



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 02:29 pm BST

PDB ID : 1SB3  
Title : Structure of 4-hydroxybenzoyl-CoA reductase from *Thauera aromatica*  
Authors : Unciuleac, M.; Warkentin, E.; Page, C.C.; Boll, M.; Ermler, U.  
Deposited on : 2004-02-10  
Resolution : 2.20 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](mailto: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.

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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 : 2.11  
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) : 2.11

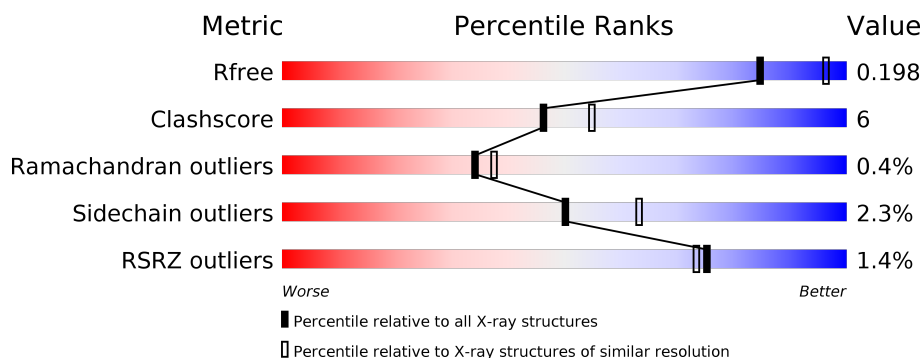
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	769	<div> <div style="width: 87%;"></div> <div style="width: 11%;"></div> <div style="width: 2%;"></div> </div>
1	D	769	<div> <div style="width: 85%;"></div> <div style="width: 13%;"></div> <div style="width: 2%;"></div> </div>
2	B	324	<div> <div style="width: 89%;"></div> <div style="width: 10%;"></div> <div style="width: 1%;"></div> </div>
2	E	324	<div> <div style="width: 86%;"></div> <div style="width: 13%;"></div> <div style="width: 1%;"></div> </div>
3	C	161	<div> <div style="width: 85%;"></div> <div style="width: 13%;"></div> <div style="width: 2%;"></div> </div>
3	F	161	<div> <div style="width: 81%;"></div> <div style="width: 15%;"></div> <div style="width: 4%;"></div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19897 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 4-hydroxybenzoyl-CoA reductase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	761	Total	C	N	O	S	0	0	0
			5716	3618	984	1085	29			
1	D	760	Total	C	N	O	S	0	0	0
			5710	3615	983	1083	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	ALA	GLY	see remark 999	UNP O33819
D	251	ALA	GLY	see remark 999	UNP O33819

- Molecule 2 is a protein called 4-hydroxybenzoyl-CoA reductase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	323	Total	C	N	O	S	0	0	0
			2407	1508	441	450	8			
2	E	323	Total	C	N	O	S	0	0	0
			2407	1508	441	450	8			

- Molecule 3 is a protein called 4-hydroxybenzoyl-CoA reductase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	161	Total	C	N	O	S	0	0	0
			1193	732	218	230	13			
3	F	157	Total	C	N	O	S	0	0	0
			1163	716	211	223	13			

There are 6 discrepancies between the modelled and reference sequences:

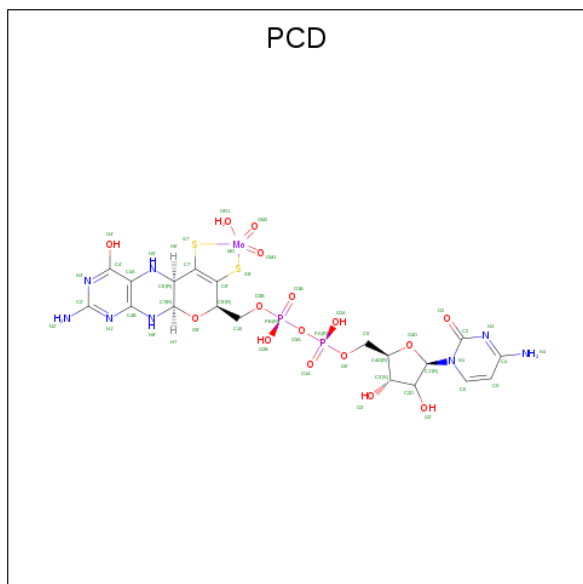
Chain	Residue	Modelled	Actual	Comment	Reference
C	142	LYS	ARG	see remark 999	UNP O33818
C	143	ILE	SER	see remark 999	UNP O33818

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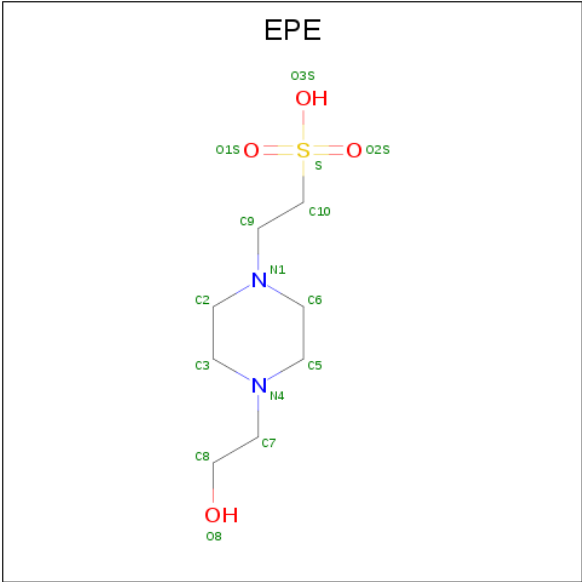
Chain	Residue	Modelled	Actual	Comment	Reference
C	144	ILE	SER	see remark 999	UNP O33818
F	142	LYS	ARG	see remark 999	UNP O33818
F	143	ILE	SER	see remark 999	UNP O33818
F	144	ILE	SER	see remark 999	UNP O33818

- Molecule 4 is (MOLYBDOPTERIN-CYTOSINE DINUCLEOTIDE-S,S)-DIOXO-AQUA-MOLYBDENUM(V) (three-letter code: PCD) (formula:  $C_{19}H_{26}MoN_8O_{16}P_2S_2$ ).



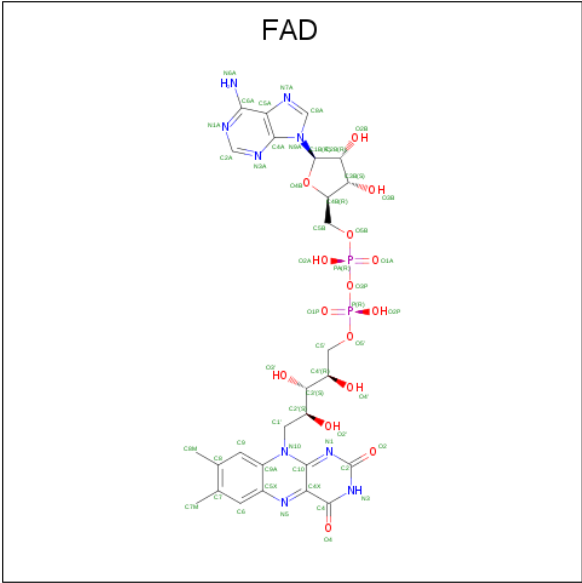
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	16	2	2		
4	D	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	16	2	2		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



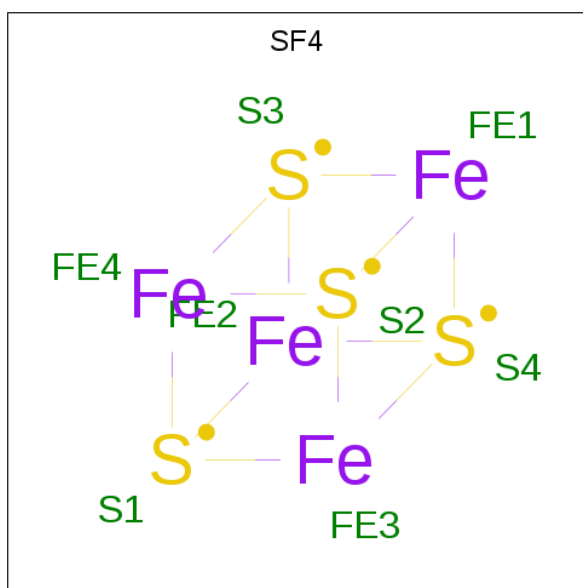
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	15	8	2	4	1	0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



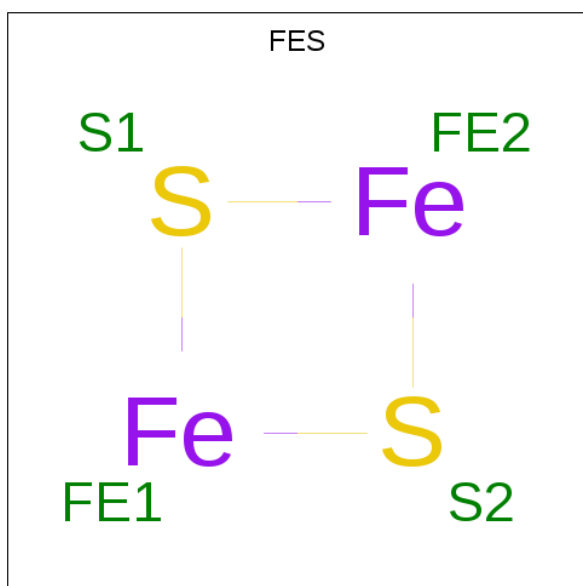
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	B	1	53	27	9	15	2	0	0
6	E	1	53	27	9	15	2	0	0

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	E	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



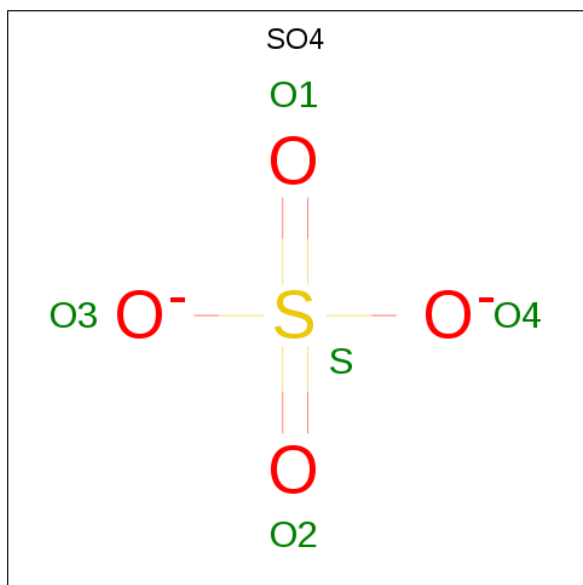
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	Fe	S	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	Fe	S	0	0
			4	2	2		
8	F	1	Total	Fe	S	0	0
			4	2	2		
8	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	319	Total	O	0	0
			319	319		
10	B	115	Total	O	0	0
			115	115		
10	C	103	Total	O	0	0
			103	103		
10	D	319	Total	O	0	0
			319	319		

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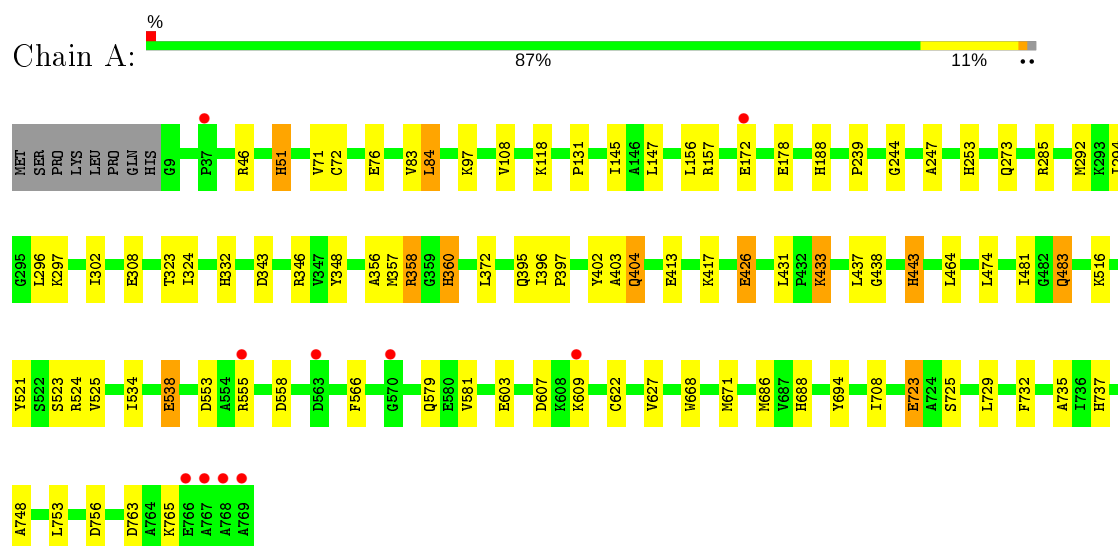
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	E	96	Total	O	0	0
			96	96		
10	F	90	Total	O	0	0
			90	90		

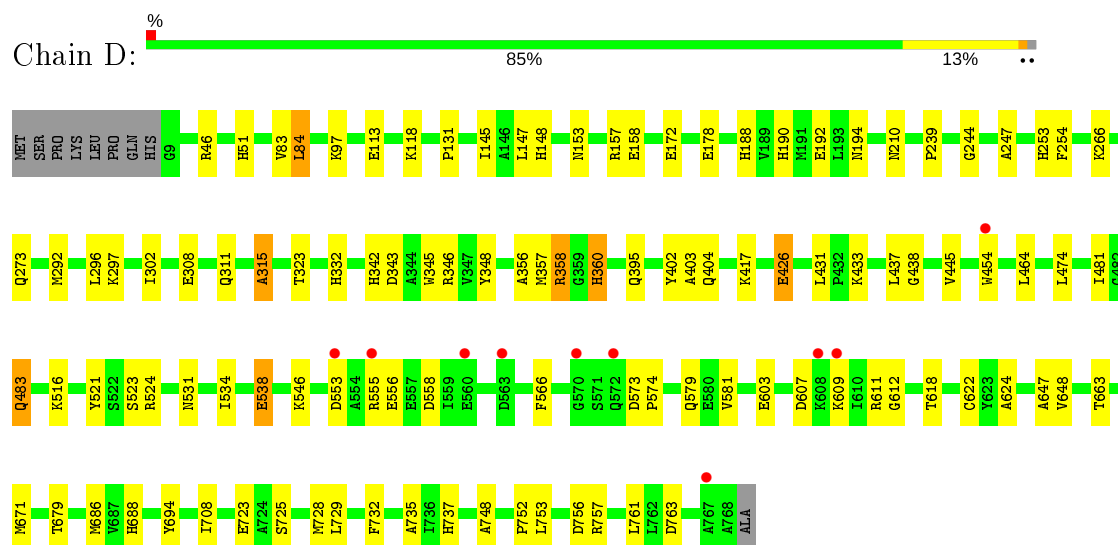
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

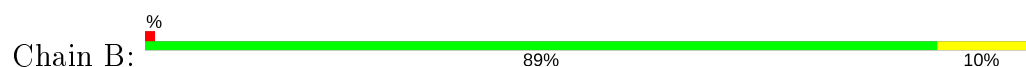
- Molecule 1: 4-hydroxybenzoyl-CoA reductase alpha subunit

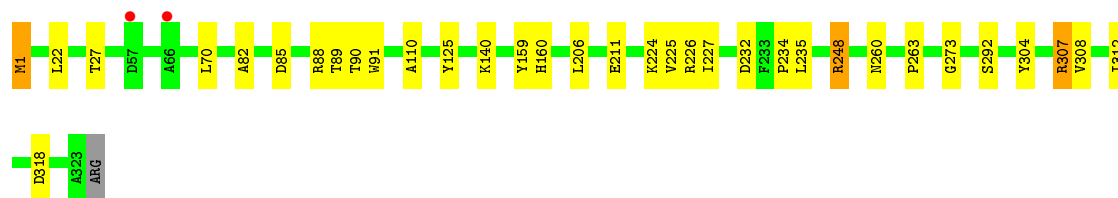


- Molecule 1: 4-hydroxybenzoyl-CoA reductase alpha subunit

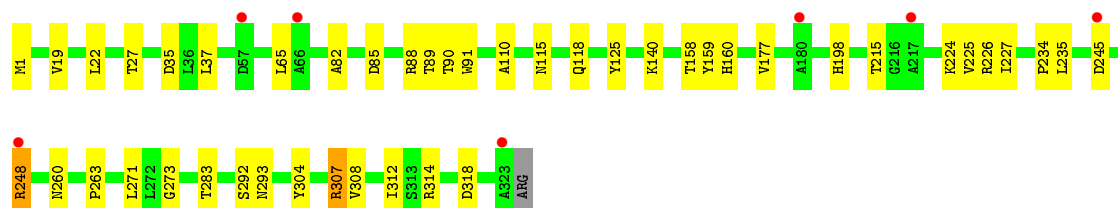
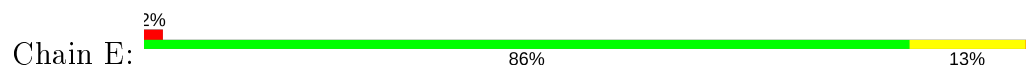


- Molecule 2: 4-hydroxybenzoyl-CoA reductase beta subunit

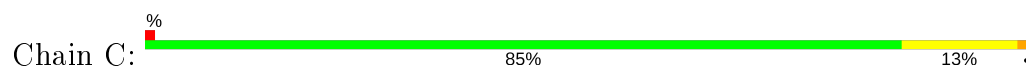




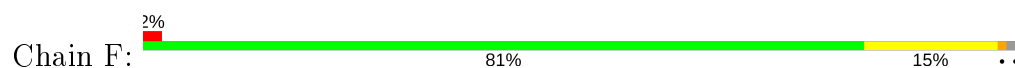
- Molecule 2: 4-hydroxybenzoyl-CoA reductase beta subunit



- Molecule 3: 4-hydroxybenzoyl-CoA reductase gamma subunit



- Molecule 3: 4-hydroxybenzoyl-CoA reductase gamma subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.62Å 150.20Å 175.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.20 19.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (19.90-2.20) 96.2 (19.90-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.26 (at 2.21Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.171 , 0.205 0.166 , 0.198	Depositor DCC
$R_{free}$ test set	7543 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19897	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SF4, FES, FAD, EPE, PCD, SO4

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	0.58	0/5823	0.76	1/7903 (0.0%)
1	D	0.57	0/5817	0.76	4/7896 (0.1%)
2	B	0.51	0/2450	0.73	0/3340
2	E	0.51	0/2450	0.73	0/3340
3	C	0.62	0/1203	0.81	1/1618 (0.1%)
3	F	0.55	0/1173	0.79	0/1580
All	All	0.56	0/18916	0.76	6/25677 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	694	TYR	N-CA-C	-6.03	94.72	111.00
1	A	694	TYR	N-CA-C	-5.94	94.97	111.00
1	D	113	GLU	OE1-CD-OE2	-5.32	116.92	123.30
3	C	112	GLU	OE1-CD-OE2	-5.06	117.22	123.30
1	D	315	ALA	N-CA-C	5.04	124.62	111.00
1	D	210	ASN	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5716	0	5769	74	0
1	D	5710	0	5764	77	0
2	B	2407	0	2434	28	0
2	E	2407	0	2434	31	0
3	C	1193	0	1225	17	0
3	F	1163	0	1198	17	0
4	A	48	0	22	7	0
4	D	48	0	22	5	0
5	A	15	0	18	0	0
6	B	53	0	31	1	0
6	E	53	0	31	3	0
7	B	8	0	0	0	0
7	E	8	0	0	0	0
8	C	8	0	0	0	0
8	F	8	0	0	0	0
9	D	5	0	0	0	0
9	E	5	0	0	0	0
10	A	319	0	0	5	0
10	B	115	0	0	1	0
10	C	103	0	0	4	0
10	D	319	0	0	9	0
10	E	96	0	0	2	0
10	F	90	0	0	2	0
All	All	19897	0	18948	239	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 6.

All (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:HG2	1:A:297:LYS:NZ	1.85	0.90
1:D:483:GLN:H	1:D:483:GLN:HE21	1.19	0.90
1:D:46:ARG:HH22	1:D:253:HIS:HE1	1.20	0.88
1:D:172:GLU:HG2	1:D:297:LYS:NZ	1.91	0.85
1:A:131:PRO:HD2	1:A:145:ILE:HD12	1.57	0.84
1:A:483:GLN:H	1:A:483:GLN:HE21	1.26	0.82
1:A:46:ARG:HH22	1:A:253:HIS:HE1	1.27	0.81
1:D:46:ARG:HH21	1:D:273:GLN:HE22	1.24	0.81
1:A:172:GLU:HG2	1:A:297:LYS:HZ1	1.45	0.80
1:D:483:GLN:HE21	1:D:483:GLN:N	1.80	0.79
1:D:417:LYS:HG2	1:D:708:ILE:HG21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HH21	1:A:273:GLN:HE22	1.30	0.79
1:D:131:PRO:HD2	1:D:145:ILE:HD12	1.63	0.79
1:A:481:ILE:H	1:A:483:GLN:HE22	1.31	0.78
1:A:607:ASP:OD1	1:A:609:LYS:HG2	1.86	0.76
1:D:607:ASP:OD1	1:D:609:LYS:HG2	1.86	0.75
1:D:172:GLU:HG2	1:D:297:LYS:HZ1	1.49	0.74
1:D:481:ILE:H	1:D:483:GLN:HE22	1.33	0.74
1:A:433:LYS:HA	1:A:433:LYS:HE3	1.71	0.72
3:C:123:ARG:HG2	3:C:123:ARG:HH11	1.54	0.72
1:A:483:GLN:HE21	1:A:483:GLN:N	1.89	0.70
1:A:737:HIS:HE1	1:A:748:ALA:O	1.74	0.69
1:D:737:HIS:HE1	1:D:748:ALA:O	1.74	0.69
1:D:83:VAL:HG13	1:D:84:LEU:HD13	1.76	0.68
1:D:433:LYS:HA	1:D:433:LYS:HE3	1.76	0.67
2:B:160:HIS:HD2	2:B:234:PRO:O	1.77	0.67
4:A:1920:PCD:MO	4:A:1920:PCD:OM1	1.66	0.67
4:D:1921:PCD:OM1	4:D:1921:PCD:MO	1.66	0.66
3:F:123:ARG:HG2	3:F:123:ARG:HH11	1.58	0.66
2:B:85:ASP:O	2:B:89:THR:HG23	1.96	0.65
1:A:83:VAL:HG13	1:A:84:LEU:HD13	1.78	0.65
3:C:123:ARG:HG2	3:C:123:ARG:NH1	2.10	0.64
2:E:85:ASP:O	2:E:89:THR:HG23	1.97	0.64
1:A:172:GLU:HG2	1:A:297:LYS:HZ3	1.61	0.64
2:B:260:ASN:HD21	2:B:292:SER:HA	1.63	0.63
3:F:123:ARG:NH1	3:F:123:ARG:HG2	2.12	0.63
1:A:686:MET:HG3	1:A:688:HIS:CE1	2.34	0.62
1:D:622:CYS:HB2	1:D:723:GLU:HG3	1.81	0.62
2:E:260:ASN:HD21	2:E:292:SER:HA	1.64	0.62
1:A:332:HIS:HB2	1:A:404:GLN:HE22	1.65	0.61
1:D:148:HIS:HE1	1:D:315:ALA:O	1.82	0.61
2:B:248:ARG:HG2	2:B:248:ARG:HH11	1.64	0.61
1:A:417:LYS:HG2	1:A:708:ILE:HG21	1.83	0.60
1:A:481:ILE:H	1:A:483:GLN:NE2	1.97	0.60
1:D:46:ARG:NH2	1:D:273:GLN:HE22	1.98	0.60
2:E:160:HIS:HD2	2:E:234:PRO:O	1.85	0.60
1:D:188:HIS:CD2	1:D:247:ALA:HB2	2.37	0.59
1:D:483:GLN:H	1:D:483:GLN:NE2	1.96	0.59
1:D:686:MET:HG3	1:D:688:HIS:CE1	2.37	0.58
2:B:224:LYS:HE2	2:B:226:ARG:HD3	1.86	0.58
1:A:188:HIS:CD2	1:A:188:HIS:H	2.22	0.58
2:B:125:TYR:CZ	2:B:140:LYS:HE3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:HIS:HB2	1:D:404:GLN:HE22	1.69	0.57
2:E:308:VAL:O	2:E:312:ILE:HG12	2.04	0.57
1:D:579:GLN:NE2	10:D:2051:HOH:O	2.35	0.56
3:F:66:HIS:HD2	10:F:2004:HOH:O	1.87	0.56
1:A:555:ARG:HB2	1:A:558:ASP:OD1	2.05	0.56
2:E:125:TYR:CZ	2:E:140:LYS:HE3	2.41	0.56
1:A:566:PHE:CD1	1:A:581:VAL:HG21	2.41	0.56
1:D:763:ASP:OD2	2:E:307:ARG:NH1	2.39	0.55
1:D:190:HIS:HD2	1:D:192:GLU:O	1.90	0.55
2:E:118:GLN:O	2:E:198:HIS:HE1	1.88	0.55
2:E:22:LEU:HD23	2:E:27:THR:HG22	1.88	0.55
1:D:481:ILE:H	1:D:483:GLN:NE2	2.02	0.55
2:B:160:HIS:HE1	10:B:1927:HOH:O	1.90	0.55
1:D:323:THR:OG1	1:D:360:HIS:HE1	1.89	0.55
1:D:725:SER:HB2	4:D:1921:PCD:H7	1.89	0.55
1:D:332:HIS:HD2	10:D:2026:HOH:O	1.90	0.55
2:B:22:LEU:HD23	2:B:27:THR:HG22	1.88	0.54
1:D:188:HIS:H	1:D:188:HIS:CD2	2.25	0.54
1:D:737:HIS:CE1	1:D:748:ALA:O	2.59	0.54
3:C:18:VAL:O	3:C:66:HIS:HE1	1.91	0.54
2:B:88:ARG:HH11	2:B:88:ARG:HG2	1.73	0.54
1:D:188:HIS:CG	1:D:247:ALA:HB2	2.42	0.54
1:A:622:CYS:HB2	1:A:723:GLU:HG3	1.89	0.54
1:A:294:ILE:HG13	1:A:372:LEU:HD23	1.90	0.53
1:A:46:ARG:NH2	1:A:273:GLN:HE22	2.01	0.53
1:A:737:HIS:CE1	1:A:748:ALA:O	2.59	0.53
2:B:1:MET:HE1	10:C:1991:HOH:O	2.08	0.53
1:D:148:HIS:HD2	10:D:2136:HOH:O	1.91	0.53
1:A:323:THR:OG1	1:A:360:HIS:HE1	1.92	0.53
2:E:1:MET:HE2	10:F:1943:HOH:O	2.08	0.53
1:A:147:LEU:HD22	1:A:348:TYR:HB3	1.91	0.53
1:D:308:GLU:HA	1:D:343:ASP:O	2.09	0.53
1:A:402:TYR:O	1:A:403:ALA:HB3	2.09	0.53
1:A:671:MET:HA	1:A:732:PHE:CD2	2.44	0.53
2:E:245:ASP:O	2:E:248:ARG:HG3	2.08	0.52
3:C:66:HIS:HD2	10:C:1984:HOH:O	1.92	0.52
1:A:285:ARG:HH11	1:A:285:ARG:HG3	1.74	0.52
1:D:402:TYR:O	1:D:403:ALA:HB3	2.10	0.52
2:E:225:VAL:HG23	2:E:312:ILE:HD13	1.91	0.52
2:E:224:LYS:HE2	2:E:226:ARG:HD3	1.92	0.51
1:A:188:HIS:CD2	1:A:247:ALA:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:HIS:HE1	1:A:356:ALA:O	1.93	0.51
1:A:443:HIS:HD2	10:A:2118:HOH:O	1.93	0.51
2:E:88:ARG:HH11	2:E:88:ARG:HG2	1.75	0.51
2:E:160:HIS:HE1	10:E:1972:HOH:O	1.94	0.51
3:F:87:LYS:HZ3	3:F:157:GLU:HB3	1.76	0.51
1:D:296:LEU:HD23	1:D:302:ILE:HA	1.93	0.51
1:D:763:ASP:CG	2:E:307:ARG:HH12	2.14	0.51
2:E:304:TYR:O	2:E:308:VAL:HG22	2.10	0.51
1:D:51:HIS:HE1	1:D:97:LYS:CE	2.24	0.50
2:B:308:VAL:O	2:B:312:ILE:HG12	2.11	0.50
1:D:454:TRP:HZ3	10:D:2237:HOH:O	1.94	0.50
2:E:159:TYR:CD2	2:E:263:PRO:HD3	2.46	0.50
1:D:752:PRO:O	1:D:757:ARG:HD2	2.12	0.49
1:A:296:LEU:HD23	1:A:302:ILE:HA	1.93	0.49
1:A:763:ASP:OD2	2:B:307:ARG:NH1	2.45	0.49
1:D:172:GLU:HG2	1:D:297:LYS:HZ3	1.72	0.49
2:E:35:ASP:HB2	6:E:1901:FAD:H2'	1.93	0.49
2:E:271:LEU:HD21	2:E:283:THR:HB	1.94	0.49
1:A:188:HIS:CG	1:A:247:ALA:HB2	2.48	0.49
1:A:725:SER:HB2	4:A:1920:PCD:H7	1.94	0.49
2:B:227:ILE:HG13	2:B:235:LEU:HD11	1.94	0.49
1:D:188:HIS:HE1	1:D:356:ALA:O	1.95	0.49
1:A:534:ILE:O	1:A:538:GLU:HG2	2.13	0.49
1:A:671:MET:HA	1:A:732:PHE:CE2	2.48	0.49
1:A:521:TYR:O	1:A:524:ARG:HG2	2.12	0.48
1:D:147:LEU:HD22	1:D:348:TYR:HB3	1.95	0.48
2:E:248:ARG:NH2	2:E:273:GLY:O	2.46	0.48
3:C:17:LEU:HG	3:F:17:LEU:HG	1.95	0.48
1:A:51:HIS:HE1	1:A:97:LYS:NZ	2.12	0.48
2:B:159:TYR:CD2	2:B:263:PRO:HD3	2.48	0.48
1:D:729:LEU:C	1:D:729:LEU:HD23	2.33	0.48
3:F:156:CYS:O	3:F:156:CYS:SG	2.72	0.48
1:A:156:LEU:HD13	1:A:348:TYR:OH	2.14	0.48
1:A:431:LEU:HD11	1:A:437:LEU:HG	1.95	0.47
1:D:153:ASN:HB2	10:D:2098:HOH:O	2.14	0.47
3:C:6:ARG:HG2	3:C:15:GLU:HG3	1.97	0.47
2:B:82:ALA:O	2:B:88:ARG:HD2	2.13	0.47
1:D:748:ALA:HA	1:D:761:LEU:HD11	1.96	0.47
1:D:131:PRO:HD2	1:D:145:ILE:CD1	2.39	0.47
1:D:332:HIS:HE1	10:D:2238:HOH:O	1.98	0.47
3:F:145:LYS:NZ	3:F:145:LYS:HB2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:LEU:HD11	2:B:206:LEU:HD21	1.97	0.47
2:B:248:ARG:CG	2:B:248:ARG:HH11	2.28	0.47
2:B:225:VAL:HG23	2:B:312:ILE:HD13	1.96	0.47
2:B:1:MET:HE2	10:C:1910:HOH:O	2.14	0.47
1:D:534:ILE:O	1:D:538:GLU:HG2	2.15	0.47
1:D:679:THR:HB	1:D:688:HIS:CE1	2.49	0.47
3:F:82:GLN:HA	3:F:82:GLN:NE2	2.30	0.47
1:A:51:HIS:HE1	1:A:97:LYS:CE	2.28	0.46
10:C:1985:HOH:O	1:D:266:LYS:HE3	2.15	0.46
1:D:426:GLU:N	1:D:426:GLU:OE1	2.48	0.46
2:E:158:THR:HB	2:E:160:HIS:CE1	2.50	0.46
3:F:105:PRO:O	3:F:109:MET:HG2	2.15	0.46
1:A:357:MET:O	1:A:358:ARG:C	2.54	0.46
3:C:118:ASN:O	3:C:121:PRO:HD3	2.16	0.46
1:D:431:LEU:HD11	1:D:437:LEU:HG	1.96	0.46
3:F:18:VAL:O	3:F:66:HIS:HE1	1.99	0.46
1:A:308:GLU:HA	1:A:343:ASP:O	2.15	0.46
1:A:426:GLU:HG2	10:A:2168:HOH:O	2.15	0.46
1:D:624:ALA:HB2	1:D:648:VAL:HG12	1.98	0.46
3:C:151:ALA:O	3:C:155:LEU:HB2	2.15	0.46
3:C:5:LEU:HG	3:C:7:LEU:HD23	1.98	0.46
2:E:90:THR:HB	2:E:91:TRP:CE3	2.50	0.46
3:F:122:SER:OG	3:F:125:GLU:HG3	2.16	0.45
1:A:748:ALA:CB	1:A:753:LEU:HD22	2.46	0.45
4:D:1921:PCD:O5'	4:D:1921:PCD:H6	2.17	0.45
1:A:763:ASP:CG	2:B:307:ARG:HH12	2.19	0.45
1:D:438:GLY:HA3	1:D:735:ALA:O	2.16	0.45
1:D:521:TYR:O	1:D:524:ARG:HG2	2.17	0.45
1:D:445:VAL:HB	1:D:618:THR:HB	1.99	0.45
1:A:396:ILE:HA	1:A:397:PRO:C	2.37	0.45
1:A:72:CYS:HA	1:A:76:GLU:OE2	2.17	0.45
1:A:483:GLN:H	1:A:483:GLN:NE2	2.05	0.45
1:A:438:GLY:HA3	1:A:735:ALA:O	2.17	0.45
3:C:57:PRO:HD3	3:C:113:ALA:HB1	1.98	0.45
1:A:483:GLN:HG3	4:A:1920:PCD:H5'2	1.98	0.45
2:E:82:ALA:O	2:E:88:ARG:HD2	2.16	0.45
3:F:118:ASN:O	3:F:121:PRO:HD3	2.17	0.45
3:F:6:ARG:HG2	3:F:15:GLU:HG3	1.98	0.45
1:A:178:GLU:HA	1:A:292:MET:O	2.16	0.44
1:A:332:HIS:HE1	10:A:2209:HOH:O	2.00	0.44
2:B:70:LEU:O	2:B:211:GLU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:ALA:HB1	6:B:1900:FAD:H4'	2.00	0.44
3:F:52:LEU:CD2	3:F:113:ALA:HB2	2.48	0.44
1:A:417:LYS:CG	1:A:708:ILE:HG21	2.47	0.44
1:D:357:MET:O	1:D:358:ARG:C	2.57	0.43
1:D:566:PHE:CD1	1:D:581:VAL:HG21	2.53	0.43
1:A:481:ILE:N	1:A:483:GLN:HE22	2.09	0.43
1:A:579:GLN:NE2	10:A:2027:HOH:O	2.42	0.43
1:A:725:SER:CB	4:A:1920:PCD:H7	2.48	0.43
2:E:215:THR:HG21	10:E:1948:HOH:O	2.19	0.43
1:A:765:LYS:HG2	1:A:765:LYS:O	2.19	0.43
2:E:110:ALA:HB1	6:E:1901:FAD:H4'	2.01	0.43
1:D:725:SER:CB	4:D:1921:PCD:H7	2.48	0.43
1:D:342:HIS:HD2	10:D:2122:HOH:O	2.01	0.43
1:A:521:TYR:HB2	10:A:2071:HOH:O	2.17	0.42
1:A:433:LYS:CA	1:A:433:LYS:HE3	2.44	0.42
3:C:65:ALA:O	3:C:68:VAL:HG22	2.19	0.42
1:D:531:ASN:HA	1:D:531:ASN:HD22	1.64	0.42
1:A:729:LEU:HD23	1:A:729:LEU:C	2.39	0.42
1:D:194:ASN:HB3	1:D:254:PHE:CZ	2.55	0.42
1:A:413:GLU:O	1:A:417:LYS:HB2	2.19	0.42
2:E:227:ILE:HG13	2:E:235:LEU:HD11	2.01	0.42
1:D:671:MET:HA	1:D:732:PHE:CE2	2.55	0.42
1:D:253:HIS:HD2	10:D:2024:HOH:O	2.02	0.42
1:D:555:ARG:HB2	1:D:558:ASP:OD1	2.19	0.42
1:D:417:LYS:CG	1:D:708:ILE:HG21	2.39	0.42
2:B:304:TYR:O	2:B:308:VAL:HG22	2.18	0.42
2:B:90:THR:HB	2:B:91:TRP:CE3	2.54	0.42
1:D:663:THR:HG23	1:D:728:MET:HG3	2.02	0.42
1:A:668:TRP:CG	3:C:139:GLY:HA2	2.54	0.42
1:A:464:LEU:HD23	1:A:474:LEU:HA	2.02	0.42
3:C:105:PRO:O	3:C:109:MET:HG2	2.20	0.41
1:D:748:ALA:CB	1:D:753:LEU:HD22	2.50	0.41
1:D:523:SER:HA	4:D:1921:PCD:O1B	2.20	0.41
1:D:647:ALA:HA	1:D:708:ILE:O	2.20	0.41
4:A:1920:PCD:H6	4:A:1920:PCD:O5'	2.20	0.41
3:C:145:LYS:NZ	3:C:145:LYS:HB2	2.35	0.41
1:D:464:LEU:HD23	1:D:474:LEU:HA	2.02	0.41
1:D:612:GLY:HA2	10:D:1970:HOH:O	2.20	0.41
1:D:178:GLU:HA	1:D:292:MET:O	2.20	0.41
2:E:19:VAL:HG21	2:E:177:VAL:HG12	2.01	0.41
1:A:404:GLN:HE21	1:A:404:GLN:HB2	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:GLY:O	1:A:627:VAL:HA	2.20	0.41
2:E:314:ARG:HE	2:E:314:ARG:HB3	1.52	0.41
2:E:115:ASN:HB2	6:E:1901:FAD:O4'	2.21	0.41
2:E:37:LEU:HA	2:E:37:LEU:HD23	1.88	0.41
1:A:71:VAL:HG22	1:A:108:VAL:HG23	2.03	0.41
1:A:324:ILE:HB	1:A:346:ARG:HB2	2.03	0.41
3:F:65:ALA:O	3:F:68:VAL:HG22	2.20	0.41
1:A:525:VAL:HB	4:A:1920:PCD:O2B	2.21	0.41
1:A:426:GLU:OE1	1:A:426:GLU:N	2.54	0.41
2:B:226:ARG:HD2	2:B:232:ASP:HB2	2.03	0.41
1:D:573:ASP:HA	1:D:574:PRO:HD3	1.88	0.41
1:A:523:SER:HA	4:A:1920:PCD:O1B	2.20	0.40
3:C:21:ASN:HD22	3:C:21:ASN:H	1.67	0.40
3:F:17:LEU:HD23	3:F:17:LEU:HA	1.83	0.40
2:B:248:ARG:NH2	2:B:273:GLY:O	2.55	0.40
3:C:52:LEU:CD2	3:C:113:ALA:HB2	2.50	0.40
1:D:756:ASP:HA	2:E:304:TYR:CD1	2.56	0.40
3:C:17:LEU:HD11	3:F:4:ILE:HG12	2.04	0.40
1:A:756:ASP:HA	2:B:304:TYR:CD1	2.56	0.40
2:B:88:ARG:HG2	2:B:88:ARG:NH1	2.35	0.40
1:D:158:GLU:HG2	1:D:345:TRP:CD1	2.56	0.40
1:D:311:GLN:NE2	1:D:346:ARG:HH11	2.19	0.40
1:D:546:LYS:HE2	1:D:556:GLU:OE2	2.21	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	759/769 (99%)	733 (97%)	22 (3%)	4 (0%)	29	31
1	D	758/769 (99%)	731 (96%)	23 (3%)	4 (0%)	29	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	321/324 (99%)	312 (97%)	9 (3%)	0	100	100
2	E	321/324 (99%)	308 (96%)	13 (4%)	0	100	100
3	C	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
3	F	155/161 (96%)	150 (97%)	4 (3%)	1 (1%)	25	26
All	All	2473/2508 (99%)	2388 (97%)	76 (3%)	9 (0%)	34	37

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	HIS
1	A	358	ARG
1	D	358	ARG
1	D	360	HIS
1	D	244	GLY
1	A	239	PRO
1	D	239	PRO
1	A	244	GLY
3	F	43	GLY

### 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	589/597 (99%)	574 (98%)	15 (2%)	47	60
1	D	589/597 (99%)	578 (98%)	11 (2%)	57	71
2	B	242/243 (100%)	238 (98%)	4 (2%)	60	74
2	E	242/243 (100%)	237 (98%)	5 (2%)	53	67
3	C	128/128 (100%)	124 (97%)	4 (3%)	40	51
3	F	126/128 (98%)	121 (96%)	5 (4%)	31	40
All	All	1916/1936 (99%)	1872 (98%)	44 (2%)	50	63

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	84	LEU
1	A	118	LYS
1	A	157	ARG
1	A	395	GLN
1	A	404	GLN
1	A	426	GLU
1	A	433	LYS
1	A	443	HIS
1	A	483	GLN
1	A	516	LYS
1	A	538	GLU
1	A	553	ASP
1	A	603	GLU
1	A	723	GLU
2	B	1	MET
2	B	248	ARG
2	B	307	ARG
2	B	318	ASP
3	C	7	LEU
3	C	21	ASN
3	C	145	LYS
3	C	158	GLU
1	D	84	LEU
1	D	118	LYS
1	D	157	ARG
1	D	395	GLN
1	D	426	GLU
1	D	483	GLN
1	D	516	LYS
1	D	538	GLU
1	D	553	ASP
1	D	603	GLU
1	D	611	ARG
2	E	65	LEU
2	E	248	ARG
2	E	293	ASN
2	E	307	ARG
2	E	318	ASP
3	F	7	LEU
3	F	21	ASN
3	F	145	LYS
3	F	155	LEU

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Mol	Chain	Res	Type
3	F	157	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	188	HIS
1	A	220	HIS
1	A	253	HIS
1	A	273	GLN
1	A	311	GLN
1	A	332	HIS
1	A	360	HIS
1	A	395	GLN
1	A	404	GLN
1	A	443	HIS
1	A	483	GLN
1	A	531	ASN
1	A	579	GLN
1	A	626	GLN
1	A	683	ASN
1	A	737	HIS
2	B	118	GLN
2	B	126	ASN
2	B	160	HIS
2	B	260	ASN
2	B	293	ASN
3	C	21	ASN
3	C	66	HIS
3	C	82	GLN
1	D	51	HIS
1	D	148	HIS
1	D	188	HIS
1	D	190	HIS
1	D	220	HIS
1	D	253	HIS
1	D	273	GLN
1	D	311	GLN
1	D	332	HIS
1	D	342	HIS
1	D	360	HIS
1	D	404	GLN

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Mol	Chain	Res	Type
1	D	483	GLN
1	D	531	ASN
1	D	626	GLN
1	D	683	ASN
1	D	737	HIS
2	E	118	GLN
2	E	126	ASN
2	E	160	HIS
2	E	198	HIS
2	E	260	ASN
2	E	293	ASN
3	F	21	ASN
3	F	66	HIS
3	F	82	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

13 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	PCD	A	1920	-	36,53,53	1.96	8 (22%)	41,86,86	5.24	20 (48%)
7	SF4	B	1910	2	0,12,12	0.00	-	-		
8	FES	F	1917	3	0,4,4	0.00	-	-		
5	EPE	A	1111	-	15,15,15	2.14	5 (33%)	18,20,20	1.81	4 (22%)
9	SO4	D	1112	-	4,4,4	0.14	0	6,6,6	0.16	0
4	PCD	D	1921	-	36,53,53	1.66	5 (13%)	41,86,86	5.25	18 (43%)
8	FES	C	1908	3	0,4,4	0.00	-	-		
9	SO4	E	1113	-	4,4,4	0.24	0	6,6,6	0.17	0
7	SF4	E	1911	2	0,12,12	0.00	-	-		
6	FAD	B	1900	-	51,58,58	2.53	16 (31%)	60,89,89	2.27	12 (20%)
8	FES	C	1907	3	0,4,4	0.00	-	-		
8	FES	F	1918	3	0,4,4	0.00	-	-		
6	FAD	E	1901	-	51,58,58	2.57	19 (37%)	60,89,89	2.47	17 (28%)

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	PCD	A	1920	-	-	4/20/78/78	0/6/6/6
7	SF4	B	1910	2	-	-	0/6/5/5
6	FAD	E	1901	-	-	6/30/50/50	0/6/6/6
4	PCD	D	1921	-	-	5/20/78/78	0/6/6/6
8	FES	C	1908	3	-	-	0/1/1/1
7	SF4	E	1911	2	-	-	0/6/5/5
8	FES	F	1917	3	-	-	0/1/1/1
6	FAD	B	1900	-	-	7/30/50/50	0/6/6/6
8	FES	C	1907	3	-	-	0/1/1/1
5	EPE	A	1111	-	-	4/9/19/19	0/1/1/1
8	FES	F	1918	3	-	-	0/1/1/1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1901	FAD	C4X-C10	7.74	1.46	1.38
6	B	1900	FAD	C4X-C10	7.45	1.46	1.38
6	E	1901	FAD	O4B-C1B	7.32	1.51	1.41
6	E	1901	FAD	C9A-N10	6.80	1.47	1.38
4	A	1920	PCD	C6'-N5'	5.71	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1900	FAD	O4B-C1B	5.65	1.49	1.41
6	B	1900	FAD	C9A-N10	5.61	1.46	1.38
6	B	1900	FAD	C10-N1	5.20	1.39	1.33
5	A	1111	EPE	O3S-S	5.16	1.65	1.47
4	D	1921	PCD	C6'-N5'	4.71	1.51	1.45
6	B	1900	FAD	C4X-N5	4.67	1.40	1.33
4	A	1920	PCD	C5-C4	4.64	1.52	1.41
4	D	1921	PCD	C5-C4	4.42	1.51	1.41
6	E	1901	FAD	C10-N1	4.42	1.38	1.33
6	B	1900	FAD	C1'-N10	4.41	1.52	1.48
6	E	1901	FAD	C4-C4X	4.35	1.48	1.41
6	B	1900	FAD	C4-N3	3.96	1.39	1.33
6	B	1900	FAD	PA-O2A	-3.87	1.37	1.55
6	E	1901	FAD	PA-O2A	-3.76	1.37	1.55
4	A	1920	PCD	O4D-C1'	3.60	1.46	1.41
6	B	1900	FAD	C4-C4X	3.51	1.47	1.41
4	A	1920	PCD	C4A-C4B	3.33	1.47	1.41
6	E	1901	FAD	C1'-N10	3.20	1.51	1.48
5	A	1111	EPE	C10-S	3.19	1.82	1.77
6	E	1901	FAD	C4A-N3A	3.13	1.40	1.35
6	B	1900	FAD	O5'-C5'	3.13	1.56	1.44
6	B	1900	FAD	C5X-N5	3.12	1.40	1.35
6	E	1901	FAD	O5'-C5'	3.11	1.56	1.44
4	D	1921	PCD	O4D-C1'	3.09	1.45	1.41
4	A	1920	PCD	C2'-N1'	3.09	1.40	1.35
5	A	1111	EPE	C9-C10	-3.02	1.44	1.52
6	E	1901	FAD	C4X-N5	3.01	1.37	1.33
6	B	1900	FAD	P-O2P	-3.00	1.41	1.55
4	A	1920	PCD	C7-C6'	2.79	1.55	1.53
6	B	1900	FAD	C2-N3	2.72	1.43	1.38
6	E	1901	FAD	C2-N1	-2.72	1.32	1.38
6	E	1901	FAD	C4-N3	2.71	1.37	1.33
6	B	1900	FAD	C8-C7	2.71	1.47	1.40
6	E	1901	FAD	C8-C7	2.53	1.47	1.40
6	E	1901	FAD	C5X-N5	2.51	1.39	1.35
6	B	1900	FAD	C2-N1	-2.48	1.33	1.38
5	A	1111	EPE	C7-N4	2.47	1.53	1.47
6	E	1901	FAD	P-O2P	-2.43	1.43	1.55
4	A	1920	PCD	C3'-C4D	2.37	1.59	1.53
4	D	1921	PCD	C4A-C4B	2.36	1.45	1.41
6	E	1901	FAD	C9A-C5X	2.32	1.47	1.42
6	E	1901	FAD	C2-N3	2.19	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1921	PCD	O4'-C4'	2.18	1.39	1.29
5	A	1111	EPE	C9-N1	2.15	1.52	1.47
6	B	1900	FAD	C2A-N3A	2.12	1.35	1.32
4	A	1920	PCD	O4'-C4'	2.08	1.39	1.29
6	E	1901	FAD	C2B-C1B	-2.07	1.50	1.53
6	E	1901	FAD	C2A-N3A	2.05	1.35	1.32

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1921	PCD	C4A-C4B-N8'	-20.64	99.25	118.13
4	A	1920	PCD	C4A-C4B-N8'	-19.90	99.93	118.13
4	D	1921	PCD	N2'-C2'-N3'	14.13	139.22	117.25
4	A	1920	PCD	N2'-C2'-N3'	13.43	138.13	117.25
4	D	1921	PCD	N2'-C2'-N1'	-10.94	100.24	117.25
4	A	1920	PCD	N2'-C2'-N1'	-10.70	100.61	117.25
6	E	1901	FAD	C1'-N10-C9A	8.78	125.20	118.29
4	A	1920	PCD	C2-N3-C4	8.67	125.13	116.34
6	E	1901	FAD	C4-N3-C2	8.36	122.20	115.14
6	B	1900	FAD	C4-N3-C2	8.28	122.13	115.14
4	D	1921	PCD	C2-N3-C4	7.85	124.30	116.34
4	A	1920	PCD	O4'-C4'-N3'	-6.98	98.92	117.30
4	D	1921	PCD	C4B-N8'-C7	6.73	136.85	123.67
6	B	1900	FAD	C1'-N10-C9A	6.66	123.53	118.29
4	A	1920	PCD	O9'-C7-C6'	-6.65	104.53	108.96
4	D	1921	PCD	O4'-C4'-N3'	-6.59	99.96	117.30
4	D	1921	PCD	C5-C4-N3	-6.45	114.28	121.72
4	A	1920	PCD	O9'-C7-N8'	6.40	115.14	108.57
4	A	1920	PCD	C3'-C2D-C1'	-6.36	91.40	100.98
4	A	1920	PCD	C4B-N8'-C7	6.34	136.09	123.67
4	D	1921	PCD	C3'-C2D-C1'	-6.20	91.64	100.98
4	A	1920	PCD	C5-C4-N3	-6.14	114.64	121.72
6	E	1901	FAD	O4'-C4'-C5'	5.57	122.43	109.92
4	D	1921	PCD	O9'-C7-N8'	5.34	114.06	108.57
6	E	1901	FAD	C1'-N10-C10	-5.24	113.72	118.41
6	B	1900	FAD	C4-C4X-C10	-5.18	116.52	119.95
4	D	1921	PCD	N4-C4-N3	5.04	124.46	116.49
4	D	1921	PCD	O9'-C7-C6'	-4.84	105.73	108.96
6	E	1901	FAD	C4-C4X-C10	-4.52	116.96	119.95
6	B	1900	FAD	O4'-C4'-C5'	4.38	119.77	109.92
6	B	1900	FAD	C1'-N10-C10	-4.37	114.50	118.41
4	A	1920	PCD	O2B-PB-O1B	4.29	133.47	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1920	PCD	N4-C4-N3	4.27	123.24	116.49
6	E	1901	FAD	C4X-C4-N3	-4.04	117.90	123.43
4	D	1921	PCD	O2B-PB-O1B	3.92	131.63	112.24
6	B	1900	FAD	C4X-C4-N3	-3.67	118.42	123.43
6	E	1901	FAD	O3'-C3'-C4'	-3.64	100.03	108.81
5	A	1111	EPE	O2S-S-C10	3.61	111.26	106.92
4	A	1920	PCD	C4A-N5'-C6'	-3.52	106.18	119.86
6	E	1901	FAD	C5X-C9A-N10	-3.49	115.19	117.72
6	B	1900	FAD	O4'-C4'-C3'	3.47	117.53	109.10
6	B	1900	FAD	O3'-C3'-C4'	-3.43	100.53	108.81
5	A	1111	EPE	O1S-S-C10	-3.43	102.79	106.92
4	D	1921	PCD	C4A-N5'-C6'	-3.38	106.73	119.86
6	E	1901	FAD	C4X-N5-C5X	3.37	120.13	116.77
6	B	1900	FAD	C4-C4X-N5	3.29	122.36	118.60
6	E	1901	FAD	C4-C4X-N5	3.19	122.24	118.60
4	D	1921	PCD	N3'-C2'-N1'	-3.11	120.54	125.42
6	B	1900	FAD	C5X-C9A-N10	-2.87	115.63	117.72
4	A	1920	PCD	O4D-C4D-C5'	2.85	118.74	109.37
6	E	1901	FAD	C2A-N1A-C6A	2.83	123.60	118.75
5	A	1111	EPE	C6-N1-C2	2.77	115.06	108.83
4	A	1920	PCD	N3'-C2'-N1'	-2.66	121.25	125.42
4	D	1921	PCD	O4D-C4D-C5'	2.65	118.08	109.37
4	A	1920	PCD	C8'-C7'-S7'	-2.63	118.66	120.15
6	E	1901	FAD	C5A-C6A-N6A	2.58	124.27	120.35
4	A	1920	PCD	C4A-C4'-N3'	2.54	131.24	124.01
4	D	1921	PCD	C4A-C4'-N3'	2.50	131.12	124.01
6	E	1901	FAD	O4'-C4'-C3'	2.48	115.12	109.10
5	A	1111	EPE	C5-N4-C3	2.47	114.40	108.83
4	A	1920	PCD	O4D-C4D-C3'	-2.43	100.31	105.11
6	B	1900	FAD	C2A-N1A-C6A	2.42	122.90	118.75
6	E	1901	FAD	N3A-C2A-N1A	-2.37	124.98	128.68
6	B	1900	FAD	N3A-C2A-N1A	-2.36	125.00	128.68
4	D	1921	PCD	O2A-PA-O1A	2.26	123.43	112.24
6	E	1901	FAD	C4'-C3'-C2'	2.25	118.05	113.36
4	D	1921	PCD	O4D-C4D-C3'	-2.22	100.72	105.11
6	E	1901	FAD	C5A-C6A-N1A	-2.17	115.42	120.35
6	E	1901	FAD	C4A-C5A-N7A	2.13	111.62	109.40
4	A	1920	PCD	O2'-C2D-C3'	2.05	118.46	111.82
4	A	1920	PCD	O2A-PA-O1A	2.03	122.29	112.24

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1920	PCD	C10-O3B-PB-O1B
5	A	1111	EPE	C10-C9-N1-C2
4	D	1921	PCD	C10-O3B-PB-O1B
6	B	1900	FAD	N10-C1'-C2'-O2'
6	B	1900	FAD	C2'-C3'-C4'-C5'
6	B	1900	FAD	O4'-C4'-C5'-O5'
6	E	1901	FAD	N10-C1'-C2'-O2'
6	E	1901	FAD	C2'-C3'-C4'-C5'
6	E	1901	FAD	O3'-C3'-C4'-C5'
6	E	1901	FAD	O4'-C4'-C5'-O5'
6	B	1900	FAD	O2'-C2'-C3'-C4'
6	B	1900	FAD	O3'-C3'-C4'-C5'
6	E	1901	FAD	O2'-C2'-C3'-C4'
5	A	1111	EPE	C8-C7-N4-C5
5	A	1111	EPE	C10-C9-N1-C6
5	A	1111	EPE	C8-C7-N4-C3
4	A	1920	PCD	C5'-O5'-PA-O3A
4	D	1921	PCD	C5'-O5'-PA-O3A
4	D	1921	PCD	C10-O3B-PB-O3A
4	A	1920	PCD	C9'-C10-O3B-PB
4	D	1921	PCD	C9'-C10-O3B-PB
6	B	1900	FAD	N10-C1'-C2'-C3'
6	E	1901	FAD	N10-C1'-C2'-C3'
4	A	1920	PCD	C10-O3B-PB-O3A
6	B	1900	FAD	PA-O3P-P-O1P
4	D	1921	PCD	C5'-O5'-PA-O1A

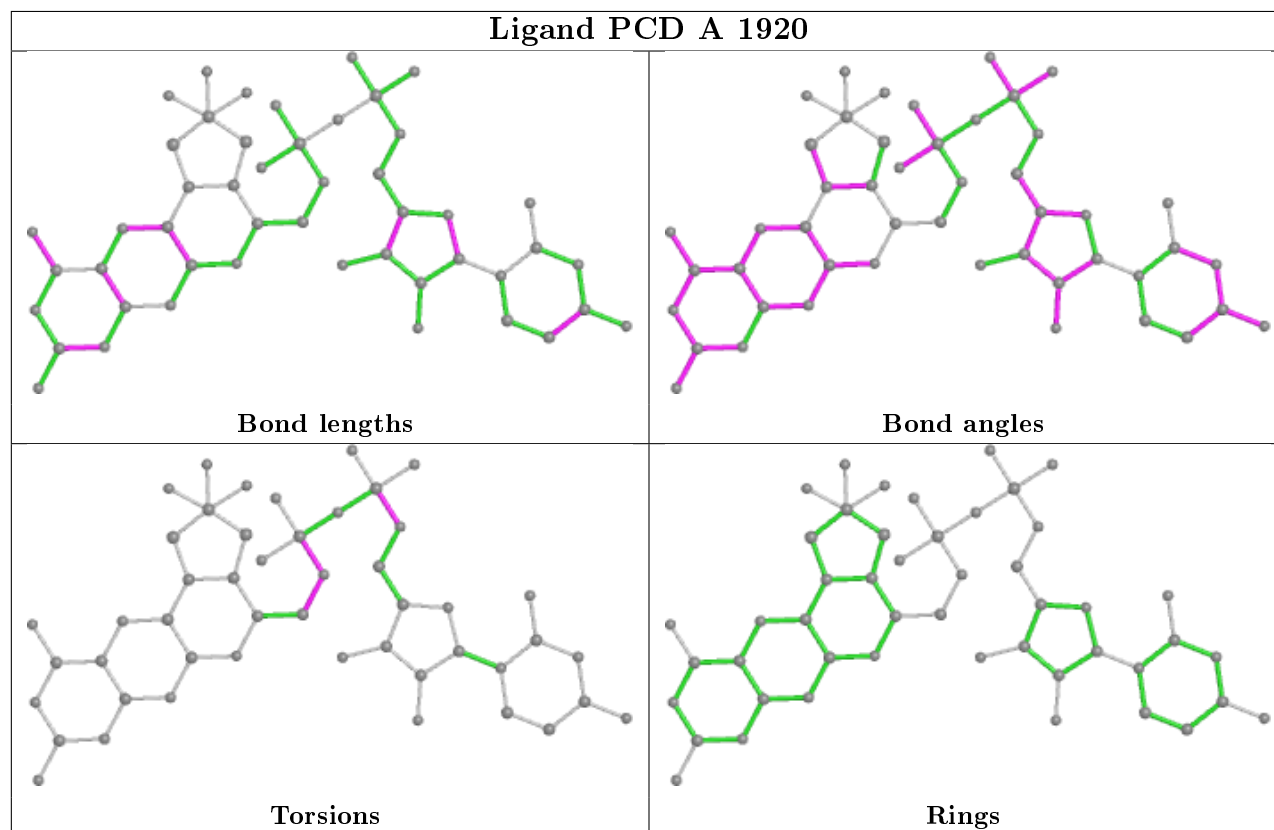
There are no ring outliers.

4 monomers are involved in 16 short contacts:

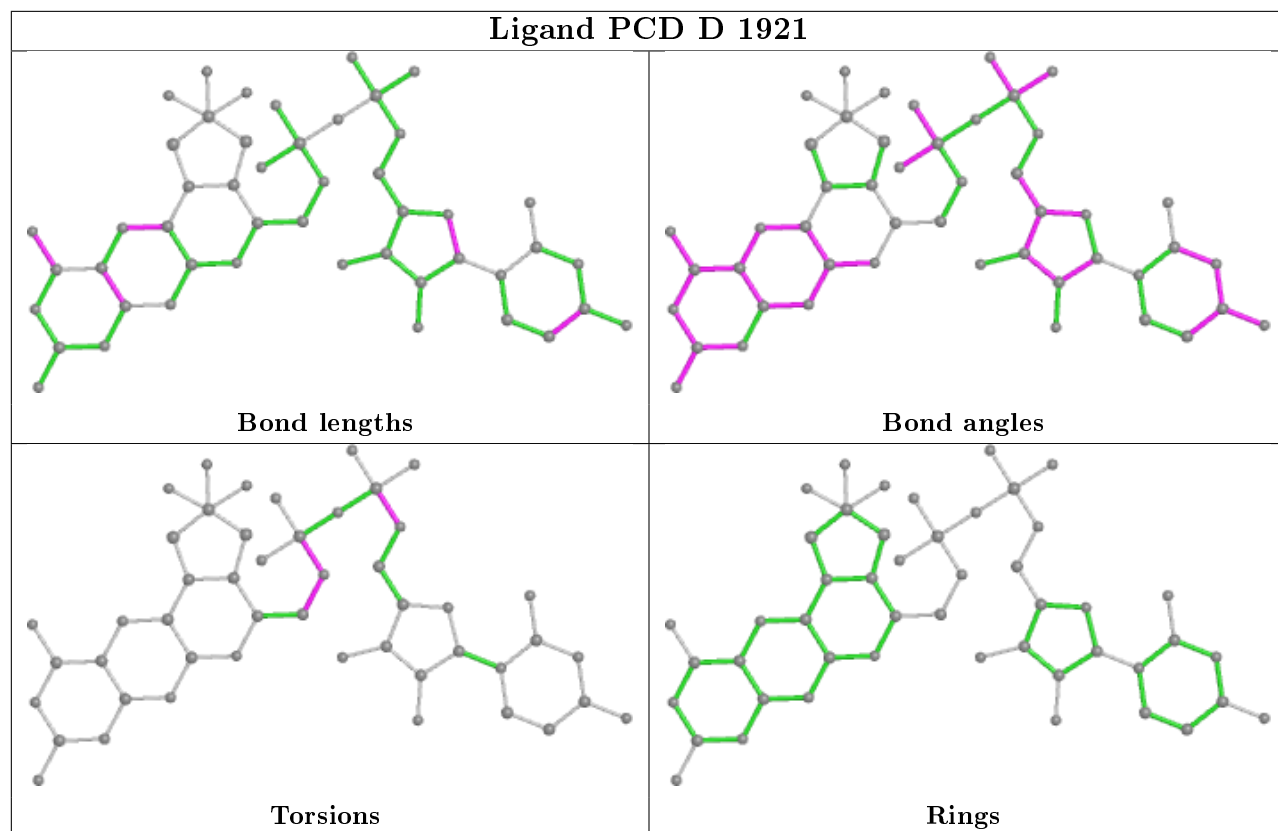
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1920	PCD	7	0
4	D	1921	PCD	5	0
6	B	1900	FAD	1	0
6	E	1901	FAD	3	0

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 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

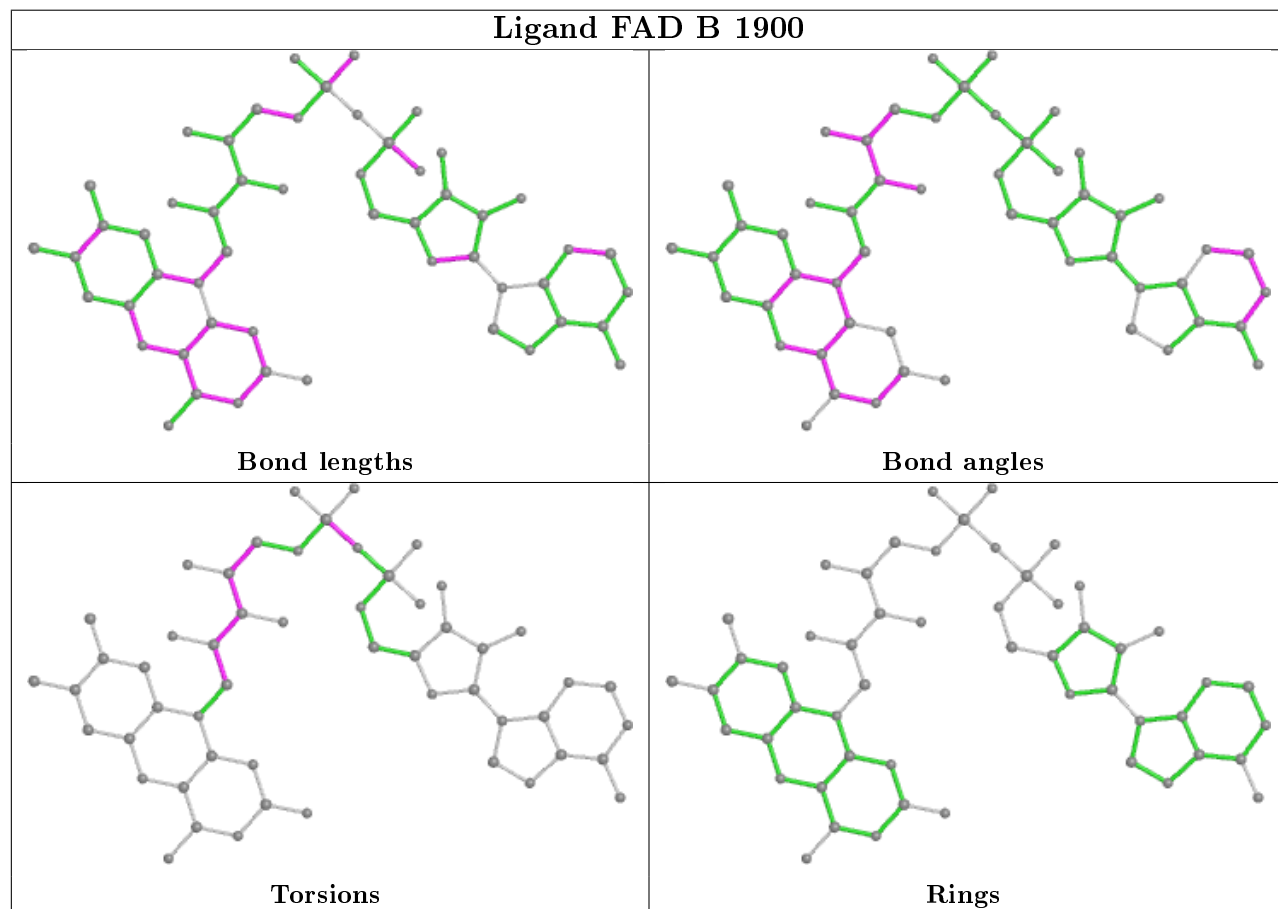
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

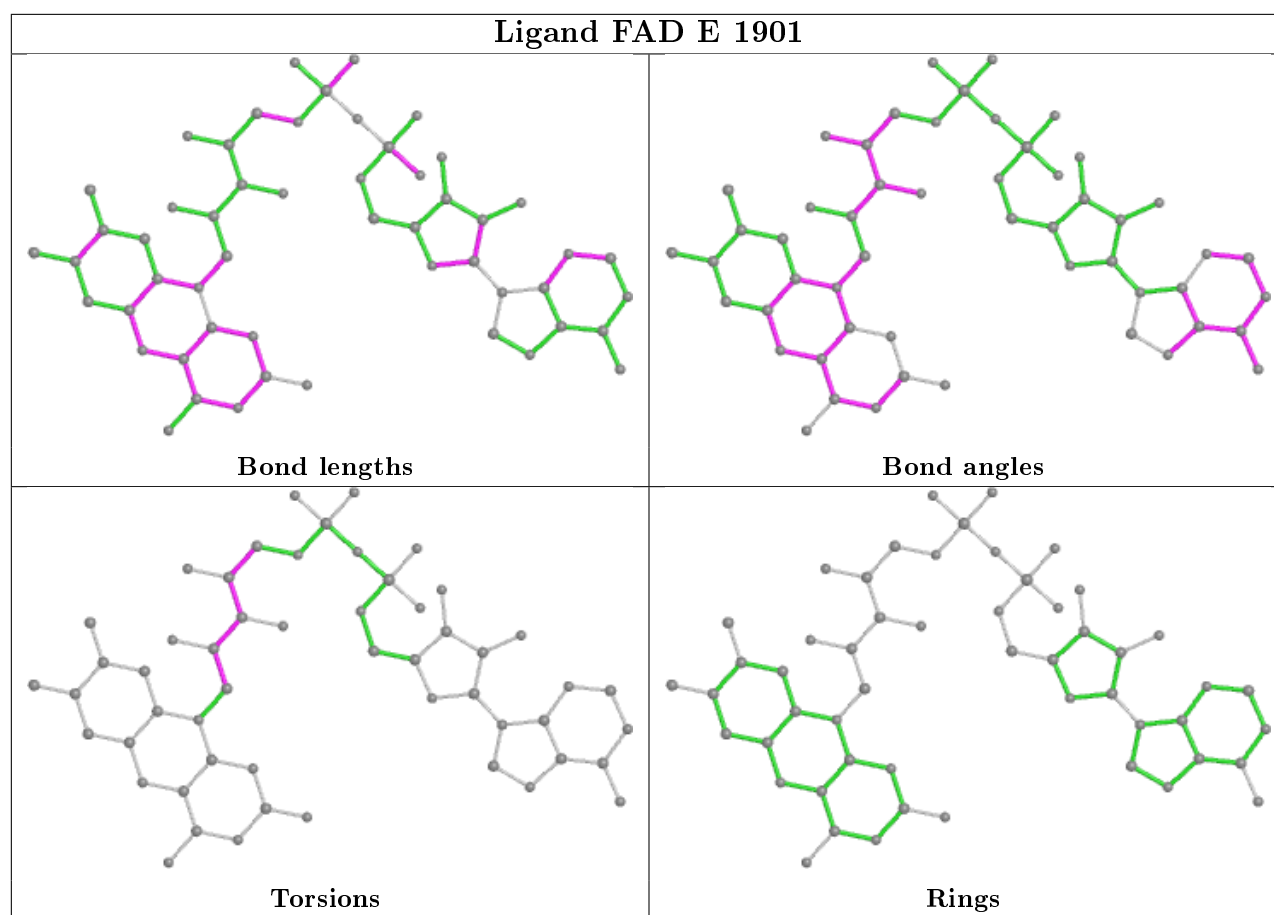


## Ligand PCD D 1921



## Ligand FAD B 1900





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	761/769 (98%)	-0.59	10 (1%) 77 75	18, 30, 55, 100	0
1	D	760/769 (98%)	-0.63	10 (1%) 77 75	16, 29, 57, 92	0
2	B	323/324 (99%)	-0.55	2 (0%) 89 88	21, 34, 59, 78	0
2	E	323/324 (99%)	-0.33	7 (2%) 62 59	21, 37, 61, 80	0
3	C	161/161 (100%)	-0.77	2 (1%) 79 77	17, 24, 46, 74	0
3	F	157/161 (97%)	-0.70	3 (1%) 66 65	19, 26, 41, 103	0
All	All	2485/2508 (99%)	-0.58	34 (1%) 75 73	16, 31, 57, 103	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	769	ALA	8.3
3	F	157	GLU	4.6
3	F	156	CYS	4.2
1	A	768	ALA	3.9
1	D	563	ASP	3.7
1	D	454	TRP	3.6
3	C	156	CYS	3.6
1	D	767	ALA	3.4
2	E	248	ARG	3.3
1	A	609	LYS	3.2
1	D	572	GLN	3.2
3	C	159	GLY	3.0
1	D	608	LYS	3.0
1	A	766	GLU	2.7
3	F	155	LEU	2.7
1	D	560	GLU	2.7
1	A	767	ALA	2.6
1	A	570	GLY	2.6
2	E	245	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	66	ALA	2.5
1	D	553	ASP	2.5
1	D	609	LYS	2.5
1	A	555	ARG	2.4
1	D	570	GLY	2.4
2	E	57	ASP	2.4
1	A	37	PRO	2.4
1	D	555	ARG	2.4
1	A	172	GLU	2.3
2	E	217	ALA	2.2
1	A	563	ASP	2.1
2	B	66	ALA	2.1
2	E	180	ALA	2.0
2	E	323	ALA	2.0
2	B	57	ASP	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

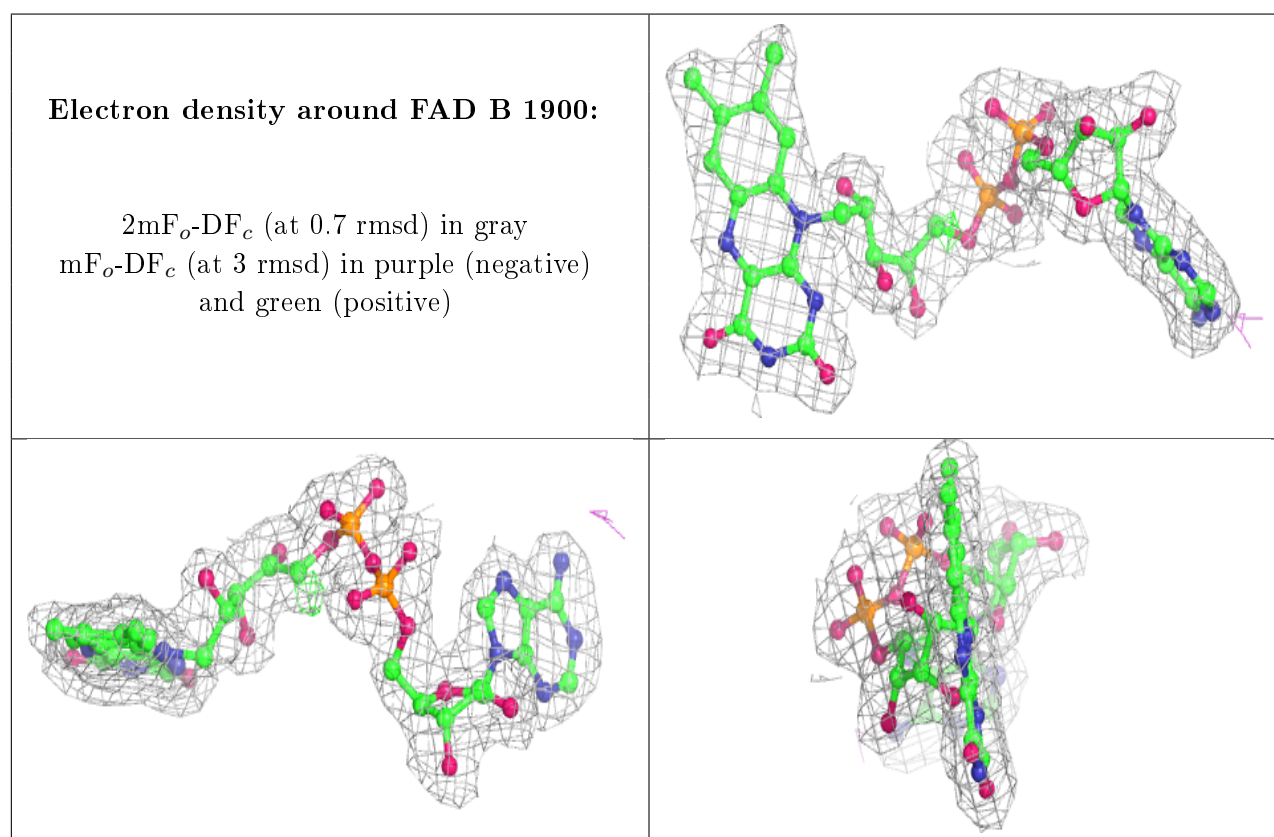
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	SO4	E	1113	5/5	0.92	0.17	41,43,46,46	5
5	EPE	A	1111	15/15	0.95	0.16	39,43,53,61	15
9	SO4	D	1112	5/5	0.96	0.15	49,49,52,53	5
6	FAD	B	1900	53/53	0.98	0.07	18,24,29,33	0
6	FAD	E	1901	53/53	0.98	0.07	23,29,32,35	0
8	FES	C	1908	4/4	0.99	0.05	20,20,22,23	0
4	PCD	A	1920	48/48	0.99	0.08	17,24,28,37	0
7	SF4	E	1911	8/8	0.99	0.05	26,29,29,29	0

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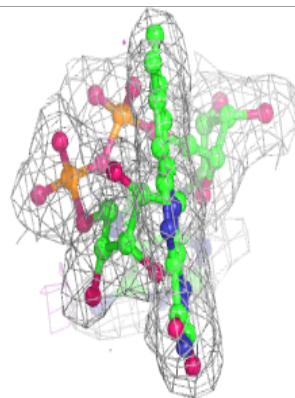
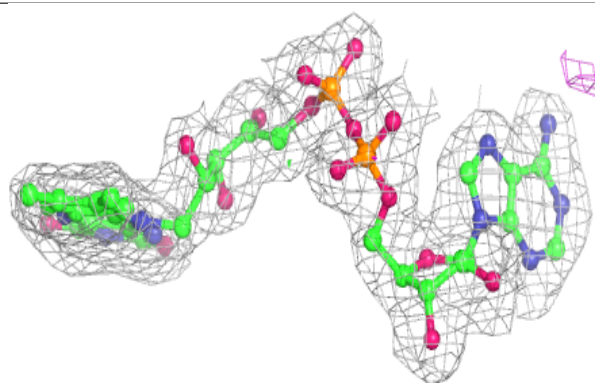
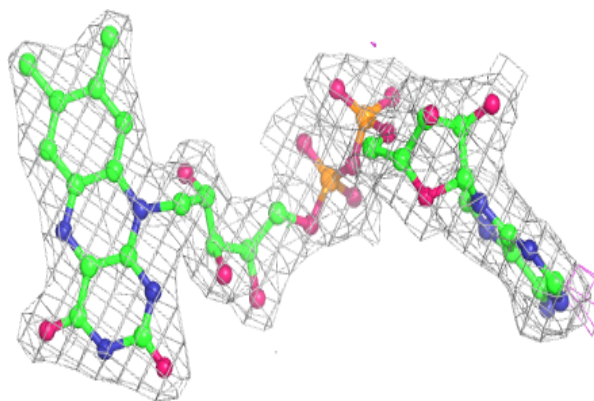
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SF4	B	1910	8/8	0.99	0.05	28,29,29,30	0
8	FES	C	1907	4/4	0.99	0.06	15,18,19,21	0
4	PCD	D	1921	48/48	0.99	0.08	18,24,29,33	0
8	FES	F	1917	4/4	1.00	0.05	19,21,23,23	0
8	FES	F	1918	4/4	1.00	0.05	23,24,24,24	0

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.

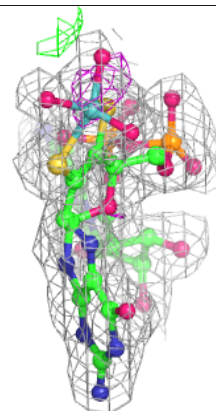
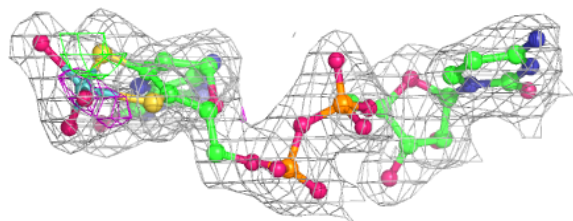
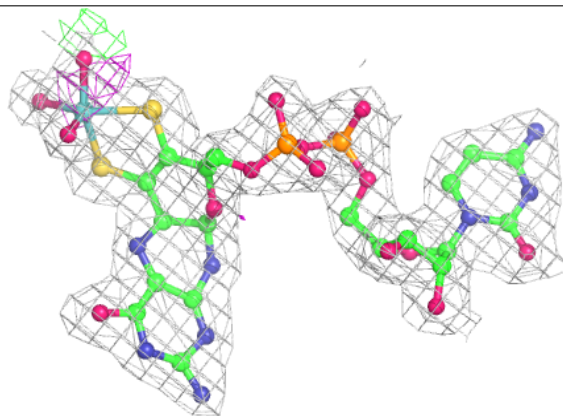


**Electron density around FAD E 1901:**

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

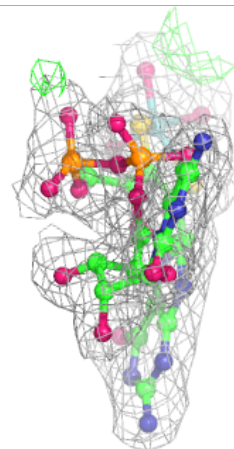
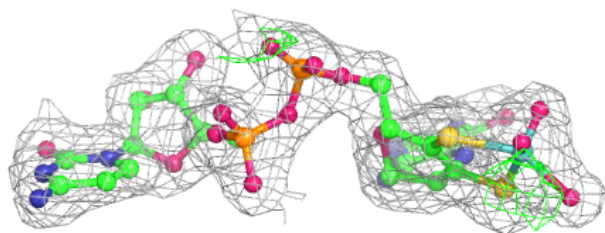
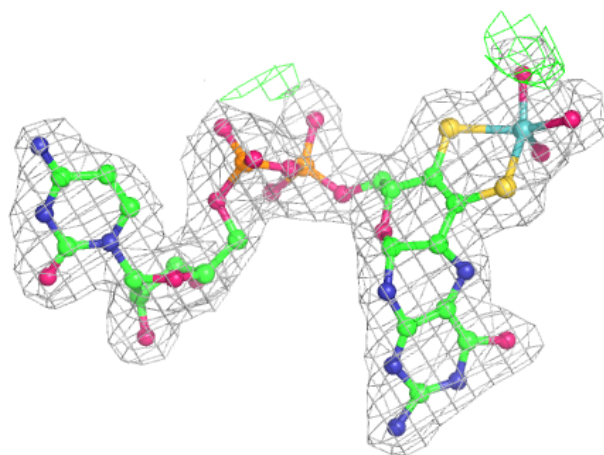
**Electron density around PCD A 1920:**

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



**Electron density around PCD D 1921:**

$2mF_o-DF_c$  (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.