



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:42 PM UTC

PDB ID : 2ISL / pdb_00002isl
Title : BluB bound to reduced flavin (FMNH₂) and molecular oxygen. (clear crystal form)
Authors : Larsen, N.A.; Taga, M.E.; Howard-Jones, A.R.; Walsh, C.T.; Walker, G.C.
Deposited on : 2006-10-17
Resolution : 2.90 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

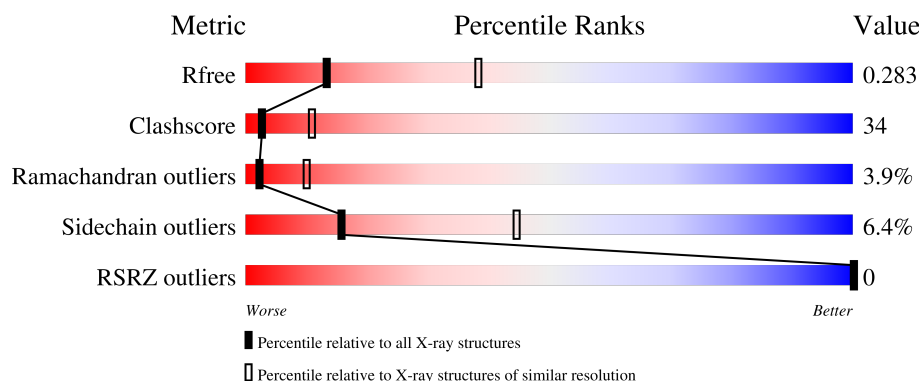
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	
1	G	230	
1	H	230	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXY	A	606	-	-	X	-
3	OXY	G	603	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14255 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:

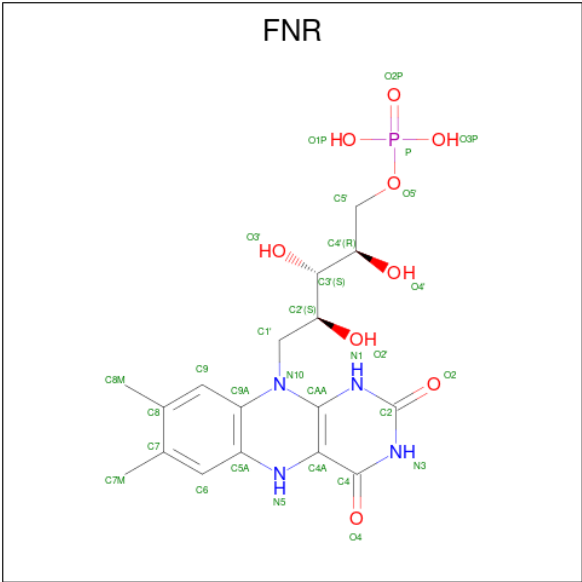
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP Q92PC8
A	-1	SER	-	cloning artifact	UNP Q92PC8
A	0	HIS	-	cloning artifact	UNP Q92PC8
B	-2	GLY	-	cloning artifact	UNP Q92PC8
B	-1	SER	-	cloning artifact	UNP Q92PC8
B	0	HIS	-	cloning artifact	UNP Q92PC8
C	-2	GLY	-	cloning artifact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



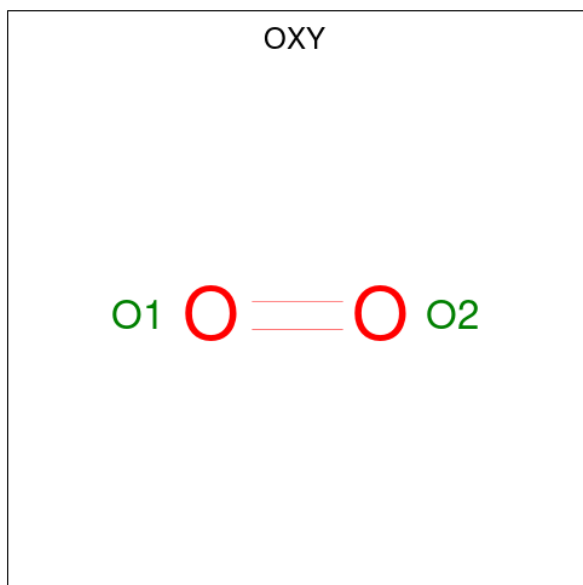
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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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 OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			2	2		
3	B	1	Total	O	0	0
			2	2		
3	C	1	Total	O	0	0
			2	2		
3	D	1	Total	O	0	0
			2	2		
3	E	1	Total	O	0	0
			2	2		
3	F	1	Total	O	0	0
			2	2		
3	G	1	Total	O	0	0
			2	2		
3	H	1	Total	O	0	0
			2	2		

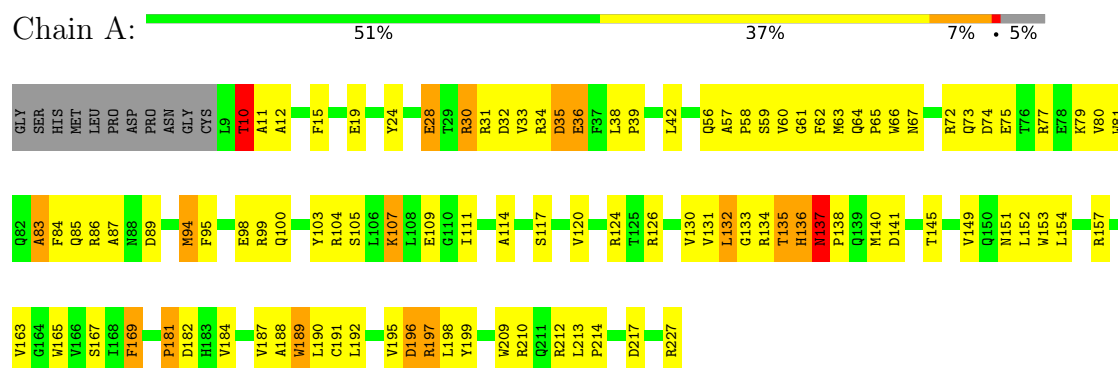
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total 12	O 12	0	0
4	B	13	Total 13	O 13	0	0
4	C	12	Total 12	O 12	0	0
4	D	10	Total 10	O 10	0	0
4	E	4	Total 4	O 4	0	0
4	F	2	Total 2	O 2	0	0
4	G	7	Total 7	O 7	0	0
4	H	3	Total 3	O 3	0	0

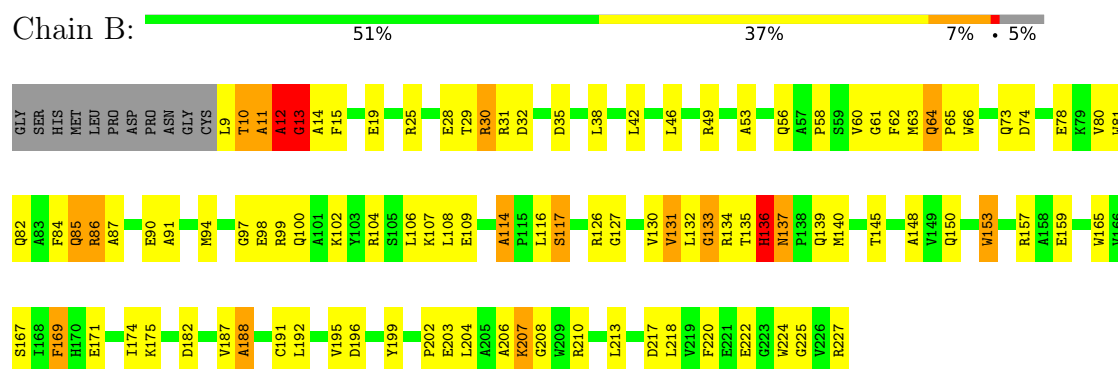
3 Residue-property plots [i](#)

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.

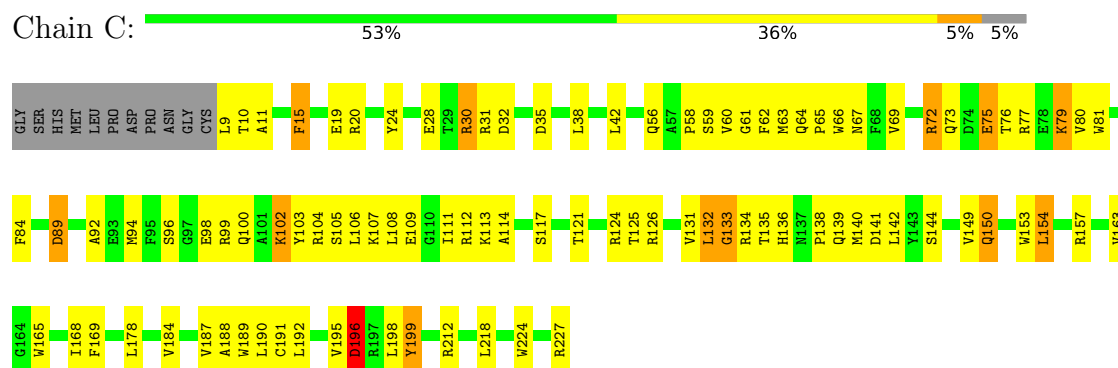
• Molecule 1: BluB



• Molecule 1: BluB

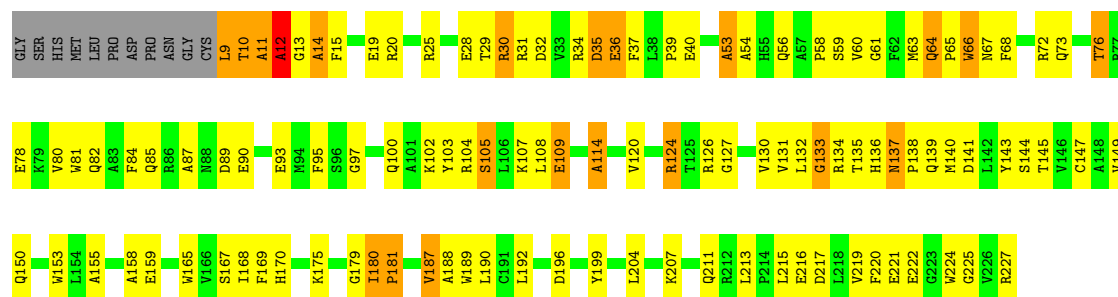


• Molecule 1: BluB



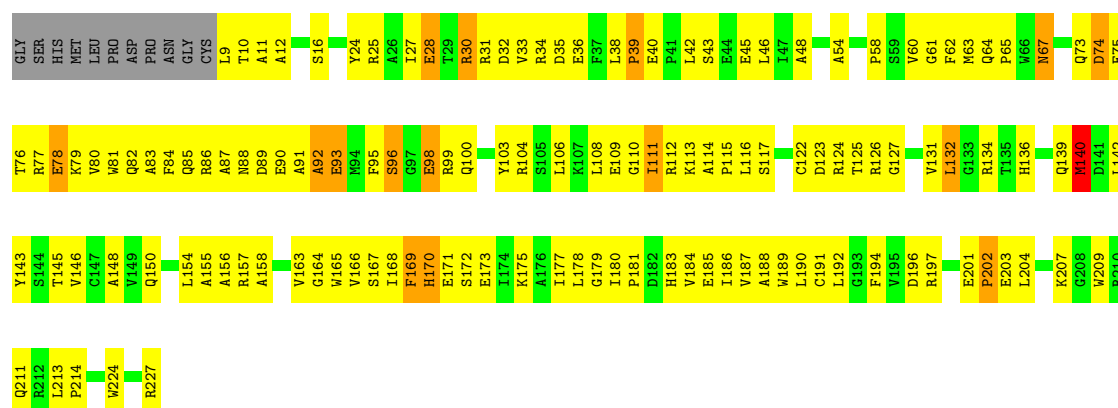
- Molecule 1: BluB

Chain D:



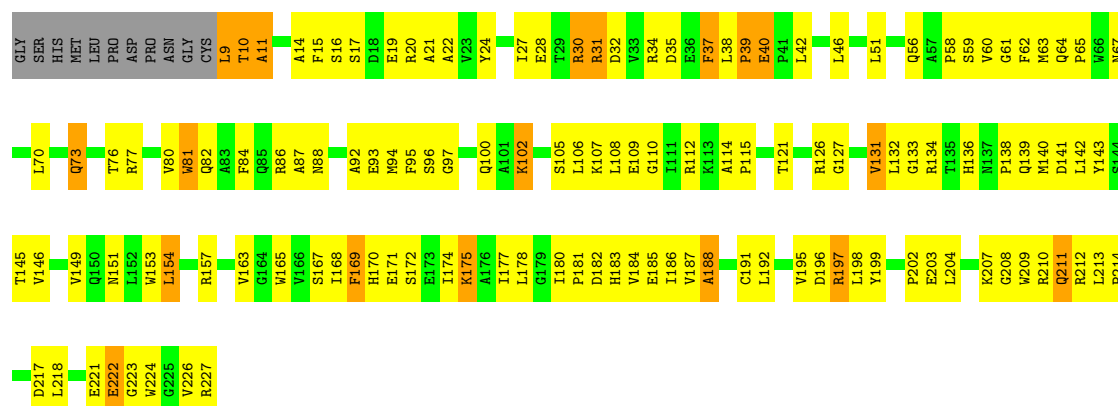
- Molecule 1: BluB

Chain E:



- Molecule 1: BluB

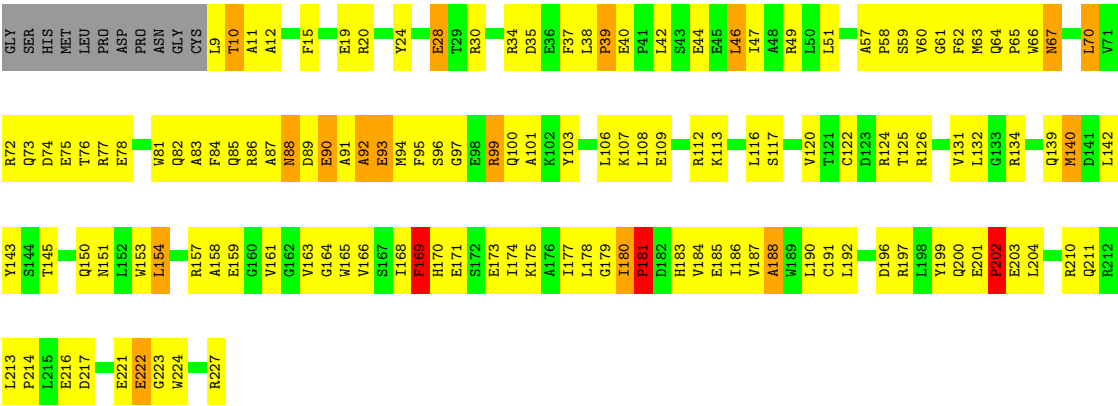
Chain F:



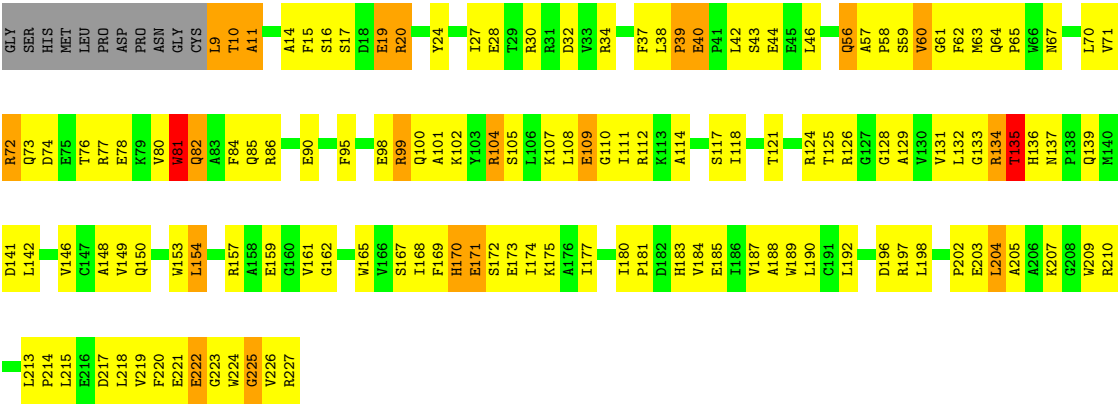
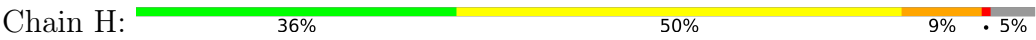
- Molecule 1: BluB

Chain G:





● Molecule 1: BluB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.07Å 173.84Å 91.98Å 90.00° 89.96° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-2.90) 96.2 (20.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.285 0.212 , 0.283	Depositor DCC
R_{free} test set	2170 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 5.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14255	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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, OXY

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	0.51	0/1780	1.03	13/2412 (0.5%)
1	B	0.54	0/1780	1.13	19/2412 (0.8%)
1	C	0.51	0/1780	1.03	10/2412 (0.4%)
1	D	0.52	0/1780	1.17	23/2412 (1.0%)
1	E	0.43	0/1780	0.98	7/2412 (0.3%)
1	F	0.43	0/1780	0.95	6/2412 (0.2%)
1	G	0.42	0/1780	0.97	6/2412 (0.2%)
1	H	0.41	0/1780	0.98	6/2412 (0.2%)
All	All	0.47	0/14240	1.03	90/19296 (0.5%)

There are no bond length outliers.

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	ASN	CA-C-N	8.71	128.45	119.56
1	D	137	ASN	C-N-CA	8.71	128.45	119.56
1	B	85	GLN	N-CA-C	-8.70	99.04	110.43
1	B	66	TRP	N-CA-C	8.42	122.99	110.52
1	D	114	ALA	CA-C-N	7.99	127.65	119.82
1	D	114	ALA	C-N-CA	7.99	127.65	119.82
1	D	64	GLN	CA-C-N	7.75	127.93	119.87
1	D	64	GLN	C-N-CA	7.75	127.93	119.87
1	D	10	THR	N-CA-C	7.43	119.87	108.42
1	D	136	HIS	N-CA-C	-7.20	105.11	114.04
1	A	32	ASP	N-CA-C	-7.19	97.53	108.67
1	D	66	TRP	N-CA-C	7.13	120.17	110.55
1	G	180	ILE	CA-C-N	6.93	128.51	119.84
1	G	180	ILE	C-N-CA	6.93	128.51	119.84
1	A	66	TRP	N-CA-C	6.93	119.91	110.55
1	B	35	ASP	N-CA-C	6.89	121.85	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	32	ASP	N-CA-C	-6.82	98.91	109.76
1	A	73	GLN	N-CA-C	6.79	120.53	110.48
1	B	32	ASP	N-CA-C	-6.79	98.19	109.46
1	E	93	GLU	N-CA-C	-6.76	104.58	114.39
1	D	105	SER	N-CA-C	-6.74	104.96	113.72
1	B	13	GLY	N-CA-C	6.71	129.07	113.18
1	C	38	LEU	CA-C-N	6.70	126.65	119.28
1	C	38	LEU	C-N-CA	6.70	126.65	119.28
1	G	88	ASN	N-CA-C	-6.61	104.16	111.36
1	A	35	ASP	N-CA-C	6.53	121.41	113.38
1	D	35	ASP	N-CA-C	6.52	122.04	113.30
1	D	170	HIS	N-CA-C	-6.50	96.64	108.02
1	C	35	ASP	N-CA-C	6.42	121.11	113.28
1	A	136	HIS	N-CA-C	-6.34	106.25	112.97
1	G	28	GLU	N-CA-C	6.23	120.14	112.54
1	B	137	ASN	CA-C-N	6.13	125.86	119.05
1	B	137	ASN	C-N-CA	6.13	125.86	119.05
1	F	10	THR	N-CA-C	6.13	118.70	108.96
1	E	28	GLU	N-CA-C	6.09	117.59	111.07
1	C	196	ASP	N-CA-C	-6.08	105.99	113.41
1	F	102	LYS	N-CA-C	-6.02	105.77	113.23
1	H	136	HIS	N-CA-C	-5.97	106.33	113.97
1	C	32	ASP	N-CA-C	-5.89	98.93	108.41
1	D	53	ALA	N-CA-C	-5.83	104.56	111.03
1	A	196	ASP	N-CA-C	-5.75	106.60	113.97
1	D	168	ILE	N-CA-C	5.74	112.35	106.21
1	B	73	GLN	N-CA-C	5.73	119.39	110.17
1	H	81	TRP	N-CA-C	-5.70	104.27	111.11
1	C	66	TRP	N-CA-C	5.69	118.94	110.52
1	B	14	ALA	N-CA-C	-5.67	101.24	110.20
1	C	113	LYS	N-CA-C	-5.65	104.59	112.45
1	B	64	GLN	CA-C-N	5.55	126.28	120.12
1	B	64	GLN	C-N-CA	5.55	126.28	120.12
1	B	218	LEU	N-CA-C	-5.52	106.44	114.12
1	C	15	PHE	N-CA-C	-5.50	103.12	110.55
1	D	180	ILE	CA-C-N	5.49	126.70	119.84
1	D	180	ILE	C-N-CA	5.49	126.70	119.84
1	H	124	ARG	N-CA-C	5.49	117.34	111.36
1	D	12	ALA	N-CA-C	5.46	122.44	110.80
1	F	188	ALA	N-CA-C	5.46	116.70	108.46
1	B	114	ALA	CA-C-N	5.45	124.64	118.97
1	B	114	ALA	C-N-CA	5.45	124.64	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	ALA	N-CA-C	-5.38	105.06	111.03
1	D	189	TRP	N-CA-C	-5.38	99.64	108.41
1	E	96	SER	N-CA-C	5.35	117.98	109.96
1	B	74	ASP	N-CA-C	5.33	117.09	111.28
1	E	33	VAL	N-CA-C	5.31	115.94	109.30
1	G	66	TRP	N-CA-C	5.30	117.36	110.53
1	D	221	GLU	N-CA-C	5.29	118.03	107.62
1	H	72	ARG	N-CA-C	5.27	121.26	114.56
1	H	10	THR	N-CA-C	5.27	116.89	108.41
1	D	11	ALA	N-CA-C	5.26	122.01	110.80
1	A	57	ALA	N-CA-C	-5.26	104.08	110.13
1	F	127	GLY	N-CA-C	-5.25	106.81	114.90
1	A	39	PRO	N-CA-C	5.24	120.72	113.65
1	C	62	PHE	N-CA-C	-5.23	104.42	111.54
1	C	199	TYR	N-CA-C	-5.23	103.13	110.50
1	B	12	ALA	N-CA-C	-5.22	99.68	110.80
1	A	67	ASN	N-CA-C	-5.20	100.82	108.99
1	D	187	VAL	N-CA-C	-5.20	106.07	111.58
1	F	208	GLY	N-CA-C	5.19	122.35	114.61
1	D	73	GLN	N-CA-C	5.19	118.20	109.95
1	G	188	ALA	N-CA-C	5.14	116.23	108.46
1	B	188	ALA	N-CA-C	5.12	117.03	108.99
1	F	96	SER	N-CA-C	5.12	118.09	109.95
1	E	170	HIS	N-CA-C	-5.10	102.31	109.96
1	B	136	HIS	N-CA-C	-5.07	105.88	113.89
1	H	134	ARG	N-CA-C	5.07	117.75	109.59
1	A	38	LEU	CA-C-N	5.07	124.85	119.28
1	A	38	LEU	C-N-CA	5.07	124.85	119.28
1	A	83	ALA	N-CA-C	-5.05	105.78	111.28
1	A	189	TRP	N-CA-C	-5.03	100.21	108.41
1	E	180	ILE	CA-C-N	5.01	126.10	119.84
1	E	180	ILE	C-N-CA	5.01	126.10	119.84

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	115	0
1	B	1741	0	1716	129	0
1	C	1741	0	1716	106	0
1	D	1741	0	1716	121	0
1	E	1741	0	1716	164	0
1	F	1741	0	1716	158	0
1	G	1741	0	1716	172	0
1	H	1741	0	1716	165	0
2	A	31	0	21	5	0
2	B	31	0	21	6	0
2	C	31	0	21	5	0
2	D	31	0	21	6	0
2	E	31	0	21	5	0
2	F	31	0	21	4	0
2	G	31	0	21	4	0
2	H	31	0	21	5	0
3	A	2	0	0	2	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	1	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	2	0
3	H	2	0	0	0	0
4	A	12	0	0	1	0
4	B	13	0	0	2	0
4	C	12	0	0	3	0
4	D	10	0	0	3	0
4	E	4	0	0	4	0
4	F	2	0	0	0	0
4	G	7	0	0	4	0
4	H	3	0	0	1	0
All	All	14255	0	13896	944	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 34.

All (944) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:VAL:HG11	1:B:134:ARG:HE	1.05	1.09
1:G:63:MET:HE2	1:G:65:PRO:HB3	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:ARG:HD2	1:E:87:ALA:N	1.72	1.04
1:E:63:MET:HE2	1:E:65:PRO:HB3	1.44	0.98
1:A:64:GLN:HE22	1:B:213:LEU:H	1.09	0.98
1:A:63:MET:HE2	1:A:65:PRO:HB3	1.44	0.97
1:G:63:MET:HG3	1:G:65:PRO:HD3	1.47	0.95
1:H:38:LEU:HB3	1:H:39:PRO:HD2	1.49	0.94
1:H:204:LEU:HD12	1:H:204:LEU:H	1.34	0.91
1:C:196:ASP:O	1:D:12:ALA:HA	1.70	0.90
1:H:81:TRP:HD1	1:H:111:ILE:HB	1.35	0.90
1:B:131:VAL:HG11	1:B:134:ARG:NE	1.85	0.90
1:E:86:ARG:HD2	1:E:87:ALA:H	1.30	0.90
1:E:86:ARG:HH21	1:E:169:PHE:HB2	1.37	0.88
1:H:17:SER:HA	1:H:20:ARG:HD3	1.53	0.88
1:G:64:GLN:HE22	1:H:213:LEU:H	1.21	0.86
1:G:96:SER:N	1:G:100:GLN:HB2	1.90	0.86
1:G:12:ALA:HB3	1:H:197:ARG:HA	1.56	0.85
1:G:174:ILE:HA	1:G:177:ILE:HD12	1.58	0.85
1:G:78:GLU:HG3	1:G:82:GLN:HE21	1.42	0.85
1:A:140:MET:HE3	2:B:501:FNR:H7M1	1.59	0.85
1:C:212:ARG:HD3	1:D:64:GLN:HE22	1.42	0.82
1:B:217:ASP:HB2	1:B:227:ARG:HH21	1.45	0.82
1:F:38:LEU:HB3	1:F:39:PRO:HD2	1.61	0.82
1:B:130:VAL:HG12	1:B:131:VAL:H	1.45	0.81
1:B:85:GLN:O	1:B:86:ARG:HB2	1.81	0.80
1:G:116:LEU:HD12	1:G:117:SER:H	1.44	0.80
1:F:82:GLN:HB3	1:F:86:ARG:NH1	1.96	0.79
1:G:106:LEU:HD13	1:G:204:LEU:HD22	1.64	0.79
1:F:39:PRO:HG2	1:F:40:GLU:H	1.45	0.79
1:F:185:GLU:HG2	1:F:186:ILE:N	1.96	0.79
1:F:32:ASP:O	1:F:34:ARG:HD2	1.83	0.78
1:C:227:ARG:HG3	1:C:227:ARG:HH11	1.47	0.78
1:F:163:VAL:HG22	1:F:192:LEU:HG	1.64	0.78
1:H:34:ARG:HH22	1:H:204:LEU:HD11	1.49	0.77
1:E:116:LEU:HD12	1:E:117:SER:H	1.49	0.77
1:H:71:VAL:HB	1:H:117:SER:HB3	1.66	0.77
1:C:134:ARG:HG3	1:C:138:PRO:HA	1.65	0.76
1:H:224:TRP:O	1:H:226:VAL:HG23	1.86	0.76
1:E:167:SER:HB3	1:F:140:MET:HE2	1.67	0.76
1:G:116:LEU:HD12	1:G:117:SER:N	2.00	0.76
1:H:37:PHE:CD2	1:H:114:ALA:HB2	2.21	0.76
1:B:203:GLU:OE2	1:B:207:LYS:HE3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:ARG:HA	1:F:11:ALA:HA	1.68	0.76
1:H:34:ARG:NH2	1:H:204:LEU:HD11	2.02	0.75
1:B:63:MET:HE2	1:B:126:ARG:HB3	1.67	0.74
2:C:504:FNR:H7M1	1:D:140:MET:HE3	1.69	0.74
1:G:95:PHE:HB2	1:G:100:GLN:HA	1.67	0.74
1:G:64:GLN:NE2	1:H:213:LEU:H	1.85	0.74
1:E:39:PRO:HA	1:E:115:PRO:HD3	1.69	0.74
1:E:123:ASP:HA	1:E:184:VAL:HG22	1.69	0.74
1:E:173:GLU:O	1:E:177:ILE:HG13	1.87	0.74
1:F:42:LEU:HB3	1:F:46:LEU:HD23	1.69	0.74
1:A:136:HIS:O	1:A:137:ASN:HB2	1.87	0.74
1:A:196:ASP:O	1:B:12:ALA:HA	1.88	0.74
1:G:74:ASP:HA	1:G:77:ARG:NE	2.03	0.73
1:A:63:MET:HG3	1:A:65:PRO:HD3	1.71	0.73
1:C:64:GLN:HE22	1:D:213:LEU:H	1.34	0.73
1:C:73:GLN:HG2	1:D:222:GLU:OE1	1.89	0.73
1:G:46:LEU:HD23	1:G:49:ARG:NH2	2.03	0.73
1:A:210:ARG:HE	1:B:63:MET:HA	1.54	0.72
1:C:195:VAL:HG21	1:C:198:LEU:HD21	1.71	0.72
1:D:63:MET:HE1	1:D:141:ASP:CB	2.19	0.72
1:E:38:LEU:HB3	1:E:40:GLU:OE1	1.89	0.72
1:H:39:PRO:HG2	1:H:40:GLU:H	1.53	0.72
1:A:167:SER:HB3	1:B:140:MET:HE2	1.69	0.72
1:H:84:PHE:HE2	1:H:109:GLU:HG2	1.54	0.71
1:G:28:GLU:HG2	1:H:56:GLN:HE22	1.55	0.71
1:G:163:VAL:HG22	1:G:192:LEU:HG	1.72	0.71
1:C:63:MET:HE3	1:C:126:ARG:O	1.89	0.71
1:G:85:GLN:HA	1:G:88:ASN:HB3	1.72	0.71
1:B:217:ASP:HB2	1:B:227:ARG:NH2	2.05	0.71
1:F:62:PHE:O	1:F:64:GLN:HG3	1.89	0.71
1:E:106:LEU:HD12	1:E:106:LEU:O	1.90	0.71
1:E:196:ASP:O	1:F:11:ALA:HB1	1.90	0.70
1:E:213:LEU:H	1:F:64:GLN:HE22	1.36	0.70
1:D:15:PHE:HB3	1:D:19:GLU:HB2	1.73	0.70
1:C:140:MET:HE2	1:D:167:SER:HB3	1.72	0.70
1:F:63:MET:HE2	1:F:65:PRO:HB3	1.71	0.70
1:D:134:ARG:HG3	1:D:138:PRO:HA	1.72	0.70
1:E:32:ASP:OD1	1:E:164:GLY:HA2	1.91	0.70
1:F:42:LEU:HD12	1:F:42:LEU:H	1.55	0.70
1:B:131:VAL:CG1	1:B:134:ARG:HE	1.96	0.70
1:F:221:GLU:O	1:F:223:GLY:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:ALA:C	1:E:93:GLU:H	1.99	0.69
1:F:95:PHE:C	1:F:100:GLN:HB2	2.16	0.69
1:E:158:ALA:HB1	1:F:20:ARG:HB3	1.74	0.69
1:H:81:TRP:O	1:H:85:GLN:HG2	1.91	0.69
1:G:83:ALA:HA	1:G:86:ARG:CZ	2.22	0.69
1:B:91:ALA:HA	1:B:94:MET:HE3	1.74	0.69
1:H:17:SER:CA	1:H:20:ARG:HD3	2.22	0.69
1:E:167:SER:CB	1:F:140:MET:HE2	2.22	0.69
1:G:125:THR:HA	1:G:134:ARG:HH22	1.58	0.69
1:H:149:VAL:HG13	1:H:190:LEU:HD11	1.74	0.69
1:E:116:LEU:HD12	1:E:117:SER:N	2.08	0.69
1:H:95:PHE:C	1:H:100:GLN:HB2	2.17	0.68
1:A:163:VAL:HG22	1:A:192:LEU:HG	1.75	0.68
1:G:46:LEU:HD23	1:G:49:ARG:HH21	1.57	0.68
1:D:102:LYS:HE3	1:D:207:LYS:O	1.94	0.68
1:C:103:TYR:HE1	1:D:132:LEU:HG	1.58	0.68
1:C:132:LEU:HD23	1:D:204:LEU:HD21	1.74	0.68
1:G:34:ARG:HH12	1:G:203:GLU:HB3	1.58	0.68
1:C:140:MET:HE2	1:D:167:SER:CB	2.24	0.68
1:A:28:GLU:CG	1:B:56:GLN:HE22	2.07	0.68
1:F:185:GLU:HG2	1:F:186:ILE:H	1.57	0.68
1:H:76:THR:O	1:H:80:VAL:HG23	1.93	0.68
1:A:165:TRP:CZ2	1:A:188:ALA:HB2	2.30	0.67
1:F:60:VAL:HG21	1:F:133:GLY:HA3	1.75	0.67
1:E:27:ILE:HG23	1:F:151:ASN:ND2	2.09	0.67
1:G:81:TRP:CH2	1:G:85:GLN:HG3	2.29	0.67
1:G:94:MET:SD	1:H:135:THR:HG21	2.34	0.67
1:F:84:PHE:CE2	1:F:109:GLU:HG2	2.29	0.67
1:H:63:MET:HE2	1:H:65:PRO:HB3	1.76	0.67
1:E:95:PHE:HB2	1:E:100:GLN:HB3	1.77	0.67
1:E:178:LEU:HD22	1:F:222:GLU:O	1.94	0.67
1:C:94:MET:HG2	1:D:130:VAL:HG11	1.78	0.66
1:E:122:CYS:HB2	1:E:145:THR:HG21	1.77	0.66
1:F:73:GLN:HE21	1:F:73:GLN:HA	1.59	0.66
1:B:135:THR:HG22	4:B:524:HOH:O	1.95	0.66
1:G:38:LEU:HB3	1:G:40:GLU:OE2	1.95	0.66
1:C:73:GLN:HG2	1:D:222:GLU:CD	2.21	0.66
1:H:60:VAL:HG21	1:H:133:GLY:HA3	1.78	0.66
1:H:204:LEU:HD12	1:H:204:LEU:N	2.11	0.65
1:F:226:VAL:HG12	1:F:227:ARG:N	2.11	0.65
1:H:134:ARG:NE	1:H:141:ASP:HB3	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:PHE:O	1:H:64:GLN:HG3	1.97	0.65
1:H:204:LEU:H	1:H:204:LEU:CD1	2.08	0.65
1:A:198:LEU:O	1:B:9:LEU:HA	1.97	0.65
1:A:28:GLU:HG2	1:B:56:GLN:HE22	1.61	0.65
1:C:60:VAL:HG22	1:C:132:LEU:O	1.96	0.65
1:H:60:VAL:CG2	1:H:133:GLY:HA3	2.27	0.65
1:F:199:TYR:CE1	1:F:203:GLU:HG3	2.31	0.65
1:G:216:GLU:HG2	1:G:217:ASP:OD2	1.96	0.65
1:A:132:LEU:HD23	1:A:133:GLY:N	2.11	0.65
1:B:202:PRO:HB3	2:B:501:FNR:H5'2	1.79	0.65
1:H:203:GLU:HG2	1:H:207:LYS:HD3	1.79	0.65
1:G:74:ASP:HA	1:G:77:ARG:HE	1.62	0.64
1:E:74:ASP:O	1:E:77:ARG:HG2	1.97	0.64
1:C:140:MET:HE3	2:D:503:FNR:H7M3	1.79	0.64
1:C:196:ASP:O	1:D:12:ALA:CA	2.46	0.64
1:E:83:ALA:O	1:E:86:ARG:HG3	1.97	0.64
1:E:64:GLN:HE22	1:F:213:LEU:H	1.44	0.64
1:E:209:TRP:CE2	1:F:132:LEU:HD11	2.33	0.64
1:H:32:ASP:O	1:H:34:ARG:HD2	1.98	0.64
1:B:132:LEU:O	1:B:134:ARG:N	2.32	0.64
1:E:175:LYS:O	1:E:179:GLY:N	2.30	0.64
1:E:60:VAL:HG11	1:E:140:MET:HB3	1.79	0.63
1:G:9:LEU:O	1:G:10:THR:HB	1.98	0.63
1:E:67:ASN:HD22	1:F:218:LEU:HB3	1.63	0.63
1:G:44:GLU:HA	1:G:47:ILE:HD12	1.81	0.63
1:D:63:MET:HE3	1:D:65:PRO:HG3	1.80	0.63
2:E:506:FNR:H6	1:F:59:SER:O	1.99	0.63
1:F:76:THR:O	1:F:80:VAL:HG23	1.98	0.63
1:G:120:VAL:O	1:G:187:VAL:HG22	1.97	0.63
1:H:42:LEU:HB3	1:H:46:LEU:HD23	1.81	0.63
1:A:227:ARG:NH1	1:H:126:ARG:HA	2.13	0.63
1:E:140:MET:HE3	2:F:505:FNR:H7M1	1.79	0.63
1:E:42:LEU:HD23	1:E:46:LEU:HD23	1.81	0.63
1:D:63:MET:HE3	1:D:65:PRO:CG	2.28	0.63
1:C:165:TRP:CZ2	1:C:188:ALA:HB2	2.34	0.62
1:H:81:TRP:CD1	1:H:111:ILE:HB	2.27	0.62
1:G:87:ALA:HB3	1:G:169:PHE:HA	1.81	0.62
1:H:165:TRP:CZ2	1:H:188:ALA:HB2	2.33	0.62
1:F:174:ILE:O	1:F:177:ILE:HG22	1.98	0.62
1:B:171:GLU:O	1:B:175:LYS:HG3	1.98	0.62
1:G:74:ASP:O	1:G:77:ARG:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:LEU:HB3	1:H:39:PRO:CD	2.27	0.62
1:G:60:VAL:O	1:G:63:MET:HG2	2.00	0.62
1:G:173:GLU:O	1:G:177:ILE:HG13	1.99	0.62
1:H:131:VAL:HG22	1:H:132:LEU:H	1.65	0.62
1:C:61:GLY:HA2	1:C:132:LEU:HB2	1.82	0.62
1:E:192:LEU:N	1:E:192:LEU:HD12	2.15	0.61
1:C:165:TRP:CZ2	1:D:140:MET:HE1	2.35	0.61
1:G:143:TYR:CE2	1:H:187:VAL:HG13	2.35	0.61
2:A:502:FNR:H7M1	1:B:140:MET:HE3	1.82	0.61
1:F:61:GLY:CA	1:F:132:LEU:HD13	2.31	0.61
1:A:227:ARG:HG3	1:A:227:ARG:HH11	1.64	0.61
1:B:175:LYS:HZ3	1:B:182:ASP:HA	1.66	0.61
1:E:171:GLU:HG2	1:E:175:LYS:HG3	1.81	0.61
1:F:60:VAL:CG2	1:F:133:GLY:HA3	2.30	0.61
1:A:60:VAL:HG22	1:A:132:LEU:O	2.01	0.61
1:C:20:ARG:HD2	1:D:159:GLU:OE2	2.01	0.61
1:F:175:LYS:HD2	1:F:180:ILE:HG21	1.82	0.61
1:G:87:ALA:CB	1:G:169:PHE:HA	2.30	0.61
1:C:58:PRO:HG3	1:D:153:TRP:CZ3	2.36	0.61
1:C:61:GLY:CA	1:C:132:LEU:HB2	2.31	0.61
1:E:108:LEU:HD21	1:F:132:LEU:HD23	1.82	0.61
2:A:502:FNR:H7	1:B:140:MET:CE	2.30	0.61
1:B:11:ALA:O	1:B:12:ALA:O	2.19	0.61
1:B:86:ARG:O	1:B:90:GLU:HG3	2.01	0.61
1:B:227:ARG:HG2	1:B:227:ARG:HH11	1.66	0.61
1:H:9:LEU:HD22	1:H:9:LEU:O	2.01	0.61
1:G:30:ARG:HA	1:G:157:ARG:HG3	1.83	0.60
1:D:78:GLU:HG3	1:D:82:GLN:HE21	1.65	0.60
1:G:132:LEU:HB3	3:G:603:OXY:O1	2.02	0.60
1:H:131:VAL:HG22	1:H:132:LEU:N	2.16	0.60
1:A:132:LEU:HD22	3:A:606:OXY:O1	2.02	0.60
1:E:90:GLU:HB2	1:F:136:HIS:NE2	2.16	0.60
1:A:64:GLN:NE2	1:B:213:LEU:H	1.91	0.60
1:B:165:TRP:CZ2	1:B:188:ALA:HB2	2.36	0.60
1:C:112:ARG:HG2	4:C:553:HOH:O	2.01	0.60
1:G:40:GLU:OE2	1:G:40:GLU:N	2.32	0.60
1:E:140:MET:HE2	1:F:167:SER:HB3	1.84	0.60
1:G:151:ASN:ND2	1:H:27:ILE:HG23	2.17	0.60
1:C:96:SER:N	1:C:100:GLN:HB2	2.17	0.60
1:A:31:ARG:HD2	1:A:199:TYR:O	2.02	0.59
1:A:63:MET:HE3	1:A:126:ARG:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:PHE:HB3	1:C:19:GLU:HB2	1.84	0.59
1:D:132:LEU:O	1:D:134:ARG:N	2.30	0.59
1:E:67:ASN:ND2	1:F:218:LEU:HB3	2.17	0.59
1:A:87:ALA:CB	1:A:169:PHE:HA	2.32	0.59
1:C:199:TYR:HA	1:D:9:LEU:HA	1.83	0.59
1:F:65:PRO:HA	1:F:126:ARG:HD2	1.85	0.59
1:F:227:ARG:HH11	1:F:227:ARG:HG2	1.68	0.59
1:G:154:LEU:HD23	1:H:154:LEU:HD23	1.84	0.59
1:B:100:GLN:NE2	1:B:104:ARG:HH21	2.00	0.59
1:G:15:PHE:HB2	1:G:20:ARG:HG3	1.84	0.59
1:E:84:PHE:CE1	1:E:168:ILE:HB	2.38	0.59
1:E:202:PRO:HG2	1:F:62:PHE:CZ	2.37	0.59
1:A:196:ASP:C	1:B:12:ALA:HA	2.28	0.59
4:A:548:HOH:O	1:B:132:LEU:HA	2.01	0.59
1:A:140:MET:HE3	2:B:501:FNR:C7M	2.31	0.59
1:B:9:LEU:HD12	1:B:9:LEU:N	2.17	0.59
1:B:139:GLN:HE21	1:B:139:GLN:HA	1.68	0.59
1:C:227:ARG:HH11	1:C:227:ARG:CG	2.16	0.58
1:F:175:LYS:HD2	1:F:180:ILE:CG2	2.33	0.58
1:F:61:GLY:HA2	1:F:132:LEU:HD13	1.85	0.58
1:F:131:VAL:HG12	1:F:134:ARG:H	1.67	0.58
1:F:226:VAL:HG12	1:F:227:ARG:H	1.66	0.58
1:H:205:ALA:HA	1:H:210:ARG:O	2.04	0.58
1:D:165:TRP:HA	1:D:190:LEU:HD23	1.85	0.58
1:F:24:TYR:O	1:F:28:GLU:HG3	2.03	0.58
1:G:9:LEU:HD22	1:H:197:ARG:HG3	1.85	0.58
1:G:224:TRP:CZ3	1:H:184:VAL:HG11	2.39	0.58
1:A:132:LEU:HD22	3:A:606:OXY:O2	2.03	0.58
1:E:10:THR:O	1:F:197:ARG:HG3	2.03	0.58
1:G:108:LEU:HD12	1:G:108:LEU:N	2.18	0.58
1:C:153:TRP:CZ3	1:D:58:PRO:HG3	2.38	0.58
1:C:60:VAL:CG2	1:C:133:GLY:HA3	2.33	0.58
1:D:155:ALA:O	1:D:158:ALA:HB3	2.04	0.58
1:E:42:LEU:HG	1:E:194:PHE:CE2	2.38	0.58
1:H:100:GLN:CD	1:H:104:ARG:HH21	2.12	0.58
1:D:13:GLY:O	1:D:14:ALA:CB	2.52	0.58
1:G:58:PRO:HG3	1:H:153:TRP:CZ3	2.39	0.58
1:B:25:ARG:O	1:B:29:THR:HG23	2.04	0.58
1:B:220:PHE:CE1	1:B:225:GLY:HA2	2.38	0.58
1:E:163:VAL:HG22	1:E:192:LEU:HG	1.86	0.58
1:F:38:LEU:HB3	1:F:39:PRO:CD	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLN:HB2	1:B:213:LEU:HD12	1.86	0.57
1:B:63:MET:HG3	1:B:65:PRO:HD3	1.86	0.57
1:B:130:VAL:O	1:B:131:VAL:HB	2.05	0.57
1:C:20:ARG:O	1:C:24:TYR:HD1	1.87	0.57
1:C:191:CYS:C	1:C:192:LEU:HD12	2.30	0.57
1:F:131:VAL:HG22	1:F:132:LEU:H	1.68	0.57
1:G:73:GLN:HE21	1:H:222:GLU:HG3	1.67	0.57
1:B:63:MET:CG	1:B:65:PRO:HD3	2.35	0.57
1:C:72:ARG:C	1:C:77:ARG:HH12	2.12	0.57
1:C:28:GLU:CG	1:D:56:GLN:HE22	2.17	0.57
1:C:131:VAL:HG22	1:C:132:LEU:N	2.20	0.57
1:D:132:LEU:C	1:D:134:ARG:H	2.11	0.57
1:E:65:PRO:HA	1:E:126:ARG:HD2	1.87	0.57
1:E:75:GLU:HA	1:E:78:GLU:HB2	1.87	0.57
1:F:165:TRP:CZ2	1:F:188:ALA:HB2	2.40	0.57
1:G:95:PHE:HB2	1:G:100:GLN:CA	2.33	0.57
1:B:145:THR:HG21	1:B:187:VAL:HG21	1.87	0.57
1:G:108:LEU:HB3	2:G:508:FNR:H3	1.70	0.57
1:G:165:TRP:CZ2	1:G:188:ALA:HB2	2.40	0.57
1:G:197:ARG:HA	1:H:11:ALA:HA	1.87	0.57
1:G:224:TRP:CZ2	1:H:184:VAL:HG21	2.40	0.57
1:A:15:PHE:HB3	1:A:19:GLU:HB2	1.87	0.57
1:C:94:MET:HG3	1:D:130:VAL:HG21	1.87	0.57
1:E:154:LEU:O	1:E:157:ARG:HB3	2.05	0.57
1:F:84:PHE:HZ	1:F:108:LEU:HB2	1.70	0.57
1:A:135:THR:HG21	1:B:94:MET:HE1	1.85	0.57
1:B:78:GLU:HG3	1:B:82:GLN:NE2	2.20	0.56
1:G:145:THR:CG2	1:G:187:VAL:HG21	2.35	0.56
1:H:99:ARG:HG2	1:H:99:ARG:HH11	1.70	0.56
1:C:59:SER:HA	2:D:503:FNR:H8M2	1.86	0.56
1:E:86:ARG:CZ	1:E:170:HIS:H	2.18	0.56
1:H:80:VAL:HG12	1:H:111:ILE:HD13	1.86	0.56
2:A:502:FNR:H7	1:B:140:MET:HE3	1.86	0.56
1:B:136:HIS:C	1:B:137:ASN:HD22	2.13	0.56
1:D:131:VAL:HG22	1:D:132:LEU:H	1.71	0.56
1:E:86:ARG:NH2	1:E:170:HIS:H	2.03	0.56
1:F:134:ARG:NH1	1:F:141:ASP:HB3	2.20	0.56
1:F:214:PRO:O	1:F:217:ASP:HB2	2.04	0.56
1:H:43:SER:O	1:H:46:LEU:HB3	2.05	0.56
1:H:214:PRO:O	1:H:217:ASP:HB2	2.05	0.56
1:A:103:TYR:HE1	1:B:132:LEU:HD22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:TRP:CZ3	1:B:58:PRO:HG3	2.40	0.56
1:E:224:TRP:CH2	1:F:184:VAL:HG21	2.40	0.56
1:H:221:GLU:O	1:H:223:GLY:N	2.34	0.56
1:C:9:LEU:N	4:C:535:HOH:O	2.38	0.56
1:F:63:MET:HE3	1:F:126:ARG:O	2.06	0.56
1:A:167:SER:CB	1:B:140:MET:HE2	2.34	0.56
1:C:114:ALA:HB1	1:C:192:LEU:O	2.05	0.56
1:D:15:PHE:O	1:D:20:ARG:NH1	2.38	0.56
1:D:63:MET:HE1	1:D:141:ASP:HB2	1.86	0.56
1:E:38:LEU:O	1:E:40:GLU:N	2.39	0.56
1:C:139:GLN:HE22	1:D:139:GLN:NE2	2.03	0.56
1:E:165:TRP:HD1	1:E:166:VAL:N	2.03	0.56
1:F:67:ASN:HB2	1:F:121:THR:OG1	2.06	0.56
1:F:73:GLN:HA	1:F:73:GLN:NE2	2.20	0.56
1:G:35:ASP:HB2	1:G:107:LYS:HD3	1.87	0.56
1:E:150:GLN:HE21	1:E:154:LEU:CD1	2.18	0.55
1:E:197:ARG:HB3	1:F:11:ALA:HB2	1.88	0.55
1:G:12:ALA:N	4:G:541:HOH:O	2.39	0.55
1:H:77:ARG:HB2	1:H:111:ILE:HG22	1.87	0.55
1:D:78:GLU:O	1:D:82:GLN:HG3	2.06	0.55
1:F:95:PHE:HB2	1:F:100:GLN:HA	1.89	0.55
1:F:73:GLN:HE21	1:F:73:GLN:CA	2.19	0.55
1:G:125:THR:CA	1:G:134:ARG:HH22	2.20	0.55
1:E:58:PRO:HG3	1:F:153:TRP:CZ3	2.42	0.55
1:G:159:GLU:O	1:G:161:VAL:HG23	2.06	0.55
1:A:131:VAL:HG12	1:A:134:ARG:HE	1.71	0.55
1:E:86:ARG:NH2	1:E:170:HIS:N	2.55	0.55
1:E:87:ALA:CB	1:E:169:PHE:HA	2.37	0.55
1:E:209:TRP:NE1	1:F:132:LEU:HD11	2.22	0.55
1:H:84:PHE:CE2	1:H:109:GLU:HG2	2.40	0.55
1:H:171:GLU:OE2	1:H:185:GLU:HG3	2.06	0.55
1:A:120:VAL:O	1:A:187:VAL:HG12	2.07	0.55
1:E:63:MET:HE2	1:E:65:PRO:CB	2.29	0.55
1:E:142:LEU:O	1:E:146:VAL:HG23	2.07	0.55
1:G:84:PHE:CE1	1:G:168:ILE:HB	2.42	0.55
1:A:195:VAL:HG21	1:A:198:LEU:HD21	1.89	0.55
1:E:9:LEU:HD23	1:E:9:LEU:N	2.21	0.55
1:G:143:TYR:OH	1:H:142:LEU:HD13	2.07	0.55
1:H:86:ARG:NH2	1:H:173:GLU:OE1	2.39	0.55
1:H:221:GLU:HG3	1:H:227:ARG:O	2.07	0.55
1:A:80:VAL:HG21	1:A:189:TRP:CH2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ARG:HH11	1:C:20:ARG:HB2	1.72	0.55
1:G:179:GLY:O	1:G:181:PRO:HD3	2.06	0.55
1:H:9:LEU:O	1:H:9:LEU:HD13	2.07	0.54
1:A:149:VAL:HG13	1:A:190:LEU:HD11	1.87	0.54
1:D:145:THR:HG21	1:D:187:VAL:HG21	1.90	0.54
1:F:134:ARG:HE	1:F:138:PRO:HA	1.72	0.54
1:D:220:PHE:CE1	1:D:225:GLY:HA2	2.42	0.54
1:E:165:TRP:CZ2	1:E:188:ALA:HB2	2.43	0.54
1:A:184:VAL:HG21	1:B:224:TRP:CH2	2.43	0.54
1:G:64:GLN:HE22	1:H:213:LEU:N	1.98	0.54
1:C:125:THR:O	1:F:227:ARG:HG3	2.07	0.54
1:D:25:ARG:O	1:D:29:THR:HG23	2.07	0.54
1:G:108:LEU:HD22	1:G:168:ILE:HD11	1.90	0.54
1:A:63:MET:HA	1:B:210:ARG:HE	1.73	0.54
1:A:75:GLU:HG2	1:A:79:LYS:HE2	1.90	0.54
1:A:103:TYR:CE1	1:B:132:LEU:HD22	2.42	0.54
1:D:31:ARG:HD2	1:D:199:TYR:O	2.08	0.54
1:C:131:VAL:O	1:C:135:THR:HG23	2.07	0.54
1:E:30:ARG:HH22	1:F:58:PRO:HB3	1.72	0.54
1:G:70:LEU:HD23	1:G:70:LEU:N	2.23	0.54
1:H:183:HIS:CD2	1:H:184:VAL:HG23	2.42	0.54
1:C:28:GLU:HA	1:D:56:GLN:NE2	2.23	0.54
1:G:140:MET:HE2	1:H:165:TRP:NE1	2.23	0.54
1:A:94:MET:HE3	4:B:524:HOH:O	2.08	0.53
1:E:179:GLY:O	1:F:224:TRP:HB3	2.07	0.53
1:A:227:ARG:HB2	1:H:125:THR:HB	1.90	0.53
1:B:131:VAL:CG1	1:B:134:ARG:HB3	2.38	0.53
1:B:191:CYS:C	1:B:192:LEU:HD12	2.32	0.53
1:F:174:ILE:HA	1:F:177:ILE:HG22	1.91	0.53
1:H:117:SER:OG	1:H:189:TRP:CZ2	2.56	0.53
1:G:213:LEU:H	1:H:64:GLN:HE22	1.56	0.53
1:C:150:GLN:HG2	1:D:147:CYS:SG	2.49	0.53
1:E:60:VAL:HB	1:E:132:LEU:O	2.08	0.53
1:D:149:VAL:HG13	1:D:190:LEU:HD11	1.91	0.53
1:D:227:ARG:HG2	1:D:227:ARG:HH11	1.73	0.53
1:G:171:GLU:OE1	1:G:175:LYS:HD2	2.09	0.53
2:G:508:FNR:H8M1	1:H:59:SER:HA	1.91	0.53
1:G:60:VAL:HG22	1:G:132:LEU:O	2.09	0.53
1:G:124:ARG:NH1	1:G:142:LEU:HG	2.23	0.53
1:C:102:LYS:HE3	1:C:102:LYS:HA	1.91	0.53
1:D:134:ARG:CG	1:D:138:PRO:HA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:GLU:OE2	1:F:185:GLU:HG3	2.09	0.53
1:F:84:PHE:HD1	1:F:168:ILE:O	1.91	0.53
1:A:132:LEU:HD13	1:B:204:LEU:HD21	1.91	0.52
1:A:56:GLN:HE22	1:B:28:GLU:HG2	1.74	0.52
1:B:11:ALA:C	1:B:12:ALA:O	2.50	0.52
1:B:85:GLN:O	1:B:86:ARG:CB	2.53	0.52
1:B:130:VAL:HG12	1:B:131:VAL:N	2.20	0.52
1:G:153:TRP:CZ3	1:H:58:PRO:HG3	2.44	0.52
1:A:58:PRO:HG3	1:B:153:TRP:CZ3	2.44	0.52
1:G:178:LEU:HD22	1:H:222:GLU:O	2.10	0.52
1:H:16:SER:O	1:H:17:SER:C	2.51	0.52
1:E:124:ARG:O	1:E:134:ARG:NH2	2.43	0.52
1:E:139:GLN:OE1	1:F:142:LEU:HD13	2.09	0.52
1:F:95:PHE:O	1:F:100:GLN:HB2	2.10	0.52
1:G:122:CYS:SG	1:G:142:LEU:HD23	2.49	0.52
1:G:184:VAL:HG11	1:H:224:TRP:CH2	2.44	0.52
1:C:67:ASN:HB2	1:C:121:THR:OG1	2.10	0.52
1:D:63:MET:HE3	1:D:65:PRO:HD3	1.92	0.52
1:D:108:LEU:O	1:D:109:GLU:HB3	2.10	0.52
1:A:24:TYR:O	1:A:28:GLU:HB2	2.09	0.52
1:C:196:ASP:O	1:D:12:ALA:N	2.43	0.52
1:E:38:LEU:CB	1:E:40:GLU:OE1	2.58	0.52
1:G:222:GLU:HG2	1:H:73:GLN:HE22	1.75	0.52
1:B:131:VAL:HG22	1:B:132:LEU:N	2.25	0.52
1:C:64:GLN:NE2	1:D:213:LEU:H	2.04	0.52
1:D:67:ASN:HB2	4:D:526:HOH:O	2.08	0.52
1:E:54:ALA:HB1	1:E:148:ALA:HB1	1.91	0.52
1:G:20:ARG:O	1:G:24:TYR:HD1	1.93	0.52
1:E:77:ARG:O	1:E:80:VAL:HB	2.10	0.52
1:F:9:LEU:N	1:F:9:LEU:HD23	2.25	0.52
1:F:39:PRO:CG	1:F:40:GLU:H	2.20	0.52
1:G:88:ASN:HA	1:G:168:ILE:HG21	1.91	0.52
1:E:96:SER:O	1:E:99:ARG:HB2	2.10	0.51
1:G:92:ALA:HB2	1:G:103:TYR:CD2	2.45	0.51
1:G:108:LEU:HD22	1:G:168:ILE:CD1	2.39	0.51
1:A:196:ASP:O	1:B:12:ALA:CA	2.57	0.51
1:F:80:VAL:O	1:F:81:TRP:C	2.53	0.51
1:F:204:LEU:HG	1:F:209:TRP:HB3	1.91	0.51
1:G:64:GLN:O	1:G:126:ARG:NH1	2.38	0.51
1:H:39:PRO:O	1:H:40:GLU:C	2.54	0.51
1:E:61:GLY:O	1:E:62:PHE:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:TRP:CZ2	1:F:112:ARG:NH2	2.79	0.51
1:C:59:SER:HA	1:C:144:SER:OG	2.10	0.51
1:H:38:LEU:CB	1:H:39:PRO:HD2	2.32	0.51
1:G:139:GLN:NE2	1:G:143:TYR:OH	2.44	0.51
1:H:24:TYR:O	1:H:28:GLU:HG3	2.09	0.51
1:E:9:LEU:HB2	1:F:198:LEU:O	2.11	0.51
1:E:86:ARG:NH2	1:E:169:PHE:HB2	2.17	0.51
1:G:196:ASP:O	1:H:11:ALA:HB1	2.11	0.51
1:G:202:PRO:HB3	2:G:508:FNR:H5'1	1.93	0.51
1:H:98:GLU:O	1:H:101:ALA:HB3	2.10	0.51
1:G:34:ARG:NH1	1:G:203:GLU:HB3	2.25	0.51
1:E:203:GLU:O	1:E:207:LYS:HD3	2.11	0.51
1:G:63:MET:SD	1:G:131:VAL:HG21	2.50	0.51
1:G:91:ALA:O	1:G:93:GLU:N	2.42	0.51
1:H:203:GLU:HG2	1:H:207:LYS:CD	2.41	0.51
1:A:56:GLN:NE2	1:B:28:GLU:HG2	2.25	0.51
1:D:34:ARG:HH21	2:D:503:FNR:HN1	1.58	0.51
1:E:103:TYR:CE1	1:E:108:LEU:HD11	2.46	0.51
1:D:30:ARG:C	1:D:31:ARG:HG2	2.36	0.51
1:F:145:THR:O	1:F:149:VAL:HG23	2.10	0.51
2:C:504:FNR:H8M2	1:D:59:SER:HA	1.93	0.50
1:E:189:TRP:O	1:E:190:LEU:HD23	2.11	0.50
1:E:30:ARG:NH2	1:F:58:PRO:HD3	2.25	0.50
1:G:47:ILE:O	1:G:51:LEU:HG	2.11	0.50
1:G:140:MET:HE2	1:H:165:TRP:HE1	1.75	0.50
1:G:202:PRO:HG2	1:H:62:PHE:CZ	2.46	0.50
1:A:227:ARG:HG3	1:H:125:THR:O	2.12	0.50
1:C:56:GLN:OE1	1:D:28:GLU:HG2	2.12	0.50
1:E:85:GLN:O	1:E:88:ASN:HB3	2.12	0.50
1:C:28:GLU:HG2	1:D:56:GLN:HE22	1.77	0.50
1:E:39:PRO:HB3	1:E:113:LYS:O	2.11	0.50
1:E:155:ALA:O	1:E:156:ALA:C	2.55	0.50
1:F:87:ALA:CB	1:F:169:PHE:HA	2.42	0.50
1:A:95:PHE:O	1:A:100:GLN:NE2	2.44	0.50
1:D:95:PHE:O	1:D:100:GLN:NE2	2.42	0.50
1:F:42:LEU:HD12	1:F:42:LEU:N	2.24	0.50
1:G:99:ARG:C	1:G:101:ALA:H	2.18	0.50
1:A:42:LEU:N	1:A:42:LEU:HD12	2.27	0.50
1:C:163:VAL:HG22	1:C:192:LEU:HG	1.93	0.50
1:A:131:VAL:CG1	1:A:134:ARG:HE	2.24	0.50
1:A:165:TRP:CZ2	1:B:140:MET:HE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:ILE:HG23	1:F:151:ASN:HD22	1.77	0.50
1:E:90:GLU:HB2	1:F:136:HIS:CE1	2.47	0.50
1:E:191:CYS:C	1:E:192:LEU:HD12	2.37	0.50
1:B:139:GLN:HA	1:B:139:GLN:NE2	2.27	0.49
1:C:140:MET:HE1	1:D:165:TRP:NE1	2.27	0.49
1:E:143:TYR:CE2	1:F:187:VAL:HG13	2.47	0.49
1:F:106:LEU:HD23	1:F:207:LYS:HE3	1.93	0.49
1:G:221:GLU:O	1:G:223:GLY:N	2.43	0.49
1:C:20:ARG:HB2	1:C:20:ARG:NH1	2.27	0.49
1:F:84:PHE:O	1:F:88:ASN:N	2.44	0.49
1:B:42:LEU:HB3	1:B:46:LEU:HD23	1.95	0.49
1:D:9:LEU:HD23	1:D:10:THR:H	1.76	0.49
1:F:177:ILE:HG23	1:F:178:LEU:HG	1.94	0.49
1:H:220:PHE:CE1	1:H:225:GLY:HA2	2.47	0.49
1:A:75:GLU:O	1:A:79:LYS:HG3	2.12	0.49
1:G:39:PRO:HD3	4:G:527:HOH:O	2.11	0.49
1:G:124:ARG:O	1:G:134:ARG:NH2	2.45	0.49
1:G:132:LEU:HD23	3:G:603:OXY:O2	2.12	0.49
1:C:124:ARG:NE	1:C:141:ASP:OD2	2.33	0.49
1:H:74:ASP:O	1:H:78:GLU:HB2	2.13	0.49
1:H:84:PHE:CE2	1:H:109:GLU:HB3	2.48	0.49
1:H:202:PRO:O	1:H:205:ALA:HB3	2.13	0.49
1:C:63:MET:HE2	1:C:65:PRO:HB3	1.94	0.49
1:C:131:VAL:HG13	1:C:134:ARG:HB3	1.93	0.49
1:E:73:GLN:O	1:E:76:THR:HB	2.12	0.49
1:F:92:ALA:O	1:F:94:MET:N	2.37	0.49
1:F:131:VAL:HG12	1:F:134:ARG:HB2	1.94	0.49
1:G:9:LEU:HA	1:H:198:LEU:O	2.13	0.49
1:G:30:ARG:NH2	1:H:58:PRO:HD3	2.27	0.49
1:G:174:ILE:HD13	1:G:177:ILE:HD12	1.94	0.49
1:D:60:VAL:HG23	1:D:133:GLY:HA3	1.95	0.49
1:E:73:GLN:HB2	1:E:76:THR:OG1	2.13	0.49
1:F:84:PHE:CZ	1:F:108:LEU:HB2	2.48	0.49
1:G:63:MET:O	1:G:64:GLN:C	2.56	0.49
1:G:201:GLU:O	1:G:202:PRO:C	2.56	0.49
1:G:221:GLU:HB2	1:G:227:ARG:OXT	2.13	0.49
1:B:60:VAL:CG2	1:B:133:GLY:HA3	2.43	0.49
1:D:68:PHE:CD1	1:D:120:VAL:HG22	2.48	0.49
1:G:171:GLU:OE2	1:G:186:ILE:HB	2.12	0.49
1:H:170:HIS:O	1:H:171:GLU:C	2.56	0.49
1:A:83:ALA:HA	1:A:86:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:MET:HE2	1:B:167:SER:HB3	1.94	0.48
1:E:64:GLN:OE1	1:F:213:LEU:HG	2.13	0.48
1:E:84:PHE:HE1	1:E:168:ILE:HB	1.77	0.48
1:H:134:ARG:NH2	1:H:141:ASP:CG	2.71	0.48
1:A:114:ALA:HB1	1:A:192:LEU:O	2.13	0.48
1:E:9:LEU:O	1:E:9:LEU:HG	2.12	0.48
1:G:61:GLY:HA2	1:G:132:LEU:HB2	1.94	0.48
1:B:99:ARG:O	1:B:100:GLN:C	2.55	0.48
1:C:89:ASP:O	1:C:92:ALA:HB3	2.13	0.48
1:E:165:TRP:CD1	1:E:166:VAL:N	2.81	0.48
1:G:113:LYS:HG2	4:G:527:HOH:O	2.13	0.48
1:A:80:VAL:HG12	1:A:111:ILE:HD13	1.96	0.48
1:C:106:LEU:HB3	1:C:108:LEU:HD21	1.95	0.48
1:E:197:ARG:HA	1:F:11:ALA:CA	2.40	0.48
1:F:63:MET:C	1:F:64:GLN:HG3	2.38	0.48
1:G:83:ALA:O	1:G:86:ARG:HG2	2.13	0.48
1:H:137:ASN:OD1	1:H:139:GLN:HB2	2.13	0.48
1:B:107:LYS:HE2	1:B:109:GLU:O	2.13	0.48
1:C:138:PRO:O	1:C:141:ASP:OD1	2.31	0.48
1:D:89:ASP:O	1:D:93:GLU:HG3	2.14	0.48
1:E:9:LEU:N	4:E:572:HOH:O	2.46	0.48
1:A:72:ARG:N	1:B:222:GLU:OE2	2.46	0.48
1:A:134:ARG:O	1:A:135:THR:CB	2.61	0.48
1:B:38:LEU:HD23	1:B:195:VAL:HA	1.96	0.48
1:B:206:ALA:C	1:B:208:GLY:H	2.21	0.48
1:F:31:ARG:HE	1:F:31:ARG:HA	1.78	0.48
1:F:37:PHE:CD2	1:F:114:ALA:HB2	2.48	0.48
1:G:83:ALA:HA	1:G:86:ARG:NE	2.28	0.48
1:G:158:ALA:HA	1:H:15:PHE:CD1	2.48	0.48
1:H:197:ARG:HG2	1:H:197:ARG:HH11	1.79	0.48
1:A:63:MET:CG	1:A:65:PRO:HD3	2.42	0.48
1:D:59:SER:HA	1:D:144:SER:HB3	1.96	0.48
1:E:110:GLY:O	1:E:114:ALA:N	2.37	0.48
1:H:86:ARG:O	1:H:90:GLU:HG3	2.13	0.48
1:E:30:ARG:HA	1:E:157:ARG:HD3	1.96	0.48
1:G:191:CYS:C	1:G:192:LEU:HD12	2.39	0.48
1:C:94:MET:CG	1:D:130:VAL:HG11	2.44	0.48
1:D:107:LYS:HE2	1:D:109:GLU:O	2.14	0.48
1:C:94:MET:HG2	1:D:130:VAL:CG1	2.43	0.48
1:E:108:LEU:CD2	1:F:132:LEU:HD23	2.43	0.48
1:A:64:GLN:HE22	1:B:213:LEU:N	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG11	1:B:94:MET:SD	2.54	0.47
1:C:73:GLN:CG	1:D:222:GLU:OE1	2.61	0.47
2:C:504:FNR:H7	1:D:140:MET:HE2	1.96	0.47
1:F:163:VAL:HA	1:F:191:CYS:O	2.14	0.47
1:G:89:ASP:O	1:G:91:ALA:N	2.47	0.47
1:H:168:ILE:HG13	2:H:507:FNR:O4	2.14	0.47
1:F:132:LEU:H	1:F:132:LEU:HD12	1.78	0.47
1:G:61:GLY:CA	1:G:132:LEU:HB2	2.44	0.47
1:G:224:TRP:CH2	1:H:184:VAL:HG21	2.49	0.47
1:A:140:MET:HE1	1:B:165:TRP:CZ2	2.49	0.47
1:E:136:HIS:CD2	1:F:87:ALA:HB1	2.50	0.47
1:A:84:PHE:CE2	1:A:109:GLU:HG2	2.50	0.47
1:A:191:CYS:C	1:A:192:LEU:HD12	2.39	0.47
1:B:61:GLY:HA2	1:B:132:LEU:HD12	1.95	0.47
1:F:202:PRO:HB3	2:F:505:FNR:H5'2	1.96	0.47
1:H:162:GLY:O	1:H:192:LEU:HA	2.15	0.47
1:E:63:MET:O	1:E:64:GLN:C	2.57	0.47
1:G:86:ARG:NE	1:G:173:GLU:OE1	2.47	0.47
1:B:9:LEU:O	1:B:10:THR:HB	2.15	0.47
1:C:30:ARG:HG2	1:C:154:LEU:HD12	1.95	0.47
1:E:79:LYS:HA	1:E:82:GLN:NE2	2.29	0.47
1:F:92:ALA:C	1:F:94:MET:H	2.20	0.47
1:B:87:ALA:CB	1:B:169:PHE:HA	2.45	0.47
1:B:169:PHE:HD1	1:B:169:PHE:O	1.97	0.47
1:E:165:TRP:HD1	1:E:166:VAL:H	1.62	0.47
1:G:67:ASN:ND2	1:H:218:LEU:O	2.48	0.47
1:H:223:GLY:O	1:H:226:VAL:HB	2.15	0.47
1:A:152:LEU:C	1:A:152:LEU:HD23	2.40	0.47
1:A:209:TRP:CZ2	1:B:132:LEU:HD21	2.50	0.47
1:E:78:GLU:O	1:E:82:GLN:HG3	2.14	0.47
1:E:171:GLU:CD	1:E:175:LYS:HD2	2.40	0.47
1:F:32:ASP:CG	2:F:505:FNR:H1'1	2.40	0.47
1:G:200:GLN:HG3	1:H:9:LEU:N	2.30	0.47
1:H:57:ALA:HB2	1:H:148:ALA:HA	1.97	0.47
1:A:192:LEU:HD12	1:A:192:LEU:N	2.29	0.47
1:E:28:GLU:HG2	1:F:56:GLN:HE22	1.80	0.47
1:E:64:GLN:NE2	1:F:213:LEU:H	2.10	0.47
1:F:39:PRO:O	1:F:40:GLU:C	2.58	0.47
1:C:69:VAL:HG11	1:C:178:LEU:HD13	1.97	0.47
1:C:140:MET:HE3	2:D:503:FNR:C7M	2.44	0.47
1:F:82:GLN:HB3	1:F:86:ARG:HH12	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:ALA:O	1:H:196:ASP:O	2.33	0.47
1:G:192:LEU:HD12	1:G:192:LEU:N	2.30	0.47
1:H:204:LEU:HB3	1:H:209:TRP:HB3	1.97	0.47
1:H:220:PHE:O	1:H:221:GLU:HG2	2.16	0.47
1:A:135:THR:C	1:A:137:ASN:H	2.22	0.46
1:B:30:ARG:C	1:B:31:ARG:HG2	2.40	0.46
1:C:75:GLU:O	1:C:79:LYS:HG2	2.14	0.46
1:E:127:GLY:HA2	1:F:210:ARG:NH1	2.30	0.46
1:F:131:VAL:CG1	1:F:134:ARG:H	2.28	0.46
1:C:134:ARG:CG	1:C:138:PRO:HA	2.41	0.46
1:E:171:GLU:HG2	1:E:175:LYS:CG	2.43	0.46
1:F:183:HIS:ND1	1:F:184:VAL:HG23	2.30	0.46
1:G:72:ARG:HB3	1:G:72:ARG:HH11	1.81	0.46
1:G:145:THR:HG21	1:G:187:VAL:HG21	1.97	0.46
1:A:10:THR:HG22	1:A:11:ALA:O	2.15	0.46
1:A:103:TYR:C	1:A:105:SER:H	2.23	0.46
1:E:64:GLN:NE2	1:F:212:ARG:HD3	2.30	0.46
1:H:16:SER:O	1:H:20:ARG:HD2	2.16	0.46
1:H:61:GLY:C	1:H:63:MET:N	2.70	0.46
1:D:39:PRO:O	1:D:40:GLU:C	2.59	0.46
1:E:31:ARG:NE	2:E:506:FNR:O3P	2.38	0.46
1:E:146:VAL:HB	1:F:146:VAL:HG11	1.96	0.46
1:H:82:GLN:HA	1:H:85:GLN:HG2	1.98	0.46
1:H:100:GLN:HG2	1:H:104:ARG:HH21	1.81	0.46
1:A:212:ARG:HA	1:B:64:GLN:HE22	1.81	0.46
1:G:30:ARG:HH21	1:H:58:PRO:HD3	1.80	0.46
1:D:131:VAL:HG13	1:D:132:LEU:O	2.16	0.46
1:B:116:LEU:HD12	1:B:117:SER:H	1.81	0.46
1:B:127:GLY:HA2	1:G:217:ASP:OD2	2.15	0.46
1:D:30:ARG:NH1	1:D:31:ARG:HA	2.30	0.46
1:D:132:LEU:HB3	3:D:601:OXY:O1	2.16	0.46
1:E:40:GLU:O	1:E:115:PRO:CB	2.63	0.46
1:E:114:ALA:CB	1:E:191:CYS:HB3	2.45	0.46
1:E:122:CYS:CB	1:E:145:THR:HG21	2.45	0.46
1:E:189:TRP:C	1:E:190:LEU:HD23	2.41	0.46
1:E:201:GLU:O	1:E:202:PRO:C	2.58	0.46
1:H:15:PHE:HD2	1:H:19:GLU:HB3	1.80	0.46
1:H:107:LYS:O	1:H:108:LEU:HD23	2.16	0.46
1:B:42:LEU:N	1:B:42:LEU:HD12	2.31	0.46
1:A:81:TRP:O	1:A:84:PHE:HB3	2.16	0.46
1:B:131:VAL:HG13	1:B:134:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LYS:NZ	1:B:182:ASP:HA	2.30	0.46
1:E:125:THR:HG23	1:E:183:HIS:HB2	1.98	0.46
1:E:136:HIS:NE2	1:F:87:ALA:HB1	2.31	0.46
1:E:140:MET:HE2	1:F:167:SER:CB	2.45	0.46
1:B:227:ARG:HH11	1:B:227:ARG:CG	2.29	0.46
1:C:77:ARG:HD2	1:C:111:ILE:O	2.15	0.46
1:C:99:ARG:HB3	4:C:533:HOH:O	2.15	0.46
1:C:149:VAL:HG13	1:C:190:LEU:HD11	1.98	0.46
1:F:131:VAL:HG13	1:F:132:LEU:N	2.31	0.46
1:G:74:ASP:OD1	1:G:75:GLU:N	2.49	0.46
1:A:131:VAL:HG22	1:A:132:LEU:N	2.31	0.45
1:A:152:LEU:HD23	1:A:152:LEU:O	2.16	0.45
1:C:80:VAL:HG21	1:C:189:TRP:CH2	2.51	0.45
1:C:227:ARG:CG	1:C:227:ARG:NH1	2.76	0.45
1:D:60:VAL:HG22	1:D:132:LEU:O	2.15	0.45
1:D:63:MET:HE3	1:D:65:PRO:CD	2.45	0.45
1:D:103:TYR:C	1:D:103:TYR:CD2	2.95	0.45
1:D:150:GLN:HA	1:D:150:GLN:OE1	2.15	0.45
1:E:81:TRP:HA	1:E:111:ILE:HD12	1.98	0.45
1:H:9:LEU:HB3	4:H:558:HOH:O	2.14	0.45
1:E:45:GLU:O	1:E:48:ALA:HB3	2.16	0.45
1:G:73:GLN:HG3	1:H:222:GLU:CD	2.41	0.45
1:C:140:MET:HE1	1:D:165:TRP:CE2	2.52	0.45
1:G:197:ARG:HB3	1:H:11:ALA:HB2	1.98	0.45
1:H:100:GLN:CG	1:H:104:ARG:HH21	2.29	0.45
1:D:124:ARG:NE	1:D:141:ASP:OD2	2.50	0.45
1:E:131:VAL:HG13	1:E:131:VAL:O	2.17	0.45
1:G:81:TRP:NE1	1:G:112:ARG:CZ	2.80	0.45
1:G:217:ASP:OD2	1:G:217:ASP:N	2.49	0.45
1:H:61:GLY:HA3	1:H:132:LEU:HB2	1.99	0.45
1:E:36:GLU:CD	1:E:36:GLU:N	2.74	0.45
1:F:77:ARG:O	1:F:80:VAL:HB	2.16	0.45
1:G:157:ARG:O	1:G:157:ARG:HD3	2.15	0.45
1:C:140:MET:HE2	1:D:167:SER:HB2	1.97	0.45
1:E:125:THR:HA	1:E:134:ARG:HH12	1.81	0.45
1:E:204:LEU:HD21	1:F:132:LEU:HD22	1.97	0.45
1:G:81:TRP:CE2	1:G:112:ARG:CZ	3.00	0.45
1:H:67:ASN:HB2	1:H:121:THR:OG1	2.16	0.45
1:C:218:LEU:HD13	1:D:66:TRP:O	2.17	0.45
1:E:204:LEU:N	1:E:204:LEU:HD12	2.32	0.45
1:F:139:GLN:O	1:F:142:LEU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:HIS:HB2	1:G:173:GLU:OE2	2.16	0.45
1:H:167:SER:N	2:H:507:FNR:O4	2.50	0.45
1:A:34:ARG:HH21	2:A:502:FNR:HN1	1.65	0.45
1:D:63:MET:O	1:D:64:GLN:C	2.60	0.45
1:D:81:TRP:O	1:D:84:PHE:HB3	2.17	0.45
1:E:25:ARG:HG2	1:F:15:PHE:CZ	2.51	0.45
1:F:35:ASP:O	1:F:35:ASP:CG	2.60	0.45
1:F:143:TYR:CD1	1:F:143:TYR:N	2.83	0.45
1:G:38:LEU:C	1:G:40:GLU:H	2.25	0.45
1:H:39:PRO:CG	1:H:40:GLU:H	2.28	0.45
1:H:215:LEU:O	1:H:219:VAL:HG23	2.17	0.45
1:C:72:ARG:C	1:C:77:ARG:NH1	2.75	0.45
1:D:9:LEU:N	4:D:513:HOH:O	2.49	0.45
1:D:76:THR:O	1:D:80:VAL:HG23	2.17	0.45
1:F:175:LYS:HA	1:F:180:ILE:HB	1.98	0.45
1:G:125:THR:O	1:G:126:ARG:C	2.59	0.45
1:H:173:GLU:O	1:H:177:ILE:HG13	2.16	0.45
1:A:213:LEU:H	1:B:64:GLN:HE22	1.63	0.45
1:B:60:VAL:C	1:B:62:PHE:H	2.24	0.45
1:B:145:THR:O	1:B:148:ALA:HB3	2.16	0.45
1:E:24:TYR:O	1:E:28:GLU:HB2	2.17	0.45
1:E:34:ARG:HG3	1:E:34:ARG:HH11	1.82	0.45
1:E:80:VAL:HG21	1:E:189:TRP:CH2	2.52	0.45
1:F:15:PHE:HD2	1:F:19:GLU:HB3	1.82	0.45
1:G:28:GLU:HG2	1:H:56:GLN:NE2	2.28	0.45
1:H:77:ARG:NH1	1:H:114:ALA:O	2.50	0.45
1:H:146:VAL:O	1:H:149:VAL:N	2.50	0.45
1:A:30:ARG:HH21	1:B:58:PRO:N	2.15	0.44
1:A:214:PRO:HB2	1:G:210:ARG:HH12	1.82	0.44
1:E:32:ASP:OD2	2:E:506:FNR:H1'1	2.17	0.44
1:E:123:ASP:N	4:E:530:HOH:O	2.41	0.44
1:F:102:LYS:HD2	1:F:105:SER:OG	2.16	0.44
1:H:71:VAL:HG21	1:H:189:TRP:CH2	2.52	0.44
1:H:84:PHE:CD2	1:H:109:GLU:HB3	2.52	0.44
1:A:33:VAL:HG13	1:A:36:GLU:HG2	1.99	0.44
1:B:65:PRO:HA	1:B:126:ARG:HD2	1.99	0.44
1:C:96:SER:CA	1:C:100:GLN:HB2	2.47	0.44
1:D:30:ARG:HH12	1:D:31:ARG:HA	1.82	0.44
1:E:92:ALA:HB1	1:E:104:ARG:HE	1.83	0.44
1:F:226:VAL:CG1	1:F:227:ARG:N	2.79	0.44
2:A:502:FNR:C7M	1:B:140:MET:HE3	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:GLU:O	1:F:172:SER:C	2.61	0.44
1:G:154:LEU:CD2	1:H:154:LEU:HD23	2.45	0.44
1:H:109:GLU:H	1:H:109:GLU:HG3	1.62	0.44
1:A:36:GLU:N	1:A:36:GLU:CD	2.75	0.44
1:B:99:ARG:O	1:B:102:LYS:N	2.50	0.44
1:B:199:TYR:CZ	1:B:203:GLU:HG3	2.52	0.44
1:E:150:GLN:HE21	1:E:154:LEU:HD11	1.82	0.44
1:E:204:LEU:HD21	1:F:132:LEU:CD2	2.48	0.44
1:C:140:MET:HE1	1:D:165:TRP:CZ2	2.52	0.44
1:D:39:PRO:HG2	1:D:40:GLU:OE2	2.17	0.44
1:D:196:ASP:N	4:D:540:HOH:O	2.39	0.44
1:F:61:GLY:HA3	1:F:132:LEU:HD13	1.98	0.44
1:D:37:PHE:CD2	1:D:114:ALA:HB2	2.53	0.44
1:D:114:ALA:HB1	1:D:192:LEU:O	2.18	0.44
1:H:15:PHE:HB3	1:H:19:GLU:CB	2.47	0.44
1:A:59:SER:CA	2:B:501:FNR:H8M1	2.48	0.44
1:A:213:LEU:H	1:B:64:GLN:NE2	2.16	0.44
1:C:80:VAL:O	1:C:81:TRP:C	2.60	0.44
1:F:131:VAL:HG12	1:F:134:ARG:CB	2.47	0.44
1:G:131:VAL:HG22	1:G:134:ARG:HD3	2.00	0.44
1:H:111:ILE:HD11	1:H:169:PHE:CZ	2.52	0.44
1:A:227:ARG:HH11	1:A:227:ARG:CG	2.30	0.44
1:B:108:LEU:O	1:B:109:GLU:HB3	2.17	0.44
1:C:103:TYR:O	1:C:105:SER:N	2.51	0.44
1:C:192:LEU:HD12	1:C:192:LEU:N	2.32	0.44
1:E:81:TRP:CE2	1:E:112:ARG:CZ	3.00	0.44
1:E:146:VAL:HG11	1:F:146:VAL:HB	2.00	0.44
1:H:111:ILE:HD11	1:H:169:PHE:HZ	1.83	0.44
1:C:136:HIS:CD2	1:D:87:ALA:HB1	2.52	0.44
1:C:168:ILE:HG13	2:C:504:FNR:O4	2.18	0.44
1:E:42:LEU:HD23	1:E:46:LEU:CD2	2.45	0.44
1:E:80:VAL:HG12	1:E:111:ILE:HD13	1.99	0.44
1:F:175:LYS:NZ	1:F:175:LYS:HB3	2.32	0.44
1:H:171:GLU:O	1:H:172:SER:C	2.61	0.44
1:A:134:ARG:O	1:A:135:THR:HB	2.17	0.43
1:B:145:THR:CG2	1:B:187:VAL:HG21	2.47	0.43
1:C:58:PRO:HD3	1:D:30:ARG:HH21	1.83	0.43
1:D:68:PHE:HD1	1:D:120:VAL:HG22	1.81	0.43
1:D:165:TRP:CZ2	1:D:188:ALA:HB2	2.53	0.43
2:E:506:FNR:H7M1	1:F:140:MET:HE3	1.99	0.43
1:A:12:ALA:O	1:B:196:ASP:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:PHE:O	1:B:87:ALA:HB3	2.18	0.43
1:E:86:ARG:O	1:E:90:GLU:HG3	2.19	0.43
1:H:141:ASP:CG	1:H:142:LEU:N	2.75	0.43
1:H:175:LYS:HE3	1:H:180:ILE:CG2	2.48	0.43
1:C:140:MET:HE3	2:D:503:FNR:H7	1.99	0.43
1:E:91:ALA:C	1:E:93:GLU:N	2.68	0.43
1:E:91:ALA:O	1:E:93:GLU:N	2.50	0.43
1:F:16:SER:O	1:F:17:SER:C	2.60	0.43
1:G:81:TRP:CZ2	1:G:85:GLN:HG3	2.52	0.43
1:G:89:ASP:C	1:G:91:ALA:N	2.76	0.43
1:A:35:ASP:CG	1:A:107:LYS:HE2	2.43	0.43
1:A:157:ARG:NH1	1:B:13:GLY:O	2.48	0.43
1:E:12:ALA:O	1:F:196:ASP:HA	2.19	0.43
1:A:214:PRO:HB2	1:G:210:ARG:NH1	2.33	0.43
1:C:42:LEU:HD12	1:C:42:LEU:N	2.32	0.43
1:G:145:THR:HG22	1:G:187:VAL:HG21	1.99	0.43
1:G:150:GLN:HG2	1:H:150:GLN:HB3	2.00	0.43
1:H:30:ARG:NH2	2:H:507:FNR:O2P	2.51	0.43
1:H:171:GLU:O	1:H:174:ILE:N	2.46	0.43
1:G:124:ARG:C	1:G:134:ARG:NH2	2.76	0.43
1:G:134:ARG:O	1:G:134:ARG:HG2	2.18	0.43
1:A:140:MET:HE2	1:B:167:SER:CB	2.49	0.43
1:A:98:GLU:HG3	1:A:99:ARG:N	2.33	0.43
1:C:84:PHE:CE2	1:C:109:GLU:HG2	2.53	0.43
1:D:84:PHE:HB2	1:D:169:PHE:HE2	1.84	0.43
1:E:10:THR:OG1	1:E:11:ALA:N	2.50	0.43
1:E:61:GLY:C	1:E:63:MET:N	2.75	0.43
1:E:86:ARG:NH1	1:E:170:HIS:HB2	2.34	0.43
1:E:165:TRP:CD1	1:E:166:VAL:H	2.36	0.43
1:F:224:TRP:O	1:F:224:TRP:CD1	2.71	0.43
1:G:9:LEU:O	1:G:10:THR:CB	2.67	0.43
1:A:165:TRP:CE2	1:B:140:MET:HE1	2.54	0.43
1:F:51:LEU:HD11	1:F:70:LEU:HD21	2.01	0.43
1:G:95:PHE:HE2	1:G:103:TYR:CD2	2.37	0.43
1:G:199:TYR:HA	1:H:9:LEU:HA	2.01	0.43
1:H:217:ASP:HA	1:H:227:ARG:NH2	2.34	0.43
1:A:95:PHE:CE1	1:B:130:VAL:HB	2.54	0.43
1:A:145:THR:CG2	1:A:187:VAL:HG11	2.49	0.43
1:C:76:THR:O	1:C:80:VAL:HG23	2.19	0.43
1:C:102:LYS:O	1:C:103:TYR:C	2.62	0.43
1:C:144:SER:OG	2:D:503:FNR:H8M2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:THR:CG2	1:D:187:VAL:HG21	2.48	0.43
1:H:30:ARG:HA	1:H:157:ARG:HD3	2.01	0.43
1:H:100:GLN:CD	1:H:104:ARG:NH2	2.76	0.43
1:C:10:THR:OG1	1:C:11:ALA:N	2.52	0.42
1:C:224:TRP:CD1	1:D:181:PRO:HD3	2.53	0.42
1:E:30:ARG:HH22	1:F:58:PRO:CB	2.31	0.42
1:E:171:GLU:OE1	1:E:186:ILE:HG13	2.19	0.42
1:G:78:GLU:CG	1:G:82:GLN:HE21	2.20	0.42
1:H:102:LYS:O	1:H:105:SER:OG	2.32	0.42
1:A:140:MET:HE1	1:B:165:TRP:CE2	2.53	0.42
1:A:217:ASP:CG	1:G:210:ARG:HH22	2.27	0.42
1:D:36:GLU:CD	1:D:36:GLU:N	2.77	0.42
1:D:126:ARG:CG	1:D:127:GLY:N	2.82	0.42
1:F:30:ARG:HA	1:F:157:ARG:HD3	2.01	0.42
1:G:57:ALA:HB1	1:G:58:PRO:HD2	2.00	0.42
1:G:84:PHE:O	1:G:88:ASN:N	2.52	0.42
1:E:9:LEU:N	1:E:9:LEU:CD2	2.82	0.42
1:E:86:ARG:HH12	1:E:170:HIS:HB2	1.85	0.42
1:G:59:SER:OG	1:G:62:PHE:HA	2.19	0.42
1:G:76:THR:O	1:G:76:THR:HG22	2.19	0.42
1:G:222:GLU:CD	1:H:73:GLN:OE1	2.61	0.42
1:A:59:SER:HA	2:B:501:FNR:H8M1	2.00	0.42
1:A:63:MET:HA	1:B:210:ARG:NE	2.33	0.42
1:A:132:LEU:HD23	1:A:133:GLY:H	1.83	0.42
1:D:215:LEU:O	1:D:219:VAL:HG23	2.20	0.42
1:F:19:GLU:O	1:F:20:ARG:C	2.63	0.42
1:F:19:GLU:O	1:F:22:ALA:N	2.52	0.42
1:F:42:LEU:HD23	1:F:46:LEU:CD2	2.49	0.42
1:F:108:LEU:HA	2:F:505:FNR:O2	2.19	0.42
1:F:170:HIS:O	1:F:171:GLU:C	2.62	0.42
1:G:81:TRP:CD1	1:G:112:ARG:NE	2.88	0.42
1:H:84:PHE:CE1	1:H:168:ILE:HB	2.54	0.42
1:B:49:ARG:HH21	1:B:159:GLU:CD	2.27	0.42
1:B:81:TRP:O	1:B:84:PHE:HB3	2.19	0.42
1:C:30:ARG:HG2	1:C:154:LEU:CD1	2.49	0.42
1:C:132:LEU:O	1:C:134:ARG:N	2.43	0.42
1:D:9:LEU:HD23	1:D:10:THR:N	2.35	0.42
1:E:67:ASN:HD22	1:E:67:ASN:HA	1.51	0.42
1:H:81:TRP:CD2	1:H:85:GLN:NE2	2.87	0.42
1:H:204:LEU:HD13	2:H:507:FNR:O4'	2.19	0.42
1:B:157:ARG:O	1:B:157:ARG:NH1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:LEU:C	1:C:134:ARG:H	2.24	0.42
1:E:67:ASN:HB2	4:E:530:HOH:O	2.18	0.42
1:G:197:ARG:HA	1:H:11:ALA:CA	2.49	0.42
1:A:197:ARG:HA	1:B:11:ALA:O	2.20	0.42
1:B:15:PHE:HB3	1:B:19:GLU:HB2	2.01	0.42
1:B:98:GLU:OE2	1:B:98:GLU:HA	2.19	0.42
1:D:13:GLY:O	1:D:14:ALA:HB3	2.19	0.42
1:G:10:THR:OG1	1:G:11:ALA:N	2.53	0.42
1:A:12:ALA:N	1:B:196:ASP:O	2.52	0.42
1:A:181:PRO:HD3	1:B:224:TRP:CD1	2.55	0.42
1:B:114:ALA:HB1	1:B:192:LEU:O	2.20	0.42
1:C:227:ARG:HG3	1:C:227:ARG:NH1	2.24	0.42
1:E:87:ALA:HB3	1:E:169:PHE:HA	2.01	0.42
1:E:172:SER:O	1:E:173:GLU:C	2.63	0.42
1:G:42:LEU:HD11	1:G:46:LEU:HD12	2.00	0.42
1:A:124:ARG:NE	1:A:141:ASP:OD2	2.47	0.42
1:A:213:LEU:HD12	1:B:64:GLN:HB2	2.01	0.42
1:B:90:GLU:O	1:B:91:ALA:C	2.63	0.42
1:D:60:VAL:CG2	1:D:133:GLY:HA3	2.49	0.42
1:D:131:VAL:HG22	1:D:132:LEU:N	2.33	0.42
1:G:157:ARG:HD3	1:G:157:ARG:C	2.45	0.42
1:H:214:PRO:HG2	1:H:217:ASP:CG	2.44	0.42
1:A:61:GLY:O	1:A:62:PHE:C	2.63	0.42
1:A:74:ASP:OD1	1:A:77:ARG:NH2	2.52	0.42
1:H:44:GLU:OE1	1:H:72:ARG:NH2	2.53	0.42
1:D:144:SER:O	1:D:147:CYS:HB2	2.19	0.41
1:H:70:LEU:HD23	1:H:118:ILE:HG23	2.02	0.41
1:A:151:ASN:OD1	1:B:150:GLN:NE2	2.51	0.41
1:E:227:ARG:HG2	1:E:227:ARG:HH11	1.85	0.41
1:F:107:LYS:HD2	1:F:107:LYS:HA	1.90	0.41
1:G:84:PHE:CE2	1:G:109:GLU:HB3	2.55	0.41
1:G:165:TRP:HD1	1:G:166:VAL:N	2.17	0.41
1:H:117:SER:OG	1:H:189:TRP:CE2	2.73	0.41
1:C:99:ARG:HA	1:C:99:ARG:HD2	1.90	0.41
1:D:53:ALA:O	1:D:54:ALA:C	2.63	0.41
1:D:180:ILE:HA	1:D:181:PRO:HD3	1.83	0.41
1:F:114:ALA:HA	1:F:115:PRO:HD3	1.92	0.41
1:G:15:PHE:HB3	1:G:19:GLU:HB2	2.02	0.41
1:B:31:ARG:HH21	1:B:202:PRO:HG3	1.85	0.41
1:B:80:VAL:HG13	1:B:174:ILE:CD1	2.51	0.41
1:F:132:LEU:HD12	1:F:132:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:SER:HA	1:G:190:LEU:O	2.20	0.41
1:G:221:GLU:C	1:G:223:GLY:H	2.27	0.41
1:H:77:ARG:HD2	1:H:111:ILE:O	2.19	0.41
1:A:134:ARG:HD2	1:A:138:PRO:HA	2.02	0.41
1:C:157:ARG:HH12	1:D:14:ALA:H	1.67	0.41
1:D:103:TYR:C	1:D:105:SER:H	2.28	0.41
1:D:108:LEU:O	1:D:109:GLU:CB	2.68	0.41
1:E:40:GLU:HB3	4:E:543:HOH:O	2.19	0.41
1:E:213:LEU:HA	1:E:214:PRO:HD3	1.87	0.41
1:F:221:GLU:O	1:F:222:GLU:C	2.63	0.41
1:G:38:LEU:O	1:G:40:GLU:N	2.53	0.41
1:G:183:HIS:CD2	1:G:183:HIS:H	2.38	0.41
1:G:185:GLU:HG2	1:G:186:ILE:N	2.35	0.41
1:C:184:VAL:HG21	1:D:224:TRP:CH2	2.55	0.41
1:E:62:PHE:HE2	1:F:211:GLN:C	2.29	0.41
1:F:92:ALA:C	1:F:94:MET:N	2.78	0.41
1:G:103:TYR:HE1	1:G:108:LEU:HD21	1.85	0.41
1:H:32:ASP:CG	2:H:507:FNR:H1'1	2.45	0.41
1:H:159:GLU:O	1:H:161:VAL:HG23	2.20	0.41
1:G:164:GLY:HA3	4:G:532:HOH:O	2.20	0.41
1:B:102:LYS:O	1:B:106:LEU:HG	2.21	0.41
1:B:131:VAL:HG11	1:B:134:ARG:HB3	2.03	0.41
1:D:175:LYS:O	1:D:179:GLY:N	2.53	0.41
1:E:30:ARG:NH2	1:F:58:PRO:CD	2.83	0.41
1:H:42:LEU:HD23	1:H:46:LEU:CD2	2.50	0.41
1:H:99:ARG:HD2	1:H:209:TRP:CZ3	2.55	0.41
1:H:128:GLY:O	1:H:129:ALA:C	2.63	0.41
1:A:103:TYR:O	1:A:105:SER:N	2.53	0.41
1:A:140:MET:HE1	1:B:165:TRP:NE1	2.36	0.41
1:A:140:MET:CE	2:B:501:FNR:H7M1	2.40	0.41
1:B:63:MET:O	1:B:64:GLN:C	2.64	0.41
1:B:87:ALA:HB2	1:B:169:PHE:HA	2.02	0.41
1:C:81:TRP:O	1:C:84:PHE:HB3	2.21	0.41
1:C:142:LEU:HD13	1:D:143:TYR:OH	2.21	0.41
2:C:504:FNR:H7	1:D:140:MET:CE	2.50	0.41
1:D:84:PHE:HB2	1:D:169:PHE:CE2	2.56	0.41
1:D:109:GLU:C	1:D:109:GLU:CD	2.88	0.41
1:D:137:ASN:HA	1:D:138:PRO:HD2	1.86	0.41
1:E:60:VAL:HG11	1:E:140:MET:CB	2.50	0.41
1:E:89:ASP:C	1:E:91:ALA:N	2.75	0.41
2:E:506:FNR:N5	1:F:60:VAL:HG23	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:ILE:HA	1:F:154:LEU:HD11	2.02	0.41
1:F:195:VAL:O	1:F:195:VAL:HG23	2.20	0.41
1:G:92:ALA:HB2	1:G:103:TYR:CE2	2.56	0.41
1:G:131:VAL:CG2	1:G:134:ARG:HD3	2.51	0.41
1:G:213:LEU:HA	1:G:214:PRO:HD3	1.83	0.41
1:D:87:ALA:HA	1:D:90:GLU:HG3	2.03	0.41
1:F:102:LYS:O	1:F:106:LEU:HG	2.20	0.41
1:G:96:SER:CA	1:G:100:GLN:HB2	2.51	0.41
1:H:80:VAL:O	1:H:81:TRP:C	2.64	0.41
1:B:99:ARG:HA	1:B:99:ARG:HD2	1.92	0.40
1:D:60:VAL:O	1:D:60:VAL:HG13	2.21	0.40
1:G:30:ARG:NH2	1:H:58:PRO:CD	2.84	0.40
1:H:15:PHE:HB3	1:H:19:GLU:HB3	2.04	0.40
1:A:85:GLN:O	1:A:86:ARG:C	2.63	0.40
1:D:61:GLY:HA2	1:D:132:LEU:HB2	2.03	0.40
1:F:39:PRO:CG	1:F:40:GLU:N	2.84	0.40
1:G:61:GLY:O	1:G:62:PHE:C	2.65	0.40
2:G:508:FNR:H6	1:H:59:SER:O	2.21	0.40
1:H:60:VAL:HG22	1:H:133:GLY:HA3	2.01	0.40
1:H:63:MET:HG2	1:H:65:PRO:HB3	2.04	0.40
1:H:71:VAL:HG21	1:H:189:TRP:HH2	1.87	0.40
1:A:131:VAL:HG22	1:A:132:LEU:H	1.86	0.40
1:C:24:TYR:O	1:C:28:GLU:HB2	2.21	0.40
1:D:217:ASP:OD2	1:F:210:ARG:NH2	2.55	0.40
1:E:109:GLU:C	1:E:109:GLU:OE2	2.64	0.40
1:G:174:ILE:O	1:G:175:LYS:C	2.64	0.40
1:A:28:GLU:HG3	1:B:56:GLN:NE2	2.37	0.40
1:B:10:THR:O	1:B:11:ALA:HB3	2.21	0.40
1:E:117:SER:HA	1:E:190:LEU:O	2.21	0.40
1:E:150:GLN:HE21	1:E:154:LEU:HD13	1.83	0.40
1:G:89:ASP:O	1:G:90:GLU:C	2.63	0.40
1:C:131:VAL:CG2	1:C:132:LEU:N	2.84	0.40
1:C:134:ARG:HH11	1:C:141:ASP:CG	2.30	0.40
1:D:78:GLU:HG3	1:D:82:GLN:NE2	2.34	0.40
1:E:43:SER:HB2	1:E:45:GLU:OE2	2.22	0.40
1:E:145:THR:OG1	1:E:187:VAL:HG21	2.21	0.40
1:F:20:ARG:O	1:F:21:ALA:C	2.63	0.40
1:F:95:PHE:O	1:F:100:GLN:HG3	2.21	0.40
1:G:28:GLU:CG	1:H:56:GLN:HE22	2.30	0.40
1:G:180:ILE:HG22	1:G:184:VAL:O	2.22	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%)	201 (93%)	11 (5%)	5 (2%)	5	19
1	B	217/230 (94%)	196 (90%)	12 (6%)	9 (4%)	2	9
1	C	217/230 (94%)	200 (92%)	15 (7%)	2 (1%)	14	41
1	D	217/230 (94%)	190 (88%)	18 (8%)	9 (4%)	2	9
1	E	217/230 (94%)	182 (84%)	25 (12%)	10 (5%)	2	7
1	F	217/230 (94%)	178 (82%)	28 (13%)	11 (5%)	1	6
1	G	217/230 (94%)	180 (83%)	26 (12%)	11 (5%)	1	6
1	H	217/230 (94%)	184 (85%)	22 (10%)	11 (5%)	1	6
All	All	1736/1840 (94%)	1511 (87%)	157 (9%)	68 (4%)	2	10

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	137	ASN
1	B	12	ALA
1	B	86	ARG
1	B	133	GLY
1	D	11	ALA
1	D	12	ALA
1	D	14	ALA
1	D	181	PRO
1	E	16	SER
1	E	111	ILE
1	F	11	ALA
1	F	181	PRO
1	F	222	GLU
1	G	10	THR
1	G	181	PRO
1	G	222	GLU

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Mol	Chain	Res	Type
1	H	11	ALA
1	H	135	THR
1	A	104	ARG
1	A	135	THR
1	B	10	THR
1	B	131	VAL
1	D	97	GLY
1	D	133	GLY
1	E	39	PRO
1	E	74	ASP
1	E	132	LEU
1	E	169	PHE
1	F	14	ALA
1	F	39	PRO
1	F	93	GLU
1	F	97	GLY
1	F	131	VAL
1	G	90	GLU
1	G	93	GLU
1	G	169	PHE
1	H	14	ALA
1	H	171	GLU
1	H	181	PRO
1	B	13	GLY
1	C	104	ARG
1	E	92	ALA
1	G	39	PRO
1	G	92	ALA
1	G	97	GLY
1	H	110	GLY
1	B	11	ALA
1	B	97	GLY
1	D	104	ARG
1	D	109	GLU
1	H	40	GLU
1	A	181	PRO
1	C	133	GLY
1	D	124	ARG
1	E	140	MET
1	E	181	PRO
1	F	37	PHE
1	F	40	GLU

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Mol	Chain	Res	Type
1	H	39	PRO
1	H	222	GLU
1	B	207	LYS
1	E	98	GLU
1	G	37	PHE
1	H	19	GLU
1	F	110	GLY
1	H	225	GLY
1	G	202	PRO

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%)	164 (92%)	14 (8%)	11	34
1	B	178/187 (95%)	173 (97%)	5 (3%)	38	72
1	C	178/187 (95%)	162 (91%)	16 (9%)	9	28
1	D	178/187 (95%)	168 (94%)	10 (6%)	19	50
1	E	178/187 (95%)	169 (95%)	9 (5%)	21	53
1	F	178/187 (95%)	166 (93%)	12 (7%)	15	43
1	G	178/187 (95%)	168 (94%)	10 (6%)	19	50
1	H	178/187 (95%)	163 (92%)	15 (8%)	10	31
All	All	1424/1496 (95%)	1333 (94%)	91 (6%)	16	44

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	28	GLU
1	A	30	ARG
1	A	36	GLU
1	A	89	ASP
1	A	94	MET

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Mol	Chain	Res	Type
1	A	107	LYS
1	A	117	SER
1	A	132	LEU
1	A	137	ASN
1	A	154	LEU
1	A	169	PHE
1	A	182	ASP
1	A	197	ARG
1	B	30	ARG
1	B	117	SER
1	B	136	HIS
1	B	153	TRP
1	B	169	PHE
1	C	30	ARG
1	C	31	ARG
1	C	72	ARG
1	C	75	GLU
1	C	79	LYS
1	C	89	ASP
1	C	98	GLU
1	C	102	LYS
1	C	107	LYS
1	C	117	SER
1	C	132	LEU
1	C	150	GLN
1	C	154	LEU
1	C	169	PHE
1	C	187	VAL
1	C	196	ASP
1	D	9	LEU
1	D	30	ARG
1	D	35	ASP
1	D	36	GLU
1	D	72	ARG
1	D	76	THR
1	D	85	GLN
1	D	135	THR
1	D	211	GLN
1	D	216	GLU
1	E	30	ARG
1	E	35	ASP
1	E	67	ASN

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Mol	Chain	Res	Type
1	E	78	GLU
1	E	98	GLU
1	E	140	MET
1	E	185	GLU
1	E	202	PRO
1	E	211	GLN
1	F	9	LEU
1	F	10	THR
1	F	30	ARG
1	F	31	ARG
1	F	73	GLN
1	F	81	TRP
1	F	154	LEU
1	F	169	PHE
1	F	175	LYS
1	F	182	ASP
1	F	197	ARG
1	F	211	GLN
1	G	46	LEU
1	G	67	ASN
1	G	70	LEU
1	G	99	ARG
1	G	140	MET
1	G	154	LEU
1	G	169	PHE
1	G	181	PRO
1	G	202	PRO
1	G	211	GLN
1	H	9	LEU
1	H	10	THR
1	H	20	ARG
1	H	56	GLN
1	H	60	VAL
1	H	81	TRP
1	H	82	GLN
1	H	99	ARG
1	H	104	ARG
1	H	109	GLU
1	H	112	ARG
1	H	135	THR
1	H	154	LEU
1	H	170	HIS

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Mol	Chain	Res	Type
1	H	204	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	64	GLN
1	A	73	GLN
1	A	100	GLN
1	A	139	GLN
1	A	150	GLN
1	A	211	GLN
1	B	56	GLN
1	B	64	GLN
1	B	73	GLN
1	B	82	GLN
1	B	100	GLN
1	B	137	ASN
1	B	139	GLN
1	B	200	GLN
1	C	64	GLN
1	C	100	GLN
1	C	137	ASN
1	C	139	GLN
1	D	56	GLN
1	D	82	GLN
1	D	139	GLN
1	E	64	GLN
1	E	67	ASN
1	E	73	GLN
1	E	82	GLN
1	E	85	GLN
1	E	100	GLN
1	E	150	GLN
1	E	151	ASN
1	E	170	HIS
1	E	200	GLN
1	E	211	GLN
1	F	64	GLN
1	F	73	GLN
1	F	100	GLN
1	F	139	GLN

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Mol	Chain	Res	Type
1	F	151	ASN
1	F	170	HIS
1	F	211	GLN
1	G	64	GLN
1	G	67	ASN
1	G	73	GLN
1	G	82	GLN
1	G	139	GLN
1	G	150	GLN
1	G	170	HIS
1	H	56	GLN
1	H	64	GLN
1	H	85	GLN
1	H	151	ASN
1	H	183	HIS
1	H	211	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](#)

16 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	B	501	-	32,33,33	1.74	7 (21%)	41,50,50	1.10	2 (4%)
2	FNR	F	505	-	32,33,33	1.78	7 (21%)	41,50,50	0.99	2 (4%)
3	OXY	D	601	-	1,1,1	1.04	0	-		
2	FNR	E	506	-	32,33,33	1.72	7 (21%)	41,50,50	0.93	2 (4%)
3	OXY	F	608	-	1,1,1	1.18	0	-		
3	OXY	G	603	-	1,1,1	1.11	0	-		
3	OXY	H	604	-	1,1,1	1.12	0	-		
3	OXY	A	606	-	1,1,1	1.17	0	-		
2	FNR	D	503	-	32,33,33	1.85	8 (25%)	41,50,50	1.01	1 (2%)
2	FNR	A	502	-	32,33,33	1.76	7 (21%)	41,50,50	1.09	2 (4%)
3	OXY	B	602	-	1,1,1	1.09	0	-		
2	FNR	C	504	-	32,33,33	1.80	8 (25%)	41,50,50	1.08	2 (4%)
3	OXY	E	607	-	1,1,1	1.16	0	-		
2	FNR	G	508	-	32,33,33	1.66	6 (18%)	41,50,50	1.10	2 (4%)
3	OXY	C	605	-	1,1,1	1.17	0	-		
2	FNR	H	507	-	32,33,33	1.78	9 (28%)	41,50,50	0.98	2 (4%)

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	B	501	-	-	5/18/18/18	0/3/3/3
2	FNR	F	505	-	-	3/18/18/18	0/3/3/3
2	FNR	E	506	-	-	1/18/18/18	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	-	-	6/18/18/18	0/3/3/3
2	FNR	G	508	-	-	7/18/18/18	0/3/3/3
2	FNR	H	507	-	-	5/18/18/18	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	FNR	C2-N3	4.61	1.45	1.37
2	D	503	FNR	C5A-C9A	4.47	1.45	1.40
2	F	505	FNR	C2-N3	4.42	1.44	1.37
2	D	503	FNR	C2-N3	4.22	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FNR	C2-N3	4.14	1.44	1.37
2	F	505	FNR	C5A-C9A	4.07	1.45	1.40
2	E	506	FNR	C2-N3	4.05	1.44	1.37
2	G	508	FNR	C2-N3	4.02	1.44	1.37
2	C	504	FNR	C2-N3	4.00	1.44	1.37
2	H	507	FNR	C5A-C9A	3.99	1.45	1.40
2	H	507	FNR	C2-N3	3.99	1.44	1.37
2	C	504	FNR	C5A-C9A	3.96	1.44	1.40
2	E	506	FNR	C5A-C9A	3.90	1.44	1.40
2	F	505	FNR	C6-C5A	3.85	1.45	1.39
2	B	501	FNR	C6-C5A	3.80	1.45	1.39
2	D	503	FNR	C6-C5A	3.75	1.45	1.39
2	G	508	FNR	C6-C5A	3.74	1.45	1.39
2	A	502	FNR	C5A-C9A	3.68	1.44	1.40
2	G	508	FNR	C5A-C9A	3.67	1.44	1.40
2	G	508	FNR	C4A-C4	3.64	1.52	1.41
2	B	501	FNR	C4A-C4	3.58	1.52	1.41
2	H	507	FNR	C6-C5A	3.56	1.45	1.39
2	F	505	FNR	C4A-C4	3.52	1.52	1.41
2	H	507	FNR	C4A-C4	3.47	1.52	1.41
2	E	506	FNR	C6-C5A	3.46	1.45	1.39
2	C	504	FNR	C5'-C4'	3.42	1.56	1.51
2	C	504	FNR	C6-C5A	3.42	1.44	1.39
2	C	504	FNR	C4A-C4	3.34	1.51	1.41
2	E	506	FNR	C4A-C4	3.26	1.51	1.41
2	D	503	FNR	C4A-C4	3.22	1.51	1.41
2	B	501	FNR	C5A-C9A	3.15	1.44	1.40
2	A	502	FNR	C4A-C4	3.05	1.51	1.41
2	A	502	FNR	C6-C5A	2.96	1.44	1.39
2	C	504	FNR	P-O1P	-2.95	1.43	1.54
2	A	502	FNR	P-O1P	-2.93	1.43	1.54
2	A	502	FNR	C5'-C4'	2.91	1.55	1.51
2	H	507	FNR	P-O1P	-2.71	1.44	1.54
2	D	503	FNR	P-O1P	-2.63	1.45	1.54
2	D	503	FNR	CAA-N10	2.54	1.42	1.38
2	B	501	FNR	C2'-C3'	-2.52	1.49	1.53
2	E	506	FNR	P-O1P	-2.50	1.45	1.54
2	G	508	FNR	P-O1P	-2.50	1.45	1.54
2	H	507	FNR	C9-C9A	2.49	1.43	1.39
2	H	507	FNR	C5'-C4'	2.46	1.55	1.51
2	B	501	FNR	C9-C9A	2.41	1.43	1.39
2	F	505	FNR	C9-C9A	2.38	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	FNR	C9-C9A	2.37	1.43	1.39
2	G	508	FNR	C9-C9A	2.34	1.43	1.39
2	F	505	FNR	P-O1P	-2.34	1.46	1.54
2	C	504	FNR	C9-C9A	2.29	1.43	1.39
2	D	503	FNR	C2'-C3'	-2.28	1.49	1.53
2	B	501	FNR	P-O1P	-2.27	1.46	1.54
2	E	506	FNR	C9-C9A	2.19	1.43	1.39
2	D	503	FNR	C9-C9A	2.18	1.43	1.39
2	F	505	FNR	C8-C7	2.17	1.46	1.40
2	C	504	FNR	CAA-N10	2.09	1.42	1.38
2	E	506	FNR	C8-C7	2.08	1.45	1.40
2	H	507	FNR	CAA-N10	2.07	1.42	1.38
2	H	507	FNR	C8-C7	2.03	1.45	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	504	FNR	O3P-P-O5'	3.04	114.59	106.67
2	A	502	FNR	O3P-P-O5'	2.85	114.10	106.67
2	F	505	FNR	O3P-P-O5'	2.47	113.10	106.67
2	G	508	FNR	O3P-P-O5'	2.44	113.03	106.67
2	A	502	FNR	C9A-C5A-N5	2.41	122.30	119.37
2	C	504	FNR	C9A-C5A-N5	2.35	122.23	119.37
2	B	501	FNR	O3P-P-O5'	2.34	112.78	106.67
2	D	503	FNR	C9A-C5A-N5	2.24	122.10	119.37
2	H	507	FNR	C9A-C5A-N5	2.22	122.08	119.37
2	B	501	FNR	C9A-C5A-N5	2.12	121.96	119.37
2	H	507	FNR	O3P-P-O5'	2.11	112.17	106.67
2	G	508	FNR	C9A-C5A-N5	2.10	121.93	119.37
2	E	506	FNR	C9A-C5A-N5	2.10	121.92	119.37
2	F	505	FNR	C9A-C5A-N5	2.07	121.89	119.37
2	E	506	FNR	O3P-P-O5'	2.04	112.00	106.67

There are no chirality outliers.

All (35) 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	A	502	FNR	C5'-O5'-P-O1P
2	A	502	FNR	C5'-O5'-P-O2P
2	A	502	FNR	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
2	B	501	FNR	C3'-C4'-C5'-O5'
2	B	501	FNR	O4'-C4'-C5'-O5'
2	B	501	FNR	C5'-O5'-P-O1P
2	B	501	FNR	C5'-O5'-P-O2P
2	B	501	FNR	C5'-O5'-P-O3P
2	C	504	FNR	C3'-C4'-C5'-O5'
2	C	504	FNR	O4'-C4'-C5'-O5'
2	C	504	FNR	C5'-O5'-P-O1P
2	C	504	FNR	C5'-O5'-P-O2P
2	C	504	FNR	C5'-O5'-P-O3P
2	F	505	FNR	C5'-O5'-P-O1P
2	F	505	FNR	C5'-O5'-P-O3P
2	G	508	FNR	C2'-C3'-C4'-O4'
2	G	508	FNR	C2'-C3'-C4'-C5'
2	G	508	FNR	O3'-C3'-C4'-O4'
2	G	508	FNR	O3'-C3'-C4'-C5'
2	G	508	FNR	C5'-O5'-P-O1P
2	H	507	FNR	C3'-C4'-C5'-O5'
2	H	507	FNR	C5'-O5'-P-O1P
2	H	507	FNR	C5'-O5'-P-O2P
2	H	507	FNR	C5'-O5'-P-O3P
2	F	505	FNR	C5'-O5'-P-O2P
2	H	507	FNR	O4'-C4'-C5'-O5'
2	G	508	FNR	C5'-O5'-P-O3P
2	G	508	FNR	C5'-O5'-P-O2P
2	A	502	FNR	O2'-C2'-C3'-C4'
2	A	502	FNR	C4'-C5'-O5'-P
2	C	504	FNR	C4'-C5'-O5'-P
2	A	502	FNR	O2'-C2'-C3'-O3'
2	E	506	FNR	C4'-C5'-O5'-P

There are no ring outliers.

11 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FNR	6	0
2	F	505	FNR	4	0
3	D	601	OXY	1	0
2	E	506	FNR	5	0
3	G	603	OXY	2	0
3	A	606	OXY	2	0
2	D	503	FNR	6	0

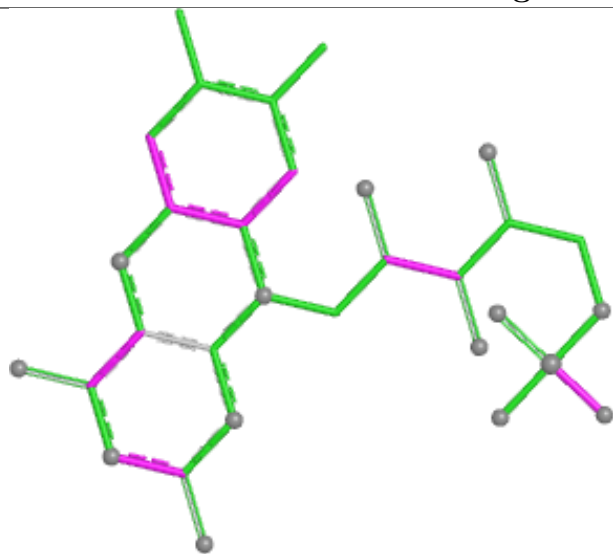
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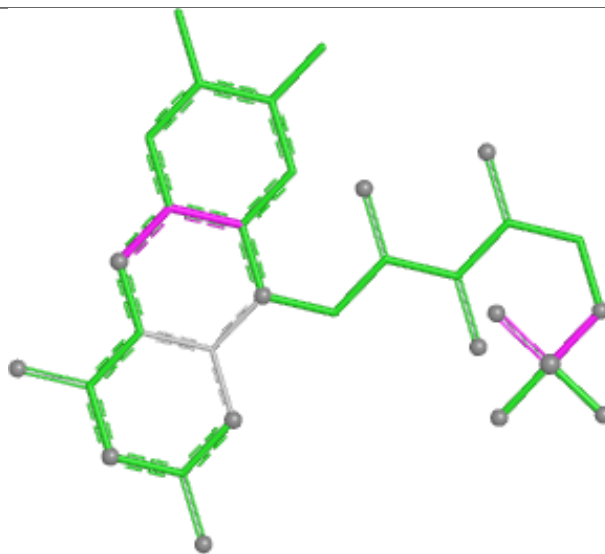
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	FNR	5	0
2	C	504	FNR	5	0
2	G	508	FNR	4	0
2	H	507	FNR	5	0

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.

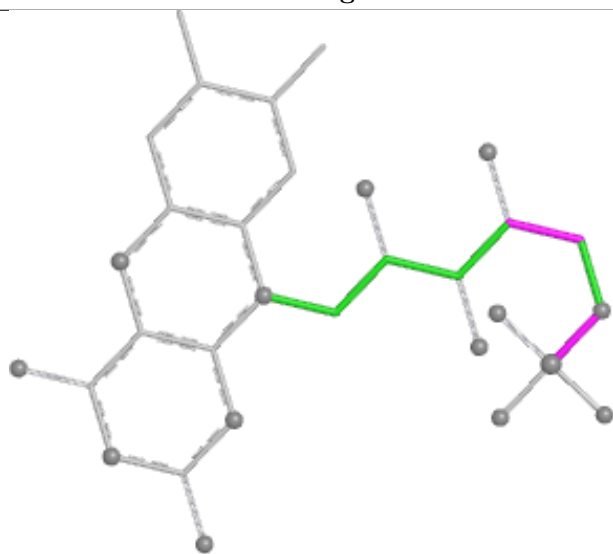
Ligand FNR B 501



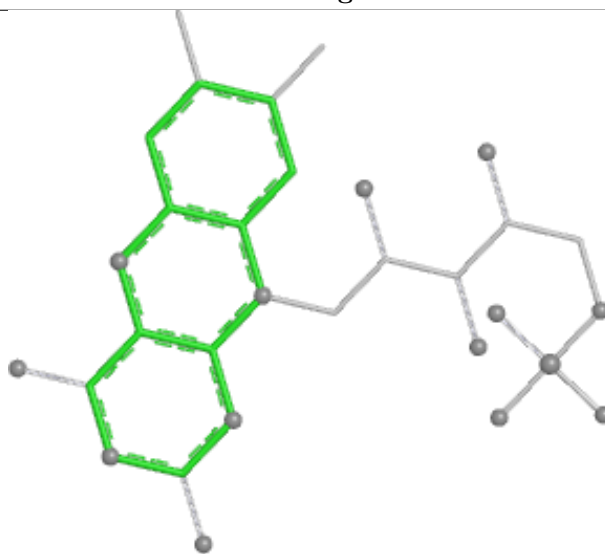
Bond lengths



Bond angles

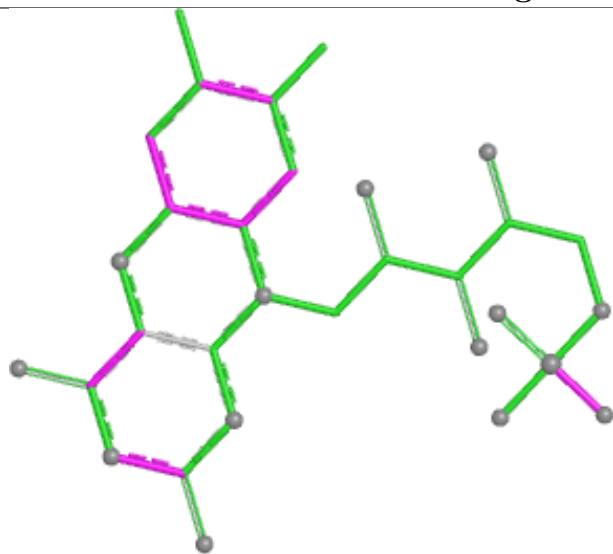


Torsions

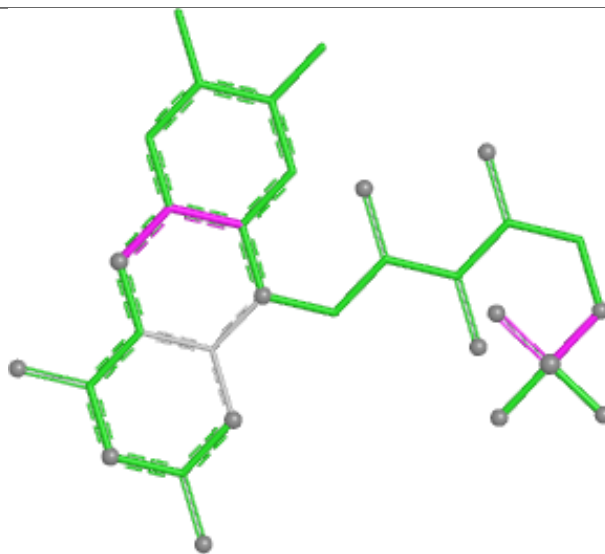


Rings

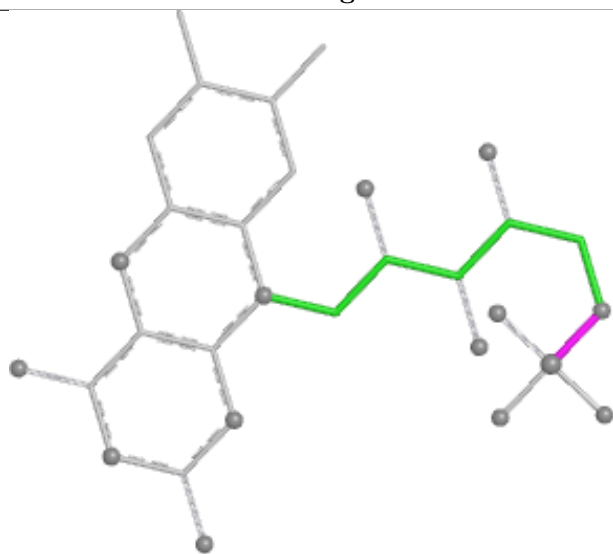
Ligand FNR F 505



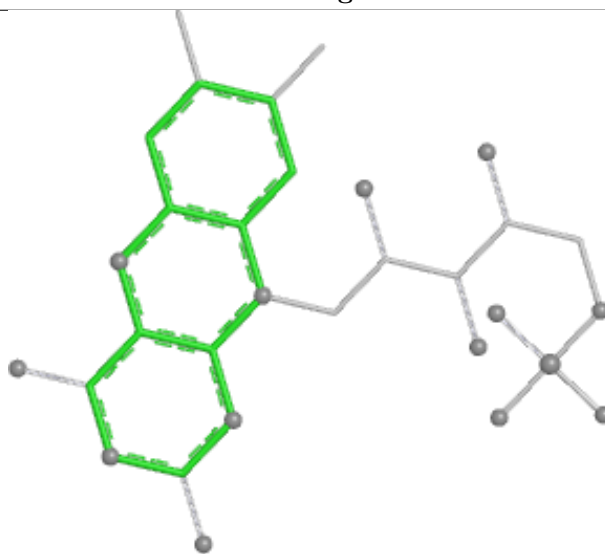
Bond lengths



Bond angles

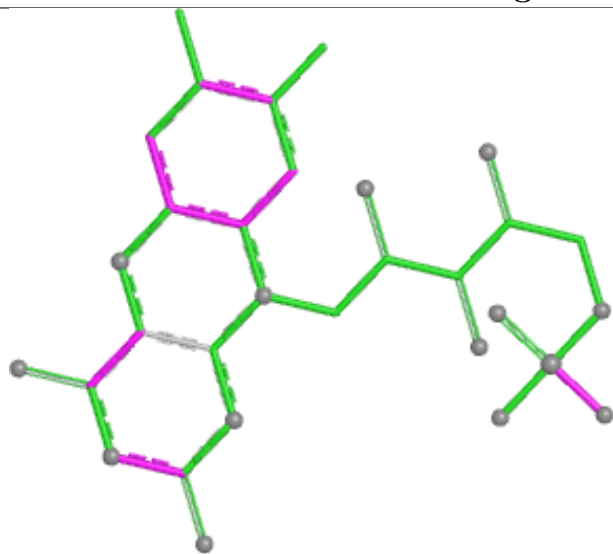


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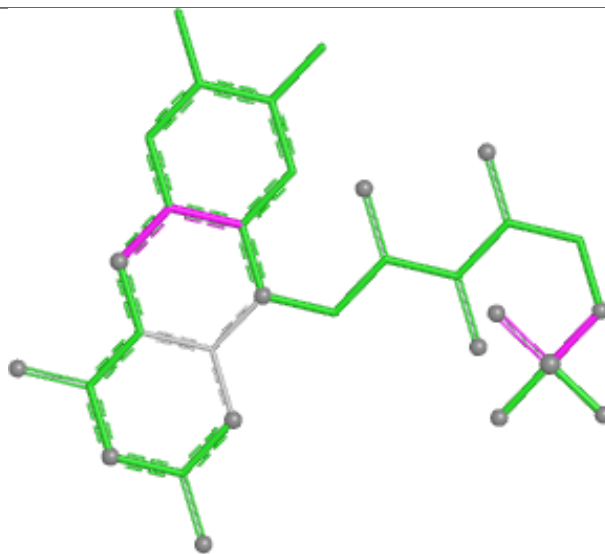


Rings

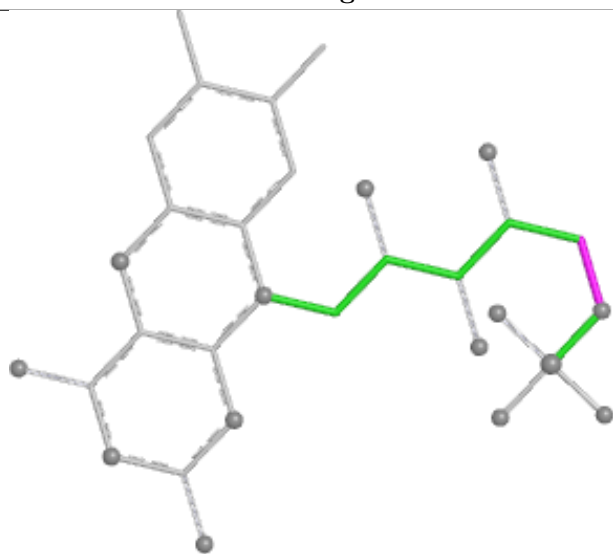
Ligand FNR E 506



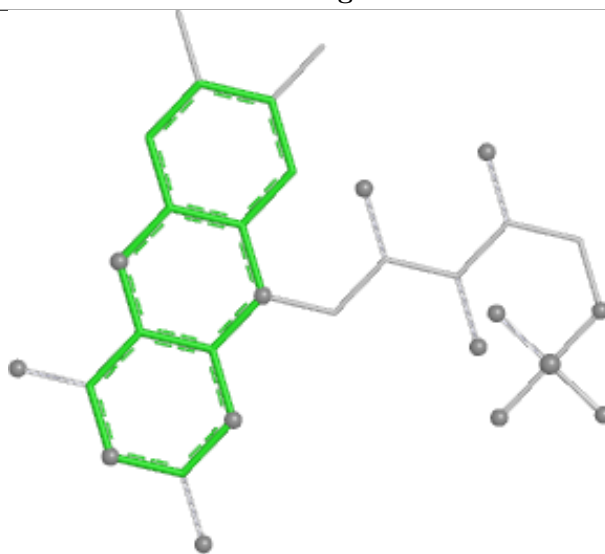
Bond lengths



Bond angles

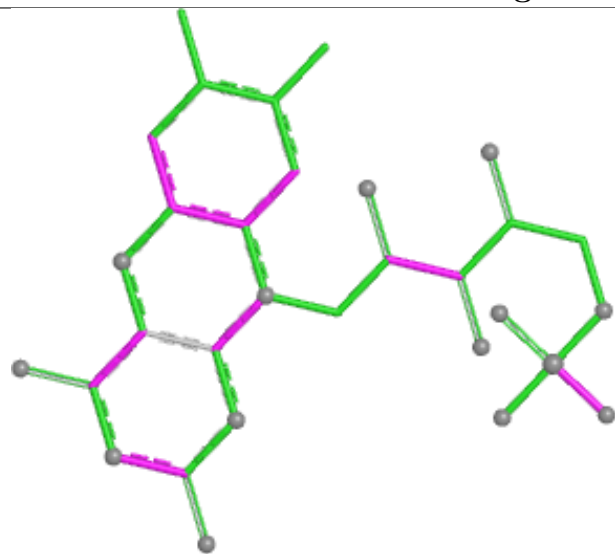


Torsions

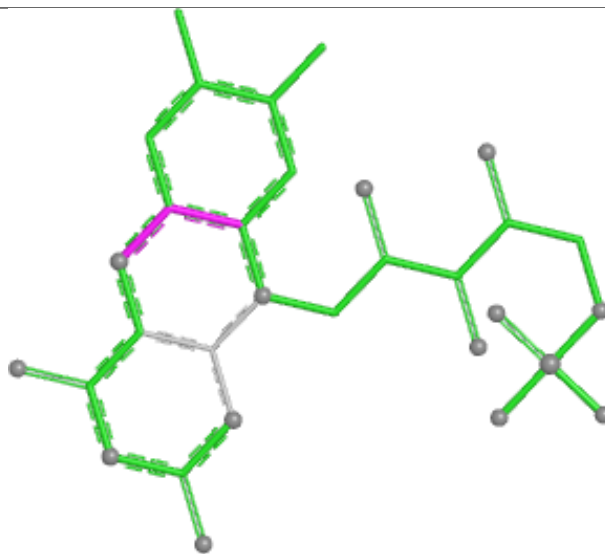


Rings

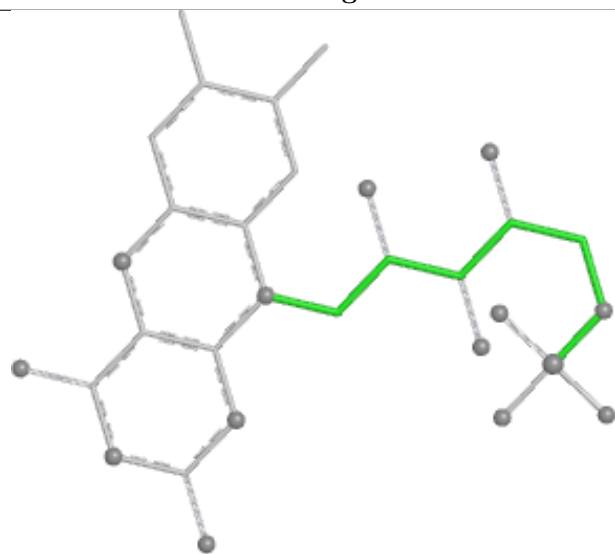
Ligand FNR D 503



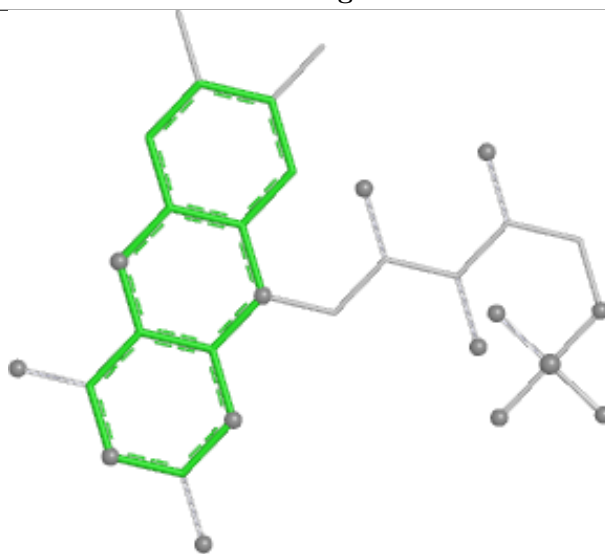
Bond lengths



Bond angles

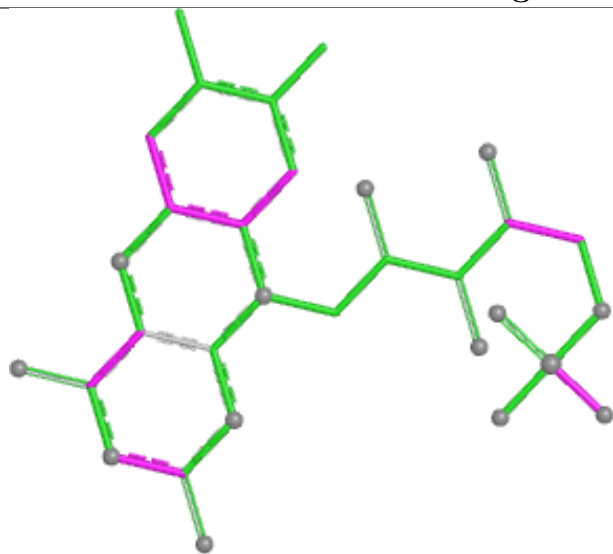


Torsions

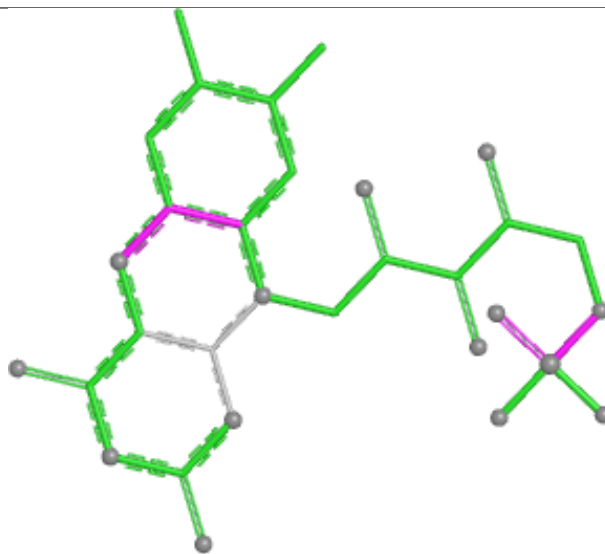


Rings

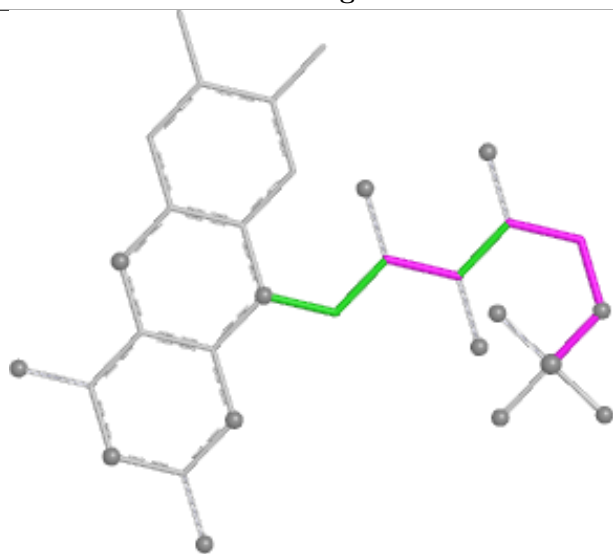
Ligand FNR A 502



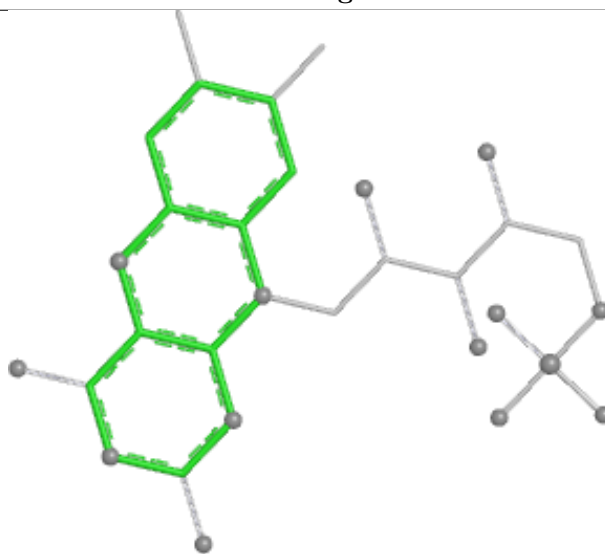
Bond lengths



Bond angles

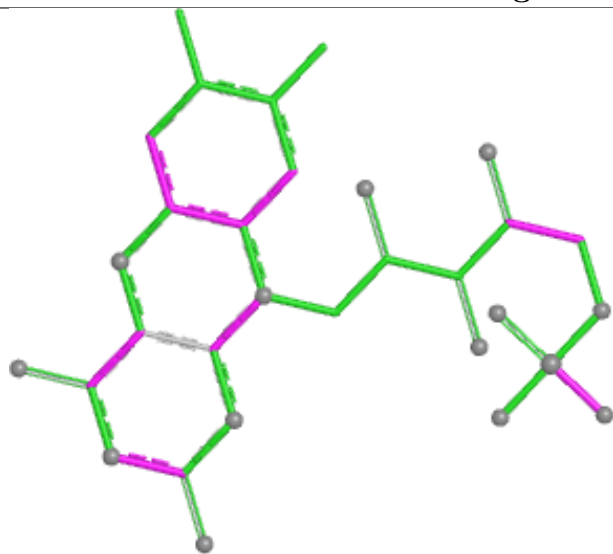


Torsions

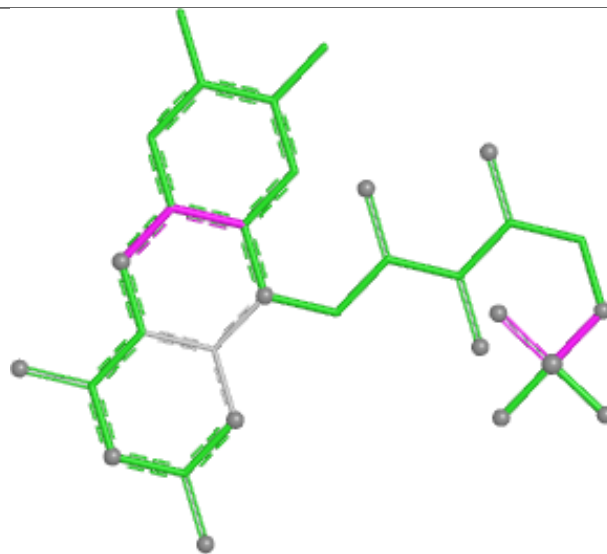


Rings

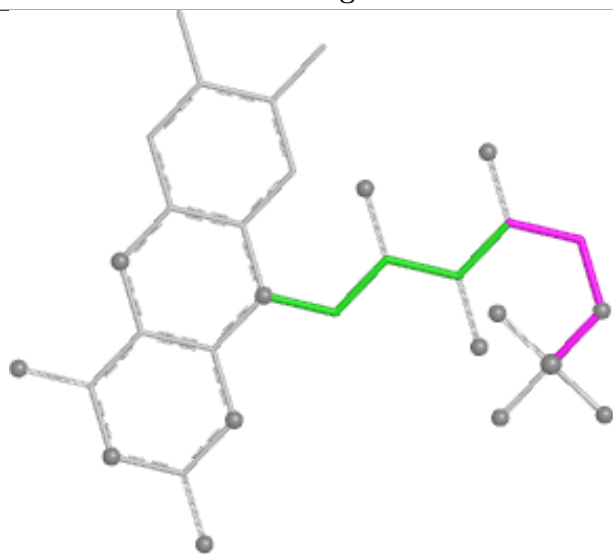
Ligand FNR C 504



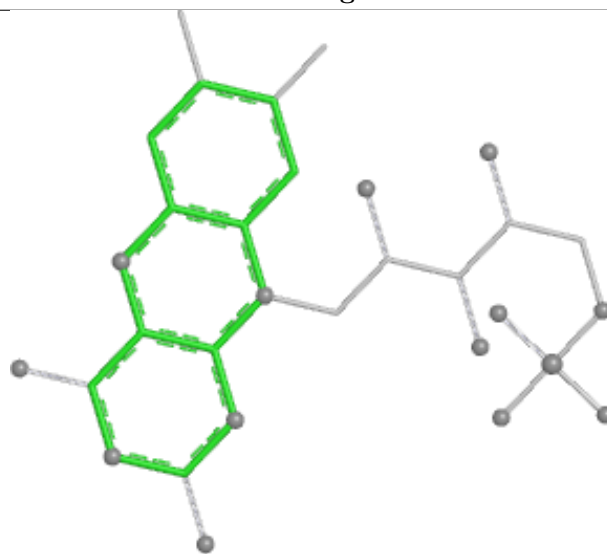
Bond lengths



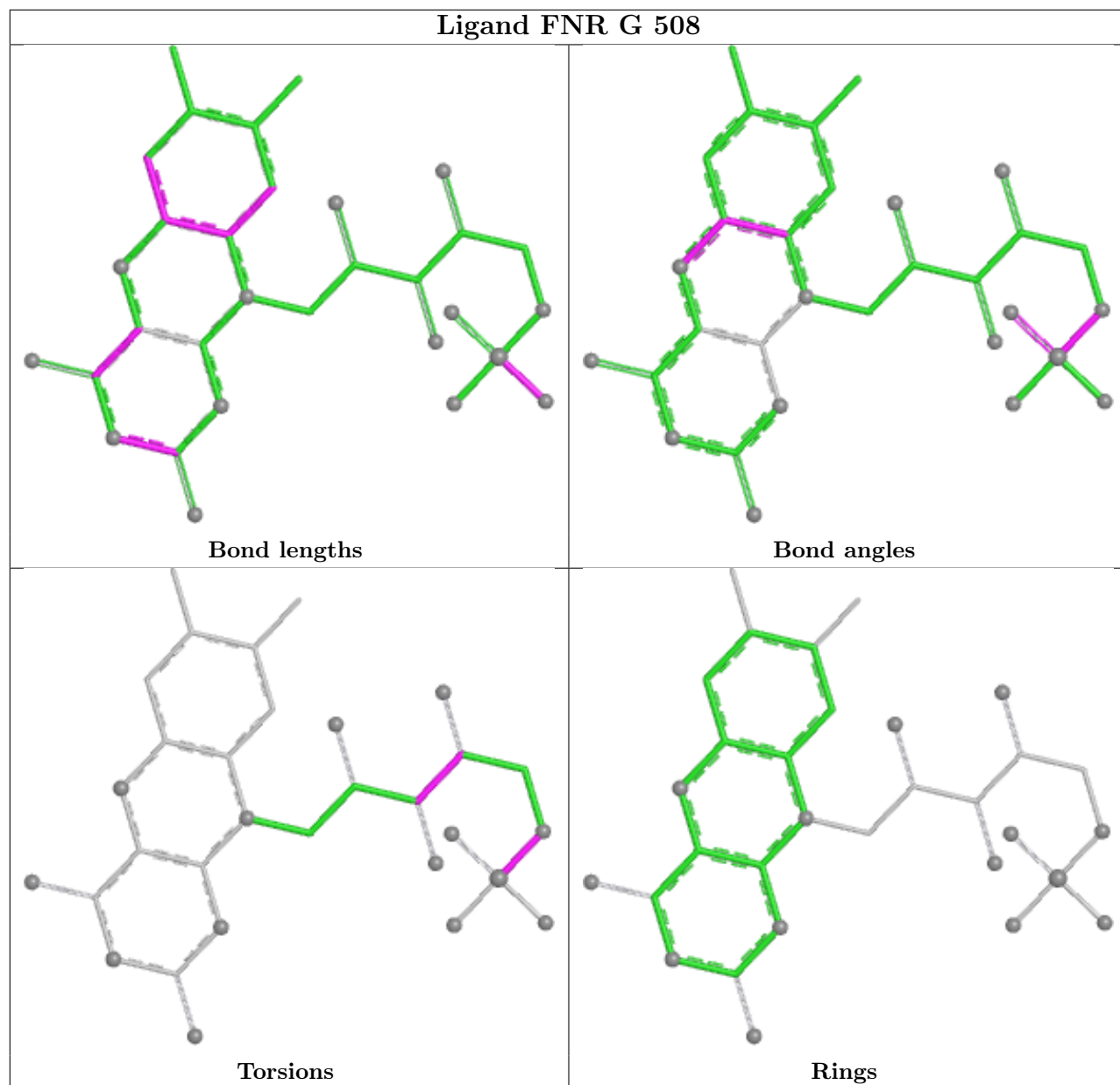
Bond angles

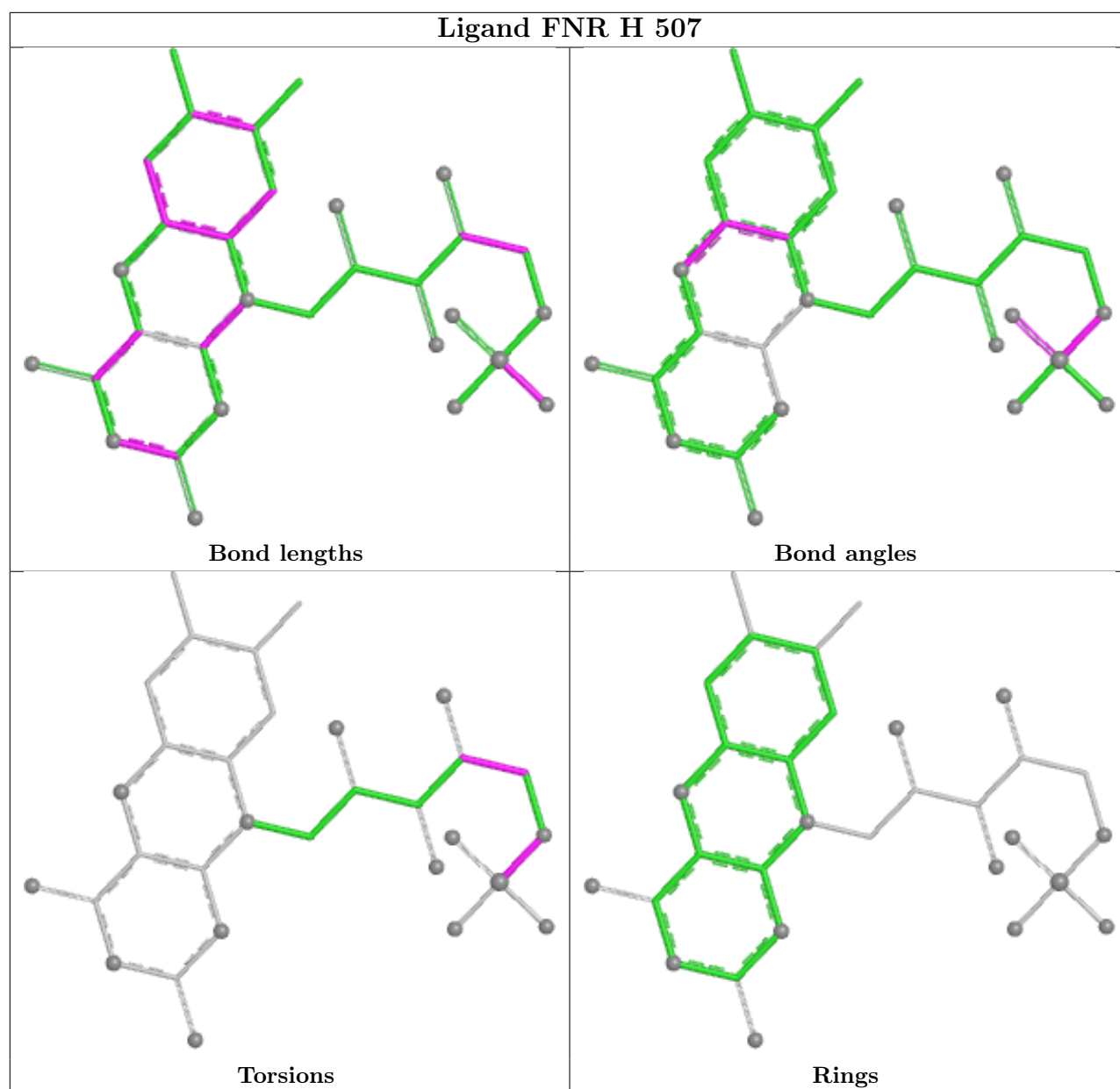


Torsions



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%)	-1.67	0 100 100	5, 19, 49, 71	0
1	B	219/230 (95%)	-1.63	0 100 100	7, 23, 50, 75	0
1	C	219/230 (95%)	-1.64	0 100 100	6, 18, 48, 67	0
1	D	219/230 (95%)	-1.61	0 100 100	6, 22, 50, 78	0
1	E	219/230 (95%)	-1.41	0 100 100	22, 50, 83, 88	0
1	F	219/230 (95%)	-1.39	0 100 100	23, 47, 76, 88	0
1	G	219/230 (95%)	-1.36	0 100 100	19, 48, 83, 89	0
1	H	219/230 (95%)	-1.38	0 100 100	21, 48, 79, 89	0
All	All	1752/1840 (95%)	-1.51	0 100 100	5, 32, 77, 89	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](#)

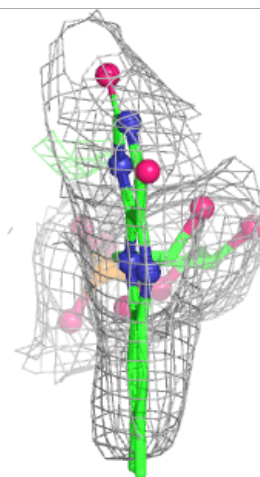
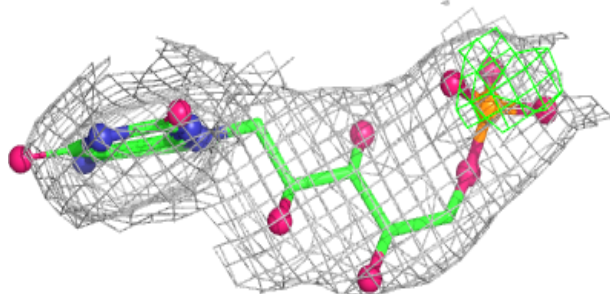
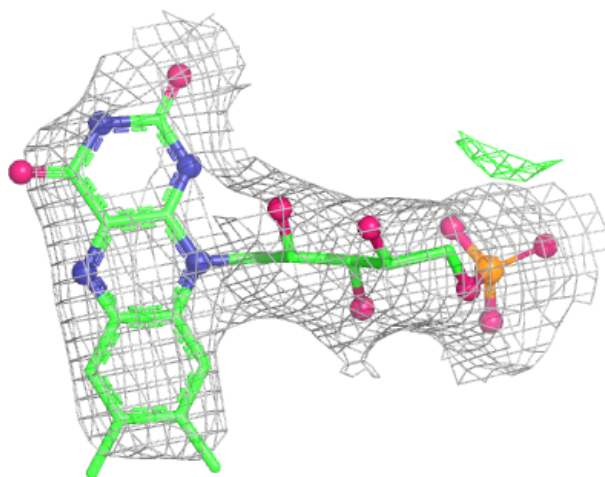
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
3	OXY	F	608	2/2	0.97	0.06	33,33,33,35	0
3	OXY	H	604	2/2	0.98	0.09	32,32,32,32	0
2	FNR	E	506	31/31	0.99	0.04	44,50,52,54	0
2	FNR	F	505	31/31	0.99	0.03	37,44,47,50	0
2	FNR	G	508	31/31	0.99	0.04	38,45,49,50	0
3	OXY	A	606	2/2	0.99	0.07	21,21,21,22	0
3	OXY	C	605	2/2	0.99	0.09	18,18,18,19	0
3	OXY	E	607	2/2	0.99	0.05	25,25,25,26	0
2	FNR	A	502	31/31	0.99	0.03	18,25,29,30	0
2	FNR	D	503	31/31	0.99	0.03	20,24,26,28	0
2	FNR	C	504	31/31	1.00	0.03	23,28,30,30	0
3	OXY	D	601	2/2	1.00	0.03	10,10,10,11	0
2	FNR	H	507	31/31	1.00	0.03	34,39,41,43	0
2	FNR	B	501	31/31	1.00	0.03	23,28,31,31	0
3	OXY	G	603	2/2	1.00	0.03	27,27,27,27	0
3	OXY	B	602	2/2	1.00	0.03	8,8,8,9	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.

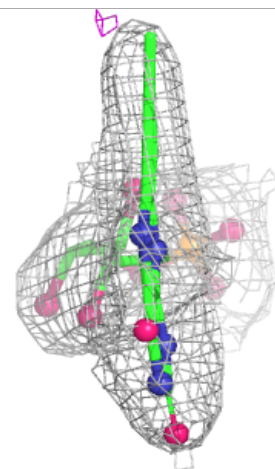
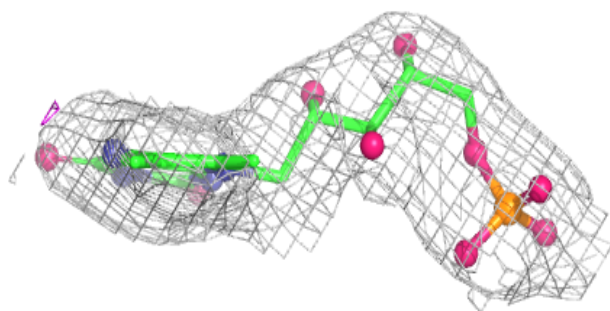
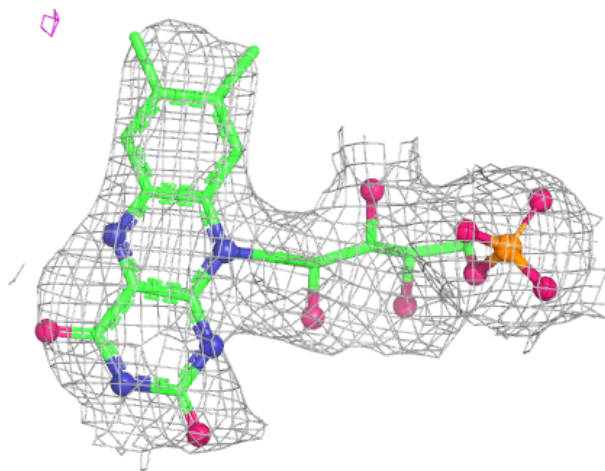
Electron density around FNR E 506:

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



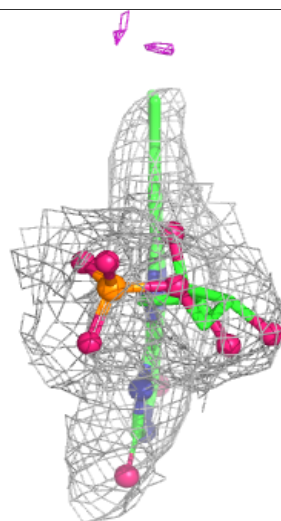
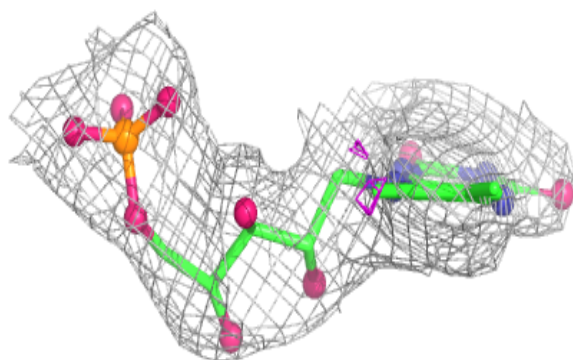
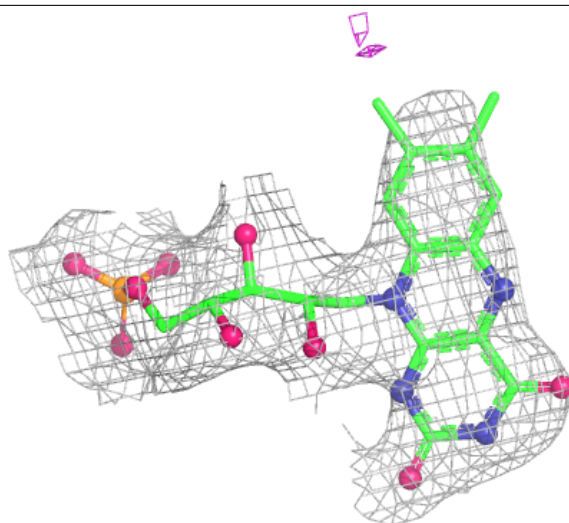
Electron density around FNR F 505:

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



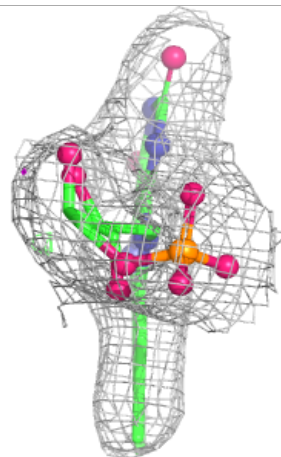
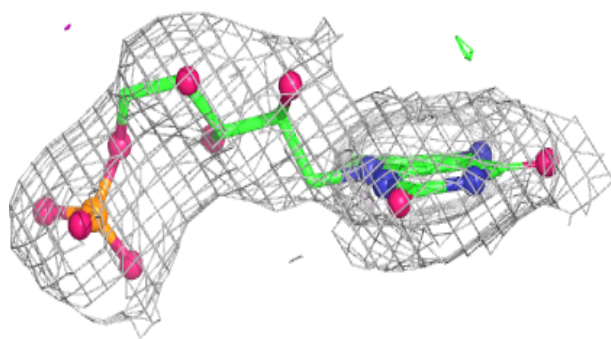
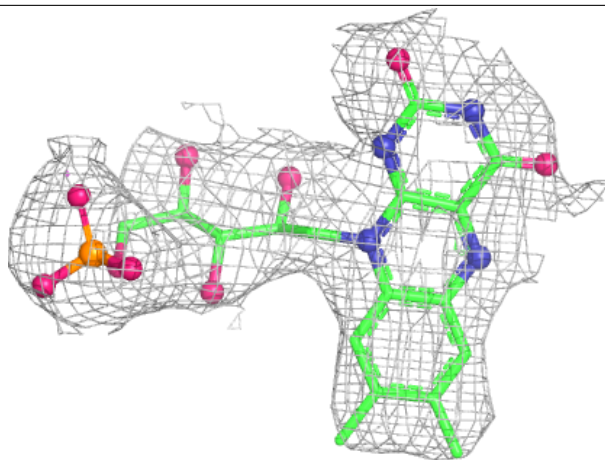
Electron density around FNR G 508:

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



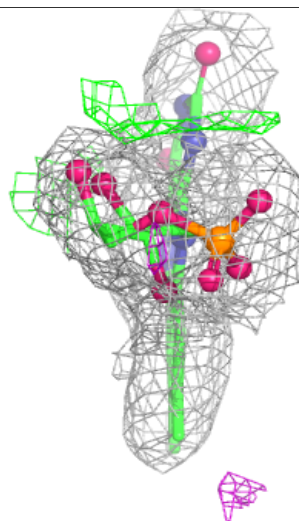
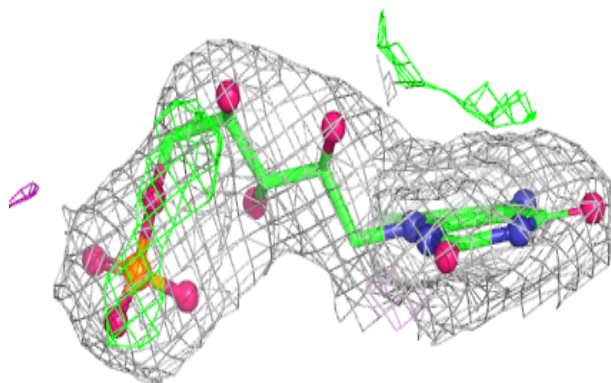
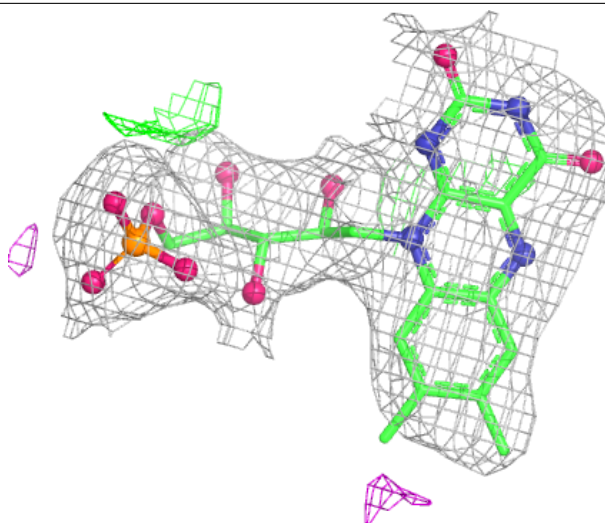
Electron density around FNR A 502:

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



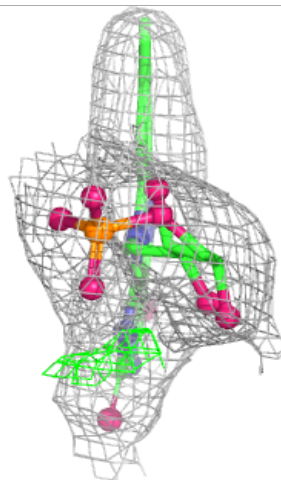
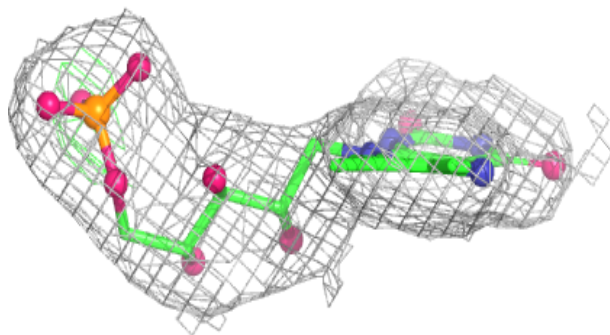
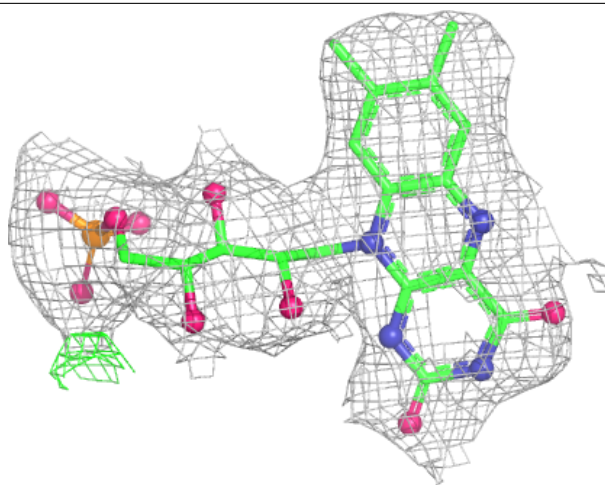
Electron density around FNR D 503:

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



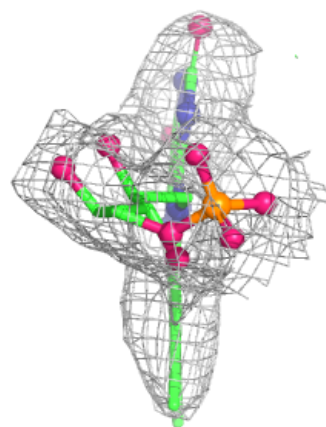
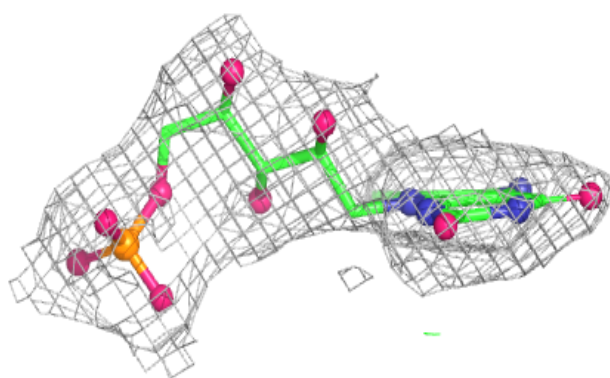
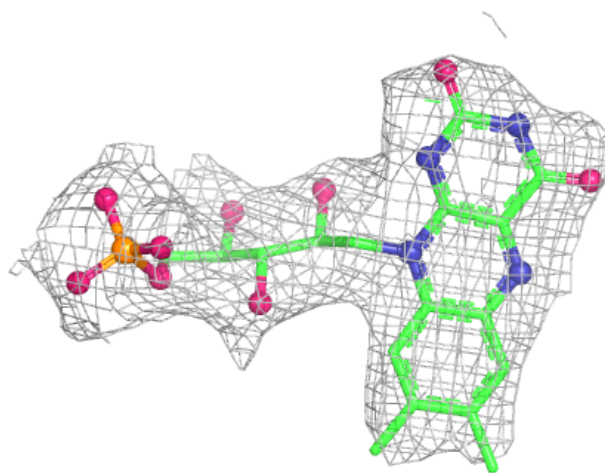
Electron density around FNR C 504:

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



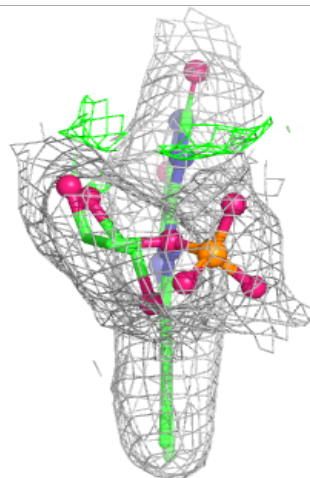
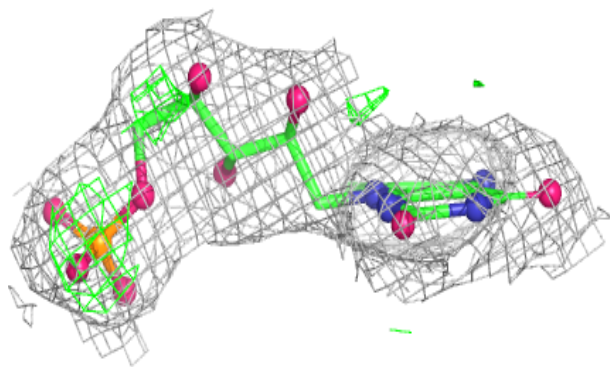
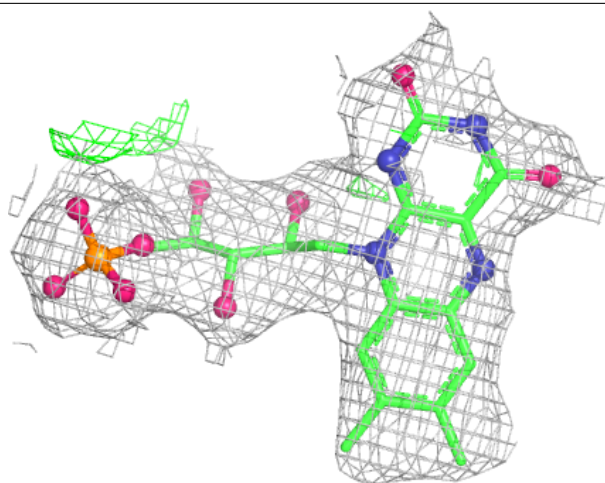
Electron density around FNR H 507:

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



Electron density around FNR 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.