



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:05 AM UTC

PDB ID : 2R4J / pdb_00002r4j
Title : Crystal structure of Escherichia coli SeMet substituted Glycerol-3-phosphate Dehydrogenase in complex with DHAP
Authors : Yeh, J.I.; Du, S.; Chinte, U.
Deposited on : 2007-08-31
Resolution : 1.96 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

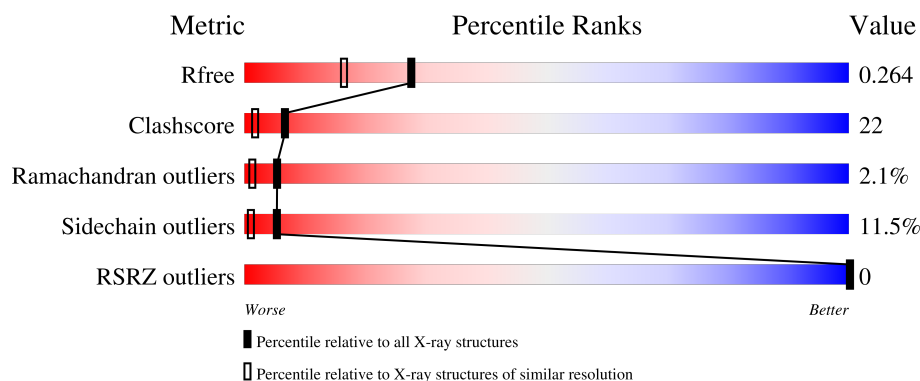
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	501	
1	B	501	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	1957	-	-	X	-
5	EDO	A	1958	-	-	X	-
5	EDO	A	1959	-	-	X	-
5	EDO	B	807	-	-	X	-
5	EDO	B	813	-	-	X	-
6	IMD	A	1960	-	-	X	-
6	IMD	A	1961	-	-	X	-
6	IMD	A	1963	-	-	X	-
6	IMD	A	1966	-	-	X	-
7	13P	A	1968	-	X	-	-
7	13P	B	816	-	X	X	-
9	TAM	B	812	-	-	X	-

2 Entry composition [i](#)

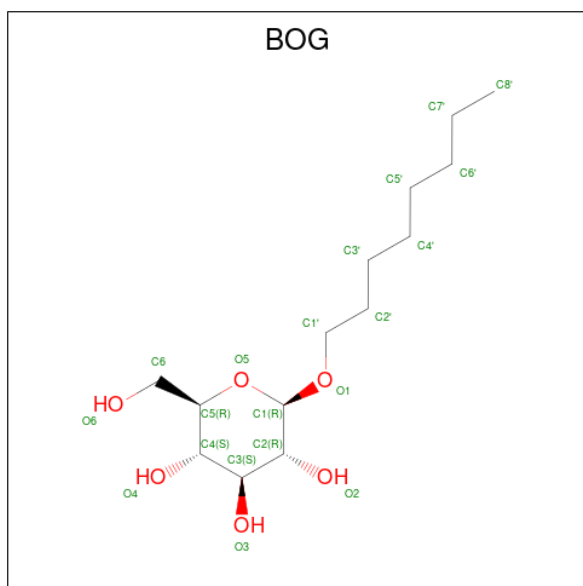
There are 10 unique types of molecules in this entry. The entry contains 8645 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aerobic glycerol-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	Se	0	0	0
			3953	2510	703	727	6	7			
1	B	497	Total	C	N	O	S	Se	0	0	0
			3981	2527	710	731	6	7			

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



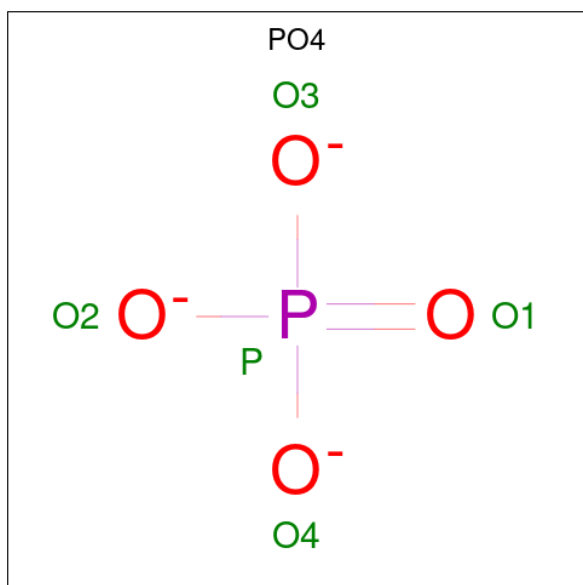
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		

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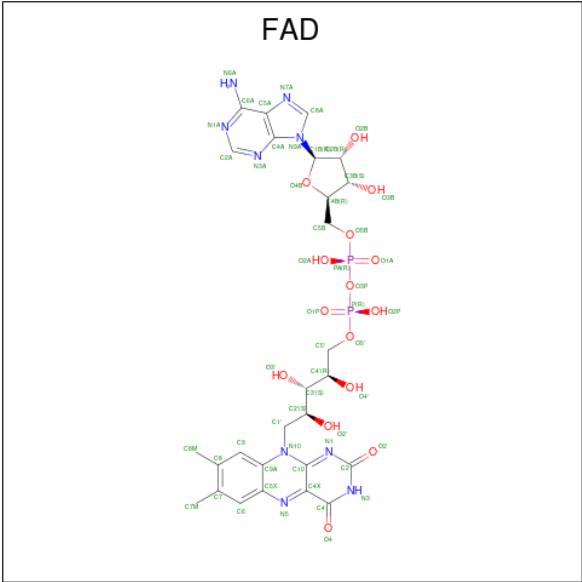
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



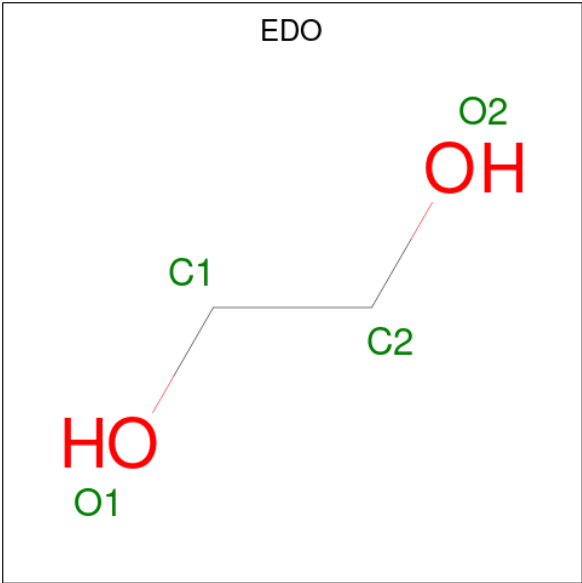
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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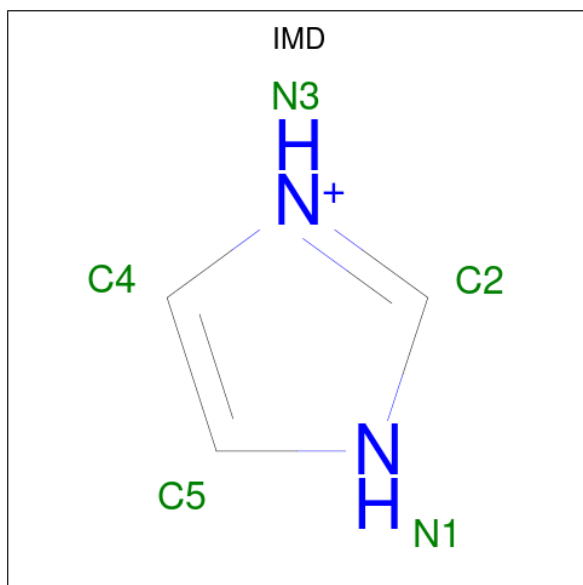
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0

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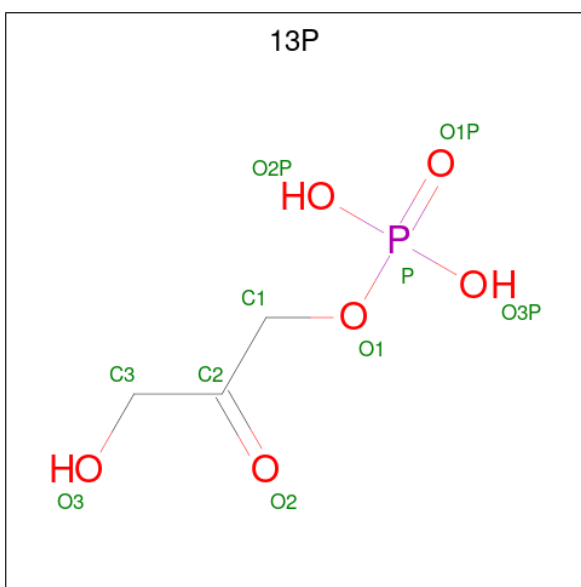
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



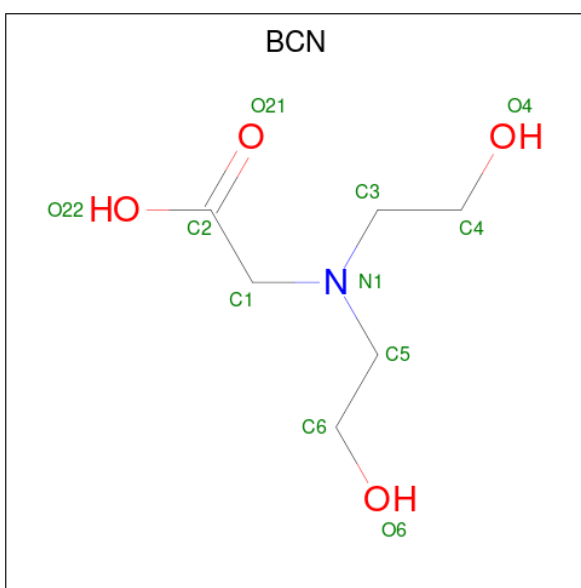
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			5	3	2		
6	A	1	Total	C	N	0	0
			5	3	2		
6	A	1	Total	C	N	0	0
			5	3	2		
6	A	1	Total	C	N	0	0
			5	3	2		
6	A	1	Total	C	N	0	0
			5	3	2		
6	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 7 is 1,3-DIHYDROXYACETONEPHOSPHATE (CCD ID: 13P) (formula: $C_3H_7O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			10	3	6	1		
7	B	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 8 is BICINE (CCD ID: BCN) (formula: $C_6H_{13}NO_4$).



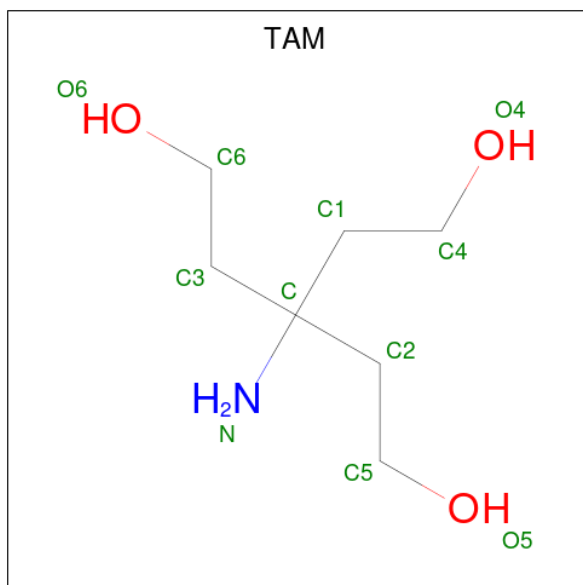
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			11	6	1	4		
8	B	1	Total	C	N	O	0	0
			11	6	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 9 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			11	7	1	3		

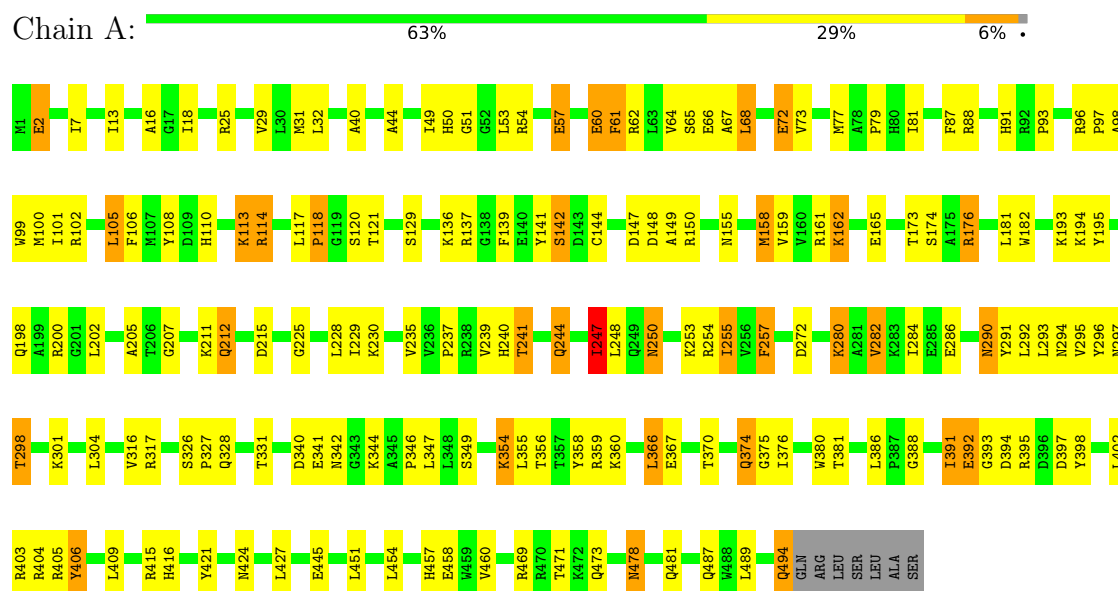
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	140	Total	O	0	0
			140	140		
10	B	137	Total	O	0	0
			137	137		

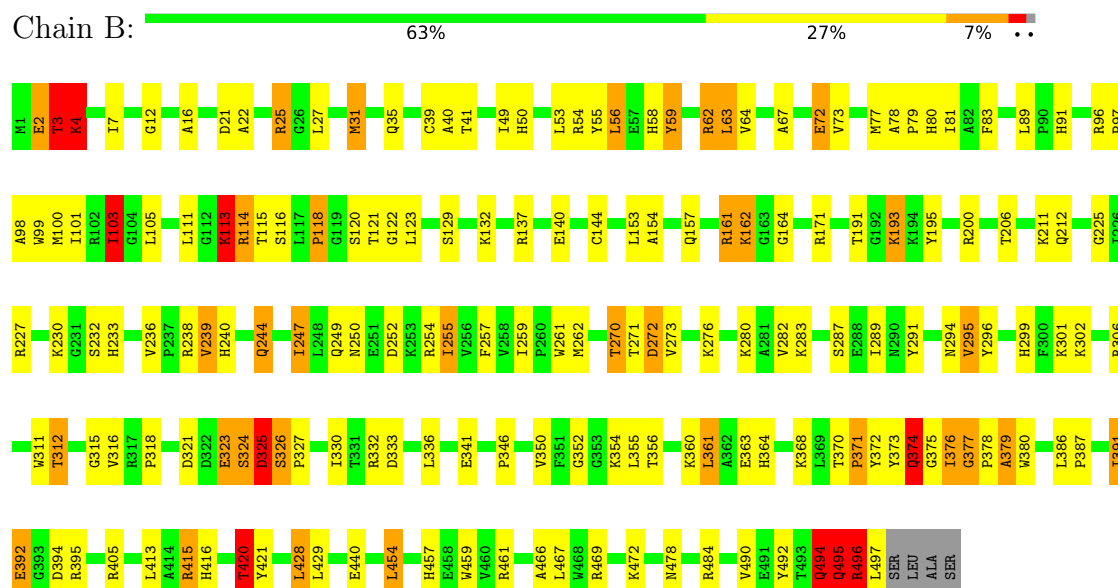
3 Residue-property plots

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: Aerobic glycerol-3-phosphate dehydrogenase



• Molecule 1: Aerobic glycerol-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	113.92Å 114.14Å 193.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.96 10.00 – 1.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-1.96) 91.1 (10.00-1.96)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	133.85 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.211 , 0.263 0.220 , 0.264	Depositor DCC
R_{free} test set	4126 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.450 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8645	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 13P, EDO, BOG, TAM, PO4, FAD, BCN, IMD

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	1.37	12/4041 (0.3%)	1.30	24/5461 (0.4%)
1	B	1.37	11/4069 (0.3%)	1.32	23/5498 (0.4%)
All	All	1.37	23/8110 (0.3%)	1.31	47/10959 (0.4%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	ILE	CA-CB	-8.40	1.44	1.54
1	A	295	VAL	C-O	8.40	1.33	1.24
1	B	12	GLY	N-CA	-7.38	1.38	1.44
1	A	471	THR	N-CA	7.23	1.55	1.46
1	B	7	ILE	CA-CB	-6.71	1.46	1.54
1	B	289	ILE	CA-C	-6.14	1.45	1.52
1	B	154	ALA	CA-CB	-6.07	1.44	1.53
1	B	289	ILE	C-O	-6.05	1.17	1.24
1	B	295	VAL	C-O	6.03	1.31	1.24
1	B	466	ALA	CA-CB	5.94	1.63	1.53
1	A	451	LEU	C-O	-5.91	1.17	1.24
1	B	495	GLN	CA-C	-5.86	1.45	1.52
1	A	87	PHE	CA-C	-5.63	1.45	1.52
1	B	374	GLN	N-CA	5.55	1.53	1.46
1	A	158	MSE	SE-CE	-5.43	1.79	1.95
1	A	205	ALA	CA-CB	5.22	1.60	1.53
1	A	207	GLY	N-CA	5.21	1.51	1.44
1	A	235	VAL	C-O	5.12	1.29	1.24
1	A	18	ILE	CA-CB	5.11	1.60	1.54
1	A	158	MSE	CG-SE	5.05	2.10	1.95
1	B	206	THR	CA-CB	-5.02	1.45	1.53
1	B	454	LEU	N-CA	5.02	1.52	1.46
1	A	257	PHE	N-CA	5.01	1.51	1.45

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	TYR	N-CA-C	-11.39	100.10	114.56
1	A	388	GLY	N-CA-C	-7.95	104.59	114.92
1	B	236	VAL	CA-C-N	-7.91	111.46	119.92
1	B	236	VAL	C-N-CA	-7.91	111.46	119.92
1	A	247	ILE	CB-CA-C	-7.50	100.11	110.77
1	B	326	SER	CA-C-N	7.37	126.90	119.24
1	B	326	SER	C-N-CA	7.37	126.90	119.24
1	B	494	GLN	N-CA-C	-7.32	105.21	112.97
1	B	25	ARG	N-CA-C	-7.22	102.49	113.89
1	A	81	ILE	N-CA-C	7.04	119.80	112.83
1	A	406	TYR	CA-C-N	-6.95	112.74	120.45
1	A	406	TYR	C-N-CA	-6.95	112.74	120.45
1	B	3	THR	CA-C-N	6.94	134.19	121.70
1	B	3	THR	C-N-CA	6.94	134.19	121.70
1	B	113	LYS	N-CA-C	6.94	125.58	110.80
1	A	355	LEU	N-CA-C	-6.79	103.96	111.36
1	B	103	ILE	CB-CA-C	-6.72	103.23	112.24
1	A	173	THR	N-CA-C	-6.69	105.74	114.04
1	A	120	SER	N-CA-C	6.68	119.92	110.50
1	B	132	LYS	CA-C-N	6.53	126.30	119.05
1	B	132	LYS	C-N-CA	6.53	126.30	119.05
1	A	174	SER	N-CA-C	6.37	118.45	108.96
1	B	206	THR	N-CA-C	6.26	120.54	113.02
1	B	374	GLN	N-CA-C	6.12	123.84	110.80
1	A	72	GLU	N-CA-C	6.06	118.84	111.82
1	A	13	ILE	N-CA-C	5.95	116.69	110.62
1	B	164	GLY	N-CA-C	-5.93	103.06	112.66
1	A	225	GLY	N-CA-C	-5.86	103.42	112.85
1	B	191	THR	N-CA-C	5.54	119.89	113.18
1	A	79	PRO	CA-C-N	-5.50	113.28	120.44
1	A	79	PRO	C-N-CA	-5.50	113.28	120.44
1	A	142	SER	N-CA-C	5.49	118.67	109.95
1	B	225	GLY	N-CA-C	-5.46	104.33	113.02
1	A	61	PHE	N-CA-C	5.45	117.22	111.28
1	A	290	ASN	N-CA-C	-5.37	105.59	111.82
1	B	420	THR	CB-CA-C	5.34	118.47	110.08
1	A	317	ARG	CA-C-N	-5.33	113.18	119.84
1	A	317	ARG	C-N-CA	-5.33	113.18	119.84
1	A	25	ARG	N-CA-C	-5.31	105.86	114.09
1	B	211	LYS	CA-C-N	-5.24	112.74	120.28
1	B	211	LYS	C-N-CA	-5.24	112.74	120.28
1	A	284	ILE	CA-C-N	-5.19	113.75	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	ILE	C-N-CA	-5.19	113.75	123.03
1	B	83	PHE	N-CA-C	5.16	114.23	108.25
1	B	122	GLY	N-CA-C	-5.10	104.83	112.89
1	A	29	VAL	N-CA-C	5.04	116.22	108.71
1	B	255	ILE	N-CA-CB	-5.02	101.92	111.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3953	0	3903	151	0
1	B	3981	0	3935	182	0
2	A	80	0	112	7	0
2	B	40	0	56	10	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	53	0	31	1	0
4	B	53	0	31	1	0
5	A	44	0	66	28	0
5	B	60	0	90	24	0
6	A	25	0	25	21	0
6	B	5	0	5	1	0
7	A	10	0	5	0	0
7	B	10	0	5	4	0
8	A	11	0	12	1	0
8	B	22	0	24	5	0
9	B	11	0	17	7	0
10	A	140	0	0	9	0
10	B	137	0	0	13	0
All	All	8645	0	8317	359	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 22.

All (359) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LEU:HD21	1:B:376:ILE:CD1	1.54	1.37
1:B:374:GLN:CB	1:B:375:GLY:HA3	1.59	1.27
1:B:467:LEU:HA	10:B:938:HOH:O	1.37	1.22
5:B:813:EDO:H22	10:B:869:HOH:O	1.37	1.20
1:B:428:LEU:HD12	1:B:428:LEU:O	1.36	1.20
5:A:1959:EDO:H21	6:A:1963:IMD:H5	1.22	1.17
1:A:237:PRO:HG3	6:A:1966:IMD:N3	1.60	1.16
1:B:361:LEU:HD12	1:B:361:LEU:O	1.44	1.14
1:A:51:GLY:HA3	1:A:68:LEU:HD13	1.29	1.12
1:A:374:GLN:CB	1:A:375:GLY:HA3	1.78	1.12
1:A:237:PRO:HG3	6:A:1966:IMD:HN3	1.02	1.11
1:A:341:GLU:CG	1:A:342:ASN:H	1.63	1.11
1:B:374:GLN:HB2	1:B:375:GLY:CA	1.79	1.10
1:A:374:GLN:HB2	1:A:375:GLY:HA3	1.28	1.10
5:A:1957:EDO:H11	6:A:1960:IMD:H5	1.29	1.10
1:B:361:LEU:HD12	1:B:361:LEU:C	1.77	1.09
1:A:237:PRO:CG	6:A:1966:IMD:HN3	1.66	1.07
5:B:807:EDO:H11	5:B:808:EDO:O1	1.55	1.06
1:B:50:HIS:CE1	1:B:354:LYS:NZ	2.24	1.06
1:A:341:GLU:HG3	1:A:342:ASN:N	1.65	1.05
1:B:27:LEU:HD21	1:B:376:ILE:HD12	1.13	1.05
5:A:1959:EDO:H21	6:A:1963:IMD:C5	1.86	1.04
1:B:428:LEU:HD12	1:B:428:LEU:C	1.82	1.03
1:A:158:MSE:CE	1:A:161:ARG:HD2	1.87	1.03
1:B:113:LYS:HB3	1:B:114:ARG:HA	1.41	1.02
1:B:50:HIS:HE1	1:B:354:LYS:NZ	1.58	1.01
1:A:158:MSE:HE1	1:A:161:ARG:HD2	1.02	0.99
1:A:294:ASN:O	1:A:298:THR:HG23	1.62	0.97
1:A:457:HIS:C	6:A:1963:IMD:H4	1.89	0.97
5:A:1959:EDO:C2	6:A:1963:IMD:H5	1.95	0.97
1:A:176:ARG:HG2	1:A:176:ARG:HH11	1.29	0.96
1:A:341:GLU:HG3	1:A:342:ASN:H	0.81	0.95
1:B:62:ARG:HD3	1:B:333:ASP:OD2	1.66	0.95
1:A:158:MSE:HE1	1:A:161:ARG:CD	1.96	0.95
5:A:1957:EDO:C1	6:A:1960:IMD:H5	1.97	0.93
1:B:73:VAL:HG12	1:B:77:MSE:CE	1.96	0.93
1:A:297:ASN:HD21	1:A:304:LEU:H	1.05	0.93
1:B:467:LEU:HD23	10:B:938:HOH:O	1.68	0.92
1:B:50:HIS:CE1	1:B:354:LYS:CE	2.53	0.91
1:B:27:LEU:CD2	1:B:376:ILE:HD12	2.00	0.91
1:A:141:TYR:OH	1:A:247:ILE:CD1	2.21	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ILE:HG23	1:B:376:ILE:O	1.70	0.88
1:B:374:GLN:HB2	1:B:375:GLY:HA3	0.88	0.88
1:B:315:GLY:HA2	5:B:813:EDO:H11	1.56	0.88
1:B:73:VAL:HG12	1:B:77:MSE:HE1	1.55	0.87
1:B:27:LEU:CD2	1:B:376:ILE:CD1	2.49	0.85
1:A:51:GLY:HA3	1:A:68:LEU:CD1	2.06	0.84
1:A:176:ARG:HH11	1:A:176:ARG:CG	1.91	0.83
1:B:50:HIS:HE1	1:B:354:LYS:HZ1	1.25	0.83
1:B:315:GLY:CA	5:B:813:EDO:H11	2.09	0.83
1:B:212:GLN:HG2	5:B:810:EDO:H22	1.59	0.82
1:A:158:MSE:HE3	1:A:158:MSE:HA	1.61	0.82
1:A:445:GLU:HB2	6:A:1960:IMD:H2	1.61	0.82
1:B:323:GLU:O	1:B:324:SER:HB3	1.80	0.82
1:B:27:LEU:HD11	1:B:376:ILE:HD11	1.60	0.82
1:B:361:LEU:C	1:B:361:LEU:CD1	2.52	0.82
1:B:374:GLN:CB	1:B:375:GLY:CA	2.43	0.82
1:A:478:ASN:ND2	1:A:481:GLN:H	1.78	0.80
1:A:487:GLN:HG2	10:A:2079:HOH:O	1.80	0.80
1:A:374:GLN:CB	1:A:375:GLY:CA	2.59	0.80
1:B:161:ARG:HB2	9:B:812:TAM:O5	1.81	0.79
1:A:141:TYR:OH	1:A:247:ILE:HD11	1.82	0.79
1:B:50:HIS:HE1	1:B:354:LYS:CE	1.93	0.79
1:B:59:TYR:CE2	2:B:800:BOG:H5'2	2.17	0.79
1:A:392:GLU:CA	1:A:392:GLU:OE1	2.30	0.78
1:B:416:HIS:O	1:B:420:THR:HG23	1.83	0.78
1:A:280:LYS:HE2	1:A:280:LYS:HA	1.65	0.78
1:B:56:LEU:HD13	1:B:64:VAL:HG21	1.66	0.78
1:B:262:MSE:HE2	5:B:807:EDO:H12	1.67	0.77
1:B:50:HIS:CE1	1:B:354:LYS:HZ3	2.03	0.76
1:A:392:GLU:OE1	1:A:392:GLU:HA	1.84	0.75
1:B:113:LYS:CB	1:B:114:ARG:HA	2.12	0.75
1:B:364:HIS:HB2	10:B:885:HOH:O	1.86	0.75
1:A:254:ARG:HD2	1:A:328:GLN:HB3	1.68	0.74
1:B:316:VAL:H	5:B:813:EDO:C1	2.00	0.74
1:B:157:GLN:HG2	9:B:812:TAM:N	2.01	0.74
1:B:27:LEU:HD21	1:B:376:ILE:HD11	1.67	0.74
1:B:361:LEU:O	1:B:361:LEU:CD1	2.30	0.74
1:A:96:ARG:NE	2:A:800:BOG:H5	2.02	0.73
1:B:114:ARG:O	1:B:114:ARG:HG2	1.88	0.73
1:A:97:PRO:HD2	1:A:100:MET:HE3	1.70	0.73
1:A:374:GLN:HB3	1:A:375:GLY:HA3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:SER:O	1:B:325:ASP:HB2	1.87	0.72
1:B:336:LEU:HD12	1:B:364:HIS:HD2	1.52	0.72
1:B:99:TRP:O	1:B:103:ILE:HG12	1.90	0.71
1:B:376:ILE:O	1:B:376:ILE:CG2	2.38	0.71
1:A:202:LEU:HD23	1:A:347:LEU:HD13	1.71	0.71
1:A:424:ASN:ND2	6:A:1961:IMD:H4	2.06	0.70
1:B:129:SER:O	1:B:301:LYS:HE2	1.91	0.69
1:A:176:ARG:HG2	1:A:176:ARG:NH1	2.06	0.69
1:B:299:HIS:HE1	10:B:882:HOH:O	1.75	0.68
1:B:50:HIS:CE1	1:B:354:LYS:HE2	2.28	0.68
1:B:113:LYS:HB3	1:B:114:ARG:CA	2.20	0.68
1:A:53:LEU:HG	2:A:800:BOG:H2	1.76	0.68
1:B:114:ARG:NH1	1:B:118:PRO:O	2.26	0.68
1:B:72:GLU:OE2	1:B:114:ARG:HB2	1.93	0.68
1:A:370:THR:HG23	1:A:376:ILE:HG21	1.76	0.68
1:B:428:LEU:C	1:B:428:LEU:CD1	2.58	0.68
1:B:378:PRO:O	1:B:379:ALA:O	2.12	0.67
1:A:406:TYR:HE1	10:A:2045:HOH:O	1.76	0.67
5:B:806:EDO:H21	10:B:958:HOH:O	1.95	0.67
1:B:250:ASN:ND2	1:B:291:TYR:CZ	2.63	0.67
1:B:405:ARG:HG3	10:B:894:HOH:O	1.93	0.67
1:B:461:ARG:NH1	10:B:942:HOH:O	2.29	0.66
5:A:1958:EDO:C2	10:A:2097:HOH:O	2.44	0.66
1:B:496:ARG:O	1:B:497:LEU:HG	1.96	0.66
1:B:336:LEU:HD12	1:B:364:HIS:CD2	2.30	0.66
1:A:254:ARG:NE	1:A:272:ASP:OD2	2.27	0.65
1:A:392:GLU:OE1	1:A:392:GLU:N	2.30	0.65
1:B:492:TYR:HB2	6:B:819:IMD:H4	1.79	0.65
1:A:51:GLY:CA	1:A:68:LEU:HD13	2.17	0.65
1:B:2:GLU:O	1:B:4:LYS:HB2	1.97	0.65
1:A:290:ASN:HA	5:A:1956:EDO:H12	1.79	0.64
1:A:181:LEU:HD23	10:A:2063:HOH:O	1.98	0.64
1:B:50:HIS:CE1	1:B:354:LYS:HZ1	2.04	0.64
1:A:478:ASN:HD22	1:A:478:ASN:C	2.06	0.63
1:A:50:HIS:NE2	1:A:354:LYS:NZ	2.44	0.62
1:B:273:VAL:HG13	8:B:820:BCN:H32	1.80	0.62
1:B:324:SER:OG	1:B:325:ASP:N	2.23	0.62
1:A:97:PRO:CD	1:A:100:MET:HE3	2.30	0.62
1:A:403:ARG:NH1	1:A:409:LEU:O	2.28	0.62
1:B:428:LEU:O	1:B:428:LEU:CD1	2.30	0.62
1:A:117:LEU:O	1:A:118:PRO:O	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PRO:HB3	2:A:1950:BOG:H2	1.82	0.61
1:B:378:PRO:O	1:B:379:ALA:C	2.43	0.61
1:A:54:ARG:HA	2:A:800:BOG:O6	2.01	0.61
1:B:373:TYR:HB2	1:B:376:ILE:HD13	1.82	0.61
1:B:287:SER:CB	8:B:821:BCN:H62	2.30	0.61
1:B:73:VAL:CG1	1:B:77:MSE:HE1	2.30	0.61
1:B:239:VAL:HG12	1:B:240:HIS:CD2	2.36	0.60
1:B:421:TYR:OH	1:B:454:LEU:HD21	2.00	0.60
1:B:440:GLU:OE2	1:B:484:ARG:NH1	2.34	0.60
1:B:16:ALA:HA	1:B:31:MSE:HE2	1.82	0.60
1:B:59:TYR:CE2	2:B:800:BOG:C5'	2.84	0.60
1:B:323:GLU:O	1:B:324:SER:CB	2.48	0.59
1:B:316:VAL:H	5:B:813:EDO:H11	1.66	0.59
1:A:297:ASN:ND2	1:A:304:LEU:H	1.89	0.59
1:B:370:THR:HG23	1:B:376:ILE:HG21	1.84	0.59
1:A:391:ILE:O	1:A:393:GLY:N	2.30	0.59
1:B:262:MSE:HE2	5:B:807:EDO:C1	2.33	0.59
1:A:239:VAL:HG23	1:A:240:HIS:CD2	2.38	0.59
1:A:394:ASP:HB3	1:A:397:ASP:HB2	1.84	0.58
1:A:148:ASP:OD1	1:A:149:ALA:N	2.35	0.58
1:A:250:ASN:OD1	1:A:291:TYR:CZ	2.56	0.58
1:A:290:ASN:CA	5:A:1956:EDO:H12	2.34	0.58
1:A:137:ARG:HH22	2:A:700:BOG:H5	1.68	0.57
1:A:406:TYR:CE1	10:A:2045:HOH:O	2.52	0.57
1:A:141:TYR:CZ	1:A:247:ILE:HD11	2.40	0.57
1:B:161:ARG:HB2	9:B:812:TAM:HO5	1.68	0.57
1:B:316:VAL:N	5:B:813:EDO:H11	2.20	0.57
1:A:341:GLU:CG	1:A:342:ASN:N	2.36	0.57
1:B:254:ARG:HH21	7:B:816:13P:H12	1.70	0.56
5:A:1958:EDO:H21	10:A:2097:HOH:O	2.04	0.56
1:B:73:VAL:CG1	1:B:77:MSE:CE	2.77	0.56
1:B:62:ARG:HG3	1:B:63:LEU:N	2.20	0.56
1:B:405:ARG:NH2	10:B:947:HOH:O	2.37	0.56
1:A:211:LYS:NZ	1:A:215:ASP:OD2	2.37	0.56
1:A:391:ILE:C	1:A:393:GLY:H	2.13	0.56
1:A:370:THR:HG23	1:A:376:ILE:CG2	2.36	0.55
1:A:454:LEU:HB3	1:A:460:VAL:HG21	1.87	0.55
5:B:804:EDO:H21	10:B:924:HOH:O	2.04	0.55
1:B:262:MSE:HE1	5:B:807:EDO:O2	2.07	0.55
1:B:103:ILE:CD1	2:B:700:BOG:H6'2	2.37	0.55
1:B:301:LYS:NZ	10:B:933:HOH:O	2.29	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:HG22	1:A:105:LEU:HD22	1.88	0.55
1:A:473:GLN:NE2	5:A:1957:EDO:H21	2.22	0.55
1:B:262:MSE:CE	5:B:807:EDO:H12	2.36	0.55
1:A:72:GLU:OE2	1:A:114:ARG:HB2	2.07	0.54
5:B:811:EDO:H11	9:B:812:TAM:H62	1.88	0.54
1:A:57:GLU:HB2	2:A:800:BOG:O6	2.08	0.54
1:A:97:PRO:HG2	1:A:100:MET:HB2	1.90	0.54
1:A:469:ARG:NH1	5:A:1953:EDO:O2	2.40	0.54
1:B:373:TYR:CB	1:B:376:ILE:HD13	2.36	0.54
1:A:230:LYS:HD3	1:A:282:VAL:HG23	1.87	0.54
1:A:286:GLU:OE1	1:A:286:GLU:HA	2.07	0.54
1:B:376:ILE:O	1:B:377:GLY:C	2.49	0.54
1:A:494:GLN:HA	1:A:494:GLN:OE1	2.06	0.54
1:B:25:ARG:HD3	1:B:377:GLY:O	2.08	0.54
1:B:157:GLN:HG2	9:B:812:TAM:HN2	1.70	0.54
1:B:391:ILE:C	1:B:392:GLU:HG2	2.32	0.53
1:A:193:LYS:HD2	1:A:195:TYR:CZ	2.43	0.53
1:A:155:ASN:O	1:A:159:VAL:HG23	2.09	0.53
1:B:457:HIS:C	5:B:811:EDO:H21	2.34	0.53
1:A:374:GLN:HB2	1:A:375:GLY:CA	2.19	0.52
1:B:376:ILE:O	1:B:377:GLY:O	2.28	0.52
1:A:229:ILE:HD12	1:A:327:PRO:HB3	1.92	0.52
1:B:101:ILE:HG23	2:B:800:BOG:H61	1.92	0.52
1:B:97:PRO:HD2	1:B:100:MET:SD	2.50	0.52
1:B:232:SER:O	1:B:270:THR:HG22	2.10	0.52
1:B:120:SER:HA	1:B:140:GLU:O	2.10	0.52
1:A:97:PRO:HB2	1:A:99:TRP:CD1	2.45	0.51
1:A:50:HIS:NE2	1:A:354:LYS:CE	2.74	0.51
1:B:478:ASN:OD1	1:B:478:ASN:C	2.52	0.51
1:B:27:LEU:CD1	1:B:376:ILE:HD11	2.38	0.51
1:A:54:ARG:HG2	10:A:2109:HOH:O	2.11	0.51
1:A:64:VAL:HG12	1:A:68:LEU:HD22	1.91	0.51
1:B:58:HIS:O	1:B:59:TYR:O	2.27	0.51
1:B:311:TRP:C	1:B:312:THR:CG2	2.84	0.51
1:A:340:ASP:HB2	1:A:344:LYS:O	2.11	0.50
1:A:129:SER:O	1:A:301:LYS:HE2	2.12	0.50
1:B:296:TYR:C	1:B:296:TYR:CD2	2.89	0.50
1:A:40:ALA:O	5:A:1965:EDO:O1	2.28	0.50
1:A:114:ARG:O	1:A:114:ARG:HG2	2.09	0.50
1:A:296:TYR:CD1	1:A:296:TYR:C	2.89	0.50
1:B:97:PRO:HG2	1:B:100:MET:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1958:EDO:H22	10:A:2097:HOH:O	2.07	0.50
1:B:272:ASP:HB2	5:B:802:EDO:H21	1.94	0.50
5:A:1953:EDO:H12	5:A:1965:EDO:O2	2.12	0.50
1:B:490:VAL:O	1:B:494:GLN:HB2	2.10	0.50
5:B:807:EDO:H11	5:B:808:EDO:HO1	1.72	0.50
1:B:324:SER:O	1:B:325:ASP:CB	2.58	0.50
1:A:478:ASN:HD21	1:A:481:GLN:H	1.55	0.49
1:A:478:ASN:HD22	1:A:481:GLN:H	1.57	0.49
1:B:27:LEU:HD21	1:B:376:ILE:HD13	1.77	0.49
1:B:227:ARG:HG2	1:B:321:ASP:HB2	1.93	0.49
1:A:200:ARG:O	1:A:346:PRO:HD2	2.12	0.49
5:A:1959:EDO:H11	6:A:1961:IMD:H2	1.94	0.49
1:B:49:ILE:HB	1:B:144:CYS:HB2	1.94	0.49
1:B:252:ASP:OD1	1:B:254:ARG:HB2	2.12	0.49
1:A:193:LYS:HE3	1:A:195:TYR:OH	2.12	0.49
1:A:294:ASN:ND2	5:A:1955:EDO:O2	2.46	0.49
1:A:237:PRO:CG	6:A:1966:IMD:N3	2.43	0.49
1:A:424:ASN:HD21	6:A:1961:IMD:H4	1.75	0.49
1:B:212:GLN:CG	5:B:810:EDO:H22	2.37	0.49
1:A:96:ARG:HE	2:A:800:BOG:H5	1.78	0.49
1:A:316:VAL:HG22	5:A:1958:EDO:H11	1.95	0.49
1:B:39:CYS:HA	1:B:469:ARG:HD3	1.95	0.49
1:B:287:SER:HB3	8:B:821:BCN:H62	1.95	0.49
1:B:2:GLU:O	1:B:4:LYS:HD2	2.13	0.48
1:B:55:TYR:OH	7:B:816:13P:O1P	2.24	0.48
1:B:67:ALA:HB1	1:B:356:THR:HG21	1.94	0.48
1:B:311:TRP:O	1:B:312:THR:HG22	2.12	0.48
1:B:336:LEU:CD2	1:B:350:VAL:HG22	2.43	0.48
1:A:416:HIS:ND1	5:A:1957:EDO:H11	2.27	0.48
1:A:391:ILE:C	1:A:393:GLY:N	2.71	0.48
1:B:21:ASP:O	1:B:22:ALA:C	2.56	0.48
1:B:59:TYR:HE2	2:B:800:BOG:C5'	2.25	0.48
1:B:459:TRP:CE2	5:B:811:EDO:H12	2.49	0.48
1:A:457:HIS:CA	6:A:1963:IMD:H4	2.44	0.48
1:A:16:ALA:HA	1:A:31:MSE:HE2	1.95	0.48
1:A:421:TYR:OH	1:A:454:LEU:HD21	2.14	0.47
1:A:469:ARG:NH1	1:A:469:ARG:HG3	2.28	0.47
1:B:54:ARG:HA	2:B:800:BOG:O2	2.14	0.47
1:B:336:LEU:HD22	1:B:350:VAL:HG22	1.95	0.47
1:B:495:GLN:C	1:B:497:LEU:H	2.22	0.47
1:A:106:PHE:HE2	5:A:1964:EDO:HO1	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:HB3	1:A:254:ARG:NH1	2.30	0.47
1:B:3:THR:HA	1:B:4:LYS:HB2	1.97	0.47
1:A:114:ARG:NH2	1:A:118:PRO:O	2.47	0.47
1:A:158:MSE:HE3	1:A:161:ARG:HB3	1.97	0.47
1:A:358:TYR:C	1:A:358:TYR:CD2	2.93	0.47
1:A:241:THR:O	1:A:241:THR:CG2	2.63	0.47
1:A:61:PHE:O	1:A:62:ARG:C	2.57	0.47
1:A:88:ARG:NE	1:A:244:GLN:HG3	2.30	0.47
1:B:193:LYS:HD3	1:B:195:TYR:CZ	2.49	0.47
1:B:440:GLU:CD	1:B:484:ARG:NH1	2.73	0.47
7:B:816:13P:O3P	7:B:816:13P:H31	2.15	0.47
1:A:67:ALA:HB1	1:A:356:THR:HG21	1.95	0.46
1:A:255:ILE:H	1:A:255:ILE:HG13	1.58	0.46
1:B:59:TYR:HE2	2:B:800:BOG:H5'2	1.73	0.46
1:B:457:HIS:HD2	9:B:812:TAM:O6	1.98	0.46
1:A:458:GLU:N	6:A:1963:IMD:H4	2.29	0.46
5:A:1957:EDO:H12	6:A:1960:IMD:H5	1.93	0.46
8:A:1969:BCN:H62	8:A:1969:BCN:H11	1.55	0.46
1:B:370:THR:O	1:B:371:PRO:C	2.57	0.46
1:B:415:ARG:HH11	1:B:415:ARG:HG2	1.80	0.46
1:A:293:LEU:HB2	5:A:1956:EDO:H21	1.98	0.46
1:A:298:THR:HG22	5:A:1955:EDO:O1	2.15	0.46
1:B:270:THR:HG21	4:B:600:FAD:HM71	1.97	0.46
1:B:58:HIS:O	1:B:59:TYR:C	2.59	0.46
1:B:378:PRO:C	1:B:379:ALA:O	2.59	0.46
1:B:415:ARG:HG2	1:B:415:ARG:NH1	2.31	0.45
1:B:96:ARG:HH11	1:B:249:GLN:HE21	1.65	0.45
1:A:106:PHE:O	1:A:110:HIS:CD2	2.70	0.45
1:A:416:HIS:ND1	5:A:1957:EDO:C1	2.80	0.45
1:B:497:LEU:HD23	1:B:497:LEU:HA	1.85	0.45
4:A:600:FAD:H4B	4:A:600:FAD:O2A	2.17	0.45
1:B:200:ARG:O	1:B:346:PRO:HD2	2.16	0.45
1:A:469:ARG:HG3	1:A:469:ARG:HH11	1.82	0.45
8:B:821:BCN:O4	8:B:821:BCN:H12	2.17	0.45
1:A:106:PHE:O	1:A:110:HIS:HD2	2.00	0.45
5:A:1959:EDO:C1	6:A:1961:IMD:H2	2.47	0.45
1:B:73:VAL:O	1:B:77:MSE:HE3	2.16	0.45
1:B:244:GLN:HE21	1:B:244:GLN:HB2	1.61	0.45
1:B:364:HIS:NE2	1:B:368:LYS:NZ	2.65	0.45
1:B:370:THR:O	1:B:372:TYR:N	2.50	0.45
1:A:254:ARG:HD2	1:A:328:GLN:CB	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LYS:HE3	1:B:113:LYS:H	1.82	0.44
1:B:232:SER:O	1:B:270:THR:CG2	2.66	0.44
1:A:359:ARG:NH1	1:A:381:THR:OG1	2.45	0.44
1:B:103:ILE:HD13	2:B:700:BOG:H6'2	1.99	0.44
1:B:336:LEU:HD21	1:B:361:LEU:CD1	2.47	0.44
1:B:386:LEU:O	1:B:387:PRO:C	2.60	0.44
1:B:77:MSE:HG2	1:B:386:LEU:HG	1.98	0.44
1:B:89:LEU:HD12	1:B:247:ILE:O	2.17	0.44
1:A:97:PRO:O	1:A:98:ALA:C	2.60	0.44
1:B:59:TYR:HE2	2:B:800:BOG:C6'	2.31	0.44
1:B:227:ARG:HG2	1:B:321:ASP:CB	2.48	0.44
1:B:262:MSE:CE	5:B:807:EDO:C1	2.93	0.44
1:B:40:ALA:O	1:B:41:THR:C	2.58	0.44
1:B:250:ASN:ND2	1:B:291:TYR:CE1	2.86	0.44
1:B:261:TRP:CZ2	1:B:472:LYS:HD2	2.53	0.44
1:B:294:ASN:ND2	5:B:803:EDO:O1	2.51	0.44
1:A:77:MSE:HE2	1:A:386:LEU:HG	2.00	0.43
1:B:254:ARG:HH21	7:B:816:13P:C1	2.30	0.43
1:B:233:HIS:CE1	1:B:270:THR:HG23	2.53	0.43
1:A:117:LEU:HD22	1:A:142:SER:HB3	2.00	0.43
1:A:147:ASP:CG	1:A:150:ARG:HG3	2.44	0.43
1:B:100:MET:HE2	2:B:800:BOG:H2'1	2.01	0.43
1:B:3:THR:HA	1:B:4:LYS:CB	2.49	0.43
5:B:803:EDO:H21	5:B:817:EDO:H11	2.01	0.43
1:A:91:HIS:CE1	1:A:98:ALA:HB2	2.54	0.42
1:A:366:LEU:HD13	1:A:366:LEU:HA	1.92	0.42
1:B:323:GLU:CB	10:B:912:HOH:O	2.67	0.42
1:A:44:ALA:HB2	5:A:1965:EDO:C2	2.49	0.42
1:A:247:ILE:HG23	1:A:257:PHE:CE1	2.54	0.42
1:B:295:VAL:O	1:B:299:HIS:HD2	2.02	0.42
8:B:820:BCN:H31	8:B:820:BCN:H62	1.64	0.42
1:A:139:PHE:N	1:A:139:PHE:CD2	2.87	0.42
1:A:158:MSE:HE3	1:A:158:MSE:CA	2.41	0.42
1:A:248:LEU:O	1:A:255:ILE:HA	2.19	0.42
1:B:232:SER:N	1:B:270:THR:HG22	2.34	0.42
1:B:259:ILE:HG21	1:B:259:ILE:HD13	1.83	0.42
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.79	0.42
1:A:374:GLN:HB3	1:A:375:GLY:CA	2.39	0.42
1:A:415:ARG:HD3	10:A:2077:HOH:O	2.18	0.42
1:A:457:HIS:HA	6:A:1963:IMD:C4	2.50	0.42
1:A:212:GLN:HE21	1:A:212:GLN:HB3	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1959:EDO:O1	6:A:1961:IMD:N1	2.53	0.42
1:B:80:HIS:CD2	1:B:81:ILE:HG23	2.54	0.42
1:A:478:ASN:ND2	1:A:478:ASN:C	2.77	0.42
1:B:91:HIS:NE2	1:B:98:ALA:HB2	2.35	0.42
1:B:157:GLN:NE2	9:B:812:TAM:H41	2.35	0.42
1:A:241:THR:O	1:A:241:THR:HG22	2.20	0.42
1:A:68:LEU:HD11	1:A:108:TYR:CE2	2.55	0.41
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.77	0.41
1:B:270:THR:HB	1:B:271:THR:H	1.40	0.41
1:A:66:GLU:HG3	1:A:360:LYS:HD2	2.02	0.41
5:A:1959:EDO:H21	6:A:1963:IMD:C4	2.46	0.41
1:B:77:MSE:HE3	1:B:77:MSE:HB2	1.96	0.41
1:B:257:PHE:HB3	1:B:259:ILE:HG13	2.03	0.41
1:A:405:ARG:HD3	5:A:1962:EDO:O2	2.20	0.41
1:A:254:ARG:HB3	1:A:254:ARG:CZ	2.51	0.41
1:A:254:ARG:HG3	1:A:328:GLN:CD	2.45	0.41
1:A:158:MSE:O	1:A:162:LYS:HG3	2.20	0.41
1:B:171:ARG:HD2	5:B:815:EDO:O2	2.21	0.41
1:B:326:SER:HA	1:B:327:PRO:HD3	1.89	0.41
1:A:73:VAL:O	1:A:77:MSE:HG3	2.21	0.41
1:B:162:LYS:HZ3	1:B:162:LYS:HG2	1.61	0.41
1:B:230:LYS:HD3	1:B:282:VAL:HG23	2.03	0.41
1:B:299:HIS:CE1	10:B:882:HOH:O	2.61	0.41
1:B:416:HIS:CE1	1:B:420:THR:HG21	2.56	0.41
1:B:318:PRO:O	1:B:352:GLY:HA2	2.21	0.41
1:B:327:PRO:HA	1:B:330:ILE:HD12	2.02	0.41
1:A:49:ILE:HB	1:A:144:CYS:HB2	2.03	0.40
1:A:60:GLU:OE1	1:A:331:THR:OG1	2.31	0.40
1:A:176:ARG:CG	1:A:176:ARG:NH1	2.61	0.40
1:B:78:ALA:N	1:B:79:PRO:CD	2.85	0.40
1:A:182:TRP:O	1:A:198:GLN:HA	2.21	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	492/501 (98%)	456 (93%)	30 (6%)	6 (1%)	10	4
1	B	495/501 (99%)	454 (92%)	26 (5%)	15 (3%)	3	0
All	All	987/1002 (98%)	910 (92%)	56 (6%)	21 (2%)	5	1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	LYS
1	A	118	PRO
1	B	113	LYS
1	B	118	PRO
1	B	324	SER
1	B	325	ASP
1	B	379	ALA
1	B	59	TYR
1	B	495	GLN
1	B	496	ARG
1	A	374	GLN
1	B	380	TRP
1	A	2	GLU
1	A	380	TRP
1	B	4	LYS
1	B	115	THR
1	B	374	GLN
1	A	354	LYS
1	B	371	PRO
1	B	377	GLY
1	B	376	ILE

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	413/412 (100%)	374 (91%)	39 (9%)	8	2
1	B	416/412 (101%)	360 (86%)	56 (14%)	4	0
All	All	829/824 (101%)	734 (88%)	95 (12%)	5	1

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	32	LEU
1	A	57	GLU
1	A	60	GLU
1	A	65	SER
1	A	68	LEU
1	A	102	ARG
1	A	105	LEU
1	A	113	LYS
1	A	114	ARG
1	A	121	THR
1	A	136	LYS
1	A	162	LYS
1	A	165	GLU
1	A	176	ARG
1	A	194	LYS
1	A	212	GLN
1	A	241	THR
1	A	244	GLN
1	A	247	ILE
1	A	250	ASN
1	A	253	LYS
1	A	255	ILE
1	A	280	LYS
1	A	282	VAL
1	A	298	THR
1	A	326	SER
1	A	349	SER
1	A	366	LEU
1	A	367	GLU
1	A	391	ILE
1	A	392	GLU
1	A	395	ARG
1	A	402	LEU
1	A	404	ARG

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Mol	Chain	Res	Type
1	A	427	LEU
1	A	478	ASN
1	A	489	LEU
1	A	494	GLN
1	B	2	GLU
1	B	3	THR
1	B	4	LYS
1	B	31	MSE
1	B	35	GLN
1	B	53	LEU
1	B	56	LEU
1	B	62	ARG
1	B	63	LEU
1	B	72	GLU
1	B	103	ILE
1	B	105	LEU
1	B	111	LEU
1	B	113	LYS
1	B	114	ARG
1	B	116	SER
1	B	121	THR
1	B	123	LEU
1	B	137	ARG
1	B	153	LEU
1	B	161	ARG
1	B	162	LYS
1	B	193	LYS
1	B	238	ARG
1	B	239	VAL
1	B	244	GLN
1	B	247	ILE
1	B	255	ILE
1	B	270	THR
1	B	272	ASP
1	B	276	LYS
1	B	280	LYS
1	B	283	LYS
1	B	302	LYS
1	B	306	ARG
1	B	312	THR
1	B	323	GLU
1	B	325	ASP

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Mol	Chain	Res	Type
1	B	332	ARG
1	B	341	GLU
1	B	355	LEU
1	B	360	LYS
1	B	361	LEU
1	B	363	GLU
1	B	391	ILE
1	B	392	GLU
1	B	394	ASP
1	B	395	ARG
1	B	413	LEU
1	B	415	ARG
1	B	420	THR
1	B	428	LEU
1	B	429	LEU
1	B	494	GLN
1	B	495	GLN
1	B	496	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	91	HIS
1	A	110	HIS
1	A	128	ASN
1	A	212	GLN
1	A	240	HIS
1	A	244	GLN
1	A	250	ASN
1	A	297	ASN
1	A	328	GLN
1	A	364	HIS
1	A	424	ASN
1	A	444	HIS
1	A	478	ASN
1	A	482	GLN
1	B	50	HIS
1	B	157	GLN
1	B	240	HIS
1	B	244	GLN
1	B	249	GLN

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Mol	Chain	Res	Type
1	B	294	ASN
1	B	299	HIS
1	B	424	ASN
1	B	457	HIS
1	B	494	GLN
1	B	495	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](#)

48 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	$\# Z > 2$
5	EDO	B	811	-	3,3,3	0.29	0	2,2,2	0.77	0
5	EDO	A	1957	-	3,3,3	1.08	0	2,2,2	0.77	0
5	EDO	A	1954	-	3,3,3	0.55	0	2,2,2	0.29	0
6	IMD	B	819	-	5,5,5	0.74	0	5,5,5	0.26	0
9	TAM	B	812	-	10,10,10	1.04	0	12,12,12	2.58	7 (58%)
2	BOG	A	700	-	20,20,20	0.77	1 (5%)	25,25,25	1.14	2 (8%)
6	IMD	A	1966	-	5,5,5	0.80	0	5,5,5	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	1951	-	4,4,4	0.69	0	6,6,6	0.72	0
2	BOG	A	800	-	20,20,20	0.64	1 (5%)	25,25,25	1.56	5 (20%)
5	EDO	B	803	-	3,3,3	0.80	0	2,2,2	0.72	0
5	EDO	B	808	-	3,3,3	0.83	0	2,2,2	0.35	0
2	BOG	B	800	-	20,20,20	0.57	0	25,25,25	1.22	2 (8%)
6	IMD	A	1961	-	5,5,5	0.76	0	5,5,5	0.37	0
5	EDO	A	1962	-	3,3,3	0.52	0	2,2,2	0.37	0
5	EDO	B	818	-	3,3,3	0.53	0	2,2,2	0.31	0
6	IMD	A	1967	-	5,5,5	0.81	0	5,5,5	0.26	0
5	EDO	B	805	-	3,3,3	0.52	0	2,2,2	0.66	0
5	EDO	B	802	-	3,3,3	0.93	0	2,2,2	0.82	0
4	FAD	A	600	-	58,58,58	1.92	22 (37%)	85,89,89	1.72	22 (25%)
5	EDO	A	1959	-	3,3,3	0.66	0	2,2,2	0.51	0
2	BOG	A	1949	-	20,20,20	0.98	1 (5%)	25,25,25	0.92	1 (4%)
5	EDO	A	1955	-	3,3,3	0.66	0	2,2,2	0.39	0
5	EDO	A	1965	-	3,3,3	0.59	0	2,2,2	0.64	0
2	BOG	B	700	-	20,20,20	0.82	1 (5%)	25,25,25	1.09	2 (8%)
5	EDO	A	1953	-	3,3,3	0.62	0	2,2,2	0.91	0
4	FAD	B	600	-	58,58,58	1.92	17 (29%)	85,89,89	1.92	22 (25%)
5	EDO	B	815	-	3,3,3	0.34	0	2,2,2	0.88	0
7	13P	B	816	-	9,9,9	4.34	6 (66%)	10,12,12	3.70	4 (40%)
5	EDO	B	804	-	3,3,3	0.50	0	2,2,2	0.87	0
7	13P	A	1968	-	9,9,9	4.45	6 (66%)	10,12,12	4.01	4 (40%)
5	EDO	B	806	-	3,3,3	1.10	0	2,2,2	0.31	0
5	EDO	B	810	-	3,3,3	0.56	0	2,2,2	0.44	0
5	EDO	B	807	-	3,3,3	0.97	0	2,2,2	0.55	0
6	IMD	A	1963	-	5,5,5	0.83	0	5,5,5	0.23	0
5	EDO	A	1956	-	3,3,3	0.48	0	2,2,2	0.24	0
5	EDO	B	817	-	3,3,3	0.62	0	2,2,2	0.33	0
2	BOG	A	1950	-	20,20,20	0.98	1 (5%)	25,25,25	1.68	5 (20%)
5	EDO	A	1958	-	3,3,3	0.49	0	2,2,2	0.25	0
3	PO4	B	801	-	4,4,4	0.51	0	6,6,6	1.02	0
6	IMD	A	1960	-	5,5,5	0.79	0	5,5,5	1.10	0
8	BCN	B	820	-	10,10,10	1.01	0	11,11,11	2.20	3 (27%)
5	EDO	A	1952	-	3,3,3	0.71	0	2,2,2	0.21	0
8	BCN	A	1969	-	10,10,10	1.03	0	11,11,11	2.05	4 (36%)
5	EDO	B	809	-	3,3,3	0.56	0	2,2,2	0.41	0
5	EDO	B	813	-	3,3,3	0.25	0	2,2,2	0.83	0
8	BCN	B	821	-	10,10,10	1.16	1 (10%)	11,11,11	2.25	4 (36%)
5	EDO	A	1964	-	3,3,3	0.53	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	814	-	3,3,3	0.72	0	2,2,2	0.21	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
5	EDO	B	811	-	-	1/1/1/1	-
5	EDO	A	1957	-	-	1/1/1/1	-
5	EDO	A	1954	-	-	0/1/1/1	-
6	IMD	B	819	-	-	-	0/1/1/1
9	TAM	B	812	-	-	5/12/12/12	-
2	BOG	A	700	-	-	7/11/31/31	0/1/1/1
6	IMD	A	1966	-	-	-	0/1/1/1
2	BOG	A	800	-	-	8/11/31/31	0/1/1/1
5	EDO	B	803	-	-	1/1/1/1	-
5	EDO	B	808	-	-	1/1/1/1	-
2	BOG	B	800	-	-	6/11/31/31	0/1/1/1
6	IMD	A	1961	-	-	-	0/1/1/1
5	EDO	A	1962	-	-	1/1/1/1	-
5	EDO	B	818	-	-	1/1/1/1	-
6	IMD	A	1967	-	-	-	0/1/1/1
5	EDO	B	805	-	-	1/1/1/1	-
5	EDO	B	802	-	-	1/1/1/1	-
4	FAD	A	600	-	-	5/34/50/50	0/6/6/6
5	EDO	A	1959	-	-	0/1/1/1	-
2	BOG	A	1949	-	-	6/11/31/31	0/1/1/1
5	EDO	A	1955	-	-	1/1/1/1	-
5	EDO	A	1965	-	-	1/1/1/1	-
2	BOG	B	700	-	-	5/11/31/31	0/1/1/1
5	EDO	A	1953	-	-	0/1/1/1	-
4	FAD	B	600	-	-	0/34/50/50	0/6/6/6
5	EDO	B	815	-	-	1/1/1/1	-
7	13P	B	816	-	-	7/8/8/8	-
5	EDO	B	804	-	-	1/1/1/1	-
7	13P	A	1968	-	-	7/8/8/8	-
5	EDO	B	806	-	-	1/1/1/1	-
5	EDO	B	810	-	-	1/1/1/1	-
5	EDO	B	807	-	-	1/1/1/1	-
6	IMD	A	1963	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1956	-	-	1/1/1/1	-
5	EDO	B	817	-	-	1/1/1/1	-
2	BOG	A	1950	-	-	5/11/31/31	0/1/1/1
5	EDO	A	1958	-	-	1/1/1/1	-
8	BCN	B	820	-	-	7/10/10/10	-
6	IMD	A	1960	-	-	-	0/1/1/1
5	EDO	A	1952	-	-	0/1/1/1	-
8	BCN	A	1969	-	-	5/10/10/10	-
5	EDO	B	809	-	-	1/1/1/1	-
5	EDO	B	813	-	-	1/1/1/1	-
8	BCN	B	821	-	-	7/10/10/10	-
5	EDO	A	1964	-	-	1/1/1/1	-
5	EDO	B	814	-	-	0/1/1/1	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	816	13P	O1-C1	8.37	1.51	1.43
7	A	1968	13P	O1-C1	7.95	1.51	1.43
7	A	1968	13P	O2-C2	6.41	1.33	1.21
7	B	816	13P	C1-C2	5.90	1.61	1.50
7	B	816	13P	O2-C2	5.69	1.31	1.21
7	A	1968	13P	C1-C2	5.63	1.61	1.50
4	B	600	FAD	C6-C7	-5.34	1.32	1.39
4	B	600	FAD	C4X-N5	4.59	1.40	1.30
4	B	600	FAD	C10-N1	4.48	1.42	1.33
4	B	600	FAD	C4'-C3'	-4.20	1.46	1.53
7	A	1968	13P	C3-C2	4.17	1.61	1.50
4	A	600	FAD	C5A-N7A	-4.12	1.31	1.39
4	A	600	FAD	PA-O3P	-3.94	1.55	1.59
7	B	816	13P	C3-C2	3.70	1.59	1.50
7	A	1968	13P	O3-C3	3.53	1.53	1.41
4	B	600	FAD	C1'-N10	3.29	1.55	1.47
2	A	1949	BOG	O1-C1	3.13	1.45	1.40
2	A	1950	BOG	O1-C1	3.10	1.45	1.40
4	A	600	FAD	PA-O2A	-3.03	1.41	1.55
7	B	816	13P	O3-C3	2.96	1.51	1.41
4	A	600	FAD	O4'-C4'	-2.96	1.37	1.43
4	B	600	FAD	C4-N3	-2.91	1.33	1.38
2	B	700	BOG	O1-C1	2.88	1.45	1.40
4	B	600	FAD	O4B-C4B	-2.81	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	FAD	P-O2P	-2.79	1.42	1.55
4	B	600	FAD	PA-O5B	-2.78	1.48	1.59
4	A	600	FAD	P-O1P	-2.76	1.41	1.50
4	A	600	FAD	O2'-C2'	-2.75	1.37	1.43
4	A	600	FAD	C9A-C5X	-2.73	1.36	1.41
4	A	600	FAD	O2-C2	-2.72	1.19	1.24
7	B	816	13P	P-O1	2.70	1.68	1.60
4	A	600	FAD	C6-C7	-2.58	1.36	1.39
4	B	600	FAD	C9A-C5X	-2.49	1.37	1.41
7	A	1968	13P	P-O1	2.49	1.68	1.60
4	A	600	FAD	C9A-N10	-2.47	1.36	1.41
4	A	600	FAD	O4B-C4B	-2.47	1.39	1.45
4	A	600	FAD	C5X-N5	-2.39	1.35	1.39
4	A	600	FAD	PA-O5B	-2.39	1.50	1.59
4	A	600	FAD	C6-C5X	-2.37	1.36	1.40
4	A	600	FAD	C4X-C10	-2.37	1.37	1.44
4	A	600	FAD	O3'-C3'	-2.36	1.37	1.43
2	A	700	BOG	O1-C1	2.36	1.44	1.40
4	B	600	FAD	PA-O1A	2.33	1.58	1.50
4	A	600	FAD	C4-N3	-2.25	1.34	1.38
4	A	600	FAD	C4X-N5	2.23	1.35	1.30
4	B	600	FAD	C9-C9A	-2.22	1.36	1.39
4	A	600	FAD	C8M-C8	-2.19	1.46	1.51
4	B	600	FAD	C5'-C4'	2.16	1.54	1.51
4	B	600	FAD	P-O2P	-2.16	1.45	1.55
8	B	821	BCN	C1-C2	2.15	1.55	1.51
2	A	800	BOG	O1-C1	2.15	1.43	1.40
4	B	600	FAD	C4X-C10	-2.09	1.38	1.44
4	B	600	FAD	C8M-C8	-2.08	1.47	1.51
4	B	600	FAD	C7M-C7	-2.06	1.47	1.51
4	A	600	FAD	C9-C8	-2.06	1.36	1.39
4	A	600	FAD	O3B-C3B	-2.02	1.37	1.43
4	B	600	FAD	PA-O2A	-2.01	1.46	1.55

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1968	13P	O3P-P-O1	-8.90	83.48	106.67
7	B	816	13P	O3P-P-O1	-8.01	85.77	106.67
7	B	816	13P	O2P-P-O1	6.43	123.44	106.67
7	A	1968	13P	O2P-P-O1	6.28	123.05	106.67
4	A	600	FAD	C5A-C4A-N3A	-5.83	118.68	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1950	BOG	C3-C4-C5	5.08	119.44	110.23
8	B	821	BCN	C1-N1-C5	4.95	123.85	111.91
8	B	820	BCN	C1-N1-C3	4.86	123.63	111.91
4	B	600	FAD	N3A-C2A-N1A	-4.85	121.25	128.58
8	A	1969	BCN	C5-N1-C3	4.74	122.72	111.44
7	A	1968	13P	O1-P-O1P	-4.54	94.16	106.44
4	A	600	FAD	O2A-PA-O5B	-4.53	87.04	107.57
7	B	816	13P	O3P-P-O1P	4.47	128.24	110.83
4	A	600	FAD	N3A-C2A-N1A	-4.38	121.96	128.58
9	B	812	TAM	C3-C-C2	-4.24	103.02	110.50
4	B	600	FAD	C9A-C5X-N5	-4.22	117.97	122.45
7	A	1968	13P	O3P-P-O1P	4.20	127.21	110.83
4	B	600	FAD	O2'-C2'-C3'	-4.16	99.51	109.25
4	B	600	FAD	C5X-N5-C4X	4.13	124.77	118.09
9	B	812	TAM	C3-C-N	-4.00	98.18	108.22
4	B	600	FAD	C10-C4X-N5	-3.94	116.75	124.81
4	B	600	FAD	C4-C4X-N5	3.92	123.62	118.21
4	B	600	FAD	O4-C4-N3	-3.70	113.15	120.11
4	A	600	FAD	N3A-C4A-N9A	3.60	133.29	127.17
4	A	600	FAD	C2A-N3A-C4A	3.51	120.40	111.83
9	B	812	TAM	C5-C2-C	3.50	120.10	115.97
8	B	820	BCN	C5-N1-C3	3.50	119.77	111.44
8	B	821	BCN	C2-C1-N1	3.46	124.73	113.77
2	B	800	BOG	C1-C2-C3	3.45	117.28	110.01
4	B	600	FAD	C5A-N7A-C8A	3.43	108.84	103.45
2	A	800	BOG	O5-C5-C4	3.36	115.76	109.70
2	A	800	BOG	C3-C4-C5	3.36	116.33	110.23
9	B	812	TAM	C2-C-N	3.33	116.59	108.22
2	A	1950	BOG	C4-C3-C2	3.13	116.33	110.83
2	A	800	BOG	C4-C3-C2	3.11	116.29	110.83
4	B	600	FAD	O3'-C3'-C2'	-3.09	101.91	108.93
4	B	600	FAD	C5A-C4A-N3A	-3.08	122.47	126.72
4	B	600	FAD	N9A-C8A-N7A	-3.04	109.62	113.94
8	B	821	BCN	C1-N1-C3	3.03	119.22	111.91
4	A	600	FAD	C5A-N7A-C8A	3.01	108.19	103.45
2	A	1950	BOG	O5-C5-C4	2.99	115.08	109.70
2	B	700	BOG	O5-C5-C6	2.94	113.72	106.44
4	B	600	FAD	C9-C9A-N10	2.89	125.74	121.85
8	A	1969	BCN	C1-N1-C5	2.87	118.83	111.91
4	A	600	FAD	O5B-C5B-C4B	2.87	118.77	108.99
2	A	800	BOG	O3-C3-C4	-2.86	103.63	110.38
4	B	600	FAD	C1'-C2'-C3'	-2.76	102.16	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	FAD	C4A-C5A-N7A	-2.72	107.47	110.58
8	A	1969	BCN	C1-N1-C3	2.71	118.44	111.91
4	B	600	FAD	C2A-N3A-C4A	2.68	118.38	111.83
4	B	600	FAD	C9A-N10-C10	2.61	124.72	120.75
2	A	1950	BOG	O1-C1-C2	2.56	112.16	108.27
4	A	600	FAD	C4X-C4-N3	2.54	119.73	113.25
7	B	816	13P	O1-P-O1P	-2.52	99.64	106.44
4	A	600	FAD	O4-C4-N3	-2.48	115.44	120.11
4	B	600	FAD	C4A-C5A-N7A	-2.48	107.74	110.58
8	B	820	BCN	C2-C1-N1	2.44	121.52	113.77
4	A	600	FAD	O5B-PA-O1A	2.44	118.60	108.94
2	A	700	BOG	C1-O5-C5	2.42	118.44	113.72
4	B	600	FAD	O5'-P-O1P	-2.41	99.38	108.94
9	B	812	TAM	C2-C-C1	2.41	114.75	110.50
9	B	812	TAM	C6-C3-C	-2.39	113.15	115.97
4	B	600	FAD	C4X-C10-N1	-2.39	118.72	124.59
2	A	1949	BOG	O1-C1-C2	2.38	111.88	108.27
4	A	600	FAD	C10-C4X-N5	-2.35	120.02	124.81
2	A	800	BOG	O5-C1-C2	-2.35	105.55	110.37
2	B	800	BOG	C4-C3-C2	2.33	114.92	110.83
2	A	1950	BOG	O4-C4-C3	-2.31	104.93	110.38
4	B	600	FAD	C4X-C4-N3	2.31	119.12	113.25
4	A	600	FAD	O4-C4-C4X	-2.30	120.47	126.53
8	B	821	BCN	C5-N1-C3	2.29	116.90	111.44
4	A	600	FAD	N9A-C8A-N7A	-2.26	110.72	113.94
2	A	700	BOG	O2-C2-C1	2.24	115.42	110.08
4	A	600	FAD	C4X-C10-N10	2.20	119.64	116.48
4	B	600	FAD	C2B-C3B-C4B	2.19	106.84	102.61
4	B	600	FAD	C4'-C3'-C2'	-2.19	109.93	113.57
9	B	812	TAM	C3-C-C1	2.18	114.36	110.50
4	A	600	FAD	C9A-C5X-N5	-2.17	120.15	122.45
4	A	600	FAD	O4'-C4'-C3'	2.16	114.31	109.25
4	A	600	FAD	C8M-C8-C7	-2.12	116.44	120.76
8	A	1969	BCN	C6-C5-N1	-2.11	106.03	113.44
4	A	600	FAD	C4-C4X-N5	2.07	121.07	118.21
2	B	700	BOG	O5-C1-O1	2.07	114.93	110.04
4	A	600	FAD	C4-N3-C2	-2.06	121.99	125.64
4	A	600	FAD	C6A-C5A-C4A	2.04	119.96	117.18
4	A	600	FAD	C5A-C4A-N9A	2.02	108.02	105.81
4	B	600	FAD	N3A-C4A-N9A	2.02	130.61	127.17

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	BOG	O5-C1-O1-C1'
2	A	800	BOG	C2'-C1'-O1-C1
4	A	600	FAD	N10-C1'-C2'-O2'
4	A	600	FAD	O4'-C4'-C5'-O5'
7	A	1968	13P	C1-O1-P-O2P
7	A	1968	13P	C1-O1-P-O3P
7	A	1968	13P	C2-C1-O1-P
7	A	1968	13P	O1-C1-C2-O2
7	A	1968	13P	C1-C2-C3-O3
7	A	1968	13P	O2-C2-C3-O3
7	B	816	13P	C1-O1-P-O1P
7	B	816	13P	C1-O1-P-O2P
7	B	816	13P	C1-O1-P-O3P
7	B	816	13P	C2-C1-O1-P
7	B	816	13P	O1-C1-C2-O2
7	B	816	13P	C1-C2-C3-O3
7	B	816	13P	O2-C2-C3-O3
8	B	820	BCN	C6-C5-N1-C3
8	B	820	BCN	N1-C1-C2-O21
8	B	820	BCN	N1-C1-C2-O22
8	B	821	BCN	N1-C1-C2-O21
8	B	821	BCN	N1-C1-C2-O22
9	B	812	TAM	N-C-C2-C5
8	B	820	BCN	N1-C3-C4-O4
2	A	800	BOG	O5-C5-C6-O6
2	B	700	BOG	O5-C5-C6-O6
8	B	820	BCN	C4-C3-N1-C1
2	A	1950	BOG	O5-C5-C6-O6
2	B	700	BOG	C4-C5-C6-O6
8	A	1969	BCN	N1-C1-C2-O22
2	A	800	BOG	C4-C5-C6-O6
2	A	800	BOG	C2-C1-O1-C1'
2	A	1950	BOG	C4-C5-C6-O6
2	A	700	BOG	C4-C5-C6-O6
8	A	1969	BCN	N1-C1-C2-O21
2	A	700	BOG	O1-C1'-C2'-C3'
2	A	700	BOG	O5-C5-C6-O6
8	A	1969	BCN	C6-C5-N1-C1
2	B	800	BOG	C2-C1-O1-C1'
2	B	800	BOG	O5-C1-O1-C1'
2	A	700	BOG	C3'-C4'-C5'-C6'
2	A	1949	BOG	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
2	A	700	BOG	C2'-C3'-C4'-C5'
8	B	820	BCN	N1-C5-C6-O6
2	A	1949	BOG	C2'-C3'-C4'-C5'
5	B	802	EDO	O1-C1-C2-O2
5	B	809	EDO	O1-C1-C2-O2
5	B	811	EDO	O1-C1-C2-O2
8	B	821	BCN	C2-C1-N1-C5
2	A	1949	BOG	C1'-C2'-C3'-C4'
2	B	700	BOG	C3'-C4'-C5'-C6'
2	B	800	BOG	C3'-C4'-C5'-C6'
2	A	1949	BOG	O1-C1'-C2'-C3'
9	B	812	TAM	C1-C-C2-C5
9	B	812	TAM	C3-C-C2-C5
5	A	1956	EDO	O1-C1-C2-O2
5	A	1962	EDO	O1-C1-C2-O2
5	B	815	EDO	O1-C1-C2-O2
2	A	800	BOG	C3'-C4'-C5'-C6'
2	B	700	BOG	C1'-C2'-C3'-C4'
7	A	1968	13P	C1-O1-P-O1P
2	A	700	BOG	C5'-C6'-C7'-C8'
2	A	1949	BOG	C5'-C6'-C7'-C8'
2	A	800	BOG	C1'-C2'-C3'-C4'
2	A	700	BOG	O5-C1-O1-C1'
2	B	700	BOG	C5'-C6'-C7'-C8'
5	B	810	EDO	O1-C1-C2-O2
5	B	813	EDO	O1-C1-C2-O2
8	B	820	BCN	C2-C1-N1-C5
8	A	1969	BCN	N1-C3-C4-O4
2	B	800	BOG	C5'-C6'-C7'-C8'
2	B	800	BOG	C4'-C5'-C6'-C7'
9	B	812	TAM	C-C3-C6-O6
2	B	800	BOG	O1-C1'-C2'-C3'
2	A	1950	BOG	C4'-C5'-C6'-C7'
2	A	1950	BOG	C2'-C1'-O1-C1
8	B	821	BCN	N1-C5-C6-O6
4	A	600	FAD	C4B-C5B-O5B-PA
2	A	800	BOG	C5'-C6'-C7'-C8'
9	B	812	TAM	C2-C-C1-C4
5	A	1964	EDO	O1-C1-C2-O2
4	A	600	FAD	C5B-O5B-PA-O1A
8	B	821	BCN	C6-C5-N1-C1
5	B	804	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	818	EDO	O1-C1-C2-O2
2	A	1949	BOG	C2'-C1'-O1-C1
5	A	1957	EDO	O1-C1-C2-O2
5	A	1965	EDO	O1-C1-C2-O2
5	B	806	EDO	O1-C1-C2-O2
5	A	1955	EDO	O1-C1-C2-O2
5	B	808	EDO	O1-C1-C2-O2
5	B	817	EDO	O1-C1-C2-O2
2	A	1950	BOG	O1-C1'-C2'-C3'
8	A	1969	BCN	C4-C3-N1-C5
5	A	1958	EDO	O1-C1-C2-O2
5	B	803	EDO	O1-C1-C2-O2
8	B	821	BCN	C4-C3-N1-C5
8	B	821	BCN	C2-C1-N1-C3
4	A	600	FAD	O4B-C4B-C5B-O5B
5	B	805	EDO	O1-C1-C2-O2
5	B	807	EDO	O1-C1-C2-O2

There are no ring outliers.

37 monomers are involved in 99 short contacts:

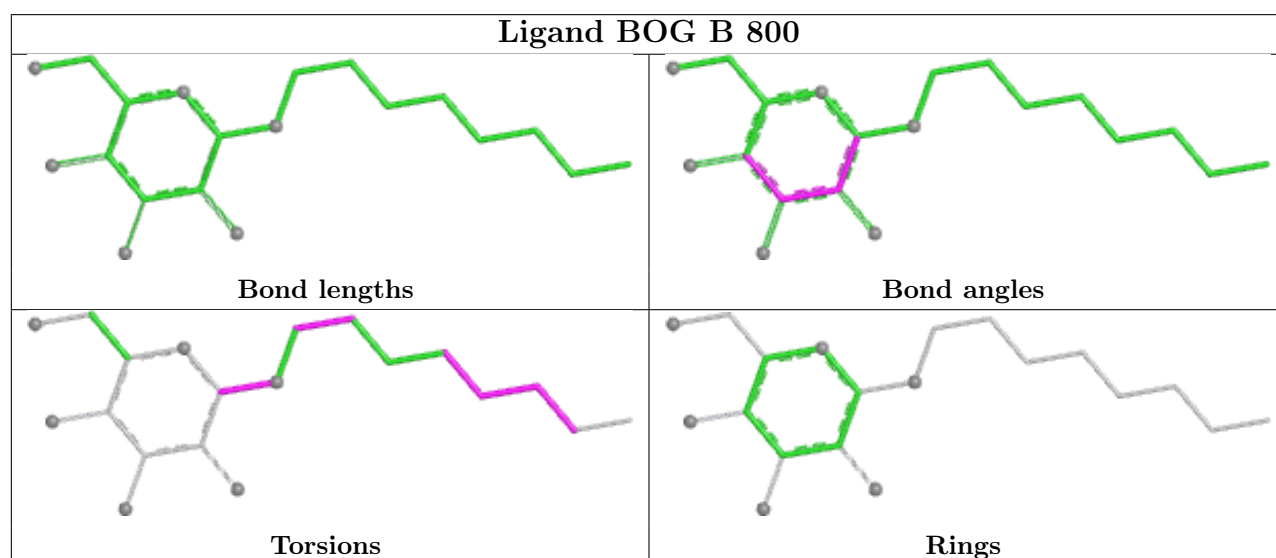
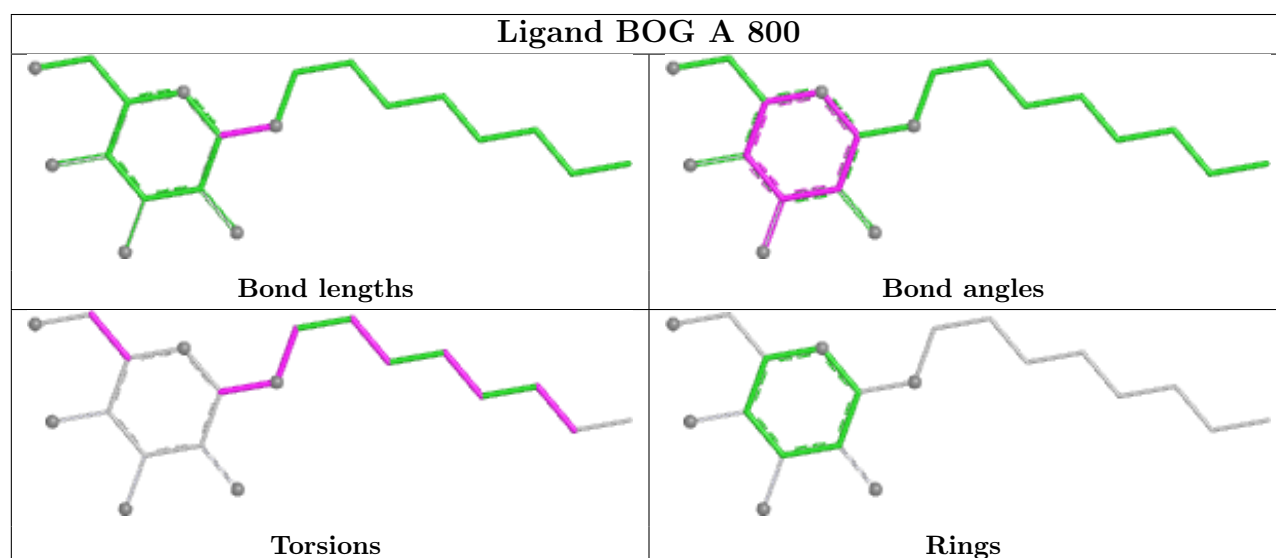
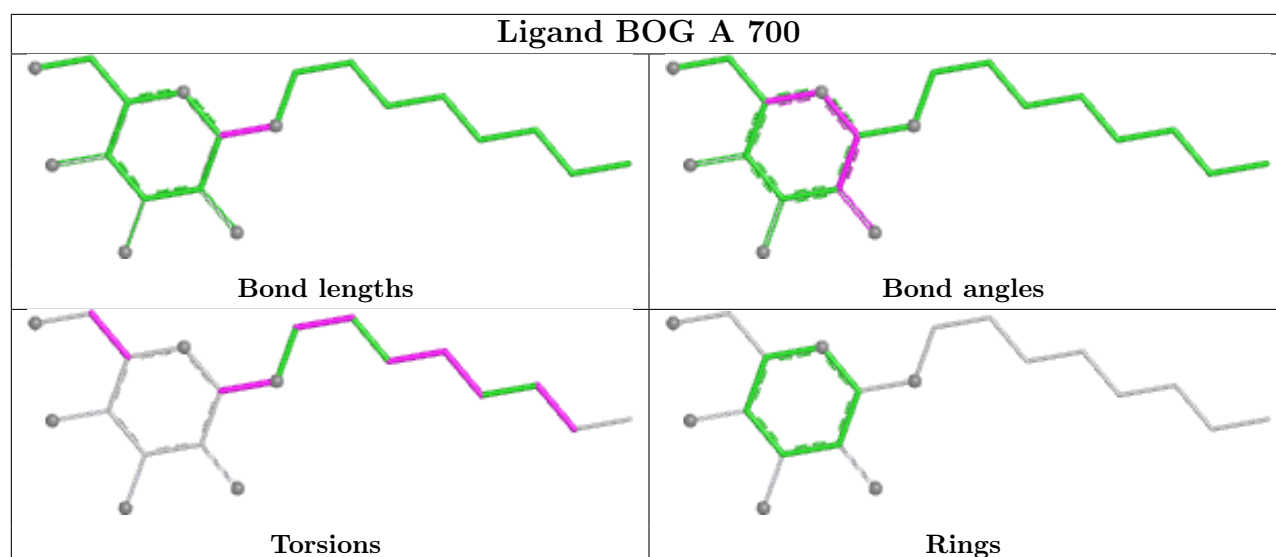
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	811	EDO	3	0
5	A	1957	EDO	6	0
6	B	819	IMD	1	0
9	B	812	TAM	7	0
2	A	700	BOG	1	0
6	A	1966	IMD	4	0
2	A	800	BOG	5	0
5	B	803	EDO	2	0
5	B	808	EDO	2	0
2	B	800	BOG	8	0
6	A	1961	IMD	5	0
5	A	1962	EDO	1	0
5	B	802	EDO	1	0
4	A	600	FAD	1	0
5	A	1959	EDO	7	0
5	A	1955	EDO	2	0
5	A	1965	EDO	3	0
2	B	700	BOG	2	0
5	A	1953	EDO	2	0
4	B	600	FAD	1	0

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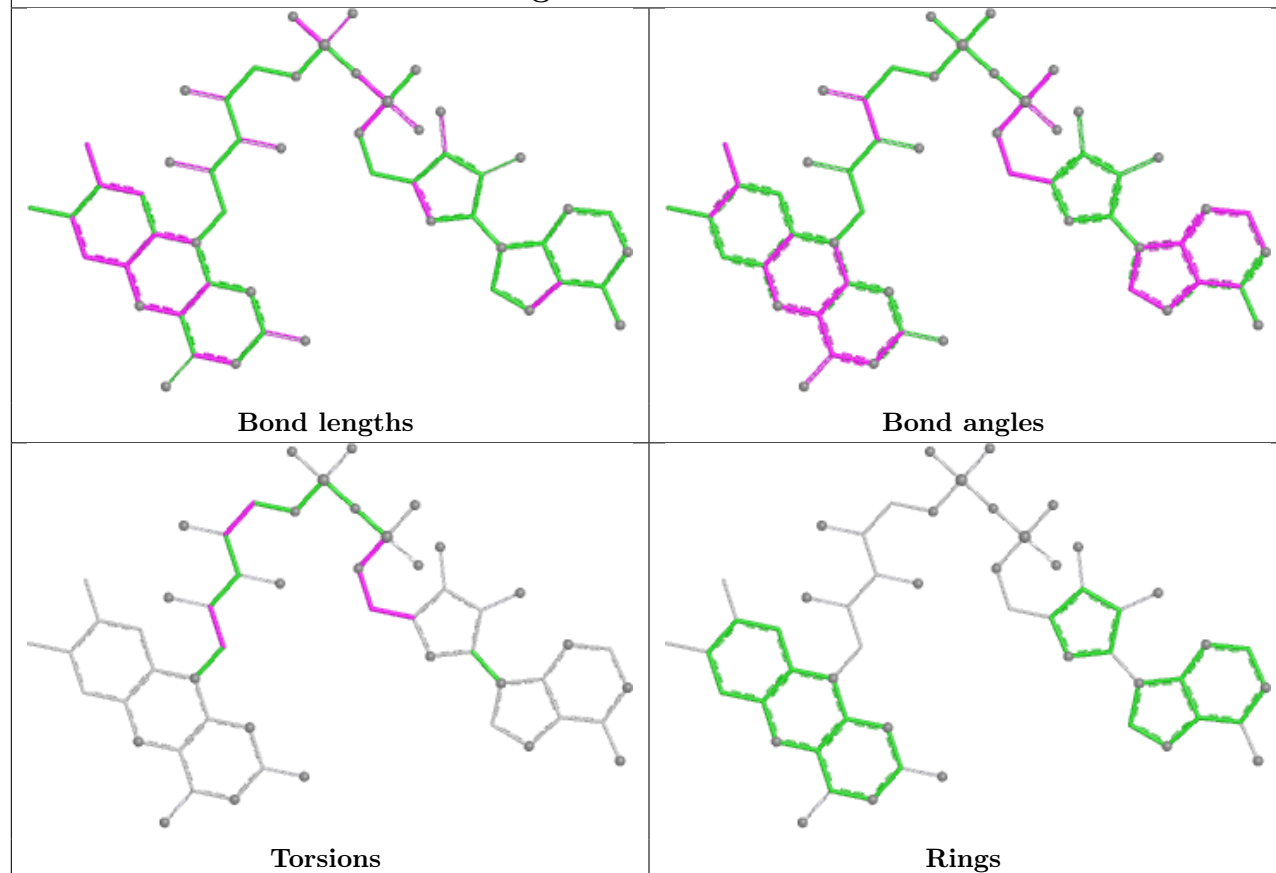
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	815	EDO	1	0
7	B	816	13P	4	0
5	B	804	EDO	1	0
5	B	806	EDO	1	0
5	B	810	EDO	2	0
5	B	807	EDO	7	0
6	A	1963	IMD	8	0
5	A	1956	EDO	3	0
5	B	817	EDO	1	0
2	A	1950	BOG	1	0
5	A	1958	EDO	4	0
6	A	1960	IMD	4	0
8	B	820	BCN	2	0
8	A	1969	BCN	1	0
5	B	813	EDO	6	0
8	B	821	BCN	3	0
5	A	1964	EDO	1	0

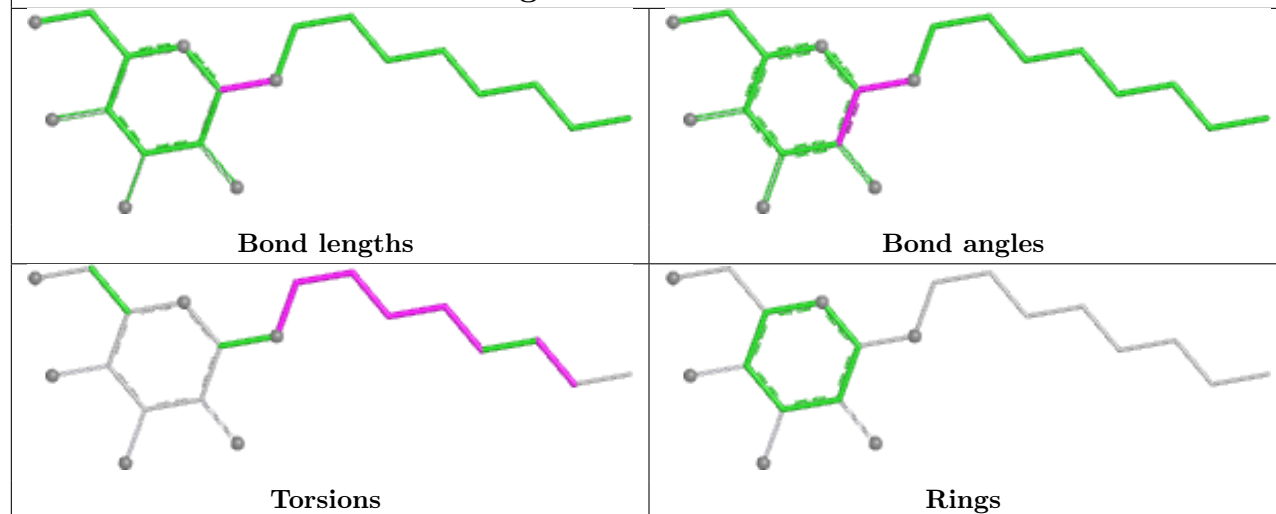
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

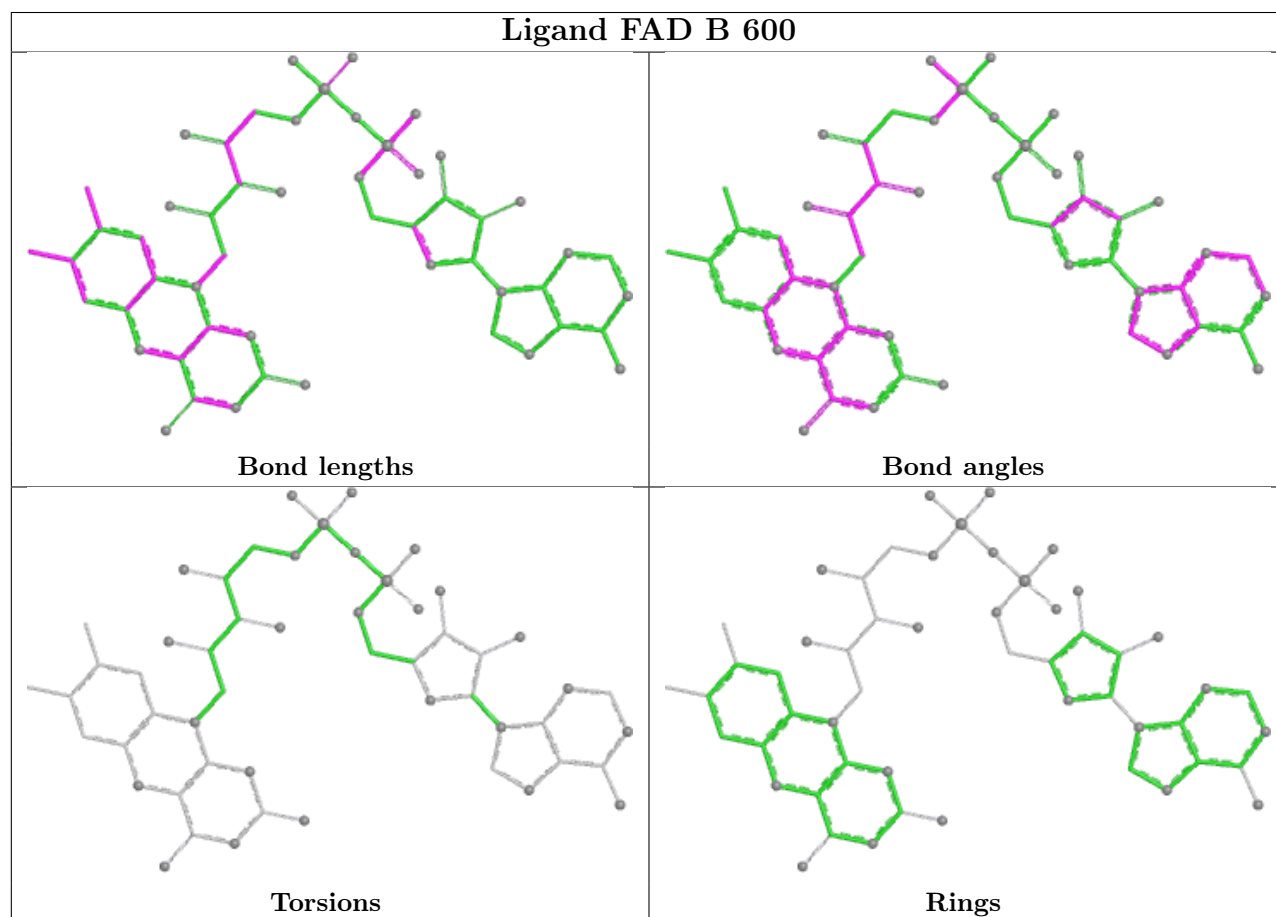
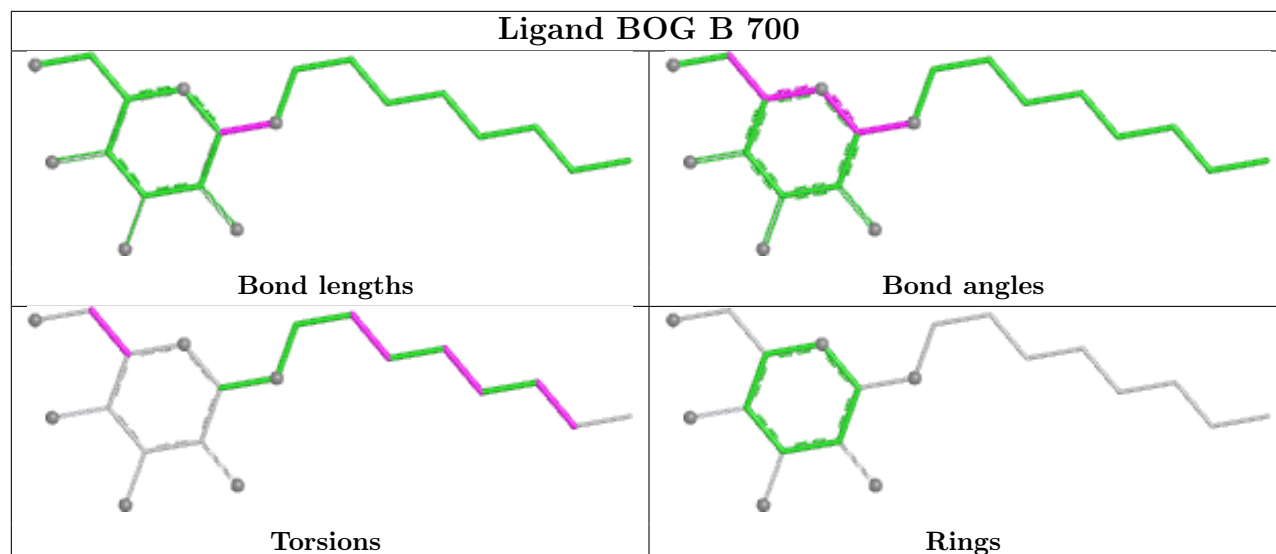


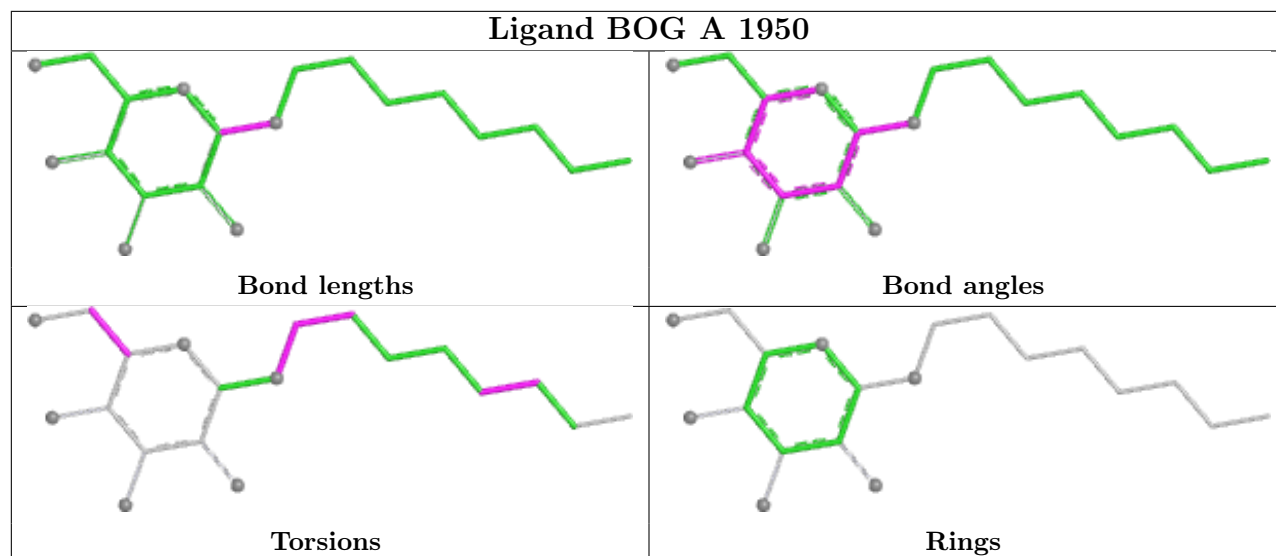
Ligand FAD A 600



Ligand BOG A 1949







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/501 (97%)	-1.04	0 100 100	20, 41, 65, 84	0
1	B	490/501 (97%)	-1.06	0 100 100	19, 41, 66, 98	0
All	All	977/1002 (97%)	-1.05	0 100 100	19, 41, 66, 98	0

There are no RSRZ outliers to report.

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
2	BOG	A	1950	20/20	0.94	0.08	90,93,94,95	0
5	EDO	B	818	4/4	0.94	0.06	72,75,75,75	0
5	EDO	A	1955	4/4	0.96	0.08	38,50,50,52	0
2	BOG	A	700	20/20	0.97	0.06	86,91,94,94	0
2	BOG	B	800	20/20	0.97	0.13	133,136,139,140	0
5	EDO	A	1953	4/4	0.97	0.08	32,45,46,47	0
5	EDO	A	1954	4/4	0.97	0.07	64,65,65,66	0

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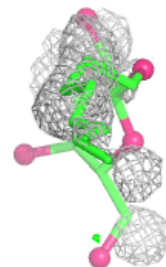
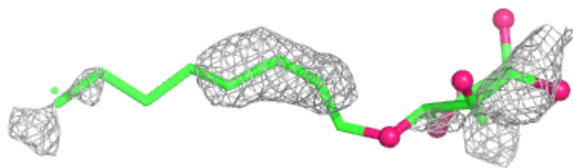
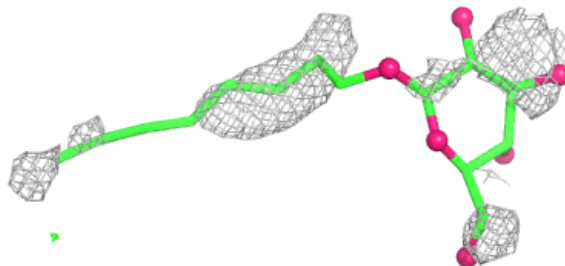
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BOG	A	800	20/20	0.97	0.14	131,136,138,138	0
5	EDO	A	1962	4/4	0.97	0.08	70,71,72,74	0
5	EDO	B	805	4/4	0.97	0.07	63,64,64,68	0
5	EDO	B	810	4/4	0.97	0.07	53,53,54,58	0
2	BOG	A	1949	20/20	0.97	0.08	92,95,97,97	0
6	IMD	A	1966	5/5	0.97	0.05	70,70,72,72	0
6	IMD	B	819	5/5	0.97	0.05	78,78,79,81	0
8	BCN	A	1969	11/11	0.97	0.07	63,76,79,79	0
8	BCN	B	820	11/11	0.97	0.06	64,69,72,74	0
3	PO4	A	1951	5/5	0.98	0.04	84,84,84,85	0
5	EDO	B	808	4/4	0.98	0.06	52,56,57,60	0
5	EDO	A	1956	4/4	0.98	0.09	41,44,50,54	0
5	EDO	B	814	4/4	0.98	0.06	54,56,56,56	0
5	EDO	B	817	4/4	0.98	0.07	55,62,65,66	0
5	EDO	A	1957	4/4	0.98	0.06	43,48,48,49	0
6	IMD	A	1960	5/5	0.98	0.06	58,58,60,60	0
6	IMD	A	1963	5/5	0.98	0.06	42,47,49,50	0
3	PO4	B	801	5/5	0.98	0.05	68,68,70,71	0
5	EDO	A	1964	4/4	0.98	0.05	64,66,66,67	0
5	EDO	B	803	4/4	0.98	0.05	47,49,52,53	0
5	EDO	B	804	4/4	0.98	0.06	49,49,51,52	0
2	BOG	B	700	20/20	0.99	0.05	63,71,77,79	0
5	EDO	B	811	4/4	0.99	0.09	36,43,44,49	0
5	EDO	B	813	4/4	0.99	0.07	36,39,41,43	0
5	EDO	A	1965	4/4	0.99	0.06	37,37,42,42	0
5	EDO	B	815	4/4	0.99	0.04	54,57,59,62	0
5	EDO	B	802	4/4	0.99	0.10	38,44,48,50	0
4	FAD	B	600	53/53	0.99	0.02	19,25,29,32	0
5	EDO	A	1958	4/4	0.99	0.12	32,34,40,46	0
6	IMD	A	1961	5/5	0.99	0.04	73,73,74,74	0
5	EDO	A	1959	4/4	0.99	0.04	43,48,49,52	0
5	EDO	B	806	4/4	0.99	0.08	34,45,50,55	0
6	IMD	A	1967	5/5	0.99	0.06	63,64,65,67	0
5	EDO	B	807	4/4	0.99	0.05	46,47,50,52	0
7	13P	A	1968	10/10	0.99	0.04	28,38,43,44	0
7	13P	B	816	10/10	0.99	0.04	28,40,45,45	0
5	EDO	A	1952	4/4	0.99	0.07	63,63,64,64	0
5	EDO	B	809	4/4	0.99	0.05	65,66,67,68	0
8	BCN	B	821	11/11	0.99	0.06	58,64,70,70	0
9	TAM	B	812	11/11	0.99	0.06	56,63,66,70	0
4	FAD	A	600	53/53	1.00	0.02	18,26,29,36	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.

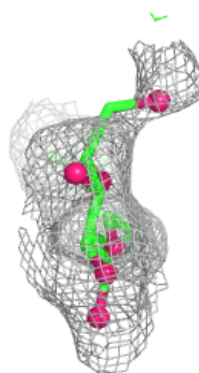
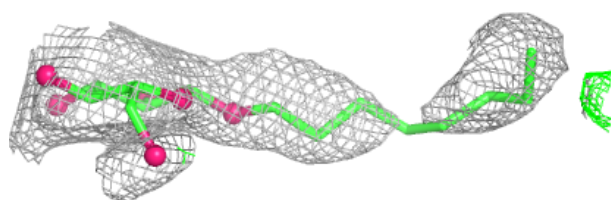
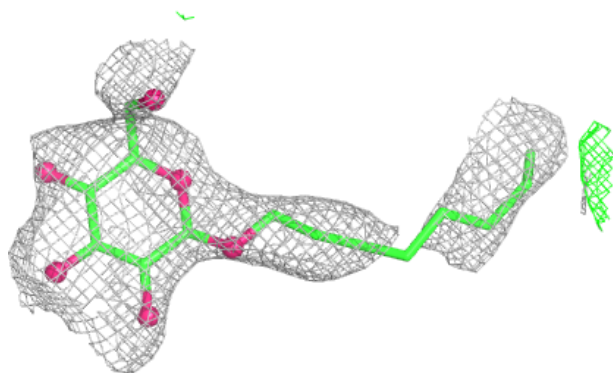
Electron density around BOG A 1950:

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

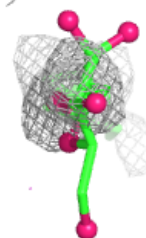
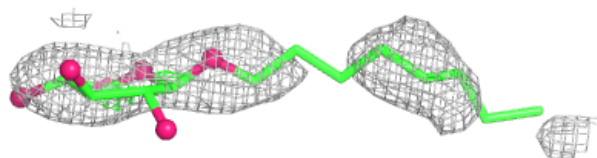
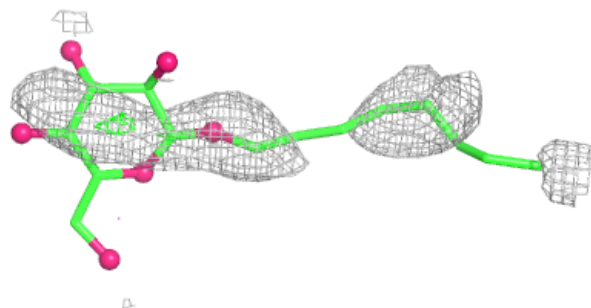


Electron density around BOG A 700:

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

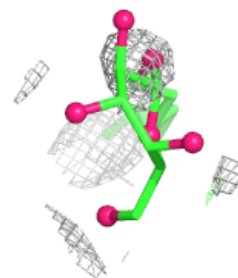
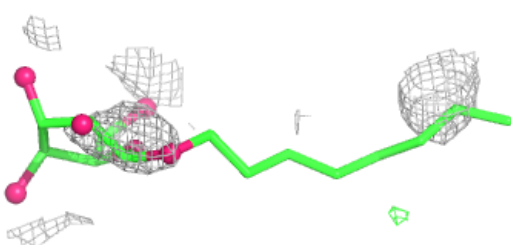
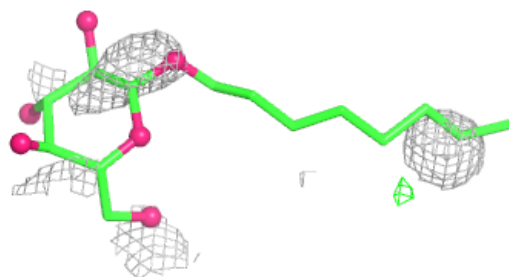
**Electron density around BOG B 800:**

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

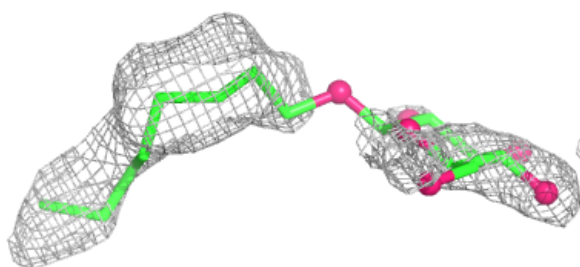
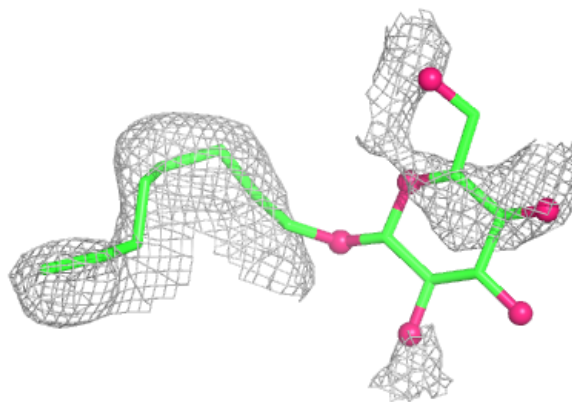


Electron density around BOG A 800:

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

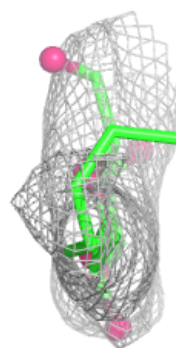
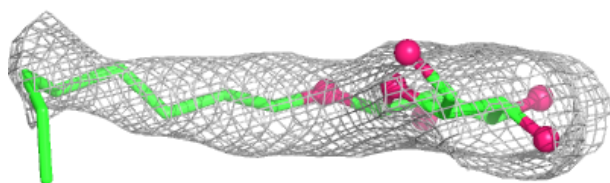
**Electron density around BOG A 1949:**

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and green (positive)

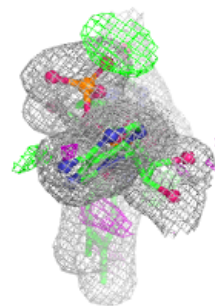
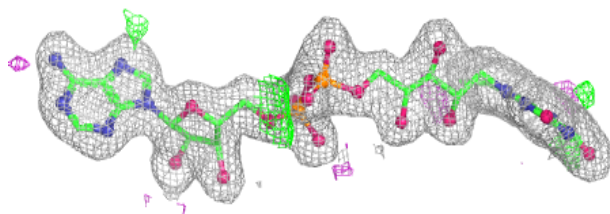
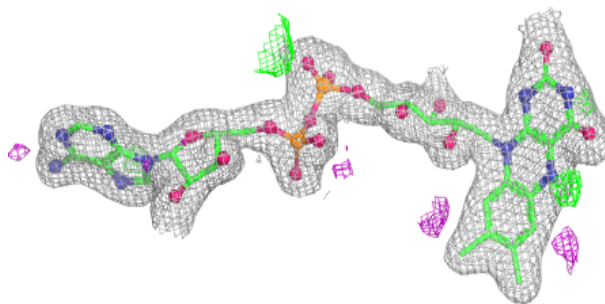


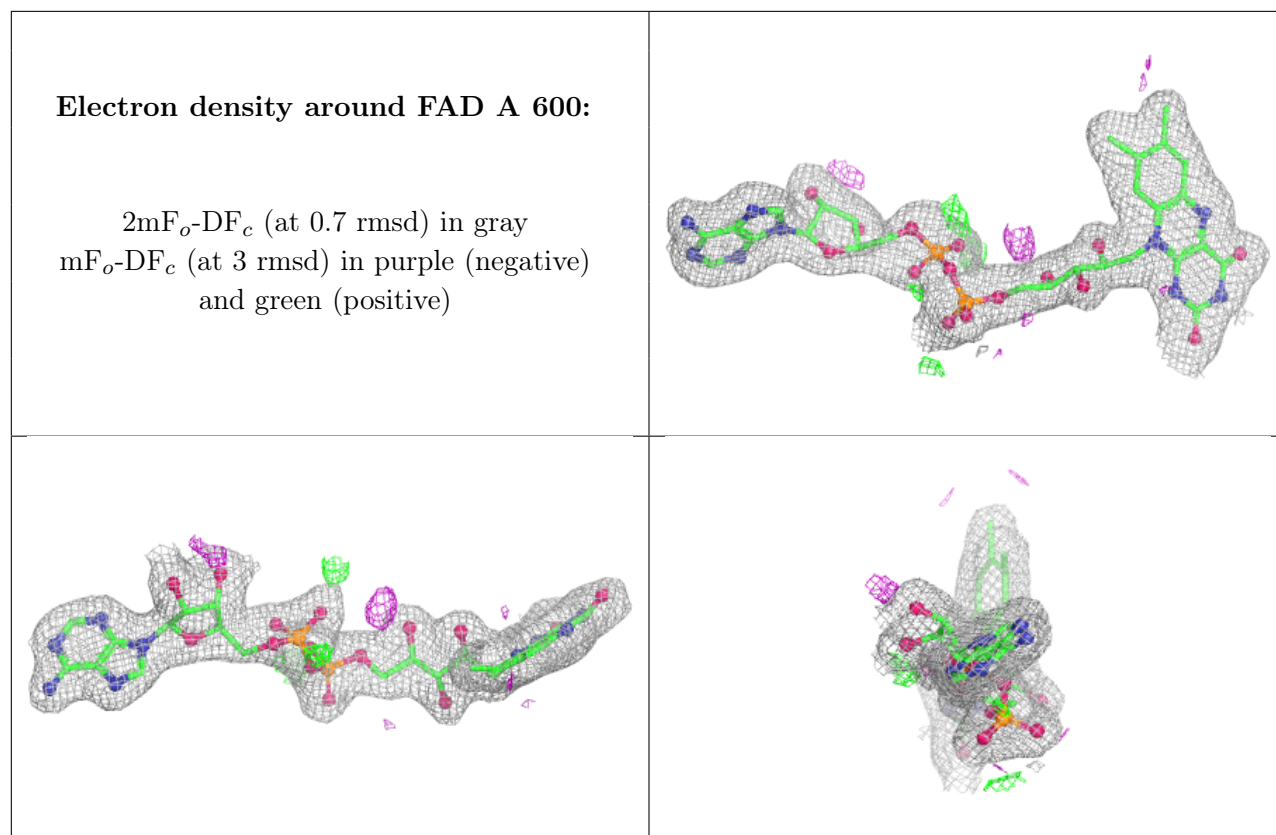
Electron density around BOG B 700:

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

**Electron density around FAD B 600:**

$2mF_o-DF_c$ (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.