



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:01 PM UTC

PDB ID : 3FY4 / pdb_00003fy4
Title : (6-4) Photolyase Crystal Structure
Authors : Hitomi, K.; Arvai, A.S.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2009-01-21
Resolution : 2.70 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

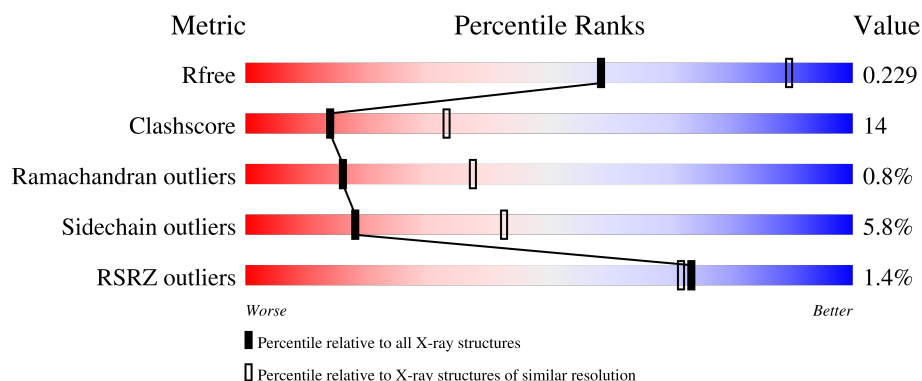
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	537	% 62% 31% • •
1	B	537	% 65% 29% • •
1	C	537	% 69% 23% • •

2 Entry composition [i](#)

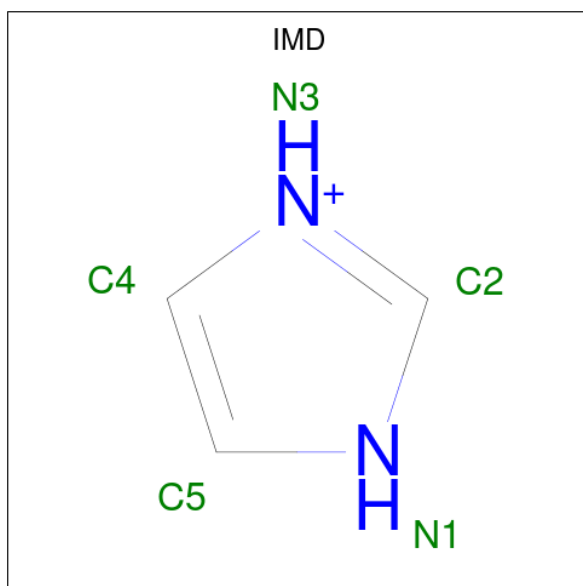
There are 6 unique types of molecules in this entry. The entry contains 13491 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-4 photolyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4194	2709	702	759	24			
1	B	521	Total	C	N	O	S	0	0	0
			4178	2697	699	758	24			
1	C	520	Total	C	N	O	S	0	0	0
			4181	2702	700	755	24			

- Molecule 2 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



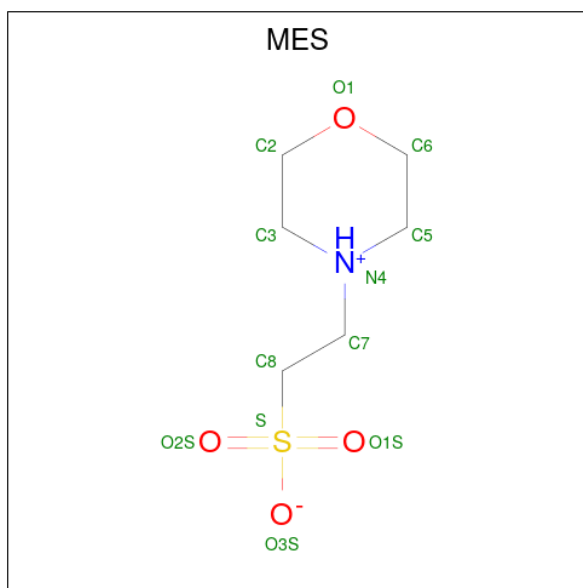
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			5	3	2		
2	A	1	Total	C	N	0	0
			5	3	2		
2	A	1	Total	C	N	0	0
			5	3	2		

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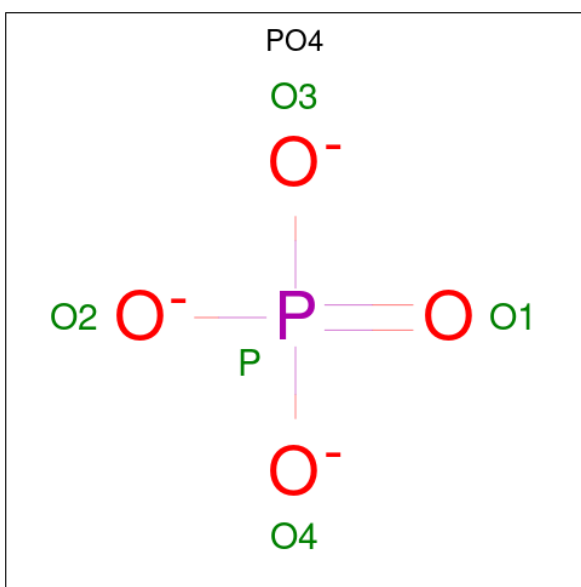
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		
2	C	1	Total	C	N	0	0
			5	3	2		
2	C	1	Total	C	N	0	0
			5	3	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



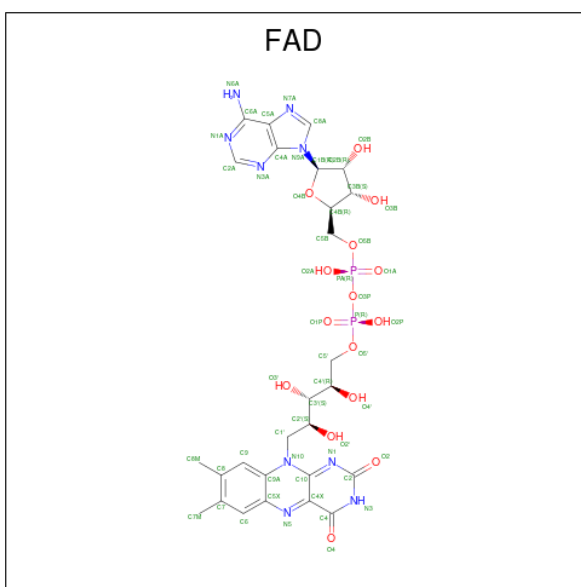
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	P 1	0	0
4	B	1	Total 5	O 4	P 1	0	0
4	C	1	Total 5	O 4	P 1	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

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

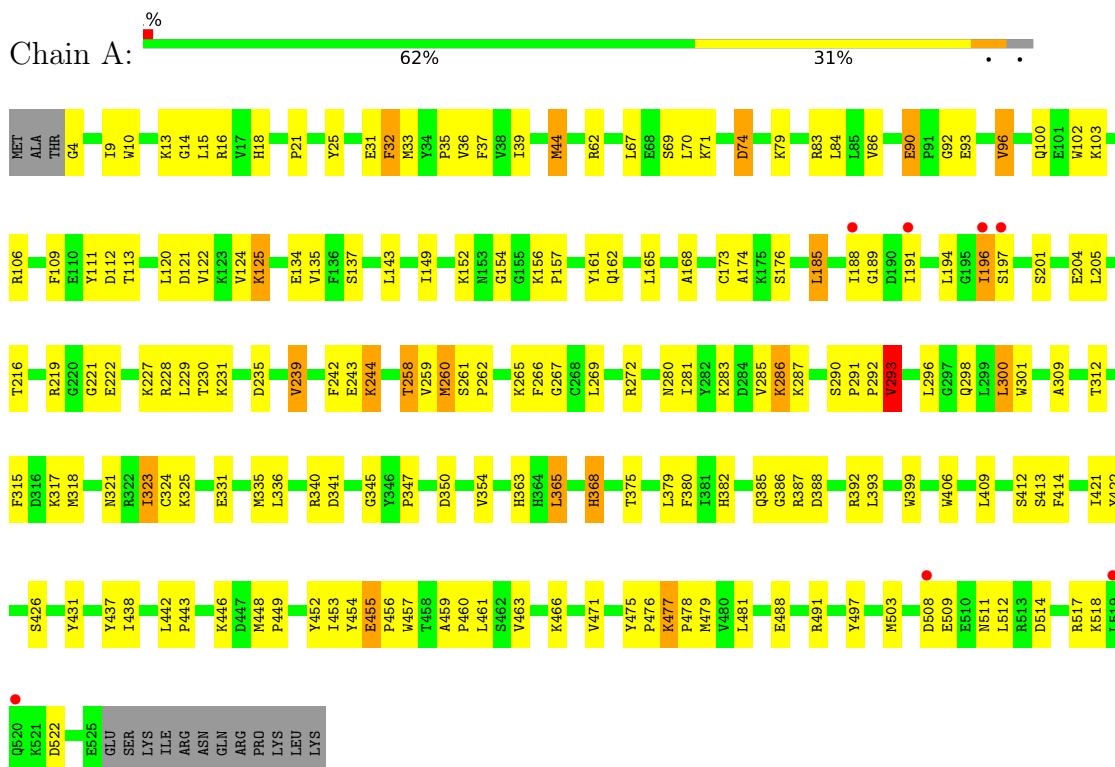
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	244	Total	O	0	0
			244	244		
6	B	187	Total	O	0	0
			187	187		
6	C	247	Total	O	0	0
			247	247		

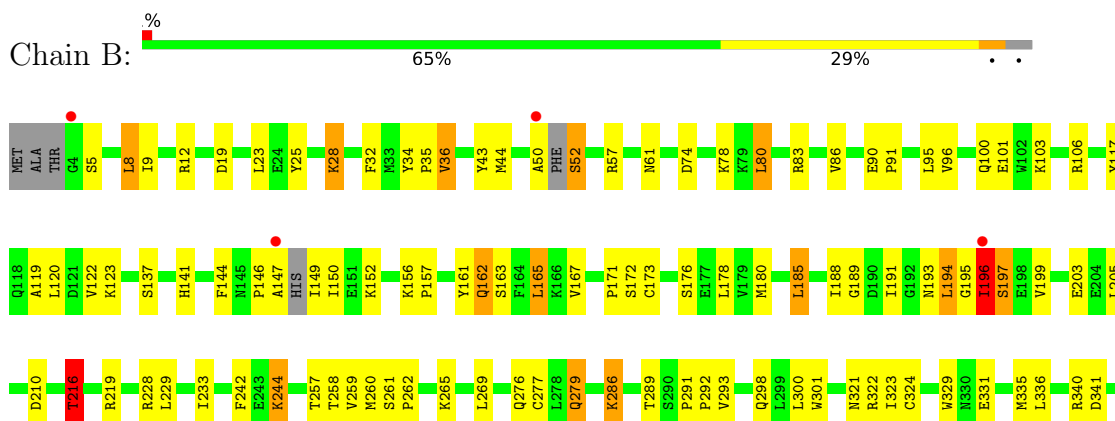
3 Residue-property plots

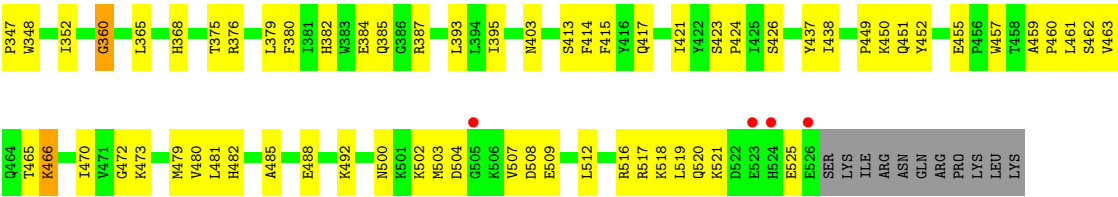
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 6-4 photolyase

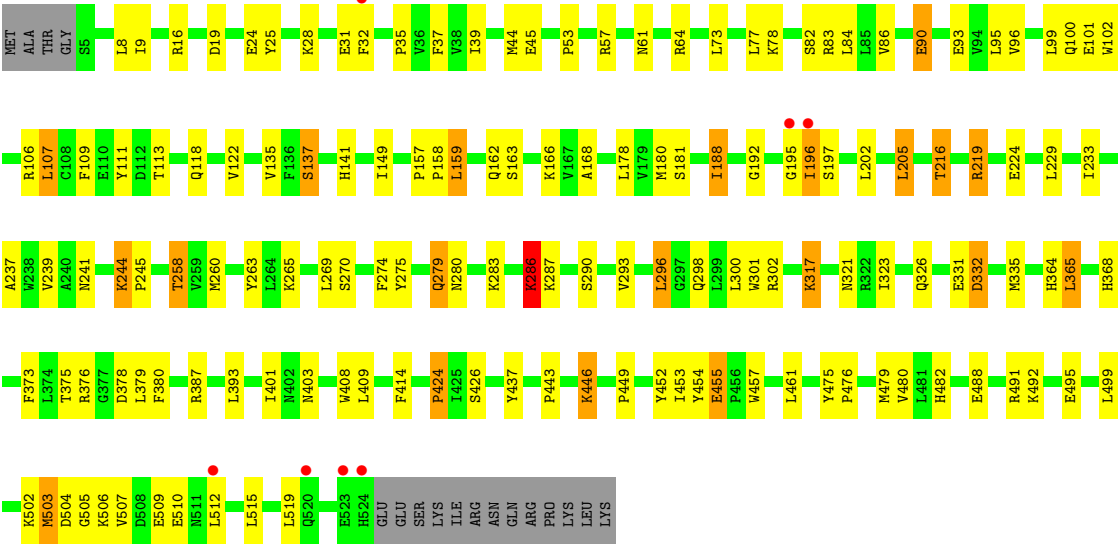


- Molecule 1: 6-4 photolyase





● Molecule 1: 6-4 photolyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.45Å 139.03Å 143.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.38 – 2.70 55.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.6 (55.38-2.70) 95.7 (55.38-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.202 , 0.237 0.195 , 0.229	Depositor DCC
R_{free} test set	3137 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13491	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: PO4, FAD, IMD, MES

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	0.44	0/4319	0.93	14/5846 (0.2%)
1	B	0.43	0/4299	0.93	18/5816 (0.3%)
1	C	0.44	0/4306	0.95	18/5829 (0.3%)
All	All	0.43	0/12924	0.94	50/17491 (0.3%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	331	GLU	N-CA-C	-8.26	96.30	109.59
1	C	216	THR	N-CA-C	-7.83	99.28	110.08
1	A	426	SER	N-CA-C	7.48	122.16	112.89
1	B	137	SER	CA-C-N	7.32	127.48	120.31
1	B	137	SER	C-N-CA	7.32	127.48	120.31
1	C	258	THR	N-CA-C	7.18	119.97	111.71
1	B	426	SER	N-CA-C	7.16	120.50	111.69
1	A	258	THR	N-CA-C	6.85	119.58	111.71
1	B	197	SER	N-CA-C	6.50	119.05	109.24
1	B	331	GLU	N-CA-C	-6.47	98.86	109.40
1	C	141	HIS	N-CA-C	-6.31	105.74	113.50
1	B	258	THR	N-CA-C	6.25	120.16	112.54
1	C	159	LEU	N-CA-C	6.18	120.08	112.54
1	C	293	VAL	N-CA-C	6.09	118.66	111.05
1	A	293	VAL	N-CA-C	5.98	120.41	112.04
1	B	421	ILE	N-CA-C	5.84	116.35	108.17
1	C	290	SER	CA-C-N	-5.84	114.36	120.38
1	C	290	SER	C-N-CA	-5.84	114.36	120.38
1	A	137	SER	CA-C-N	5.77	126.25	120.14
1	A	137	SER	C-N-CA	5.77	126.25	120.14
1	A	323	ILE	N-CA-C	5.70	118.47	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	426	SER	N-CA-C	5.67	120.47	113.50
1	B	472	GLY	N-CA-C	-5.63	107.90	115.21
1	C	296	LEU	N-CA-C	-5.55	105.38	111.82
1	A	331	GLU	N-CA-C	-5.52	99.68	109.06
1	B	293	VAL	N-CA-C	5.52	117.99	111.09
1	A	216	THR	N-CA-C	-5.51	102.47	110.08
1	B	291	PRO	N-CA-C	-5.49	105.20	110.47
1	A	122	VAL	N-CA-C	-5.46	105.39	110.53
1	A	412	SER	N-CA-C	-5.41	106.85	113.50
1	A	229	LEU	N-CA-C	-5.39	105.30	111.07
1	C	137	SER	CA-C-N	5.39	125.37	120.03
1	C	137	SER	C-N-CA	5.39	125.37	120.03
1	A	260	MET	N-CA-C	-5.37	106.73	113.28
1	B	52	SER	CA-C-N	5.28	125.58	119.93
1	B	52	SER	C-N-CA	5.28	125.58	119.93
1	A	296	LEU	N-CA-C	-5.28	105.69	111.82
1	A	44	MET	N-CA-C	5.27	119.84	113.41
1	B	360	GLY	N-CA-C	-5.26	107.98	115.30
1	B	141	HIS	N-CA-C	-5.25	107.25	113.97
1	B	216	THR	N-CA-C	-5.24	102.85	110.08
1	C	181	SER	N-CA-C	5.23	116.23	108.60
1	B	423	SER	CA-C-N	5.15	124.95	119.28
1	B	423	SER	C-N-CA	5.15	124.95	119.28
1	C	44	MET	N-CA-C	5.09	119.49	113.12
1	C	424	PRO	N-CA-C	-5.08	107.78	114.03
1	B	509	GLU	N-CA-C	5.05	116.48	110.97
1	C	437	TYR	N-CA-C	-5.05	105.47	110.97
1	C	376	ARG	N-CA-C	5.03	119.17	113.19
1	C	45	GLU	N-CA-C	5.00	117.68	110.28

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	4194	0	4108	143	0
1	B	4178	0	4092	120	0
1	C	4181	0	4099	102	0
2	A	15	0	15	0	0
2	B	25	0	25	1	0
2	C	10	0	10	4	0
3	A	12	0	13	3	0
3	B	12	0	13	3	0
3	C	12	0	13	3	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	A	53	0	31	1	0
5	B	53	0	31	0	0
5	C	53	0	31	0	0
6	A	244	0	0	7	0
6	B	187	0	0	2	0
6	C	247	0	0	2	0
All	All	13491	0	12481	365	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 14.

All (365) 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:C:286:LYS:H	1:C:286:LYS:HD3	1.19	1.06
1:A:4:GLY:N	1:A:103:LYS:HZ3	1.64	0.94
1:A:285:VAL:HG23	1:A:286:LYS:H	1.29	0.93
1:C:387:ARG:HH11	1:C:403:ASN:HD21	1.18	0.86
1:A:508:ASP:HB3	1:A:511:ASN:HD22	1.43	0.83
1:A:165:LEU:HD21	1:A:300:LEU:HG	1.59	0.82
1:C:286:LYS:HD3	1:C:286:LYS:N	1.95	0.81
1:A:368:HIS:NE2	3:A:920:MES:H22	1.98	0.79
1:B:178:LEU:HB2	1:B:180:MET:HE3	1.67	0.76
1:A:31:GLU:HG3	1:A:32:PHE:CD2	2.21	0.76
1:B:91:PRO:HB2	1:B:120:LEU:HD21	1.68	0.76
1:A:318:MET:HE2	1:A:382:HIS:HE2	1.51	0.74
1:A:285:VAL:O	1:A:286:LYS:HB3	1.85	0.74
1:C:96:VAL:O	1:C:100:GLN:HG2	1.88	0.74
1:C:387:ARG:HH11	1:C:403:ASN:ND2	1.86	0.73
1:B:162:GLN:H	1:B:162:GLN:NE2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ARG:HG3	1:C:401:ILE:HD11	1.71	0.73
1:B:8:LEU:C	1:B:8:LEU:HD12	2.15	0.72
1:C:317:LYS:NZ	1:C:317:LYS:HB3	2.05	0.71
1:C:245:PRO:HG3	3:C:920:MES:O3S	1.91	0.71
1:C:387:ARG:NH1	1:C:403:ASN:HD21	1.88	0.71
1:A:196:ILE:HD12	1:A:196:ILE:H	1.56	0.70
1:C:286:LYS:HG2	1:C:287:LYS:H	1.54	0.70
1:C:408:TRP:HE1	2:C:901:IMD:H2	1.57	0.70
1:A:10:TRP:HB3	1:A:109:PHE:HB3	1.74	0.70
1:A:113:THR:OG1	6:A:3245:HOH:O	2.10	0.70
1:A:286:LYS:HG2	1:A:287:LYS:N	2.05	0.70
1:B:80:LEU:HD23	1:B:185:LEU:HD22	1.75	0.69
1:C:488:GLU:HG3	1:C:492:LYS:HE3	1.74	0.69
1:A:106:ARG:HD3	1:A:134:GLU:OE2	1.92	0.68
1:B:292:PRO:HB2	3:B:920:MES:O3S	1.91	0.68
1:C:443:PRO:O	1:C:446:LYS:HB2	1.93	0.68
1:B:74:ASP:OD2	1:B:78:LYS:HE2	1.94	0.68
1:A:508:ASP:HB3	1:A:511:ASN:ND2	2.08	0.68
1:B:86:VAL:O	1:B:197:SER:HB3	1.94	0.68
1:A:121:ASP:O	1:A:125:LYS:HB2	1.93	0.67
1:C:364:HIS:NE2	3:C:920:MES:H32	2.09	0.67
1:C:19:ASP:HB2	1:C:180:MET:HE1	1.77	0.67
1:B:228:ARG:NH1	1:B:259:VAL:HB	2.09	0.67
1:B:340:ARG:HD2	1:B:341:ASP:OD1	1.95	0.67
1:B:28:LYS:HB2	1:B:28:LYS:NZ	2.10	0.67
1:B:455:GLU:HA	1:B:457:TRP:CZ3	2.29	0.67
1:A:286:LYS:HG2	1:A:287:LYS:H	1.59	0.67
1:C:286:LYS:H	1:C:286:LYS:CD	2.01	0.66
1:A:25:TYR:CE1	1:A:106:ARG:HD2	2.30	0.66
1:A:191:ILE:HG21	1:A:196:ILE:HG12	1.77	0.66
1:A:86:VAL:O	1:A:197:SER:HB3	1.96	0.66
1:A:318:MET:HE2	1:A:382:HIS:NE2	2.10	0.66
1:A:188:ILE:HG23	1:A:189:GLY:H	1.59	0.66
1:A:379:LEU:HD22	1:A:479:MET:HE2	1.78	0.66
1:C:24:GLU:HG2	1:C:28:LYS:HE2	1.78	0.65
1:B:382:HIS:CE1	1:B:384:GLU:HG3	2.32	0.65
1:A:285:VAL:HG23	1:A:286:LYS:N	2.08	0.65
1:B:19:ASP:HB2	1:B:180:MET:HE1	1.79	0.65
1:A:9:ILE:HG23	1:A:35:PRO:HA	1.78	0.65
1:B:119:ALA:O	1:B:122:VAL:HG12	1.97	0.64
1:A:239:VAL:HG21	1:A:281:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:HIS:NE2	3:B:920:MES:H22	2.13	0.64
1:A:188:ILE:HG23	1:A:189:GLY:N	2.14	0.63
1:B:9:ILE:HG23	1:B:35:PRO:HA	1.81	0.63
1:B:147:ALA:O	1:B:149:ILE:N	2.31	0.62
1:C:326:GLN:HB3	1:C:512:LEU:HD11	1.82	0.61
1:B:61:ASN:ND2	1:B:216:THR:HG22	2.16	0.60
1:C:244:LYS:HG3	1:C:298:GLN:OE1	2.01	0.60
1:A:453:ILE:HG23	1:A:454:TYR:CD1	2.36	0.60
1:C:25:TYR:CE1	1:C:106:ARG:HD3	2.36	0.60
1:A:286:LYS:CG	1:A:287:LYS:N	2.64	0.60
1:A:4:GLY:HA3	1:A:31:GLU:OE2	2.01	0.60
1:B:260:MET:HE2	1:B:269:LEU:HD22	1.83	0.60
1:A:201:SER:OG	1:A:204:GLU:HG3	2.02	0.59
1:A:228:ARG:NH1	1:A:259:VAL:HB	2.18	0.59
1:B:375:THR:O	1:B:380:PHE:HA	2.03	0.59
1:B:452:TYR:CD2	1:B:459:ALA:HA	2.38	0.59
1:B:260:MET:CE	1:B:269:LEU:HD22	2.33	0.58
1:B:516:ARG:O	1:B:520:GLN:CG	2.50	0.58
1:A:13:LYS:O	1:A:267:GLY:HA3	2.04	0.58
1:A:379:LEU:CD2	1:A:479:MET:HE2	2.34	0.58
1:B:242:PHE:O	1:B:289:THR:HG21	2.03	0.58
1:B:286:LYS:HE2	1:B:286:LYS:H	1.69	0.58
1:A:165:LEU:CD2	1:A:300:LEU:HG	2.33	0.57
1:B:8:LEU:HD13	1:B:36:VAL:HG13	1.87	0.57
1:A:460:PRO:HD2	1:A:463:VAL:HG21	1.87	0.57
1:A:514:ASP:O	1:A:517:ARG:CG	2.52	0.57
1:B:387:ARG:HD2	1:B:387:ARG:O	2.05	0.57
1:A:477:LYS:NZ	1:A:477:LYS:HB3	2.20	0.57
1:A:31:GLU:HG3	1:A:32:PHE:HD2	1.69	0.57
1:A:32:PHE:CD2	1:A:32:PHE:N	2.73	0.56
1:A:32:PHE:HD2	1:A:32:PHE:N	2.03	0.56
1:A:111:TYR:OH	1:A:113:THR:HG22	2.06	0.56
1:B:229:LEU:O	1:B:233:ILE:HG12	2.05	0.56
1:B:321:ASN:HB3	1:B:324:CYS:HB3	1.87	0.56
1:B:101:GLU:HG2	1:B:194:LEU:HD13	1.87	0.56
1:C:280:ASN:O	1:C:283:LYS:HG2	2.05	0.56
1:A:431:TYR:HE2	6:A:3312:HOH:O	1.88	0.56
1:A:74:ASP:HB2	1:A:84:LEU:HB3	1.88	0.56
1:B:188:ILE:N	1:B:188:ILE:HD12	2.21	0.56
1:A:460:PRO:HB2	1:A:463:VAL:HG23	1.87	0.56
1:C:86:VAL:O	1:C:197:SER:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLU:HG3	1:C:93:GLU:H	1.71	0.55
1:A:13:LYS:O	1:A:266:PHE:O	2.23	0.55
1:A:173:CYS:HA	1:A:176:SER:HB3	1.87	0.55
1:A:292:PRO:HB2	3:A:920:MES:O3S	2.06	0.55
1:C:244:LYS:HG3	1:C:298:GLN:CD	2.32	0.55
1:B:336:LEU:HD22	1:B:385:GLN:HG2	1.89	0.55
1:B:25:TYR:CE1	1:B:106:ARG:HD2	2.42	0.55
1:B:191:ILE:HG21	1:B:196:ILE:HB	1.89	0.55
1:A:448:MET:SD	1:A:449:PRO:HD2	2.47	0.54
1:A:111:TYR:CE1	1:A:113:THR:HG23	2.42	0.54
1:A:461:LEU:HD13	1:A:461:LEU:O	2.08	0.54
1:C:503:MET:HB2	1:C:507:VAL:HG22	1.89	0.54
1:A:452:TYR:CD2	1:A:459:ALA:HA	2.42	0.54
1:B:80:LEU:HB3	1:B:185:LEU:HB2	1.89	0.54
1:A:340:ARG:HD2	1:A:341:ASP:OD1	2.08	0.54
1:B:360:GLY:HA3	1:B:395:ILE:HG23	1.90	0.54
1:B:450:LYS:H	1:B:450:LYS:CD	2.20	0.54
1:A:457:TRP:CE3	1:A:478:PRO:HG3	2.43	0.54
1:A:452:TYR:CE2	1:A:459:ALA:HA	2.43	0.54
1:B:508:ASP:OD2	1:B:508:ASP:C	2.51	0.54
1:A:96:VAL:O	1:A:100:GLN:HG2	2.08	0.53
1:A:244:LYS:HG3	1:A:298:GLN:OE1	2.08	0.53
1:A:317:LYS:O	1:A:321:ASN:HB2	2.09	0.53
1:C:279:GLN:HA	1:C:279:GLN:OE1	2.08	0.53
1:C:9:ILE:HG23	1:C:35:PRO:HA	1.90	0.53
1:A:67:LEU:O	1:A:71:LYS:HG3	2.08	0.53
1:B:5:SER:HB2	1:B:103:LYS:O	2.08	0.53
1:B:502:LYS:C	1:B:504:ASP:H	2.17	0.53
1:C:8:LEU:HD23	1:C:8:LEU:C	2.34	0.53
1:C:502:LYS:C	1:C:504:ASP:H	2.16	0.53
1:A:39:ILE:HG23	1:A:44:MET:HG3	1.90	0.53
1:A:149:ILE:HD12	1:A:168:ALA:HA	1.90	0.53
1:B:500:ASN:HA	1:B:507:VAL:CG2	2.39	0.53
1:B:450:LYS:H	1:B:450:LYS:HD2	1.73	0.53
1:A:125:LYS:HD2	1:A:135:VAL:HG11	1.91	0.52
1:B:460:PRO:HB2	1:B:463:VAL:HG23	1.91	0.52
1:B:517:ARG:O	1:B:520:GLN:HB2	2.09	0.52
1:C:495:GLU:OE1	1:C:519:LEU:HD21	2.10	0.52
1:B:28:LYS:HB2	1:B:28:LYS:HZ2	1.75	0.52
1:C:275:TYR:CE1	1:C:296:LEU:HD11	2.45	0.52
1:C:317:LYS:HB3	1:C:317:LYS:HZ2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:LEU:HD22	1:C:269:LEU:HD11	1.92	0.52
1:C:379:LEU:CD2	1:C:479:MET:HE2	2.40	0.52
1:B:387:ARG:HD2	1:B:387:ARG:C	2.34	0.52
1:C:83:ARG:HB3	1:C:188:ILE:HD12	1.92	0.52
1:B:228:ARG:HG2	1:B:260:MET:SD	2.50	0.51
1:C:258:THR:HB	1:C:260:MET:HG2	1.92	0.51
1:B:244:LYS:HE3	1:B:257:THR:HG21	1.90	0.51
1:A:227:LYS:HE3	1:A:231:LYS:HZ1	1.75	0.51
1:B:50:ALA:O	1:B:52:SER:N	2.43	0.51
1:C:449:PRO:HG2	1:C:452:TYR:HD1	1.75	0.51
1:B:460:PRO:HD2	1:B:463:VAL:HG21	1.93	0.51
1:C:178:LEU:HB3	1:C:180:MET:HE3	1.93	0.51
1:B:462:SER:O	1:B:466:LYS:HB2	2.11	0.51
1:B:492:LYS:HG2	1:B:519:LEU:HD22	1.93	0.51
1:B:521:LYS:O	1:B:525:GLU:HG2	2.10	0.51
1:A:335:MET:HE2	1:A:379:LEU:HB3	1.92	0.51
1:B:244:LYS:HG3	1:B:298:GLN:CD	2.36	0.51
1:A:290:SER:HB3	1:A:291:PRO:HD2	1.92	0.50
1:A:321:ASN:OD1	1:A:323:ILE:HG12	2.11	0.50
1:B:8:LEU:CD1	1:B:36:VAL:HG13	2.40	0.50
1:B:28:LYS:O	1:B:106:ARG:NH2	2.44	0.50
1:A:503:MET:HE1	1:A:511:ASN:ND2	2.26	0.50
1:C:499:LEU:HD23	1:C:515:LEU:HD22	1.92	0.50
1:A:239:VAL:HG11	1:A:281:ILE:HD12	1.92	0.50
1:B:449:PRO:O	1:B:450:LYS:C	2.55	0.50
1:B:286:LYS:H	1:B:286:LYS:CE	2.24	0.50
1:C:368:HIS:CG	1:C:409:LEU:HD11	2.46	0.50
1:A:33:MET:HE1	1:A:185:LEU:HG	1.94	0.50
1:A:239:VAL:HG21	1:A:281:ILE:CD1	2.41	0.50
1:B:146:PRO:O	1:B:150:ILE:HG13	2.12	0.49
1:C:35:PRO:HD2	1:C:188:ILE:HD11	1.94	0.49
1:B:163:SER:O	1:B:167:VAL:HG23	2.12	0.49
1:B:352:ILE:HA	1:B:437:TYR:OH	2.13	0.49
1:C:260:MET:HE2	1:C:269:LEU:HD22	1.94	0.49
1:A:102:TRP:CZ2	1:A:194:LEU:HD12	2.48	0.49
1:A:227:LYS:HE3	1:A:231:LYS:NZ	2.28	0.49
1:C:178:LEU:CB	1:C:180:MET:HE3	2.43	0.49
1:A:382:HIS:HB3	1:A:385:GLN:HG2	1.94	0.49
1:A:21:PRO:HD2	6:A:3157:HOH:O	2.12	0.49
1:A:157:PRO:HG2	6:A:3590:HOH:O	2.13	0.49
1:C:57:ARG:HG3	1:C:57:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:ASP:OD1	1:C:335:MET:HE2	2.13	0.49
1:B:279:GLN:OE1	1:B:279:GLN:HA	2.11	0.49
1:C:492:LYS:NZ	2:C:902:IMD:HN1	2.10	0.49
1:A:259:VAL:HG12	1:A:259:VAL:O	2.12	0.49
1:B:91:PRO:CB	1:B:120:LEU:HD21	2.40	0.49
1:B:195:GLY:O	1:B:196:ILE:C	2.55	0.49
1:B:518:LYS:HD3	1:B:518:LYS:C	2.38	0.49
1:C:25:TYR:CD1	1:C:106:ARG:HD3	2.46	0.49
1:A:368:HIS:CG	1:A:409:LEU:HD11	2.47	0.49
1:A:517:ARG:CG	1:A:518:LYS:N	2.76	0.49
1:B:335:MET:HE2	1:B:479:MET:HE2	1.94	0.49
1:C:118:GLN:O	1:C:122:VAL:HG23	2.12	0.49
1:A:161:TYR:CE2	1:A:292:PRO:HB3	2.48	0.48
1:A:325:LYS:HD2	1:A:497:TYR:CE1	2.48	0.48
1:A:260:MET:CE	1:A:269:LEU:HD22	2.44	0.48
1:B:162:GLN:HG3	6:B:3474:HOH:O	2.13	0.48
1:C:16:ARG:NE	1:C:270:SER:HB2	2.28	0.48
1:B:156:LYS:NZ	1:B:322:ARG:HD3	2.28	0.48
1:A:69:SER:HA	1:A:221:GLY:HA2	1.96	0.48
1:A:121:ASP:O	1:A:125:LYS:HE3	2.13	0.48
1:A:438:ILE:HG23	1:A:442:LEU:HD12	1.95	0.48
1:C:149:ILE:CD1	1:C:168:ALA:HA	2.43	0.48
1:A:365:LEU:O	1:A:368:HIS:HB2	2.13	0.48
1:B:480:VAL:HG22	1:B:485:ALA:HB2	1.95	0.48
1:A:14:GLY:O	1:A:16:ARG:N	2.44	0.48
1:B:413:SER:O	1:B:414:PHE:HB2	2.13	0.48
1:C:180:MET:HA	1:C:180:MET:HE2	1.95	0.48
1:A:503:MET:HE1	1:A:511:ASN:HD21	1.79	0.48
1:B:321:ASN:OD1	1:B:323:ILE:HG12	2.14	0.48
1:C:195:GLY:O	1:C:196:ILE:C	2.57	0.48
1:A:437:TYR:HB3	6:A:3164:HOH:O	2.13	0.47
1:B:375:THR:OG1	1:B:376:ARG:N	2.45	0.47
1:C:499:LEU:HD12	1:C:499:LEU:O	2.15	0.47
1:C:77:LEU:HD12	1:C:84:LEU:HB2	1.96	0.47
1:C:503:MET:CB	1:C:507:VAL:HG22	2.43	0.47
1:B:348:TRP:O	1:B:352:ILE:HG13	2.15	0.47
1:A:162:GLN:H	1:A:162:GLN:CD	2.21	0.47
1:A:449:PRO:HG2	1:A:452:TYR:HD1	1.79	0.47
1:B:301:TRP:CZ2	3:B:920:MES:H71	2.50	0.47
1:C:163:SER:O	1:C:166:LYS:HB3	2.15	0.47
1:A:345:GLY:O	1:A:347:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ARG:HH21	1:C:106:ARG:HG3	1.79	0.47
1:B:335:MET:HE2	1:B:379:LEU:HD22	1.96	0.47
1:A:228:ARG:NH1	1:A:258:THR:O	2.48	0.46
1:B:165:LEU:HD11	1:B:300:LEU:HG	1.96	0.46
1:C:25:TYR:CZ	1:C:106:ARG:NH2	2.83	0.46
1:C:488:GLU:CD	1:C:491:ARG:HE	2.23	0.46
1:A:149:ILE:CD1	1:A:168:ALA:HA	2.46	0.46
1:A:347:PRO:HG2	1:A:456:PRO:HD3	1.98	0.46
1:C:31:GLU:HB3	1:C:32:PHE:CD1	2.51	0.46
1:B:12:ARG:HB3	1:B:117:TYR:CE2	2.50	0.46
1:B:156:LYS:HB3	1:B:157:PRO:HD2	1.98	0.46
1:B:244:LYS:HG3	1:B:298:GLN:OE1	2.15	0.46
1:C:453:ILE:HG23	1:C:454:TYR:CD1	2.51	0.46
1:A:243:GLU:HG2	1:A:293:VAL:HG21	1.97	0.46
1:B:466:LYS:O	1:B:466:LYS:HD3	2.15	0.46
1:C:101:GLU:CG	1:C:192:GLY:HA3	2.45	0.46
1:A:156:LYS:HB3	1:A:157:PRO:HD2	1.97	0.46
1:A:312:THR:O	1:A:315:PHE:HB2	2.16	0.46
1:A:471:VAL:HA	1:A:475:TYR:O	2.15	0.45
1:B:101:GLU:OE1	1:B:193:ASN:HB3	2.16	0.45
1:C:102:TRP:HE1	1:C:192:GLY:H	1.64	0.45
1:A:477:LYS:HB3	1:A:477:LYS:HZ2	1.81	0.45
1:C:301:TRP:CZ2	3:C:920:MES:H81	2.50	0.45
1:C:504:ASP:O	1:C:506:LYS:N	2.45	0.45
1:C:205:LEU:HD12	1:C:205:LEU:HA	1.80	0.45
1:B:452:TYR:CE2	1:B:460:PRO:HD3	2.51	0.45
1:B:43:TYR:CE1	1:B:57:ARG:HD3	2.52	0.45
1:C:53:PRO:HA	6:C:3655:HOH:O	2.16	0.45
1:A:244:LYS:HG3	1:A:298:GLN:CD	2.41	0.45
1:A:258:THR:HB	1:A:260:MET:HG2	1.99	0.45
1:A:309:ALA:HB1	1:A:399:TRP:CZ3	2.52	0.45
1:B:96:VAL:O	1:B:100:GLN:HG3	2.17	0.45
1:C:99:LEU:HD12	1:C:99:LEU:HA	1.85	0.45
1:B:415:PHE:CZ	1:B:417:GLN:HB2	2.53	0.45
1:A:235:ASP:O	1:A:239:VAL:HG12	2.17	0.44
1:B:165:LEU:HD11	1:B:300:LEU:CG	2.48	0.44
1:B:461:LEU:HD12	1:B:461:LEU:O	2.16	0.44
1:C:237:ALA:O	1:C:241:ASN:ND2	2.50	0.44
1:B:171:PRO:O	1:B:173:CYS:N	2.44	0.44
1:B:122:VAL:HG13	1:B:123:LYS:N	2.33	0.44
1:C:321:ASN:OD1	1:C:323:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LYS:HD3	1:B:286:LYS:N	2.33	0.44
1:A:13:LYS:HB2	6:A:3247:HOH:O	2.16	0.44
1:A:508:ASP:OD1	1:A:509:GLU:N	2.50	0.44
1:C:286:LYS:HG2	1:C:287:LYS:N	2.29	0.44
1:C:449:PRO:HG2	1:C:452:TYR:CD1	2.52	0.44
1:C:455:GLU:HA	1:C:457:TRP:CZ3	2.53	0.44
1:A:508:ASP:CB	1:A:511:ASN:HD22	2.24	0.44
1:A:363:HIS:HE1	1:A:365:LEU:HD22	1.83	0.44
1:B:191:ILE:CD1	1:B:196:ILE:HD12	2.47	0.44
1:A:454:TYR:C	1:A:455:GLU:HG2	2.42	0.43
1:C:475:TYR:CD1	1:C:476:PRO:HD2	2.53	0.43
1:B:161:TYR:OH	1:B:300:LEU:HB2	2.18	0.43
1:C:229:LEU:O	1:C:233:ILE:HG12	2.19	0.43
1:A:33:MET:O	1:A:188:ILE:HA	2.18	0.43
1:B:152:LYS:HD2	1:B:167:VAL:O	2.18	0.43
1:B:466:LYS:NZ	6:B:3633:HOH:O	2.50	0.43
1:C:509:GLU:HG3	1:C:510:GLU:N	2.33	0.43
1:B:261:SER:OG	1:B:262:PRO:HD3	2.18	0.43
1:C:111:TYR:CE1	1:C:113:THR:HG23	2.54	0.43
1:C:408:TRP:NE1	2:C:901:IMD:H2	2.31	0.43
1:A:191:ILE:HG22	1:A:191:ILE:O	2.19	0.43
1:A:260:MET:HE2	1:A:269:LEU:HD22	2.00	0.43
1:A:443:PRO:O	1:A:446:LYS:HB2	2.19	0.43
1:B:516:ARG:HG3	1:B:516:ARG:HH11	1.83	0.43
1:C:78:LYS:HA	1:C:82:SER:O	2.18	0.43
1:A:191:ILE:HG21	1:A:196:ILE:CG1	2.47	0.43
1:A:386:GLY:HA3	1:A:406:TRP:CH2	2.54	0.43
1:B:86:VAL:HG21	1:B:199:VAL:HG22	2.00	0.43
1:B:347:PRO:HB2	1:B:438:ILE:HD13	2.00	0.43
1:B:452:TYR:CE2	1:B:459:ALA:HA	2.53	0.43
1:B:329:TRP:CG	1:B:382:HIS:HA	2.54	0.42
1:B:387:ARG:C	1:B:387:ARG:CD	2.92	0.42
1:B:500:ASN:HA	1:B:507:VAL:HG23	2.01	0.42
1:C:57:ARG:HG3	1:C:57:ARG:NH1	2.34	0.42
1:C:25:TYR:OH	1:C:106:ARG:NH2	2.52	0.42
1:C:502:LYS:C	1:C:504:ASP:N	2.73	0.42
1:B:188:ILE:HG22	1:B:189:GLY:O	2.20	0.42
1:C:424:PRO:HD3	1:C:482:HIS:CE1	2.55	0.42
1:B:25:TYR:CZ	1:B:106:ARG:NH1	2.87	0.42
1:A:321:ASN:HB3	1:A:324:CYS:HB3	2.02	0.42
1:C:224:GLU:HG2	6:C:3114:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLY:O	1:A:96:VAL:HG13	2.19	0.42
1:A:375:THR:O	1:A:380:PHE:HA	2.20	0.42
1:A:477:LYS:O	1:A:478:PRO:C	2.63	0.42
1:C:37:PHE:O	1:C:86:VAL:HA	2.19	0.42
1:C:107:LEU:HB3	1:C:135:VAL:HG22	2.02	0.42
1:A:120:LEU:O	1:A:124:VAL:HG23	2.20	0.42
1:C:157:PRO:HA	1:C:158:PRO:HD3	1.91	0.42
1:A:62:ARG:HH12	1:A:392:ARG:HA	1.84	0.41
1:A:301:TRP:CZ2	3:A:920:MES:H71	2.55	0.41
1:A:421:ILE:HG22	1:A:422:TYR:O	2.20	0.41
1:A:90:GLU:HG3	1:A:93:GLU:H	1.84	0.41
1:A:413:SER:O	1:A:414:PHE:HB2	2.20	0.41
1:B:233:ILE:HD11	2:B:906:IMD:N1	2.35	0.41
1:C:373:PHE:O	1:C:378:ASP:HB2	2.19	0.41
1:A:227:LYS:O	1:A:230:THR:HB	2.20	0.41
1:A:261:SER:HB3	1:A:262:PRO:CD	2.50	0.41
1:A:475:TYR:CD1	1:A:476:PRO:HD2	2.55	0.41
1:B:5:SER:HA	1:B:32:PHE:CZ	2.54	0.41
1:B:276:GLN:O	1:B:277:CYS:C	2.63	0.41
1:A:18:HIS:ND1	1:A:222:GLU:OE2	2.34	0.41
1:B:188:ILE:N	1:B:188:ILE:CD1	2.83	0.41
1:B:387:ARG:NH1	1:B:403:ASN:OD1	2.47	0.41
1:A:350:ASP:O	1:A:354:VAL:HG23	2.20	0.41
1:B:144:PHE:O	1:B:146:PRO:HD3	2.20	0.41
1:C:64:ARG:HH11	1:C:64:ARG:HG3	1.86	0.41
1:C:162:GLN:OE1	1:C:162:GLN:N	2.43	0.41
1:C:274:PHE:HD2	1:C:274:PHE:O	2.04	0.41
1:C:379:LEU:HD21	1:C:479:MET:HE2	2.03	0.41
1:A:336:LEU:HD13	1:A:385:GLN:HB3	2.03	0.41
1:C:95:LEU:O	1:C:99:LEU:HB2	2.20	0.41
1:C:260:MET:CE	1:C:269:LEU:HD22	2.50	0.41
1:C:375:THR:O	1:C:380:PHE:HA	2.21	0.41
1:A:152:LYS:C	1:A:154:GLY:H	2.29	0.41
1:A:387:ARG:HD2	1:A:387:ARG:C	2.46	0.41
1:C:93:GLU:O	1:C:96:VAL:HG22	2.19	0.41
1:C:219:ARG:O	1:C:263:TYR:OH	2.31	0.41
1:A:111:TYR:CG	1:A:112:ASP:N	2.89	0.41
1:A:242:PHE:HB3	6:A:3143:HOH:O	2.21	0.41
1:A:261:SER:HB3	1:A:262:PRO:HD3	2.03	0.41
1:A:387:ARG:NE	1:A:388:ASP:OD2	2.50	0.41
1:A:461:LEU:HD13	1:A:461:LEU:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:HD13	1:B:36:VAL:CG1	2.49	0.41
1:B:261:SER:N	1:B:262:PRO:HD2	2.36	0.41
1:B:465:THR:OG1	1:B:470:ILE:HD11	2.21	0.41
1:C:408:TRP:CE3	1:C:414:PHE:HB3	2.55	0.41
1:B:424:PRO:HD3	1:B:482:HIS:CE1	2.56	0.41
1:C:37:PHE:HE2	1:C:39:ILE:HD13	1.86	0.41
1:A:36:VAL:HG12	1:A:37:PHE:N	2.36	0.40
1:A:196:ILE:H	1:A:196:ILE:CD1	2.18	0.40
1:A:261:SER:HB2	5:A:900:FAD:C5'	2.51	0.40
1:A:453:ILE:HG23	1:A:454:TYR:HD1	1.82	0.40
1:B:32:PHE:HD2	1:B:34:TYR:HE1	1.69	0.40
1:A:280:ASN:O	1:A:283:LYS:HG2	2.21	0.40
1:B:259:VAL:O	1:B:259:VAL:HG12	2.21	0.40
1:B:382:HIS:HE1	1:B:384:GLU:HG3	1.84	0.40
1:B:460:PRO:HD2	1:B:463:VAL:CG2	2.51	0.40
1:B:194:LEU:HD12	1:B:194:LEU:HA	1.91	0.40
1:C:492:LYS:HZ2	2:C:902:IMD:HN1	1.67	0.40
1:A:488:GLU:OE2	1:A:491:ARG:NH1	2.54	0.40
1:C:109:PHE:O	1:C:137:SER:HA	2.20	0.40
1:C:365:LEU:HD12	1:C:365:LEU:HA	1.86	0.40
1:A:143:LEU:HD23	1:A:272:ARG:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	520/537 (97%)	471 (91%)	46 (9%)	3 (1%)	21	44
1	B	515/537 (96%)	471 (92%)	38 (7%)	6 (1%)	10	27
1	C	518/537 (96%)	486 (94%)	28 (5%)	4 (1%)	16	37
All	All	1553/1611 (96%)	1428 (92%)	112 (7%)	13 (1%)	16	37

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	LYS
1	B	172	SER
1	B	176	SER
1	B	286	LYS
1	B	451	GLN
1	A	15	LEU
1	B	503	MET
1	A	174	ALA
1	C	332	ASP
1	B	196	ILE
1	C	196	ILE
1	C	286	LYS
1	C	505	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	453/473 (96%)	427 (94%)	26 (6%)	18	43
1	B	451/473 (95%)	422 (94%)	29 (6%)	16	38
1	C	452/473 (96%)	428 (95%)	24 (5%)	20	46
All	All	1356/1419 (96%)	1277 (94%)	79 (6%)	18	42

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	PHE
1	A	70	LEU
1	A	74	ASP
1	A	79	LYS
1	A	83	ARG
1	A	90	GLU
1	A	96	VAL
1	A	125	LYS

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Mol	Chain	Res	Type
1	A	185	LEU
1	A	196	ILE
1	A	205	LEU
1	A	219	ARG
1	A	239	VAL
1	A	244	LYS
1	A	265	LYS
1	A	293	VAL
1	A	300	LEU
1	A	365	LEU
1	A	368	HIS
1	A	393	LEU
1	A	455	GLU
1	A	466	LYS
1	A	477	LYS
1	A	481	LEU
1	A	512	LEU
1	A	522	ASP
1	B	8	LEU
1	B	23	LEU
1	B	28	LYS
1	B	36	VAL
1	B	44	MET
1	B	80	LEU
1	B	83	ARG
1	B	90	GLU
1	B	95	LEU
1	B	162	GLN
1	B	165	LEU
1	B	185	LEU
1	B	194	LEU
1	B	196	ILE
1	B	203	GLU
1	B	205	LEU
1	B	210	ASP
1	B	216	THR
1	B	219	ARG
1	B	244	LYS
1	B	265	LYS
1	B	279	GLN
1	B	365	LEU
1	B	393	LEU

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Mol	Chain	Res	Type
1	B	466	LYS
1	B	473	LYS
1	B	481	LEU
1	B	488	GLU
1	B	512	LEU
1	C	61	ASN
1	C	73	LEU
1	C	90	GLU
1	C	107	LEU
1	C	159	LEU
1	C	188	ILE
1	C	202	LEU
1	C	205	LEU
1	C	216	THR
1	C	219	ARG
1	C	239	VAL
1	C	244	LYS
1	C	265	LYS
1	C	279	GLN
1	C	286	LYS
1	C	300	LEU
1	C	317	LYS
1	C	365	LEU
1	C	393	LEU
1	C	446	LYS
1	C	455	GLU
1	C	461	LEU
1	C	480	VAL
1	C	503	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	193	ASN
1	A	314	ASN
1	A	385	GLN
1	A	511	ASN
1	B	61	ASN
1	B	100	GLN
1	B	153	ASN
1	B	162	GLN

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Mol	Chain	Res	Type
1	B	314	ASN
1	B	402	ASN
1	B	405	ASN
1	B	440	HIS
1	B	451	GLN
1	C	61	ASN
1	C	193	ASN
1	C	241	ASN
1	C	326	GLN
1	C	402	ASN
1	C	403	ASN
1	C	440	HIS
1	C	468	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
2	IMD	B	903	-	5,5,5	0.95	0	5,5,5	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	A	930	-	4,4,4	1.68	1 (25%)	6,6,6	0.46	0
4	PO4	C	930	-	4,4,4	1.67	1 (25%)	6,6,6	0.46	0
5	FAD	A	900	-	58,58,58	1.73	12 (20%)	85,89,89	1.61	17 (20%)
5	FAD	B	900	-	58,58,58	1.74	14 (24%)	85,89,89	1.65	17 (20%)
2	IMD	B	904	-	5,5,5	1.01	0	5,5,5	0.22	0
2	IMD	A	902	-	5,5,5	1.05	0	5,5,5	0.15	0
4	PO4	B	930	-	4,4,4	1.68	1 (25%)	6,6,6	0.47	0
2	IMD	B	906	-	5,5,5	0.93	0	5,5,5	0.19	0
3	MES	C	920	-	12,12,12	1.36	3 (25%)	15,16,16	0.75	0
5	FAD	C	900	-	58,58,58	1.78	14 (24%)	85,89,89	1.61	15 (17%)
2	IMD	A	901	-	5,5,5	0.94	0	5,5,5	0.22	0
3	MES	A	920	-	12,12,12	1.59	3 (25%)	15,16,16	0.76	1 (6%)
2	IMD	C	902	-	5,5,5	1.04	0	5,5,5	0.18	0
2	IMD	B	901	-	5,5,5	0.95	0	5,5,5	0.19	0
3	MES	B	920	-	12,12,12	1.67	4 (33%)	15,16,16	0.82	0
2	IMD	A	905	-	5,5,5	0.98	0	5,5,5	0.17	0
2	IMD	C	901	-	5,5,5	0.94	0	5,5,5	0.25	0
2	IMD	B	905	-	5,5,5	0.99	0	5,5,5	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	920	-	-	0/6/14/14	0/1/1/1
2	IMD	A	901	-	-	-	0/1/1/1
2	IMD	B	903	-	-	-	0/1/1/1
2	IMD	B	904	-	-	-	0/1/1/1
5	FAD	A	900	-	-	2/34/50/50	0/6/6/6
2	IMD	C	902	-	-	-	0/1/1/1
3	MES	B	920	-	-	0/6/14/14	0/1/1/1
2	IMD	B	901	-	-	-	0/1/1/1
2	IMD	B	906	-	-	-	0/1/1/1
2	IMD	A	902	-	-	-	0/1/1/1
5	FAD	B	900	-	-	3/34/50/50	0/6/6/6
3	MES	C	920	-	-	2/6/14/14	0/1/1/1
2	IMD	A	905	-	-	-	0/1/1/1
2	IMD	B	905	-	-	-	0/1/1/1
2	IMD	C	901	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	C	900	-	-	2/34/50/50	0/6/6/6

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	900	FAD	C4X-N5	4.77	1.41	1.30
5	C	900	FAD	C2A-N1A	4.69	1.42	1.33
5	B	900	FAD	C2A-N1A	4.52	1.42	1.33
5	A	900	FAD	C2A-N1A	4.32	1.41	1.33
5	B	900	FAD	C4X-N5	4.31	1.40	1.30
5	C	900	FAD	C4X-N5	4.24	1.39	1.30
5	B	900	FAD	C10-N1	4.19	1.41	1.33
5	C	900	FAD	C2A-N3A	4.18	1.41	1.33
5	A	900	FAD	C10-N1	4.07	1.41	1.33
5	C	900	FAD	C10-N1	4.01	1.41	1.33
5	B	900	FAD	C2A-N3A	3.69	1.40	1.33
5	A	900	FAD	C2A-N3A	3.57	1.40	1.33
5	C	900	FAD	C9-C8	3.54	1.44	1.39
3	B	920	MES	C7-N4	3.25	1.54	1.47
5	B	900	FAD	P-O3P	3.22	1.63	1.59
5	A	900	FAD	C10-N10	3.15	1.44	1.37
3	A	920	MES	C7-N4	3.03	1.54	1.47
5	A	900	FAD	C6-C7	2.99	1.43	1.39
5	B	900	FAD	C6-C5X	2.93	1.44	1.40
5	B	900	FAD	C10-N10	2.86	1.43	1.37
5	A	900	FAD	C9-C9A	2.85	1.44	1.39
5	B	900	FAD	C6-C7	2.85	1.43	1.39
3	A	920	MES	C5-N4	2.82	1.54	1.46
3	B	920	MES	C5-N4	2.80	1.54	1.46
5	C	900	FAD	C10-N10	2.73	1.43	1.37
5	C	900	FAD	C6-C7	2.70	1.43	1.39
5	B	900	FAD	C1'-N10	2.68	1.54	1.47
5	C	900	FAD	C9-C9A	2.66	1.43	1.39
5	A	900	FAD	C9A-C5X	2.65	1.45	1.41
5	A	900	FAD	C6-C5X	2.65	1.44	1.40
5	A	900	FAD	P-O3P	2.62	1.62	1.59
5	C	900	FAD	P-O3P	2.58	1.62	1.59
5	B	900	FAD	C9A-C5X	2.56	1.45	1.41
5	C	900	FAD	C6-C5X	2.55	1.43	1.40
5	B	900	FAD	C9-C8	2.55	1.43	1.39
5	A	900	FAD	C9-C8	2.52	1.43	1.39
5	B	900	FAD	C9-C9A	2.51	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	920	MES	C5-N4	2.51	1.53	1.46
3	A	920	MES	C3-N4	2.49	1.53	1.46
5	A	900	FAD	C1'-N10	2.47	1.53	1.47
5	C	900	FAD	C9A-C5X	2.40	1.45	1.41
5	C	900	FAD	C8A-N7A	2.36	1.36	1.31
3	B	920	MES	C3-N4	2.35	1.53	1.46
3	C	920	MES	C3-N4	2.29	1.53	1.46
5	C	900	FAD	C5A-N7A	-2.20	1.35	1.39
5	C	900	FAD	C1'-N10	2.13	1.53	1.47
3	C	920	MES	C7-N4	2.11	1.52	1.47
3	B	920	MES	C8-S	2.07	1.80	1.77
5	B	900	FAD	C2'-C3'	2.07	1.57	1.53
4	B	930	PO4	P-O3	-2.03	1.48	1.54
5	B	900	FAD	C1'-C2'	2.03	1.55	1.52
4	A	930	PO4	P-O3	-2.02	1.48	1.54
4	C	930	PO4	P-O3	-2.01	1.48	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	900	FAD	N3A-C2A-N1A	-5.15	120.78	128.58
5	C	900	FAD	N3A-C2A-N1A	-5.04	120.96	128.58
5	A	900	FAD	N3A-C2A-N1A	-4.97	121.06	128.58
5	B	900	FAD	N9A-C8A-N7A	-4.94	106.93	113.94
5	C	900	FAD	N9A-C8A-N7A	-4.71	107.26	113.94
5	A	900	FAD	N9A-C8A-N7A	-4.64	107.35	113.94
5	C	900	FAD	C5A-N7A-C8A	4.52	110.55	103.45
5	A	900	FAD	C5A-N7A-C8A	4.35	110.29	103.45
5	B	900	FAD	C5A-N7A-C8A	4.35	110.28	103.45
5	B	900	FAD	C4X-C10-N10	3.36	121.29	116.48
5	A	900	FAD	C5A-C4A-N3A	-3.33	122.14	126.72
5	C	900	FAD	C5A-C4A-N3A	-3.32	122.15	126.72
5	A	900	FAD	C4X-C10-N10	3.25	121.13	116.48
5	C	900	FAD	C4X-C10-N10	3.20	121.06	116.48
5	B	900	FAD	C5A-C4A-N3A	-3.13	122.41	126.72
5	A	900	FAD	C4A-C5A-N7A	-3.03	107.12	110.58
5	C	900	FAD	C4A-C5A-N7A	-3.02	107.13	110.58
5	B	900	FAD	C4A-N9A-C8A	2.95	108.84	105.74
5	B	900	FAD	O2-C2-N1	-2.89	117.00	121.80
5	B	900	FAD	C10-C4X-N5	-2.88	118.92	124.81
5	B	900	FAD	C4A-C5A-N7A	-2.87	107.30	110.58
5	A	900	FAD	C10-C4X-N5	-2.85	118.99	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	900	FAD	C4-N3-C2	-2.76	120.75	125.64
5	C	900	FAD	C10-C4X-N5	-2.71	119.28	124.81
5	A	900	FAD	C2A-N3A-C4A	2.62	118.22	111.83
5	A	900	FAD	C4A-N9A-C8A	2.61	108.48	105.74
5	C	900	FAD	O2-C2-N1	-2.59	117.50	121.80
5	A	900	FAD	O2-C2-N1	-2.58	117.52	121.80
5	B	900	FAD	C2A-N3A-C4A	2.57	118.12	111.83
5	B	900	FAD	C4-N3-C2	-2.54	121.13	125.64
5	A	900	FAD	C4-N3-C2	-2.51	121.18	125.64
5	C	900	FAD	C2A-N3A-C4A	2.49	117.92	111.83
5	C	900	FAD	C4A-N9A-C8A	2.40	108.26	105.74
5	A	900	FAD	C4-C4X-N5	2.38	121.49	118.21
5	B	900	FAD	O2P-P-O3P	2.34	113.60	107.27
5	C	900	FAD	C4X-C4-N3	2.33	119.18	113.25
5	B	900	FAD	C4-C4X-N5	2.32	121.42	118.21
5	A	900	FAD	N3A-C4A-N9A	2.32	131.11	127.17
5	C	900	FAD	C9A-C5X-N5	-2.30	120.01	122.45
5	C	900	FAD	N3A-C4A-N9A	2.28	131.05	127.17
5	B	900	FAD	C9A-C5X-N5	-2.24	120.08	122.45
5	B	900	FAD	N3A-C4A-N9A	2.22	130.95	127.17
5	B	900	FAD	O2A-PA-O3P	2.22	113.27	107.27
5	A	900	FAD	C4X-C4-N3	2.19	118.83	113.25
5	A	900	FAD	C9A-C5X-N5	-2.17	120.15	122.45
5	B	900	FAD	C4X-C4-N3	2.14	118.70	113.25
5	A	900	FAD	O2P-P-O3P	2.11	112.97	107.27
5	C	900	FAD	C4-C4X-N5	2.03	121.02	118.21
3	A	920	MES	C2-C3-N4	-2.01	107.06	110.12
5	A	900	FAD	C4X-C10-N1	-2.01	119.66	124.59

There are no chirality outliers.

All (9) torsion outliers are listed below:

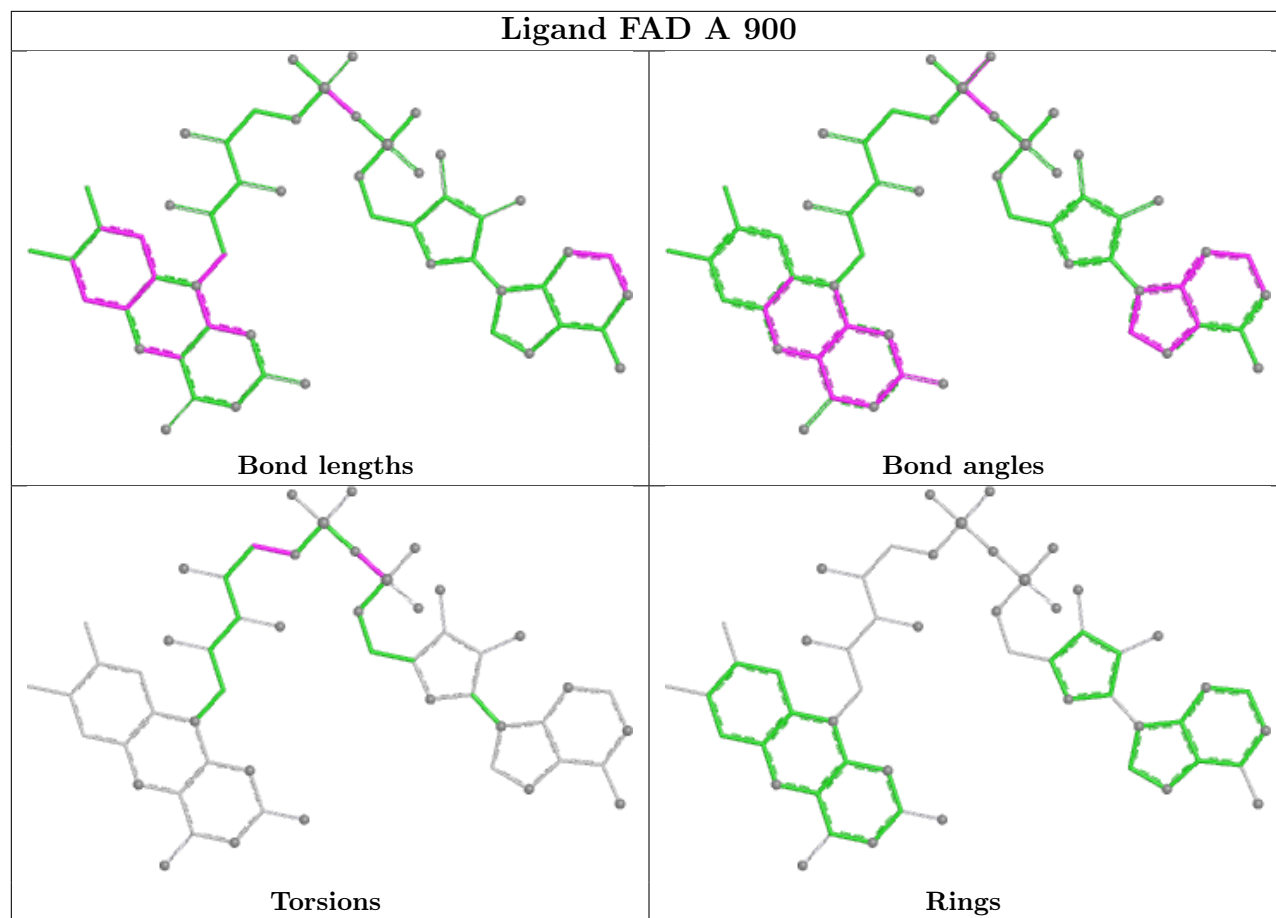
Mol	Chain	Res	Type	Atoms
3	C	920	MES	C8-C7-N4-C5
5	A	900	FAD	P-O3P-PA-O2A
3	C	920	MES	C8-C7-N4-C3
5	B	900	FAD	P-O3P-PA-O2A
5	C	900	FAD	P-O3P-PA-O2A
5	B	900	FAD	P-O3P-PA-O1A
5	B	900	FAD	C4B-C5B-O5B-PA
5	C	900	FAD	C4B-C5B-O5B-PA
5	A	900	FAD	C4'-C5'-O5'-P

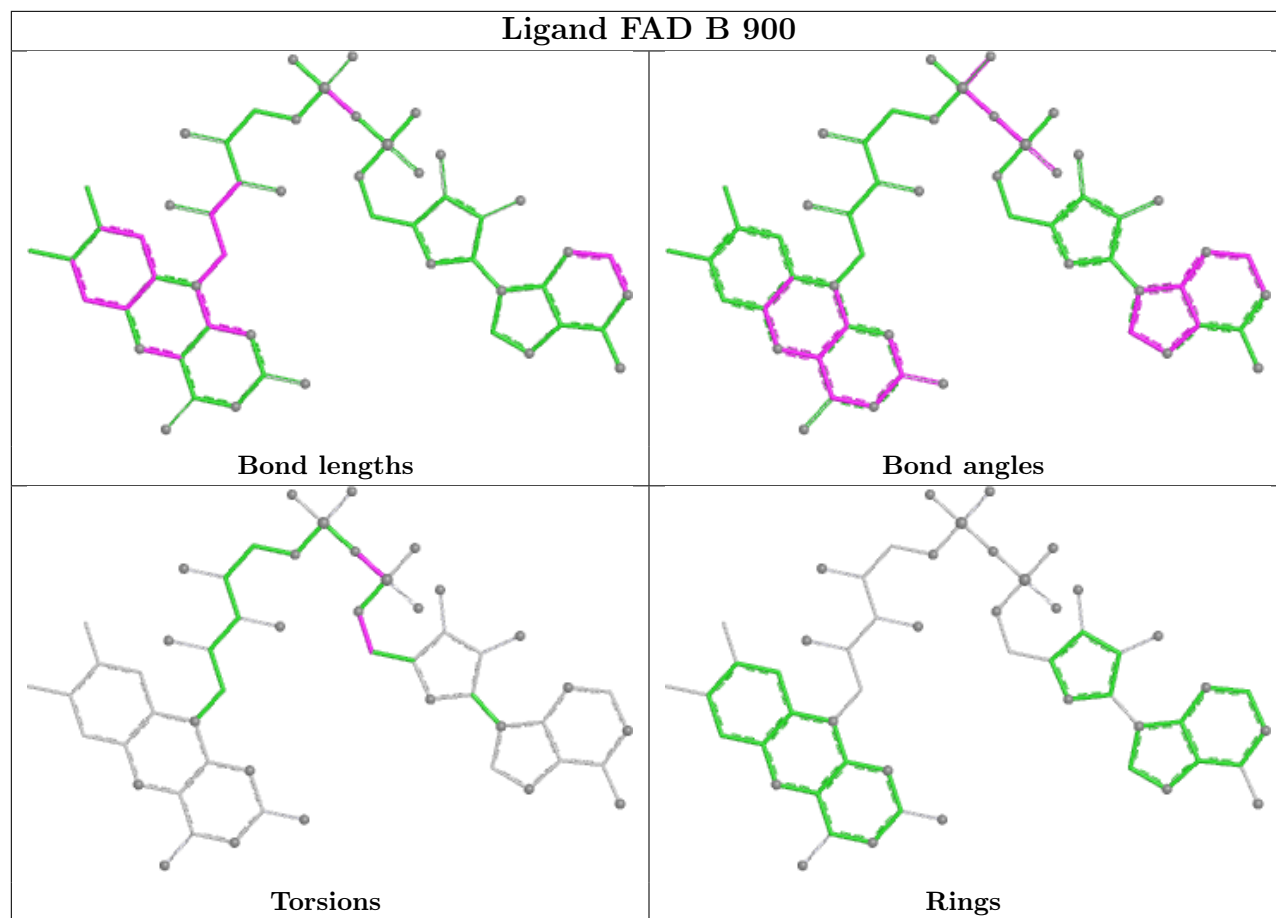
There are no ring outliers.

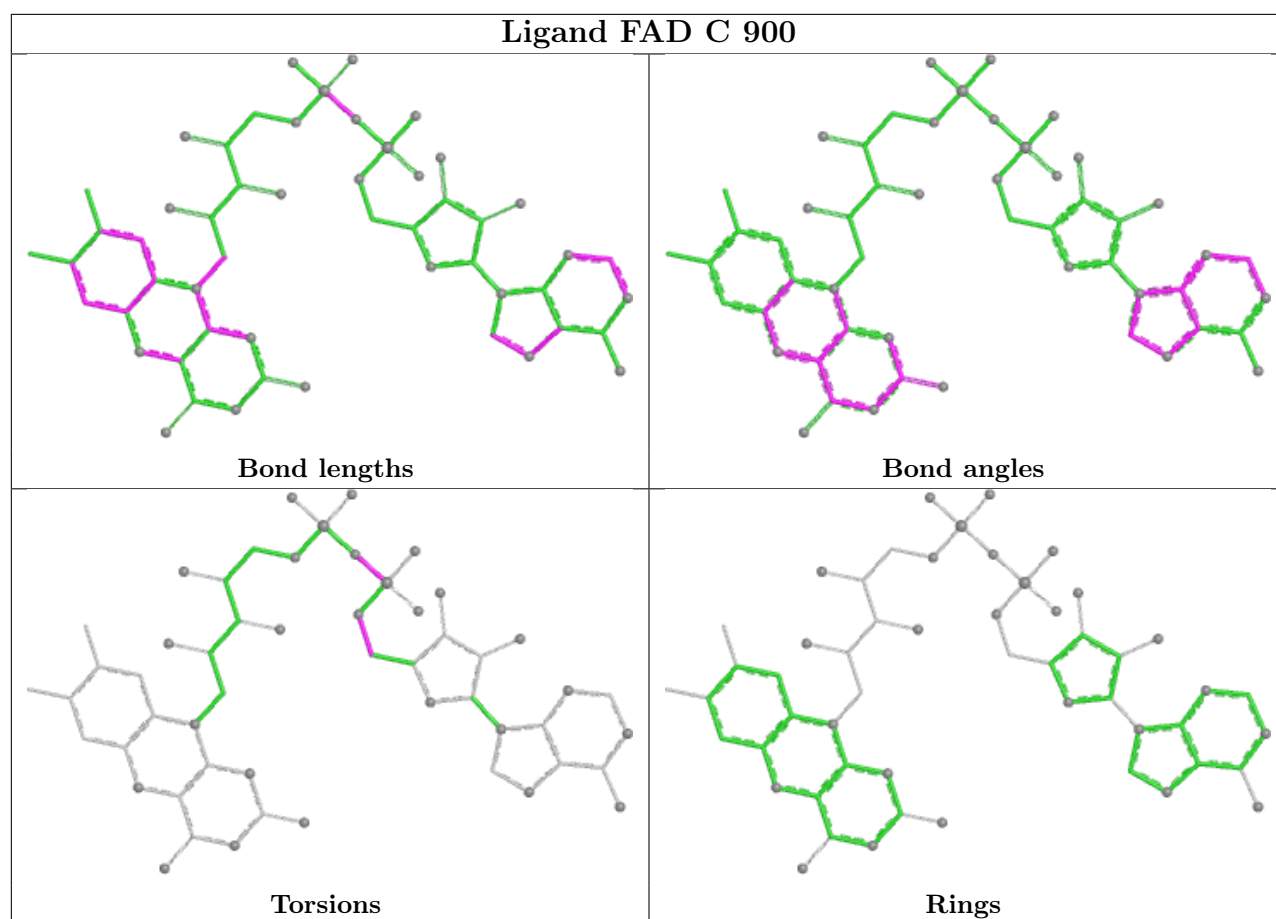
7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	900	FAD	1	0
2	B	906	IMD	1	0
3	C	920	MES	3	0
3	A	920	MES	3	0
2	C	902	IMD	2	0
3	B	920	MES	3	0
2	C	901	IMD	2	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	522/537 (97%)	-0.21	7 (1%) 75 73	18, 36, 65, 100	0
1	B	521/537 (97%)	-0.19	8 (1%) 72 70	20, 39, 67, 100	0
1	C	520/537 (96%)	-0.26	7 (1%) 75 73	16, 36, 76, 101	0
All	All	1563/1611 (97%)	-0.22	22 (1%) 73 72	16, 37, 67, 101	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	524	HIS	5.2
1	A	196	ILE	3.7
1	B	526	GLU	3.5
1	C	520	GLN	3.1
1	B	196	ILE	3.0
1	B	4	GLY	2.9
1	A	508	ASP	2.8
1	C	523	GLU	2.8
1	A	188	ILE	2.6
1	C	196	ILE	2.5
1	A	197	SER	2.3
1	C	32	PHE	2.3
1	C	195	GLY	2.3
1	B	147	ALA	2.3
1	B	524	HIS	2.3
1	A	520	GLN	2.3
1	A	519	LEU	2.2
1	B	523	GLU	2.2
1	B	50	ALA	2.1
1	B	505	GLY	2.1
1	A	191	ILE	2.1
1	C	512	LEU	2.1

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](#)

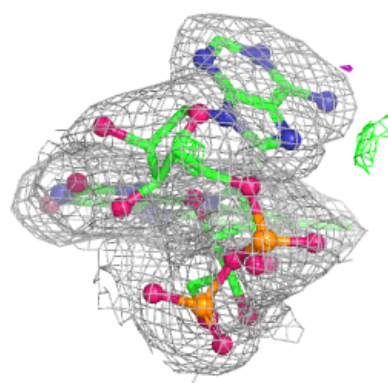
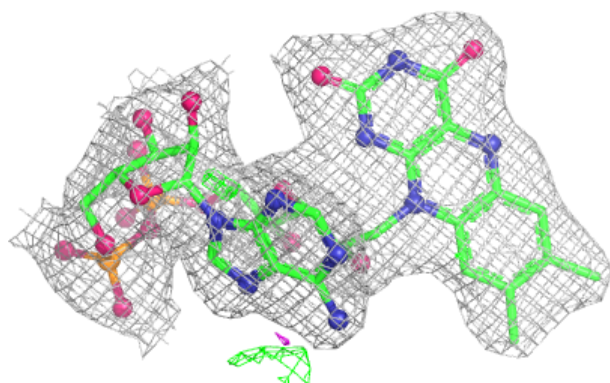
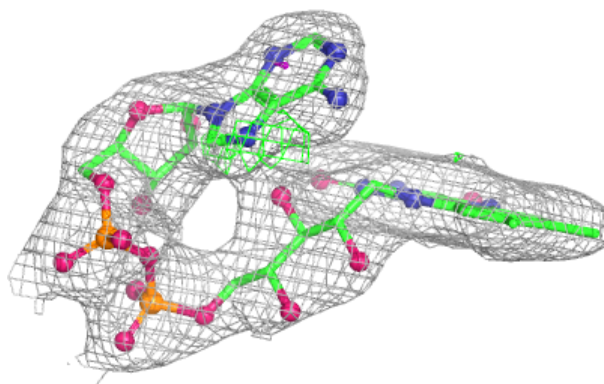
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IMD	B	904	5/5	0.71	0.24	73,74,74,74	0
2	IMD	A	905	5/5	0.74	0.32	83,84,84,84	0
2	IMD	B	903	5/5	0.77	0.28	88,88,89,89	0
4	PO4	C	930	5/5	0.77	0.24	98,98,99,100	0
2	IMD	B	905	5/5	0.78	0.26	65,66,66,67	0
4	PO4	B	930	5/5	0.79	0.20	94,96,96,96	0
2	IMD	A	902	5/5	0.80	0.20	54,56,56,56	0
2	IMD	B	906	5/5	0.80	0.28	90,90,90,90	0
3	MES	B	920	12/12	0.82	0.32	85,90,101,102	0
3	MES	A	920	12/12	0.83	0.30	85,88,97,97	0
3	MES	C	920	12/12	0.84	0.33	97,100,111,111	0
2	IMD	C	902	5/5	0.87	0.17	48,48,49,49	0
4	PO4	A	930	5/5	0.87	0.17	92,93,93,94	0
2	IMD	A	901	5/5	0.88	0.20	72,72,72,72	0
2	IMD	B	901	5/5	0.90	0.20	68,69,69,70	0
2	IMD	C	901	5/5	0.93	0.13	52,53,54,54	0
5	FAD	B	900	53/53	0.97	0.06	20,25,31,32	0
5	FAD	C	900	53/53	0.97	0.06	16,18,22,26	0
5	FAD	A	900	53/53	0.98	0.05	18,23,26,29	0

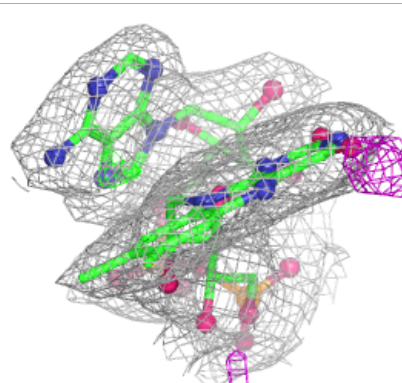
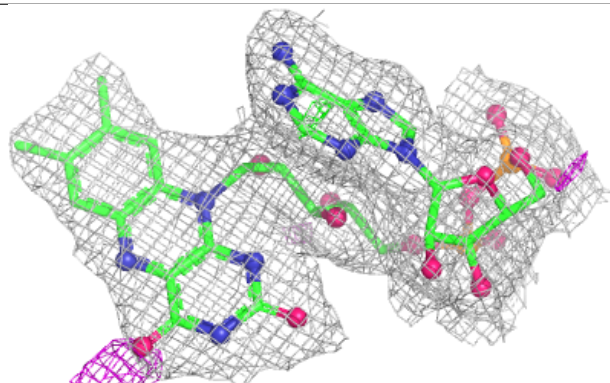
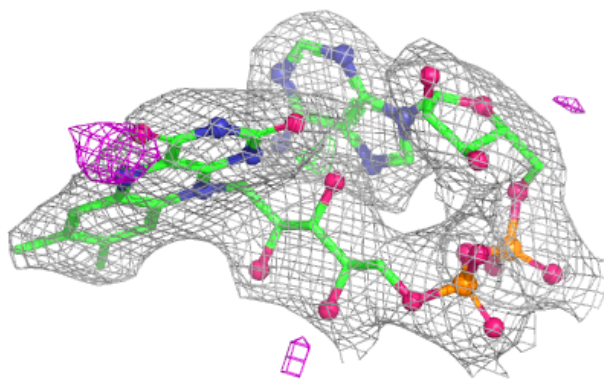
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

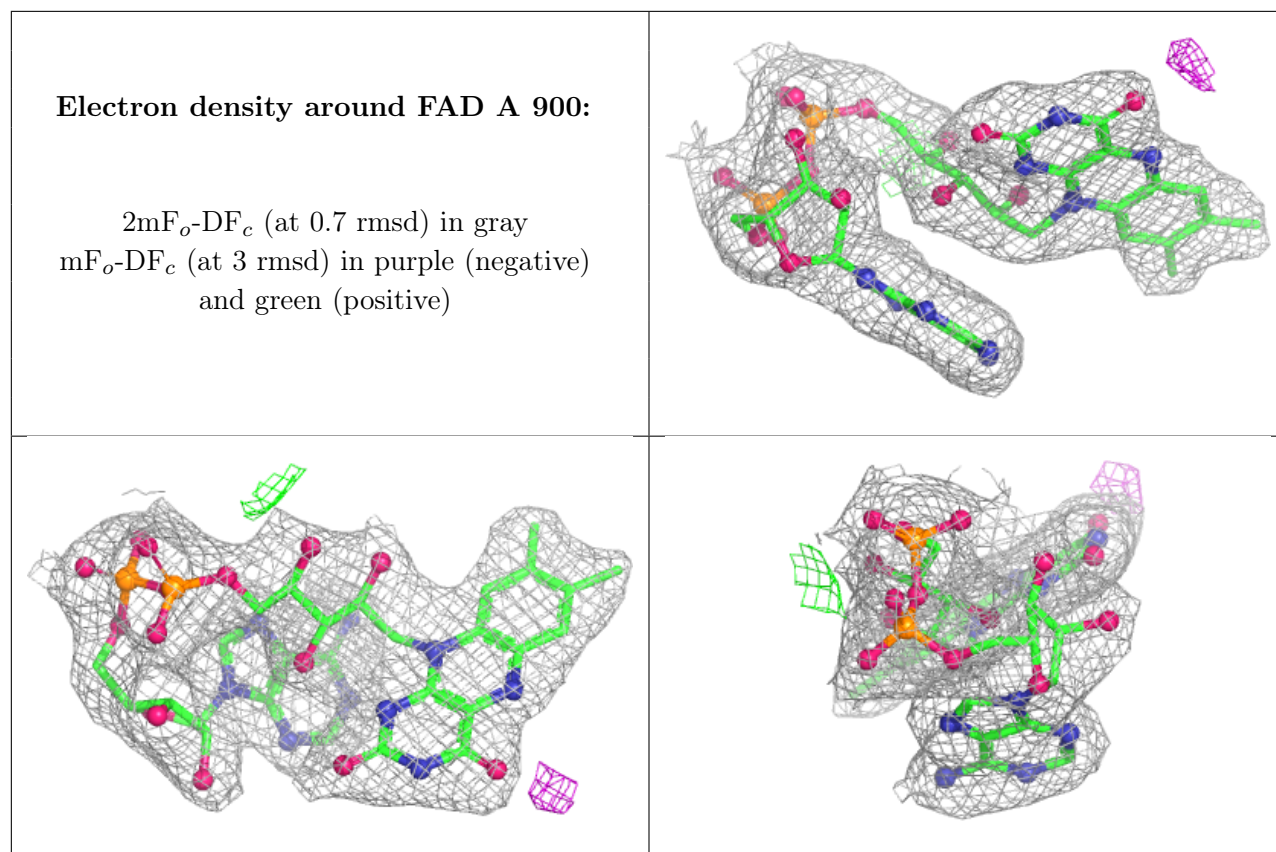
Electron density around FAD B 900:

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

**Electron density around FAD C 900:**

$2mF_o-DF_c$ (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.