



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:10 PM UTC

PDB ID : 2ISK / pdb_00002isk
Title : BluB bound to flavin anion (charge transfer complex)
Authors : Larsen, N.A.; Taga, M.E.; Howard-Jones, A.R.; Walsh, C.T.; Walker, G.C.
Deposited on : 2006-10-17
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

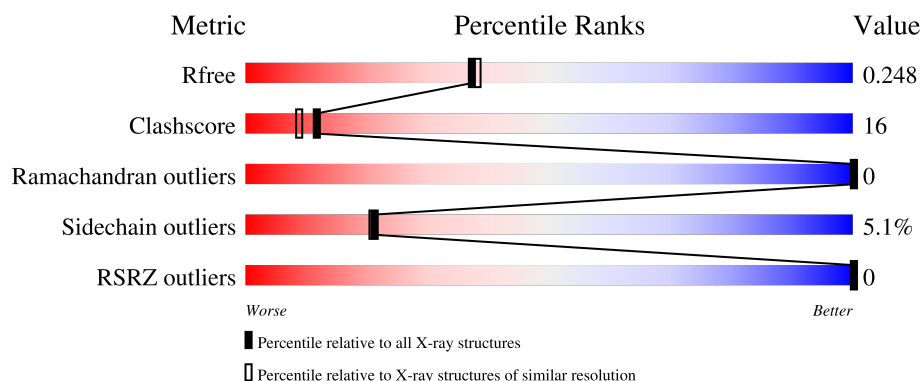
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	230	
1	B	230	
1	C	230	
1	D	230	
1	E	230	

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Mol	Chain	Length	Quality of chain
1	F	230	 73%19%• 5%
1	G	230	 69%23%• 5%
1	H	230	 72%20%• 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15127 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 BluB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	B	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	C	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	D	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	E	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	F	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	G	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	H	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			

There are 24 discrepancies between the modelled and reference sequences:

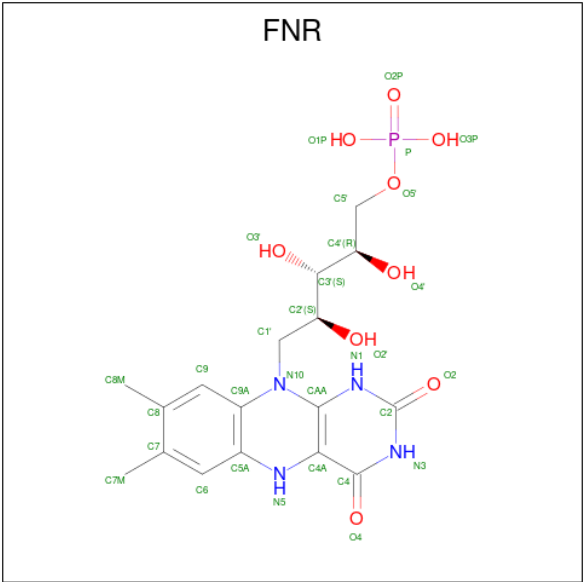
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP Q92PC8
A	-1	SER	-	cloning artifact	UNP Q92PC8
A	0	HIS	-	cloning artifact	UNP Q92PC8
B	-2	GLY	-	cloning artifact	UNP Q92PC8
B	-1	SER	-	cloning artifact	UNP Q92PC8
B	0	HIS	-	cloning artifact	UNP Q92PC8
C	-2	GLY	-	cloning artifact	UNP Q92PC8
C	-1	SER	-	cloning artifact	UNP Q92PC8
C	0	HIS	-	cloning artifact	UNP Q92PC8
D	-2	GLY	-	cloning artifact	UNP Q92PC8
D	-1	SER	-	cloning artifact	UNP Q92PC8
D	0	HIS	-	cloning artifact	UNP Q92PC8
E	-2	GLY	-	cloning artifact	UNP Q92PC8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	cloning artifact	UNP Q92PC8
E	0	HIS	-	cloning artifact	UNP Q92PC8
F	-2	GLY	-	cloning artifact	UNP Q92PC8
F	-1	SER	-	cloning artifact	UNP Q92PC8
F	0	HIS	-	cloning artifact	UNP Q92PC8
G	-2	GLY	-	cloning artifact	UNP Q92PC8
G	-1	SER	-	cloning artifact	UNP Q92PC8
G	0	HIS	-	cloning artifact	UNP Q92PC8
H	-2	GLY	-	cloning artifact	UNP Q92PC8
H	-1	SER	-	cloning artifact	UNP Q92PC8
H	0	HIS	-	cloning artifact	UNP Q92PC8

- 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: C₁₇H₂₃N₄O₉P).



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

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

- Molecule 3 is water.

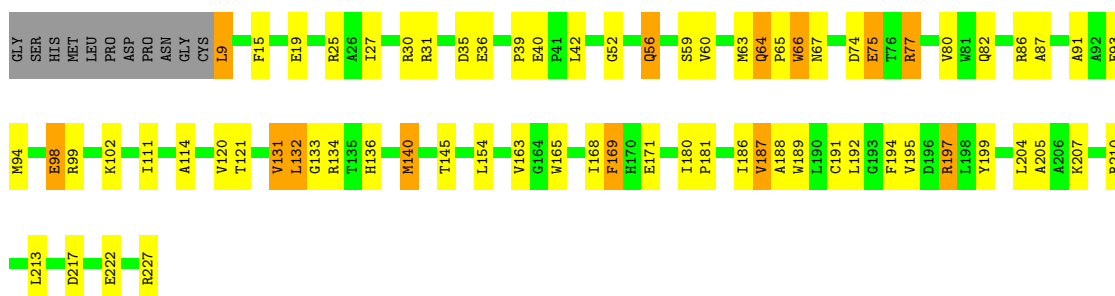
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total	O	0	0
			131	131		
3	B	105	Total	O	0	0
			105	105		
3	C	126	Total	O	0	0
			126	126		
3	D	99	Total	O	0	0
			99	99		
3	E	131	Total	O	0	0
			131	131		
3	F	125	Total	O	0	0
			125	125		
3	G	107	Total	O	0	0
			107	107		
3	H	127	Total	O	0	0
			127	127		

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.

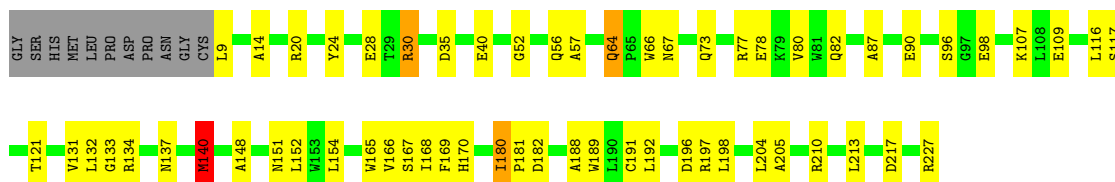
• Molecule 1: BluB

Chain A: 



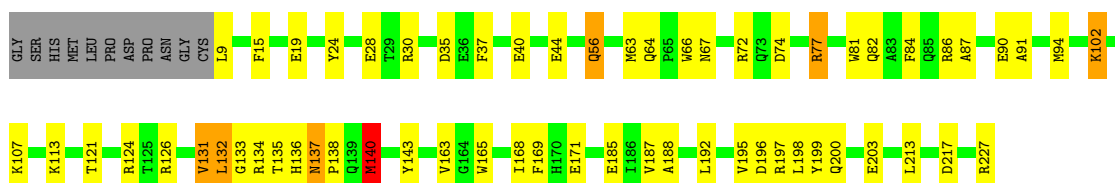
• Molecule 1: BluB

Chain B: 



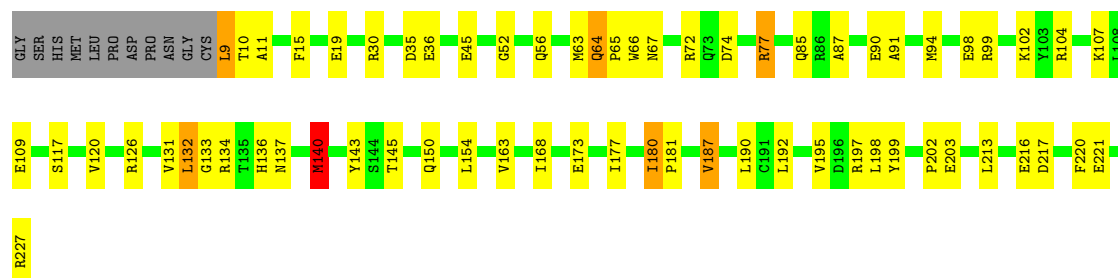
• Molecule 1: BluB

Chain C: 



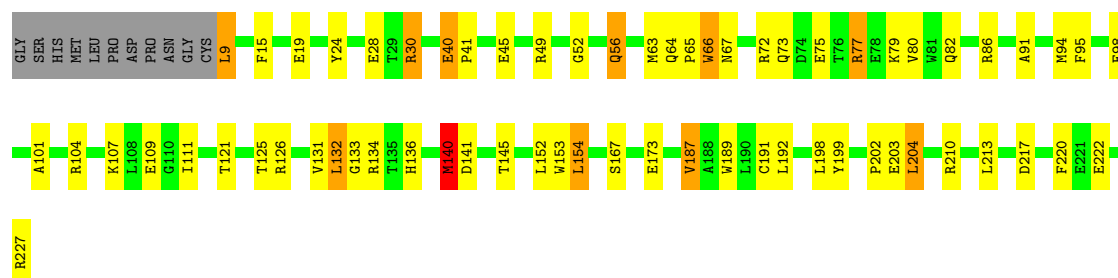
• Molecule 1: BluB

Chain D: 



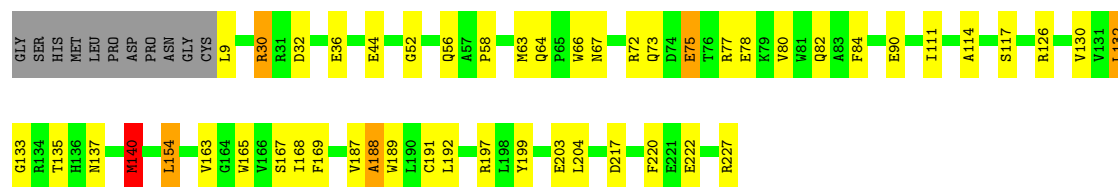
• Molecule 1: BluB

Chain E: 67% 23% 5%



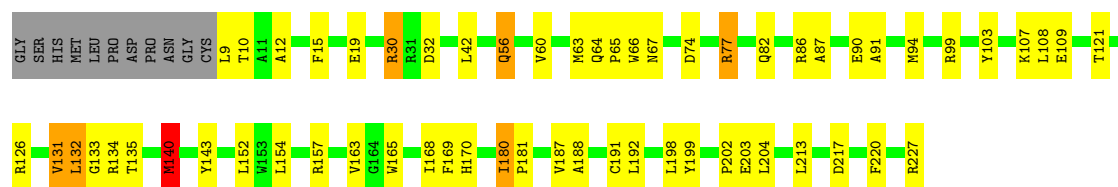
• Molecule 1: BluB

Chain F: 73% 19% 5%



• Molecule 1: BluB

Chain G: 69% 23% 5%



• Molecule 1: BluB

Chain H: 72% 20% 5%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.45Å 169.87Å 90.95Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	80.2 (20.00-2.10) 80.1 (20.00-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.250 0.202 , 0.248	Depositor DCC
R_{free} test set	4513 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.794	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 16.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15127	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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	0.43	1/1780 (0.1%)	0.94	7/2412 (0.3%)
1	B	0.41	1/1780 (0.1%)	0.94	8/2412 (0.3%)
1	C	0.41	1/1780 (0.1%)	0.92	4/2412 (0.2%)
1	D	0.41	1/1780 (0.1%)	0.95	9/2412 (0.4%)
1	E	0.43	1/1780 (0.1%)	0.93	4/2412 (0.2%)
1	F	0.42	1/1780 (0.1%)	0.92	5/2412 (0.2%)
1	G	0.40	1/1780 (0.1%)	0.90	6/2412 (0.2%)
1	H	0.38	0/1780	0.93	7/2412 (0.3%)
All	All	0.41	7/14240 (0.0%)	0.93	50/19296 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	MET	SD-CE	-7.24	1.61	1.79
1	G	140	MET	SD-CE	-6.88	1.62	1.79
1	F	140	MET	SD-CE	-6.77	1.62	1.79
1	D	140	MET	SD-CE	-6.61	1.63	1.79
1	C	140	MET	SD-CE	-6.33	1.63	1.79
1	E	140	MET	SD-CE	-6.02	1.64	1.79
1	B	140	MET	SD-CE	-5.62	1.65	1.79

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	TRP	N-CA-C	7.69	120.93	110.55
1	F	168	ILE	N-CA-C	7.56	114.30	106.21
1	H	66	TRP	N-CA-C	7.52	120.70	110.55
1	B	168	ILE	N-CA-C	7.47	114.20	106.21
1	D	64	GLN	CA-C-N	7.24	127.40	119.87
1	D	64	GLN	C-N-CA	7.24	127.40	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	168	ILE	N-CA-C	6.94	113.64	106.21
1	B	66	TRP	N-CA-C	6.91	119.87	110.55
1	H	64	GLN	CA-C-N	6.51	126.64	119.87
1	H	64	GLN	C-N-CA	6.51	126.64	119.87
1	F	137	ASN	CA-C-N	6.41	126.10	119.82
1	F	137	ASN	C-N-CA	6.41	126.10	119.82
1	B	180	ILE	CA-C-N	6.29	126.65	119.92
1	B	180	ILE	C-N-CA	6.29	126.65	119.92
1	A	66	TRP	N-CA-C	6.25	118.99	110.55
1	A	64	GLN	CA-C-N	6.23	126.35	119.87
1	A	64	GLN	C-N-CA	6.23	126.35	119.87
1	F	66	TRP	N-CA-C	6.14	118.83	110.55
1	E	66	TRP	N-CA-C	6.00	118.65	110.55
1	B	64	GLN	CA-C-N	5.96	126.07	119.87
1	B	64	GLN	C-N-CA	5.96	126.07	119.87
1	D	66	TRP	N-CA-C	5.96	119.29	110.48
1	G	168	ILE	N-CA-C	5.95	115.17	106.55
1	E	64	GLN	CA-C-N	5.93	126.03	119.87
1	E	64	GLN	C-N-CA	5.93	126.03	119.87
1	H	180	ILE	CA-C-N	5.84	126.17	119.92
1	H	180	ILE	C-N-CA	5.84	126.17	119.92
1	C	137	ASN	CA-C-N	5.83	125.54	119.82
1	C	137	ASN	C-N-CA	5.83	125.54	119.82
1	G	126	ARG	N-CA-C	-5.72	102.83	110.55
1	D	180	ILE	CA-C-N	5.58	125.89	119.92
1	D	180	ILE	C-N-CA	5.58	125.89	119.92
1	A	39	PRO	N-CA-C	5.56	121.91	114.18
1	B	137	ASN	CA-C-N	5.54	125.25	119.82
1	B	137	ASN	C-N-CA	5.54	125.25	119.82
1	H	137	ASN	CA-C-N	5.48	125.19	119.82
1	H	137	ASN	C-N-CA	5.48	125.19	119.82
1	A	111	ILE	N-CA-C	5.46	116.85	110.62
1	C	168	ILE	N-CA-C	5.44	114.43	106.55
1	G	180	ILE	CA-C-N	5.44	126.20	120.11
1	G	180	ILE	C-N-CA	5.44	126.20	120.11
1	A	168	ILE	N-CA-C	5.40	115.02	106.32
1	G	66	TRP	N-CA-C	5.27	118.28	110.48
1	D	35	ASP	N-CA-C	5.24	120.33	112.94
1	A	35	ASP	N-CA-C	5.15	120.20	113.30
1	G	32	ASP	N-CA-C	-5.09	100.22	108.41
1	F	188	ALA	N-CA-C	5.05	116.74	108.76
1	E	111	ILE	N-CA-C	5.03	116.35	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	ASN	CA-C-N	5.00	125.07	119.87
1	D	137	ASN	C-N-CA	5.00	125.07	119.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1741	0	1716	81	0
1	B	1741	0	1716	64	0
1	C	1741	0	1716	61	0
1	D	1741	0	1716	64	0
1	E	1741	0	1716	68	0
1	F	1741	0	1716	49	0
1	G	1741	0	1716	70	0
1	H	1741	0	1716	55	0
2	A	31	0	22	4	0
2	B	31	0	22	5	0
2	C	31	0	22	2	0
2	D	31	0	22	4	0
2	E	31	0	22	3	0
2	F	31	0	22	5	0
2	G	31	0	22	3	0
2	H	31	0	22	5	0
3	A	131	0	0	9	0
3	B	105	0	0	10	0
3	C	126	0	0	5	0
3	D	99	0	0	3	0
3	E	131	0	0	5	0
3	F	125	0	0	4	0
3	G	107	0	0	8	0
3	H	127	0	0	7	0
All	All	15127	0	13904	447	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 16.

All (447) 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:D:91:ALA:HA	1:D:94:MET:HE3	1.28	1.10
1:E:91:ALA:HA	1:E:94:MET:HE3	1.32	1.08
1:H:91:ALA:HA	1:H:94:MET:HE3	1.36	1.07
2:C:504:FNR:H7M1	1:D:140:MET:HE2	1.37	1.05
1:C:140:MET:HE2	2:D:503:FNR:H7M1	1.36	1.03
2:E:506:FNR:H7M1	1:F:140:MET:HE3	1.40	1.03
2:A:502:FNR:H7M1	1:B:140:MET:HE3	1.41	0.98
1:D:145:THR:HG21	1:D:187:VAL:HG11	1.43	0.97
1:A:91:ALA:HA	1:A:94:MET:HE3	1.46	0.97
1:E:145:THR:HG21	1:E:187:VAL:HG11	1.48	0.96
1:H:67:ASN:HD21	1:H:126:ARG:HH22	1.10	0.95
1:E:67:ASN:HD21	1:E:126:ARG:HH22	1.14	0.94
1:D:67:ASN:HD21	1:D:126:ARG:HH22	0.96	0.94
1:A:140:MET:HE2	1:B:167:SER:HB3	1.50	0.93
1:E:167:SER:HB3	1:F:140:MET:HE2	1.48	0.92
1:A:145:THR:HG21	1:A:187:VAL:HG11	1.51	0.90
1:A:140:MET:HE2	1:B:167:SER:CB	2.02	0.90
1:A:140:MET:HE3	2:B:501:FNR:H7	1.52	0.90
1:B:131:VAL:HG13	1:B:134:ARG:HB3	1.52	0.88
1:D:67:ASN:HD21	1:D:126:ARG:NH2	1.73	0.87
1:G:140:MET:HE2	2:H:507:FNR:H7M1	1.55	0.87
1:A:64:GLN:HE22	1:B:213:LEU:H	1.22	0.86
1:E:131:VAL:HG13	1:E:134:ARG:HB3	1.59	0.85
1:G:82:GLN:NE2	1:G:86:ARG:HH21	1.75	0.85
1:A:145:THR:CG2	1:A:187:VAL:HG11	2.08	0.83
1:G:131:VAL:HG13	1:G:134:ARG:HB3	1.61	0.83
1:D:67:ASN:ND2	1:D:126:ARG:HH22	1.75	0.82
1:C:67:ASN:HD21	1:C:126:ARG:HH22	1.25	0.82
1:A:213:LEU:H	1:B:64:GLN:HE22	1.28	0.81
1:B:196:ASP:O	1:B:197:ARG:HD2	1.80	0.81
1:E:140:MET:HE3	2:F:505:FNR:H7M3	1.61	0.80
1:H:74:ASP:HA	1:H:77:ARG:NH1	1.97	0.80
1:C:217:ASP:HA	1:C:227:ARG:HH21	1.46	0.80
1:C:64:GLN:HE22	1:D:213:LEU:H	1.28	0.79
1:F:67:ASN:HD21	1:F:126:ARG:HH22	1.24	0.79
1:C:74:ASP:HA	1:C:77:ARG:NH1	1.99	0.78
1:C:131:VAL:HG13	1:C:134:ARG:HB3	1.65	0.77
1:H:150:GLN:O	1:H:154:LEU:HD13	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:MET:HA	1:C:140:MET:HE3	1.69	0.75
1:E:67:ASN:HD21	1:E:126:ARG:NH2	1.86	0.74
1:H:74:ASP:HA	1:H:77:ARG:HH12	1.53	0.74
1:G:213:LEU:H	1:H:64:GLN:HE22	1.36	0.73
1:A:75:GLU:HB2	3:A:770:HOH:O	1.88	0.73
1:F:36:GLU:HG3	1:F:197:ARG:CZ	2.19	0.72
1:D:150:GLN:O	1:D:154:LEU:HD13	1.88	0.72
1:G:91:ALA:HA	1:G:94:MET:HE3	1.71	0.72
1:D:74:ASP:HA	1:D:77:ARG:NH1	2.05	0.72
1:G:64:GLN:HE22	1:H:213:LEU:H	1.35	0.72
1:E:24:TYR:O	1:E:28:GLU:HG3	1.89	0.72
2:A:502:FNR:H7M1	1:B:140:MET:CE	2.16	0.72
1:E:222:GLU:HG3	1:F:73:GLN:NE2	2.05	0.72
1:H:150:GLN:NE2	1:H:154:LEU:HD11	2.04	0.71
1:E:140:MET:HE3	2:F:505:FNR:C7M	2.20	0.71
1:A:222:GLU:HG3	1:B:73:GLN:NE2	2.05	0.71
1:B:30:ARG:NH1	2:B:501:FNR:O2P	2.24	0.71
1:C:74:ASP:HA	1:C:77:ARG:HH12	1.55	0.71
1:G:77:ARG:HD3	3:G:644:HOH:O	1.90	0.71
1:D:150:GLN:NE2	1:D:154:LEU:HD11	2.06	0.70
1:E:145:THR:HG21	1:E:187:VAL:CG1	2.21	0.70
1:H:9:LEU:N	1:H:9:LEU:HD23	2.07	0.70
1:E:213:LEU:H	1:F:64:GLN:HE22	1.39	0.70
1:G:163:VAL:HG22	1:G:192:LEU:HG	1.74	0.70
1:C:217:ASP:HA	1:C:227:ARG:NH2	2.06	0.69
1:A:140:MET:CE	1:B:167:SER:HB3	2.22	0.69
1:F:130:VAL:O	3:F:758:HOH:O	2.10	0.69
1:D:145:THR:CG2	1:D:187:VAL:HG11	2.19	0.69
1:H:217:ASP:HA	3:H:773:HOH:O	1.92	0.69
1:E:167:SER:CB	1:F:140:MET:HE2	2.24	0.68
1:G:63:MET:HE2	1:G:65:PRO:HB3	1.76	0.68
1:A:98:GLU:HG3	1:A:99:ARG:N	2.08	0.67
1:H:67:ASN:HD21	1:H:126:ARG:NH2	1.89	0.67
1:H:67:ASN:ND2	1:H:126:ARG:HH22	1.88	0.67
1:G:87:ALA:CB	1:G:169:PHE:HA	2.24	0.67
1:E:217:ASP:HA	1:E:227:ARG:HH21	1.58	0.67
1:A:227:ARG:HH11	1:A:227:ARG:HG2	1.58	0.67
1:E:154:LEU:HD23	1:F:154:LEU:HD23	1.76	0.67
1:A:140:MET:HE2	1:B:167:SER:HB2	1.78	0.66
1:E:67:ASN:ND2	1:E:126:ARG:HH22	1.88	0.66
1:A:25:ARG:NH2	3:B:790:HOH:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:VAL:HG22	1:D:192:LEU:HG	1.77	0.66
1:B:204:LEU:HD13	3:B:543:HOH:O	1.95	0.66
1:G:227:ARG:HG2	1:G:227:ARG:HH11	1.61	0.66
1:G:82:GLN:HE22	1:G:86:ARG:HH21	1.44	0.65
1:C:67:ASN:HD21	1:C:126:ARG:NH2	1.95	0.65
1:E:125:THR:HB	1:G:227:ARG:HG2	1.78	0.65
1:C:140:MET:CE	1:C:143:TYR:HD2	2.11	0.64
1:G:74:ASP:HA	1:G:77:ARG:NH1	2.12	0.64
1:C:87:ALA:CB	1:C:169:PHE:HA	2.28	0.64
1:C:197:ARG:HB2	1:D:9:LEU:CD2	2.28	0.64
1:B:80:VAL:HG21	1:B:189:TRP:CH2	2.33	0.64
1:F:217:ASP:HA	1:F:227:ARG:HH21	1.62	0.64
1:B:217:ASP:HA	1:B:227:ARG:NH2	2.14	0.63
1:A:63:MET:HE2	1:A:65:PRO:HB3	1.81	0.62
1:B:131:VAL:HG11	1:B:134:ARG:NE	2.14	0.62
1:C:67:ASN:ND2	1:C:126:ARG:HH22	1.95	0.62
1:C:77:ARG:HD3	3:C:563:HOH:O	2.00	0.62
1:F:67:ASN:HD21	1:F:126:ARG:NH2	1.97	0.62
1:H:41:PRO:HG3	3:H:763:HOH:O	2.00	0.62
1:A:74:ASP:HA	1:A:77:ARG:NH1	2.15	0.61
1:C:67:ASN:HB2	1:C:121:THR:OG1	2.01	0.61
1:E:9:LEU:HD23	1:E:9:LEU:N	2.15	0.61
1:G:140:MET:CE	2:H:507:FNR:H7M1	2.28	0.61
1:H:150:GLN:HE21	1:H:154:LEU:HD11	1.66	0.61
1:D:98:GLU:OE2	1:D:102:LYS:HE3	2.01	0.60
1:F:80:VAL:HG21	1:F:189:TRP:CH2	2.36	0.60
1:H:77:ARG:HD3	3:H:594:HOH:O	2.02	0.60
1:E:125:THR:HB	1:G:227:ARG:NH1	2.16	0.59
1:G:170:HIS:HA	3:G:1561:HOH:O	2.02	0.59
1:E:80:VAL:HG21	1:E:189:TRP:CH2	2.38	0.59
1:A:213:LEU:H	1:B:64:GLN:NE2	1.98	0.59
1:A:199:TYR:CE2	1:B:9:LEU:HD12	2.38	0.59
1:C:64:GLN:NE2	1:D:213:LEU:H	1.99	0.59
1:D:140:MET:CE	1:D:143:TYR:HD2	2.15	0.59
1:E:145:THR:CG2	1:E:187:VAL:HG11	2.29	0.59
1:B:14:ALA:O	3:B:790:HOH:O	2.16	0.58
1:E:77:ARG:HD3	3:E:562:HOH:O	2.01	0.58
1:D:227:ARG:HG2	1:D:227:ARG:HH11	1.67	0.58
1:C:15:PHE:HB3	1:C:19:GLU:HB2	1.86	0.58
1:D:87:ALA:O	1:D:90:GLU:HB3	2.04	0.58
1:H:227:ARG:HG2	1:H:227:ARG:HH11	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:CYS:C	1:E:192:LEU:HD12	2.28	0.58
1:A:140:MET:HE1	1:B:165:TRP:NE1	2.18	0.58
1:B:14:ALA:N	3:B:790:HOH:O	2.36	0.58
1:F:227:ARG:HH11	1:F:227:ARG:HG2	1.68	0.58
1:G:82:GLN:NE2	1:G:86:ARG:NH2	2.50	0.58
1:C:35:ASP:HB2	1:C:107:LYS:HD3	1.84	0.58
1:A:64:GLN:NE2	1:B:213:LEU:H	1.95	0.58
1:B:131:VAL:CG1	1:B:134:ARG:NE	2.67	0.58
1:F:114:ALA:HB1	1:F:192:LEU:O	2.04	0.58
1:B:90:GLU:OE1	1:B:170:HIS:NE2	2.37	0.57
1:D:120:VAL:O	1:D:187:VAL:HG13	2.03	0.57
1:D:145:THR:HG21	1:D:187:VAL:CG1	2.28	0.57
1:H:30:ARG:NH1	2:H:507:FNR:O2P	2.38	0.57
1:H:80:VAL:HG21	1:H:189:TRP:CH2	2.38	0.57
1:D:140:MET:HE3	1:D:143:TYR:CD2	2.39	0.57
1:C:197:ARG:HB2	1:D:9:LEU:HD23	1.87	0.57
1:H:199:TYR:CZ	1:H:203:GLU:HG3	2.39	0.57
1:B:24:TYR:O	1:B:28:GLU:HG3	2.05	0.57
1:G:131:VAL:CG1	1:G:134:ARG:NE	2.67	0.57
1:A:52:GLY:O	1:A:56:GLN:HG2	2.05	0.57
1:D:150:GLN:HE21	1:D:154:LEU:HD11	1.68	0.57
1:A:9:LEU:N	1:A:9:LEU:HD23	2.20	0.57
1:D:107:LYS:HE2	1:D:109:GLU:O	2.04	0.57
1:E:132:LEU:HD23	1:E:133:GLY:N	2.19	0.57
1:E:140:MET:HE2	1:F:167:SER:HB3	1.85	0.57
3:G:1083:HOH:O	1:H:71:VAL:HG13	2.05	0.57
1:H:165:TRP:CZ2	1:H:188:ALA:HB2	2.40	0.57
1:G:131:VAL:HG11	1:G:134:ARG:NE	2.20	0.56
1:D:132:LEU:HD23	1:D:133:GLY:N	2.20	0.56
1:G:99:ARG:HD3	3:G:932:HOH:O	2.05	0.56
1:H:113:LYS:HE3	3:H:1225:HOH:O	2.05	0.56
1:D:140:MET:HE3	1:D:140:MET:HA	1.86	0.56
1:B:14:ALA:C	3:B:790:HOH:O	2.49	0.56
1:G:140:MET:CE	1:G:143:TYR:HD2	2.19	0.56
1:D:74:ASP:HA	1:D:77:ARG:HH12	1.69	0.56
1:F:67:ASN:ND2	1:F:126:ARG:HH22	2.00	0.56
1:G:56:GLN:OE1	1:H:28:GLU:HG2	2.06	0.56
1:C:77:ARG:HH11	1:C:77:ARG:HB2	1.69	0.55
1:C:163:VAL:HG22	1:C:192:LEU:HG	1.87	0.55
1:G:191:CYS:C	1:G:192:LEU:HD12	2.31	0.55
1:A:197:ARG:HB2	1:B:9:LEU:CD2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:VAL:CG1	1:C:134:ARG:NE	2.70	0.55
1:E:107:LYS:HE2	1:E:109:GLU:O	2.07	0.55
1:F:163:VAL:HG22	1:F:192:LEU:HG	1.86	0.55
1:B:67:ASN:HB2	1:B:121:THR:OG1	2.07	0.55
1:E:63:MET:HE2	1:E:65:PRO:HB3	1.88	0.55
1:F:197:ARG:HG2	1:F:197:ARG:HH11	1.71	0.55
1:G:132:LEU:HD23	1:G:133:GLY:N	2.21	0.55
1:B:204:LEU:HD22	2:B:501:FNR:O4'	2.07	0.55
1:E:94:MET:HE1	1:F:135:THR:HB	1.88	0.55
1:G:87:ALA:HB2	1:G:169:PHE:HA	1.89	0.55
1:A:91:ALA:CA	1:A:94:MET:HE3	2.30	0.55
1:E:15:PHE:HB3	1:E:19:GLU:HB2	1.89	0.55
1:G:227:ARG:HG2	1:G:227:ARG:NH1	2.21	0.55
1:H:220:PHE:HE1	1:H:227:ARG:NH1	2.05	0.54
1:A:25:ARG:CZ	3:B:790:HOH:O	2.55	0.54
1:C:140:MET:HE1	1:C:143:TYR:HD2	1.73	0.54
1:C:200:GLN:HG2	1:D:10:THR:HG22	1.90	0.54
1:E:220:PHE:HE1	1:E:227:ARG:NH1	2.06	0.54
1:B:217:ASP:HA	1:B:227:ARG:HH21	1.72	0.54
1:D:140:MET:CE	1:D:143:TYR:CD2	2.91	0.53
1:E:204:LEU:HD21	1:F:132:LEU:HD13	1.90	0.53
1:A:140:MET:HE3	2:B:501:FNR:C6	2.32	0.53
1:C:165:TRP:CZ2	1:C:188:ALA:HB2	2.42	0.53
1:A:197:ARG:HB2	1:B:9:LEU:HD21	1.91	0.53
1:B:131:VAL:HG11	1:B:134:ARG:CZ	2.38	0.53
1:C:171:GLU:OE2	1:C:185:GLU:HG3	2.08	0.53
1:G:64:GLN:NE2	1:H:213:LEU:H	2.05	0.53
1:G:15:PHE:HB3	1:G:19:GLU:HB2	1.91	0.53
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.25	0.52
1:C:140:MET:CE	1:C:143:TYR:CD2	2.91	0.52
1:B:132:LEU:HD23	1:B:133:GLY:N	2.25	0.52
1:A:77:ARG:HH11	1:A:77:ARG:HB2	1.75	0.52
1:A:132:LEU:HD23	1:A:133:GLY:N	2.24	0.52
1:H:77:ARG:HH11	1:H:77:ARG:HB2	1.74	0.52
1:F:30:ARG:NH1	2:F:505:FNR:O2P	2.31	0.52
2:G:508:FNR:H7M1	1:H:140:MET:SD	2.49	0.52
1:C:24:TYR:O	1:C:28:GLU:HG3	2.10	0.52
1:G:140:MET:HE3	1:G:143:TYR:CD2	2.44	0.52
1:B:87:ALA:O	1:B:90:GLU:HG2	2.09	0.52
1:A:217:ASP:HA	1:A:227:ARG:HH21	1.74	0.52
1:D:173:GLU:O	1:D:177:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:ARG:O	1:F:77:ARG:NH2	2.43	0.52
1:C:72:ARG:HG3	3:C:1135:HOH:O	2.10	0.51
1:C:102:LYS:HE2	3:C:1164:HOH:O	2.10	0.51
1:G:132:LEU:HD22	3:H:509:HOH:O	2.10	0.51
1:G:227:ARG:NE	3:G:685:HOH:O	2.39	0.51
1:E:132:LEU:HD22	3:F:1645:HOH:O	2.09	0.51
1:E:75:GLU:O	1:E:79:LYS:HG3	2.11	0.51
1:A:98:GLU:HG3	1:A:99:ARG:H	1.75	0.51
1:C:132:LEU:HD23	1:C:133:GLY:N	2.26	0.51
1:C:213:LEU:H	1:D:64:GLN:HE22	1.59	0.51
1:G:140:MET:HE3	1:G:143:TYR:HD2	1.74	0.51
1:A:74:ASP:HA	1:A:77:ARG:HH12	1.76	0.51
1:B:131:VAL:CG1	1:B:134:ARG:HB3	2.33	0.51
1:C:140:MET:HE3	1:C:143:TYR:CD2	2.45	0.51
1:C:35:ASP:OD1	1:C:107:LYS:HE3	2.11	0.51
1:F:191:CYS:C	1:F:192:LEU:HD12	2.35	0.51
1:B:77:ARG:CB	1:B:77:ARG:HH11	2.24	0.50
1:C:37:PHE:O	1:C:113:LYS:HE2	2.11	0.50
1:C:199:TYR:CZ	1:C:203:GLU:HG3	2.46	0.50
1:F:204:LEU:HD22	2:F:505:FNR:O4'	2.11	0.50
1:D:131:VAL:CG2	1:D:134:ARG:HB3	2.40	0.50
1:D:220:PHE:HE1	1:D:227:ARG:HH12	1.59	0.50
1:B:107:LYS:HE2	1:B:109:GLU:O	2.11	0.50
1:C:227:ARG:HG2	1:C:227:ARG:HH11	1.76	0.50
1:B:166:VAL:O	1:B:169:PHE:HE1	1.95	0.50
1:C:90:GLU:OE2	1:D:136:HIS:HE1	1.94	0.50
1:G:30:ARG:NH1	2:G:508:FNR:O3P	2.41	0.50
1:A:77:ARG:HD3	3:A:593:HOH:O	2.12	0.50
1:B:205:ALA:HA	1:B:210:ARG:O	2.11	0.50
1:B:166:VAL:HG12	1:B:169:PHE:CE1	2.47	0.50
1:D:197:ARG:HH11	1:D:197:ARG:HG2	1.76	0.50
1:A:191:CYS:C	1:A:192:LEU:HD12	2.36	0.50
1:F:36:GLU:HA	1:F:197:ARG:NH2	2.27	0.50
1:C:81:TRP:O	1:C:84:PHE:HB3	2.12	0.50
1:E:52:GLY:O	1:E:56:GLN:HG3	2.12	0.50
1:F:220:PHE:HE1	1:F:227:ARG:HH12	1.59	0.49
1:A:80:VAL:HG21	1:A:189:TRP:CH2	2.47	0.49
1:G:90:GLU:OE2	1:H:136:HIS:HE1	1.94	0.49
1:G:67:ASN:HB2	1:G:121:THR:OG1	2.12	0.49
1:G:82:GLN:O	1:G:86:ARG:HG2	2.12	0.49
1:E:227:ARG:HG2	1:E:227:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:THR:O	1:G:227:ARG:CZ	2.60	0.49
1:B:191:CYS:C	1:B:192:LEU:HD12	2.38	0.48
1:E:9:LEU:HB3	1:F:199:TYR:HA	1.95	0.48
1:A:82:GLN:O	1:A:86:ARG:HG3	2.13	0.48
1:E:131:VAL:CG1	1:E:134:ARG:NE	2.76	0.48
1:A:102:LYS:HE2	1:A:207:LYS:O	2.14	0.48
1:E:95:PHE:HZ	3:F:758:HOH:O	1.97	0.48
1:E:213:LEU:H	1:F:64:GLN:NE2	2.07	0.48
1:A:15:PHE:HB3	1:A:19:GLU:HB2	1.95	0.48
1:G:165:TRP:CZ2	1:G:188:ALA:HB2	2.49	0.48
2:C:504:FNR:H5'1	3:C:579:HOH:O	2.13	0.48
1:A:77:ARG:CZ	3:A:898:HOH:O	2.62	0.47
1:B:52:GLY:O	1:B:56:GLN:HG2	2.13	0.47
1:D:217:ASP:HA	1:D:227:ARG:HH21	1.78	0.47
1:B:35:ASP:HB2	1:B:107:LYS:HD3	1.95	0.47
1:A:120:VAL:O	1:A:187:VAL:HG12	2.14	0.47
3:E:510:HOH:O	1:F:132:LEU:HD22	2.13	0.47
1:F:227:ARG:HG2	1:F:227:ARG:NH1	2.30	0.47
1:G:10:THR:O	1:H:197:ARG:HA	2.14	0.47
1:G:135:THR:HB	1:H:94:MET:HE1	1.96	0.47
1:G:199:TYR:HA	1:H:9:LEU:HB3	1.97	0.47
1:H:67:ASN:HB2	1:H:121:THR:OG1	2.14	0.47
1:H:173:GLU:HB3	3:H:1432:HOH:O	2.14	0.47
1:A:195:VAL:HG23	3:A:1133:HOH:O	2.14	0.47
1:F:220:PHE:HE1	1:F:227:ARG:NH1	2.13	0.47
1:E:131:VAL:HG13	1:E:134:ARG:CB	2.36	0.47
1:E:153:TRP:CZ3	1:F:58:PRO:HG3	2.51	0.46
1:G:30:ARG:HG2	1:G:154:LEU:HD23	1.97	0.46
1:G:60:VAL:HG22	1:G:132:LEU:O	2.16	0.46
1:A:25:ARG:NH1	3:B:790:HOH:O	2.48	0.46
1:B:131:VAL:HG13	1:B:134:ARG:CB	2.36	0.46
1:C:131:VAL:HG11	1:C:134:ARG:NE	2.29	0.46
1:D:77:ARG:HD3	3:D:665:HOH:O	2.14	0.46
1:G:202:PRO:HG3	2:G:508:FNR:O1P	2.16	0.46
1:A:132:LEU:HD22	3:B:1644:HOH:O	2.16	0.46
1:C:195:VAL:HG21	1:C:198:LEU:HD21	1.97	0.46
1:H:40:GLU:HG2	1:H:194:PHE:CD2	2.51	0.46
1:D:134:ARG:O	1:D:134:ARG:HG2	2.15	0.46
1:E:131:VAL:HG11	1:E:134:ARG:NE	2.31	0.46
1:G:152:LEU:HD23	1:G:152:LEU:C	2.41	0.46
1:G:227:ARG:NH2	3:G:685:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:MET:HE1	1:B:165:TRP:HE1	1.80	0.46
1:A:87:ALA:CB	1:A:169:PHE:HA	2.45	0.45
1:E:210:ARG:HA	3:E:1138:HOH:O	2.16	0.45
1:A:42:LEU:N	1:A:42:LEU:HD12	2.31	0.45
1:D:154:LEU:CD1	1:D:154:LEU:N	2.79	0.45
1:D:221:GLU:HG3	1:D:227:ARG:O	2.16	0.45
1:A:131:VAL:HG13	1:A:134:ARG:HB3	1.98	0.45
1:D:52:GLY:O	1:D:56:GLN:HG2	2.16	0.45
1:F:132:LEU:HD23	1:F:133:GLY:N	2.31	0.45
1:G:131:VAL:HG11	1:G:134:ARG:CZ	2.45	0.45
1:B:198:LEU:HD23	3:B:1367:HOH:O	2.15	0.45
1:E:45:GLU:HG2	1:E:49:ARG:HH12	1.80	0.45
1:G:140:MET:HE2	1:H:165:TRP:CZ2	2.52	0.45
1:A:9:LEU:HB2	1:B:198:LEU:O	2.17	0.45
1:A:136:HIS:NE2	1:B:90:GLU:OE1	2.50	0.45
1:A:67:ASN:HB2	1:A:121:THR:OG1	2.15	0.45
1:B:182:ASP:HB2	3:B:816:HOH:O	2.17	0.45
1:C:140:MET:HE2	2:D:503:FNR:C7M	2.26	0.45
1:E:67:ASN:HB2	1:E:121:THR:OG1	2.17	0.45
1:F:36:GLU:HG2	1:F:197:ARG:HG3	1.99	0.45
1:B:116:LEU:HD12	1:B:117:SER:H	1.82	0.45
1:C:131:VAL:HG11	1:C:134:ARG:CZ	2.46	0.45
1:E:98:GLU:O	1:E:101:ALA:HB3	2.17	0.45
1:F:77:ARG:HD3	1:F:111:ILE:O	2.16	0.45
1:F:220:PHE:CE1	1:F:227:ARG:NH1	2.84	0.45
1:D:227:ARG:HG2	1:D:227:ARG:NH1	2.28	0.45
1:E:199:TYR:CZ	1:E:203:GLU:HG3	2.52	0.45
1:G:30:ARG:HA	1:G:157:ARG:HD3	1.99	0.45
1:A:59:SER:HA	2:B:501:FNR:H8M2	1.99	0.44
1:A:134:ARG:O	1:A:134:ARG:HG2	2.17	0.44
3:A:807:HOH:O	1:B:20:ARG:HD2	2.18	0.44
1:C:124:ARG:HG3	3:C:1418:HOH:O	2.17	0.44
1:A:66:TRP:HA	1:A:121:THR:O	2.18	0.44
1:E:131:VAL:CG1	1:E:134:ARG:HB3	2.40	0.44
1:F:36:GLU:HG3	1:F:197:ARG:NE	2.31	0.44
1:F:63:MET:HE3	1:F:126:ARG:O	2.17	0.44
1:C:87:ALA:HB2	1:C:169:PHE:HA	2.00	0.44
1:E:40:GLU:H	1:E:40:GLU:HG2	1.50	0.44
1:E:91:ALA:CA	1:E:94:MET:HE3	2.24	0.44
1:C:136:HIS:NE2	1:D:90:GLU:OE2	2.50	0.44
1:G:15:PHE:HB3	1:G:19:GLU:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:GLN:HE21	1:G:82:GLN:HB3	1.61	0.44
1:G:140:MET:CE	1:G:143:TYR:CD2	3.00	0.44
1:A:165:TRP:CZ2	1:A:188:ALA:HB2	2.52	0.44
1:E:82:GLN:O	1:E:86:ARG:HG3	2.17	0.44
1:D:197:ARG:HG2	1:D:197:ARG:NH1	2.33	0.44
1:H:45:GLU:H	1:H:45:GLU:CD	2.26	0.44
1:D:199:TYR:CZ	1:D:203:GLU:HG3	2.53	0.44
1:A:145:THR:HG22	1:A:187:VAL:HG11	1.95	0.44
1:A:163:VAL:HG22	1:A:192:LEU:HG	1.99	0.44
1:B:165:TRP:CZ2	1:B:188:ALA:HB2	2.53	0.44
1:H:9:LEU:N	1:H:9:LEU:CD2	2.79	0.44
1:D:117:SER:HA	1:D:190:LEU:O	2.17	0.43
1:E:136:HIS:HE1	1:F:90:GLU:OE2	2.01	0.43
1:E:152:LEU:C	1:E:152:LEU:HD23	2.42	0.43
1:E:198:LEU:C	1:F:9:LEU:HD12	2.43	0.43
1:G:140:MET:HE3	1:G:140:MET:HA	2.00	0.43
1:G:217:ASP:HA	3:G:685:HOH:O	2.18	0.43
1:H:220:PHE:CE1	1:H:227:ARG:NH1	2.85	0.43
1:A:40:GLU:OE1	1:E:173:GLU:OE2	2.36	0.43
1:A:140:MET:HE1	1:B:165:TRP:CE2	2.53	0.43
1:E:40:GLU:HA	1:E:41:PRO:HD3	1.92	0.43
1:G:42:LEU:N	1:G:42:LEU:HD12	2.33	0.43
1:A:60:VAL:HG22	1:A:132:LEU:O	2.18	0.43
1:E:104:ARG:NH2	3:E:728:HOH:O	2.41	0.43
1:B:57:ALA:HB2	1:B:148:ALA:HA	2.01	0.43
1:B:180:ILE:HA	1:B:181:PRO:HD3	1.79	0.43
1:C:135:THR:HB	1:D:94:MET:HE1	1.99	0.43
1:G:103:TYR:CE1	1:H:132:LEU:HG	2.54	0.43
1:G:140:MET:HG3	2:H:507:FNR:C7M	2.47	0.43
1:A:31:ARG:HD2	1:A:199:TYR:O	2.18	0.43
1:E:66:TRP:HA	1:E:121:THR:O	2.18	0.43
1:E:73:GLN:HG3	1:F:222:GLU:CD	2.44	0.43
1:F:199:TYR:CZ	1:F:203:GLU:HG3	2.54	0.43
1:G:107:LYS:HE2	1:G:109:GLU:O	2.18	0.43
1:A:36:GLU:N	1:A:36:GLU:CD	2.77	0.43
1:B:9:LEU:HD23	1:B:9:LEU:C	2.43	0.43
1:B:152:LEU:HD23	1:B:152:LEU:C	2.44	0.43
1:F:78:GLU:O	1:F:82:GLN:HG3	2.18	0.43
1:H:145:THR:HG21	1:H:187:VAL:HG21	2.01	0.43
1:A:36:GLU:HG2	1:B:9:LEU:HD11	2.00	0.43
1:A:120:VAL:O	1:A:187:VAL:CG1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:PRO:HG3	2:D:503:FNR:O1P	2.17	0.43
1:G:74:ASP:HA	1:G:77:ARG:HH12	1.84	0.43
1:C:86:ARG:HA	1:C:86:ARG:HD3	1.90	0.43
1:A:180:ILE:HA	1:A:181:PRO:HD3	1.83	0.43
1:F:52:GLY:O	1:F:56:GLN:HG2	2.19	0.42
1:F:227:ARG:HE	1:H:128:GLY:HA2	1.84	0.42
1:A:180:ILE:HD12	1:A:186:ILE:HD11	2.01	0.42
1:B:78:GLU:HG3	1:B:82:GLN:HE21	1.84	0.42
1:D:10:THR:OG1	1:D:11:ALA:N	2.51	0.42
1:D:203:GLU:HB2	3:D:791:HOH:O	2.18	0.42
1:H:45:GLU:CD	1:H:45:GLU:N	2.77	0.42
1:H:152:LEU:C	1:H:152:LEU:HD23	2.44	0.42
1:E:45:GLU:CG	1:E:49:ARG:HH12	2.32	0.42
1:G:108:LEU:HD13	1:H:132:LEU:HD21	2.01	0.42
1:H:197:ARG:NH1	3:H:762:HOH:O	2.52	0.42
1:G:12:ALA:O	1:H:196:ASP:HA	2.19	0.42
1:G:220:PHE:CE1	1:G:227:ARG:NH2	2.87	0.42
1:A:205:ALA:HA	1:A:210:ARG:O	2.20	0.42
2:A:502:FNR:C7M	1:B:140:MET:HG3	2.49	0.42
1:D:154:LEU:N	1:D:154:LEU:HD12	2.35	0.42
1:H:102:LYS:HB2	1:H:102:LYS:HE3	1.88	0.42
1:A:204:LEU:HD12	2:A:502:FNR:O4'	2.20	0.42
1:D:45:GLU:H	1:D:45:GLU:CD	2.28	0.42
1:G:99:ARG:HD2	1:G:99:ARG:HA	1.86	0.42
1:H:204:LEU:HD22	2:H:507:FNR:O4'	2.19	0.42
1:C:82:GLN:OE1	1:C:86:ARG:NH2	2.52	0.42
1:D:216:GLU:HG2	1:D:217:ASP:N	2.35	0.42
1:E:202:PRO:HB3	2:E:506:FNR:H5'2	2.01	0.42
1:F:32:ASP:CG	2:F:505:FNR:H1'1	2.45	0.42
1:A:56:GLN:HE21	1:A:56:GLN:HB3	1.62	0.42
1:A:99:ARG:HD2	1:A:99:ARG:HA	1.78	0.42
1:C:197:ARG:HB2	1:D:9:LEU:HD21	2.02	0.42
1:D:15:PHE:HB3	1:D:19:GLU:HB2	2.01	0.41
1:F:75:GLU:HG3	3:F:1450:HOH:O	2.19	0.41
1:F:165:TRP:CZ2	1:F:188:ALA:HB2	2.55	0.41
1:G:9:LEU:HD23	1:G:9:LEU:N	2.35	0.41
1:G:198:LEU:O	1:H:9:LEU:HB2	2.20	0.41
1:A:194:PHE:CB	1:E:86:ARG:HD3	2.50	0.41
1:A:210:ARG:HG3	3:A:1528:HOH:O	2.20	0.41
1:C:196:ASP:OD1	1:C:197:ARG:HG2	2.19	0.41
1:D:36:GLU:O	1:D:195:VAL:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ARG:HD3	3:D:1142:HOH:O	2.20	0.41
1:G:213:LEU:H	1:H:64:GLN:NE2	2.12	0.41
1:D:180:ILE:HA	1:D:181:PRO:HD3	1.80	0.41
1:G:180:ILE:HA	1:G:181:PRO:HD3	1.80	0.41
1:H:117:SER:HA	1:H:190:LEU:O	2.20	0.41
1:D:220:PHE:CE1	1:D:227:ARG:NH1	2.88	0.41
1:A:99:ARG:NH2	3:A:1528:HOH:O	2.53	0.41
1:D:63:MET:HE2	1:D:65:PRO:HB3	2.02	0.41
3:G:1083:HOH:O	1:H:73:GLN:HB2	2.20	0.41
1:A:9:LEU:N	1:A:9:LEU:CD2	2.84	0.41
1:A:171:GLU:CD	3:A:1011:HOH:O	2.64	0.41
1:C:9:LEU:HD12	1:D:198:LEU:C	2.46	0.41
1:E:63:MET:SD	1:E:141:ASP:HB3	2.60	0.41
1:G:199:TYR:CZ	1:G:203:GLU:HG3	2.56	0.41
1:A:227:ARG:HB3	3:A:1053:HOH:O	2.21	0.41
1:C:77:ARG:HH11	1:C:77:ARG:CB	2.33	0.41
1:C:91:ALA:O	1:C:94:MET:HB2	2.21	0.41
1:C:137:ASN:HA	1:C:138:PRO:HD2	1.94	0.41
1:D:132:LEU:HD23	1:D:132:LEU:C	2.46	0.41
1:E:30:ARG:NH1	2:E:506:FNR:O2P	2.46	0.41
1:E:192:LEU:HD12	1:E:192:LEU:N	2.35	0.41
1:C:91:ALA:HA	1:C:94:MET:HE3	2.02	0.41
1:E:72:ARG:NH2	3:E:1203:HOH:O	2.53	0.41
1:H:227:ARG:HG2	1:H:227:ARG:NH1	2.34	0.41
1:A:36:GLU:CG	1:B:9:LEU:HD11	2.51	0.40
1:B:196:ASP:C	1:B:197:ARG:HD2	2.44	0.40
1:C:56:GLN:HE21	1:C:56:GLN:HB3	1.64	0.40
1:H:132:LEU:HD23	1:H:133:GLY:N	2.35	0.40
1:A:114:ALA:HB1	1:A:192:LEU:O	2.21	0.40
1:C:40:GLU:O	1:C:40:GLU:HG3	2.20	0.40
1:C:140:MET:HG3	2:D:503:FNR:C7M	2.51	0.40
1:D:85:GLN:OE1	1:D:85:GLN:HA	2.21	0.40
1:D:131:VAL:HG23	1:D:134:ARG:HB3	2.03	0.40
1:E:63:MET:HE3	1:E:126:ARG:O	2.21	0.40
1:G:192:LEU:HD12	1:G:192:LEU:N	2.36	0.40
1:A:213:LEU:N	1:B:64:GLN:HE22	2.07	0.40
1:F:84:PHE:HB2	1:F:169:PHE:CE2	2.56	0.40
1:H:168:ILE:O	1:H:168:ILE:HG22	2.20	0.40
1:A:27:ILE:HG23	1:B:151:ASN:ND2	2.36	0.40
1:C:63:MET:HE3	1:C:126:ARG:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/230 (94%)	211 (97%)	6 (3%)	0	100	100
1	B	217/230 (94%)	216 (100%)	1 (0%)	0	100	100
1	C	217/230 (94%)	210 (97%)	7 (3%)	0	100	100
1	D	217/230 (94%)	213 (98%)	4 (2%)	0	100	100
1	E	217/230 (94%)	212 (98%)	5 (2%)	0	100	100
1	F	217/230 (94%)	215 (99%)	2 (1%)	0	100	100
1	G	217/230 (94%)	213 (98%)	4 (2%)	0	100	100
1	H	217/230 (94%)	213 (98%)	4 (2%)	0	100	100
All	All	1736/1840 (94%)	1703 (98%)	33 (2%)	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	178/187 (95%)	165 (93%)	13 (7%)	13	10
1	B	178/187 (95%)	172 (97%)	6 (3%)	32	35
1	C	178/187 (95%)	169 (95%)	9 (5%)	21	21
1	D	178/187 (95%)	170 (96%)	8 (4%)	24	25
1	E	178/187 (95%)	168 (94%)	10 (6%)	19	18
1	F	178/187 (95%)	170 (96%)	8 (4%)	24	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	178/187 (95%)	170 (96%)	8 (4%)	24	25
1	H	178/187 (95%)	168 (94%)	10 (6%)	19	18
All	All	1424/1496 (95%)	1352 (95%)	72 (5%)	21	21

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	30	ARG
1	A	56	GLN
1	A	75	GLU
1	A	77	ARG
1	A	93	GLU
1	A	98	GLU
1	A	131	VAL
1	A	132	LEU
1	A	154	LEU
1	A	169	PHE
1	A	187	VAL
1	A	197	ARG
1	B	30	ARG
1	B	40	GLU
1	B	96	SER
1	B	98	GLU
1	B	140	MET
1	B	154	LEU
1	C	30	ARG
1	C	44	GLU
1	C	56	GLN
1	C	77	ARG
1	C	102	LYS
1	C	131	VAL
1	C	132	LEU
1	C	140	MET
1	C	187	VAL
1	D	9	LEU
1	D	30	ARG
1	D	72	ARG
1	D	77	ARG
1	D	99	ARG
1	D	132	LEU

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Mol	Chain	Res	Type
1	D	140	MET
1	D	187	VAL
1	E	9	LEU
1	E	30	ARG
1	E	40	GLU
1	E	56	GLN
1	E	77	ARG
1	E	132	LEU
1	E	140	MET
1	E	154	LEU
1	E	187	VAL
1	E	204	LEU
1	F	30	ARG
1	F	44	GLU
1	F	75	GLU
1	F	117	SER
1	F	132	LEU
1	F	140	MET
1	F	154	LEU
1	F	187	VAL
1	G	30	ARG
1	G	56	GLN
1	G	77	ARG
1	G	131	VAL
1	G	132	LEU
1	G	140	MET
1	G	187	VAL
1	G	204	LEU
1	H	9	LEU
1	H	18	ASP
1	H	30	ARG
1	H	40	GLU
1	H	56	GLN
1	H	77	ARG
1	H	99	ARG
1	H	132	LEU
1	H	169	PHE
1	H	204	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	64	GLN
1	A	85	GLN
1	A	150	GLN
1	B	64	GLN
1	B	73	GLN
1	B	82	GLN
1	B	211	GLN
1	C	56	GLN
1	C	64	GLN
1	C	67	ASN
1	C	88	ASN
1	C	211	GLN
1	D	64	GLN
1	D	67	ASN
1	D	82	GLN
1	D	136	HIS
1	D	139	GLN
1	D	150	GLN
1	E	67	ASN
1	E	85	GLN
1	E	136	HIS
1	E	150	GLN
1	F	56	GLN
1	F	64	GLN
1	F	67	ASN
1	F	73	GLN
1	F	85	GLN
1	F	150	GLN
1	G	64	GLN
1	G	82	GLN
1	G	136	HIS
1	G	150	GLN
1	G	211	GLN
1	H	56	GLN
1	H	64	GLN
1	H	67	ASN
1	H	88	ASN
1	H	136	HIS
1	H	150	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	E	506	-	32,33,33	2.17	13 (40%)	41,50,50	1.49	7 (17%)
2	FNR	F	505	-	32,33,33	2.19	13 (40%)	41,50,50	1.53	7 (17%)
2	FNR	H	507	-	32,33,33	2.08	13 (40%)	41,50,50	1.57	7 (17%)
2	FNR	G	508	-	32,33,33	2.00	11 (34%)	41,50,50	1.84	11 (26%)
2	FNR	D	503	-	32,33,33	2.04	12 (37%)	41,50,50	1.88	12 (29%)
2	FNR	A	502	-	32,33,33	2.14	11 (34%)	41,50,50	2.39	13 (31%)
2	FNR	C	504	-	32,33,33	2.15	13 (40%)	41,50,50	2.42	12 (29%)
2	FNR	B	501	-	32,33,33	2.15	12 (37%)	41,50,50	1.54	7 (17%)

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	E	506	-	-	2/18/18/18	0/3/3/3
2	FNR	F	505	-	-	2/18/18/18	0/3/3/3
2	FNR	H	507	-	-	2/18/18/18	0/3/3/3
2	FNR	G	508	-	-	0/18/18/18	0/3/3/3
2	FNR	D	503	-	-	0/18/18/18	0/3/3/3
2	FNR	A	502	-	-	8/18/18/18	0/3/3/3
2	FNR	C	504	-	-	7/18/18/18	0/3/3/3
2	FNR	B	501	-	-	2/18/18/18	0/3/3/3

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	506	FNR	C4A-N5	4.78	1.45	1.35
2	C	504	FNR	C4A-N5	4.73	1.45	1.35
2	A	502	FNR	C4A-N5	4.68	1.45	1.35
2	D	503	FNR	C4'-C3'	4.54	1.61	1.53
2	F	505	FNR	C4A-N5	4.46	1.44	1.35
2	D	503	FNR	C4A-N5	4.30	1.44	1.35
2	B	501	FNR	C4A-N5	4.25	1.44	1.35
2	H	507	FNR	C5A-C9A	4.25	1.45	1.40
2	H	507	FNR	C4A-N5	4.18	1.44	1.35
2	E	506	FNR	C6-C7	4.00	1.45	1.39
2	G	508	FNR	C4A-N5	3.96	1.43	1.35
2	D	503	FNR	C6-C7	3.94	1.45	1.39
2	C	504	FNR	C6-C7	3.93	1.45	1.39
2	A	502	FNR	C6-C7	3.89	1.44	1.39
2	F	505	FNR	C6-C7	3.86	1.44	1.39
2	G	508	FNR	C9-C9A	3.72	1.45	1.39
2	F	505	FNR	C5A-C9A	3.70	1.44	1.40
2	B	501	FNR	C6-C7	3.63	1.44	1.39
2	E	506	FNR	C5A-C9A	3.63	1.44	1.40
2	E	506	FNR	C9-C9A	3.59	1.45	1.39
2	C	504	FNR	C2'-C3'	-3.57	1.47	1.53
2	H	507	FNR	C6-C7	3.56	1.44	1.39
2	B	501	FNR	C9-C9A	3.55	1.45	1.39
2	F	505	FNR	C9-C9A	3.49	1.45	1.39
2	G	508	FNR	C4'-C3'	3.47	1.59	1.53
2	G	508	FNR	C9A-N10	3.46	1.47	1.41
2	B	501	FNR	CAA-N10	3.41	1.44	1.38
2	G	508	FNR	C6-C7	3.38	1.44	1.39
2	B	501	FNR	C5A-C9A	3.32	1.44	1.40
2	D	503	FNR	C9-C9A	3.30	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	FNR	C9-C9A	3.27	1.44	1.39
2	H	507	FNR	CAA-N10	3.25	1.44	1.38
2	C	504	FNR	C9-C9A	3.21	1.44	1.39
2	F	505	FNR	C9A-N10	3.18	1.46	1.41
2	A	502	FNR	C6-C5A	3.14	1.44	1.39
2	A	502	FNR	C2'-C3'	-3.12	1.48	1.53
2	A	502	FNR	C5A-C9A	3.04	1.43	1.40
2	H	507	FNR	C9-C9A	3.03	1.44	1.39
2	C	504	FNR	CAA-N10	3.02	1.43	1.38
2	E	506	FNR	CAA-N10	3.02	1.43	1.38
2	C	504	FNR	C5A-C9A	3.02	1.43	1.40
2	B	501	FNR	C5'-C4'	2.98	1.55	1.51
2	D	503	FNR	CAA-N10	2.95	1.43	1.38
2	F	505	FNR	CAA-N10	2.94	1.43	1.38
2	B	501	FNR	C9A-N10	2.92	1.46	1.41
2	A	502	FNR	CAA-N10	2.92	1.43	1.38
2	E	506	FNR	C9A-N10	2.89	1.46	1.41
2	A	502	FNR	C5'-C4'	-2.87	1.47	1.51
2	E	506	FNR	C6-C5A	2.86	1.44	1.39
2	A	502	FNR	C4-N3	2.81	1.44	1.38
2	G	508	FNR	CAA-N10	2.80	1.43	1.38
2	F	505	FNR	C6-C5A	2.80	1.43	1.39
2	C	504	FNR	C6-C5A	2.80	1.43	1.39
2	E	506	FNR	C4-N3	2.73	1.44	1.38
2	D	503	FNR	C4-N3	2.72	1.44	1.38
2	B	501	FNR	C4'-C3'	2.71	1.58	1.53
2	F	505	FNR	C4-N3	2.71	1.43	1.38
2	C	504	FNR	C5'-C4'	-2.70	1.48	1.51
2	H	507	FNR	C6-C5A	2.68	1.43	1.39
2	D	503	FNR	C5A-N5	2.60	1.44	1.39
2	C	504	FNR	C1'-C2'	2.60	1.56	1.52
2	A	502	FNR	C9A-N10	2.59	1.45	1.41
2	F	505	FNR	C5'-C4'	2.59	1.55	1.51
2	H	507	FNR	C9A-N10	2.58	1.45	1.41
2	D	503	FNR	O3'-C3'	2.56	1.49	1.43
2	B	501	FNR	C4-N3	2.56	1.43	1.38
2	C	504	FNR	C4-N3	2.56	1.43	1.38
2	F	505	FNR	C4'-C3'	2.55	1.57	1.53
2	B	501	FNR	C1'-C2'	2.54	1.56	1.52
2	C	504	FNR	C9A-N10	2.54	1.45	1.41
2	G	508	FNR	C5A-N5	2.50	1.44	1.39
2	F	505	FNR	C1'-C2'	2.49	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	FNR	C5A-N5	2.42	1.44	1.39
2	D	503	FNR	C6-C5A	2.41	1.43	1.39
2	F	505	FNR	C5A-N5	2.38	1.43	1.39
2	B	501	FNR	C5A-N5	2.38	1.43	1.39
2	E	506	FNR	C4'-C3'	2.38	1.57	1.53
2	B	501	FNR	C6-C5A	2.37	1.43	1.39
2	E	506	FNR	C5A-N5	2.35	1.43	1.39
2	H	507	FNR	C1'-C2'	2.34	1.55	1.52
2	C	504	FNR	C5A-N5	2.32	1.43	1.39
2	H	507	FNR	C5'-C4'	2.32	1.55	1.51
2	E	506	FNR	C8M-C8	2.27	1.55	1.51
2	G	508	FNR	C4-N3	2.25	1.43	1.38
2	H	507	FNR	C5A-N5	2.25	1.43	1.39
2	C	504	FNR	C8M-C8	2.23	1.55	1.51
2	H	507	FNR	C4-N3	2.23	1.43	1.38
2	D	503	FNR	C9A-N10	2.21	1.45	1.41
2	H	507	FNR	C8M-C8	2.18	1.55	1.51
2	H	507	FNR	C4'-C3'	2.15	1.57	1.53
2	G	508	FNR	O3'-C3'	2.13	1.48	1.43
2	G	508	FNR	C8-C7	2.11	1.46	1.40
2	D	503	FNR	C5A-C9A	2.08	1.42	1.40
2	G	508	FNR	C5A-C9A	2.08	1.42	1.40
2	F	505	FNR	C8M-C8	2.07	1.54	1.51
2	D	503	FNR	C8M-C8	2.06	1.54	1.51
2	E	506	FNR	O3'-C3'	2.05	1.48	1.43
2	E	506	FNR	C5'-C4'	2.03	1.54	1.51

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	504	FNR	C5'-C4'-C3'	-8.80	95.62	112.22
2	A	502	FNR	C5'-C4'-C3'	-8.31	96.55	112.22
2	A	502	FNR	O1P-P-O5'	-5.85	91.42	106.67
2	C	504	FNR	O1P-P-O5'	-5.55	92.21	106.67
2	G	508	FNR	C5'-C4'-C3'	-5.20	102.40	112.22
2	D	503	FNR	C5'-C4'-C3'	-5.13	102.54	112.22
2	B	501	FNR	C4-N3-C2	-4.57	120.07	126.37
2	C	504	FNR	C4'-C3'-C2'	4.46	120.99	113.57
2	F	505	FNR	C4-N3-C2	-4.45	120.24	126.37
2	E	506	FNR	C4-N3-C2	-4.44	120.25	126.37
2	D	503	FNR	C4-N3-C2	-4.39	120.32	126.37
2	C	504	FNR	C4-N3-C2	-4.38	120.34	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	FNR	C4-N3-C2	-4.37	120.35	126.37
2	H	507	FNR	C4-N3-C2	-4.32	120.42	126.37
2	G	508	FNR	C4-N3-C2	-4.08	120.75	126.37
2	A	502	FNR	C4'-C3'-C2'	4.01	120.24	113.57
2	B	501	FNR	N3-C2-N1	3.54	121.30	115.74
2	H	507	FNR	N3-C2-N1	3.49	121.23	115.74
2	F	505	FNR	N3-C2-N1	3.45	121.16	115.74
2	G	508	FNR	C4'-C3'-C2'	3.45	119.31	113.57
2	D	503	FNR	C4'-C3'-C2'	3.37	119.18	113.57
2	C	504	FNR	N3-C2-N1	3.34	120.99	115.74
2	A	502	FNR	N3-C2-N1	3.34	120.99	115.74
2	A	502	FNR	O3P-P-O2P	3.33	123.80	110.83
2	E	506	FNR	N3-C2-N1	3.32	120.96	115.74
2	C	504	FNR	O3P-P-O2P	3.24	123.47	110.83
2	D	503	FNR	N3-C2-N1	3.18	120.74	115.74
2	G	508	FNR	N3-C2-N1	3.11	120.64	115.74
2	C	504	FNR	O4'-C4'-C5'	2.98	116.55	109.99
2	G	508	FNR	O4'-C4'-C5'	2.97	116.54	109.99
2	A	502	FNR	C1'-C2'-C3'	-2.90	101.81	109.66
2	D	503	FNR	O3P-P-O5'	-2.88	99.16	106.67
2	A	502	FNR	O4'-C4'-C5'	2.88	116.33	109.99
2	C	504	FNR	C1'-C2'-C3'	-2.87	101.88	109.66
2	D	503	FNR	C8M-C8-C9	-2.83	114.59	119.57
2	E	506	FNR	O1P-P-O5'	-2.81	99.35	106.67
2	H	507	FNR	O1P-P-O5'	-2.80	99.36	106.67
2	F	505	FNR	O1P-P-O5'	-2.56	99.99	106.67
2	H	507	FNR	C8M-C8-C9	-2.53	115.12	119.57
2	G	508	FNR	O3'-C3'-C2'	-2.50	103.25	108.93
2	A	502	FNR	C8M-C8-C9	-2.48	115.20	119.57
2	B	501	FNR	C8M-C8-C9	-2.43	115.29	119.57
2	E	506	FNR	C8M-C8-C9	-2.42	115.31	119.57
2	G	508	FNR	C4A-C4-N3	2.39	118.70	112.13
2	F	505	FNR	C8M-C8-C9	-2.39	115.37	119.57
2	D	503	FNR	C4A-C4-N3	2.37	118.65	112.13
2	G	508	FNR	C6-C5A-C9A	2.37	122.39	119.80
2	F	505	FNR	O3P-P-O2P	2.37	120.07	110.83
2	G	508	FNR	C8M-C8-C9	-2.36	115.41	119.57
2	H	507	FNR	O3P-P-O2P	2.36	120.03	110.83
2	C	504	FNR	C8M-C8-C9	-2.33	115.46	119.57
2	E	506	FNR	O4-C4-C4A	-2.31	121.69	127.26
2	D	503	FNR	O4-C4-C4A	-2.30	121.71	127.26
2	B	501	FNR	O3P-P-O2P	2.30	119.79	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	503	FNR	C8M-C8-C7	2.30	125.45	120.76
2	E	506	FNR	C4A-C4-N3	2.29	118.41	112.13
2	E	506	FNR	O3P-P-O2P	2.28	119.72	110.83
2	A	502	FNR	O3P-P-O5'	2.27	112.59	106.67
2	A	502	FNR	C4A-C4-N3	2.26	118.35	112.13
2	C	504	FNR	C4A-C4-N3	2.26	118.33	112.13
2	D	503	FNR	O4'-C4'-C5'	2.25	114.96	109.99
2	C	504	FNR	O3P-P-O5'	2.25	112.54	106.67
2	C	504	FNR	O4-C4-C4A	-2.23	121.88	127.26
2	H	507	FNR	O4-C4-C4A	-2.22	121.91	127.26
2	A	502	FNR	O4-C4-C4A	-2.21	121.93	127.26
2	H	507	FNR	C4A-C4-N3	2.19	118.14	112.13
2	F	505	FNR	O4-C4-C4A	-2.17	122.02	127.26
2	G	508	FNR	C1'-C2'-C3'	-2.17	103.77	109.66
2	F	505	FNR	C4A-C4-N3	2.15	118.04	112.13
2	B	501	FNR	C4A-C4-N3	2.15	118.03	112.13
2	B	501	FNR	O4-C4-C4A	-2.15	122.09	127.26
2	B	501	FNR	O1P-P-O5'	-2.11	101.16	106.67
2	D	503	FNR	C1'-N10-C9A	-2.11	116.54	120.63
2	A	502	FNR	O4'-C4'-C3'	2.10	114.16	109.25
2	G	508	FNR	O4-C4-C4A	-2.04	122.33	127.26
2	D	503	FNR	C1'-C2'-C3'	-2.01	104.22	109.66

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	FNR	C3'-C4'-C5'-O5'
2	A	502	FNR	O4'-C4'-C5'-O5'
2	B	501	FNR	C3'-C4'-C5'-O5'
2	B	501	FNR	O4'-C4'-C5'-O5'
2	C	504	FNR	C3'-C4'-C5'-O5'
2	C	504	FNR	O4'-C4'-C5'-O5'
2	E	506	FNR	C3'-C4'-C5'-O5'
2	E	506	FNR	O4'-C4'-C5'-O5'
2	F	505	FNR	C3'-C4'-C5'-O5'
2	F	505	FNR	O4'-C4'-C5'-O5'
2	H	507	FNR	C3'-C4'-C5'-O5'
2	H	507	FNR	O4'-C4'-C5'-O5'
2	A	502	FNR	C2'-C3'-C4'-O4'
2	A	502	FNR	C2'-C3'-C4'-C5'
2	C	504	FNR	C2'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
2	A	502	FNR	O3'-C3'-C4'-O4'
2	A	502	FNR	O3'-C3'-C4'-C5'
2	C	504	FNR	C2'-C3'-C4'-C5'
2	A	502	FNR	C5'-O5'-P-O3P
2	C	504	FNR	C5'-O5'-P-O3P
2	C	504	FNR	O3'-C3'-C4'-O4'
2	C	504	FNR	O3'-C3'-C4'-C5'
2	A	502	FNR	O2'-C2'-C3'-C4'

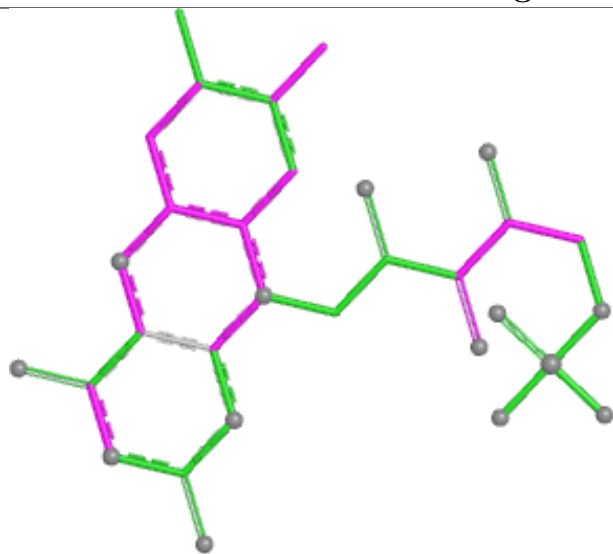
There are no ring outliers.

8 monomers are involved in 31 short contacts:

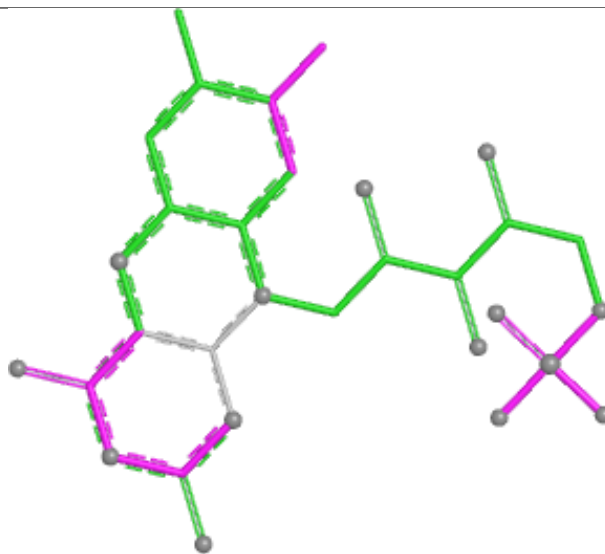
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	506	FNR	3	0
2	F	505	FNR	5	0
2	H	507	FNR	5	0
2	G	508	FNR	3	0
2	D	503	FNR	4	0
2	A	502	FNR	4	0
2	C	504	FNR	2	0
2	B	501	FNR	5	0

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.

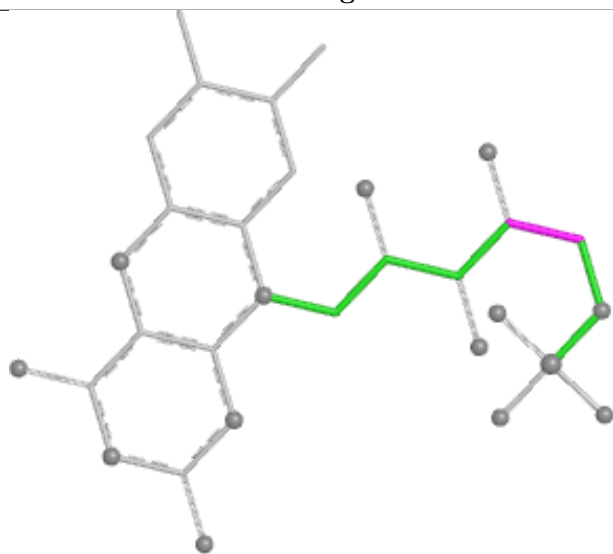
Ligand FNR E 506



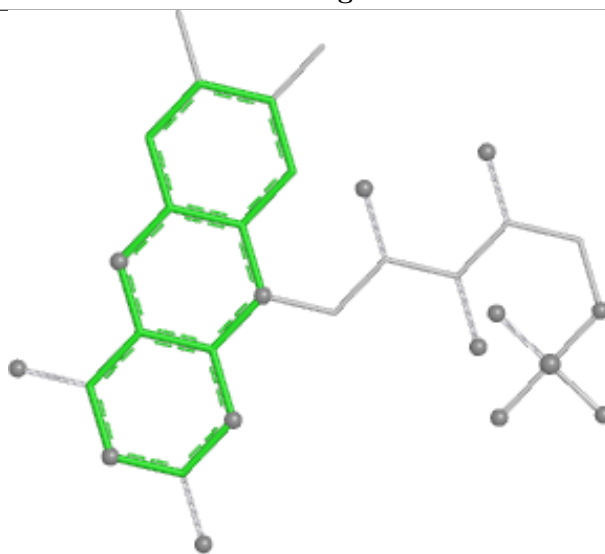
Bond lengths



Bond angles

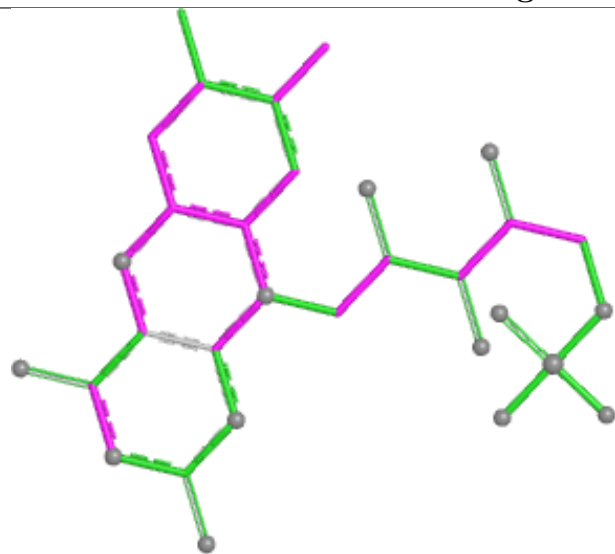


Torsions

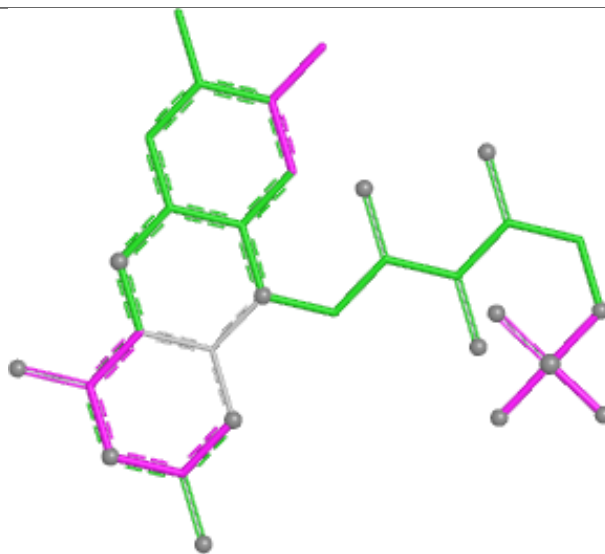


Rings

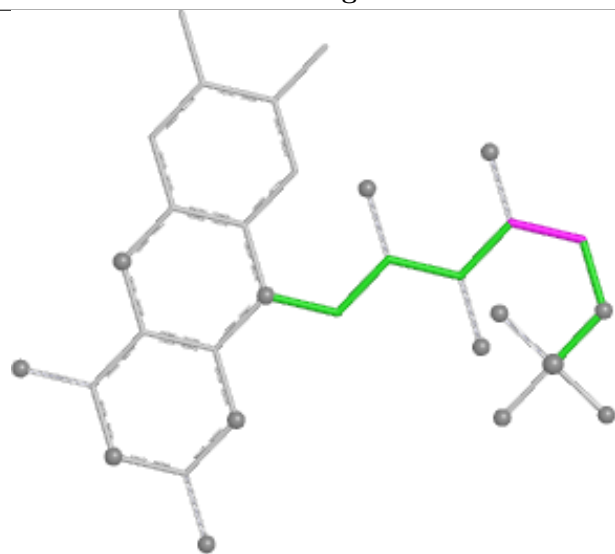
Ligand FNR F 505



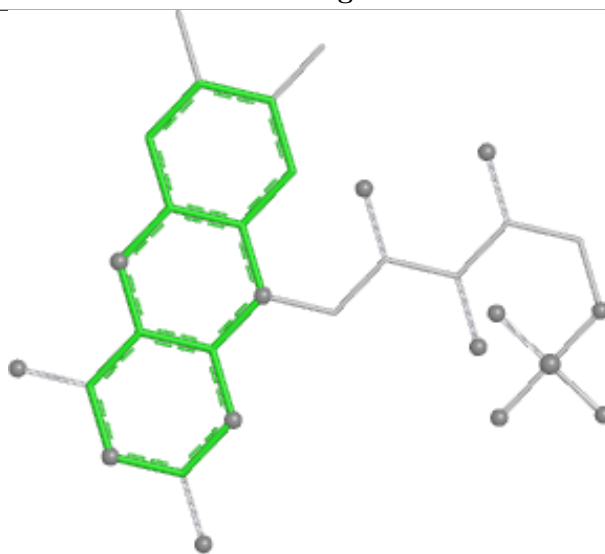
Bond lengths



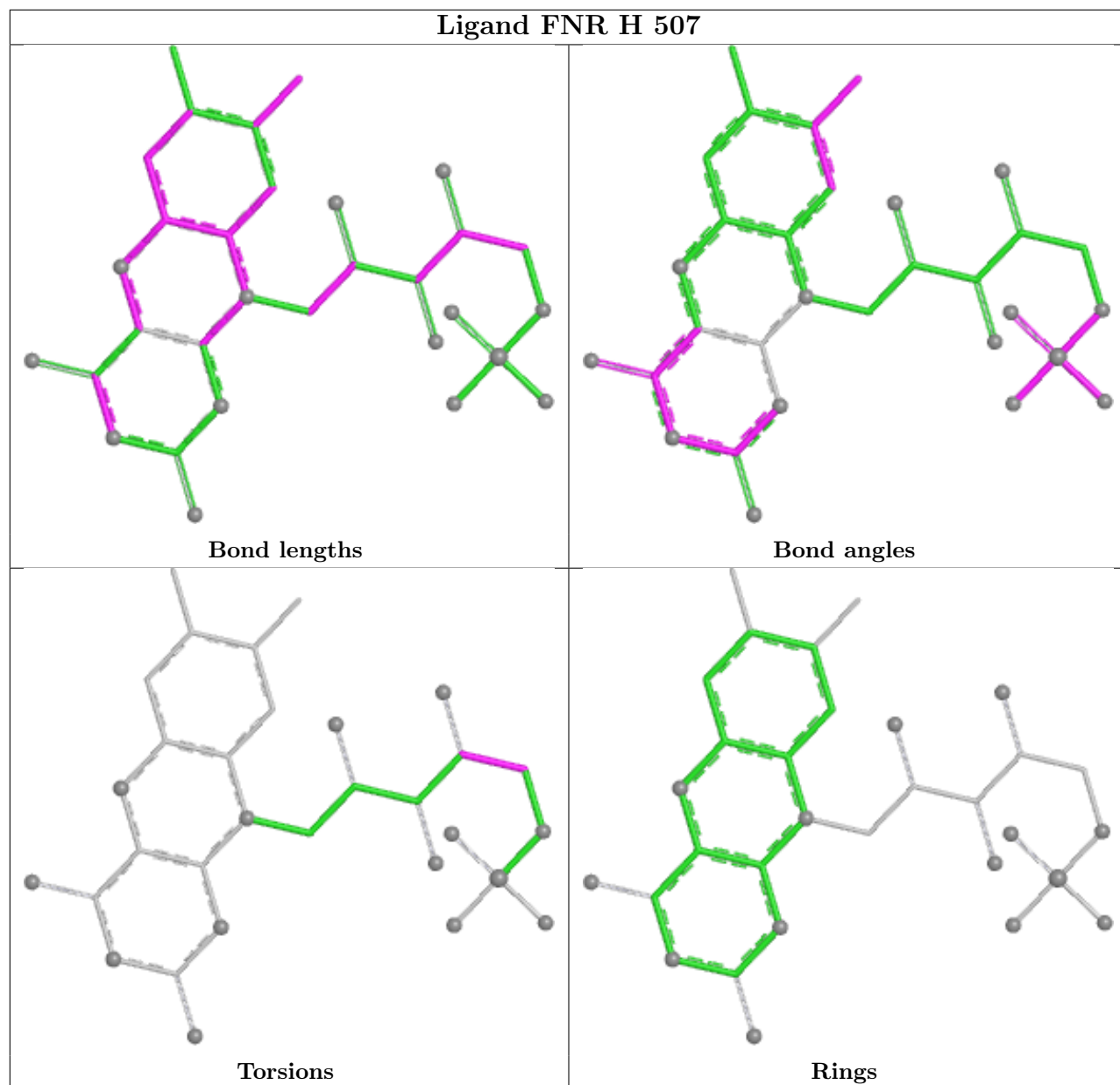
Bond angles

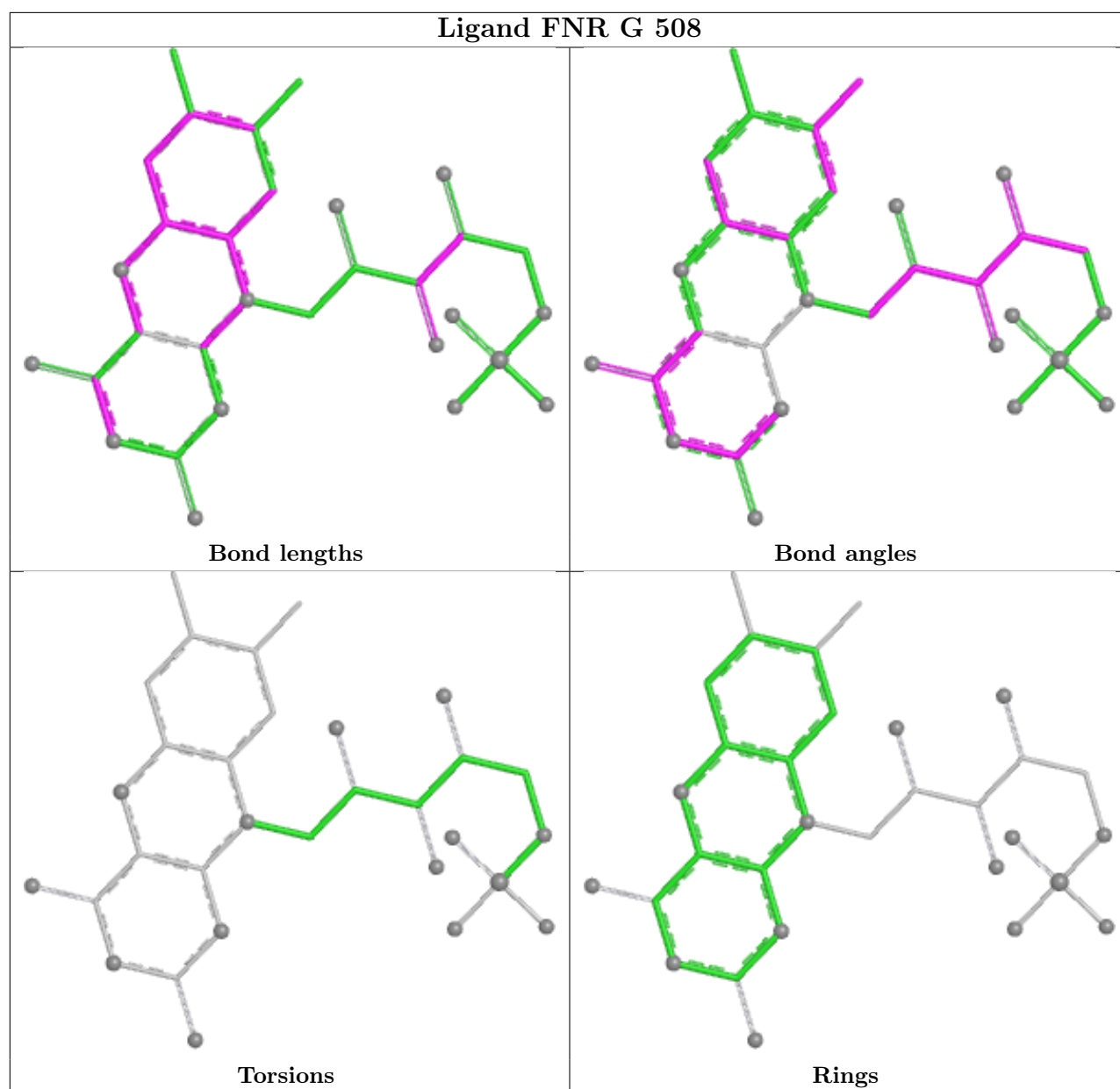


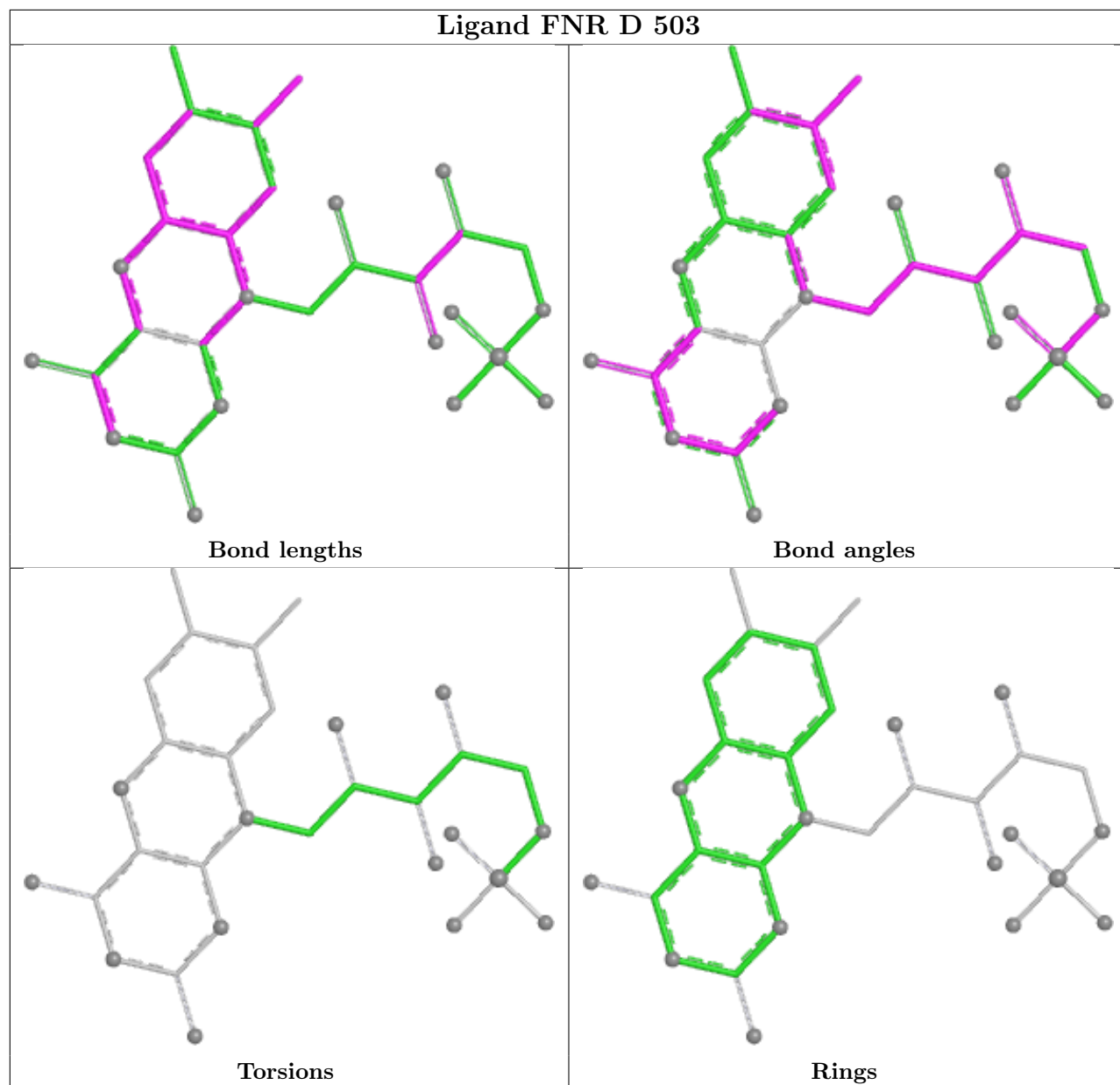
Torsions

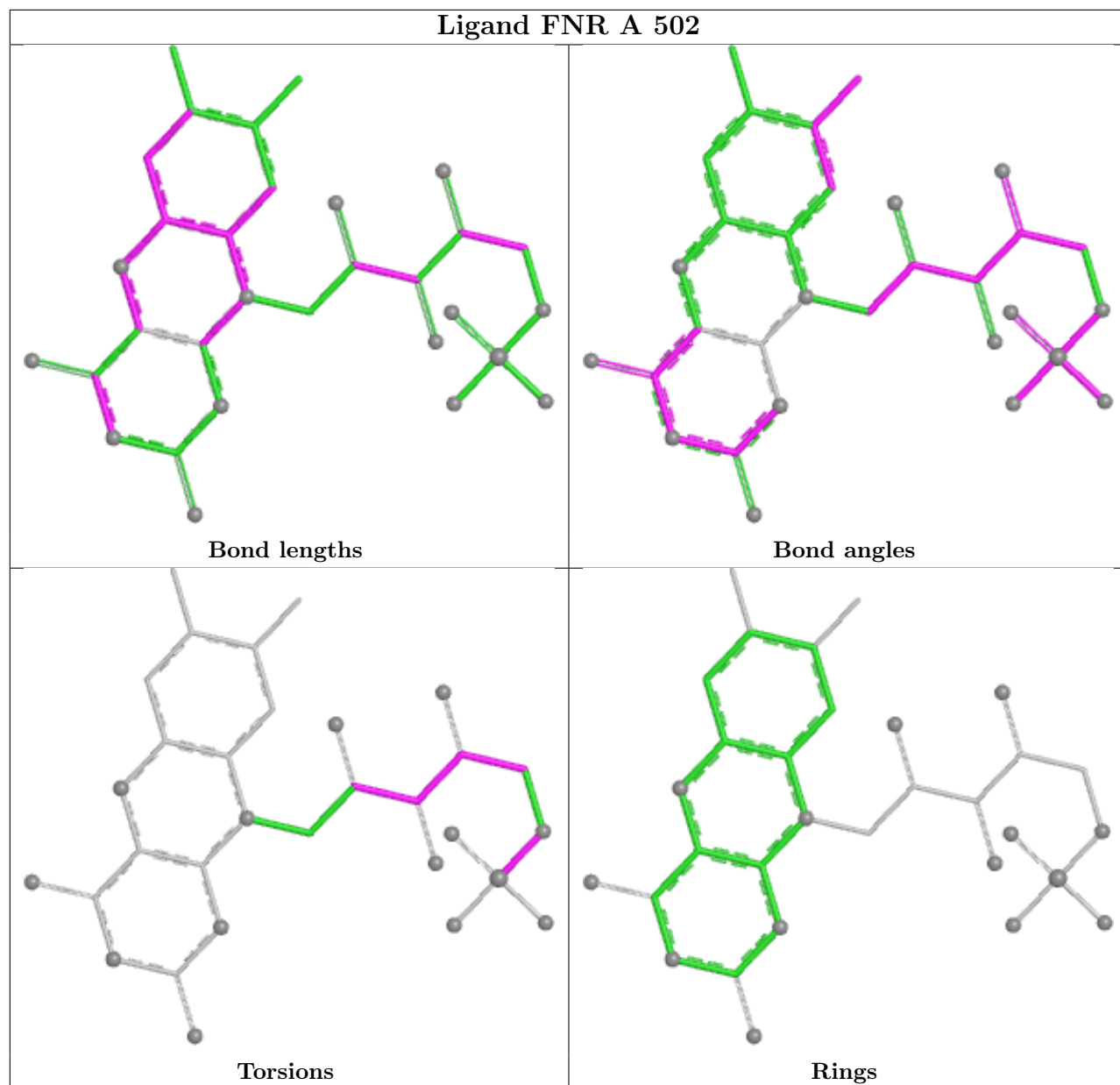


Rings

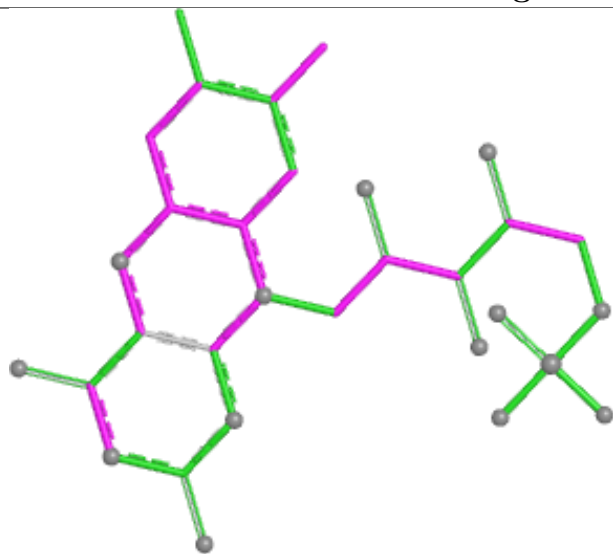




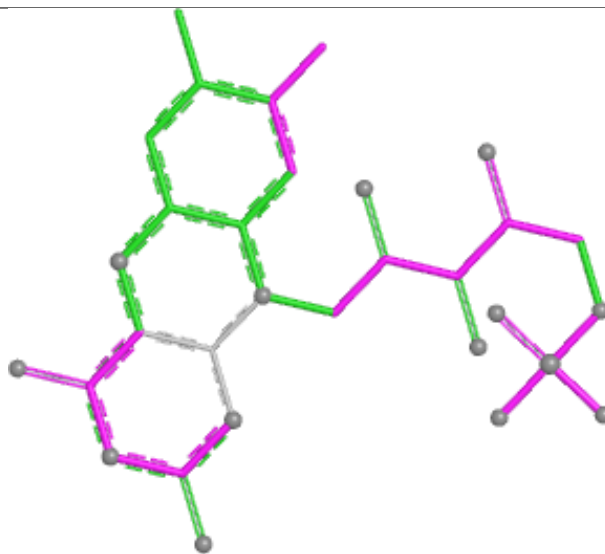




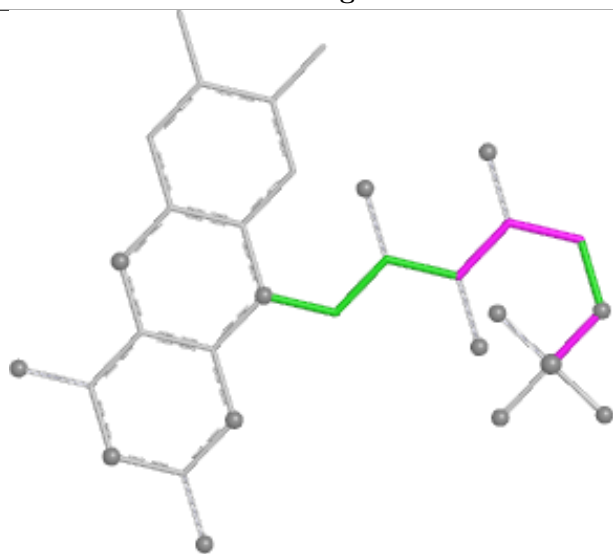
Ligand FNR C 504



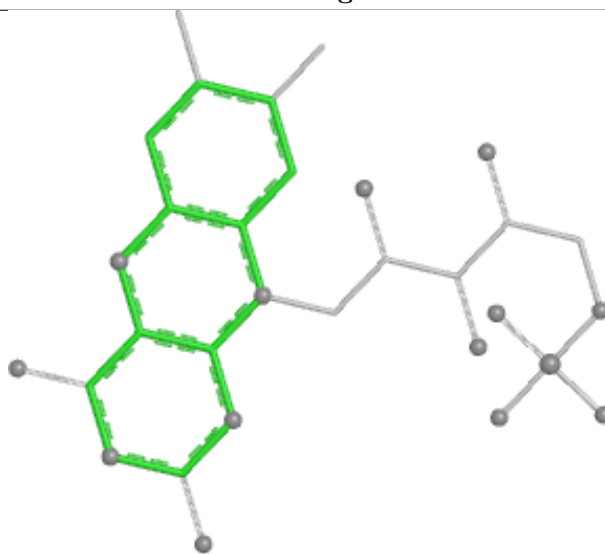
Bond lengths



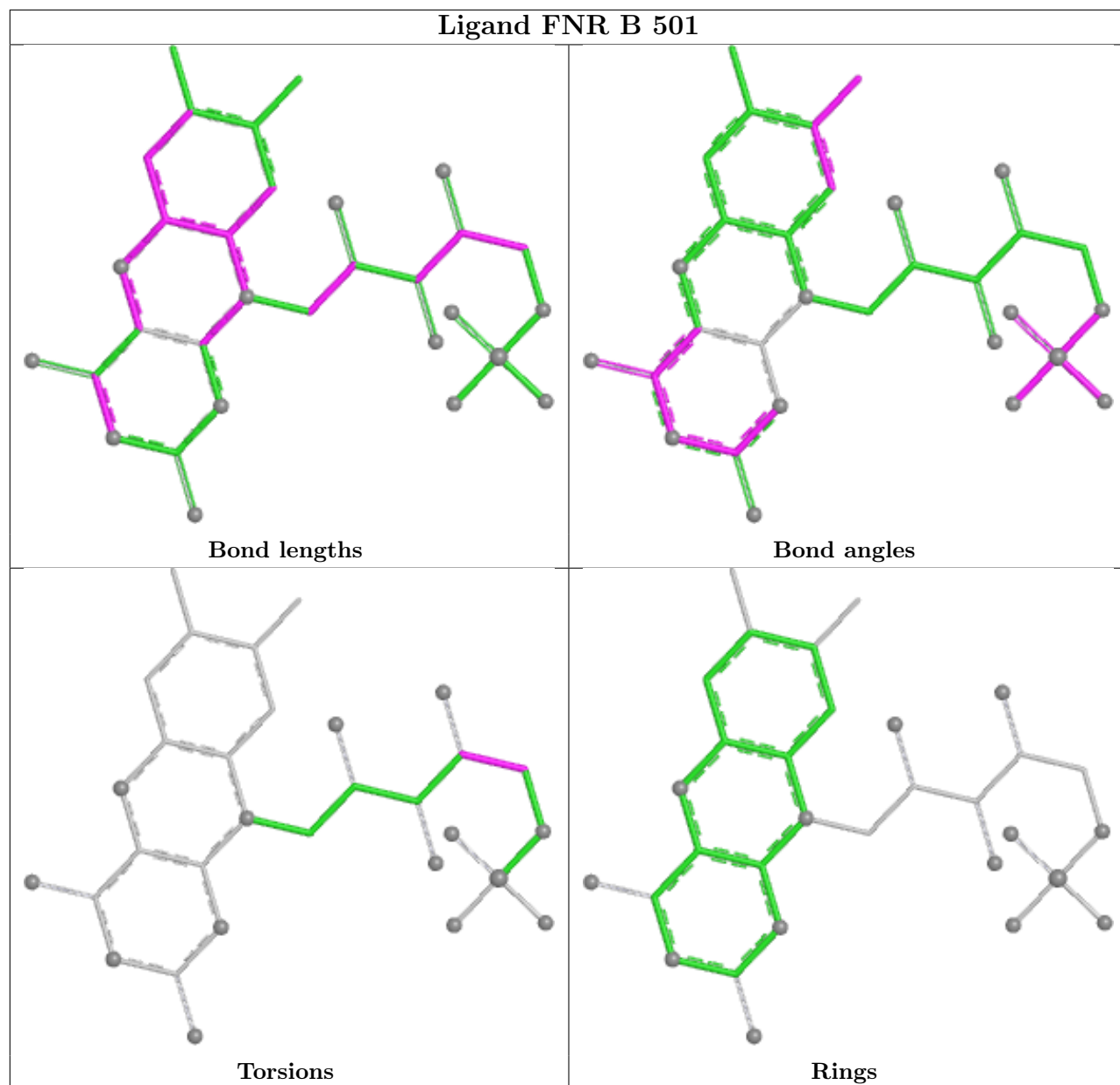
Bond angles



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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	219/230 (95%)	-1.48	0 100 100	9, 16, 30, 42	0
1	B	219/230 (95%)	-1.49	0 100 100	9, 18, 29, 43	0
1	C	219/230 (95%)	-1.44	0 100 100	11, 20, 36, 48	0
1	D	219/230 (95%)	-1.46	0 100 100	11, 19, 31, 39	0
1	E	219/230 (95%)	-1.49	0 100 100	9, 16, 28, 38	0
1	F	219/230 (95%)	-1.47	0 100 100	10, 18, 30, 42	0
1	G	219/230 (95%)	-1.45	0 100 100	12, 20, 37, 46	0
1	H	219/230 (95%)	-1.47	0 100 100	11, 19, 31, 42	0
All	All	1752/1840 (95%)	-1.47	0 100 100	9, 18, 32, 48	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

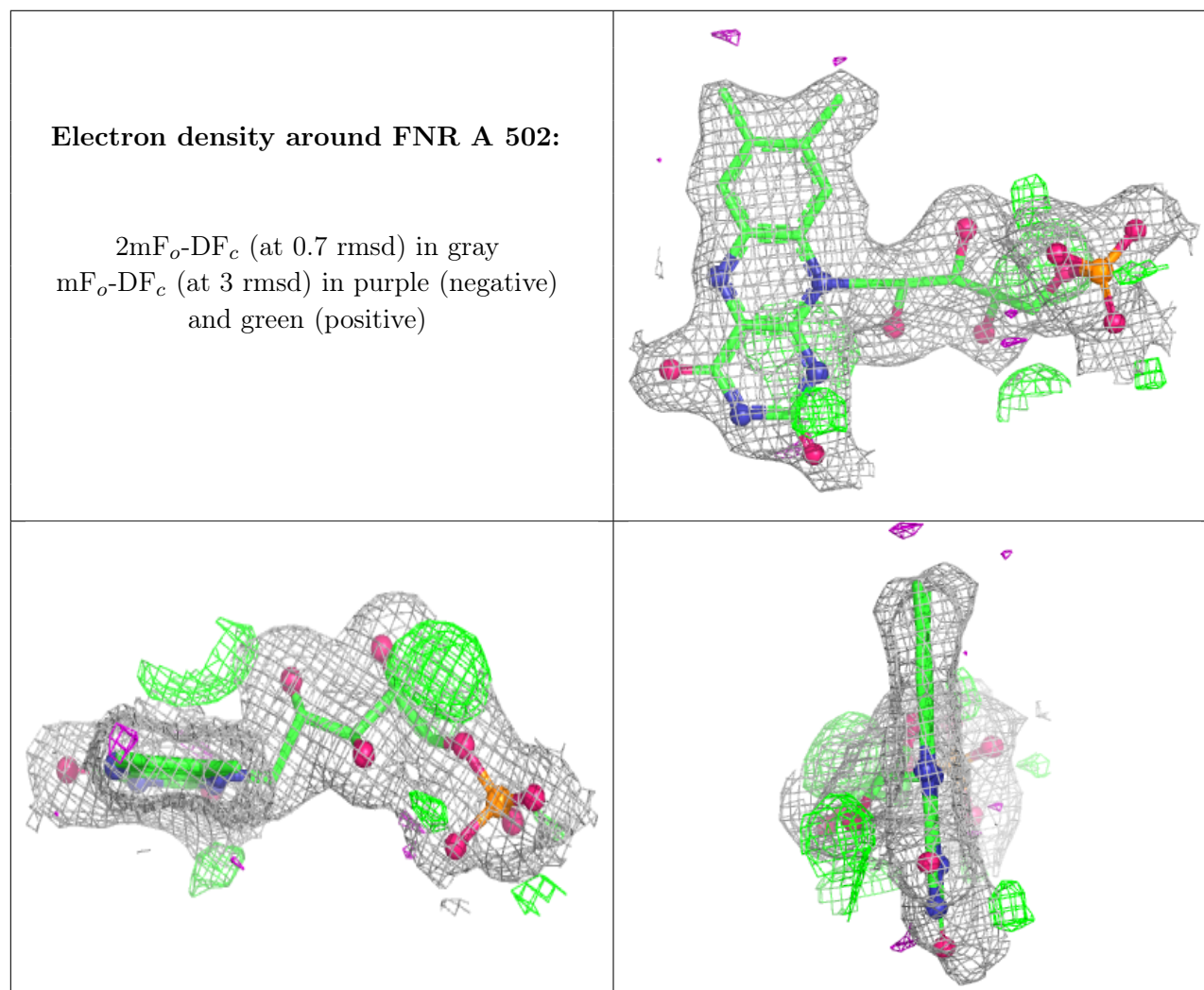
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

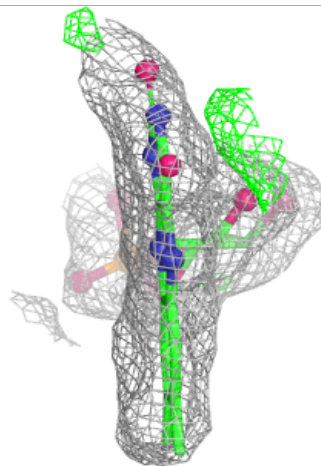
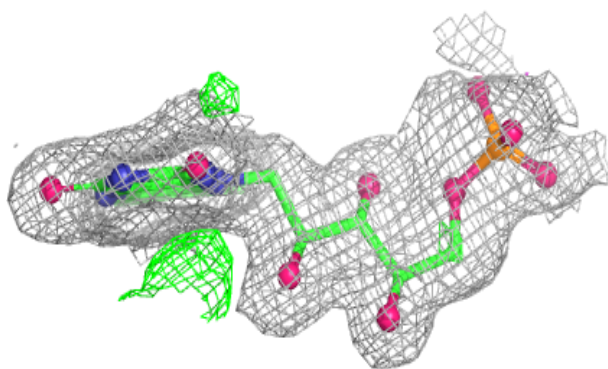
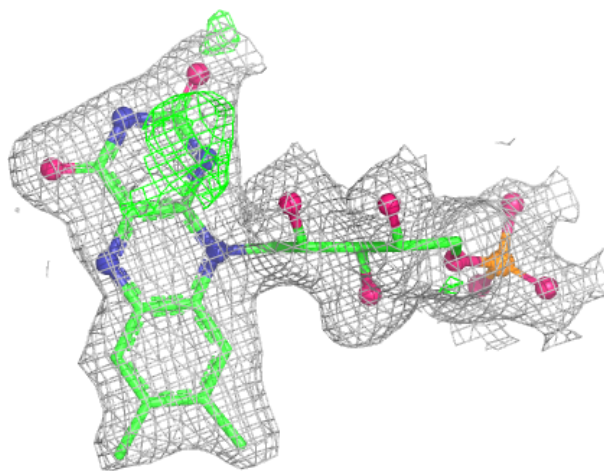
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FNR	A	502	31/31	0.99	0.03	12,17,20,24	0
2	FNR	B	501	31/31	0.99	0.03	13,17,24,27	0
2	FNR	C	504	31/31	0.99	0.03	14,18,23,27	0
2	FNR	D	503	31/31	0.99	0.03	11,17,28,31	0
2	FNR	E	506	31/31	0.99	0.03	12,17,31,36	0
2	FNR	F	505	31/31	0.99	0.03	14,17,24,28	0
2	FNR	G	508	31/31	0.99	0.03	10,15,30,32	0
2	FNR	H	507	31/31	0.99	0.03	8,13,27,31	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.



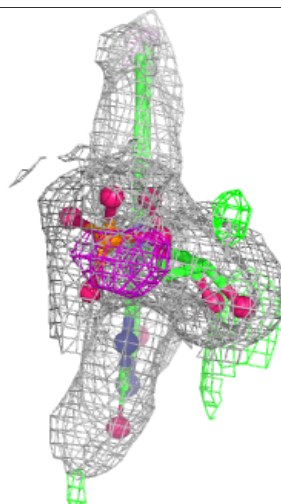
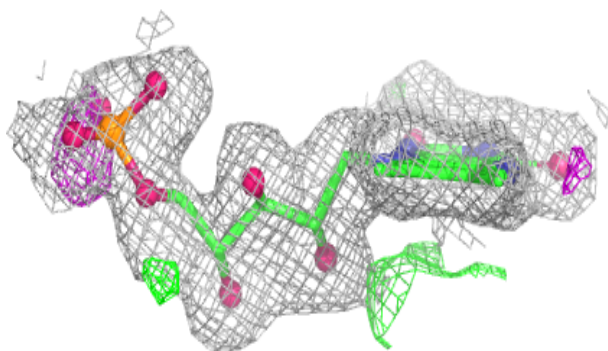
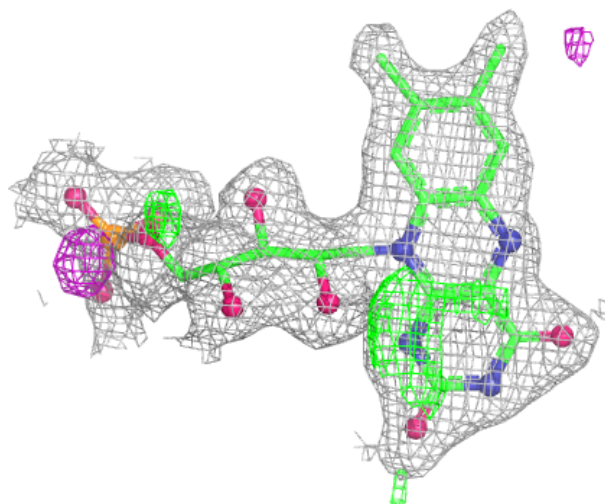
Electron density around FNR B 501:

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



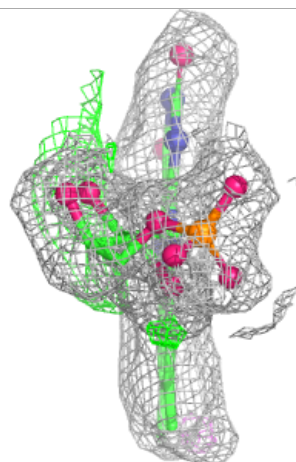
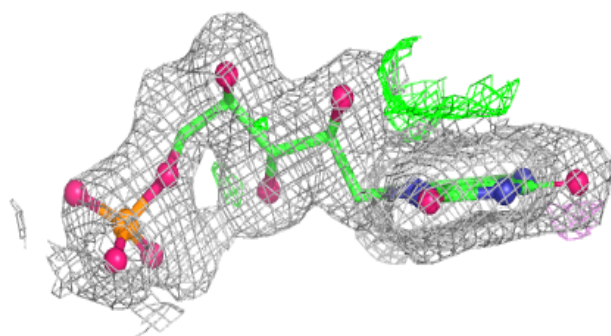
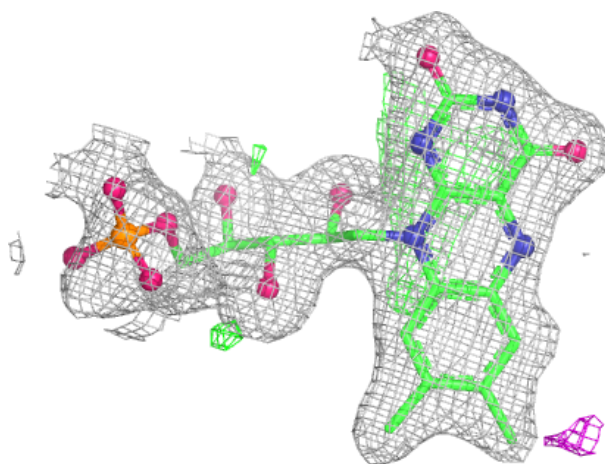
Electron density around FNR C 504:

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



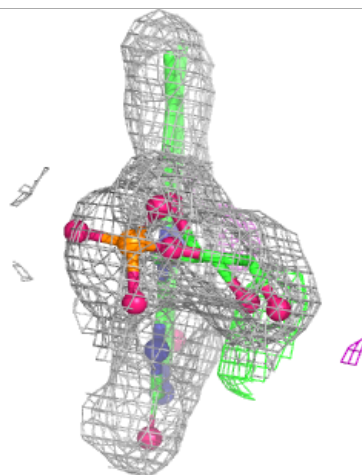
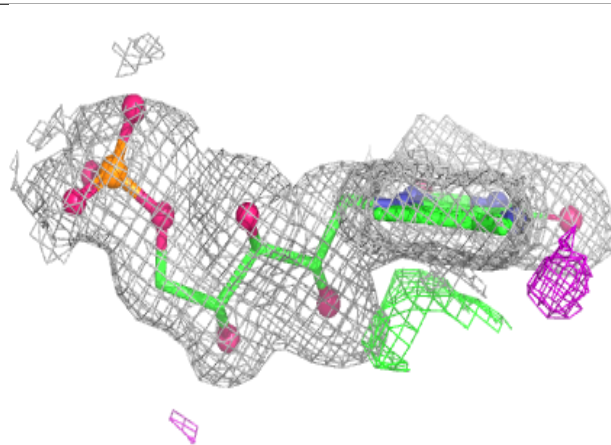
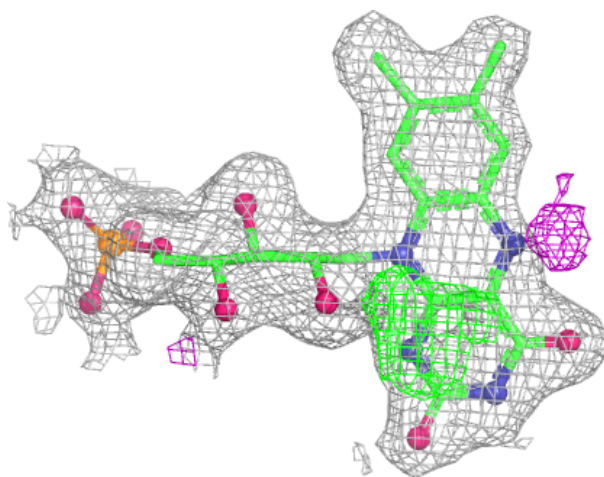
Electron density around FNR D 503:

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



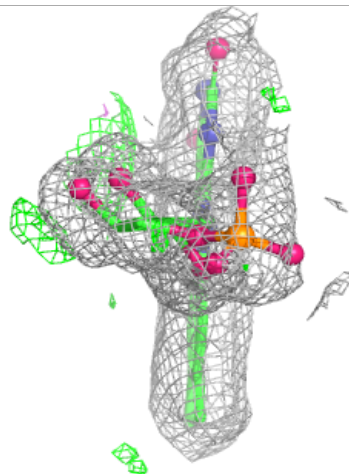
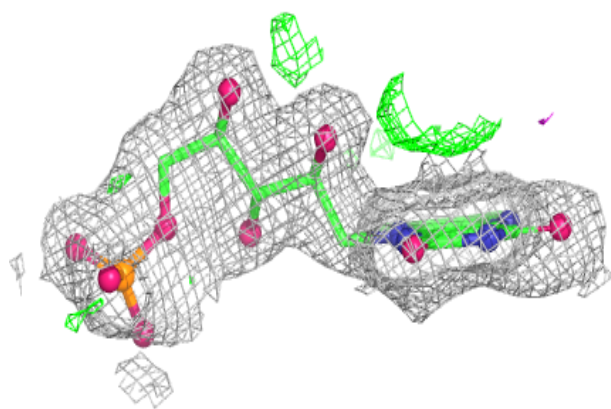
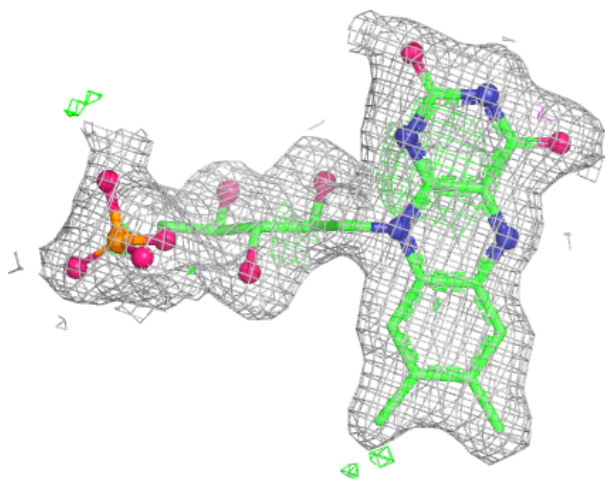
Electron density around FNR E 506:

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



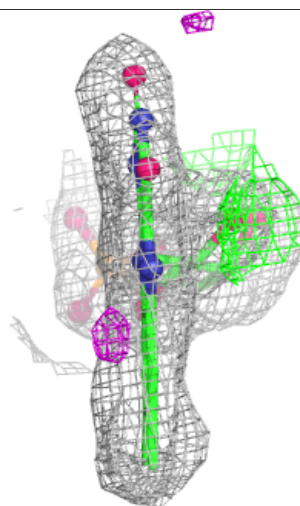
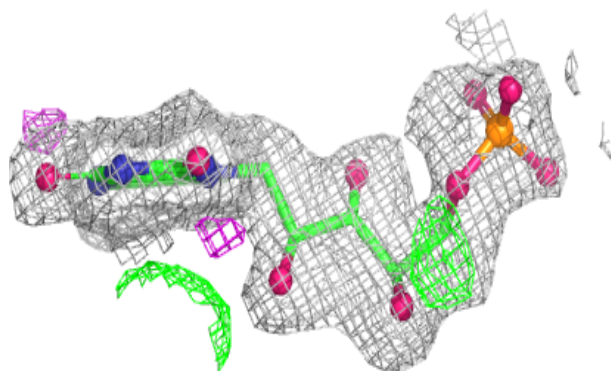
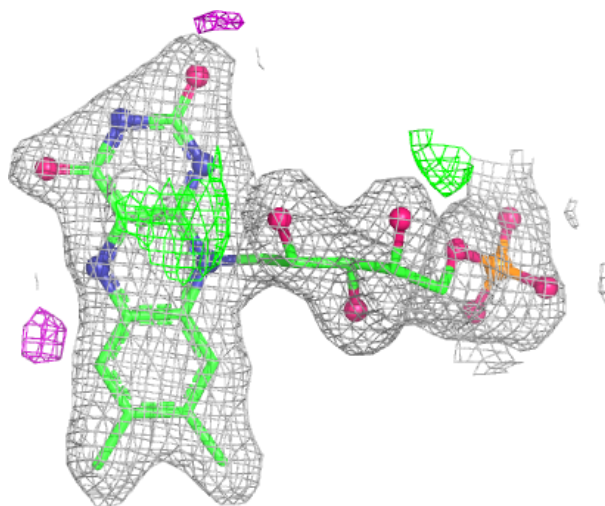
Electron density around FNR F 505:

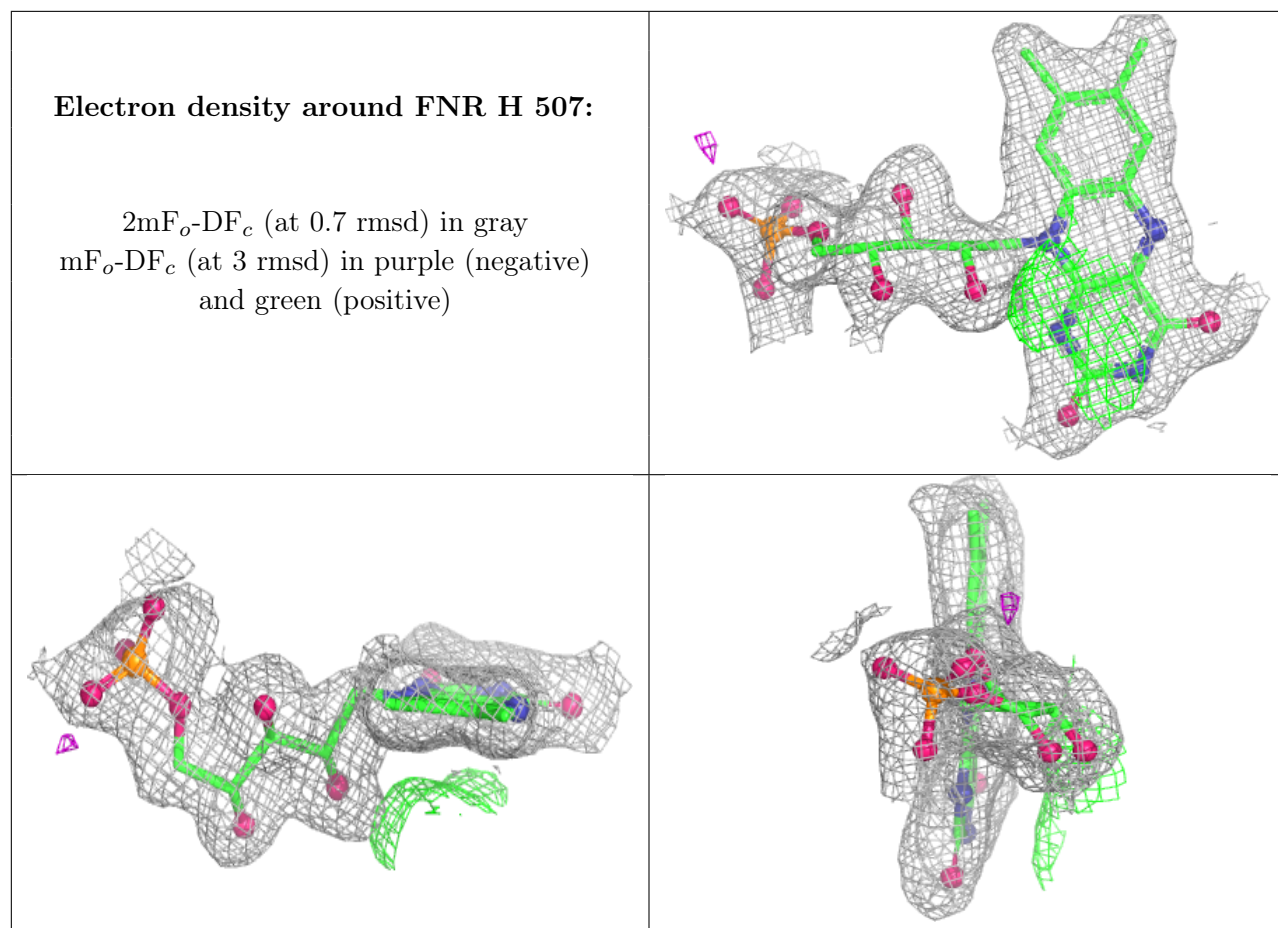
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FNR G 508:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.