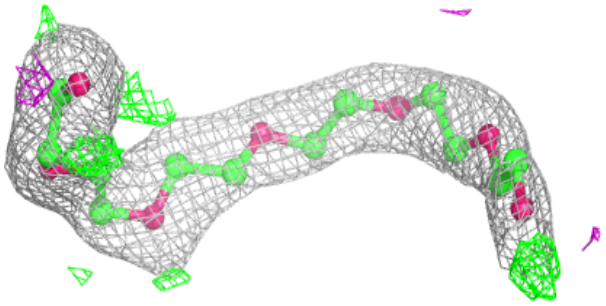


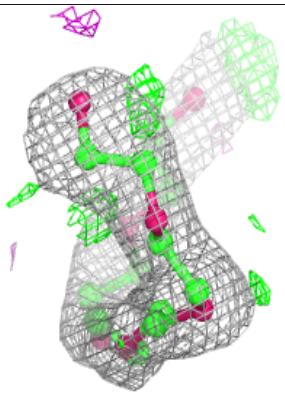


Electron density around P6G C 601:

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

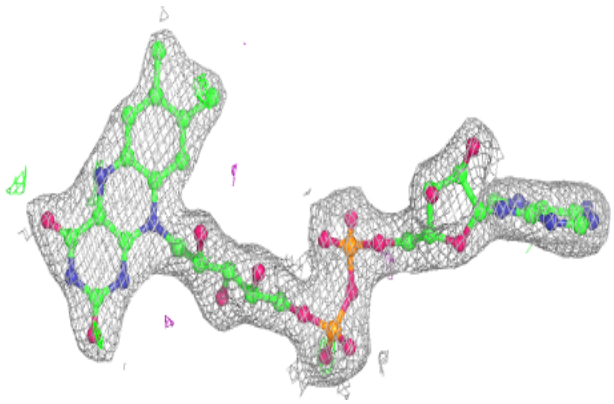


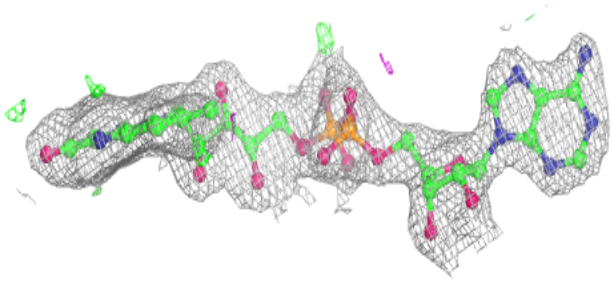


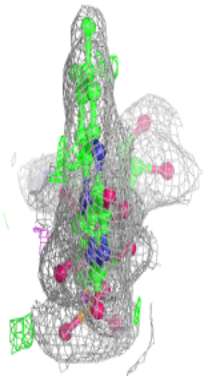


Electron density around FAD C 602:

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

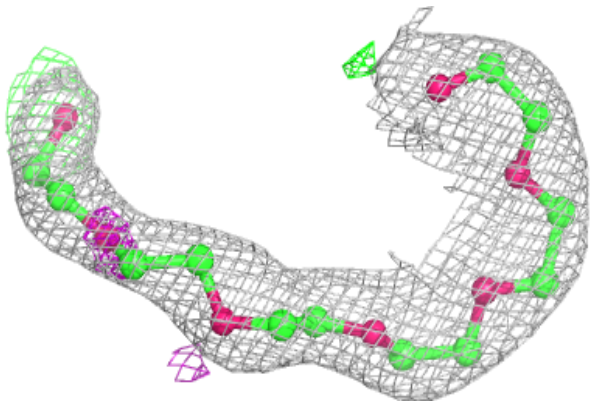


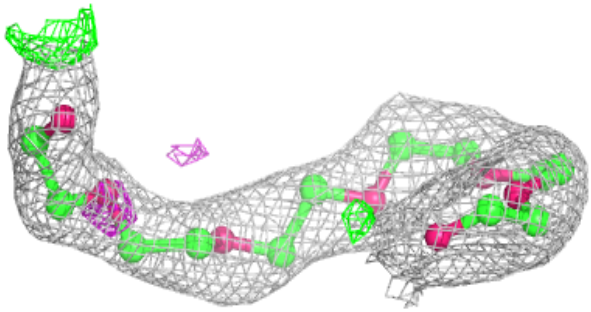


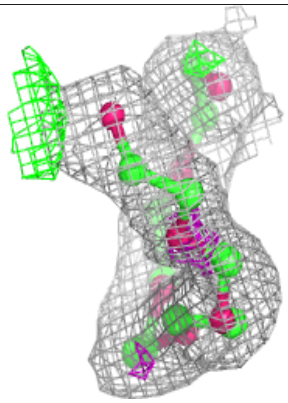


Electron density around P6G A 601:

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

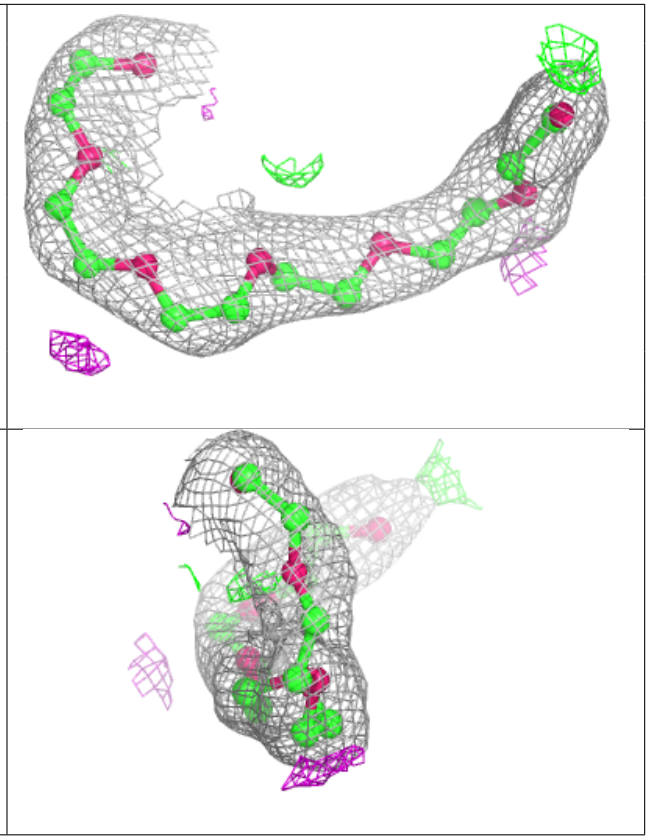






Electron density around P6G B 601:

$2mF_o$-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.