



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:35 AM UTC

PDB ID : 1RM6 / pdb_00001rm6
Title : Structure of 4-hydroxybenzoyl-CoA reductase from *Thauera aromatica*
Authors : Unciuleac, M.; Warkentin, E.; Page, C.C.; Dutton, P.L.; Boll, M.; Ermler, U.
Deposited on : 2003-11-27
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

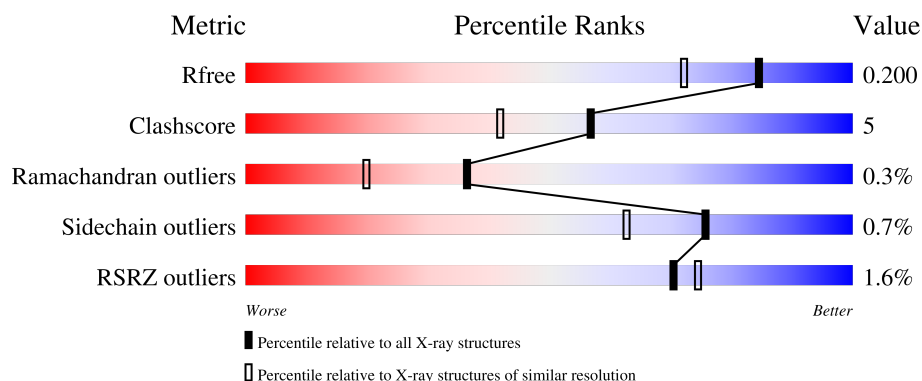
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	769	% 88% 11% .
1	D	769	2% 88% 10% .
2	B	324	92% 7% .
2	E	324	3% 90% 10% .
3	C	161	% 84% 13% .

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Mol	Chain	Length	Quality of chain
3	F	161	% 84% 12% ..

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 21258 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	17	0
			5794	3667	993	1103	31			
1	D	760	Total	C	N	O	S	0	18	0
			5782	3660	994	1098	30			

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	9	0
			2438	1528	444	458	8			
2	E	323	Total	C	N	O	S	0	6	0
			2427	1521	446	452	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	157	Total	C	N	O	S	0	4	0
			1186	729	219	225	13			
3	F	157	Total	C	N	O	S	0	3	0
			1177	725	215	224	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

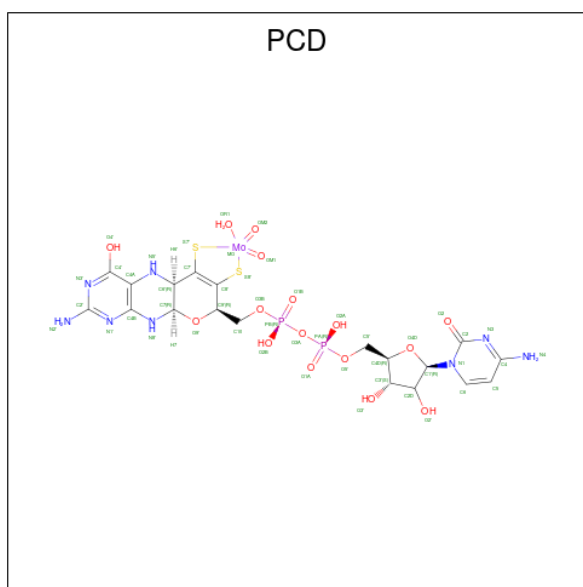
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

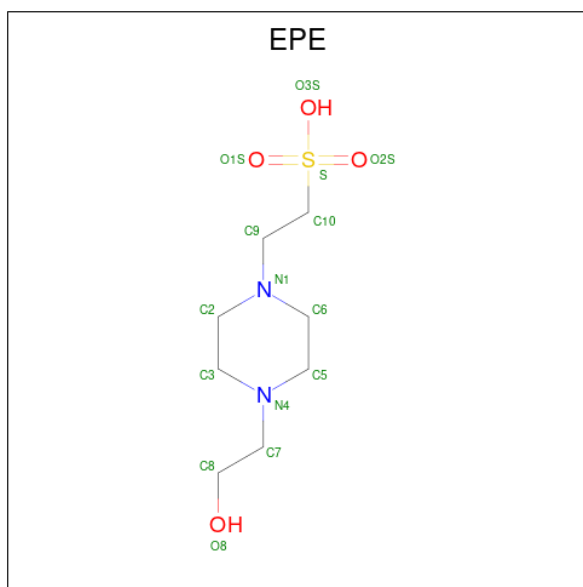
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0

- Molecule 6 is (MOLYBDOPTERIN-CYTOSINE DINUCLEOTIDE-S,S)-DIOXO-AQUA-MOLYBDENUM(V) (CCD ID: PCD) (formula: C₁₉H₂₆MoN₈O₁₆P₂S₂).



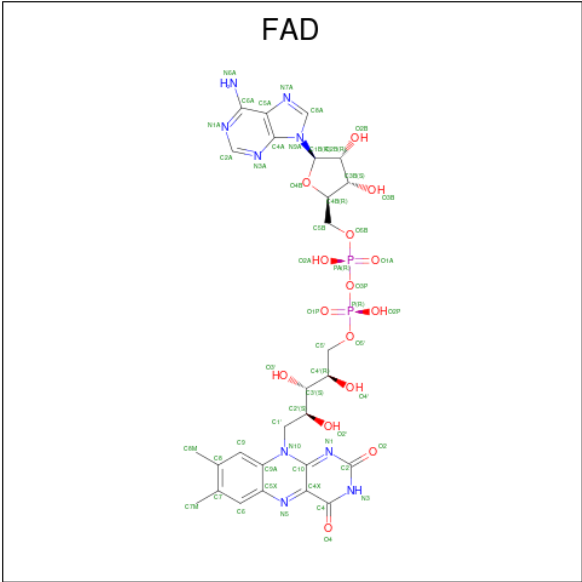
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	A	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	16	2	2		
6	D	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	16	2	2		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



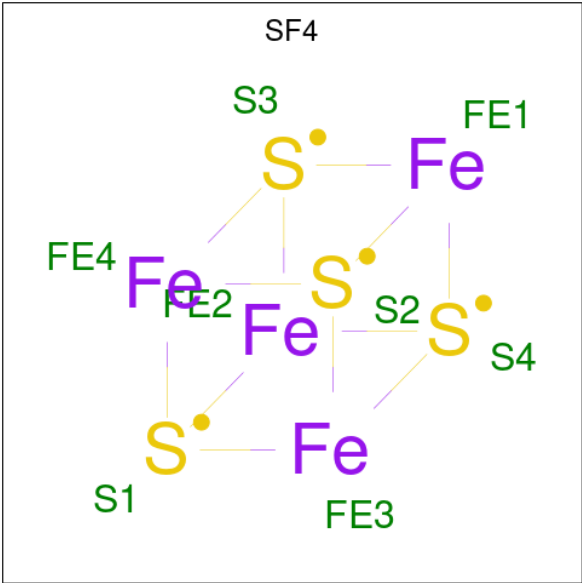
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



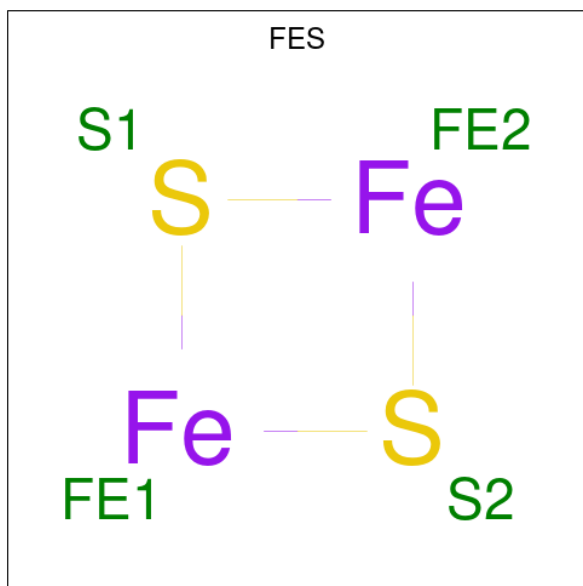
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
8	E	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Fe S	0	1
			16	8 8		
9	E	1	Total	Fe S	0	1
			16	8 8		

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 11 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total	K	0	0
			1	1		

- Molecule 12 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	630	Total	O	0	0
			630	630		
13	B	290	Total	O	0	0
			290	290		
13	C	172	Total	O	0	0
			172	172		
13	D	663	Total	O	0	0
			663	663		
13	E	233	Total	O	0	0
			233	233		
13	F	146	Total	O	0	0
			146	146		

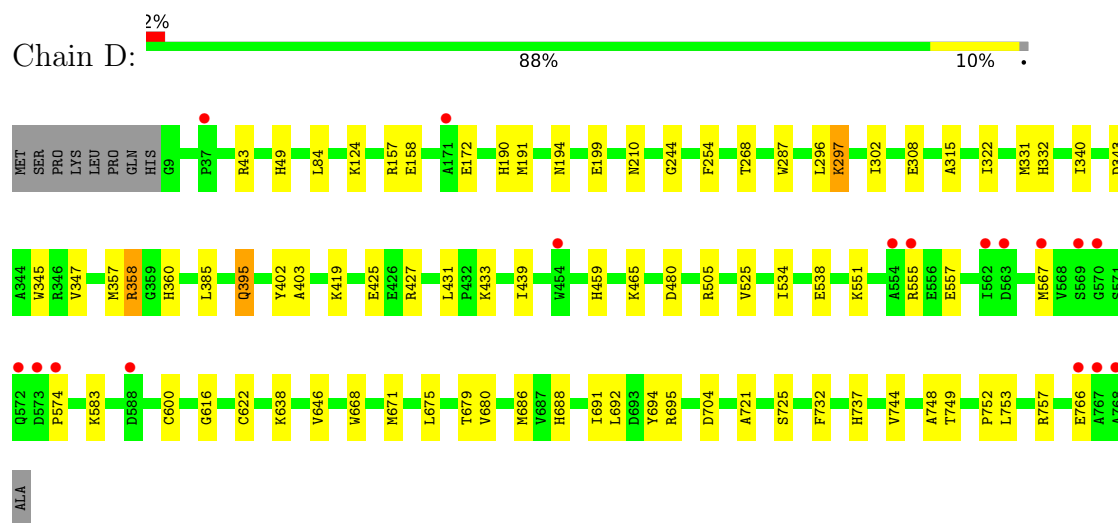
3 Residue-property plots [i](#)

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.

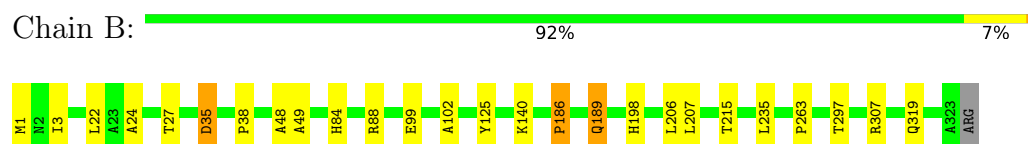
- Molecule 1: 4-hydroxybenzoyl-CoA reductase alpha subunit



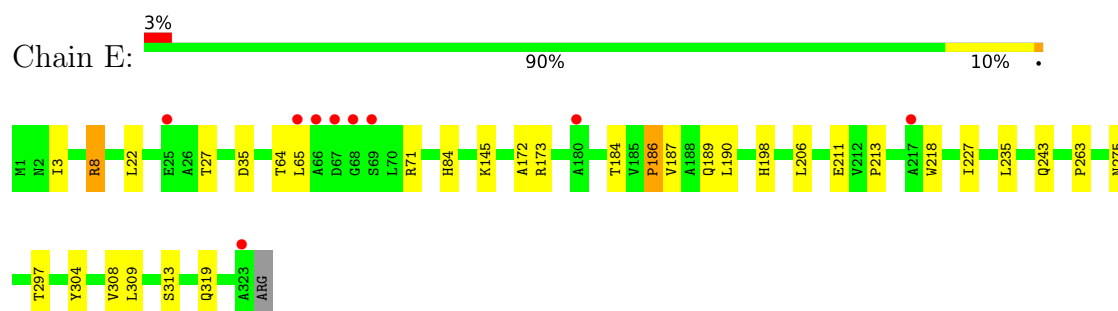
- Molecule 1: 4-hydroxybenzoyl-CoA reductase alpha subunit



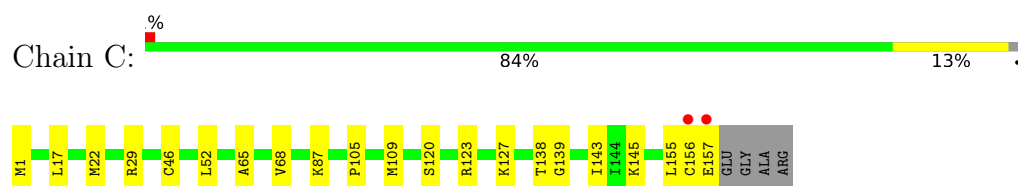
- Molecule 2: 4-hydroxybenzoyl-CoA reductase beta subunit



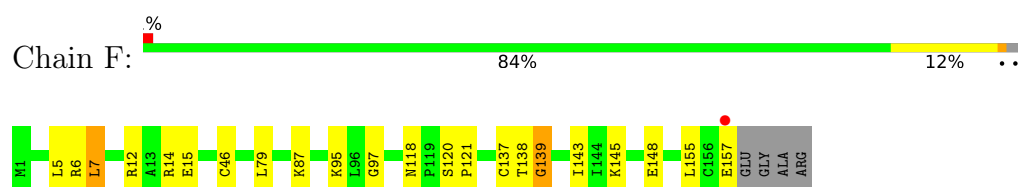
- Molecule 2: 4-hydroxybenzoyl-CoA reductase beta subunit



- 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, α , β , γ	113.02Å 151.84Å 174.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 1.60 19.91 – 1.60	Depositor EDS
% Data completeness (in resolution range)	86.0 (19.91-1.60) 86.1 (19.91-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.152 , 0.173 (Not available) , 0.200	Depositor DCC
R_{free} test set	16885 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.3	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	0.97	EDS
Total number of atoms	21258	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: SF4, K, NA, SO4, CL, PCD, FES, FAD, EPE

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	0.76	2/5959 (0.0%)	1.03	20/8086 (0.2%)
1	D	0.76	2/5967 (0.0%)	1.03	21/8094 (0.3%)
2	B	0.71	0/2518	1.02	11/3431 (0.3%)
2	E	0.69	0/2499	1.03	10/3405 (0.3%)
3	C	0.71	0/1210	1.03	4/1628 (0.2%)
3	F	0.75	0/1199	1.07	7/1614 (0.4%)
All	All	0.74	4/19352 (0.0%)	1.03	73/26258 (0.3%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	191	MET	SD-CE	-7.72	1.60	1.79
1	A	191	MET	SD-CE	-6.70	1.62	1.79
1	D	646	VAL	CA-CB	5.55	1.61	1.54
1	A	77	THR	CA-CB	5.07	1.59	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	MET	N-CA-C	-9.74	101.39	113.18
1	A	315	ALA	N-CA-C	9.41	124.77	113.28
1	D	315	ALA	N-CA-C	9.18	124.48	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	331	MET	N-CA-C	-8.93	102.38	113.18
1	A	525	VAL	N-CA-C	8.35	118.38	110.53
1	D	695	ARG	N-CA-C	7.73	121.69	109.39
2	E	263	PRO	N-CA-C	-7.61	98.30	111.32
1	A	695	ARG	N-CA-C	7.61	121.48	109.39
1	D	525	VAL	N-CA-C	7.41	117.49	110.53
2	B	235	LEU	N-CA-C	-7.32	103.01	112.23
2	B	263	PRO	N-CA-C	-7.27	98.89	111.32
3	C	138	THR	N-CA-C	7.21	122.17	113.23
1	D	427	ARG	N-CA-C	6.83	122.28	113.88
1	D	694	TYR	N-CA-C	-6.66	96.82	108.20
2	B	48	ALA	N-CA-C	-6.62	105.02	113.23
1	D	704	ASP	N-CA-C	-6.60	100.71	110.48
1	D	431	LEU	CA-C-N	6.46	126.44	119.78
1	D	431	LEU	C-N-CA	6.46	126.44	119.78
2	B	198	HIS	N-CA-C	6.42	120.97	113.20
2	E	3	ILE	N-CA-C	6.33	117.21	109.30
1	D	287	TRP	N-CA-C	-6.31	101.08	110.23
3	F	138	THR	N-CA-C	6.16	120.87	113.23
2	B	3	ILE	N-CA-C	6.15	117.68	109.37
2	E	186	PRO	N-CA-C	-6.14	101.56	111.14
2	B	186	PRO	N-CA-C	-6.08	101.65	111.14
1	A	675	LEU	N-CA-C	6.04	121.31	113.88
1	D	297	LYS	N-CA-C	-5.96	101.70	110.52
2	E	313	SER	N-CA-C	-5.95	104.87	111.36
1	D	616	GLY	N-CA-C	-5.93	106.85	114.85
1	D	347	VAL	N-CA-C	5.92	116.40	108.11
1	D	675	LEU	N-CA-C	5.85	121.30	114.04
2	E	198	HIS	N-CA-C	5.83	120.39	113.16
3	F	46	CYS	N-CA-C	5.82	121.82	114.31
1	A	297	LYS	N-CA-C	-5.71	102.06	110.52
2	B	102	ALA	CB-CA-C	-5.70	109.99	116.54
1	D	692	LEU	N-CA-C	-5.68	105.12	112.68
1	A	210	ASN	N-CA-C	-5.67	99.94	109.07
3	F	79	LEU	N-CA-C	5.60	117.46	111.36
1	D	210	ASN	N-CA-C	-5.58	99.80	108.90
1	A	743	ALA	N-CA-C	5.57	117.16	111.14
1	A	190	HIS	N-CA-C	-5.55	102.18	110.23
1	D	744	VAL	N-CA-C	5.53	118.51	113.20
1	A	391	ASN	N-CA-C	5.50	119.69	112.92
1	A	692	LEU	N-CA-C	-5.49	105.38	112.68
3	C	143	ILE	N-CA-C	-5.40	105.27	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	ALA	N-CA-C	5.36	118.63	111.24
1	A	287	TRP	N-CA-C	-5.30	102.20	110.10
2	E	297	THR	N-CA-C	-5.30	106.81	113.28
2	B	215	THR	N-CA-C	5.29	119.44	112.89
1	A	694	TYR	N-CA-C	-5.26	97.96	107.75
2	E	235	LEU	N-CA-C	-5.26	105.72	111.82
3	F	137	CYS	N-CA-C	5.26	119.75	112.45
3	F	143	ILE	N-CA-C	-5.25	105.42	110.72
1	A	36	ALA	CA-C-N	5.23	125.28	119.32
1	A	36	ALA	C-N-CA	5.23	125.28	119.32
3	C	46	CYS	N-CA-C	5.23	121.05	114.31
3	C	29	ARG	N-CA-C	5.22	117.05	111.36
1	A	704	ASP	N-CA-C	-5.22	102.76	110.48
2	B	297	THR	N-CA-C	-5.21	106.92	113.28
1	A	39	ALA	N-CA-C	5.19	117.75	109.96
3	F	97	GLY	N-CA-C	-5.19	107.48	115.73
2	E	190	LEU	N-CA-C	-5.19	106.46	112.89
1	D	622	CYS	N-CA-C	-5.17	101.27	109.96
1	D	190	HIS	N-CA-C	-5.17	102.73	110.23
2	B	207	LEU	N-CA-C	-5.17	101.34	109.25
1	A	363	VAL	N-CA-C	5.11	115.33	110.53
1	D	480	ASP	N-CA-C	-5.10	100.85	108.96
2	B	35	ASP	N-CA-C	-5.09	106.76	113.12
2	E	213	PRO	N-CA-C	5.09	116.91	110.70
3	F	139	GLY	N-CA-C	-5.06	108.01	115.30
1	D	721	ALA	N-CA-C	5.04	117.61	110.50
2	E	309	LEU	N-CA-C	-5.01	105.82	111.28
1	A	347	VAL	N-CA-C	5.00	115.17	108.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	TYR	Sidechain

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	5794	0	5838	45	0
1	D	5782	0	5834	49	0
2	B	2438	0	2459	19	0
2	E	2427	0	2463	24	0
3	C	1186	0	1230	21	0
3	F	1177	0	1221	27	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	48	0	21	3	0
6	D	48	0	21	2	0
7	A	45	0	54	4	0
7	D	15	0	18	0	0
8	B	53	0	30	1	0
8	E	53	0	31	1	0
9	B	16	0	0	0	0
9	E	16	0	0	0	0
10	C	8	0	0	0	0
10	F	8	0	0	0	0
11	D	1	0	0	0	0
12	D	5	0	0	0	0
13	A	630	0	0	8	0
13	B	290	0	0	3	0
13	C	172	0	0	4	0
13	D	663	0	0	13	0
13	E	233	0	0	6	0
13	F	146	0	0	10	0
All	All	21258	0	19220	178	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 5.

All (178) 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)
2:E:173[A]:ARG:NH1	2:E:184:THR:HG21	1.85	0.91
1:A:178[B]:GLU:OE1	1:A:291:LYS:HD2	1.76	0.86
3:F:145[A]:LYS:HG2	13:F:9545:HOH:O	1.76	0.86
3:C:145[B]:LYS:HE2	13:C:7445:HOH:O	1.78	0.83
2:E:145:LYS:HE3	13:E:7688:HOH:O	1.79	0.83
3:C:145[A]:LYS:HE2	13:C:6769:HOH:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:PRO:HB2	2:B:189[B]:GLN:HE21	1.48	0.79
2:B:186:PRO:HB2	2:B:189[A]:GLN:HE21	1.49	0.76
1:D:199[B]:GLU:CD	13:D:6860:HOH:O	2.29	0.75
3:F:145[B]:LYS:HD3	13:F:6470:HOH:O	1.85	0.75
1:D:419:LYS:HE2	1:D:425:GLU:HG3	1.66	0.74
3:C:123[B]:ARG:HB2	3:C:123[B]:ARG:HH11	1.50	0.74
3:C:87:LYS:HZ2	3:C:157:GLU:HG3	1.51	0.74
1:D:425:GLU:HG2	13:D:7454:HOH:O	1.86	0.73
6:D:920:PCD:MO	6:D:920:PCD:OM1	1.60	0.73
2:E:65:LEU:HD12	2:E:65:LEU:N	2.04	0.72
3:F:145[B]:LYS:HG2	13:F:7433:HOH:O	1.89	0.71
1:A:131:PRO:HD2	1:A:145:ILE:HD12	1.73	0.71
1:A:459:HIS:HB3	1:A:528[B]:MET:HE3	1.72	0.71
1:D:172:GLU:HG2	1:D:297:LYS:HZ3	1.56	0.70
2:B:27[B]:THR:HG22	2:B:49:ALA:HB3	1.74	0.70
3:F:145[B]:LYS:CG	13:F:7433:HOH:O	2.38	0.69
1:A:199[B]:GLU:CD	13:A:6771:HOH:O	2.36	0.68
3:C:87:LYS:NZ	3:C:157:GLU:HG3	2.08	0.67
1:A:750[B]:ASP:OD1	1:A:757:ARG:NE	2.29	0.66
2:B:1:MET:HE1	3:C:22:MET:HE3	1.77	0.66
3:C:87:LYS:NZ	3:C:157:GLU:CG	2.59	0.66
3:F:87:LYS:HE2	3:F:157:GLU:HB2	1.77	0.65
1:A:763:ASP:CG	2:B:307:ARG:HH12	2.05	0.65
3:C:145[B]:LYS:HE3	13:C:7692:HOH:O	1.96	0.65
2:E:275:ASN:HB3	13:E:7103:HOH:O	1.97	0.65
3:C:123[B]:ARG:HB2	3:C:123[B]:ARG:NH1	2.11	0.64
2:E:65:LEU:HD11	2:E:71:ARG:HB2	1.79	0.64
1:D:172:GLU:HG2	1:D:297:LYS:NZ	2.11	0.64
1:A:763:ASP:OD2	2:B:307:ARG:NH1	2.30	0.64
1:D:49:HIS:HD2	13:D:9006:HOH:O	1.80	0.64
1:D:433:LYS:HA	13:D:7298:HOH:O	1.97	0.63
1:D:557:GLU:H	1:D:557:GLU:CD	2.06	0.63
1:D:748[B]:ALA:CB	1:D:753:LEU:HD22	2.29	0.62
2:B:1:MET:HG2	13:B:9337:HOH:O	1.98	0.62
1:A:602[A]:THR:HG23	13:A:9185:HOH:O	1.99	0.61
6:A:920:PCD:OM1	6:A:920:PCD:MO	1.71	0.61
1:D:748[B]:ALA:HB1	1:D:753:LEU:HD22	1.82	0.61
1:A:111[B]:ILE:HG13	3:F:12:ARG:HH21	1.66	0.60
3:C:17:LEU:HD23	3:F:15:GLU:HG2	1.82	0.60
1:D:555:ARG:HB2	1:D:557:GLU:OE2	2.01	0.60
1:D:124:LYS:HE3	13:D:9146:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157[B]:ARG:NH1	13:D:7119:HOH:O	2.35	0.60
3:F:145[B]:LYS:HE3	3:F:148:GLU:OE1	2.02	0.60
2:E:304:TYR:O	2:E:308[A]:VAL:HG22	2.01	0.59
1:D:385:LEU:HG	1:D:439:ILE:HD13	1.84	0.59
1:D:638[B]:LYS:HE3	2:E:227:ILE:O	2.04	0.58
3:C:87:LYS:HZ1	3:C:157:GLU:HG2	1.68	0.57
2:B:99[B]:GLU:HG3	13:B:6539:HOH:O	2.04	0.57
2:E:22:LEU:HD11	2:E:206:LEU:HD21	1.87	0.56
1:A:459:HIS:HB3	1:A:528[B]:MET:CE	2.36	0.56
2:E:173[A]:ARG:HH12	2:E:184:THR:HG21	1.68	0.55
3:C:120[B]:SER:OG	3:C:155:LEU:HD21	2.07	0.55
1:D:737:HIS:CD2	1:D:748[B]:ALA:O	2.60	0.55
2:E:64:THR:C	2:E:65:LEU:HD12	2.32	0.55
1:D:679:THR:HB	1:D:688:HIS:CE1	2.42	0.55
1:A:679:THR:HB	1:A:688:HIS:CE1	2.42	0.54
2:E:186:PRO:HB2	2:E:189[B]:GLN:OE1	2.07	0.54
1:A:111[B]:ILE:HG13	3:F:12:ARG:NH2	2.22	0.54
1:D:534:ILE:O	1:D:538[B]:GLU:HG2	2.07	0.54
1:A:38:ASP:OD2	1:A:38:ASP:N	2.41	0.54
1:A:560:GLU:HG3	1:A:569:SER:HB3	1.89	0.54
3:C:17:LEU:CD2	3:F:15:GLU:HG2	2.37	0.53
1:A:768:ALA:O	1:A:769:ALA:C	2.53	0.52
1:A:431:LEU:HD11	1:A:437:LEU:HG	1.92	0.52
2:B:1:MET:HE1	3:C:22:MET:CE	2.39	0.52
2:E:65:LEU:HD11	2:E:71:ARG:CB	2.39	0.52
1:A:465:LYS:HD2	1:A:465:LYS:C	2.34	0.52
3:C:87:LYS:HZ1	3:C:157:GLU:CG	2.23	0.52
1:D:199[B]:GLU:HG2	1:D:268:THR:HG23	1.92	0.52
1:A:199[B]:GLU:HG2	1:A:268:THR:HG23	1.91	0.52
1:D:505[B]:ARG:NH1	13:D:9226:HOH:O	2.32	0.52
2:E:65:LEU:N	2:E:65:LEU:CD1	2.71	0.51
1:D:43:ARG:HD2	13:D:7280:HOH:O	2.11	0.50
3:F:6:ARG:NH1	13:F:7134:HOH:O	2.33	0.50
2:E:319:GLN:HB2	13:E:7328:HOH:O	2.13	0.49
1:A:748[B]:ALA:CB	1:A:753:LEU:HD22	2.42	0.49
2:B:24:ALA:HB3	2:B:27[B]:THR:HG21	1.94	0.49
1:A:608:LYS:HE3	1:A:609:LYS:HE2	1.93	0.49
2:E:304:TYR:CZ	2:E:308[A]:VAL:HG11	2.47	0.49
1:D:419:LYS:CE	1:D:425:GLU:HG3	2.38	0.48
1:A:686:MET:HG3	1:A:688:HIS:CE1	2.47	0.48
3:F:145[B]:LYS:HG3	13:F:9545:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLU:HG2	1:A:345:TRP:CD1	2.49	0.48
1:A:439:ILE:HD12	1:A:626:GLN:O	2.14	0.47
1:A:668:TRP:CG	3:C:139:GLY:HA2	2.50	0.47
2:B:22:LEU:HD11	2:B:206:LEU:HD21	1.96	0.47
3:F:95:LYS:NZ	3:F:145[A]:LYS:NZ	2.62	0.47
1:A:188:HIS:CG	1:A:247:ALA:HB2	2.49	0.47
1:A:505[B]:ARG:NH1	13:A:9124:HOH:O	2.34	0.47
1:A:583:LYS:HG2	13:A:6893:HOH:O	2.14	0.47
3:C:52:LEU:HG	3:C:109:MET:HE3	1.97	0.47
3:F:12:ARG:NH2	13:F:6915:HOH:O	2.47	0.47
1:A:737:HIS:HD2	1:A:748[B]:ALA:O	1.97	0.46
2:B:1:MET:HE2	13:C:6226:HOH:O	2.15	0.46
1:D:567:MET:SD	1:D:574:PRO:O	2.74	0.46
1:D:84:LEU:HD21	1:D:322:ILE:HD12	1.98	0.46
1:D:194:ASN:HB3	1:D:254:PHE:CZ	2.50	0.46
1:D:752:PRO:O	1:D:757:ARG:HD2	2.15	0.46
2:E:84:HIS:HE1	13:E:9303:HOH:O	1.97	0.46
2:B:35:ASP:HB2	8:B:900:FAD:H2'	1.97	0.46
1:D:551:LYS:HE2	13:D:7002:HOH:O	2.15	0.46
1:A:432:PRO:HG2	1:A:435:ARG:HD3	1.97	0.46
2:B:84:HIS:O	2:B:88:ARG:HG3	2.15	0.46
1:D:158:GLU:HG2	1:D:345:TRP:CD1	2.51	0.46
1:D:505[B]:ARG:NH2	13:D:9226:HOH:O	2.41	0.46
2:B:186:PRO:HB2	2:B:189[A]:GLN:NE2	2.25	0.46
1:A:737:HIS:CD2	1:A:748[B]:ALA:O	2.68	0.46
2:E:35:ASP:HB2	8:E:900:FAD:H2'	1.98	0.45
2:E:319:GLN:NE2	13:E:7328:HOH:O	2.48	0.45
1:A:500:ARG:NH2	13:A:7043:HOH:O	2.50	0.45
2:B:99[B]:GLU:CG	13:B:6539:HOH:O	2.64	0.45
3:F:118:ASN:O	3:F:121:PRO:HD3	2.16	0.45
3:F:145[A]:LYS:CG	13:F:9545:HOH:O	2.47	0.45
1:D:686:MET:HG3	1:D:688:HIS:CE1	2.52	0.45
1:D:583[B]:LYS:HG2	13:D:6930:HOH:O	2.16	0.45
1:D:749[A]:THR:N	13:D:9389:HOH:O	2.42	0.45
1:D:465:LYS:HD2	1:D:465:LYS:C	2.43	0.44
3:F:145[B]:LYS:CG	13:F:9545:HOH:O	2.66	0.44
1:D:459:HIS:HD1	1:D:600:CYS:H	1.66	0.44
1:D:680:VAL:H	1:D:688:HIS:HD1	1.66	0.44
2:E:8:ARG:NH1	13:E:9540:HOH:O	2.51	0.44
1:A:308:GLU:HA	1:A:343:ASP:O	2.18	0.43
3:C:105:PRO:O	3:C:109:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:173[A]:ARG:NH2	2:E:211:GLU:OE2	2.44	0.43
3:F:95:LYS:HD2	3:F:145[A]:LYS:HZ3	1.82	0.43
1:A:176:ILE:HD12	7:A:932:EPE:H92	2.01	0.43
7:A:932:EPE:H32	13:A:6551:HOH:O	2.17	0.43
1:D:668:TRP:CG	3:F:139:GLY:HA2	2.53	0.43
1:A:750[B]:ASP:CG	13:A:7036:HOH:O	2.61	0.43
3:F:7:LEU:HD13	3:F:14:ARG:HB2	2.00	0.43
1:D:332:HIS:CE1	1:D:340:ILE:HD12	2.54	0.43
1:D:725:SER:HB2	6:D:920:PCD:H7	2.01	0.43
1:D:49:HIS:HE1	13:D:7610:HOH:O	2.02	0.43
1:D:557:GLU:CD	1:D:557:GLU:N	2.76	0.43
1:A:176:ILE:HD12	7:A:932:EPE:C2	2.49	0.43
3:F:145[B]:LYS:HG3	13:F:7433:HOH:O	2.10	0.43
1:A:748[B]:ALA:HB1	1:A:753:LEU:HD22	2.00	0.42
1:A:622:CYS:HB3	1:A:723:GLU:OE1	2.20	0.42
2:E:218:TRP:CD2	2:E:243:GLN:HG3	2.54	0.42
3:C:123[A]:ARG:NH1	3:C:127:LYS:NZ	2.67	0.42
3:C:87:LYS:NZ	3:C:157:GLU:HG2	2.28	0.42
1:D:84:LEU:HD21	1:D:322:ILE:CD1	2.50	0.42
1:D:395:GLN:HE21	1:D:395:GLN:HB3	1.69	0.42
1:A:505[B]:ARG:NH2	13:A:9124:HOH:O	2.48	0.42
2:B:125:TYR:CZ	2:B:140[A]:LYS:HE3	2.54	0.42
1:D:296:LEU:HD23	1:D:302:ILE:HA	2.02	0.42
1:D:357:MET:O	1:D:358:ARG:C	2.63	0.42
6:A:920:PCD:O5'	6:A:920:PCD:H6	2.20	0.42
1:D:308:GLU:HA	1:D:343:ASP:O	2.18	0.42
2:E:22:LEU:HD23	2:E:27:THR:HG22	2.02	0.42
3:F:145[B]:LYS:CE	3:F:148:GLU:OE1	2.65	0.42
2:E:172:ALA:O	2:E:187[A]:VAL:HG23	2.20	0.41
3:F:5:LEU:HG	3:F:7:LEU:HD12	2.00	0.41
1:A:496:VAL:HG13	1:A:538[A]:GLU:OE2	2.20	0.41
1:A:573:ASP:HA	1:A:574:PRO:HD3	1.91	0.41
1:D:737:HIS:HD2	1:D:748[B]:ALA:O	2.00	0.41
2:E:172:ALA:C	2:E:187[A]:VAL:HG23	2.44	0.41
1:A:454:TRP:CD2	7:A:930:EPE:H21	2.56	0.41
1:A:560:GLU:CG	1:A:569:SER:HB3	2.49	0.41
2:B:186:PRO:HB2	2:B:189[B]:GLN:NE2	2.26	0.41
1:D:671:MET:HA	1:D:732:PHE:CE2	2.54	0.41
1:A:725:SER:HB2	6:A:920:PCD:H7	2.03	0.41
3:F:95:LYS:HZ2	3:F:145[A]:LYS:NZ	2.18	0.41
3:F:120[B]:SER:OG	3:F:155:LEU:HD11	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:TYR:O	1:A:403:ALA:HB3	2.22	0.41
1:D:402:TYR:O	1:D:403:ALA:HB3	2.22	0.40
3:C:65:ALA:O	3:C:68:VAL:HG22	2.21	0.40
1:A:438:GLY:O	1:A:627:VAL:HA	2.21	0.40
1:D:748[B]:ALA:HB3	1:D:753:LEU:HD22	2.02	0.40
3:F:95:LYS:HZ2	3:F:145[A]:LYS:HE2	1.86	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	776/769 (101%)	755 (97%)	17 (2%)	4 (0%)	24	10
1	D	776/769 (101%)	752 (97%)	21 (3%)	3 (0%)	30	14
2	B	330/324 (102%)	325 (98%)	5 (2%)	0	100	100
2	E	327/324 (101%)	321 (98%)	6 (2%)	0	100	100
3	C	159/161 (99%)	155 (98%)	3 (2%)	1 (1%)	21	7
3	F	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
All	All	2526/2508 (101%)	2463 (98%)	55 (2%)	8 (0%)	36	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	HIS
3	C	156	CYS
1	D	360	HIS
1	A	358	ARG
1	D	358	ARG
1	D	244	GLY

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Mol	Chain	Res	Type
1	A	244	GLY
1	A	239	PRO

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	567/597 (95%)	562 (99%)	5 (1%)	70	55
1	D	606/597 (102%)	603 (100%)	3 (0%)	81	70
2	B	250/243 (103%)	246 (98%)	4 (2%)	55	33
2	E	248/243 (102%)	247 (100%)	1 (0%)	84	75
3	C	130/128 (102%)	129 (99%)	1 (1%)	73	59
3	F	129/128 (101%)	128 (99%)	1 (1%)	73	59
All	All	1930/1936 (100%)	1915 (99%)	15 (1%)	76	59

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LYS
1	A	395	GLN
1	A	583	LYS
1	A	691	ILE
1	A	766	GLU
2	B	38	PRO
2	B	189[A]	GLN
2	B	189[B]	GLN
2	B	319	GLN
3	C	1	MET
1	D	395	GLN
1	D	691	ILE
1	D	766	GLU
2	E	8	ARG
3	F	7	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	ASN
1	A	626	GLN
1	A	737	HIS
2	B	135	ASN
2	B	243	GLN
2	B	293	ASN
1	D	49	HIS
1	D	210	ASN
1	D	395	GLN
1	D	626	GLN
1	D	683	ASN
1	D	716	ASN
2	E	84	HIS
2	E	135	ASN
2	E	243	GLN
2	E	293	ASN
2	E	319	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 5 are monoatomic - leaving 17 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$
8	FAD	B	900	-	58,58,58	1.78	13 (22%)	85,89,89	1.49	11 (12%)
6	PCD	A	920	-	41,53,53	1.86	8 (19%)	55,86,86	3.49	24 (43%)
7	EPE	D	931	-	15,15,15	1.95	5 (33%)	19,20,20	1.45	3 (15%)
9	SF4	B	910[A]	2	0,12,12	-	-	-	-	-
10	FES	F	908	3	0,4,4	-	-	-	-	-
6	PCD	D	920	-	41,53,53	1.72	6 (14%)	55,86,86	3.50	23 (41%)
9	SF4	B	910[B]	2	0,12,12	-	-	-	-	-
12	SO4	D	773	-	4,4,4	0.35	0	6,6,6	0.07	0
9	SF4	E	910[B]	2	0,12,12	-	-	-	-	-
9	SF4	E	910[A]	2	0,12,12	-	-	-	-	-
7	EPE	A	933	-	15,15,15	1.93	3 (20%)	19,20,20	1.64	5 (26%)
7	EPE	A	930	-	15,15,15	1.81	2 (13%)	19,20,20	1.50	4 (21%)
7	EPE	A	932	-	15,15,15	2.06	4 (26%)	19,20,20	1.64	6 (31%)
10	FES	C	908	3	0,4,4	-	-	-	-	-
8	FAD	E	900	-	58,58,58	1.78	12 (20%)	85,89,89	1.60	15 (17%)
10	FES	C	907	3	0,4,4	-	-	-	-	-
10	FES	F	907	3	0,4,4	-	-	-	-	-

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
8	FAD	B	900	-	-	7/34/50/50	0/6/6/6
6	PCD	A	920	-	-	2/22/78/78	0/6/6/6
7	EPE	D	931	-	-	4/9/19/19	0/1/1/1
9	SF4	B	910[A]	2	-	-	0/6/5/5
10	FES	F	908	3	-	-	0/1/1/1
6	PCD	D	920	-	-	2/22/78/78	0/6/6/6
9	SF4	B	910[B]	2	-	-	0/6/5/5
9	SF4	E	910[B]	2	-	-	0/6/5/5
9	SF4	E	910[A]	2	-	-	0/6/5/5
7	EPE	A	933	-	-	5/9/19/19	0/1/1/1
7	EPE	A	930	-	-	3/9/19/19	0/1/1/1
7	EPE	A	932	-	-	4/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FES	C	908	3	-	-	0/1/1/1
8	FAD	E	900	-	-	6/34/50/50	0/6/6/6
10	FES	C	907	3	-	-	0/1/1/1
10	FES	F	907	3	-	-	0/1/1/1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	920	PCD	PA-O3A	6.15	1.66	1.59
6	D	920	PCD	PA-O3A	5.81	1.65	1.59
8	B	900	FAD	P-O3P	-5.74	1.53	1.59
8	E	900	FAD	P-O3P	-5.54	1.53	1.59
6	D	920	PCD	C6'-N5'	5.19	1.52	1.45
7	A	932	EPE	O3S-S	5.00	1.66	1.47
6	A	920	PCD	C6'-N5'	4.90	1.52	1.45
7	A	930	EPE	O3S-S	4.84	1.65	1.47
7	A	933	EPE	O3S-S	4.80	1.65	1.47
7	D	931	EPE	O3S-S	4.60	1.64	1.47
7	A	933	EPE	C9-C10	-3.73	1.42	1.52
7	A	930	EPE	C9-C10	-3.73	1.42	1.52
8	E	900	FAD	O4B-C1B	3.73	1.50	1.42
6	A	920	PCD	C5-C4	3.71	1.51	1.42
8	B	900	FAD	C1'-C2'	3.58	1.57	1.52
8	E	900	FAD	C10-N1	3.58	1.40	1.33
7	A	932	EPE	C9-C10	-3.56	1.43	1.52
8	B	900	FAD	C4X-N5	3.39	1.38	1.30
8	B	900	FAD	C9A-N10	3.38	1.47	1.41
6	D	920	PCD	C5-C4	3.37	1.50	1.42
6	A	920	PCD	C2'-N1'	3.35	1.41	1.35
6	A	920	PCD	C4A-C4B	3.24	1.47	1.41
8	B	900	FAD	O4B-C1B	3.19	1.49	1.42
8	B	900	FAD	O5'-C5'	3.14	1.56	1.44
8	E	900	FAD	O5'-C5'	3.14	1.56	1.44
8	E	900	FAD	PA-O2A	-3.12	1.40	1.55
8	E	900	FAD	C5A-C6A	3.12	1.49	1.41
7	D	931	EPE	C9-C10	-2.89	1.44	1.52
7	A	932	EPE	C7-N4	2.79	1.53	1.47
8	E	900	FAD	C4X-N5	2.70	1.36	1.30
8	B	900	FAD	PA-O2A	-2.63	1.43	1.55
6	D	920	PCD	C2'-N1'	2.56	1.39	1.35
6	A	920	PCD	C4-N3	2.55	1.39	1.34
8	B	900	FAD	O3B-C3B	-2.47	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	900	FAD	C5A-C6A	2.47	1.47	1.41
8	B	900	FAD	P-O2P	-2.41	1.44	1.55
7	A	932	EPE	C10-S	2.41	1.81	1.77
6	D	920	PCD	C4A-C4B	2.41	1.45	1.41
8	E	900	FAD	C9A-C5X	2.40	1.45	1.41
8	E	900	FAD	C1'-C2'	2.37	1.56	1.52
6	A	920	PCD	C7-C6'	2.36	1.55	1.53
8	E	900	FAD	O4-C4	-2.33	1.19	1.23
8	B	900	FAD	C6-C5X	2.27	1.43	1.40
8	B	900	FAD	C10-N1	2.25	1.37	1.33
7	D	931	EPE	C2-N1	2.24	1.53	1.46
7	D	931	EPE	C7-N4	2.24	1.52	1.47
7	D	931	EPE	C10-S	2.20	1.80	1.77
8	B	900	FAD	C8-C7	2.18	1.46	1.40
8	E	900	FAD	C8-C7	2.17	1.46	1.40
6	D	920	PCD	C4A-N5'	2.14	1.43	1.38
6	A	920	PCD	C4A-N5'	2.10	1.43	1.38
8	E	900	FAD	PA-O3P	2.08	1.61	1.59
7	A	933	EPE	C10-S	2.06	1.80	1.77

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	920	PCD	N2'-C2'-N3'	12.87	136.52	117.22
6	D	920	PCD	N2'-C2'-N3'	12.07	135.32	117.22
6	D	920	PCD	C7-C6'-N5'	10.26	117.95	107.87
6	A	920	PCD	N2'-C2'-N1'	-10.08	102.11	117.22
6	A	920	PCD	C7-C6'-N5'	9.80	117.50	107.87
6	D	920	PCD	N2'-C2'-N1'	-9.77	102.57	117.22
6	D	920	PCD	O4'-C4'-N3'	-7.06	98.74	117.24
6	D	920	PCD	O9'-C7-C6'	-7.06	104.25	108.96
6	A	920	PCD	O9'-C7-N8'	6.68	114.67	108.61
6	A	920	PCD	O4'-C4'-N3'	-6.34	100.64	117.24
6	D	920	PCD	C4B-N8'-C7	6.16	135.72	123.62
8	B	900	FAD	O3'-C3'-C4'	-5.45	96.55	108.93
8	E	900	FAD	O3'-C3'-C4'	-5.38	96.71	108.93
6	A	920	PCD	C4B-N8'-C7	5.17	133.77	123.62
8	B	900	FAD	O4'-C4'-C5'	5.07	121.17	109.99
8	E	900	FAD	O4B-C1B-N9A	-4.90	98.67	108.09
8	E	900	FAD	O4'-C4'-C5'	4.63	120.21	109.99
6	D	920	PCD	C2D-C1'-N1	4.54	125.89	113.25
6	A	920	PCD	C3'-C2D-C1'	-4.53	92.90	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	920	PCD	C3'-C2D-C1'	-4.44	93.07	101.46
8	B	900	FAD	O4B-C1B-N9A	-4.10	100.22	108.09
6	D	920	PCD	C4A-N5'-C6'	-4.07	104.03	119.86
6	A	920	PCD	C2D-C1'-N1	4.03	124.47	113.25
6	A	920	PCD	C4A-N5'-C6'	-3.90	104.71	119.86
6	A	920	PCD	C5-C4-N3	-3.73	115.04	121.32
6	D	920	PCD	N4-C4-N3	3.62	124.38	117.91
6	D	920	PCD	O2B-PB-O1B	3.60	129.19	112.44
7	A	933	EPE	C10-C9-N1	3.60	125.98	112.36
6	D	920	PCD	C5-C4-N3	-3.58	115.29	121.32
7	D	931	EPE	C10-C9-N1	3.39	125.18	112.36
8	E	900	FAD	C5X-C9A-N10	-3.31	114.97	117.97
6	A	920	PCD	O2-C2-N1	3.28	125.32	118.90
6	A	920	PCD	O2B-PB-O1B	3.23	127.46	112.44
8	E	900	FAD	C5'-C4'-C3'	3.17	118.20	112.22
7	A	930	EPE	C5-N4-C3	3.17	115.67	108.84
7	A	932	EPE	C10-C9-N1	3.17	124.35	112.36
6	D	920	PCD	C4A-C4'-N3'	3.14	131.84	123.91
6	A	920	PCD	C8'-C7'-S7'	-3.03	118.43	120.15
6	A	920	PCD	N4-C4-N3	3.01	123.28	117.91
7	A	933	EPE	C6-N1-C2	2.95	115.19	108.84
7	A	930	EPE	C10-C9-N1	2.91	123.39	112.36
8	B	900	FAD	O4'-C4'-C3'	2.89	116.01	109.25
6	D	920	PCD	O9'-C7-N8'	2.89	111.23	108.61
6	A	920	PCD	C4A-C4'-N3'	2.88	131.19	123.91
6	A	920	PCD	C7'-C8'-S8'	2.85	121.77	120.15
7	A	932	EPE	C6-N1-C2	2.83	114.94	108.84
6	D	920	PCD	O2-C2-N1	2.81	124.40	118.90
6	A	920	PCD	O2-C2-N3	-2.75	117.99	122.33
8	E	900	FAD	O4'-C4'-C3'	2.71	115.60	109.25
7	A	930	EPE	C6-N1-C2	2.71	114.69	108.84
6	D	920	PCD	O4D-C4D-C3'	-2.69	99.81	105.15
6	A	920	PCD	N3'-C2'-N1'	-2.68	121.37	125.48
8	B	900	FAD	C2A-N1A-C6A	2.65	123.08	118.73
7	A	932	EPE	O2S-S-C10	2.64	110.72	106.73
8	E	900	FAD	C4X-C10-N10	2.63	120.25	116.48
7	D	931	EPE	C6-N1-C2	2.62	114.49	108.84
8	E	900	FAD	C4-N3-C2	-2.62	121.00	125.64
6	A	920	PCD	C6-N1-C2	2.60	124.84	120.46
7	A	930	EPE	O2S-S-C10	2.58	110.63	106.73
7	A	933	EPE	C5-N4-C3	2.58	114.40	108.84
7	A	932	EPE	C5-N4-C3	2.54	114.32	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	920	PCD	O3A-PB-O1B	-2.54	103.06	110.70
6	A	920	PCD	O4D-C4D-C5'	2.51	117.37	109.33
6	D	920	PCD	C6-N1-C2	2.50	124.68	120.46
8	E	900	FAD	C2B-C1B-N9A	2.48	119.47	113.30
8	E	900	FAD	C2A-N1A-C6A	2.47	122.79	118.73
6	D	920	PCD	O4D-C4D-C5'	2.46	117.22	109.33
6	A	920	PCD	O4D-C4D-C3'	-2.46	100.27	105.15
6	A	920	PCD	O9'-C7-C6'	-2.44	107.34	108.96
8	B	900	FAD	C5'-C4'-C3'	2.42	116.78	112.22
6	D	920	PCD	C4-N3-C2	2.41	124.05	120.26
8	B	900	FAD	C5X-C9A-N10	-2.41	115.79	117.97
8	B	900	FAD	C2B-C1B-N9A	2.39	119.25	113.30
6	A	920	PCD	C4-N3-C2	2.39	124.02	120.26
7	A	933	EPE	O1S-S-C10	-2.35	103.18	106.73
8	E	900	FAD	O2A-PA-O1A	2.31	123.20	112.44
8	B	900	FAD	O2'-C2'-C3'	-2.28	103.92	109.25
7	D	931	EPE	C5-N4-C3	2.28	113.74	108.84
6	D	920	PCD	N3'-C2'-N1'	-2.21	122.09	125.48
6	A	920	PCD	O2A-PA-O1A	2.21	122.72	112.44
8	E	900	FAD	C10-N1-C2	2.20	121.62	116.85
6	D	920	PCD	O2A-PA-O1A	2.17	122.54	112.44
7	A	933	EPE	O2S-S-C10	2.17	110.00	106.73
8	B	900	FAD	C4-C4X-N5	2.14	121.16	118.21
8	B	900	FAD	C10-N1-C2	2.13	121.47	116.85
6	D	920	PCD	O2-C2-N3	-2.12	118.99	122.33
7	A	932	EPE	C7-N4-C3	2.08	116.78	111.24
8	E	900	FAD	C9A-C5X-N5	2.06	124.64	122.45
8	E	900	FAD	C4X-C10-N1	-2.02	119.64	124.59
7	A	932	EPE	O1S-S-C10	-2.02	103.68	106.73
8	E	900	FAD	C8M-C8-C9	-2.01	116.04	119.57

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	920	PCD	C10-O3B-PB-O1B
6	D	920	PCD	C10-O3B-PB-O1B
7	A	932	EPE	C10-C9-N1-C2
7	A	932	EPE	C10-C9-N1-C6
8	B	900	FAD	N10-C1'-C2'-O2'
8	B	900	FAD	N10-C1'-C2'-C3'
8	B	900	FAD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
8	E	900	FAD	C2'-C3'-C4'-C5'
8	E	900	FAD	O4'-C4'-C5'-O5'
7	A	932	EPE	C8-C7-N4-C3
8	B	900	FAD	C2'-C3'-C4'-C5'
7	A	933	EPE	N4-C7-C8-O8
8	B	900	FAD	O3'-C3'-C4'-C5'
7	A	930	EPE	C8-C7-N4-C5
7	A	932	EPE	C8-C7-N4-C5
7	A	933	EPE	C8-C7-N4-C5
7	D	931	EPE	C8-C7-N4-C5
7	D	931	EPE	N4-C7-C8-O8
7	A	933	EPE	C10-C9-N1-C6
7	D	931	EPE	C8-C7-N4-C3
7	A	933	EPE	C8-C7-N4-C3
8	B	900	FAD	O2'-C2'-C3'-C4'
8	E	900	FAD	O2'-C2'-C3'-C4'
7	A	930	EPE	C8-C7-N4-C3
8	E	900	FAD	N10-C1'-C2'-O2'
8	E	900	FAD	N10-C1'-C2'-C3'
7	A	933	EPE	C10-C9-N1-C2
8	E	900	FAD	O3'-C3'-C4'-C5'
6	A	920	PCD	C9'-C10-O3B-PB
6	D	920	PCD	C9'-C10-O3B-PB
7	A	930	EPE	C10-C9-N1-C2
7	D	931	EPE	C10-C9-N1-C6
8	B	900	FAD	PA-O3P-P-O1P

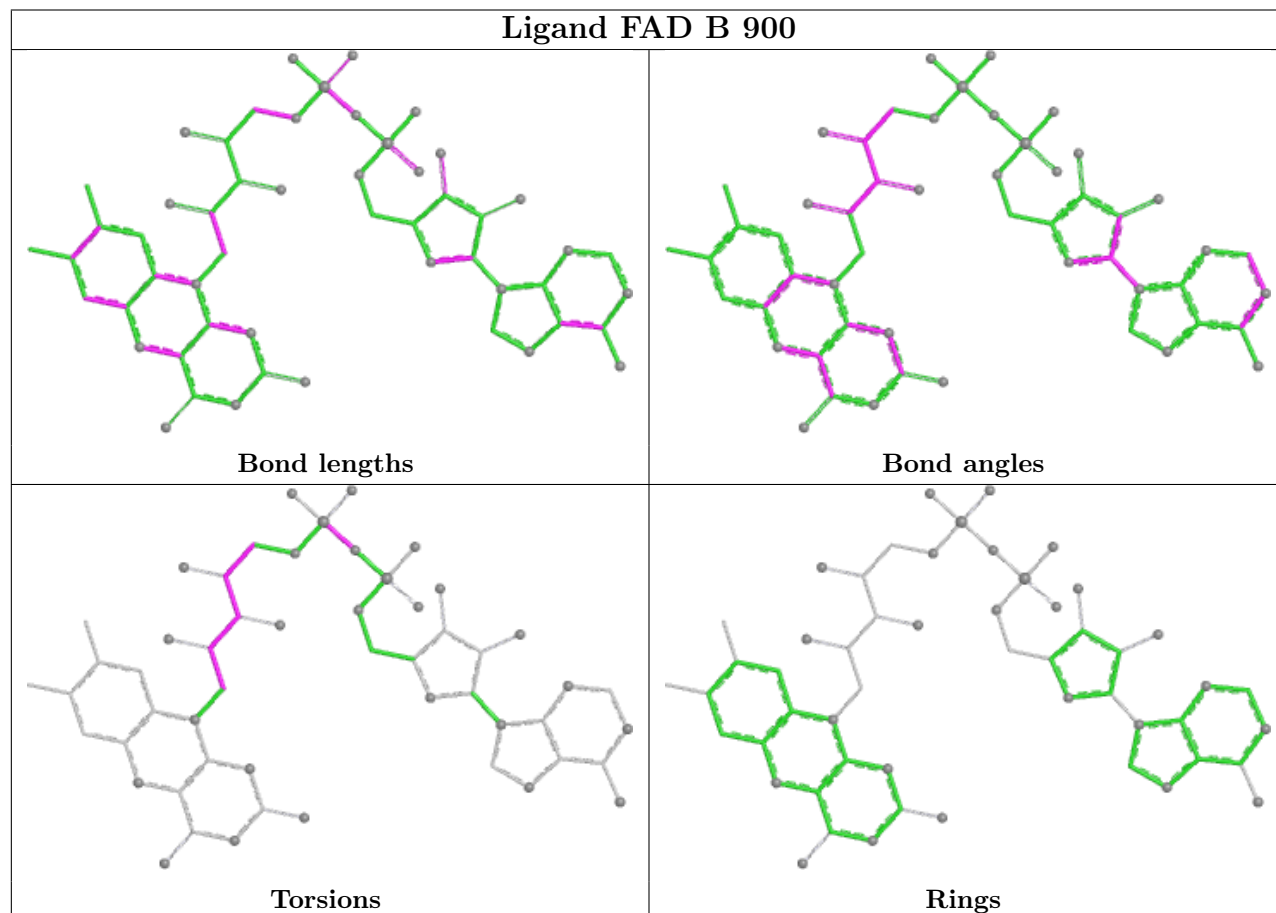
There are no ring outliers.

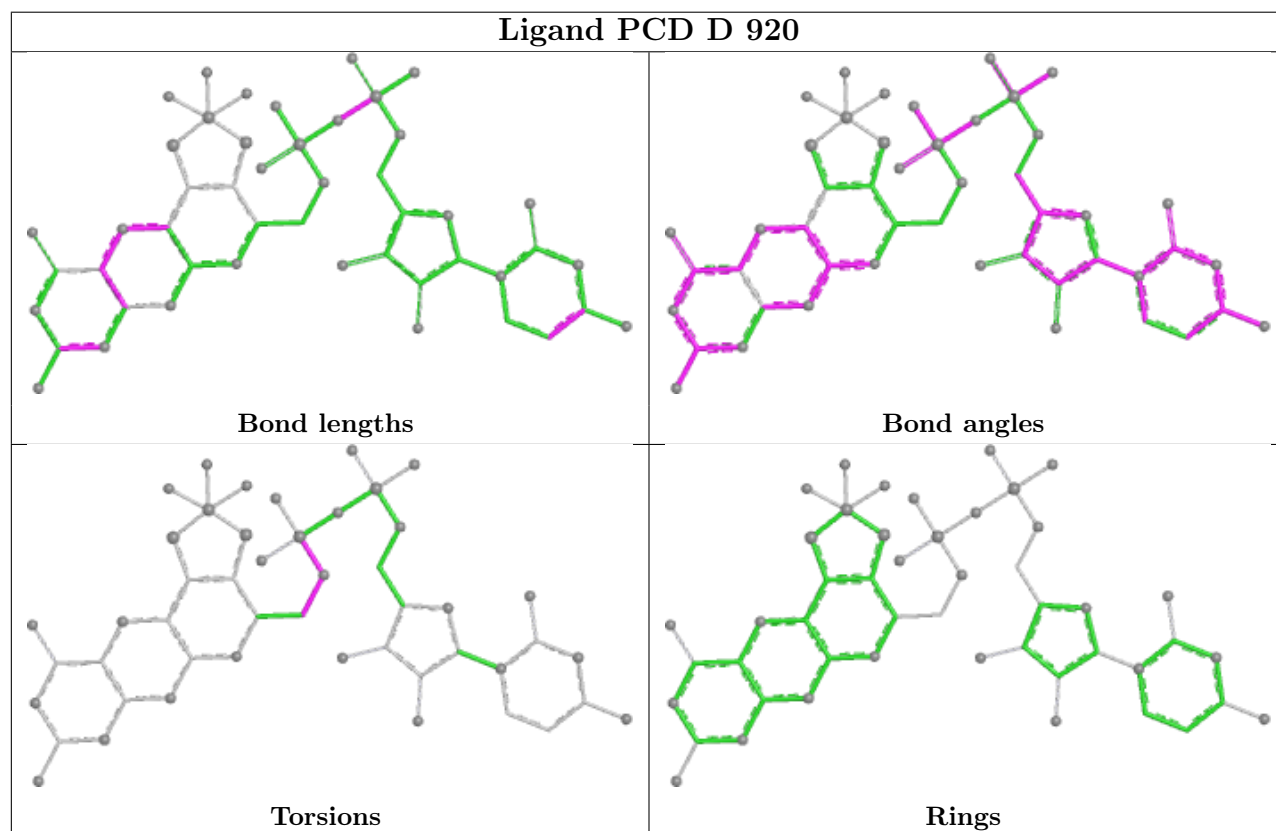
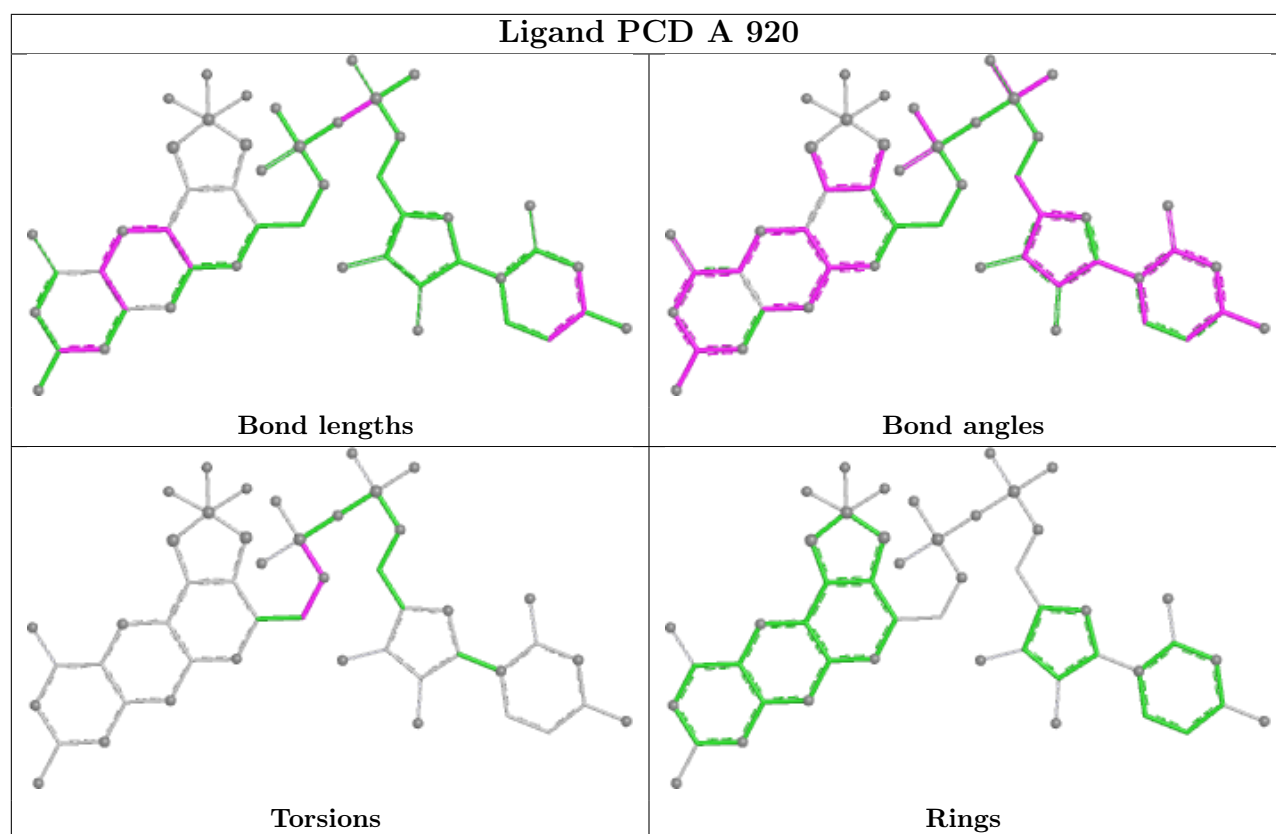
6 monomers are involved in 11 short contacts:

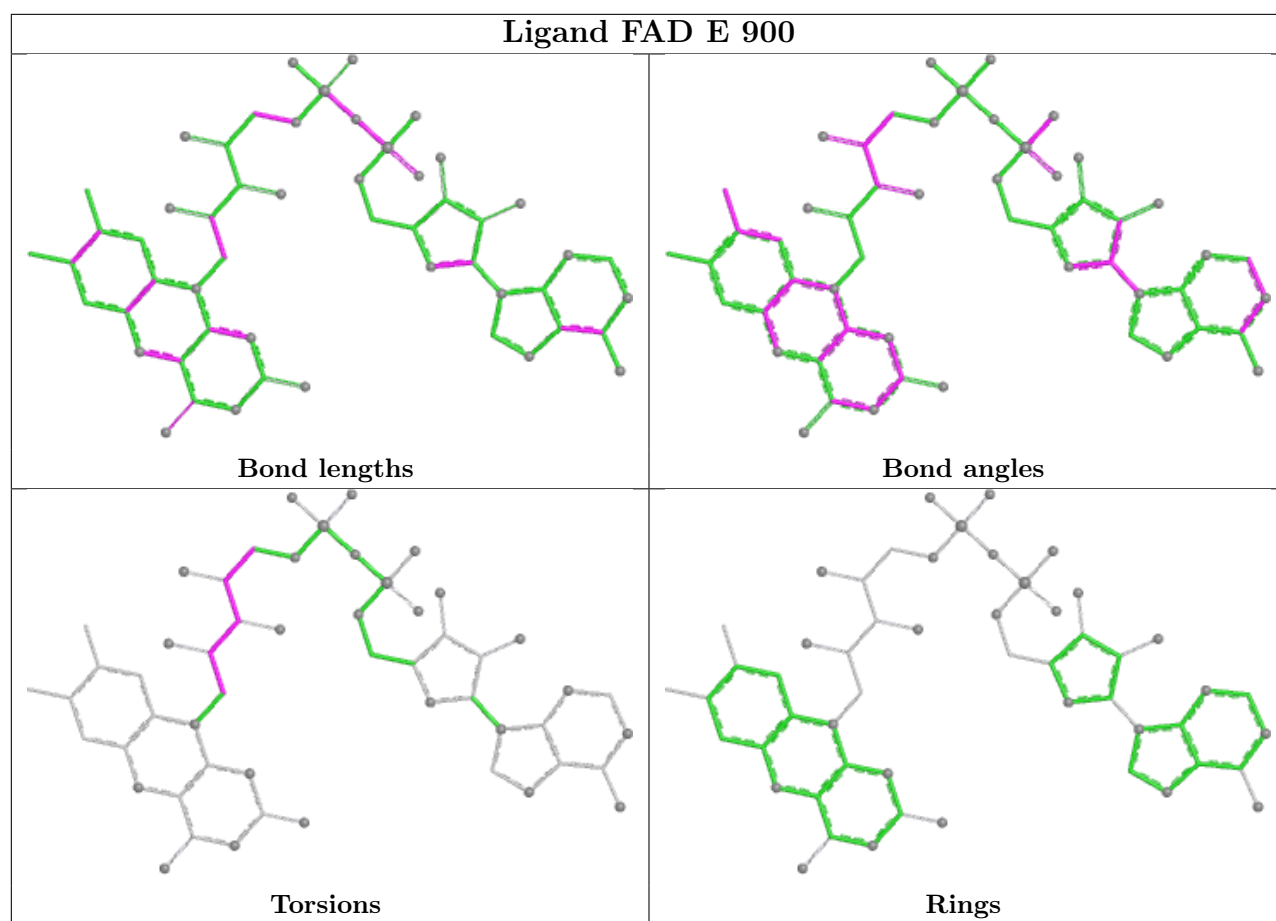
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	900	FAD	1	0
6	A	920	PCD	3	0
6	D	920	PCD	2	0
7	A	930	EPE	1	0
7	A	932	EPE	3	0
8	E	900	FAD	1	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	761/769 (98%)	-0.53	10 (1%) 75 79	7, 14, 29, 67	17 (2%)
1	D	760/769 (98%)	-0.53	17 (2%) 62 66	7, 14, 34, 76	18 (2%)
2	B	323/324 (99%)	-0.33	0 100 100	8, 17, 35, 47	9 (2%)
2	E	323/324 (99%)	0.08	9 (2%) 55 58	9, 20, 38, 53	6 (1%)
3	C	157/161 (97%)	-0.67	2 (1%) 75 79	8, 13, 25, 79	4 (2%)
3	F	157/161 (97%)	-0.67	1 (0%) 85 88	8, 13, 27, 55	3 (1%)
All	All	2481/2508 (98%)	-0.44	39 (1%) 70 74	7, 15, 33, 79	57 (2%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	454	TRP	5.3
1	D	768	ALA	5.0
2	E	66	ALA	4.7
2	E	65	LEU	4.5
3	C	156	CYS	4.2
2	E	323	ALA	3.9
1	D	562	ILE	3.8
1	A	769	ALA	3.8
1	D	574	PRO	3.7
1	D	570	GLY	3.6
1	A	767	ALA	3.4
1	D	767	ALA	3.4
1	D	766	GLU	3.3
1	A	38	ASP	3.3
1	D	37	PRO	3.2
3	F	157	GLU	3.1
1	A	768	ALA	3.1
1	A	563	ASP	3.0
1	D	569	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	562	ILE	2.9
3	C	157	GLU	2.8
1	D	563	ASP	2.8
1	A	570	GLY	2.8
2	E	67	ASP	2.7
1	D	554	ALA	2.6
1	D	572	GLN	2.5
2	E	68	GLY	2.5
1	D	171	ALA	2.4
1	A	764	ALA	2.3
2	E	25	GLU	2.3
1	D	573	ASP	2.2
1	A	766	GLU	2.2
2	E	217	ALA	2.2
1	A	569	SER	2.2
1	D	588	ASP	2.2
2	E	69	SER	2.2
2	E	180	ALA	2.0
1	D	567	MET	2.0
1	D	555	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EPE	A	932	15/15	0.77	0.39	51,53,57,58	15
7	EPE	A	933	15/15	0.78	0.35	40,55,59,60	15
12	SO4	D	773	5/5	0.83	0.29	48,51,52,53	5

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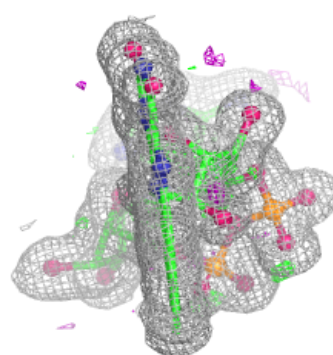
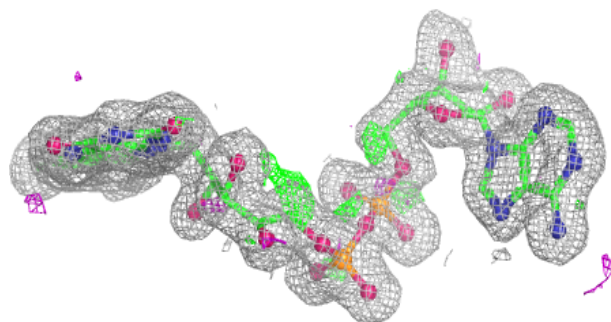
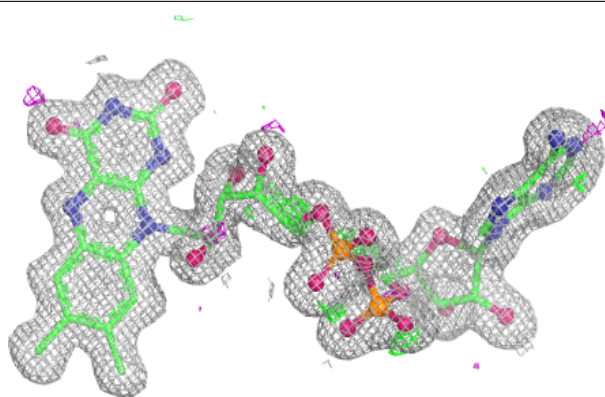
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EPE	A	930	15/15	0.92	0.15	25,31,39,41	15
7	EPE	D	931	15/15	0.94	0.14	15,33,44,53	15
5	NA	A	771	1/1	0.96	0.07	18,18,18,18	0
4	CL	D	770	1/1	0.97	0.04	14,14,14,14	1
8	FAD	E	900	53/53	0.98	0.05	9,14,20,20	0
5	NA	D	772	1/1	0.98	0.07	18,18,18,18	0
8	FAD	B	900	53/53	0.99	0.04	9,12,15,17	0
4	CL	A	770	1/1	0.99	0.03	15,15,15,15	1
9	SF4	E	910[A]	8/8	0.99	0.03	8,10,11,11	8
9	SF4	E	910[B]	8/8	0.99	0.03	9,11,13,13	8
6	PCD	A	920	48/48	0.99	0.04	7,9,12,13	0
6	PCD	D	920	48/48	1.00	0.03	6,8,10,12	0
9	SF4	B	910[A]	8/8	1.00	0.02	8,10,13,15	8
10	FES	C	907	4/4	1.00	0.02	8,9,9,9	0
10	FES	C	908	4/4	1.00	0.01	9,9,10,10	0
10	FES	F	907	4/4	1.00	0.02	7,7,8,8	0
10	FES	F	908	4/4	1.00	0.02	9,9,9,10	0
11	K	D	771	1/1	1.00	0.08	19,19,19,19	0
9	SF4	B	910[B]	8/8	1.00	0.02	6,10,11,11	8

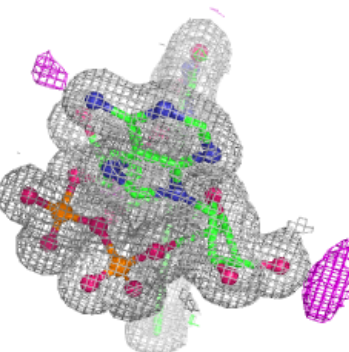
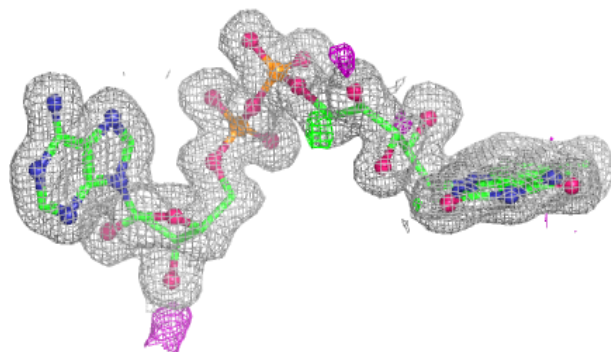
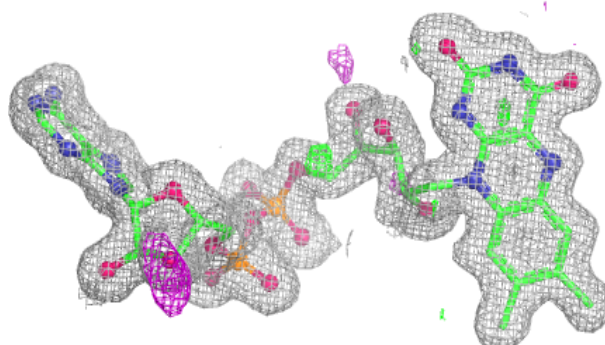
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD E 900:

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

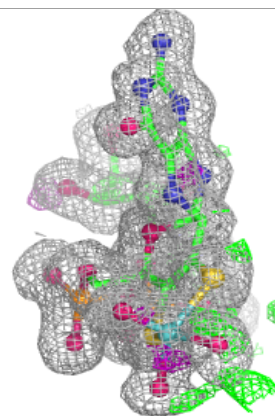
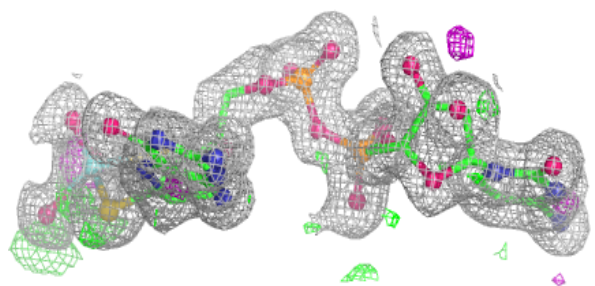
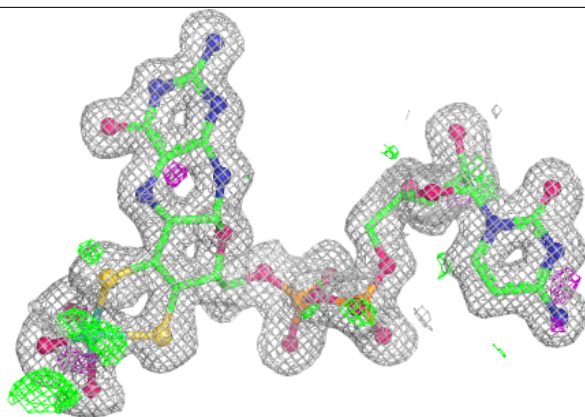
**Electron density around FAD B 900:**

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

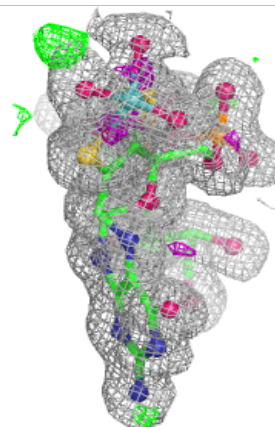
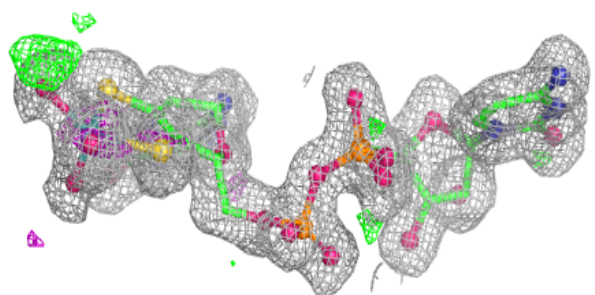
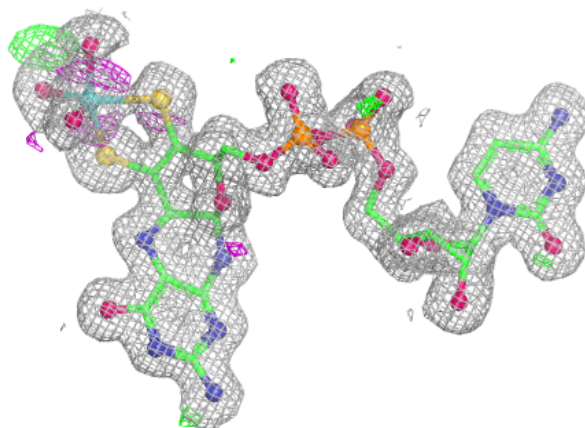


Electron density around PCD A 920:

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

**Electron density around PCD D 920:**

$2mF_o-DF_c$ (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.