



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:40 AM EDT

PDB ID : 3VKJ / pdb_00003vkj
Title : Crystal structure of Sulfolobus shibatae isopentenyl diphosphate isomerase, octameric form
Authors : Nakatani, H.; Goda, S.; Unno, H.; Nagai, T.; Yoshimura, T.; Hemmi, H.
Deposited on : 2011-11-17
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

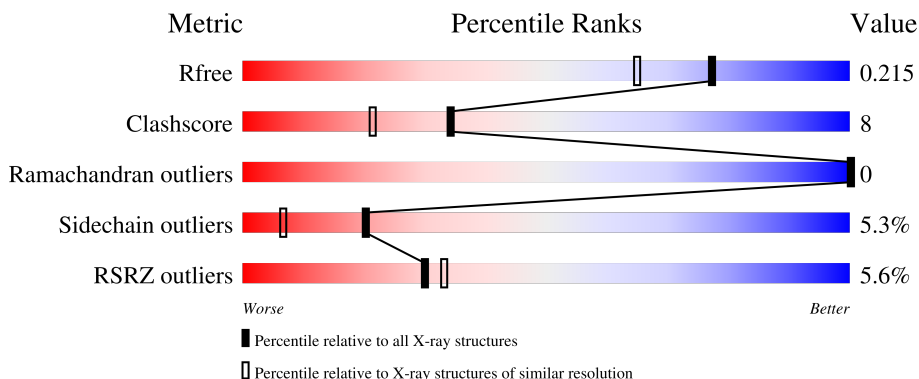
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	
1	C	368	
1	D	368	

2 Entry composition [i](#)

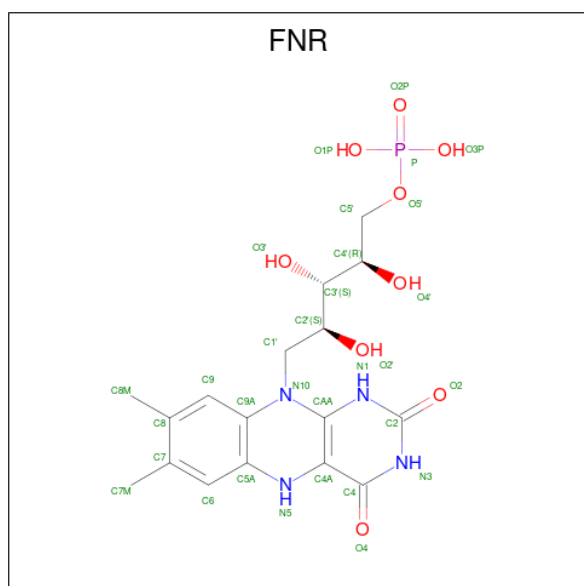
There are 3 unique types of molecules in this entry. The entry contains 12048 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isopentenyl-diphosphate delta-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2800	1795	474	520	11			
1	B	363	Total	C	N	O	S	0	0	0
			2800	1795	474	520	11			
1	C	363	Total	C	N	O	S	0	0	0
			2800	1795	474	520	11			
1	D	363	Total	C	N	O	S	0	0	0
			2800	1795	474	520	11			

- Molecule 2 is 1-DEOXY-1-(7,8-DIMETHYL-2,4-DIOXO-3,4-DIHYDRO-2H-BENZO[G]PT ERIDIN-1-ID-10(5H)-YL)-5-O-PHOSPHONATO-D-RIBITOL (CCD ID: FNR) (formula: $C_{17}H_{23}N_4O_9P$).



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

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

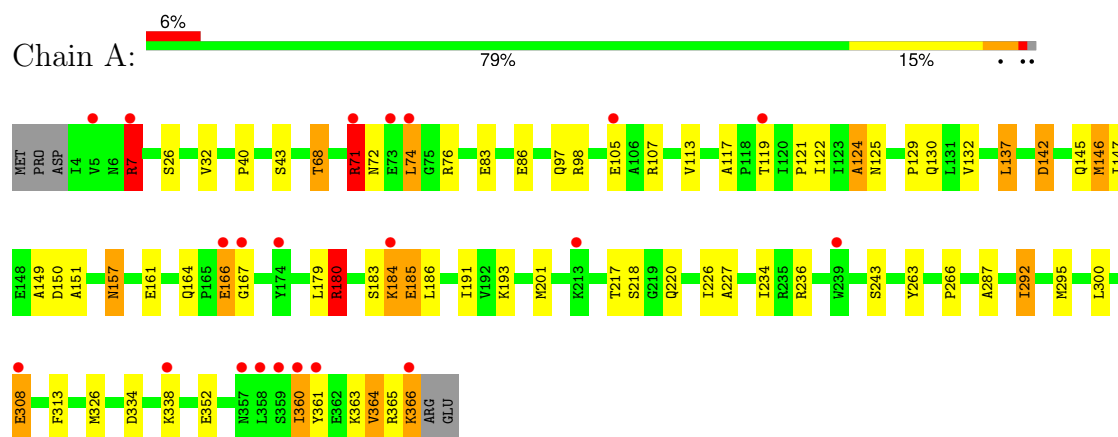
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total	O	0	0
			163	163		
3	B	174	Total	O	0	0
			174	174		
3	C	207	Total	O	0	0
			207	207		
3	D	180	Total	O	0	0
			180	180		

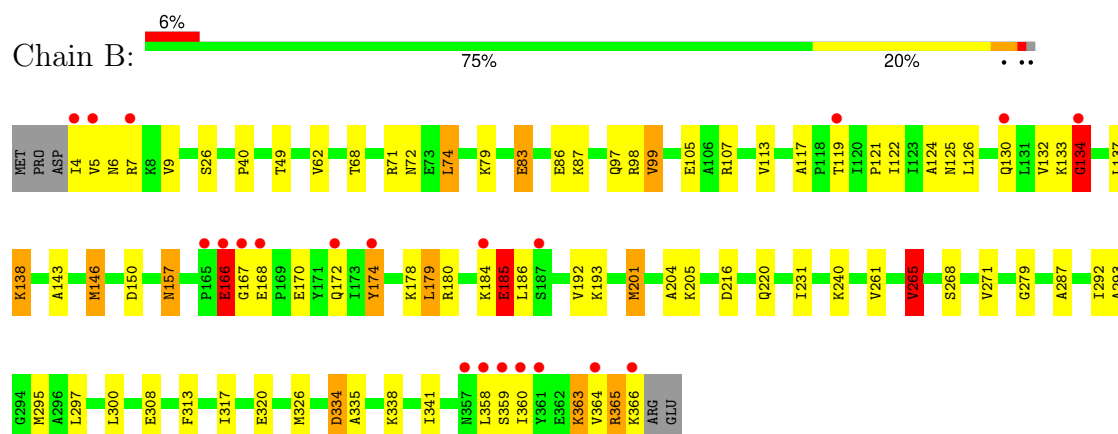
3 Residue-property plots [i](#)

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

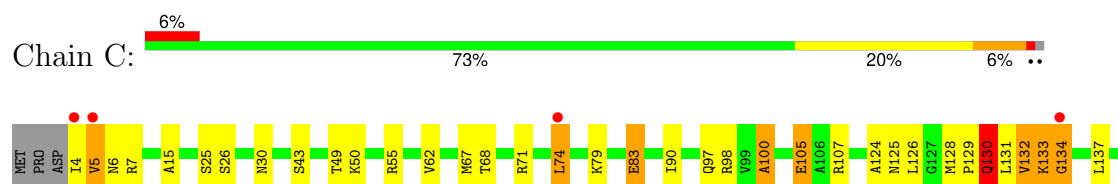
- Molecule 1: Isopentenyl-diphosphate delta-isomerase

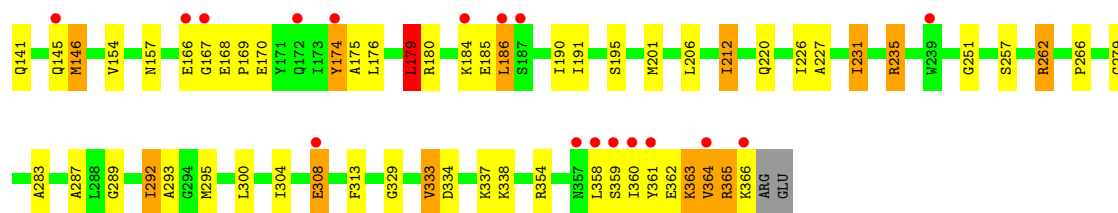


- Molecule 1: Isopentenyl-diphosphate delta-isomerase

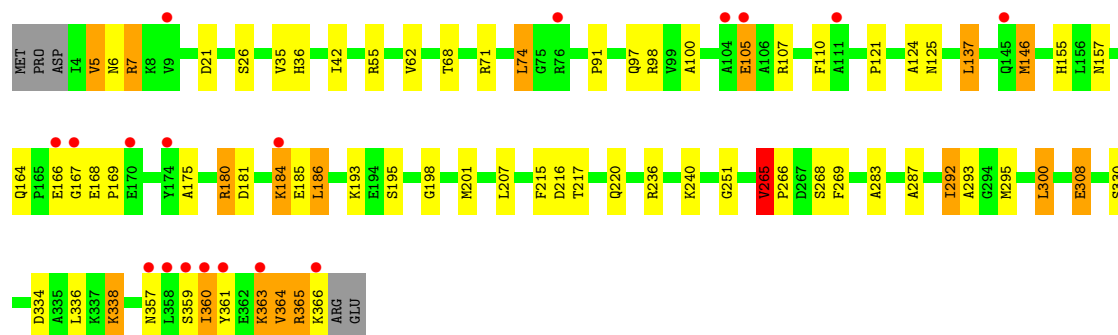
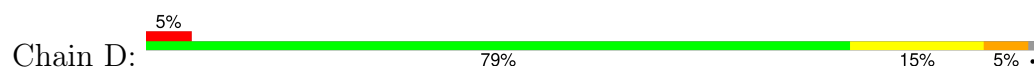


- Molecule 1: Isopentenyl-diphosphate delta-isomerase





● Molecule 1: Isopentenyl-diphosphate delta-isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.84Å 100.84Å 336.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.15 – 1.70 35.15 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.6 (35.15-1.70) 94.6 (35.15-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.217 0.184 , 0.215	Depositor DCC
R_{free} test set	9047 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12048	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FNR

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	1.74	29/2847 (1.0%)	1.55	35/3835 (0.9%)
1	B	1.77	38/2847 (1.3%)	1.59	32/3835 (0.8%)
1	C	1.80	45/2847 (1.6%)	1.79	39/3835 (1.0%)
1	D	1.77	40/2847 (1.4%)	1.54	30/3835 (0.8%)
All	All	1.77	152/11388 (1.3%)	1.62	136/15340 (0.9%)

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	B	0	2

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	134	GLY	N-CA	16.98	1.69	1.45
1	D	201	MET	SD-CE	-10.86	1.52	1.79
1	B	201	MET	SD-CE	-10.79	1.52	1.79
1	C	235	ARG	CD-NE	-9.80	1.32	1.46
1	D	167	GLY	CA-C	-9.10	1.42	1.51
1	A	167	GLY	CA-C	-9.09	1.42	1.51
1	D	146	MET	SD-CE	-9.03	1.56	1.79
1	A	164	GLN	CB-CG	-8.84	1.25	1.52
1	C	262	ARG	CD-NE	-8.82	1.33	1.46
1	D	360	ILE	CA-CB	-8.42	1.44	1.54
1	D	360	ILE	CB-CG2	-8.42	1.24	1.52
1	C	130	GLN	N-CA	8.26	1.56	1.46
1	A	201	MET	SD-CE	-8.24	1.58	1.79
1	C	167	GLY	CA-C	-8.18	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	TYR	CD2-CE2	-7.87	1.15	1.38
1	A	149	ALA	CA-CB	7.83	1.66	1.53
1	D	5	VAL	CB-CG2	-7.75	1.26	1.52
1	A	83	GLU	CB-CG	-7.70	1.29	1.52
1	C	133	LYS	C-N	-7.66	1.24	1.34
1	C	292	ILE	CB-CG1	-7.42	1.38	1.53
1	B	170	GLU	CD-OE1	-7.40	1.11	1.25
1	A	236	ARG	CZ-NH2	-7.22	1.24	1.33
1	A	292	ILE	CB-CG1	-7.22	1.39	1.53
1	C	132	VAL	CA-CB	-7.21	1.44	1.54
1	C	146	MET	SD-CE	-7.14	1.61	1.79
1	B	83	GLU	CB-CG	-7.07	1.31	1.52
1	C	235	ARG	CZ-NH2	-6.93	1.24	1.33
1	C	195	SER	C-O	6.92	1.30	1.23
1	D	184	LYS	N-CA	6.87	1.54	1.46
1	D	166	GLU	CA-C	-6.82	1.43	1.53
1	D	364	VAL	CA-CB	6.79	1.61	1.54
1	C	231	ILE	N-CA	6.78	1.54	1.46
1	B	192	VAL	CA-CB	-6.73	1.46	1.54
1	B	180	ARG	CD-NE	-6.71	1.36	1.46
1	D	292	ILE	CA-CB	-6.67	1.45	1.55
1	B	174	TYR	CB-CG	-6.67	1.36	1.51
1	B	341	ILE	C-O	6.63	1.31	1.23
1	D	7	ARG	CZ-NH2	-6.62	1.24	1.33
1	A	130	GLN	N-CA	6.57	1.54	1.46
1	C	279	GLY	N-CA	6.55	1.54	1.45
1	B	157	ASN	CG-ND2	-6.54	1.19	1.33
1	B	49	THR	N-CA	6.53	1.54	1.46
1	D	166	GLU	CB-CG	-6.47	1.33	1.52
1	B	167	GLY	CA-C	-6.47	1.46	1.51
1	D	164	GLN	CB-CG	-6.46	1.33	1.52
1	C	131	LEU	CA-C	-6.45	1.43	1.52
1	D	215	PHE	N-CA	6.44	1.54	1.45
1	B	271	VAL	N-CA	6.36	1.54	1.46
1	D	201	MET	CB-CG	-6.33	1.33	1.52
1	A	352	GLU	N-CA	6.32	1.53	1.46
1	D	42	ILE	CA-C	-6.30	1.46	1.52
1	B	201	MET	CB-CG	-6.29	1.33	1.52
1	B	124	ALA	CA-CB	6.24	1.62	1.53
1	B	204	ALA	CA-C	6.21	1.60	1.52
1	A	166	GLU	CB-CG	-6.17	1.33	1.52
1	B	87	LYS	N-CA	6.16	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	7	ARG	CZ-NH1	-6.07	1.24	1.32
1	D	157	ASN	CG-OD1	-6.06	1.12	1.23
1	B	146	MET	SD-CE	-6.04	1.64	1.79
1	D	181	ASP	N-CA	6.02	1.53	1.46
1	B	205	LYS	N-CA	6.01	1.53	1.46
1	D	330	SER	C-O	-6.00	1.16	1.23
1	A	117	ALA	CA-CB	5.99	1.60	1.53
1	A	124	ALA	CA-CB	5.89	1.61	1.53
1	C	169	PRO	C-O	5.86	1.30	1.23
1	C	145	GLN	CB-CG	-5.85	1.34	1.52
1	D	175	ALA	CA-CB	5.83	1.62	1.53
1	C	361	TYR	C-O	5.80	1.30	1.24
1	D	265	VAL	CB-CG2	-5.80	1.33	1.52
1	B	117	ALA	CA-CB	5.79	1.59	1.53
1	B	168	GLU	CA-C	-5.79	1.45	1.52
1	A	7	ARG	CB-CG	-5.76	1.35	1.52
1	A	142	ASP	CB-CG	-5.76	1.37	1.52
1	C	257	SER	C-O	5.75	1.30	1.24
1	C	43	SER	N-CA	-5.73	1.39	1.45
1	D	35	VAL	C-O	5.72	1.30	1.24
1	A	157	ASN	CG-ND2	-5.72	1.21	1.33
1	A	146	MET	SD-CE	-5.71	1.65	1.79
1	A	234	ILE	C-O	5.69	1.30	1.24
1	C	227	ALA	N-CA	5.67	1.53	1.46
1	B	231	ILE	C-O	5.66	1.30	1.24
1	B	126	LEU	N-CA	5.64	1.53	1.45
1	D	155	HIS	N-CA	5.64	1.52	1.45
1	C	132	VAL	CB-CG2	-5.63	1.33	1.52
1	C	15	ALA	CA-CB	5.63	1.62	1.53
1	B	317	ILE	N-CA	5.62	1.53	1.46
1	D	7	ARG	CB-CG	-5.60	1.35	1.52
1	C	329	GLY	N-CA	5.59	1.53	1.45
1	B	335	ALA	CA-CB	5.55	1.61	1.53
1	C	55	ARG	CZ-NH1	-5.55	1.25	1.32
1	D	198	GLY	N-CA	5.54	1.51	1.45
1	A	151	ALA	CA-CB	5.53	1.62	1.53
1	C	168	GLU	CA-C	-5.52	1.45	1.52
1	D	195	SER	C-O	5.51	1.29	1.23
1	B	240	LYS	N-CA	5.49	1.53	1.46
1	C	174	TYR	CB-CG	-5.48	1.39	1.51
1	C	201	MET	SD-CE	-5.48	1.65	1.79
1	C	49	THR	N-CA	5.48	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	5	VAL	CB-CG1	-5.46	1.34	1.52
1	D	240	LYS	N-CA	5.45	1.53	1.46
1	C	201	MET	CB-CG	-5.45	1.36	1.52
1	B	261	VAL	N-CA	5.44	1.53	1.46
1	A	236	ARG	CZ-NH1	-5.44	1.25	1.32
1	A	243	SER	N-CA	5.42	1.53	1.46
1	A	32	VAL	C-O	5.42	1.30	1.24
1	A	122	ILE	CA-CB	5.41	1.61	1.54
1	C	362	GLU	CA-CB	5.39	1.61	1.53
1	C	50	LYS	N-CA	5.38	1.52	1.45
1	D	207	LEU	CA-C	5.38	1.59	1.52
1	B	6	ASN	CG-ND2	-5.37	1.22	1.33
1	B	292	ILE	CB-CG1	-5.35	1.42	1.53
1	A	147	ILE	CA-CB	5.33	1.61	1.54
1	C	283	ALA	CA-CB	5.32	1.61	1.53
1	D	338	LYS	CA-CB	5.30	1.62	1.53
1	B	130	GLN	C-O	5.30	1.30	1.24
1	C	212	ILE	N-CA	5.28	1.52	1.46
1	B	143	ALA	N-CA	5.27	1.52	1.46
1	C	201	MET	CG-SD	5.26	1.94	1.80
1	B	292	ILE	CB-CG2	-5.26	1.35	1.52
1	C	333	VAL	CA-CB	5.26	1.61	1.54
1	A	292	ILE	N-CA	-5.25	1.40	1.46
1	B	138	LYS	CG-CD	-5.24	1.36	1.52
1	D	21	ASP	N-CA	5.24	1.52	1.46
1	B	297	LEU	N-CA	5.23	1.51	1.46
1	D	292	ILE	CB-CG1	-5.23	1.43	1.53
1	B	174	TYR	CE2-CZ	-5.21	1.25	1.38
1	C	83	GLU	N-CA	5.20	1.52	1.46
1	D	6	ASN	CG-ND2	-5.18	1.22	1.33
1	C	6	ASN	CG-ND2	-5.18	1.22	1.33
1	D	283	ALA	CA-CB	5.17	1.61	1.53
1	D	292	ILE	N-CA	-5.16	1.40	1.46
1	B	7	ARG	CB-CG	-5.16	1.36	1.52
1	D	180	ARG	CD-NE	-5.14	1.39	1.46
1	C	292	ILE	CB-CG2	5.14	1.69	1.52
1	A	161	GLU	CD-OE2	-5.13	1.15	1.25
1	D	361	TYR	C-O	5.13	1.30	1.24
1	B	172	GLN	N-CA	5.12	1.52	1.45
1	C	100	ALA	CA-CB	-5.12	1.44	1.53
1	C	304	ILE	N-CA	5.11	1.52	1.46
1	D	36	HIS	N-CA	5.10	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	336	LEU	N-CA	5.10	1.52	1.46
1	C	98	ARG	CD-NE	-5.10	1.39	1.46
1	A	364	VAL	CA-C	5.09	1.59	1.52
1	C	5	VAL	CB-CG2	-5.09	1.35	1.52
1	D	295	MET	SD-CE	-5.08	1.66	1.79
1	C	364	VAL	CA-C	5.06	1.59	1.52
1	B	170	GLU	CD-OE2	-5.06	1.15	1.25
1	B	201	MET	N-CA	5.05	1.52	1.46
1	C	226	ILE	N-CA	5.04	1.52	1.46
1	A	227	ALA	N-CA	5.04	1.52	1.46
1	A	201	MET	CB-CG	-5.02	1.37	1.52
1	A	113	VAL	CA-CB	5.01	1.59	1.54

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	LYS	CA-C-N	-25.93	92.58	123.44
1	C	133	LYS	C-N-CA	-25.93	92.58	123.44
1	C	262	ARG	NE-CZ-NH2	20.64	137.78	119.20
1	B	166	GLU	CA-C-N	-20.06	108.01	121.65
1	B	166	GLU	C-N-CA	-20.06	108.01	121.65
1	C	166	GLU	CA-C-N	-16.75	110.10	122.33
1	C	166	GLU	C-N-CA	-16.75	110.10	122.33
1	A	166	GLU	CB-CA-C	-16.42	87.62	111.76
1	D	360	ILE	CG1-CB-CG2	-15.20	65.11	110.70
1	C	235	ARG	NE-CZ-NH1	14.31	135.81	121.50
1	C	262	ARG	CD-NE-CZ	13.53	143.34	124.40
1	B	166	GLU	CB-CA-C	-13.46	92.43	111.14
1	C	166	GLU	CB-CA-C	-13.45	94.06	111.40
1	D	166	GLU	CB-CA-C	-13.18	89.63	111.51
1	A	166	GLU	CA-C-N	-11.94	102.45	121.32
1	A	166	GLU	C-N-CA	-11.94	102.45	121.32
1	C	262	ARG	NE-CZ-NH1	-11.87	109.63	121.50
1	C	235	ARG	CB-CG-CD	11.67	138.14	111.30
1	D	166	GLU	CA-C-N	-11.41	103.28	121.32
1	D	166	GLU	C-N-CA	-11.41	103.28	121.32
1	C	235	ARG	CD-NE-CZ	11.32	140.25	124.40
1	A	76	ARG	NE-CZ-NH1	-10.79	110.71	121.50
1	C	235	ARG	NE-CZ-NH2	-10.56	109.70	119.20
1	A	76	ARG	NE-CZ-NH2	10.06	128.26	119.20
1	C	98	ARG	NE-CZ-NH2	9.84	128.06	119.20
1	A	363	LYS	CD-CE-NZ	-9.80	80.54	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	GLU	N-CA-C	9.32	124.93	112.25
1	D	7	ARG	CB-CG-CD	-9.25	90.02	111.30
1	A	292	ILE	CB-CG1-CD1	-9.16	94.56	113.80
1	D	5	VAL	CB-CA-C	-9.10	102.80	111.44
1	C	98	ARG	NE-CZ-NH1	-8.94	112.56	121.50
1	D	292	ILE	CB-CG1-CD1	-8.62	95.71	113.80
1	B	71	ARG	CB-CG-CD	8.60	131.09	111.30
1	B	71	ARG	CA-CB-CG	8.57	131.24	114.10
1	B	363	LYS	N-CA-C	8.45	120.11	111.07
1	C	180	ARG	NE-CZ-NH1	-8.36	113.14	121.50
1	C	292	ILE	CB-CG1-CD1	-7.91	97.19	113.80
1	B	134	GLY	N-CA-C	7.79	126.22	114.61
1	A	363	LYS	N-CA-C	7.77	120.44	111.11
1	A	226	ILE	N-CA-C	-7.62	103.37	110.53
1	A	180	ARG	NE-CZ-NH1	7.23	128.73	121.50
1	D	184	LYS	N-CA-C	7.23	120.02	111.71
1	C	7	ARG	NE-CZ-NH2	7.20	125.68	119.20
1	C	133	LYS	O-C-N	-7.18	110.03	121.53
1	B	180	ARG	NE-CZ-NH2	-7.17	112.75	119.20
1	A	166	GLU	N-CA-C	7.10	121.20	107.71
1	D	98	ARG	CB-CG-CD	-6.99	95.23	111.30
1	D	5	VAL	CG1-CB-CG2	-6.90	95.62	110.80
1	C	166	GLU	N-CA-C	6.85	120.94	111.55
1	C	180	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	A	363	LYS	CA-CB-CG	-6.78	100.55	114.10
1	D	363	LYS	N-CA-C	6.70	118.24	111.07
1	A	292	ILE	CA-CB-CG2	6.69	121.88	110.50
1	C	206	LEU	N-CA-C	-6.66	103.95	111.14
1	A	164	GLN	CB-CA-C	6.61	119.92	109.27
1	A	236	ARG	NH1-CZ-NH2	-6.60	110.72	119.30
1	A	98	ARG	CB-CG-CD	-6.55	96.23	111.30
1	A	142	ASP	CB-CG-OD1	-6.54	103.36	118.40
1	B	292	ILE	CB-CG1-CD1	-6.53	100.09	113.80
1	B	7	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	B	179	LEU	CD1-CG-CD2	6.49	125.07	110.80
1	C	365	ARG	NE-CZ-NH1	6.47	127.97	121.50
1	D	360	ILE	CB-CA-C	-6.45	103.71	111.97
1	C	174	TYR	CE1-CZ-OH	-6.44	100.58	119.90
1	A	180	ARG	NE-CZ-NH2	-6.37	113.47	119.20
1	B	292	ILE	CB-CA-C	-6.32	99.81	111.18
1	D	360	ILE	CB-CG1-CD1	-6.31	100.54	113.80
1	C	186	LEU	CB-CG-CD1	6.23	129.40	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ARG	NE-CZ-NH2	6.22	124.80	119.20
1	A	71	ARG	CG-CD-NE	-6.19	98.38	112.00
1	B	170	GLU	OE1-CD-OE2	-6.17	108.09	122.90
1	A	68	THR	N-CA-C	6.17	116.22	108.45
1	A	71	ARG	CB-CG-CD	6.15	125.45	111.30
1	B	292	ILE	CG1-CB-CG2	-6.14	92.28	110.70
1	C	292	ILE	CA-CB-CG2	6.02	120.73	110.50
1	B	364	VAL	N-CA-C	5.89	116.08	110.42
1	D	236	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	B	98	ARG	CB-CG-CD	-5.87	97.80	111.30
1	B	365	ARG	NE-CZ-NH1	5.85	127.35	121.50
1	D	180	ARG	NE-CZ-NH1	5.84	127.34	121.50
1	A	76	ARG	CD-NE-CZ	5.83	132.56	124.40
1	D	180	ARG	CB-CG-CD	-5.83	97.90	111.30
1	A	184	LYS	N-CA-C	5.82	118.41	111.71
1	C	363	LYS	N-CA-C	5.79	118.06	111.11
1	D	357	ASN	N-CA-C	-5.78	101.09	109.59
1	D	300	LEU	CD1-CG-CD2	5.72	123.39	110.80
1	D	146	MET	CG-SD-CE	5.72	113.48	100.90
1	A	43	SER	N-CA-CB	-5.72	101.31	110.63
1	B	185	GLU	N-CA-CB	-5.69	103.03	110.88
1	D	167	GLY	N-CA-C	5.67	118.64	111.09
1	A	183	SER	N-CA-C	-5.66	105.20	111.71
1	B	133	LYS	CA-C-N	-5.66	109.79	120.77
1	B	133	LYS	C-N-CA	-5.66	109.79	120.77
1	D	217	THR	O-C-N	5.64	128.10	122.12
1	C	146	MET	CG-SD-CE	5.59	113.21	100.90
1	D	292	ILE	CA-CB-CG2	5.56	119.95	110.50
1	B	126	LEU	CA-C-N	-5.54	115.58	121.45
1	B	126	LEU	C-N-CA	-5.54	115.58	121.45
1	C	364	VAL	N-CA-C	5.54	115.74	110.42
1	B	174	TYR	CE1-CZ-OH	-5.53	103.31	119.90
1	D	7	ARG	CA-CB-CG	5.50	125.10	114.10
1	C	4	ILE	CA-C-N	-5.49	117.34	122.66
1	C	4	ILE	C-N-CA	-5.49	117.34	122.66
1	D	269	PHE	N-CA-C	-5.48	99.58	108.52
1	C	179	LEU	CD1-CG-CD2	5.48	122.85	110.80
1	D	251	GLY	CA-C-N	-5.45	118.67	122.59
1	D	251	GLY	C-N-CA	-5.45	118.67	122.59
1	A	72	ASN	N-CA-C	5.41	117.60	111.11
1	C	262	ARG	NH1-CZ-NH2	-5.39	112.30	119.30
1	A	7	ARG	CB-CA-C	-5.38	99.99	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ARG	CG-CD-NE	-5.37	100.18	112.00
1	B	99	VAL	CB-CA-C	-5.36	104.91	112.14
1	C	251	GLY	N-CA-C	5.34	117.47	112.08
1	C	67	MET	CA-C-N	-5.32	113.05	122.20
1	C	67	MET	C-N-CA	-5.32	113.05	122.20
1	B	334	ASP	N-CA-C	5.32	117.08	111.28
1	D	364	VAL	N-CA-C	5.29	115.91	110.36
1	A	7	ARG	CB-CG-CD	-5.27	99.17	111.30
1	A	191	ILE	N-CA-C	-5.26	100.74	108.11
1	A	363	LYS	CG-CD-CE	5.23	123.33	111.30
1	D	365	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	B	4	ILE	CA-C-N	-5.22	117.60	122.66
1	B	4	ILE	C-N-CA	-5.22	117.60	122.66
1	C	174	TYR	OH-CZ-CE2	5.20	135.49	119.90
1	A	164	GLN	CG-CD-NE2	-5.18	108.63	116.40
1	B	72	ASN	N-CA-C	5.17	117.32	111.11
1	D	186	LEU	CB-CG-CD1	5.17	126.21	110.70
1	B	170	GLU	CG-CD-OE2	5.16	130.26	118.40
1	B	265	VAL	CG1-CB-CG2	5.16	122.14	110.80
1	D	201	MET	CG-SD-CE	-5.15	89.56	100.90
1	B	265	VAL	CA-CB-CG1	5.06	119.00	110.40
1	A	191	ILE	CA-C-N	-5.04	116.57	122.93
1	A	191	ILE	C-N-CA	-5.04	116.57	122.93
1	C	191	ILE	N-CA-C	-5.04	101.23	108.48
1	C	354	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	C	185	GLU	CA-CB-CG	-5.01	104.08	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	134	GLY	Peptide
1	B	166	GLU	Peptide

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	2800	0	2886	32	0
1	B	2800	0	2886	34	0
1	C	2800	0	2886	61	0
1	D	2800	0	2886	45	1
2	A	31	0	22	2	0
2	B	31	0	22	2	0
2	C	31	0	22	1	0
2	D	31	0	22	0	0
3	A	163	0	0	7	0
3	B	174	0	0	4	0
3	C	207	0	0	14	1
3	D	180	0	0	7	0
All	All	12048	0	11632	175	1

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 8.

All (175) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:GLY:N	1:C:134:GLY:CA	1.69	1.56
1:A:361:TYR:HE1	3:A:614:HOH:O	1.05	1.32
1:C:133:LYS:O	1:C:134:GLY:HA3	1.30	1.25
1:C:90:ILE:CG1	3:C:593:HOH:O	1.71	1.24
1:C:133:LYS:O	1:C:134:GLY:CA	1.82	1.23
1:C:133:LYS:C	1:C:134:GLY:CA	2.13	1.21
1:C:90:ILE:HB	3:C:593:HOH:O	1.26	1.17
1:D:100:ALA:CB	1:D:146:MET:HE1	1.73	1.17
1:C:130:GLN:NE2	3:C:657:HOH:O	1.80	1.14
1:C:100:ALA:HB1	1:C:146:MET:HE1	1.22	1.13
1:C:30:ASN:OD1	3:C:598:HOH:O	1.68	1.12
1:C:107:ARG:HG2	1:C:146:MET:HE3	1.30	1.09
1:B:366:LYS:HD3	3:B:586:HOH:O	1.52	1.07
1:C:100:ALA:CB	1:C:146:MET:HE1	1.83	1.07
1:A:361:TYR:CE1	3:A:614:HOH:O	1.82	1.07
1:C:90:ILE:CD1	3:C:593:HOH:O	1.90	1.06
1:C:90:ILE:HD12	3:C:593:HOH:O	1.50	1.06
1:C:130:GLN:HG2	3:C:579:HOH:O	1.54	1.06
1:D:100:ALA:HB1	1:D:146:MET:HE1	1.43	0.96
1:C:130:GLN:OE1	3:C:579:HOH:O	1.84	0.94
1:C:107:ARG:HA	1:C:146:MET:CE	1.99	0.93
1:C:107:ARG:CG	1:C:146:MET:HE3	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ARG:NH1	3:B:576:HOH:O	2.01	0.90
1:B:338:LYS:HG2	1:B:366:LYS:HB3	1.55	0.88
1:A:184:LYS:HA	1:A:184:LYS:HE2	1.54	0.87
1:D:366:LYS:O	3:D:656:HOH:O	1.93	0.86
1:D:137:LEU:HD11	1:D:185:GLU:HG2	1.56	0.86
1:A:338:LYS:HG2	1:A:366:LYS:HB3	1.58	0.86
1:C:107:ARG:HA	1:C:146:MET:HE2	1.58	0.85
1:C:100:ALA:HB1	1:C:146:MET:CE	2.05	0.85
1:D:180:ARG:HD2	3:D:543:HOH:O	1.76	0.85
1:C:235:ARG:HD2	3:C:605:HOH:O	1.77	0.83
1:D:100:ALA:HB1	1:D:146:MET:CE	2.07	0.83
1:C:184:LYS:HA	1:C:184:LYS:HE2	1.61	0.82
1:D:265:VAL:HG23	1:D:268:SER:HB3	1.63	0.81
1:D:100:ALA:HB3	1:D:146:MET:HE1	1.65	0.79
1:C:130:GLN:CG	3:C:579:HOH:O	2.21	0.76
1:A:180:ARG:HD2	3:A:598:HOH:O	1.86	0.75
1:C:97:GLN:HE21	1:C:125:ASN:H	1.34	0.75
1:D:107:ARG:HA	1:D:146:MET:CE	2.16	0.74
1:D:107:ARG:HA	1:D:146:MET:HE3	1.69	0.73
1:C:90:ILE:CB	3:C:593:HOH:O	1.77	0.73
1:A:184:LYS:HE2	1:A:184:LYS:CA	2.19	0.72
1:D:338:LYS:HG2	1:D:366:LYS:HB3	1.71	0.72
1:D:265:VAL:CG2	1:D:268:SER:HB3	2.20	0.72
1:D:97:GLN:HE21	1:D:125:ASN:H	1.36	0.71
1:B:97:GLN:HE21	1:B:125:ASN:H	1.38	0.71
1:B:265:VAL:HG22	1:B:268:SER:HB3	1.72	0.71
1:A:97:GLN:HE21	1:A:125:ASN:H	1.39	0.70
1:C:308:GLU:HG2	3:C:530:HOH:O	1.89	0.70
1:A:137:LEU:HD11	1:A:185:GLU:HG2	1.73	0.70
1:B:184:LYS:HA	1:B:184:LYS:HE2	1.73	0.70
1:D:107:ARG:HG2	1:D:146:MET:HE3	1.74	0.70
1:C:97:GLN:HE22	1:C:124:ALA:HB1	1.57	0.69
1:C:170:GLU:OE2	3:C:655:HOH:O	2.13	0.67
1:C:231:ILE:HG22	1:C:235:ARG:HD3	1.78	0.64
1:B:107:ARG:CZ	3:B:576:HOH:O	2.39	0.64
1:B:79:LYS:O	1:B:83:GLU:HG2	1.98	0.63
1:C:262:ARG:HD2	1:C:289:GLY:O	1.97	0.63
1:C:295:MET:HE1	1:C:313:PHE:HE1	1.61	0.63
1:C:141:GLN:HG2	3:C:548:HOH:O	1.98	0.63
1:D:308:GLU:HG2	3:D:579:HOH:O	1.98	0.62
1:B:107:ARG:NE	3:B:576:HOH:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:LEU:CD1	1:D:185:GLU:HG2	2.29	0.62
1:C:132:VAL:HG12	1:C:175:ALA:HB2	1.82	0.62
1:B:137:LEU:CD2	1:B:185:GLU:HG2	2.30	0.62
1:B:68:THR:OG1	1:B:74:LEU:HG	2.00	0.61
1:B:174:TYR:CD2	1:B:174:TYR:C	2.79	0.60
1:A:97:GLN:HE22	1:A:124:ALA:HB1	1.67	0.60
1:A:365:ARG:O	1:A:366:LYS:HB2	2.02	0.58
1:C:295:MET:HE1	1:C:313:PHE:CE1	2.37	0.58
1:D:265:VAL:HG23	1:D:265:VAL:O	2.03	0.58
1:C:231:ILE:CG2	1:C:235:ARG:HD3	2.34	0.58
1:D:365:ARG:O	1:D:366:LYS:HB2	2.03	0.57
1:A:129:PRO:O	1:A:132:VAL:HG22	2.05	0.57
1:A:71:ARG:HB2	1:A:74:LEU:HD22	1.86	0.57
1:D:184:LYS:HB2	3:D:616:HOH:O	2.05	0.57
1:C:107:ARG:CA	1:C:146:MET:CE	2.81	0.56
1:D:68:THR:OG1	1:D:74:LEU:HG	2.06	0.55
1:C:97:GLN:NE2	1:C:125:ASN:H	2.05	0.55
1:C:107:ARG:CB	1:C:146:MET:HE3	2.37	0.55
1:A:308:GLU:HG2	3:A:516:HOH:O	2.07	0.55
1:A:26:SER:H	1:A:220:GLN:HE21	1.55	0.55
1:D:107:ARG:CG	1:D:146:MET:HE3	2.37	0.54
1:B:107:ARG:HG2	1:B:146:MET:HE2	1.90	0.53
1:C:174:TYR:CD2	1:C:174:TYR:C	2.87	0.53
1:A:68:THR:OG1	1:A:74:LEU:HG	2.09	0.53
1:C:68:THR:OG1	1:C:74:LEU:HG	2.08	0.53
1:C:338:LYS:HG2	1:C:366:LYS:HB3	1.90	0.52
1:A:97:GLN:NE2	1:A:125:ASN:H	2.05	0.51
1:B:97:GLN:NE2	1:B:125:ASN:H	2.08	0.51
1:B:137:LEU:HD21	1:B:185:GLU:HG2	1.92	0.51
1:D:26:SER:H	1:D:220:GLN:HE21	1.58	0.51
1:D:97:GLN:HE22	1:D:124:ALA:HB1	1.76	0.51
1:D:107:ARG:CA	1:D:146:MET:HE3	2.39	0.51
1:B:137:LEU:HD22	1:B:185:GLU:HG2	1.92	0.50
1:D:265:VAL:HG23	1:D:268:SER:CB	2.39	0.50
1:D:265:VAL:CG2	1:D:265:VAL:O	2.60	0.50
1:A:40:PRO:HG2	1:A:326:MET:HE3	1.94	0.50
1:B:26:SER:H	1:B:220:GLN:HE21	1.58	0.49
1:B:287:ALA:O	1:B:365:ARG:HD2	2.12	0.49
1:D:184:LYS:HE2	1:D:184:LYS:HA	1.95	0.49
1:D:308:GLU:H	1:D:308:GLU:CD	2.20	0.49
1:B:184:LYS:HE2	1:B:184:LYS:CA	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ARG:HG3	1:D:74:LEU:HD22	1.96	0.48
1:C:26:SER:H	1:C:220:GLN:HE21	1.62	0.47
2:A:401:FNR:H6	2:A:401:FNR:H9	1.96	0.47
1:B:105:GLU:H	1:B:105:GLU:CD	2.22	0.47
1:C:62:VAL:HA	1:C:293:ALA:O	2.15	0.47
2:C:401:FNR:H9	2:C:401:FNR:H6	1.96	0.47
1:B:134:GLY:HA2	1:B:178:LYS:NZ	2.30	0.47
1:D:184:LYS:HG3	3:D:616:HOH:O	2.14	0.47
1:D:193:LYS:HB3	1:D:216:ASP:HB3	1.96	0.47
1:D:287:ALA:O	1:D:365:ARG:HD2	2.15	0.47
1:C:184:LYS:HE2	1:C:184:LYS:CA	2.40	0.46
1:D:100:ALA:CB	1:D:146:MET:CE	2.63	0.46
1:D:110:PHE:HB2	1:D:146:MET:HE2	1.97	0.46
1:B:358:LEU:O	1:B:359:SER:C	2.58	0.46
1:D:97:GLN:NE2	1:D:125:ASN:H	2.09	0.45
1:B:121:PRO:HA	1:B:150:ASP:OD2	2.16	0.45
1:C:266:PRO:HB3	1:C:364:VAL:HG13	1.99	0.45
1:B:193:LYS:HB3	1:B:216:ASP:HB3	1.97	0.45
2:B:401:FNR:H6	2:B:401:FNR:H9	1.98	0.45
1:B:295:MET:HE1	1:B:313:PHE:HE1	1.82	0.45
1:A:121:PRO:HA	1:A:150:ASP:OD2	2.17	0.45
1:C:79:LYS:O	1:C:83:GLU:HG3	2.17	0.45
1:C:107:ARG:HA	1:C:146:MET:HE3	1.94	0.45
1:C:179:LEU:HD22	1:C:190:ILE:HD13	2.00	0.44
1:B:365:ARG:O	1:B:366:LYS:HB2	2.16	0.44
1:A:292:ILE:HG21	1:A:292:ILE:HD13	1.79	0.44
1:B:40:PRO:HG2	1:B:326:MET:HE3	2.00	0.44
1:A:180:ARG:CD	3:A:598:HOH:O	2.58	0.44
1:A:217:THR:O	1:A:218:SER:C	2.60	0.44
1:B:193:LYS:NZ	2:B:401:FNR:HN1	2.16	0.44
1:B:62:VAL:HA	1:B:293:ALA:O	2.18	0.43
1:C:25:SER:HB2	1:C:220:GLN:HE21	1.82	0.43
1:A:365:ARG:HG3	1:A:366:LYS:N	2.33	0.43
1:C:107:ARG:CA	1:C:146:MET:HE2	2.40	0.43
1:D:180:ARG:CD	3:D:543:HOH:O	2.50	0.43
1:A:266:PRO:HB3	1:A:364:VAL:HG13	2.00	0.43
1:D:91:PRO:HB3	1:D:121:PRO:HB2	2.01	0.43
1:A:263:TYR:HE1	1:A:360:ILE:HG13	1.83	0.42
1:B:86:GLU:OE2	1:B:119:THR:HG23	2.19	0.42
1:B:113:VAL:CG1	1:B:122:ILE:HD12	2.48	0.42
1:D:26:SER:H	1:D:220:GLN:NE2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:GLU:CD	1:D:105:GLU:H	2.27	0.42
1:A:193:LYS:NZ	2:A:401:FNR:HN1	2.17	0.42
1:C:105:GLU:H	1:C:105:GLU:CD	2.27	0.42
1:A:287:ALA:O	1:A:365:ARG:HD2	2.19	0.42
1:C:365:ARG:O	1:C:366:LYS:HB2	2.19	0.42
1:C:292:ILE:HG21	1:C:292:ILE:HD13	1.54	0.42
1:D:184:LYS:CB	3:D:616:HOH:O	2.66	0.42
1:B:279:GLY:HA3	1:B:320:GLU:HB2	2.01	0.42
1:A:308:GLU:CD	1:A:308:GLU:H	2.27	0.41
1:A:295:MET:HE1	1:A:313:PHE:HE1	1.84	0.41
1:B:174:TYR:HE2	1:B:178:LYS:HD2	1.85	0.41
1:C:97:GLN:HE22	1:C:124:ALA:CB	2.30	0.41
1:A:86:GLU:OE2	1:A:119:THR:HG23	2.21	0.41
1:C:126:LEU:O	1:C:154:VAL:HA	2.20	0.41
1:C:179:LEU:HD13	1:C:212:ILE:HD11	2.03	0.41
1:C:287:ALA:O	1:C:365:ARG:HD2	2.20	0.41
1:C:333:VAL:HG12	1:C:337:LYS:HE3	2.03	0.41
1:C:97:GLN:NE2	1:C:124:ALA:HB1	2.30	0.41
1:A:107:ARG:HG2	1:A:146:MET:HE2	2.01	0.41
1:B:26:SER:H	1:B:220:GLN:NE2	2.19	0.41
1:C:358:LEU:O	1:C:359:SER:C	2.63	0.41
1:D:292:ILE:HD13	1:D:292:ILE:HG21	1.78	0.41
1:D:62:VAL:HA	1:D:293:ALA:O	2.21	0.40
1:C:71:ARG:HG3	1:C:74:LEU:HD22	2.03	0.40
1:D:107:ARG:CB	1:D:146:MET:HE3	2.51	0.40
1:D:266:PRO:HB3	1:D:364:VAL:HG13	2.03	0.40
1:A:7:ARG:NH2	3:A:639:HOH:O	2.54	0.40
1:A:137:LEU:HD13	3:A:567:HOH:O	2.21	0.40
1:C:128:MET:N	1:C:129:PRO:CD	2.84	0.40
1:D:168:GLU:HA	1:D:169:PRO:HD2	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ARG:NH2	3:C:643:HOH:O[6_565]	2.04	0.16

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	361/368 (98%)	349 (97%)	12 (3%)	0	100	100
1	B	361/368 (98%)	350 (97%)	11 (3%)	0	100	100
1	C	361/368 (98%)	352 (98%)	9 (2%)	0	100	100
1	D	361/368 (98%)	354 (98%)	7 (2%)	0	100	100
All	All	1444/1472 (98%)	1405 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	297/302 (98%)	279 (94%)	18 (6%)	17	5
1	B	297/302 (98%)	279 (94%)	18 (6%)	17	5
1	C	297/302 (98%)	283 (95%)	14 (5%)	23	9
1	D	297/302 (98%)	284 (96%)	13 (4%)	25	10
All	All	1188/1208 (98%)	1125 (95%)	63 (5%)	20	7

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	71	ARG

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Mol	Chain	Res	Type
1	A	74	LEU
1	A	105	GLU
1	A	137	LEU
1	A	142	ASP
1	A	145	GLN
1	A	157	ASN
1	A	166	GLU
1	A	179	LEU
1	A	180	ARG
1	A	185	GLU
1	A	186	LEU
1	A	300	LEU
1	A	308	GLU
1	A	334	ASP
1	A	360	ILE
1	A	366	LYS
1	B	5	VAL
1	B	9	VAL
1	B	74	LEU
1	B	99	VAL
1	B	132	VAL
1	B	138	LYS
1	B	157	ASN
1	B	166	GLU
1	B	179	LEU
1	B	185	GLU
1	B	186	LEU
1	B	201	MET
1	B	265	VAL
1	B	300	LEU
1	B	308	GLU
1	B	334	ASP
1	B	360	ILE
1	B	363	LYS
1	C	5	VAL
1	C	74	LEU
1	C	105	GLU
1	C	130	GLN
1	C	137	LEU
1	C	157	ASN
1	C	176	LEU
1	C	179	LEU

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Mol	Chain	Res	Type
1	C	186	LEU
1	C	300	LEU
1	C	308	GLU
1	C	334	ASP
1	C	360	ILE
1	C	363	LYS
1	D	5	VAL
1	D	7	ARG
1	D	74	LEU
1	D	105	GLU
1	D	137	LEU
1	D	186	LEU
1	D	265	VAL
1	D	300	LEU
1	D	308	GLU
1	D	334	ASP
1	D	359	SER
1	D	360	ILE
1	D	363	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	157	ASN
1	A	220	GLN
1	A	246	ASN
1	A	312	GLN
1	B	97	GLN
1	B	157	ASN
1	B	164	GLN
1	B	220	GLN
1	B	246	ASN
1	B	312	GLN
1	C	30	ASN
1	C	97	GLN
1	C	130	GLN
1	C	157	ASN
1	C	164	GLN
1	C	220	GLN
1	C	246	ASN
1	C	312	GLN

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Mol	Chain	Res	Type
1	D	97	GLN
1	D	164	GLN
1	D	220	GLN
1	D	246	ASN
1	D	312	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FNR	A	401	-	32,33,33	1.63	6 (18%)	41,50,50	1.80	10 (24%)
2	FNR	D	401	-	32,33,33	1.55	5 (15%)	41,50,50	1.65	10 (24%)
2	FNR	C	401	-	32,33,33	1.59	7 (21%)	41,50,50	2.31	17 (41%)
2	FNR	B	401	-	32,33,33	1.36	5 (15%)	41,50,50	1.65	8 (19%)

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
2	FNR	A	401	-	-	4/18/18/18	0/3/3/3
2	FNR	D	401	-	-	4/18/18/18	0/3/3/3
2	FNR	C	401	-	-	3/18/18/18	0/3/3/3
2	FNR	B	401	-	-	4/18/18/18	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FNR	C9-C8	4.99	1.46	1.39
2	A	401	FNR	C5'-C4'	4.60	1.58	1.51
2	D	401	FNR	C9-C8	4.34	1.45	1.39
2	C	401	FNR	C5'-C4'	3.90	1.57	1.51
2	D	401	FNR	O4-C4	2.98	1.29	1.23
2	B	401	FNR	C4A-N5	2.96	1.41	1.35
2	C	401	FNR	C9-C8	2.76	1.43	1.39
2	A	401	FNR	C7M-C7	2.63	1.55	1.51
2	B	401	FNR	C1'-C2'	2.45	1.56	1.52
2	D	401	FNR	C9A-N10	2.43	1.45	1.41
2	D	401	FNR	C5'-C4'	2.39	1.55	1.51
2	C	401	FNR	C5A-C9A	-2.35	1.38	1.40
2	C	401	FNR	C4'-C3'	2.24	1.57	1.53
2	C	401	FNR	C5A-N5	-2.22	1.36	1.39
2	A	401	FNR	C9A-N10	2.18	1.44	1.41
2	B	401	FNR	C8M-C8	2.16	1.55	1.51
2	D	401	FNR	C2-N1	-2.16	1.33	1.37
2	C	401	FNR	O2-C2	2.14	1.27	1.23
2	B	401	FNR	O2'-C2'	2.12	1.47	1.43
2	A	401	FNR	O2'-C2'	2.11	1.47	1.43
2	C	401	FNR	C4A-N5	2.10	1.40	1.35
2	A	401	FNR	C4A-C4	2.04	1.48	1.41
2	B	401	FNR	O4'-C4'	2.03	1.47	1.43

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FNR	N3-C2-N1	5.68	124.67	115.74
2	C	401	FNR	C4-N3-C2	-5.66	118.57	126.37
2	C	401	FNR	C9-C9A-N10	-4.57	115.71	121.85
2	B	401	FNR	N3-C2-N1	4.37	122.60	115.74
2	A	401	FNR	C9A-C5A-N5	4.17	124.45	119.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FNR	N3-C2-N1	3.99	122.01	115.74
2	A	401	FNR	O2-C2-N1	-3.86	115.00	121.86
2	C	401	FNR	C1'-N10-C9A	3.77	127.96	120.63
2	A	401	FNR	N3-C2-N1	3.70	121.56	115.74
2	A	401	FNR	C4-N3-C2	-3.60	121.41	126.37
2	C	401	FNR	C5A-C9A-N10	3.50	121.97	118.01
2	C	401	FNR	C9A-C5A-N5	3.50	123.63	119.37
2	B	401	FNR	C5A-C9A-N10	3.21	121.65	118.01
2	A	401	FNR	O4-C4-C4A	-3.18	119.59	127.26
2	C	401	FNR	O4-C4-C4A	-3.07	119.85	127.26
2	D	401	FNR	O4-C4-C4A	-3.03	119.95	127.26
2	B	401	FNR	C5A-N5-C4A	-3.01	114.13	121.08
2	D	401	FNR	O2-C2-N1	-3.00	116.53	121.86
2	C	401	FNR	O3'-C3'-C4'	-2.99	102.13	108.93
2	C	401	FNR	C4A-C4-N3	2.97	120.29	112.13
2	D	401	FNR	C9A-C5A-N5	2.93	122.94	119.37
2	A	401	FNR	C4-C4A-N5	2.90	123.79	116.37
2	B	401	FNR	O2-C2-N1	-2.87	116.76	121.86
2	B	401	FNR	C9A-C5A-N5	2.84	122.83	119.37
2	B	401	FNR	O4-C4-C4A	-2.77	120.59	127.26
2	A	401	FNR	C5A-N5-C4A	-2.73	114.78	121.08
2	C	401	FNR	C5A-N5-C4A	-2.71	114.82	121.08
2	A	401	FNR	C4A-C4-N3	2.69	119.52	112.13
2	B	401	FNR	C9-C9A-N10	-2.58	118.39	121.85
2	A	401	FNR	C9-C9A-N10	-2.56	118.41	121.85
2	C	401	FNR	O2-C2-N3	-2.46	117.50	121.86
2	D	401	FNR	C9-C8-C7	-2.45	116.09	119.69
2	C	401	FNR	O2'-C2'-C3'	-2.41	103.60	109.25
2	C	401	FNR	C5'-C4'-C3'	-2.35	107.79	112.22
2	D	401	FNR	C4-C4A-N5	2.32	122.30	116.37
2	D	401	FNR	C4-N3-C2	-2.27	123.24	126.37
2	C	401	FNR	O2-C2-N1	-2.27	117.83	121.86
2	D	401	FNR	C6-C5A-C9A	-2.26	117.32	119.80
2	D	401	FNR	C9-C9A-N10	-2.25	118.83	121.85
2	C	401	FNR	C8M-C8-C7	2.24	125.34	120.76
2	C	401	FNR	O5'-C5'-C4'	2.23	115.31	109.36
2	C	401	FNR	C4-C4A-N5	2.23	122.06	116.37
2	A	401	FNR	C5'-C4'-C3'	-2.21	108.05	112.22
2	B	401	FNR	C1'-C2'-C3'	2.19	115.59	109.66
2	D	401	FNR	C5A-N5-C4A	-2.08	116.28	121.08

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	FNR	O3'-C3'-C4'-O4'
2	A	401	FNR	C2'-C3'-C4'-O4'
2	B	401	FNR	C2'-C3'-C4'-O4'
2	D	401	FNR	C2'-C3'-C4'-O4'
2	D	401	FNR	O3'-C3'-C4'-O4'
2	A	401	FNR	C4'-C5'-O5'-P
2	B	401	FNR	O3'-C3'-C4'-C5'
2	B	401	FNR	C4'-C5'-O5'-P
2	C	401	FNR	C4'-C5'-O5'-P
2	D	401	FNR	C4'-C5'-O5'-P
2	C	401	FNR	O3'-C3'-C4'-C5'
2	C	401	FNR	C2'-C3'-C4'-C5'
2	D	401	FNR	O3'-C3'-C4'-C5'
2	A	401	FNR	O3'-C3'-C4'-O4'
2	A	401	FNR	O3'-C3'-C4'-C5'

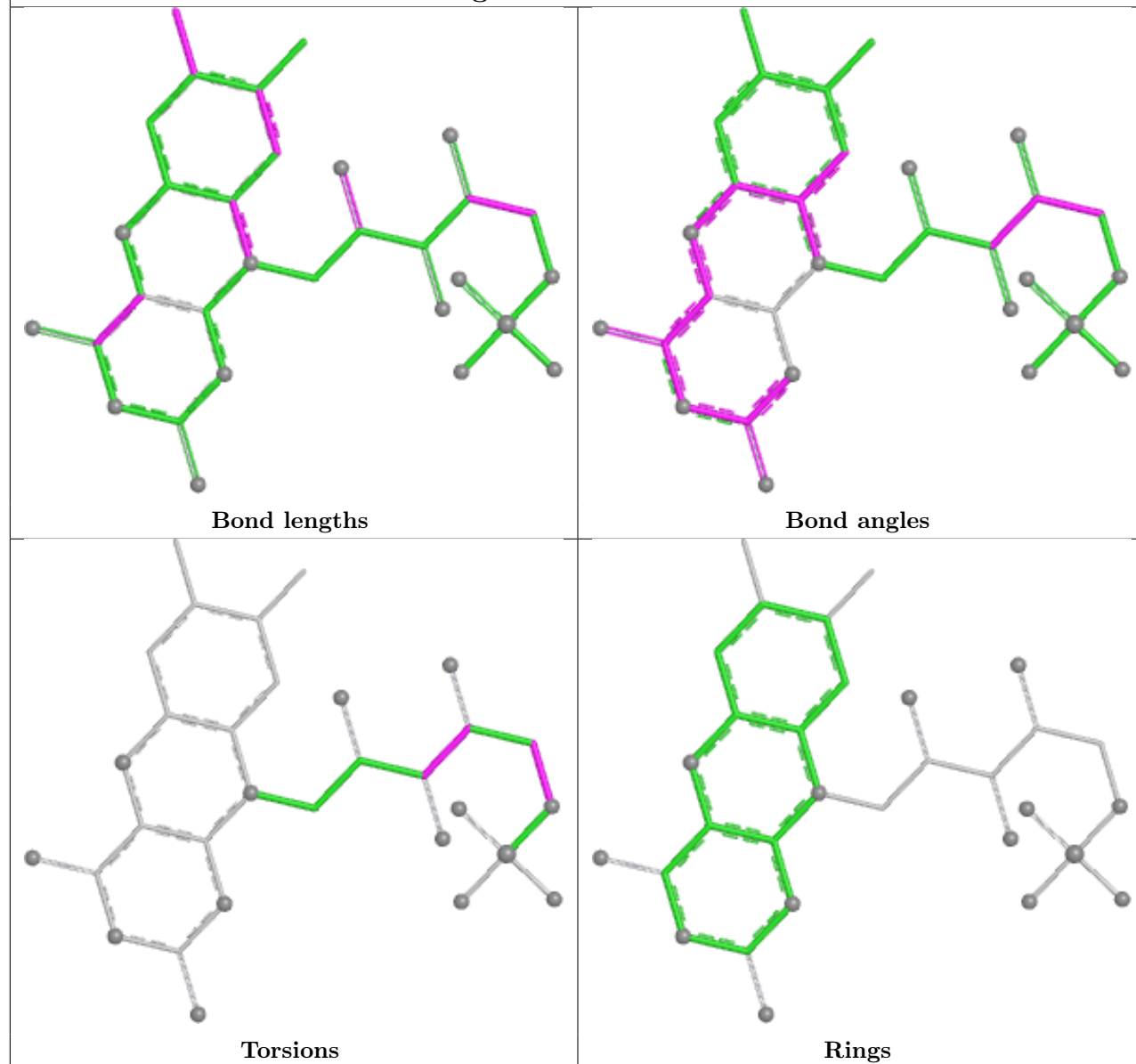
There are no ring outliers.

3 monomers are involved in 5 short contacts:

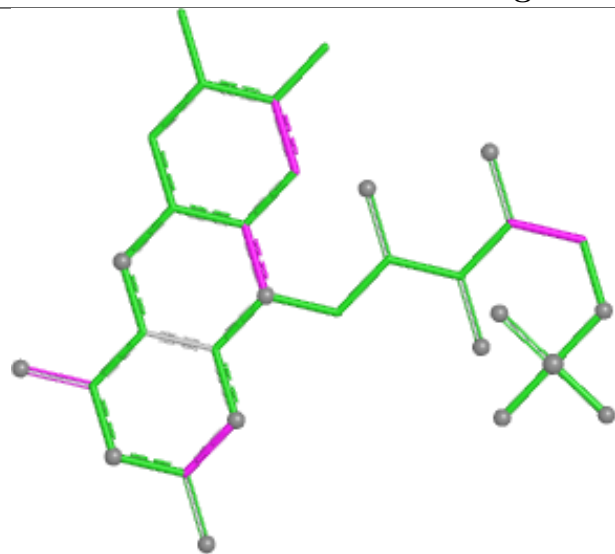
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	FNR	2	0
2	C	401	FNR	1	0
2	B	401	FNR	2	0

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

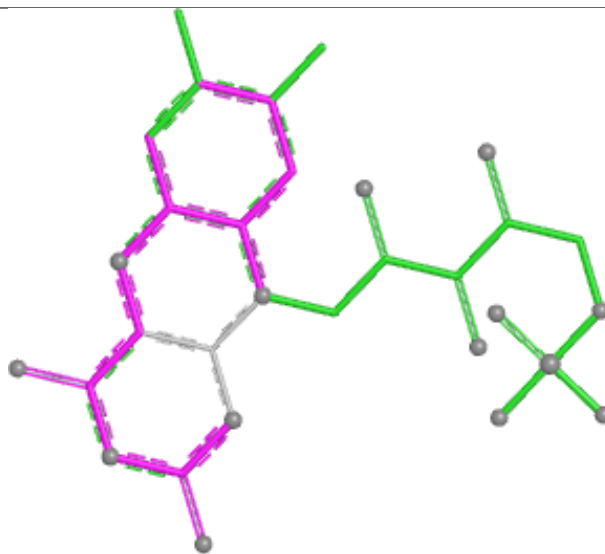
Ligand FNR A 401



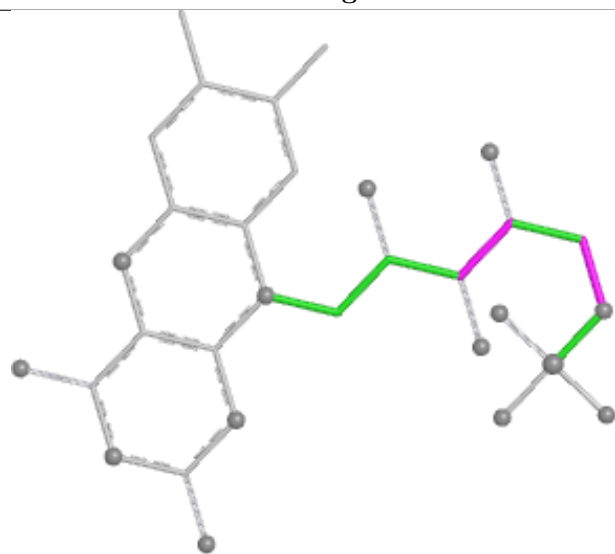
Ligand FNR D 401



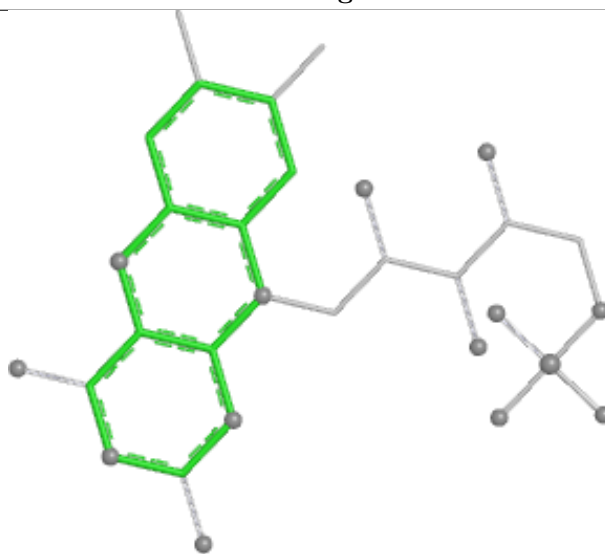
Bond lengths



Bond angles

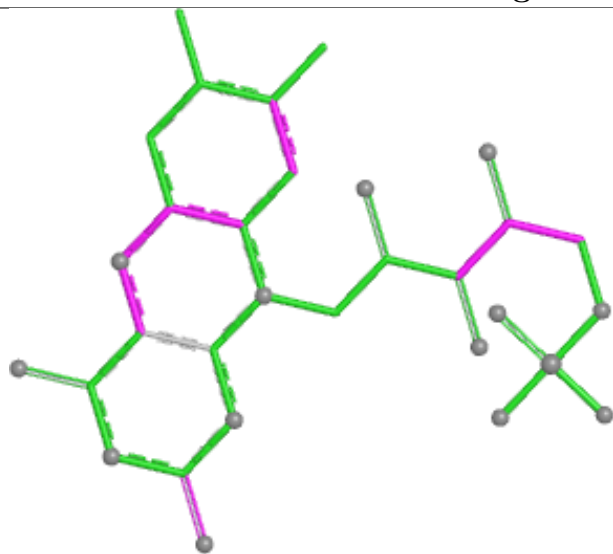


Torsions

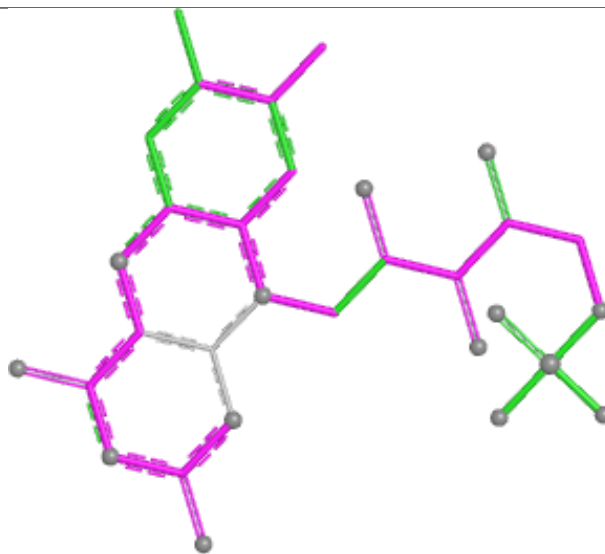


Rings

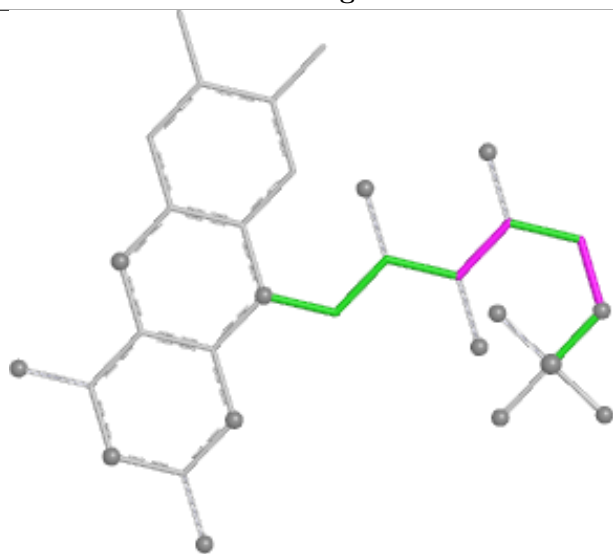
Ligand FNR C 401



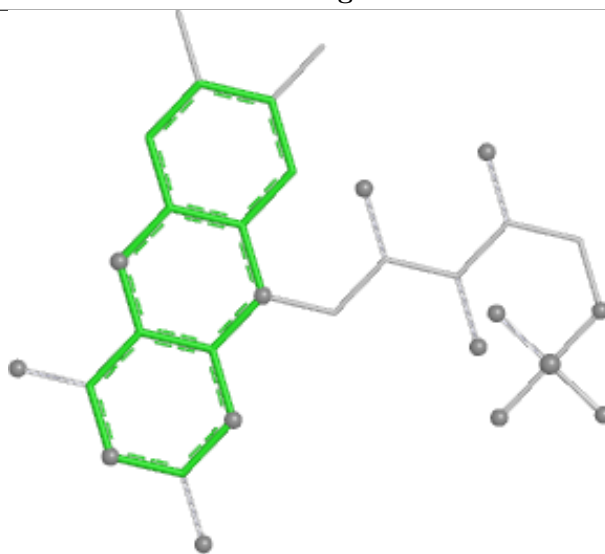
Bond lengths



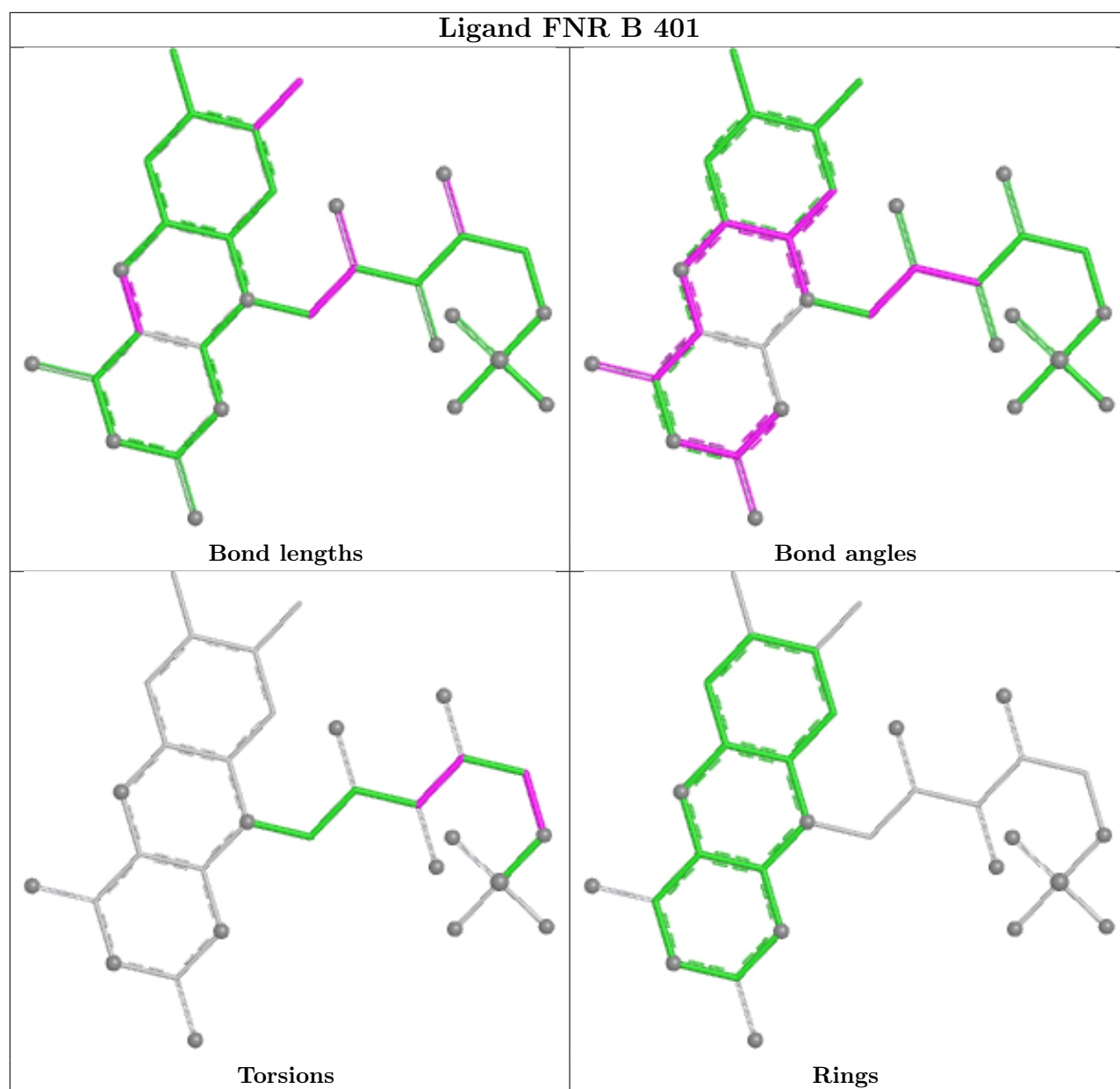
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	363/368 (98%)	0.21	21 (5%) 29 32	14, 21, 38, 50	0
1	B	363/368 (98%)	0.27	21 (5%) 29 32	14, 21, 38, 50	0
1	C	363/368 (98%)	0.22	21 (5%) 29 32	14, 20, 37, 50	0
1	D	363/368 (98%)	0.21	18 (4%) 34 38	14, 21, 38, 50	0
All	All	1452/1472 (98%)	0.23	81 (5%) 30 33	14, 21, 38, 50	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	184	LYS	5.9
1	B	134	GLY	5.6
1	B	174	TYR	5.1
1	C	5	VAL	4.9
1	C	166	GLU	4.6
1	D	167	GLY	4.6
1	A	167	GLY	4.4
1	D	359	SER	4.3
1	B	360	ILE	4.2
1	C	134	GLY	4.1
1	C	145	GLN	4.0
1	C	184	LYS	4.0
1	C	358	LEU	4.0
1	D	166	GLU	3.9
1	C	361	TYR	3.7
1	B	361	TYR	3.7
1	C	359	SER	3.4
1	A	166	GLU	3.4
1	C	357	ASN	3.4
1	B	358	LEU	3.4
1	C	167	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	166	GLU	3.3
1	C	366	LYS	3.1
1	A	359	SER	3.1
1	D	361	TYR	3.0
1	D	358	LEU	3.0
1	A	366	LYS	3.0
1	D	360	ILE	3.0
1	B	167	GLY	3.0
1	A	5	VAL	2.9
1	B	357	ASN	2.9
1	A	74	LEU	2.9
1	B	364	VAL	2.9
1	D	174	TYR	2.9
1	B	187	SER	2.9
1	A	184	LYS	2.8
1	B	359	SER	2.8
1	C	239	TRP	2.8
1	A	361	TYR	2.8
1	B	168	GLU	2.8
1	C	174	TYR	2.8
1	C	308	GLU	2.8
1	D	145	GLN	2.7
1	B	5	VAL	2.7
1	A	105	GLU	2.7
1	C	187	SER	2.7
1	D	111	ALA	2.7
1	A	357	ASN	2.6
1	C	360	ILE	2.6
1	D	170	GLU	2.6
1	B	7	ARG	2.6
1	B	366	LYS	2.5
1	C	172	GLN	2.5
1	A	358	LEU	2.4
1	B	4	ILE	2.4
1	D	9	VAL	2.4
1	A	71	ARG	2.4
1	A	308	GLU	2.4
1	D	105	GLU	2.4
1	B	184	LYS	2.4
1	D	363	LYS	2.4
1	A	7	ARG	2.3
1	A	73	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	119	THR	2.3
1	A	239	TRP	2.3
1	A	119	THR	2.3
1	D	357	ASN	2.3
1	C	364	VAL	2.3
1	C	74	LEU	2.2
1	B	172	GLN	2.2
1	A	360	ILE	2.2
1	D	76	ARG	2.2
1	B	130	GLN	2.1
1	C	186	LEU	2.1
1	C	4	ILE	2.1
1	D	104	ALA	2.1
1	B	165	PRO	2.1
1	D	366	LYS	2.1
1	A	338	LYS	2.1
1	A	174	TYR	2.1
1	A	213	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

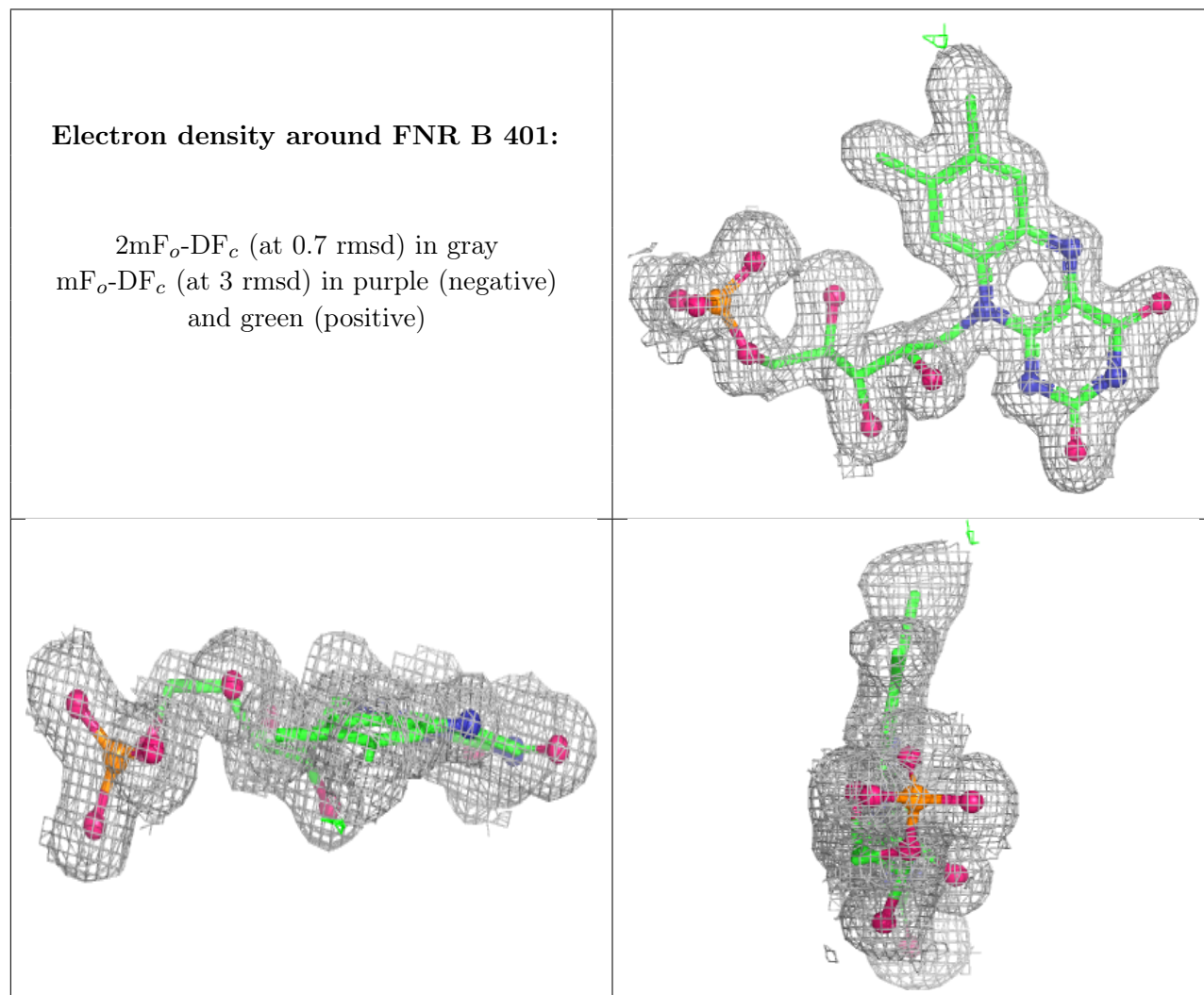
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

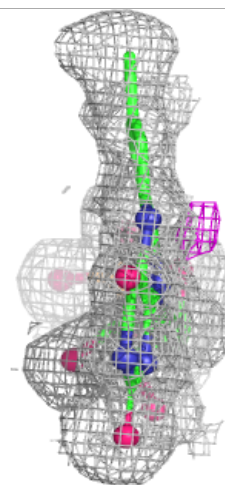
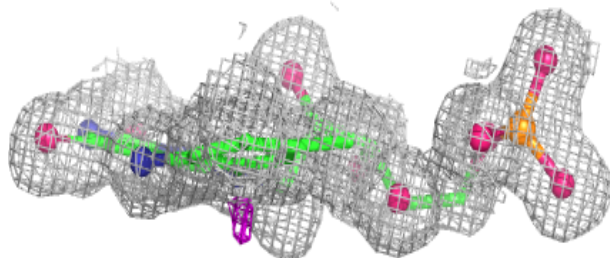
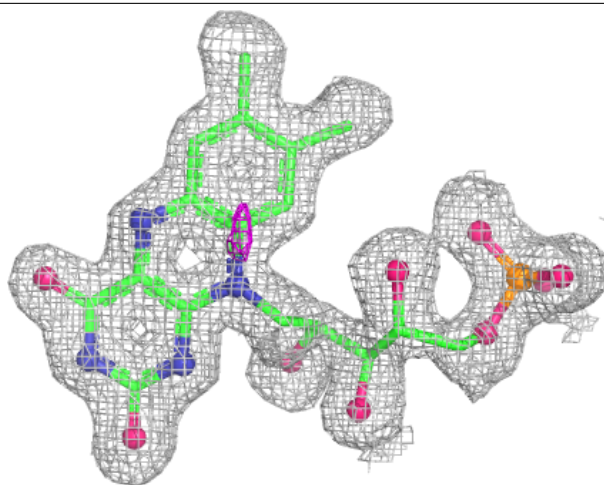
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FNR	B	401	31/31	0.98	0.05	13,17,20,22	0
2	FNR	C	401	31/31	0.98	0.05	13,15,19,20	0
2	FNR	D	401	31/31	0.98	0.05	15,16,20,23	0
2	FNR	A	401	31/31	0.99	0.04	14,17,20,21	0

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.



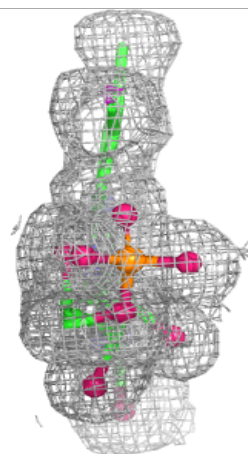
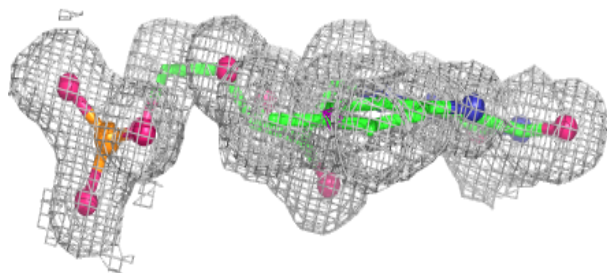
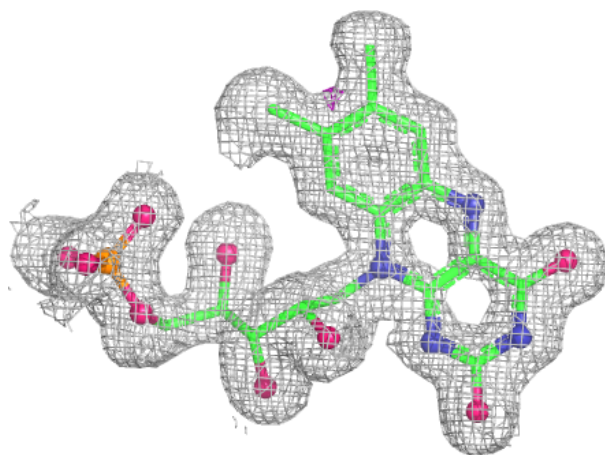
Electron density around FNR C 401:

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



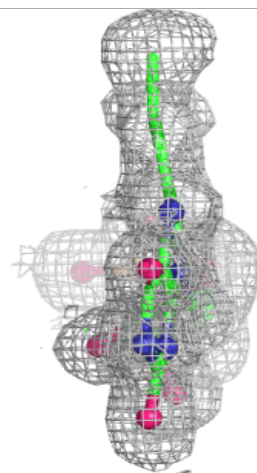
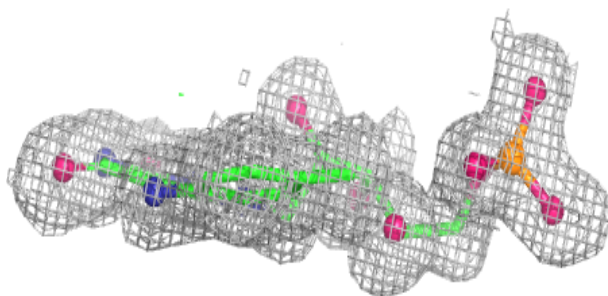
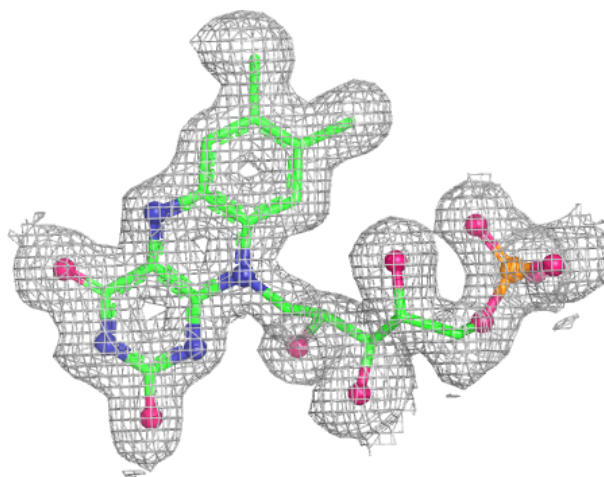
Electron density around FNR D 401:

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



Electron density around FNR 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.