



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:29 AM UTC

PDB ID : 3W88 / pdb_00003w88
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with SH-1-200
Authors : Inaoka, D.K.; Hashimoto, S.; Rocha, J.R.; Iida, M.; Tabuchi, T.; Lee, N.; Matsuoka, S.; Kuranaga, T.; Shiba, T.; Balogun, E.O.; Sakamoto, K.; Suzuki, S.; Montanari, C.A.; Nara, T.; Aoki, T.; Inoue, M.; Honma, T.; Tanaka, A.; Harada, S.; Kita, K.
Deposited on : 2013-03-12
Resolution : 1.40 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)

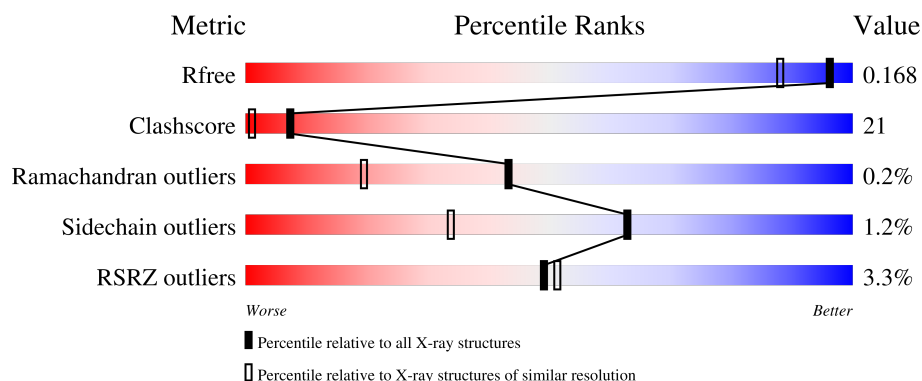
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	314	
1	B	314	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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
3	GOL	B	404[B]	-	X	-	-
3	GOL	B	412	-	-	X	-
4	CAC	A	415	-	X	-	-
4	CAC	B	413	-	X	-	-
4	CAC	B	414	-	X	-	-
6	EDO	A	423	-	-	X	-
6	EDO	A	433	-	-	X	-
6	EDO	A	434	-	-	X	-
6	EDO	A	435	-	-	X	-
6	EDO	B	416	-	-	X	-
6	EDO	B	418	-	-	X	-
6	EDO	B	424	-	-	X	-
7	PEG	A	437[A]	-	-	X	-
7	PEG	A	437[B]	-	-	X	-
7	PEG	A	438	-	-	X	-
7	PEG	A	439	-	-	X	-
7	PEG	A	440	-	-	X	-
7	PEG	B	432	-	-	X	-
7	PEG	B	433	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6466 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.

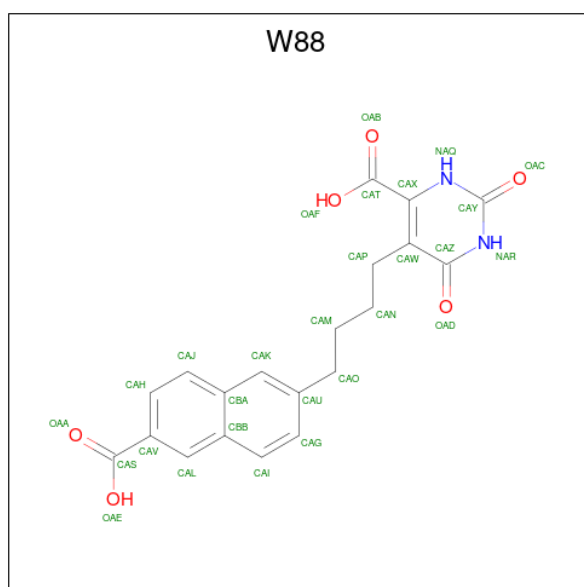
- Molecule 1 is a protein called Dihydroorotate dehydrogenase (fumarate).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	19	0
			2554	1629	427	479	19			
1	B	314	Total	C	N	O	S	0	17	0
			2533	1609	427	478	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q4D3W2
B	-1	SER	-	expression tag	UNP Q4D3W2

- Molecule 2 is 5-[4-(6-carboxynaphthalen-2-yl)butyl]-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (CCD ID: W88) (formula: C₂₀H₁₈N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	20	2	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	1
			56	40	4	12		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



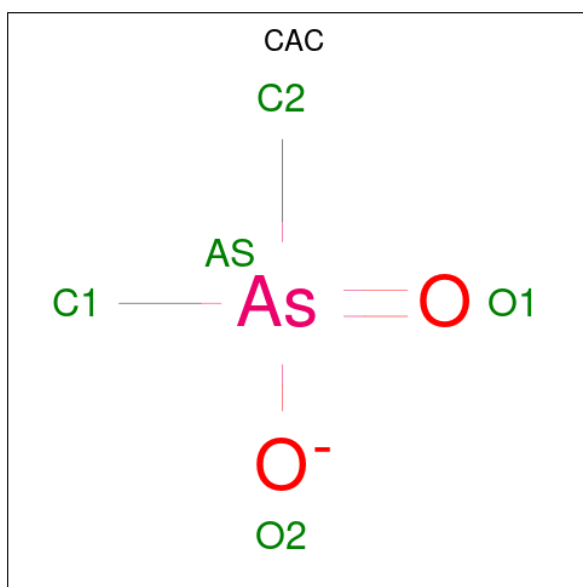
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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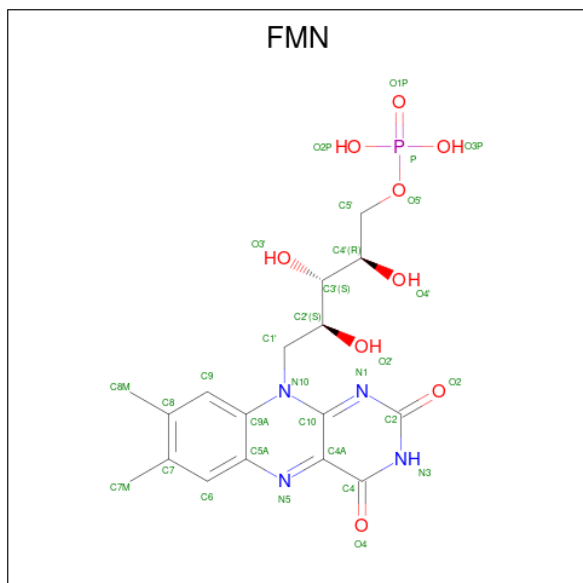
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	1
			12	6	6		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

- Molecule 4 is CACODYLATE ION (CCD ID: CAC) (formula: $\text{C}_2\text{H}_6\text{AsO}_2$).



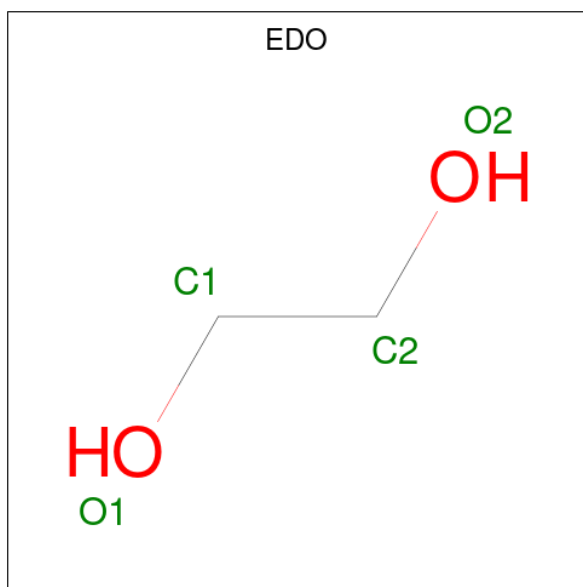
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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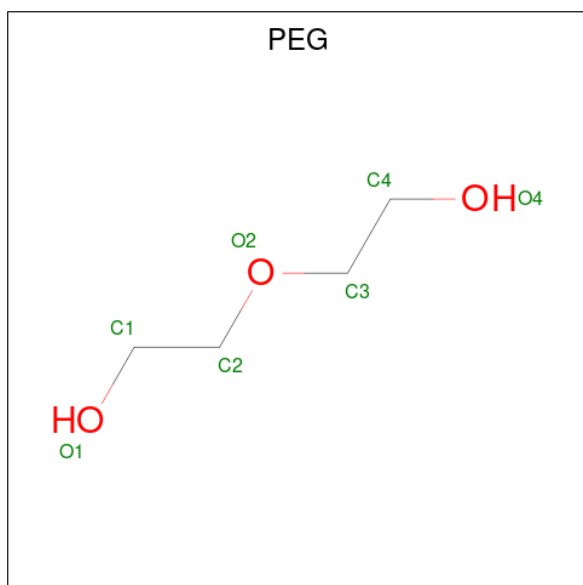
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0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

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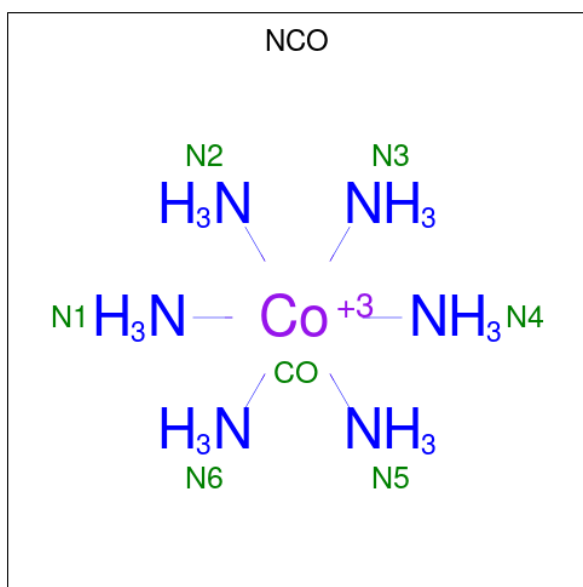
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	1
			14	8	6		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	1
			14	8	6		
7	B	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is COBALT HEXAMMINE(III) (CCD ID: NCO) (formula: $CoH_{18}N_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	Co	N	0	0
			7	1	6		
8	A	1	Total	Co	N	0	1
			14	2	12		

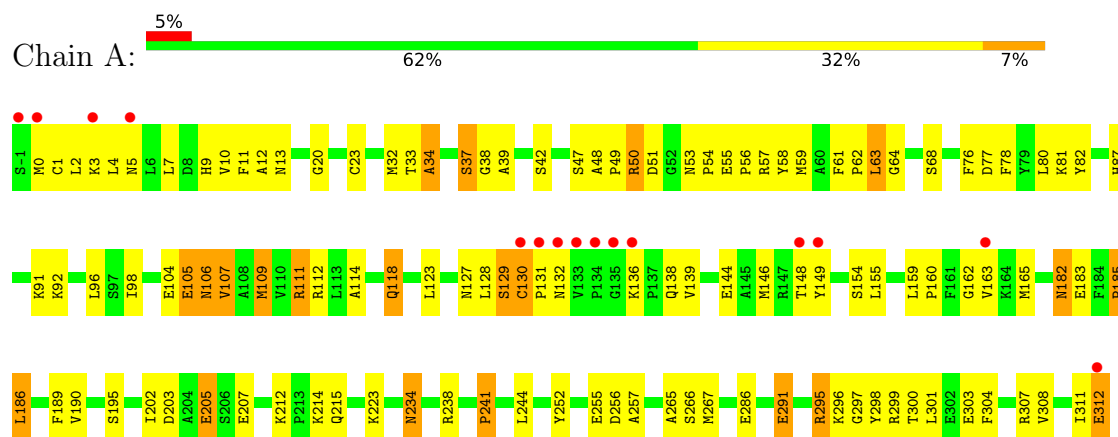
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	371	Total	O	0	10
			381	381		
9	B	440	Total	O	0	7
			447	447		

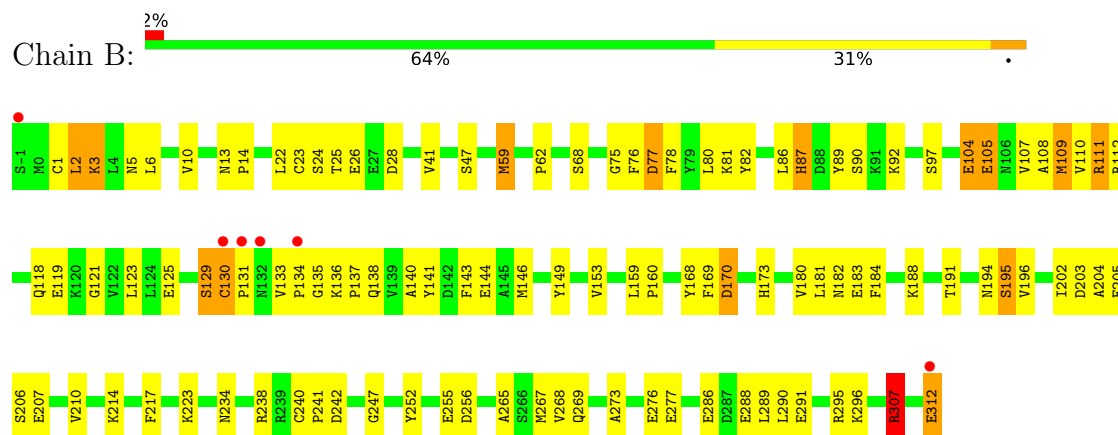
3 Residue-property plots

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: Dihydroorotate dehydrogenase (fumarate)



- Molecule 1: Dihydroorotate dehydrogenase (fumarate)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.97Å 71.52Å 129.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.96 – 1.40 36.96 – 1.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (36.96-1.40) 95.1 (36.96-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.139 , 0.166 0.143 , 0.168	Depositor DCC
R_{free} test set	5941 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	8.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6466	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6031e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EDO, W88, GOL, CAC, FMN, NCO, PEG

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	2.01	93/2606 (3.6%)	1.42	17/3524 (0.5%)
1	B	1.87	83/2585 (3.2%)	1.36	13/3496 (0.4%)
All	All	1.94	176/5191 (3.4%)	1.39	30/7020 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130[A]	CYS	C-N	16.74	1.73	1.33
1	A	130[B]	CYS	C-N	16.74	1.73	1.33
1	A	59	MET	C-O	-8.63	1.13	1.23
1	B	136	LYS	C-O	-8.61	1.15	1.24
1	A	266	SER	C-O	-8.49	1.14	1.24
1	A	48	ALA	C-O	-8.49	1.13	1.24
1	A	265	ALA	C-O	-8.46	1.13	1.23
1	A	32	MET	C-O	-8.38	1.14	1.24
1	B	107	VAL	C-O	-8.30	1.14	1.24
1	B	255	GLU	C-O	-8.29	1.14	1.24
1	B	291	GLU	C-O	-8.15	1.14	1.24
1	A	127	ASN	C-O	-8.08	1.14	1.24
1	B	104	GLU	C-O	-8.05	1.14	1.24
1	A	244	LEU	C-O	-8.03	1.14	1.23
1	B	202	ILE	C-O	-7.88	1.15	1.24
1	A	78	PHE	C-O	-7.81	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	LEU	C-O	-7.79	1.15	1.24
1	B	23	CYS	C-O	-7.76	1.18	1.23
1	A	96	LEU	CB-CG	-7.72	1.38	1.53
1	A	76	PHE	C-O	-7.68	1.15	1.24
1	A	205[A]	GLU	C-O	-7.68	1.15	1.24
1	A	205[B]	GLU	C-O	-7.68	1.15	1.24
1	A	202	ILE	C-O	-7.65	1.16	1.24
1	B	267	MET	C-O	-7.64	1.14	1.23
1	A	159	LEU	CA-C	7.61	1.59	1.52
1	A	23	CYS	C-O	-7.57	1.18	1.23
1	A	33	THR	C-O	-7.54	1.15	1.24
1	B	182	ASN	CA-C	7.48	1.62	1.52
1	A	53	ASN	C-O	-7.48	1.14	1.23
1	A	255	GLU	C-O	-7.46	1.15	1.24
1	A	136	LYS	N-CA	7.44	1.56	1.46
1	B	77	ASP	C-O	-7.44	1.15	1.24
1	A	64	GLY	C-O	-7.38	1.12	1.23
1	A	114	ALA	C-O	-7.30	1.17	1.24
1	A	298	TYR	C-O	-7.29	1.15	1.24
1	A	50	ARG	C-O	-7.25	1.15	1.23
1	A	51	ASP	C-O	-7.11	1.15	1.24
1	A	185	PRO	N-CD	7.10	1.57	1.47
1	B	170	ASP	C-O	-7.09	1.15	1.24
1	A	62	PRO	N-CD	7.06	1.57	1.47
1	A	56	PRO	N-CD	7.04	1.57	1.47
1	A	49	PRO	N-CD	7.04	1.57	1.47
1	B	204	ALA	C-O	-6.97	1.15	1.24
1	A	61	PHE	C-O	-6.96	1.17	1.24
1	A	47	SER	C-O	-6.88	1.16	1.24
1	B	59	MET	SD-CE	-6.85	1.62	1.79
1	B	196	VAL	C-O	-6.85	1.17	1.24
1	B	207	GLU	C-O	-6.84	1.14	1.23
1	A	111[A]	ARG	C-O	-6.81	1.16	1.24
1	A	111[B]	ARG	C-O	-6.81	1.16	1.24
1	A	80	LEU	C-O	-6.81	1.16	1.24
1	B	146	MET	SD-CE	-6.80	1.62	1.79
1	B	22	LEU	C-O	-6.77	1.15	1.23
1	B	78	PHE	C-O	-6.69	1.16	1.24
1	B	2	LEU	C-O	-6.68	1.14	1.23
1	A	207	GLU	C-O	-6.60	1.14	1.23
1	B	149	TYR	C-O	-6.59	1.16	1.24
1	A	63	LEU	C-O	-6.57	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	VAL	C-O	-6.56	1.16	1.24
1	B	24	SER	C-O	-6.55	1.15	1.24
1	B	111[A]	ARG	C-O	-6.53	1.16	1.24
1	B	111[B]	ARG	C-O	-6.53	1.16	1.24
1	B	90	SER	C-O	-6.50	1.15	1.24
1	B	184	PHE	CA-C	-6.50	1.44	1.52
1	A	107	VAL	C-O	-6.49	1.16	1.24
1	A	159	LEU	C-O	-6.48	1.18	1.24
1	A	267	MET	C-O	-6.48	1.15	1.23
1	B	75	GLY	C-O	-6.44	1.15	1.23
1	B	86	LEU	C-O	-6.44	1.15	1.23
1	A	77	ASP	C-O	-6.42	1.16	1.24
1	A	241	PRO	N-CD	6.40	1.56	1.47
1	B	3	LYS	CE-NZ	6.35	1.68	1.49
1	B	87	HIS	C-O	-6.35	1.16	1.23
1	A	148	THR	N-CA	6.33	1.53	1.46
1	B	110	VAL	C-O	-6.31	1.15	1.24
1	A	300	THR	C-O	-6.29	1.16	1.23
1	A	49	PRO	C-O	-6.26	1.16	1.23
1	B	194	ASN	C-O	-6.23	1.15	1.23
1	B	173	HIS	C-O	-6.20	1.16	1.24
1	A	57	ARG	C-O	-6.19	1.16	1.24
1	A	301	LEU	C-O	-6.18	1.16	1.24
1	A	81	LYS	C-O	-6.16	1.17	1.24
1	B	286	GLU	C-O	-6.15	1.17	1.24
1	A	104	GLU	C-O	-6.14	1.17	1.24
1	B	169	PHE	C-O	-6.14	1.16	1.24
1	B	76	PHE	C-O	-6.14	1.17	1.24
1	A	114	ALA	C-N	6.13	1.41	1.33
1	A	146	MET	C-O	-6.11	1.17	1.24
1	A	53	ASN	C-N	6.11	1.41	1.33
1	B	143	PHE	C-O	-6.09	1.17	1.24
1	B	140	ALA	C-O	-6.02	1.16	1.24
1	A	295	ARG	CZ-NH2	-6.00	1.25	1.33
1	B	3	LYS	C-O	-6.00	1.16	1.23
1	A	112	ARG	C-O	-5.97	1.16	1.24
1	A	13	ASN	C-O	-5.96	1.16	1.24
1	B	265	ALA	C-O	-5.96	1.16	1.23
1	A	185	PRO	C-O	-5.94	1.17	1.24
1	A	4	LEU	C-O	-5.94	1.16	1.23
1	B	105	GLU	CD-OE1	-5.91	1.14	1.25
1	A	118	GLN	CA-C	-5.90	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	GLY	CA-C	-5.89	1.46	1.52
1	B	1	CYS	C-O	-5.89	1.17	1.23
1	A	11	PHE	C-O	-5.88	1.16	1.24
1	B	195	SER	C-O	-5.88	1.16	1.23
1	B	242	ASP	C-O	-5.86	1.16	1.24
1	B	295	ARG	CZ-NH2	-5.83	1.25	1.33
1	A	257	ALA	C-O	-5.82	1.17	1.24
1	B	6	LEU	C-O	-5.81	1.16	1.23
1	B	252	TYR	C-O	-5.79	1.16	1.24
1	B	133	VAL	C-N	5.79	1.41	1.33
1	A	189	PHE	CA-C	-5.78	1.45	1.52
1	B	289	LEU	C-O	-5.78	1.17	1.24
1	A	58	TYR	C-O	-5.77	1.17	1.23
1	A	38	GLY	C-O	-5.77	1.16	1.23
1	A	303	GLU	CD-OE1	-5.76	1.14	1.25
1	B	109	MET	C-O	-5.76	1.17	1.24
1	B	141	TYR	C-O	-5.74	1.16	1.24
1	B	26	GLU	C-O	-5.69	1.17	1.24
1	B	205[A]	GLU	C-O	-5.65	1.17	1.24
1	B	205[B]	GLU	C-O	-5.65	1.17	1.24
1	A	39	ALA	C-O	-5.62	1.17	1.23
1	A	299	ARG	C-O	-5.62	1.16	1.24
1	A	304	PHE	C-O	-5.61	1.17	1.24
1	B	133	VAL	C-O	-5.60	1.17	1.24
1	A	130[A]	CYS	N-CA	5.56	1.52	1.46
1	A	130[B]	CYS	N-CA	5.56	1.52	1.46
1	A	105	GLU	C-O	-5.53	1.17	1.24
1	A	160	PRO	C-O	5.52	1.30	1.23
1	B	134	PRO	N-CD	5.52	1.55	1.47
1	A	54	PRO	N-CD	5.51	1.55	1.47
1	A	106	ASN	C-O	-5.51	1.17	1.24
1	B	25	THR	C-O	-5.50	1.16	1.23
1	B	112	ARG	C-O	-5.50	1.17	1.24
1	A	296	LYS	C-O	-5.47	1.16	1.24
1	B	206	SER	C-O	-5.45	1.16	1.24
1	A	62	PRO	C-O	-5.45	1.17	1.24
1	B	268	VAL	C-O	-5.42	1.18	1.24
1	A	12	ALA	C-O	-5.40	1.17	1.24
1	B	269	GLN	C-O	-5.40	1.17	1.23
1	A	241	PRO	C-O	-5.38	1.17	1.24
1	A	109	MET	C-O	-5.37	1.17	1.24
1	A	146	MET	SD-CE	-5.37	1.66	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	183	GLU	N-CA	5.35	1.53	1.46
1	B	130[A]	CYS	CA-C	5.35	1.59	1.53
1	B	130[B]	CYS	CA-C	5.35	1.59	1.53
1	B	144	GLU	C-O	-5.34	1.17	1.24
1	B	288	GLU	C-O	-5.32	1.17	1.24
1	B	135	GLY	C-O	-5.32	1.16	1.24
1	B	3	LYS	CD-CE	5.27	1.68	1.52
1	A	160	PRO	CA-CB	-5.26	1.46	1.53
1	A	234	ASN	CG-OD1	5.25	1.33	1.23
1	B	137	PRO	N-CD	5.24	1.55	1.47
1	A	215	GLN	CD-NE2	-5.24	1.22	1.33
1	B	89	TYR	C-O	-5.23	1.17	1.24
1	A	160	PRO	N-CA	5.22	1.53	1.47
1	A	118	GLN	C-O	-5.21	1.18	1.24
1	B	255	GLU	CD-OE1	-5.20	1.15	1.25
1	B	205[A]	GLU	CD-OE2	-5.19	1.15	1.25
1	B	205[B]	GLU	CD-OE2	-5.19	1.15	1.25
1	A	295	ARG	C-O	-5.18	1.18	1.24
1	A	255	GLU	CD-OE1	-5.17	1.15	1.25
1	A	297	GLY	C-O	-5.15	1.17	1.23
1	A	162	GLY	CA-C	-5.14	1.47	1.52
1	B	290	LEU	C-O	-5.13	1.18	1.24
1	B	307[A]	ARG	C-O	-5.12	1.17	1.24
1	B	307[B]	ARG	C-O	-5.12	1.17	1.24
1	A	129	SER	CA-C	5.09	1.59	1.52
1	B	191	THR	CA-C	-5.07	1.46	1.52
1	A	256	ASP	C-O	-5.06	1.18	1.24
1	A	186	LEU	C-O	-5.04	1.17	1.24
1	B	256	ASP	C-O	-5.04	1.18	1.24
1	B	41	VAL	N-CA	5.03	1.52	1.46
1	A	34	ALA	C-O	-5.03	1.17	1.24
1	A	37	SER	C-O	-5.03	1.17	1.23
1	B	296	LYS	C-O	-5.02	1.17	1.24
1	B	181	LEU	CA-C	-5.00	1.46	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	SER	O-C-N	-15.20	106.03	123.06
1	B	129	SER	O-C-N	-11.40	107.77	122.37
1	B	3	LYS	CD-CE-NZ	10.32	144.92	111.90
1	A	291	GLU	CB-CG-CD	9.70	129.09	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	CYS	N-CA-CB	-9.18	95.47	110.71
1	A	159	LEU	O-C-N	8.14	126.92	121.71
1	A	130[A]	CYS	O-C-N	-7.17	116.83	121.85
1	A	130[B]	CYS	O-C-N	-7.17	116.83	121.85
1	A	189	PHE	CA-C-O	6.85	129.00	121.06
1	A	123	LEU	O-C-N	-6.51	115.61	123.29
1	B	133	VAL	CA-C-N	-6.27	113.30	119.76
1	B	133	VAL	C-N-CA	-6.27	113.30	119.76
1	B	146	MET	CG-SD-CE	-6.04	87.61	100.90
1	B	3	LYS	CG-CD-CE	5.91	124.90	111.30
1	B	159	LEU	O-C-N	5.86	125.46	121.71
1	B	119	GLU	N-CA-C	5.82	117.70	111.36
1	A	144[A]	GLU	CA-C-O	5.75	126.57	119.79
1	A	144[B]	GLU	CA-C-O	5.75	126.57	119.79
1	A	42	SER	O-C-N	-5.64	116.42	122.85
1	A	136	LYS	N-CA-C	5.59	122.16	109.81
1	A	190	VAL	CA-C-O	-5.57	114.65	120.27
1	B	240	CYS	O-C-N	-5.55	116.37	121.42
1	A	53	ASN	CA-C-N	-5.43	114.37	119.85
1	A	53	ASN	C-N-CA	-5.43	114.37	119.85
1	A	55	GLU	C-N-CD	5.32	132.30	120.60
1	A	114	ALA	CA-C-O	5.31	123.43	118.44
1	B	123	LEU	O-C-N	-5.23	117.12	123.29
1	A	182	ASN	CA-C-O	-5.13	112.55	119.11
1	B	28	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	180	VAL	O-C-N	-5.03	116.98	121.91

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	SER	Mainchain

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	2554	0	2540	117	0
1	B	2533	0	2512	63	0
2	A	28	0	16	1	0
2	B	56	0	32	8	0
3	A	90	0	119	6	0
3	B	72	0	95	12	0
4	A	10	0	0	2	0
4	B	10	0	0	0	0
5	A	31	0	19	1	0
5	B	31	0	19	0	0
6	A	72	0	107	34	0
6	B	60	0	88	31	0
7	A	42	0	59	38	0
7	B	28	0	40	18	0
8	A	21	0	0	2	0
9	A	381	0	0	25	0
9	B	447	0	0	28	0
All	All	6466	0	5646	233	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 21.

All (233) 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:3:LYS:CE	1:B:3:LYS:NZ	1.68	1.54
1:A:130[A]:CYS:C	1:A:131:PRO:N	1.69	1.47
1:A:130[B]:CYS:C	1:A:131:PRO:N	1.73	1.47
1:A:1:CYS:HB2	7:A:437[B]:PEG:H22	1.33	1.11
2:B:401[A]:W88:CAI	7:B:433:PEG:H22	1.81	1.10
1:A:2:LEU:HD12	1:A:286:GLU:HG3	1.29	1.09
1:A:130[A]:CYS:SG	1:A:139:VAL:HG23	1.94	1.07
1:A:128:LEU:CD1	1:A:163[B]:VAL:HG21	1.86	1.05
1:A:1:CYS:HB2	7:A:437[A]:PEG:H22	1.32	1.04
2:B:401[A]:W88:H17	7:B:433:PEG:C2	1.91	1.01
2:B:401[A]:W88:H17	7:B:433:PEG:H22	1.01	1.00
1:A:312[A]:GLU:OE2	1:A:312[A]:GLU:HA	1.57	1.00
1:A:185:PRO:HG2	7:A:440:PEG:H22	1.44	0.96
1:A:5:ASN:HB3	6:A:433:EDO:C2	1.98	0.94
1:A:5:ASN:ND2	1:A:10[A]:VAL:HG22	1.83	0.93
1:B:130[B]:CYS:SG	1:B:131:PRO:HD2	2.09	0.93
1:A:2:LEU:HD12	1:A:286:GLU:CG	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:SER:OG	3:B:402:GOL:H11	1.73	0.89
1:A:128:LEU:HD12	1:A:163[B]:VAL:HG21	1.56	0.88
1:A:312[A]:GLU:OE2	1:A:312[A]:GLU:CA	2.18	0.88
7:A:438:PEG:H31	7:A:440:PEG:C1	2.05	0.86
6:B:429:EDO:H22	9:B:875:HOH:O	1.75	0.86
1:B:111[B]:ARG:NH2	7:B:432:PEG:C2	2.39	0.86
1:B:131:PRO:HD3	2:B:401[B]:W88:CAK	2.07	0.85
1:B:277:GLU:HB2	6:B:418:EDO:H12	1.60	0.84
7:A:438:PEG:H31	7:A:440:PEG:H12	1.57	0.84
1:A:5:ASN:HD21	1:A:10[A]:VAL:HG22	1.42	0.82
1:A:312[A]:GLU:HG3	9:B:744:HOH:O	1.78	0.82
2:B:401[A]:W88:CAI	7:B:433:PEG:C2	2.55	0.81
1:A:131:PRO:HB3	2:A:401:W88:CAI	2.12	0.80
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.30	0.80
1:A:128:LEU:CD1	1:A:163[B]:VAL:CG2	2.60	0.79
1:B:130[B]:CYS:SG	1:B:131:PRO:CD	2.71	0.79
1:A:128:LEU:HD11	1:A:163[B]:VAL:HG21	1.65	0.79
1:A:128:LEU:HG	1:A:163[B]:VAL:HG23	1.63	0.78
1:A:5:ASN:HB3	6:A:433:EDO:O2	1.84	0.77
1:A:185:PRO:HG2	7:A:440:PEG:C2	2.14	0.77
1:A:2:LEU:CD1	1:A:286:GLU:HG3	2.12	0.76
1:A:128:LEU:HG	1:A:163[B]:VAL:CG2	2.15	0.76
1:A:138[B]:GLN:HG2	1:B:170:ASP:OD2	1.86	0.76
7:B:431[B]:PEG:O1	7:B:431[B]:PEG:H32	1.76	0.75
1:A:3[C]:LYS:HZ3	1:A:3[C]:LYS:C	1.95	0.75
6:B:421:EDO:H11	9:B:584:HOH:O	1.87	0.74
1:B:59:MET:HE3	9:B:601:HOH:O	1.88	0.73
1:A:5:ASN:HB3	6:A:433:EDO:H21	1.71	0.73
1:A:185:PRO:HD2	7:A:439:PEG:H42	1.70	0.72
1:B:59:MET:CE	9:B:601:HOH:O	2.38	0.72
1:B:195:SER:OG	3:B:402:GOL:C1	2.37	0.72
6:B:429:EDO:H12	9:B:555:HOH:O	1.88	0.72
6:A:434:EDO:H12	8:A:442[B]:NCO:N1	2.05	0.72
1:A:91:LYS:O	6:A:423:EDO:H22	1.89	0.71
1:A:154:SER:CB	7:A:438:PEG:H22	2.21	0.70
1:A:63:LEU:HD11	6:B:419:EDO:H22	1.74	0.70
1:A:2:LEU:HB2	7:A:437[B]:PEG:H12	1.72	0.70
1:A:154:SER:HB3	7:A:438:PEG:H22	1.73	0.70
1:B:273:ALA:HB1	6:B:418:EDO:H11	1.75	0.69
1:B:111[B]:ARG:NH2	7:B:432:PEG:H21	2.07	0.69
1:B:47[B]:SER:O	6:B:416:EDO:H12	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:CG	1:A:149[B]:TYR:OH	2.37	0.67
1:B:111[B]:ARG:NH2	7:B:432:PEG:H22	2.09	0.67
1:A:138[B]:GLN:CG	1:B:170:ASP:OD2	2.43	0.67
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.40	0.67
1:B:131:PRO:CD	2:B:401[B]:W88:CAK	2.73	0.66
7:A:438:PEG:C3	7:A:440:PEG:C1	2.73	0.66
1:B:81:LYS:HE2	9:B:904:HOH:O	1.94	0.66
6:A:434:EDO:H22	8:A:442[A]:NCO:N6	2.10	0.65
6:B:419:EDO:H21	9:B:863:HOH:O	1.96	0.65
1:A:130[B]:CYS:C	1:A:131:PRO:CD	2.69	0.65
6:B:430:EDO:H12	9:B:940:HOH:O	1.97	0.65
7:A:439:PEG:H32	9:A:870:HOH:O	1.96	0.64
1:A:138[A]:GLN:HG3	9:A:855:HOH:O	1.97	0.64
7:A:438:PEG:H31	7:A:440:PEG:H11	1.79	0.63
1:B:111[B]:ARG:HH22	7:B:432:PEG:H22	1.63	0.63
1:A:2:LEU:H	7:A:437[A]:PEG:C2	2.12	0.62
7:A:438:PEG:C3	7:A:440:PEG:H12	2.27	0.62
1:A:154:SER:O	7:A:438:PEG:H41	1.99	0.62
1:A:128:LEU:HD12	1:A:163[A]:VAL:CG1	2.28	0.62
1:A:2:LEU:H	7:A:437[B]:PEG:C2	2.12	0.62
1:B:276:GLU:HB2	6:B:418:EDO:H22	1.81	0.62
7:A:439:PEG:C3	9:A:870:HOH:O	2.48	0.62
1:A:3[C]:LYS:C	1:A:3[C]:LYS:NZ	2.57	0.62
1:A:68[B]:SER:OG	1:A:214[B]:LYS:NZ	2.33	0.61
1:B:68[B]:SER:OG	1:B:214[B]:LYS:NZ	2.32	0.61
3:B:409:GOL:C3	9:B:693:HOH:O	2.49	0.61
6:A:420:EDO:H21	9:A:534:HOH:O	2.00	0.61
6:A:434:EDO:H11	9:A:734[A]:HOH:O	2.00	0.61
1:A:128:LEU:CG	1:A:163[B]:VAL:CG2	2.79	0.61
1:A:130[A]:CYS:C	1:A:131:PRO:CA	2.70	0.61
6:B:421:EDO:C1	9:B:584:HOH:O	2.46	0.60
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.84	0.60
6:A:427:EDO:H21	9:A:665:HOH:O	2.01	0.60
3:B:412:GOL:C1	9:B:628:HOH:O	2.49	0.60
1:B:195:SER:HB3	9:B:675:HOH:O	2.01	0.60
1:A:241:PRO:HB3	3:A:413:GOL:H12	1.84	0.60
1:A:2:LEU:H	7:A:437[B]:PEG:C1	2.15	0.59
1:A:128:LEU:CD1	1:A:163[A]:VAL:CG1	2.80	0.59
7:A:437[A]:PEG:H11	9:A:653:HOH:O	2.02	0.59
1:A:3[A]:LYS:N	7:A:437[A]:PEG:H21	2.18	0.58
1:B:5[B]:ASN:ND2	1:B:10:VAL:HG22	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:HB3	7:A:439:PEG:H12	1.85	0.58
1:A:163[A]:VAL:HG12	1:A:165:MET:SD	2.44	0.58
1:A:98[A]:ILE:O	1:A:98[A]:ILE:HG13	2.04	0.58
1:A:130[A]:CYS:C	1:A:131:PRO:CD	2.73	0.57
1:A:128:LEU:CD1	1:A:163[A]:VAL:HG13	2.35	0.57
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.88	0.57
7:A:437[B]:PEG:H11	9:A:653:HOH:O	2.04	0.57
6:A:435:EDO:C2	9:A:657:HOH:O	2.53	0.57
1:B:92:LYS:HE2	6:B:424:EDO:H12	1.86	0.57
1:B:223[B]:LYS:NZ	3:B:412:GOL:H2	2.20	0.57
4:A:416:CAC:C2	6:A:427:EDO:H11	2.35	0.56
1:A:2:LEU:HB2	7:A:437[A]:PEG:H12	1.88	0.56
1:A:182:ASN:O	6:A:435:EDO:H21	2.05	0.56
1:A:149[A]:TYR:HE1	9:A:689:HOH:O	1.89	0.55
2:B:401[A]:W88:H18	7:B:433:PEG:H12	1.88	0.55
1:A:105:GLU:HG2	1:A:109:MET:HE2	1.89	0.55
1:A:312[A]:GLU:OE2	1:A:312[A]:GLU:N	2.40	0.55
1:B:241:PRO:HA	3:B:408:GOL:H31	1.89	0.55
1:B:121:GLY:CA	6:B:423:EDO:H22	2.37	0.55
1:A:1:CYS:CB	7:A:437[A]:PEG:H22	2.23	0.54
1:A:1:CYS:CB	7:A:437[B]:PEG:H22	2.24	0.54
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.02	0.54
6:B:416:EDO:H11	9:B:539:HOH:O	2.07	0.54
1:A:130[A]:CYS:SG	1:A:139:VAL:CG2	2.85	0.54
1:A:312[A]:GLU:CG	9:B:744:HOH:O	2.48	0.54
1:B:108:ALA:CB	7:B:432:PEG:H12	2.37	0.54
1:A:128:LEU:HD12	1:A:163[B]:VAL:CG2	2.32	0.53
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.07	0.53
1:B:111[B]:ARG:HH21	7:B:432:PEG:C1	2.21	0.53
7:A:436:PEG:H21	9:B:808:HOH:O	2.08	0.53
1:B:47[B]:SER:O	6:B:416:EDO:C1	2.57	0.53
1:A:5:ASN:CB	6:A:433:EDO:O2	2.55	0.53
1:A:128:LEU:HD12	1:A:163[A]:VAL:HG11	1.90	0.53
3:A:411:GOL:H12	9:A:799:HOH:O	2.08	0.53
1:A:2:LEU:CD1	1:A:286:GLU:CG	2.78	0.52
1:A:154:SER:HB2	7:A:438:PEG:H22	1.89	0.52
1:B:62:PRO:HB3	6:B:430:EDO:H21	1.91	0.52
1:A:92:LYS:HE2	6:A:423:EDO:H11	1.92	0.51
6:A:435:EDO:C1	9:A:657:HOH:O	2.58	0.51
1:A:87:HIS:HE1	1:A:92:LYS:O	1.92	0.51
1:A:128:LEU:HG	1:A:163[A]:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:PRO:HD3	7:B:431[B]:PEG:H21	1.93	0.51
1:A:195:SER:HB3	9:A:798:HOH:O	2.11	0.50
1:B:87:HIS:HE1	1:B:92:LYS:O	1.93	0.50
1:B:203:ASP:HB2	3:B:410:GOL:H12	1.94	0.50
7:A:438:PEG:H21	7:A:440:PEG:O1	2.11	0.50
1:A:312[A]:GLU:N	1:A:312[A]:GLU:CD	2.69	0.50
6:B:422:EDO:H11	9:B:527:HOH:O	2.11	0.50
1:A:128:LEU:CD1	1:A:163[A]:VAL:HG11	2.43	0.49
1:A:308:VAL:O	6:A:418:EDO:H21	2.11	0.49
1:A:205[A]:GLU:HG2	6:B:426:EDO:H12	1.94	0.49
1:B:131:PRO:HD3	2:B:401[B]:W88:H12	1.93	0.49
6:B:429:EDO:C2	9:B:875:HOH:O	2.49	0.49
1:A:203:ASP:HB2	6:A:434:EDO:H21	1.95	0.48
1:A:223[B]:LYS:HG3	1:A:252:TYR:CE1	2.48	0.48
1:B:160:PRO:HB2	6:B:425:EDO:H22	1.95	0.48
6:A:435:EDO:H22	9:A:657:HOH:O	2.12	0.48
1:B:104:GLU:HB3	7:B:432:PEG:H31	1.95	0.48
1:A:9:HIS:HE1	9:A:522:HOH:O	1.97	0.48
1:A:138[A]:GLN:CG	9:A:855:HOH:O	2.59	0.48
4:A:415:CAC:C1	9:A:784:HOH:O	2.62	0.48
3:B:412:GOL:H11	9:B:628:HOH:O	2.14	0.48
1:A:7:LEU:O	1:A:9:HIS:HD2	1.97	0.48
1:A:212:LYS:NZ	1:B:312:GLU:HG2	2.28	0.47
1:B:130[A]:CYS:SG	9:B:832:HOH:O	2.28	0.47
1:A:182:ASN:O	6:A:435:EDO:C2	2.63	0.47
1:A:2:LEU:N	7:A:437[B]:PEG:C2	2.77	0.47
1:A:91:LYS:O	6:A:423:EDO:C2	2.61	0.47
1:A:2:LEU:N	7:A:437[A]:PEG:C2	2.77	0.47
1:A:37:SER:O	6:A:423:EDO:H11	2.14	0.47
1:B:77:ASP:H	6:B:416:EDO:H11	1.78	0.47
1:B:210:VAL:HA	3:B:410:GOL:H31	1.97	0.47
1:A:130[B]:CYS:C	1:A:131:PRO:CA	2.77	0.46
6:A:434:EDO:C1	9:A:734[A]:HOH:O	2.59	0.46
1:A:2:LEU:H	7:A:437[A]:PEG:C1	2.25	0.46
7:A:436:PEG:H21	7:A:436:PEG:H41	1.49	0.46
1:B:129:SER:HA	1:B:138:GLN:NE2	2.31	0.46
6:A:432:EDO:C1	9:A:579:HOH:O	2.64	0.46
1:B:223[A]:LYS:HE3	3:B:412:GOL:H2	1.97	0.46
1:A:34:ALA:HB3	3:A:402[A]:GOL:H11	1.97	0.46
1:A:186:LEU:HD21	7:A:440:PEG:H31	1.98	0.46
7:A:438:PEG:C3	7:A:440:PEG:H11	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASN:HB2	9:A:591:HOH:O	2.16	0.45
6:B:424:EDO:C2	9:B:634:HOH:O	2.63	0.45
1:A:106:ASN:ND2	1:A:149[B]:TYR:OH	2.49	0.45
1:B:223[B]:LYS:HZ1	3:B:412:GOL:H2	1.81	0.45
6:B:424:EDO:H21	9:B:634:HOH:O	2.16	0.45
1:A:2:LEU:N	7:A:437[A]:PEG:H21	2.31	0.45
1:A:182:ASN:O	6:A:435:EDO:C1	2.65	0.44
1:B:108:ALA:HB2	7:B:432:PEG:H12	1.98	0.44
1:A:107:VAL:O	1:A:111[A]:ARG:HG3	2.17	0.44
1:A:163[A]:VAL:CG1	1:A:165:MET:SD	3.05	0.44
1:A:130[B]:CYS:SG	1:A:131:PRO:HD2	2.59	0.43
7:B:431[B]:PEG:O1	7:B:431[B]:PEG:C3	2.55	0.43
3:A:406:GOL:O3	6:A:434:EDO:C2	2.66	0.43
6:B:416:EDO:C2	9:B:539:HOH:O	2.66	0.43
6:A:425:EDO:H21	9:A:633:HOH:O	2.18	0.43
1:B:307[B]:ARG:NH2	9:B:825:HOH:O	2.44	0.43
1:A:130[B]:CYS:O	1:A:138[B]:GLN:NE2	2.49	0.43
1:B:105:GLU:HG2	1:B:109:MET:HE2	2.01	0.43
1:B:130[B]:CYS:SG	1:B:131:PRO:N	2.90	0.43
1:A:155:LEU:HB2	7:A:438:PEG:H11	2.01	0.43
6:B:424:EDO:H11	9:B:512:HOH:O	2.19	0.43
1:A:238:ARG:NH2	6:A:418:EDO:H22	2.34	0.43
1:A:138[B]:GLN:HG3	1:B:170:ASP:OD2	2.19	0.42
1:B:188:LYS:HE3	9:B:909:HOH:O	2.19	0.42
3:A:414:GOL:H32	9:A:739:HOH:O	2.19	0.42
1:A:205[A]:GLU:HA	6:B:426:EDO:H21	2.01	0.42
1:B:2:LEU:HG	6:B:427:EDO:H12	2.00	0.42
6:B:420:EDO:H12	9:B:829:HOH:O	2.19	0.42
1:A:98[A]:ILE:O	1:A:98[A]:ILE:CG1	2.67	0.42
1:B:13:ASN:HB2	1:B:14:PRO:HD2	2.01	0.42
6:A:435:EDO:H12	9:A:657:HOH:O	2.18	0.42
1:B:241:PRO:HA	3:B:408:GOL:C3	2.49	0.42
1:B:97:SER:HA	1:B:125:GLU:O	2.20	0.42
7:B:433:PEG:H12	9:B:938[A]:HOH:O	2.19	0.42
1:A:20:GLY:HA3	5:A:417:FMN:N5	2.35	0.42
1:A:205[B]:GLU:HA	6:B:426:EDO:H21	2.02	0.42
6:A:420:EDO:C1	9:A:611:HOH:O	2.68	0.42
1:A:128:LEU:HD11	1:A:163[B]:VAL:CG2	2.43	0.41
1:A:308:VAL:O	6:A:418:EDO:C2	2.68	0.41
1:A:50:ARG:HA	6:A:420:EDO:H12	2.02	0.41
6:A:431:EDO:H22	9:A:689:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111[B]:ARG:NH2	7:B:432:PEG:C1	2.81	0.41
1:B:160:PRO:HB3	1:B:188:LYS:HG3	2.03	0.41
1:A:107:VAL:O	1:A:111[B]:ARG:HG3	2.19	0.41
1:B:77:ASP:H	6:B:416:EDO:C1	2.33	0.41
1:A:3[C]:LYS:HZ2	1:A:3[C]:LYS:HB3	1.85	0.41
1:A:307:ARG:HH22	6:A:426:EDO:H22	1.86	0.41
7:A:436:PEG:H12	1:B:168:TYR:HA	2.03	0.41
1:B:277:GLU:CB	6:B:418:EDO:H12	2.40	0.41
1:A:295:ARG:HH21	6:A:424:EDO:C1	2.34	0.40
3:A:403:GOL:H31	1:B:217:PHE:CE1	2.56	0.40
1:A:311:ILE:HG22	1:A:312[A]:GLU:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/314 (105%)	323 (98%)	6 (2%)	1 (0%)	36	16
1	B	329/314 (105%)	318 (97%)	11 (3%)	0	100	100
All	All	659/628 (105%)	641 (97%)	17 (3%)	1 (0%)	43	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	MET

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/259 (107%)	274 (99%)	4 (1%)	59	28
1	B	276/259 (107%)	272 (99%)	4 (1%)	59	28
All	All	554/518 (107%)	546 (99%)	8 (1%)	63	28

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	291	GLU
1	A	312[A]	GLU
1	A	312[B]	GLU
1	B	118	GLN
1	B	307[A]	ARG
1	B	307[B]	ARG
1	B	312	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	9	HIS
1	A	87	HIS
1	A	132	ASN
1	A	234	ASN
1	A	275	GLN
1	B	53	ASN
1	B	87	HIS
1	B	132	ASN
1	B	138	GLN
1	B	234	ASN
1	B	275	GLN

5.3.3 RNA ⓘ

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](#)

82 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	$\# Z > 2$
3	GOL	B	404[A]	-	5,5,5	0.99	0	5,5,5	0.79	0
3	GOL	A	402[A]	-	5,5,5	1.16	0	5,5,5	0.77	0
8	NCO	A	442[B]	-	6,6,6	1.32	1 (16%)	-		
5	FMN	B	415	-	33,33,33	1.41	5 (15%)	48,50,50	1.21	6 (12%)
7	PEG	A	437[B]	-	6,6,6	0.67	0	5,5,5	1.46	1 (20%)
6	EDO	A	428	-	3,3,3	0.59	0	2,2,2	0.43	0
6	EDO	B	423	-	3,3,3	0.80	0	2,2,2	0.98	0
6	EDO	B	425	-	3,3,3	0.96	0	2,2,2	0.75	0
7	PEG	B	431[B]	-	6,6,6	0.54	0	5,5,5	0.81	0
7	PEG	A	436	-	6,6,6	1.03	1 (16%)	5,5,5	1.58	2 (40%)
3	GOL	A	412	-	5,5,5	0.84	0	5,5,5	1.49	1 (20%)
7	PEG	B	432	-	6,6,6	1.30	0	5,5,5	1.66	2 (40%)
3	GOL	B	411	-	5,5,5	0.70	0	5,5,5	0.96	0
6	EDO	B	419	-	3,3,3	0.73	0	2,2,2	0.72	0
3	GOL	A	407[B]	-	5,5,5	0.38	0	5,5,5	0.73	0
6	EDO	B	417	-	3,3,3	0.23	0	2,2,2	1.17	0
7	PEG	A	440	-	6,6,6	0.51	0	5,5,5	0.96	0
6	EDO	B	427	-	3,3,3	0.65	0	2,2,2	0.59	0
6	EDO	A	431	-	3,3,3	0.76	0	2,2,2	0.36	0
3	GOL	A	402[B]	-	5,5,5	1.21	0	5,5,5	1.34	1 (20%)
6	EDO	A	433	-	3,3,3	1.14	0	2,2,2	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	412	-	5,5,5	0.65	0	5,5,5	0.96	0
6	EDO	B	426	-	3,3,3	0.52	0	2,2,2	1.08	0
6	EDO	A	426	-	3,3,3	0.51	0	2,2,2	0.34	0
3	GOL	A	403	-	5,5,5	0.95	0	5,5,5	1.23	0
3	GOL	A	411	-	5,5,5	0.87	0	5,5,5	0.84	0
3	GOL	B	407	-	5,5,5	0.68	0	5,5,5	0.81	0
2	W88	B	401[B]	-	30,30,30	1.53	5 (16%)	40,42,42	1.11	4 (10%)
8	NCO	A	441	-	6,6,6	3.11	6 (100%)	-		
3	GOL	A	408	-	5,5,5	0.41	0	5,5,5	0.58	0
6	EDO	A	434	-	3,3,3	0.45	0	2,2,2	0.83	0
3	GOL	A	410	-	5,5,5	0.91	0	5,5,5	1.46	1 (20%)
6	EDO	A	435	-	3,3,3	0.85	0	2,2,2	0.44	0
6	EDO	B	429	-	3,3,3	0.54	0	2,2,2	0.31	0
3	GOL	B	403	-	5,5,5	1.32	1 (20%)	5,5,5	1.15	0
4	CAC	B	414	-	2,4,4	2.79	2 (100%)	4,6,6	1.84	2 (50%)
6	EDO	B	420	-	3,3,3	0.57	0	2,2,2	0.14	0
3	GOL	A	405	-	5,5,5	1.47	1 (20%)	5,5,5	1.82	1 (20%)
3	GOL	A	409	-	5,5,5	0.81	0	5,5,5	1.23	1 (20%)
3	GOL	B	409	-	5,5,5	0.69	0	5,5,5	0.64	0
6	EDO	B	416	-	3,3,3	1.38	0	2,2,2	1.34	0
3	GOL	A	406	-	5,5,5	0.84	0	5,5,5	1.55	2 (40%)
4	CAC	A	415	-	2,4,4	5.64	2 (100%)	4,6,6	8.37	3 (75%)
6	EDO	B	422	-	3,3,3	0.35	0	2,2,2	0.03	0
6	EDO	A	427	-	3,3,3	0.54	0	2,2,2	0.03	0
3	GOL	B	404[B]	-	5,5,5	0.47	0	5,5,5	1.54	2 (40%)
6	EDO	B	430	-	3,3,3	0.84	0	2,2,2	0.40	0
3	GOL	A	404	-	5,5,5	0.50	0	5,5,5	0.55	0
3	GOL	B	405	-	5,5,5	0.99	0	5,5,5	1.48	1 (20%)
4	CAC	B	413	-	2,4,4	4.96	2 (100%)	4,6,6	3.97	3 (75%)
6	EDO	A	418	-	3,3,3	1.08	0	2,2,2	0.59	0
8	NCO	A	442[A]	-	6,6,6	1.01	0	-		
7	PEG	A	438	-	6,6,6	0.37	0	5,5,5	1.43	0
7	PEG	B	433	-	6,6,6	0.42	0	5,5,5	0.95	0
7	PEG	A	437[A]	-	6,6,6	0.81	0	5,5,5	1.59	1 (20%)
6	EDO	A	432	-	3,3,3	0.78	0	2,2,2	0.64	0
3	GOL	A	414	-	5,5,5	0.49	0	5,5,5	0.29	0
3	GOL	B	410	-	5,5,5	0.58	0	5,5,5	1.53	1 (20%)
7	PEG	A	439	-	6,6,6	0.73	0	5,5,5	1.78	1 (20%)
6	EDO	A	420	-	3,3,3	0.89	0	2,2,2	1.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	407[A]	-	5,5,5	0.30	0	5,5,5	0.38	0
3	GOL	B	408	-	5,5,5	1.18	1 (20%)	5,5,5	1.07	0
6	EDO	A	423	-	3,3,3	0.76	0	2,2,2	0.97	0
6	EDO	A	424	-	3,3,3	0.52	0	2,2,2	0.37	0
6	EDO	B	424	-	3,3,3	0.94	0	2,2,2	1.71	1 (50%)
6	EDO	A	422	-	3,3,3	1.00	0	2,2,2	0.41	0
6	EDO	A	430	-	3,3,3	0.61	0	2,2,2	0.51	0
6	EDO	A	419	-	3,3,3	0.52	0	2,2,2	0.40	0
4	CAC	A	416	-	2,4,4	4.58	2 (100%)	4,6,6	1.63	1 (25%)
3	GOL	B	406	-	5,5,5	0.39	0	5,5,5	0.36	0
2	W88	B	401[A]	-	30,30,30	1.75	6 (20%)	40,42,42	1.29	6 (15%)
6	EDO	B	428	-	3,3,3	0.57	0	2,2,2	0.17	0
6	EDO	B	421	-	3,3,3	0.58	0	2,2,2	0.31	0
3	GOL	A	413	-	5,5,5	0.81	0	5,5,5	1.02	0
7	PEG	B	431[A]	-	6,6,6	0.57	0	5,5,5	0.38	0
2	W88	A	401	-	30,30,30	1.74	7 (23%)	40,42,42	1.31	7 (17%)
6	EDO	A	421	-	3,3,3	0.34	0	2,2,2	1.36	0
6	EDO	B	418	-	3,3,3	0.80	0	2,2,2	0.77	0
6	EDO	A	429	-	3,3,3	0.88	0	2,2,2	0.36	0
6	EDO	A	425	-	3,3,3	0.81	0	2,2,2	0.21	0
3	GOL	B	402	-	5,5,5	0.62	0	5,5,5	1.12	0
5	FMN	A	417	-	33,33,33	1.34	3 (9%)	48,50,50	1.31	6 (12%)

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	GOL	B	404[A]	-	-	0/4/4/4	-
3	GOL	B	405	-	-	0/4/4/4	-
6	EDO	A	419	-	-	0/1/1/1	-
3	GOL	A	402[A]	-	-	0/4/4/4	-
3	GOL	A	411	-	-	4/4/4/4	-
3	GOL	B	407	-	-	2/4/4/4	-
2	W88	B	401[B]	-	-	3/15/15/15	0/3/3/3
3	GOL	B	406	-	-	2/4/4/4	-
2	W88	B	401[A]	-	-	8/15/15/15	0/3/3/3
3	GOL	A	408	-	-	0/4/4/4	-
6	EDO	A	434	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FMN	B	415	-	-	1/18/18/18	0/3/3/3
3	GOL	A	410	-	-	1/4/4/4	-
6	EDO	A	435	-	-	1/1/1/1	-
6	EDO	B	428	-	-	0/1/1/1	-
6	EDO	A	418	-	-	1/1/1/1	-
7	PEG	A	437[B]	-	-	4/4/4/4	-
6	EDO	A	428	-	-	0/1/1/1	-
7	PEG	A	438	-	-	3/4/4/4	-
6	EDO	B	423	-	-	0/1/1/1	-
7	PEG	A	437[A]	-	-	4/4/4/4	-
7	PEG	B	433	-	-	0/4/4/4	-
6	EDO	B	425	-	-	0/1/1/1	-
7	PEG	B	431[B]	-	-	3/4/4/4	-
7	PEG	A	436	-	-	2/4/4/4	-
6	EDO	B	421	-	-	1/1/1/1	-
6	EDO	B	429	-	-	1/1/1/1	-
3	GOL	A	412	-	-	0/4/4/4	-
6	EDO	A	430	-	-	1/1/1/1	-
7	PEG	B	432	-	-	3/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-
6	EDO	A	432	-	-	1/1/1/1	-
3	GOL	A	413	-	-	4/4/4/4	-
3	GOL	A	414	-	-	2/4/4/4	-
6	EDO	B	420	-	-	0/1/1/1	-
3	GOL	B	410	-	-	2/4/4/4	-
3	GOL	A	405	-	-	3/4/4/4	-
7	PEG	A	439	-	-	2/4/4/4	-
3	GOL	A	409	-	-	1/4/4/4	-
3	GOL	B	409	-	-	0/4/4/4	-
3	GOL	B	411	-	-	1/4/4/4	-
6	EDO	B	419	-	-	1/1/1/1	-
7	PEG	B	431[A]	-	-	3/4/4/4	-
3	GOL	A	407[B]	-	-	4/4/4/4	-
6	EDO	B	417	-	-	0/1/1/1	-
7	PEG	A	440	-	-	3/4/4/4	-
6	EDO	B	416	-	-	0/1/1/1	-
3	GOL	A	406	-	-	0/4/4/4	-
6	EDO	A	420	-	-	1/1/1/1	-
3	GOL	A	407[A]	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	W88	A	401	-	-	3/15/15/15	0/3/3/3
6	EDO	B	427	-	-	1/1/1/1	-
3	GOL	B	408	-	-	4/4/4/4	-
6	EDO	A	431	-	-	0/1/1/1	-
6	EDO	A	423	-	-	1/1/1/1	-
6	EDO	A	421	-	-	1/1/1/1	-
6	EDO	A	427	-	-	1/1/1/1	-
6	EDO	B	422	-	-	1/1/1/1	-
6	EDO	B	426	-	-	0/1/1/1	-
6	EDO	A	424	-	-	1/1/1/1	-
6	EDO	B	424	-	-	1/1/1/1	-
6	EDO	A	422	-	-	1/1/1/1	-
3	GOL	A	402[B]	-	-	0/4/4/4	-
6	EDO	A	429	-	-	1/1/1/1	-
6	EDO	A	425	-	-	0/1/1/1	-
3	GOL	B	404[B]	-	-	4/4/4/4	-
3	GOL	B	412	-	-	2/4/4/4	-
6	EDO	A	433	-	-	1/1/1/1	-
3	GOL	A	404	-	-	0/4/4/4	-
6	EDO	B	418	-	-	1/1/1/1	-
6	EDO	B	430	-	-	1/1/1/1	-
6	EDO	A	426	-	-	1/1/1/1	-
3	GOL	B	402	-	-	2/4/4/4	-
5	FMN	A	417	-	-	2/18/18/18	0/3/3/3
3	GOL	A	403	-	-	0/4/4/4	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	415	CAC	AS-C1	7.51	2.08	1.90
4	B	413	CAC	AS-C2	6.57	2.05	1.90
2	B	401[A]	W88	CAV-CAS	-6.14	1.36	1.49
5	A	417	FMN	C4-N3	-4.76	1.29	1.38
4	A	416	CAC	AS-C2	4.59	2.01	1.90
4	A	416	CAC	AS-C1	4.57	2.01	1.90
2	A	401	W88	CAL-CAV	3.98	1.44	1.37
8	A	441	NCO	CO-N3	3.82	2.08	1.96
5	B	415	FMN	C4-N3	-3.79	1.31	1.38
2	B	401[B]	W88	CAV-CAS	-3.64	1.41	1.49
8	A	441	NCO	CO-N5	3.56	2.08	1.96
2	B	401[B]	W88	CAO-CAU	-3.55	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	W88	CAV-CAS	-3.40	1.42	1.49
2	B	401[A]	W88	CAO-CAU	-3.34	1.42	1.51
8	A	441	NCO	CO-N6	3.25	2.07	1.96
2	A	401	W88	CAO-CAU	-3.09	1.43	1.51
5	A	417	FMN	O4-C4	3.03	1.29	1.23
2	B	401[B]	W88	OAE-CAS	-3.01	1.21	1.30
2	B	401[B]	W88	CAP-CAW	-2.94	1.43	1.51
4	B	414	CAC	AS-C2	2.83	1.97	1.90
5	B	415	FMN	C8M-C8	-2.76	1.45	1.51
8	A	441	NCO	CO-N4	2.75	2.05	1.96
4	B	414	CAC	AS-C1	2.75	1.96	1.90
4	A	415	CAC	AS-C2	2.68	1.96	1.90
2	A	401	W88	CAJ-CAH	2.66	1.42	1.36
8	A	441	NCO	CO-N2	2.59	2.05	1.96
5	B	415	FMN	C6-C5A	-2.59	1.36	1.40
2	B	401[A]	W88	CAP-CAW	-2.57	1.44	1.51
2	A	401	W88	CAI-CAG	2.51	1.42	1.36
4	B	413	CAC	AS-C1	2.45	1.96	1.90
3	A	405	GOL	C3-C2	2.43	1.61	1.51
8	A	441	NCO	CO-N1	2.42	2.04	1.96
3	B	403	GOL	O2-C2	-2.41	1.36	1.43
2	B	401[B]	W88	CAJ-CAH	2.16	1.41	1.36
5	A	417	FMN	C2'-C3'	-2.16	1.49	1.53
3	B	408	GOL	C1-C2	2.15	1.60	1.51
5	B	415	FMN	O4-C4	2.15	1.27	1.23
2	B	401[A]	W88	CAL-CAV	2.13	1.41	1.37
2	A	401	W88	OAF-CAT	-2.13	1.24	1.30
5	B	415	FMN	C9-C8	2.12	1.42	1.39
2	B	401[A]	W88	CAI-CBB	-2.10	1.37	1.42
2	A	401	W88	CAM-CAO	2.05	1.61	1.52
8	A	442[B]	NCO	CO-N5	2.05	2.03	1.96
7	A	436	PEG	O4-C4	-2.04	1.31	1.42
2	B	401[A]	W88	CAZ-CAW	-2.02	1.41	1.44

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	415	CAC	O1-AS-C1	-15.75	91.92	111.50
4	B	413	CAC	O1-AS-C1	-6.12	103.89	111.50
4	A	415	CAC	O1-AS-C2	5.16	117.92	111.50
4	B	413	CAC	O2-AS-C2	-3.99	96.16	105.84
5	A	417	FMN	C4-C4A-N5	3.63	123.22	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	439	PEG	O2-C2-C1	-3.52	94.60	110.11
3	A	405	GOL	O3-C3-C2	3.52	126.20	110.38
7	A	437[A]	PEG	C3-O2-C2	3.48	128.48	113.26
4	B	413	CAC	O2-AS-C1	3.08	113.30	105.84
5	A	417	FMN	O4-C4-C4A	-2.93	118.81	126.53
7	A	437[B]	PEG	C3-O2-C2	2.89	125.91	113.26
5	B	415	FMN	C5A-C6-C7	2.86	126.13	120.83
5	B	415	FMN	C7M-C7-C6	2.86	124.61	119.57
2	B	401[A]	W88	CAV-CAL-CBB	-2.73	116.99	121.19
2	B	401[A]	W88	CAH-CAV-CAS	-2.73	114.98	120.37
5	A	417	FMN	C4A-C4-N3	2.63	119.94	113.25
3	A	410	GOL	C3-C2-C1	-2.62	102.20	111.80
2	B	401[A]	W88	CAW-CAZ-NAR	2.62	117.69	115.70
5	A	417	FMN	C9A-C5A-N5	-2.53	119.77	122.45
4	B	414	CAC	O1-AS-C2	-2.53	108.35	111.50
3	A	402[B]	GOL	C3-C2-C1	2.53	121.08	111.80
2	B	401[B]	W88	CAI-CBB-CAL	-2.52	117.67	122.00
5	B	415	FMN	C6-C7-C8	-2.50	116.02	119.69
5	A	417	FMN	C7M-C7-C6	2.45	123.89	119.57
6	B	424	EDO	O2-C2-C1	-2.42	93.98	112.39
5	A	417	FMN	C4-C4A-C10	-2.41	112.81	116.93
2	B	401[A]	W88	CAH-CAV-CAL	2.40	122.11	119.21
2	A	401	W88	OAB-CAT-CAX	-2.38	116.05	120.20
3	B	410	GOL	O1-C1-C2	-2.37	99.71	110.38
2	B	401[B]	W88	CAW-CAZ-NAR	2.36	117.50	115.70
2	A	401	W88	NAR-CAY-NAQ	2.36	119.44	115.74
4	A	415	CAC	O2-AS-C1	2.35	111.53	105.84
2	A	401	W88	CAJ-CAH-CAV	-2.32	118.03	120.78
3	A	406	GOL	O2-C2-C1	2.32	118.78	109.18
7	B	432	PEG	O2-C2-C1	2.30	120.27	110.11
7	A	436	PEG	O2-C3-C4	-2.29	100.03	110.11
2	A	401	W88	OAE-CAS-CAV	2.28	120.69	114.84
2	B	401[B]	W88	OAE-CAS-OAA	-2.28	118.45	123.35
2	B	401[A]	W88	OAE-CAS-CAV	2.26	120.64	114.84
3	A	406	GOL	O2-C2-C3	-2.25	99.87	109.18
3	B	405	GOL	O1-C1-C2	2.25	120.50	110.38
7	B	432	PEG	O1-C1-C2	2.24	125.01	111.82
2	B	401[B]	W88	CAN-CAM-CAO	-2.21	104.49	113.74
3	A	409	GOL	O3-C3-C2	2.19	120.25	110.38
2	B	401[A]	W88	OAA-CAS-CAV	-2.18	115.74	121.46
2	A	401	W88	CAZ-NAR-CAY	-2.17	123.38	126.37
4	A	416	CAC	O2-AS-C2	-2.16	100.61	105.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	412	GOL	O2-C2-C1	2.15	118.09	109.18
2	A	401	W88	CAJ-CBA-CBB	2.09	122.49	118.91
2	A	401	W88	OAC-CAY-NAQ	-2.09	118.16	121.86
5	B	415	FMN	C9A-C5A-N5	-2.07	120.25	122.45
3	B	404[B]	GOL	O2-C2-C1	-2.07	100.59	109.18
5	B	415	FMN	O2-C2-N1	-2.05	118.39	121.80
4	B	414	CAC	O2-AS-C1	2.05	110.80	105.84
3	B	404[B]	GOL	O2-C2-C3	2.04	117.62	109.18
5	B	415	FMN	C6-C5A-N5	2.04	121.83	118.44
7	A	436	PEG	O1-C1-C2	2.04	123.81	111.82

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	W88	OAF-CAT-CAX-NAQ
2	B	401[A]	W88	OAF-CAT-CAX-NAQ
2	B	401[B]	W88	OAF-CAT-CAX-NAQ
3	A	405	GOL	O1-C1-C2-C3
3	A	405	GOL	C1-C2-C3-O3
3	A	407[B]	GOL	O1-C1-C2-C3
3	A	407[B]	GOL	C1-C2-C3-O3
3	A	411	GOL	O1-C1-C2-C3
3	A	411	GOL	C1-C2-C3-O3
3	A	411	GOL	O2-C2-C3-O3
3	A	414	GOL	C1-C2-C3-O3
3	A	414	GOL	O2-C2-C3-O3
3	B	404[B]	GOL	C1-C2-C3-O3
3	B	407	GOL	O1-C1-C2-O2
3	B	407	GOL	O1-C1-C2-C3
3	B	410	GOL	O1-C1-C2-O2
3	B	410	GOL	O1-C1-C2-C3
3	B	412	GOL	O1-C1-C2-C3
2	B	401[A]	W88	OAA-CAS-CAV-CAH
2	B	401[A]	W88	OAA-CAS-CAV-CAL
2	B	401[A]	W88	OAE-CAS-CAV-CAL
2	B	401[A]	W88	OAE-CAS-CAV-CAH
7	A	436	PEG	C4-C3-O2-C2
7	B	431[B]	PEG	C1-C2-O2-C3
3	A	405	GOL	O1-C1-C2-O2
3	A	411	GOL	O1-C1-C2-O2
3	B	404[B]	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	A	436	PEG	O1-C1-C2-O2
7	A	437[A]	PEG	O1-C1-C2-O2
7	A	438	PEG	O2-C3-C4-O4
7	A	439	PEG	O2-C3-C4-O4
7	B	431[B]	PEG	O2-C3-C4-O4
3	A	413	GOL	O1-C1-C2-C3
3	A	413	GOL	C1-C2-C3-O3
3	B	402	GOL	O1-C1-C2-C3
3	B	404[B]	GOL	O1-C1-C2-C3
3	B	406	GOL	O1-C1-C2-C3
3	B	408	GOL	O1-C1-C2-C3
3	B	408	GOL	C1-C2-C3-O3
7	A	437[B]	PEG	O1-C1-C2-O2
3	A	407[B]	GOL	O2-C2-C3-O3
3	A	413	GOL	O2-C2-C3-O3
3	B	402	GOL	O1-C1-C2-O2
3	B	412	GOL	O1-C1-C2-O2
7	A	440	PEG	C4-C3-O2-C2
7	A	439	PEG	O1-C1-C2-O2
6	A	418	EDO	O1-C1-C2-O2
6	B	427	EDO	O1-C1-C2-O2
6	B	430	EDO	O1-C1-C2-O2
7	B	432	PEG	O2-C3-C4-O4
7	A	440	PEG	O2-C3-C4-O4
2	B	401[A]	W88	CAN-CAM-CAO-CAU
3	A	407[B]	GOL	O1-C1-C2-O2
3	A	413	GOL	O1-C1-C2-O2
3	B	408	GOL	O1-C1-C2-O2
7	A	437[A]	PEG	O2-C3-C4-O4
7	B	431[A]	PEG	O2-C3-C4-O4
6	A	422	EDO	O1-C1-C2-O2
6	A	427	EDO	O1-C1-C2-O2
6	A	429	EDO	O1-C1-C2-O2
6	A	433	EDO	O1-C1-C2-O2
6	B	419	EDO	O1-C1-C2-O2
6	B	422	EDO	O1-C1-C2-O2
7	B	431[A]	PEG	C4-C3-O2-C2
3	B	404[B]	GOL	O1-C1-C2-O2
6	A	423	EDO	O1-C1-C2-O2
6	B	421	EDO	O1-C1-C2-O2
3	A	409	GOL	O2-C2-C3-O3
3	B	411	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	437[B]	PEG	C1-C2-O2-C3
7	A	438	PEG	C4-C3-O2-C2
7	A	437[B]	PEG	O2-C3-C4-O4
7	B	431[A]	PEG	C1-C2-O2-C3
6	A	432	EDO	O1-C1-C2-O2
2	A	401	W88	CAN-CAM-CAO-CAU
7	A	438	PEG	C1-C2-O2-C3
7	A	440	PEG	C1-C2-O2-C3
7	A	437[A]	PEG	C4-C3-O2-C2
7	B	431[B]	PEG	C4-C3-O2-C2
6	B	424	EDO	O1-C1-C2-O2
5	A	417	FMN	C4'-C5'-O5'-P
5	B	415	FMN	C4'-C5'-O5'-P
3	B	406	GOL	O1-C1-C2-O2
3	A	407[A]	GOL	C1-C2-C3-O3
6	A	420	EDO	O1-C1-C2-O2
6	A	426	EDO	O1-C1-C2-O2
7	B	432	PEG	C4-C3-O2-C2
6	A	430	EDO	O1-C1-C2-O2
3	A	410	GOL	O1-C1-C2-O2
6	A	421	EDO	O1-C1-C2-O2
3	B	408	GOL	O2-C2-C3-O3
7	A	437[A]	PEG	C1-C2-O2-C3
6	A	424	EDO	O1-C1-C2-O2
6	A	434	EDO	O1-C1-C2-O2
6	B	418	EDO	O1-C1-C2-O2
6	B	429	EDO	O1-C1-C2-O2
7	B	432	PEG	O1-C1-C2-O2
5	A	417	FMN	C2'-C3'-C4'-O4'
2	B	401[A]	W88	OAB-CAT-CAX-CAW
2	B	401[B]	W88	OAB-CAT-CAX-CAW
6	A	435	EDO	O1-C1-C2-O2
7	A	437[B]	PEG	C4-C3-O2-C2
2	B	401[A]	W88	OAB-CAT-CAX-NAQ
2	B	401[B]	W88	OAB-CAT-CAX-NAQ
2	A	401	W88	CAO-CAM-CAN-CAP

There are no ring outliers.

53 monomers are involved in 144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402[A]	GOL	1	0

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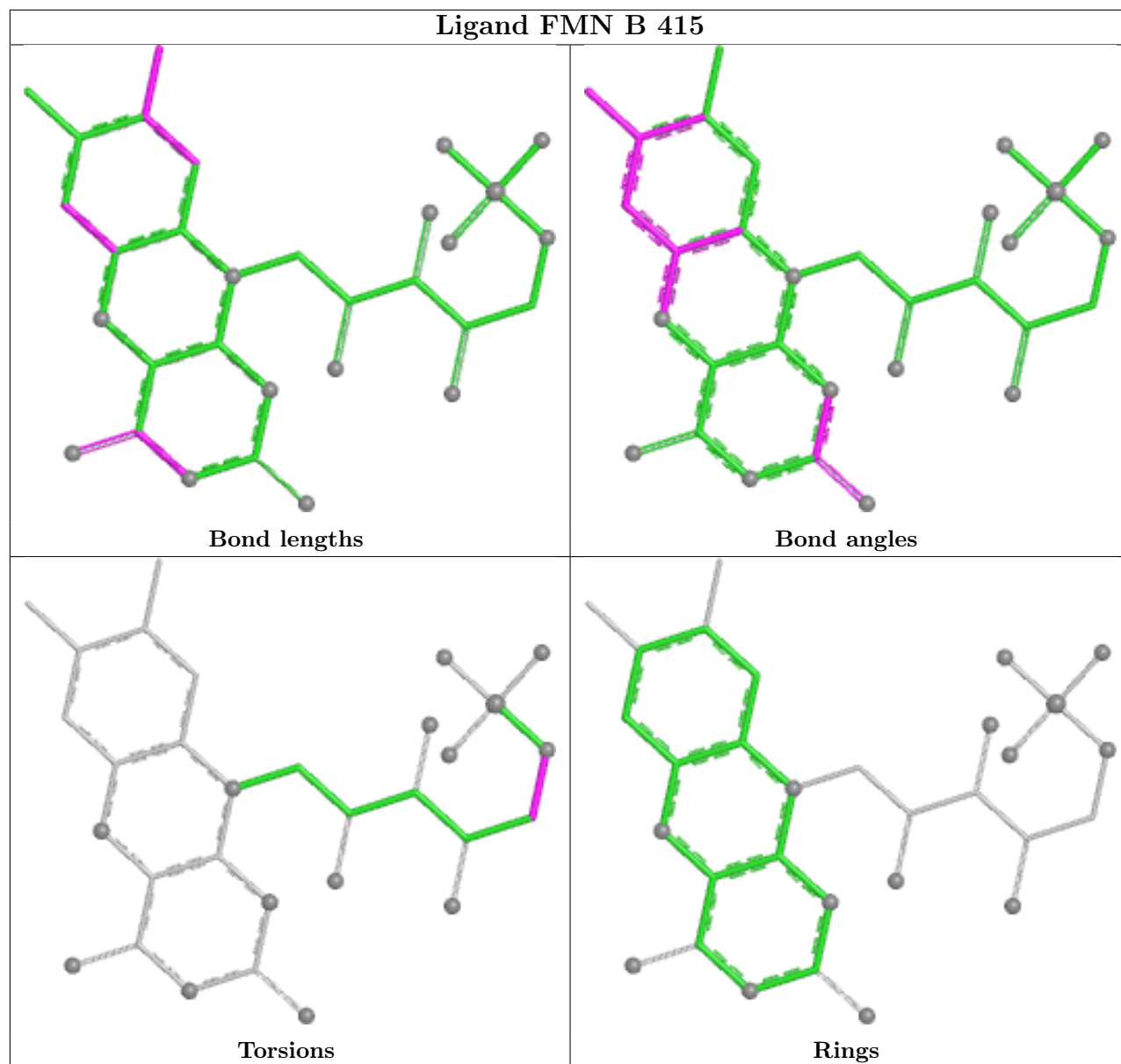
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	442[B]	NCO	1	0
7	A	437[B]	PEG	7	0
6	B	423	EDO	1	0
6	B	425	EDO	1	0
7	B	431[B]	PEG	3	0
7	A	436	PEG	3	0
7	B	432	PEG	9	0
6	B	419	EDO	2	0
7	A	440	PEG	10	0
6	B	427	EDO	1	0
6	A	431	EDO	1	0
6	A	433	EDO	4	0
3	B	412	GOL	5	0
6	B	426	EDO	3	0
6	A	426	EDO	1	0
3	A	403	GOL	1	0
3	A	411	GOL	1	0
2	B	401[B]	W88	3	0
6	A	434	EDO	6	0
6	A	435	EDO	7	0
6	B	429	EDO	3	0
6	B	420	EDO	1	0
3	B	409	GOL	1	0
6	B	416	EDO	6	0
3	A	406	GOL	1	0
4	A	415	CAC	1	0
6	B	422	EDO	1	0
6	A	427	EDO	2	0
6	B	430	EDO	2	0
6	A	418	EDO	3	0
8	A	442[A]	NCO	1	0
7	A	438	PEG	12	0
7	B	433	PEG	6	0
7	A	437[A]	PEG	9	0
6	A	432	EDO	1	0
3	A	414	GOL	1	0
3	B	410	GOL	2	0
7	A	439	PEG	4	0
6	A	420	EDO	3	0
3	B	408	GOL	2	0
6	A	423	EDO	4	0
6	A	424	EDO	1	0

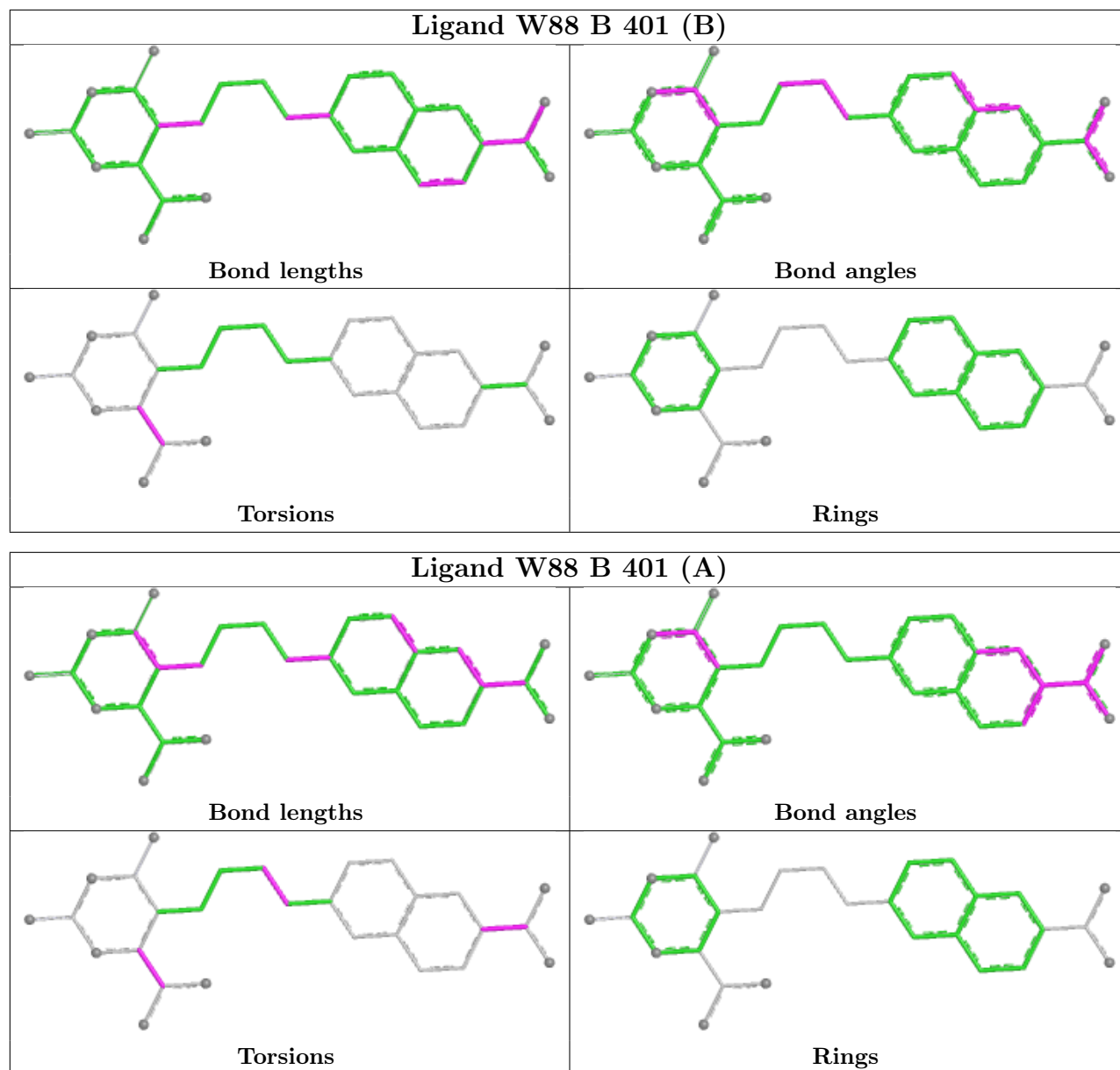
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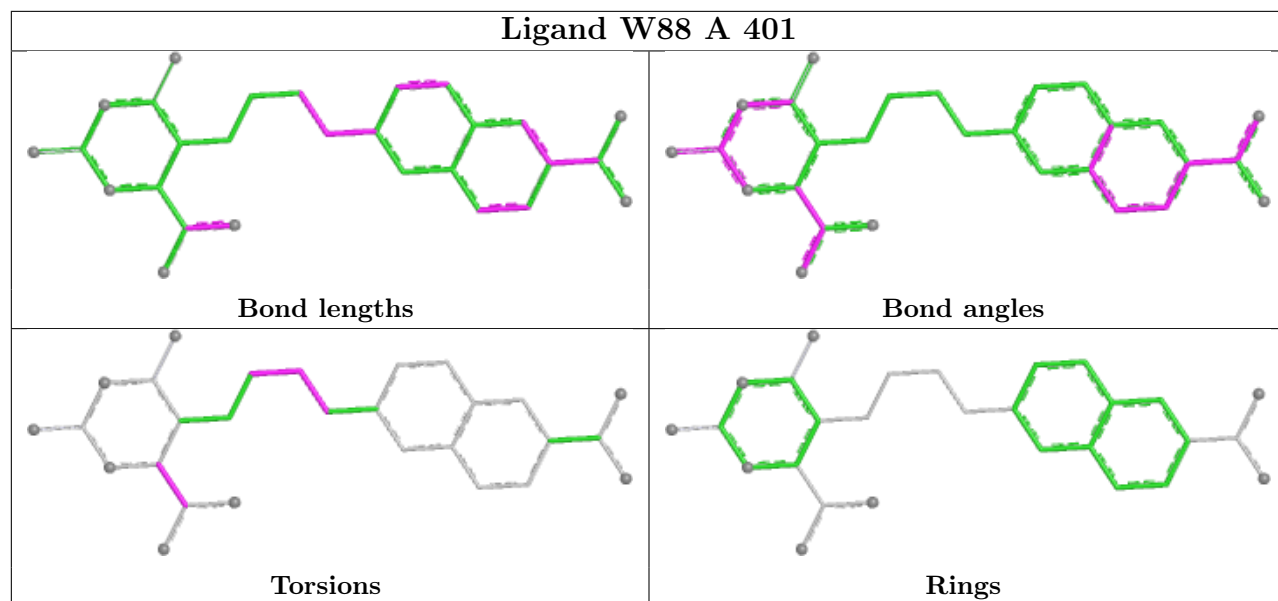
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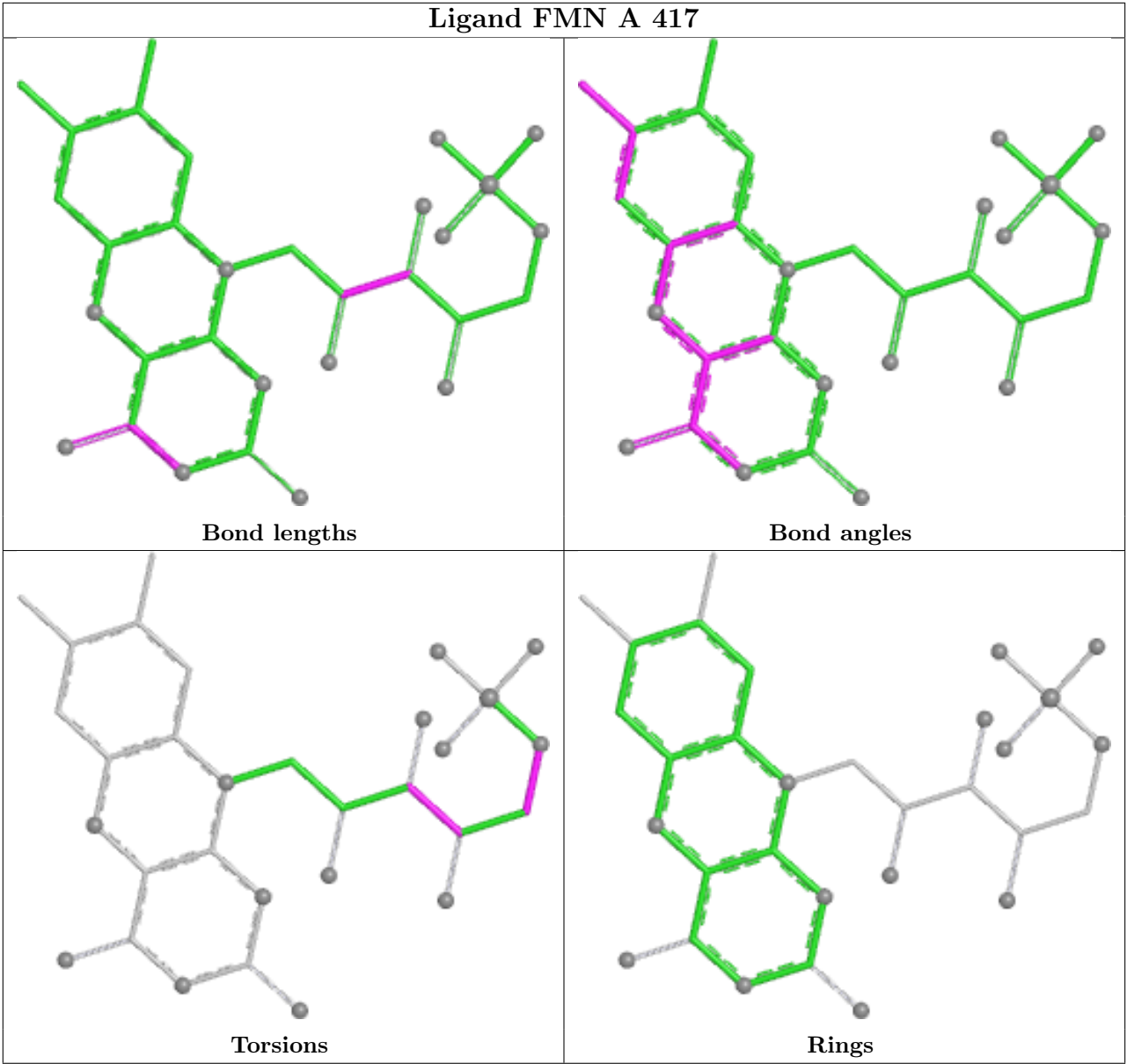
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	424	EDO	4	0
4	A	416	CAC	1	0
2	B	401[A]	W88	5	0
6	B	421	EDO	2	0
3	A	413	GOL	1	0
2	A	401	W88	1	0
6	B	418	EDO	4	0
6	A	425	EDO	1	0
3	B	402	GOL	2	0
5	A	417	FMN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	130[B]:CYS	C	131:PRO	N	1.73
1	A	130[A]:CYS	C	131:PRO	N	1.69

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	314/314 (100%)	-0.12	15 (4%) 35 38	3, 8, 25, 54	19 (6%)
1	B	314/314 (100%)	-0.36	6 (1%) 66 69	3, 8, 20, 45	17 (5%)
All	All	628/628 (100%)	-0.24	21 (3%) 49 51	3, 8, 22, 54	36 (5%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	PRO	7.0
1	A	133	VAL	6.7
1	A	134	PRO	5.1
1	A	-1	SER	4.8
1	A	130[A]	CYS	4.5
1	A	135	GLY	4.4
1	B	130[A]	CYS	3.8
1	A	132	ASN	3.6
1	B	131	PRO	3.4
1	B	-1	SER	3.2
1	B	312	GLU	3.1
1	A	312[A]	GLU	2.9
1	A	0	MET	2.8
1	A	5	ASN	2.7
1	B	134	PRO	2.4
1	A	3[A]	LYS	2.3
1	A	149[A]	TYR	2.3
1	A	136	LYS	2.2
1	A	163[A]	VAL	2.1
1	A	148	THR	2.1
1	B	132	ASN	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
7	PEG	B	431[A]	7/7	0.49	0.37	61,80,102,108	7
7	PEG	B	431[B]	7/7	0.49	0.37	23,26,27,29	7
3	GOL	A	411	6/6	0.51	0.21	46,61,66,74	0
4	CAC	B	414	5/5	0.53	0.24	142,150,164,166	0
6	EDO	A	430	4/4	0.56	0.32	63,68,70,72	0
7	PEG	A	437[A]	7/7	0.60	0.20	21,21,28,28	7
7	PEG	A	437[B]	7/7	0.60	0.20	20,21,26,27	7
6	EDO	A	419	4/4	0.61	0.23	57,59,64,65	0
6	EDO	A	422	4/4	0.65	0.21	39,56,57,59	0
6	EDO	B	420	4/4	0.66	0.18	56,61,62,63	0
6	EDO	A	431	4/4	0.67	0.18	40,52,52,58	0
3	GOL	B	411	6/6	0.67	0.18	51,52,54,55	0
6	EDO	A	427	4/4	0.69	0.15	52,53,56,58	0
6	EDO	A	428	4/4	0.70	0.20	48,50,51,56	0
3	GOL	A	408	6/6	0.70	0.20	46,51,62,64	0
6	EDO	B	428	4/4	0.72	0.17	50,52,54,56	0
6	EDO	B	430	4/4	0.72	0.14	35,37,39,44	0
6	EDO	A	435	4/4	0.74	0.16	33,37,38,44	0
6	EDO	A	429	4/4	0.74	0.18	36,39,40,44	0
3	GOL	B	402	6/6	0.75	0.16	23,33,39,39	0
3	GOL	A	407[A]	6/6	0.75	0.19	37,41,42,48	6
3	GOL	A	407[B]	6/6	0.75	0.19	20,28,29,30	6
6	EDO	B	429	4/4	0.76	0.16	33,40,45,55	0
6	EDO	B	423	4/4	0.76	0.16	39,46,46,49	0
3	GOL	B	408	6/6	0.76	0.14	30,34,38,47	0
3	GOL	A	409	6/6	0.77	0.18	30,34,38,51	0
7	PEG	A	439	7/7	0.77	0.14	24,31,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	426	4/4	0.78	0.18	54,57,60,61	0
3	GOL	B	404[B]	6/6	0.78	0.15	21,26,27,28	6
6	EDO	B	421	4/4	0.78	0.16	37,38,45,47	0
3	GOL	B	404[A]	6/6	0.78	0.15	16,18,21,25	6
6	EDO	B	417	4/4	0.79	0.16	32,35,35,41	0
6	EDO	A	425	4/4	0.79	0.14	31,35,41,41	0
3	GOL	A	414	6/6	0.79	0.16	39,50,52,56	0
7	PEG	A	440	7/7	0.81	0.12	27,33,36,43	0
7	PEG	B	432	7/7	0.81	0.14	22,26,30,34	0
6	EDO	A	418	4/4	0.82	0.15	17,24,29,30	0
3	GOL	B	407	6/6	0.83	0.14	25,40,41,45	0
6	EDO	A	432	4/4	0.83	0.12	34,40,41,42	0
6	EDO	A	433	4/4	0.83	0.13	20,25,30,36	0
6	EDO	B	422	4/4	0.83	0.15	27,32,34,35	0
6	EDO	A	423	4/4	0.83	0.13	20,23,27,38	0
3	GOL	A	412	6/6	0.84	0.14	29,40,43,44	0
6	EDO	B	419	4/4	0.84	0.12	27,31,34,35	0
7	PEG	A	438	7/7	0.84	0.11	29,32,34,34	0
6	EDO	B	426	4/4	0.84	0.14	26,34,35,39	0
3	GOL	B	409	6/6	0.85	0.12	22,37,39,40	0
3	GOL	A	413	6/6	0.85	0.13	29,37,39,40	0
3	GOL	B	412	6/6	0.85	0.14	22,32,36,49	0
3	GOL	B	406	6/6	0.85	0.12	29,40,44,54	0
3	GOL	B	410	6/6	0.86	0.11	26,30,33,37	0
3	GOL	A	403	6/6	0.86	0.11	23,23,25,29	0
7	PEG	B	433	7/7	0.86	0.14	19,29,39,46	0
6	EDO	A	424	4/4	0.87	0.14	33,34,40,42	0
6	EDO	A	421	4/4	0.87	0.14	29,30,34,38	0
6	EDO	B	427	4/4	0.87	0.14	20,28,34,38	0
3	GOL	A	410	6/6	0.88	0.11	24,27,28,41	0
6	EDO	B	416	4/4	0.88	0.10	18,23,24,35	0
4	CAC	A	416	5/5	0.88	0.25	30,34,39,43	0
6	EDO	B	425	4/4	0.88	0.12	24,29,30,30	0
3	GOL	B	405	6/6	0.88	0.12	17,22,23,26	0
6	EDO	A	434	4/4	0.88	0.12	25,25,26,29	0
3	GOL	A	405	6/6	0.89	0.12	17,21,32,32	0
6	EDO	A	420	4/4	0.90	0.11	24,29,30,31	0
3	GOL	A	406	6/6	0.90	0.11	21,27,27,30	0
2	W88	B	401[A]	28/28	0.91	0.14	6,13,34,36	28
3	GOL	B	403	6/6	0.91	0.10	22,24,26,26	0
2	W88	B	401[B]	28/28	0.91	0.14	6,14,26,29	28
4	CAC	A	415	5/5	0.92	0.26	11,17,21,22	0

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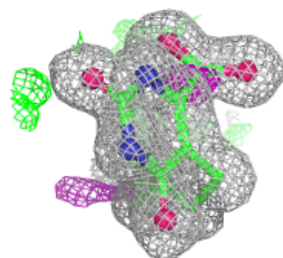
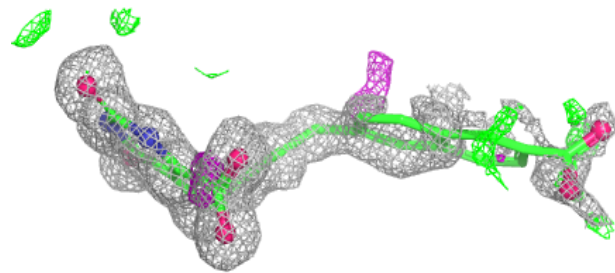
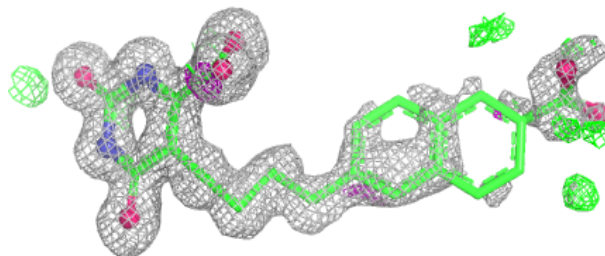
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PEG	A	436	7/7	0.93	0.13	13,25,28,33	0
6	EDO	B	424	4/4	0.93	0.24	16,22,22,27	0
4	CAC	B	413	5/5	0.94	0.22	12,16,18,20	0
3	GOL	A	402[A]	6/6	0.94	0.06	9,9,10,10	6
3	GOL	A	404	6/6	0.94	0.07	16,18,19,22	0
3	GOL	A	402[B]	6/6	0.94	0.06	9,10,11,12	6
2	W88	A	401	28/28	0.95	0.14	7,22,61,70	0
6	EDO	B	418	4/4	0.96	0.17	19,20,22,22	0
8	NCO	A	442[A]	7/7	0.96	0.13	16,17,19,21	7
8	NCO	A	442[B]	7/7	0.96	0.13	15,16,18,20	7
5	FMN	B	415	31/31	0.99	0.03	3,4,5,6	0
5	FMN	A	417	31/31	0.99	0.03	3,4,6,6	0
8	NCO	A	441	7/7	1.00	0.05	6,6,7,7	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.

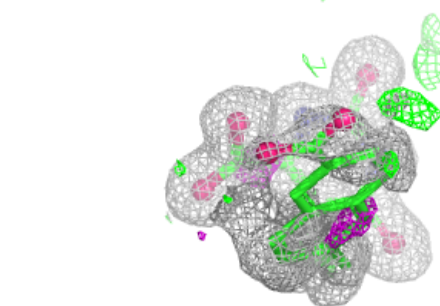
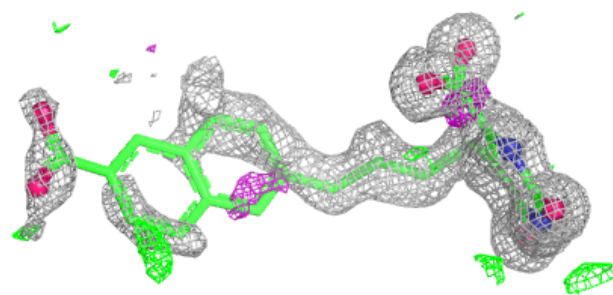
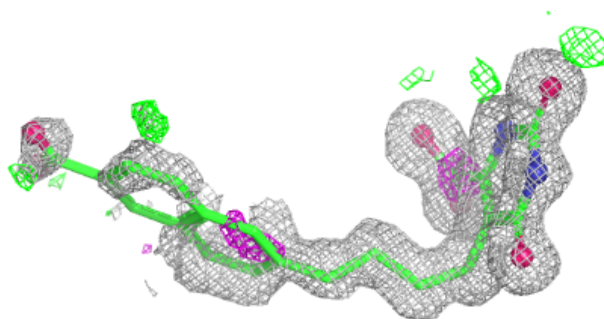
Electron density around W88 B 401 (A):

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

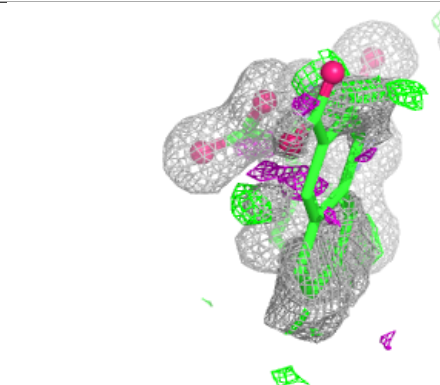
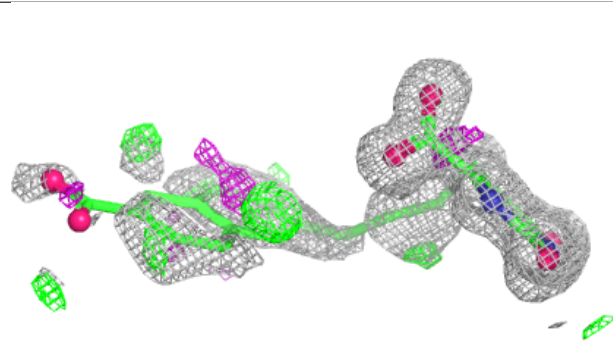
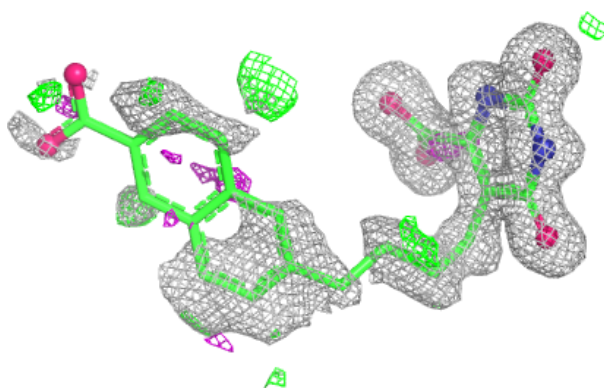


Electron density around W88 B 401 (B):

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

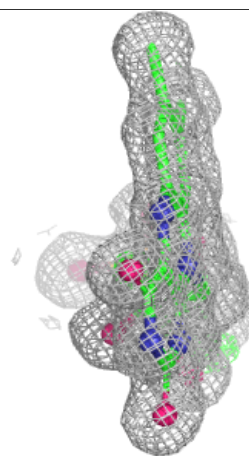
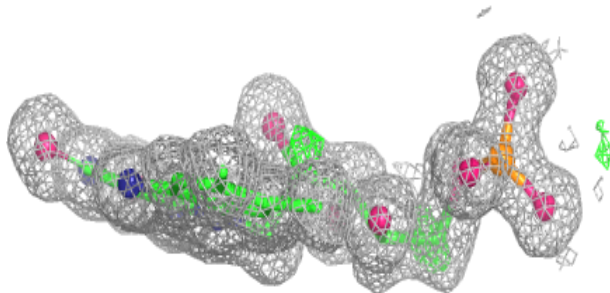
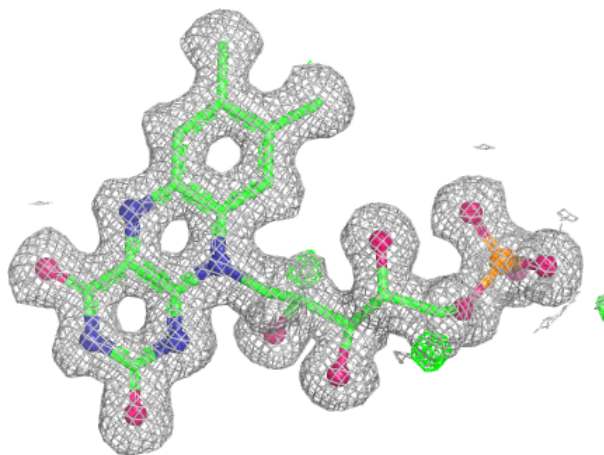
**Electron density around W88 A 401:**

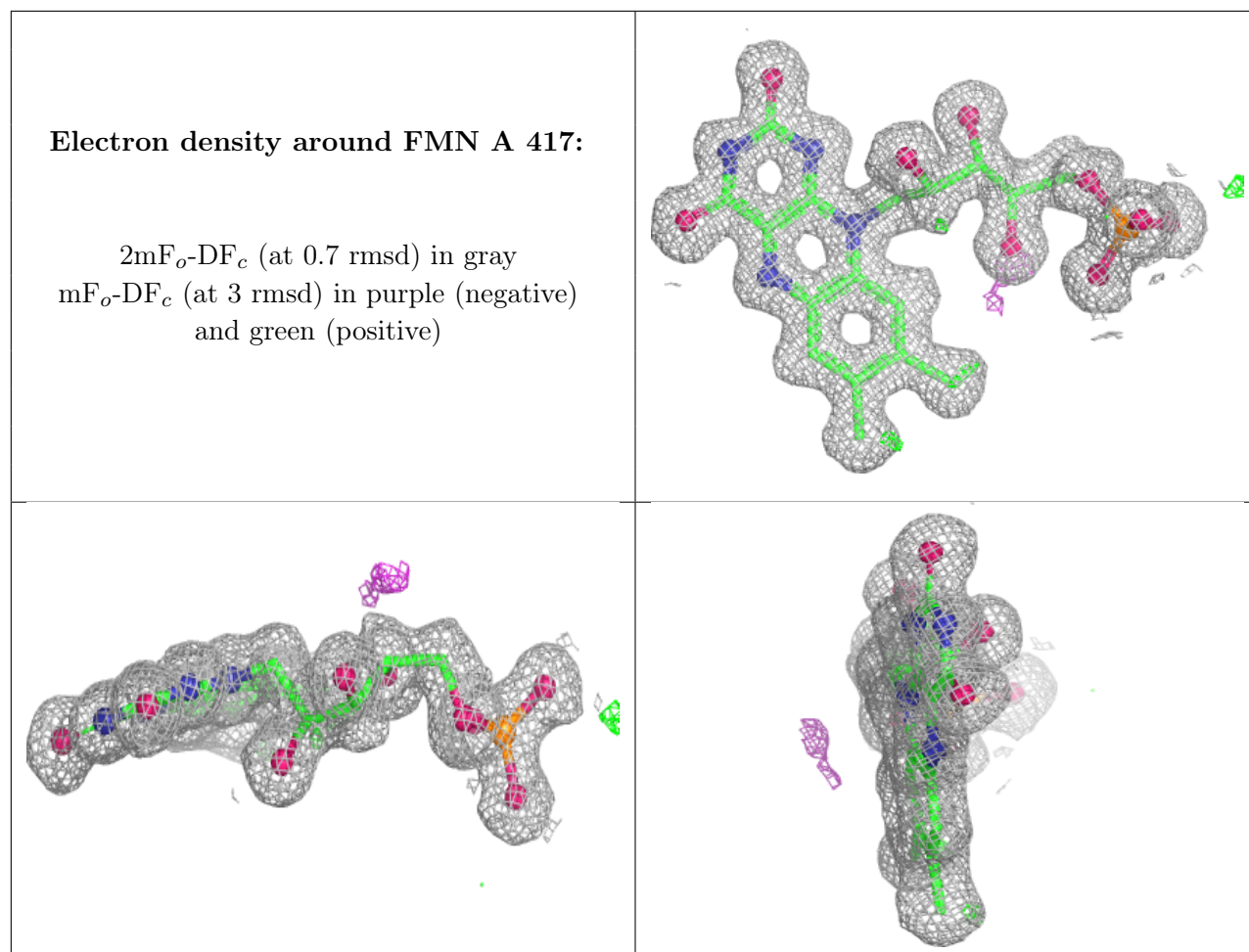
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN B 415:

$2mF_o-DF_c$ (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.