Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2024 – 04:13 PM JST

PDB ID	:	5EJD
Title	:	The crystal structure of holo T3CT
Authors	:	Zhang, J.R.; Tang, Y.; Zhou, J.H.
Deposited on	:	2015-11-01
Resolution	:	2.49 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:

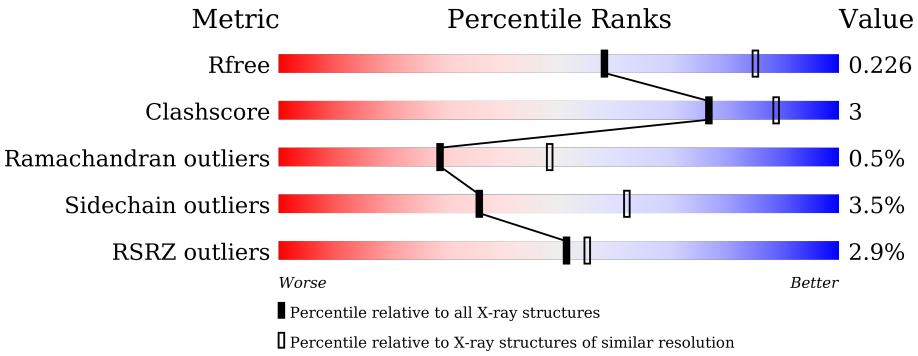
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	B	477	82% 8% • 9%
1	D	477	84% 6% • 8%
1	F	477	84% 6% • 9%
1	H	477	4% 84% 5% • 9%
1	J	477	3% 83% 7% • 9%
1	L	477	5% 82% 6% • 9%

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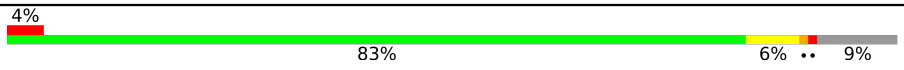
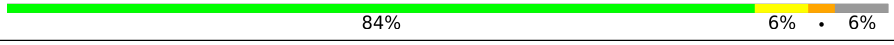
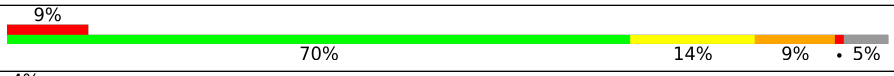
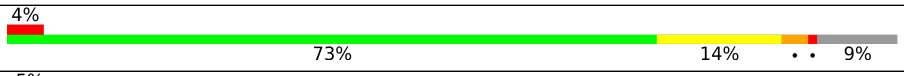
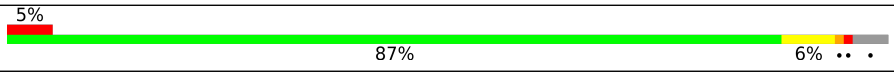
Mol	Chain	Length	Quality of chain
1	N	477	
1	P	477	
2	A	77	
2	C	77	
2	E	77	
2	G	77	
2	I	77	
2	K	77	
2	M	77	
2	O	77	

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	GOL	P	501	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 33064 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 TqaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	436	Total	C	N	O	S	0	0	0
			3486	2227	601	645	13			
1	D	437	Total	C	N	O	S	0	0	0
			3493	2232	602	646	13			
1	F	435	Total	C	N	O	S	0	0	0
			3478	2223	600	642	13			
1	H	435	Total	C	N	O	S	0	0	0
			3478	2223	600	642	13			
1	J	436	Total	C	N	O	S	0	0	0
			3486	2227	601	645	13			
1	L	435	Total	C	N	O	S	0	0	0
			3478	2223	600	642	13			
1	N	435	Total	C	N	O	S	0	0	0
			3478	2223	600	642	13			
1	P	436	Total	C	N	O	S	0	0	0
			3486	2227	601	645	13			

- Molecule 2 is a protein called TqaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	75	Total	C	N	O	S	0	0	0
			554	351	94	107	2			
2	C	74	Total	C	N	O	S	0	0	0
			547	346	93	106	2			
2	E	72	Total	C	N	O	S	0	0	0
			533	337	90	104	2			
2	G	75	Total	C	N	O	S	0	0	0
			554	351	94	107	2			
2	I	72	Total	C	N	O	S	0	0	0
			533	337	90	104	2			
2	K	73	Total	C	N	O	S	0	0	0
			536	340	90	104	2			

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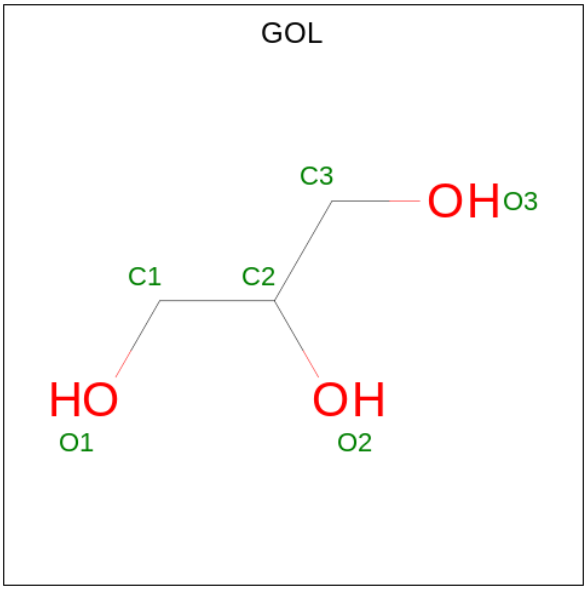
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	70	Total	C	N	O	S	0	0	0
			517	327	87	101	2			
2	O	74	Total	C	N	O	S	0	0	0
			545	345	92	106	2			

There are 8 discrepancies between the modelled and reference sequences:

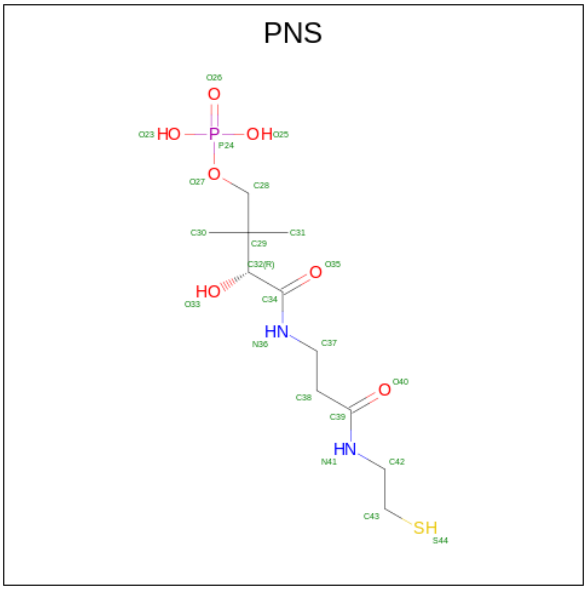
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP F1CWE4
C	1	MET	-	initiating methionine	UNP F1CWE4
E	1	MET	-	initiating methionine	UNP F1CWE4
G	1	MET	-	initiating methionine	UNP F1CWE4
I	1	MET	-	initiating methionine	UNP F1CWE4
K	1	MET	-	initiating methionine	UNP F1CWE4
M	1	MET	-	initiating methionine	UNP F1CWE4
O	1	MET	-	initiating methionine	UNP F1CWE4

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O		0	0
			6	3	3			
3	D	1	Total	C	O		0	0
			6	3	3			
3	P	1	Total	C	O		0	0
			6	3	3			

- Molecule 4 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	C	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	E	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	G	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	I	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	K	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	M	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	O	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	112	Total	O	0	0
			112	112		
5	A	15	Total	O	0	0
			15	15		
5	D	118	Total	O	0	0
			118	118		

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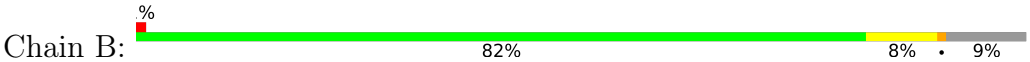
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	8	Total O 8 8	0	0
5	F	73	Total O 73 73	0	0
5	E	6	Total O 6 6	0	0
5	H	69	Total O 69 69	0	0
5	G	6	Total O 6 6	0	0
5	J	70	Total O 70 70	0	0
5	I	12	Total O 12 12	0	0
5	L	63	Total O 63 63	0	0
5	K	2	Total O 2 2	0	0
5	N	55	Total O 55 55	0	0
5	M	5	Total O 5 5	0	0
5	P	76	Total O 76 76	0	0
5	O	6	Total O 6 6	0	0

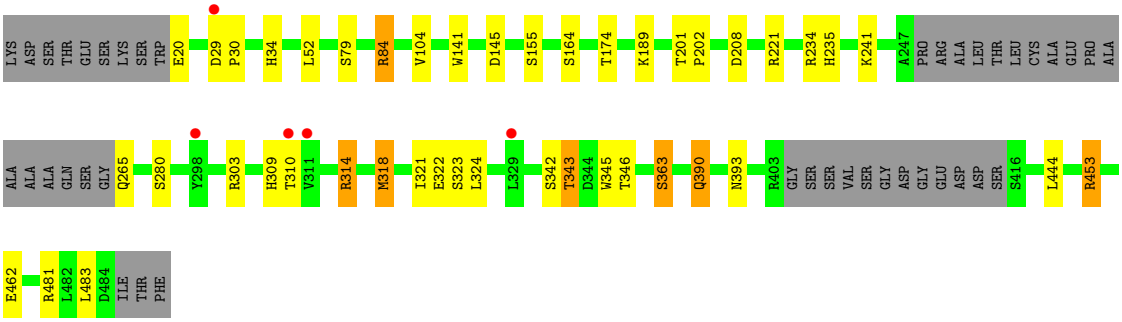
3 Residue-property plots (i)

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: TqaA

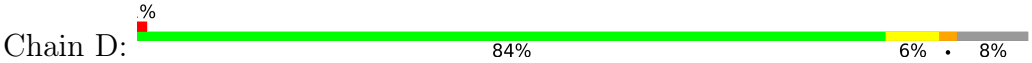
Chain B:

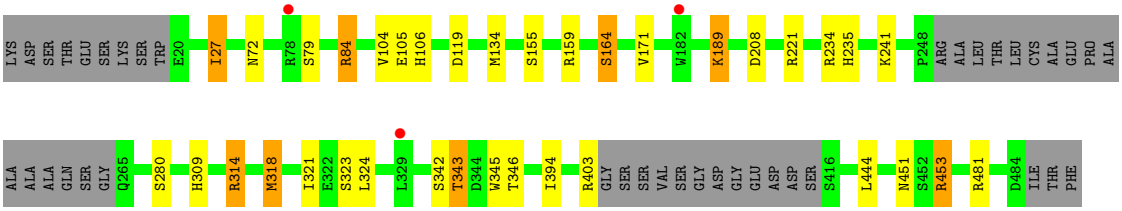




• Molecule 1: TqaA

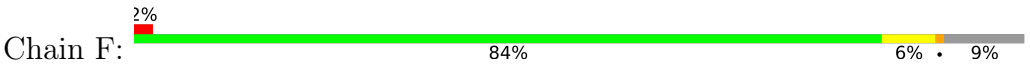
Chain D:

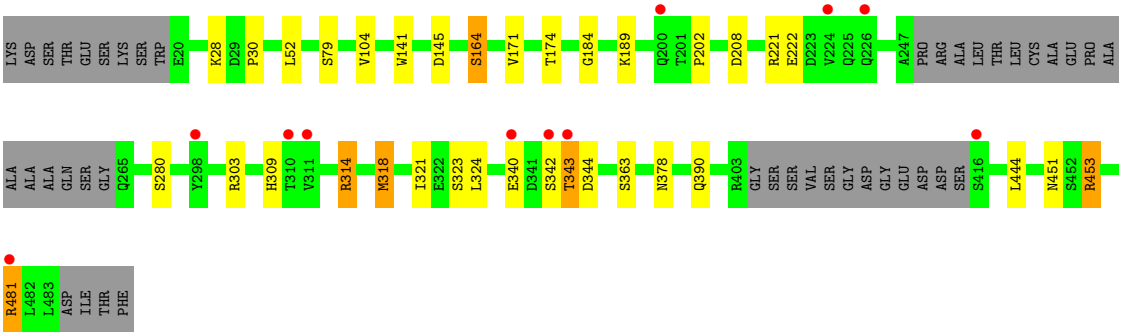




• Molecule 1: TqaA

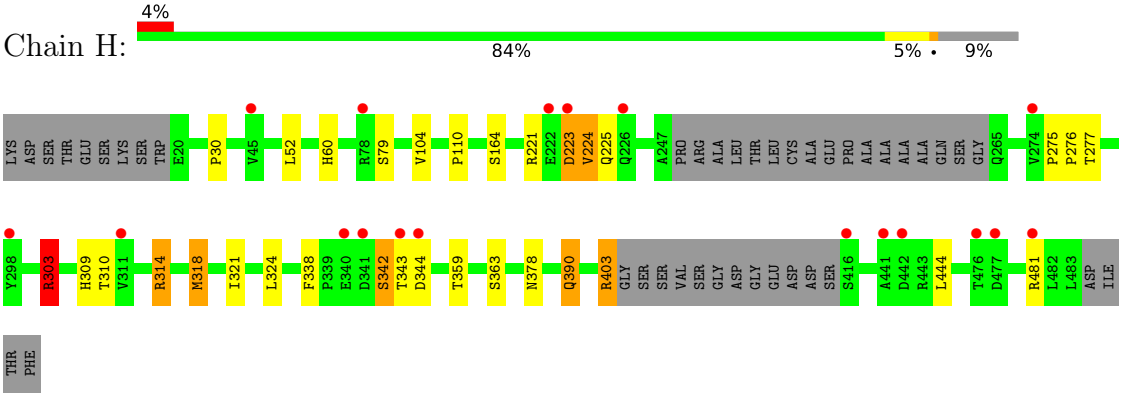
Chain F:





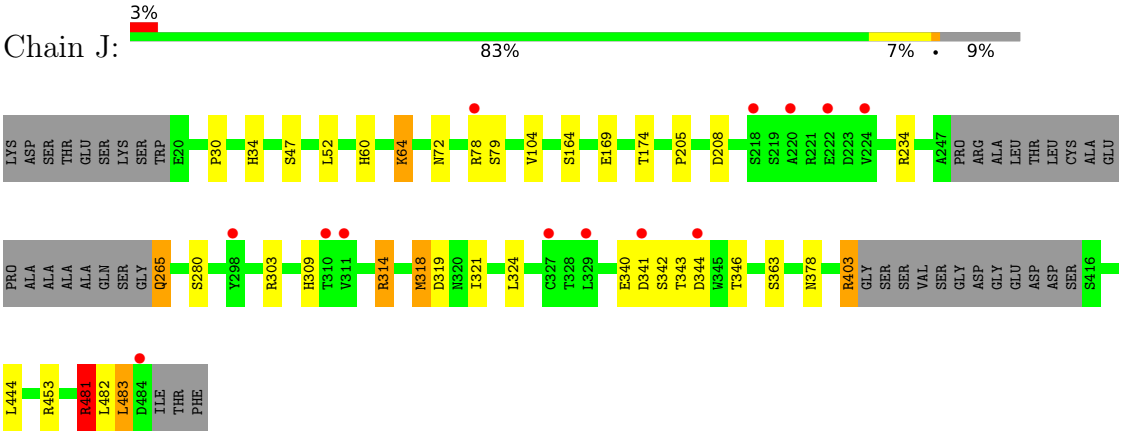
• Molecule 1: TqaA

Chain H:



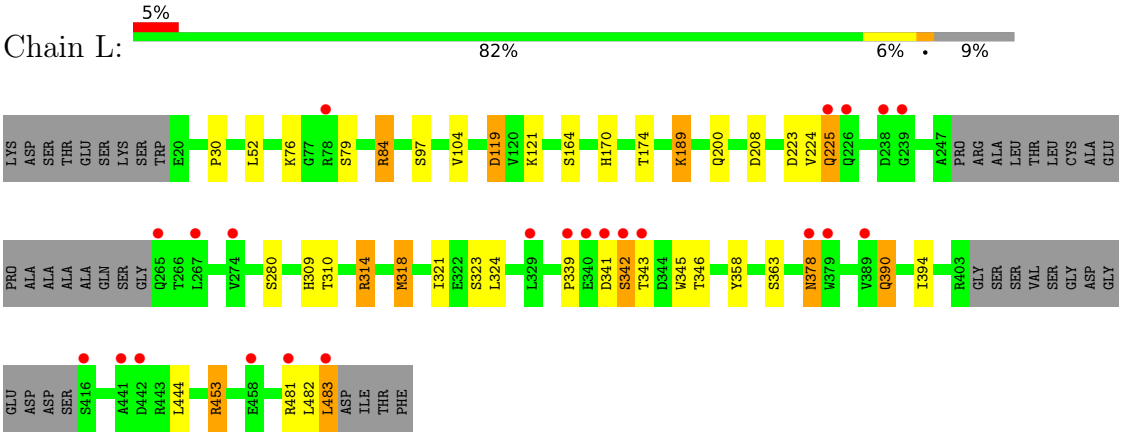
• Molecule 1: TqaA

Chain J:



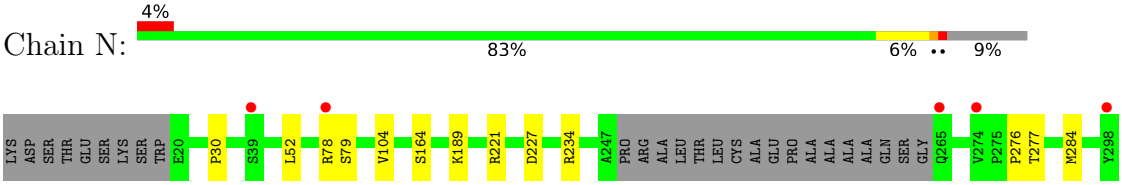
• Molecule 1: TqaA

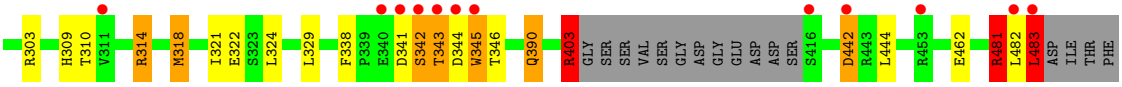
Chain L:



• Molecule 1: TqaA

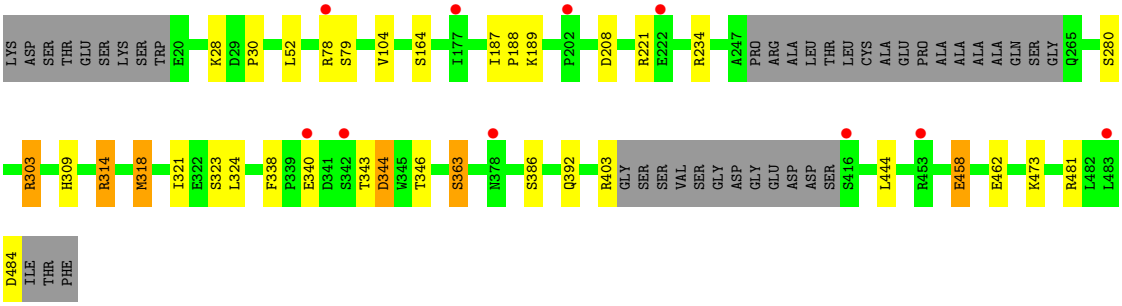
Chain N:





• Molecule 1: TqaA

Chain P:

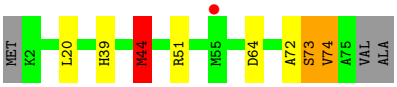


• Molecule 2: TqaA

Chain A:

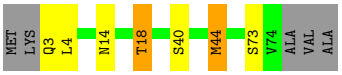
• Molecule 2: TqaA

Chain C:



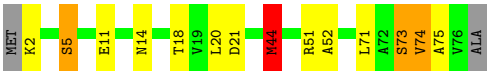
• Molecule 2: TqaA

Chain E:



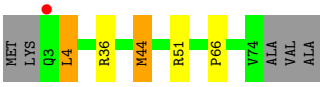
• Molecule 2: TqaA

Chain G:



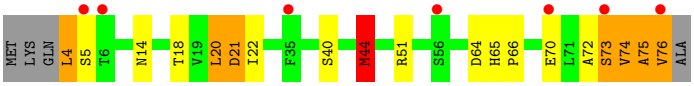
• Molecule 2: TqaA

Chain I:



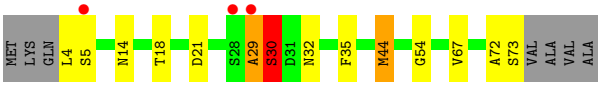
• Molecule 2: TqaA

Chain K:



• Molecule 2: TqaA

Chain M:



• Molecule 2: TqaA

Chain O:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.19Å 204.76Å 126.05Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	50.00 – 2.49 34.72 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.49) 99.3 (34.72-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.194 , 0.222 0.198 , 0.226	Depositor DCC
R_{free} test set	9162 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	33064	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, PNS

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	B	0.73	0/3582	0.82	9/4892 (0.2%)
1	D	0.73	0/3590	0.84	11/4904 (0.2%)
1	F	0.68	0/3574	0.80	7/4881 (0.1%)
1	H	0.67	0/3574	0.80	7/4881 (0.1%)
1	J	0.68	0/3582	0.83	9/4892 (0.2%)
1	L	0.68	0/3574	0.82	11/4881 (0.2%)
1	N	0.67	1/3574 (0.0%)	0.83	11/4881 (0.2%)
1	P	0.69	0/3582	0.79	5/4892 (0.1%)
2	A	0.76	0/564	0.81	2/764 (0.3%)
2	C	0.73	0/557	0.81	1/754 (0.1%)
2	E	0.68	0/543	0.75	1/736 (0.1%)
2	G	0.75	0/564	1.04	7/764 (0.9%)
2	I	0.66	0/543	0.87	4/736 (0.5%)
2	K	0.67	0/546	0.96	5/741 (0.7%)
2	M	0.69	0/527	0.93	5/714 (0.7%)
2	O	0.65	0/555	0.80	2/753 (0.3%)
All	All	0.69	1/33031 (0.0%)	0.83	97/45066 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1
2	C	0	1
2	K	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	345	TRP	CB-CG	5.96	1.60	1.50

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	442	ASP	CB-CG-OD1	9.44	126.80	118.30
1	D	314	ARG	NE-CZ-NH2	-9.35	115.62	120.30
1	H	314	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	B	314	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	D	314	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	F	314	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	J	314	ARG	NE-CZ-NH2	-8.81	115.90	120.30
1	B	314	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	J	314	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	N	314	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	P	314	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	F	314	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	N	481	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	B	208	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	H	314	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	L	314	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	L	453	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	N	390	GLN	CB-CA-C	-7.64	95.11	110.40
1	J	403	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	H	390	GLN	CB-CA-C	-7.62	95.17	110.40
1	L	314	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	N	314	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	N	341	ASP	CB-CG-OD2	7.51	125.06	118.30
1	L	390	GLN	CB-CA-C	-7.44	95.53	110.40
1	L	223	ASP	CB-CG-OD2	7.43	124.98	118.30
1	N	442	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	H	223	ASP	CB-CG-OD1	7.37	124.94	118.30
1	P	314	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	F	221	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	B	390	GLN	CB-CA-C	-7.19	96.03	110.40
2	K	4	LEU	CB-CG-CD2	6.65	122.31	111.00
2	K	21	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	L	225	GLN	N-CA-CB	6.55	122.39	110.60
1	D	453	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	D	27	ILE	CB-CA-C	-6.43	98.74	111.60
1	L	119	ASP	CB-CG-OD2	6.26	123.93	118.30
2	G	51	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	N	403	ARG	NE-CZ-NH1	6.19	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	341	ASP	CB-CG-OD2	6.17	123.85	118.30
1	N	483	LEU	CA-CB-CG	6.13	129.39	115.30
1	J	453	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	G	21	ASP	CB-CG-OD2	-6.04	112.86	118.30
2	A	44	MET	CA-CB-CG	5.99	123.48	113.30
1	D	221	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	D	84	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	M	21	ASP	CB-CG-OD1	5.91	123.62	118.30
1	N	345	TRP	CA-CB-CG	5.89	124.89	113.70
2	M	4	LEU	CB-CG-CD2	5.89	121.01	111.00
2	I	36	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	H	303	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	L	483	LEU	CA-CB-CG	5.88	128.83	115.30
1	B	29	ASP	N-CA-CB	5.88	121.18	110.60
2	K	21	ASP	CB-CG-OD1	5.80	123.52	118.30
2	I	44	MET	CB-CG-SD	5.77	129.70	112.40
1	H	378	ASN	CB-CA-C	-5.73	98.94	110.40
2	M	30	SER	N-CA-CB	5.73	119.09	110.50
1	D	235	HIS	N-CA-CB	5.68	120.82	110.60
2	G	20	LEU	N-CA-C	-5.64	95.78	111.00
2	O	21	ASP	CB-CG-OD1	5.63	123.37	118.30
2	E	44	MET	CB-CG-SD	5.63	129.29	112.40
2	C	44	MET	CB-CG-SD	5.63	129.29	112.40
1	D	84	ARG	CG-CD-NE	-5.63	99.98	111.80
2	G	44	MET	CB-CG-SD	5.60	129.20	112.40
1	H	303	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	D	119	ASP	CB-CG-OD1	5.58	123.32	118.30
2	K	44	MET	CB-CG-SD	5.58	129.12	112.40
2	M	29	ALA	N-CA-C	-5.57	95.96	111.00
1	B	84	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	N	234	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	G	20	LEU	C-N-CA	-5.54	107.85	121.70
1	L	84	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	M	21	ASP	CB-CG-OD2	-5.53	113.33	118.30
2	A	70	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	B	84	ARG	CG-CD-NE	-5.50	100.25	111.80
2	O	44	MET	CB-CG-SD	5.45	128.75	112.40
1	B	234	ARG	CG-CD-NE	-5.44	100.38	111.80
1	J	481	ARG	CB-CG-CD	-5.42	97.52	111.60
1	D	234	ARG	CG-CD-NE	-5.39	100.48	111.80
1	F	453	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	L	453	ARG	CG-CD-NE	5.37	123.07	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	208	ASP	CB-CA-C	-5.33	99.73	110.40
2	K	20	LEU	CB-CA-C	-5.30	100.13	110.20
1	J	378	ASN	CB-CA-C	-5.30	99.81	110.40
1	F	221	ARG	NE-CZ-NH2	-5.27	117.66	120.30
2	I	36	ARG	CD-NE-CZ	5.25	130.95	123.60
1	J	208	ASP	CB-CA-C	-5.25	99.91	110.40
1	B	221	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	G	21	ASP	CB-CG-OD1	5.20	122.97	118.30
1	F	378	ASN	CB-CA-C	-5.11	100.19	110.40
1	F	208	ASP	CB-CA-C	-5.10	100.21	110.40
1	P	78	ARG	CB-CG-CD	5.10	124.85	111.60
2	G	5	SER	N-CA-CB	-5.09	102.86	110.50
1	P	234	ARG	CG-CD-NE	-5.09	101.11	111.80
2	I	4	LEU	CB-CG-CD1	5.09	119.65	111.00
1	D	208	ASP	CB-CA-C	-5.05	100.30	110.40
1	L	224	VAL	C-N-CA	-5.01	109.17	121.70
1	J	234	ARG	CG-CD-NE	-5.00	101.30	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	73	SER	Peptide
2	K	74	VAL	Peptide
1	N	481	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3486	0	3415	24	0
1	D	3493	0	3422	16	0
1	F	3478	0	3411	19	0
1	H	3478	0	3411	16	0
1	J	3486	0	3415	21	0
1	L	3478	0	3411	22	0
1	N	3478	0	3411	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	3486	0	3415	18	0
2	A	554	0	542	6	0
2	C	547	0	533	8	0
2	E	533	0	515	3	0
2	G	554	0	542	8	0
2	I	533	0	515	2	0
2	K	536	0	521	12	0
2	M	517	0	498	10	0
2	O	545	0	529	2	0
3	B	6	0	8	0	0
3	D	6	0	8	0	0
3	P	6	0	8	0	0
4	A	21	0	20	1	0
4	C	21	0	21	1	0
4	E	21	0	21	3	0
4	G	21	0	21	0	0
4	I	21	0	21	0	0
4	K	21	0	21	5	0
4	M	21	0	21	1	0
4	O	21	0	21	2	0
5	A	15	0	0	0	0
5	B	112	0	0	6	0
5	C	8	0	0	1	0
5	D	118	0	0	4	0
5	E	6	0	0	0	0
5	F	73	0	0	1	0
5	G	6	0	0	0	0
5	H	69	0	0	3	0
5	I	12	0	0	1	0
5	J	70	0	0	1	0
5	K	2	0	0	0	0
5	L	63	0	0	1	0
5	M	5	0	0	0	0
5	N	55	0	0	0	0
5	O	6	0	0	0	0
5	P	76	0	0	1	0
All	All	33064	0	31697	192	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 3.

All (192) 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:J:265:GLN:N	1:J:265:GLN:OE1	1.89	1.05
1:B:201:THR:HG22	5:B:617:HOH:O	1.58	1.04
1:P:473:LYS:NZ	1:P:484:ASP:OD1	1.97	0.97
1:B:201:THR:CG2	5:B:617:HOH:O	2.09	0.94
1:B:20:GLU:N	1:B:20:GLU:OE1	2.02	0.92
1:L:453:ARG:O	1:L:453:ARG:HD2	1.72	0.88
2:C:73:SER:O	2:C:74:VAL:HG23	1.74	0.88
1:N:303:ARG:HD3	1:N:338:PHE:HB2	1.56	0.88
1:J:78:ARG:NE	1:J:169:GLU:OE2	2.08	0.86
1:F:451:ASN:OD1	1:F:453:ARG:HG2	1.78	0.84
1:J:319:ASP:OD1	2:I:51:ARG:NH2	2.15	0.80
1:D:155:SER:HB3	5:D:633:HOH:O	1.81	0.79
1:D:451:ASN:OD1	1:D:453:ARG:HG2	1.82	0.79
1:H:223:ASP:OD2	1:H:225:GLN:N	2.15	0.79
1:J:60:HIS:CE1	1:J:64:LYS:NZ	2.50	0.79
1:H:303:ARG:HD2	1:H:338:PHE:O	1.83	0.77
1:L:339:PRO:HB2	1:L:341:ASP:HB3	1.66	0.75
1:L:358:TYR:OH	4:K:101:PNS:H312	1.86	0.74
1:B:265:GLN:N	1:B:453:ARG:NH2	2.36	0.74
1:N:342:SER:O	1:N:344:ASP:N	2.21	0.74
1:H:342:SER:O	1:H:344:ASP:N	2.20	0.74
1:H:277:THR:OG1	5:H:501:HOH:O	2.06	0.74
1:J:60:HIS:CE1	1:J:64:LYS:HZ2	2.05	0.73
1:P:458:GLU:H	1:P:458:GLU:CD	1.94	0.72
2:I:66:PRO:HD2	5:I:201:HOH:O	1.92	0.70
1:L:225:GLN:O	1:L:225:GLN:HG2	1.92	0.69
1:D:105:GLU:OE2	5:D:602:HOH:O	2.12	0.68
1:N:342:SER:HB2	1:N:482:LEU:HD21	1.75	0.68
1:N:403:ARG:HD2	1:N:403:ARG:O	1.94	0.68
2:K:72:ALA:O	2:K:73:SER:OG	2.11	0.67
1:J:265:GLN:OE1	1:J:265:GLN:CA	2.42	0.67
1:J:342:SER:O	1:J:344:ASP:N	2.23	0.67
1:P:303:ARG:HG3	1:P:338:PHE:HB2	1.79	0.65
1:F:202:PRO:CG	2:M:54:GLY:O	2.44	0.65
1:H:403:ARG:HD2	1:H:403:ARG:C	2.17	0.64
2:M:29:ALA:O	2:M:30:SER:CB	2.46	0.64
1:H:359:THR:OG1	5:H:502:HOH:O	2.14	0.63
1:B:322:GLU:CB	2:A:44:MET:HE1	2.28	0.63
1:D:27:ILE:HD12	1:D:106:HIS:CE1	2.34	0.62
1:P:314:ARG:NH2	1:P:324:LEU:O	2.31	0.62
1:B:322:GLU:HB2	2:A:44:MET:CE	2.30	0.61
1:L:119:ASP:OD2	1:L:121:LYS:NZ	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:221:ARG:HD2	1:N:227:ASP:HA	1.82	0.60
2:C:72:ALA:O	2:C:73:SER:OG	2.10	0.60
2:K:65:HIS:N	2:K:66:PRO:HD3	2.17	0.60
2:K:40:SER:HB2	4:K:101:PNS:H311	1.84	0.59
1:F:202:PRO:HG3	2:M:54:GLY:O	2.01	0.59
1:H:221:ARG:O	1:H:223:ASP:O	2.21	0.59
2:K:20:LEU:O	2:K:22:ILE:N	2.35	0.59
1:F:174:THR:HG22	5:F:553:HOH:O	2.01	0.59
2:C:64:ASP:OD2	5:C:201:HOH:O	2.17	0.58
1:B:322:GLU:CB	2:A:44:MET:CE	2.81	0.58
2:M:32:ASN:HB3	2:M:35:PHE:CD2	2.39	0.57
1:B:34:HIS:C	1:B:34:HIS:CD2	2.78	0.57
1:J:265:GLN:N	1:J:265:GLN:CD	2.59	0.56
1:J:314:ARG:NH2	1:J:324:LEU:O	2.31	0.56
1:L:314:ARG:NH2	1:L:324:LEU:O	2.32	0.56
2:A:44:MET:HE3	2:A:45:LYS:HG2	1.87	0.56
1:J:303:ARG:HD2	1:J:340:GLU:HA	1.87	0.56
1:B:265:GLN:N	1:B:453:ARG:HH21	2.02	0.56
1:J:60:HIS:CE1	1:J:64:LYS:HZ1	2.24	0.56
1:F:314:ARG:NH2	1:F:324:LEU:O	2.31	0.56
1:B:314:ARG:NH2	1:B:324:LEU:O	2.33	0.55
2:M:32:ASN:HB3	2:M:35:PHE:CG	2.41	0.55
2:C:73:SER:O	2:C:74:VAL:CG2	2.53	0.55
2:K:72:ALA:O	2:K:73:SER:CB	2.53	0.55
1:B:322:GLU:HB3	2:A:44:MET:HE1	1.87	0.55
2:G:52:ALA:O	1:J:205:PRO:HD3	2.06	0.55
1:D:159:ARG:NH1	5:D:601:HOH:O	2.00	0.54
1:L:394:ILE:HD13	4:K:101:PNS:C42	2.38	0.54
1:J:78:ARG:CZ	1:J:169:GLU:OE2	2.55	0.54
1:B:393:ASN:OD1	4:A:101:PNS:H372	2.08	0.53
1:D:314:ARG:NH2	1:D:324:LEU:O	2.32	0.53
2:G:73:SER:O	2:G:74:VAL:HG13	2.09	0.53
2:M:30:SER:HA	2:M:67:VAL:HG13	1.91	0.53
1:N:314:ARG:NH2	1:N:324:LEU:O	2.31	0.53
1:L:225:GLN:O	1:L:225:GLN:CG	2.56	0.53
1:B:318:MET:HE3	1:B:321:ILE:HD12	1.91	0.52
2:K:64:ASP:C	2:K:66:PRO:HD3	2.30	0.52
1:H:318:MET:HE3	1:H:321:ILE:HD12	1.92	0.52
5:D:610:HOH:O	2:C:51:ARG:HD3	2.09	0.52
1:F:343:THR:O	1:F:481:ARG:HD3	2.10	0.52
1:D:318:MET:HE3	1:D:321:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:303:ARG:HD3	1:N:338:PHE:CB	2.32	0.52
1:L:174:THR:HG22	5:L:536:HOH:O	2.09	0.52
1:P:473:LYS:NZ	1:P:484:ASP:CG	2.64	0.51
1:H:303:ARG:HG2	1:H:338:PHE:HB2	1.92	0.51
1:H:60:HIS:CE1	1:H:110:PRO:HB3	2.46	0.51
1:L:189:LYS:HD2	1:L:323:SER:HB2	1.92	0.51
1:N:318:MET:HE3	1:N:321:ILE:HD12	1.93	0.51
2:C:72:ALA:O	2:C:73:SER:CB	2.58	0.50
1:F:342:SER:C	1:F:344:ASP:H	2.14	0.50
1:J:318:MET:HE3	1:J:321:ILE:HD12	1.92	0.50
1:L:318:MET:HE3	1:L:321:ILE:HD12	1.93	0.50
1:P:318:MET:HE3	1:P:321:ILE:HD12	1.93	0.50
1:N:322:GLU:HA	2:M:44:MET:CE	2.41	0.50
1:L:97:SER:OG	1:L:208:ASP:HB2	2.12	0.50
1:N:329:LEU:HD11	4:M:101:PNS:H431	1.94	0.50
1:L:318:MET:C	2:K:51:ARG:HH22	2.15	0.50
1:F:189:LYS:HD2	1:F:323:SER:HB2	1.94	0.50
2:E:40:SER:HB2	4:E:101:PNS:H311	1.94	0.49
1:P:363:SER:HB2	5:P:629:HOH:O	2.13	0.49
1:F:303:ARG:CZ	1:F:340:GLU:HG2	2.43	0.49
1:J:60:HIS:ND1	1:J:64:LYS:NZ	2.60	0.49
1:L:84:ARG:HH12	1:L:200:GLN:HE21	1.61	0.49
1:B:363:SER:HB2	5:B:632:HOH:O	2.12	0.49
1:D:27:ILE:HD11	1:D:106:HIS:CG	2.48	0.49
1:F:318:MET:HE3	1:F:321:ILE:HD12	1.94	0.49
1:H:223:ASP:OD2	1:H:224:VAL:N	2.45	0.49
1:N:343:THR:N	1:N:482:LEU:CD2	2.75	0.49
1:L:394:ILE:HD13	4:K:101:PNS:H422	1.93	0.49
1:H:314:ARG:NH2	1:H:324:LEU:O	2.34	0.48
1:B:174:THR:HG22	5:B:671:HOH:O	2.13	0.48
1:P:458:GLU:CD	1:P:458:GLU:N	2.66	0.48
4:K:101:PNS:O35	4:K:101:PNS:H313	2.12	0.48
1:D:189:LYS:HD2	1:D:323:SER:HB2	1.96	0.48
1:J:363:SER:HB2	5:J:531:HOH:O	2.13	0.48
1:N:482:LEU:HG	1:N:483:LEU:HD13	1.97	0.47
1:B:342:SER:O	1:B:343:THR:C	2.53	0.47
2:A:7:ASP:OD2	1:N:221:ARG:NE	2.46	0.46
1:D:394:ILE:HD13	4:C:101:PNS:H431	1.98	0.46
2:O:14:ASN:O	2:O:18:THR:HG23	2.16	0.46
1:B:189:LYS:HD2	1:B:323:SER:HB2	1.98	0.46
1:L:310:THR:OG1	1:L:390:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:346:THR:HA	1:L:481:ARG:HA	1.98	0.45
1:B:155:SER:HB3	5:B:640:HOH:O	2.16	0.45
1:H:310:THR:OG1	1:H:390:GLN:HG2	2.16	0.45
2:G:2:LYS:HB2	2:G:2:LYS:HE3	1.78	0.45
1:B:310:THR:OG1	1:B:390:GLN:HG2	2.17	0.45
1:N:346:THR:HA	1:N:481:ARG:HA	1.98	0.45
1:N:310:THR:OG1	1:N:390:GLN:HG2	2.16	0.45
2:K:75:ALA:O	2:K:76:VAL:C	2.54	0.45
1:N:30:PRO:HB3	1:N:52:LEU:HD13	1.99	0.45
1:P:344:ASP:OD2	1:P:481:ARG:CZ	2.65	0.45
2:E:3:GLN:HG3	2:E:4:LEU:N	2.31	0.45
1:H:363:SER:HB2	5:H:532:HOH:O	2.17	0.45
1:J:346:THR:HA	1:J:481:ARG:HA	1.99	0.45
2:K:44:MET:O	2:K:44:MET:HG2	2.16	0.45
2:K:14:ASN:O	2:K:18:THR:HG23	2.16	0.44
2:M:14:ASN:O	2:M:18:THR:HG23	2.16	0.44
1:D:72:ASN:HD22	1:D:134:MET:HE1	1.82	0.44
1:B:202:PRO:HA	5:B:653:HOH:O	2.18	0.44
1:F:343:THR:O	1:F:481:ARG:CD	2.65	0.44
1:N:276:PRO:HG2	1:N:284:MET:HE1	1.98	0.44
1:D:27:ILE:CD1	1:D:106:HIS:CE1	3.01	0.44
1:F:141:TRP:HA	1:F:145:ASP:HB2	2.00	0.44
2:E:14:ASN:O	2:E:18:THR:HG23	2.17	0.44
1:L:30:PRO:HB3	1:L:52:LEU:HD13	2.00	0.43
1:P:346:THR:HA	1:P:481:ARG:HA	1.99	0.43
1:F:30:PRO:HB3	1:F:52:LEU:HD13	1.99	0.43
1:D:346:THR:HA	1:D:481:ARG:HA	2.00	0.43
1:F:28:LYS:HE2	2:G:18:THR:HA	1.99	0.43
2:K:70:GLU:O	2:K:74:VAL:HG23	2.17	0.43
2:G:74:VAL:O	2:G:75:ALA:HB2	2.18	0.43
2:O:44:MET:O	2:O:44:MET:HG2	2.18	0.43
2:C:44:MET:O	2:C:44:MET:HG2	2.17	0.43
1:H:30:PRO:HB3	1:H:52:LEU:HD13	2.01	0.43
1:L:378:ASN:OD1	1:L:378:ASN:N	2.51	0.43
1:B:346:THR:HA	1:B:481:ARG:HA	2.00	0.42
1:F:390:GLN:NE2	4:E:101:PNS:H422	2.34	0.42
1:D:164:SER:HB3	1:D:171:VAL:HG22	2.01	0.42
2:K:73:SER:HA	2:K:75:ALA:HB2	2.01	0.42
1:P:392:GLN:OE1	4:O:101:PNS:C42	2.68	0.42
1:D:342:SER:O	1:D:343:THR:C	2.57	0.42
1:F:184:GLY:N	4:E:101:PNS:H432	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:14:ASN:O	2:G:18:THR:HG23	2.18	0.42
1:L:189:LYS:CD	1:L:323:SER:HB2	2.50	0.42
2:M:44:MET:O	2:M:44:MET:HG2	2.14	0.42
1:P:189:LYS:HD2	1:P:323:SER:HB2	2.01	0.42
1:P:392:GLN:OE1	4:O:101:PNS:H421	2.20	0.42
1:J:34:HIS:HE1	1:J:47:SER:OG	2.02	0.42
1:P:403:ARG:HH11	1:P:403:ARG:HG3	1.85	0.41
1:D:27:ILE:CD1	1:D:106:HIS:CD2	3.02	0.41
2:G:44:MET:O	2:G:44:MET:HG2	2.15	0.41
2:G:71:LEU:O	2:G:73:SER:O	2.38	0.41
1:J:483:LEU:CD1	1:J:483:LEU:N	2.83	0.41
2:C:20:LEU:O	1:P:28:LYS:O	2.38	0.41
1:B:241:LYS:HA	1:B:241:LYS:HD2	1.65	0.41
1:F:164:SER:HB3	1:F:171:VAL:HG22	2.01	0.41
1:L:76:LYS:HE2	1:L:170:HIS:CD2	2.56	0.41
1:B:30:PRO:HB3	1:B:52:LEU:HD13	2.02	0.41
1:F:342:SER:O	1:F:343:THR:OG1	2.30	0.41
2:M:30:SER:HA	2:M:67:VAL:CG1	2.49	0.41
1:P:187:ILE:CG2	1:P:188:PRO:HD3	2.51	0.40
1:F:342:SER:O	1:F:344:ASP:N	2.47	0.40
1:L:481:ARG:O	1:L:483:LEU:N	2.54	0.40
1:B:141:TRP:HA	1:B:145:ASP:HB2	2.03	0.40
1:J:30:PRO:HB3	1:J:52:LEU:HD13	2.03	0.40
1:P:30:PRO:HB3	1:P:52:LEU:HD13	2.02	0.40
1:H:275:PRO:HA	1:H:276:PRO:HD3	1.92	0.40
1:J:482:LEU:HD22	1:J:482:LEU:N	2.36	0.40
1:P:221:ARG:HH11	1:P:221:ARG:HG3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	430/477 (90%)	421 (98%)	8 (2%)	1 (0%)	47	68
1	D	431/477 (90%)	421 (98%)	9 (2%)	1 (0%)	47	68
1	F	429/477 (90%)	416 (97%)	12 (3%)	1 (0%)	47	68
1	H	429/477 (90%)	419 (98%)	9 (2%)	1 (0%)	47	68
1	J	430/477 (90%)	419 (97%)	10 (2%)	1 (0%)	47	68
1	L	429/477 (90%)	417 (97%)	9 (2%)	3 (1%)	22	39
1	N	429/477 (90%)	418 (97%)	9 (2%)	2 (0%)	29	48
1	P	430/477 (90%)	420 (98%)	9 (2%)	1 (0%)	47	68
2	A	73/77 (95%)	73 (100%)	0	0	100	100
2	C	72/77 (94%)	69 (96%)	2 (3%)	1 (1%)	11	20
2	E	70/77 (91%)	68 (97%)	1 (1%)	1 (1%)	11	20
2	G	73/77 (95%)	69 (94%)	3 (4%)	1 (1%)	11	20
2	I	70/77 (91%)	69 (99%)	1 (1%)	0	100	100
2	K	71/77 (92%)	67 (94%)	1 (1%)	3 (4%)	3	3
2	M	68/77 (88%)	66 (97%)	0	2 (3%)	4	6
2	O	72/77 (94%)	71 (99%)	1 (1%)	0	100	100
All	All	4006/4432 (90%)	3903 (97%)	84 (2%)	19 (0%)	29	48

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	74	VAL
1	F	343	THR
2	E	73	SER
1	N	343	THR
1	L	482	LEU
2	M	30	SER
1	H	343	THR
1	J	343	THR
1	L	342	SER
2	K	21	ASP
2	M	72	ALA
1	D	343	THR
1	L	343	THR
2	K	75	ALA
2	G	74	VAL
2	K	73	SER

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Mol	Chain	Res	Type
1	N	342	SER
1	P	343	THR
1	B	343	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	394/425 (93%)	379 (96%)	15 (4%)	33	58
1	D	395/425 (93%)	383 (97%)	12 (3%)	41	68
1	F	393/425 (92%)	383 (98%)	10 (2%)	47	73
1	H	393/425 (92%)	382 (97%)	11 (3%)	43	70
1	J	394/425 (93%)	380 (96%)	14 (4%)	35	61
1	L	393/425 (92%)	381 (97%)	12 (3%)	40	67
1	N	393/425 (92%)	379 (96%)	14 (4%)	35	61
1	P	394/425 (93%)	380 (96%)	14 (4%)	35	61
2	A	57/58 (98%)	54 (95%)	3 (5%)	22	43
2	C	56/58 (97%)	54 (96%)	2 (4%)	35	61
2	E	55/58 (95%)	53 (96%)	2 (4%)	35	61
2	G	57/58 (98%)	53 (93%)	4 (7%)	15	29
2	I	55/58 (95%)	53 (96%)	2 (4%)	35	61
2	K	55/58 (95%)	51 (93%)	4 (7%)	14	27
2	M	53/58 (91%)	50 (94%)	3 (6%)	20	39
2	O	56/58 (97%)	51 (91%)	5 (9%)	9	19
All	All	3593/3864 (93%)	3466 (96%)	127 (4%)	36	62

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	79	SER

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Mol	Chain	Res	Type
1	B	84	ARG
1	B	104	VAL
1	B	164	SER
1	B	235	HIS
1	B	280	SER
1	B	303	ARG
1	B	309	HIS
1	B	318	MET
1	B	345	TRP
1	B	363	SER
1	B	444	LEU
1	B	453	ARG
1	B	462	GLU
1	B	483	LEU
2	A	11	GLU
2	A	39	HIS
2	A	44	MET
1	D	79	SER
1	D	84	ARG
1	D	104	VAL
1	D	164	SER
1	D	189	LYS
1	D	241	LYS
1	D	280	SER
1	D	309	HIS
1	D	318	MET
1	D	345	TRP
1	D	403	ARG
1	D	444	LEU
2	C	39	HIS
2	C	44	MET
1	F	79	SER
1	F	104	VAL
1	F	164	SER
1	F	222	GLU
1	F	280	SER
1	F	309	HIS
1	F	318	MET
1	F	363	SER
1	F	444	LEU
1	F	481	ARG
2	E	18	THR

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Mol	Chain	Res	Type
2	E	44	MET
1	H	79	SER
1	H	104	VAL
1	H	164	SER
1	H	224	VAL
1	H	303	ARG
1	H	309	HIS
1	H	318	MET
1	H	342	SER
1	H	403	ARG
1	H	444	LEU
1	H	481	ARG
2	G	5	SER
2	G	11	GLU
2	G	44	MET
2	G	73	SER
1	J	64	LYS
1	J	72	ASN
1	J	79	SER
1	J	104	VAL
1	J	164	SER
1	J	174	THR
1	J	265	GLN
1	J	280	SER
1	J	309	HIS
1	J	318	MET
1	J	403	ARG
1	J	444	LEU
1	J	481	ARG
1	J	483	LEU
2	I	4	LEU
2	I	44	MET
1	L	79	SER
1	L	104	VAL
1	L	164	SER
1	L	189	LYS
1	L	280	SER
1	L	309	HIS
1	L	318	MET
1	L	342	SER
1	L	345	TRP
1	L	363	SER

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Mol	Chain	Res	Type
1	L	378	ASN
1	L	444	LEU
2	K	4	LEU
2	K	5	SER
2	K	44	MET
2	K	76	VAL
1	N	78	ARG
1	N	79	SER
1	N	104	VAL
1	N	164	SER
1	N	189	LYS
1	N	277	THR
1	N	309	HIS
1	N	318	MET
1	N	345	TRP
1	N	403	ARG
1	N	442	ASP
1	N	444	LEU
1	N	462	GLU
1	N	483	LEU
2	M	5	SER
2	M	44	MET
2	M	73	SER
1	P	79	SER
1	P	104	VAL
1	P	164	SER
1	P	280	SER
1	P	303	ARG
1	P	309	HIS
1	P	318	MET
1	P	340	GLU
1	P	344	ASP
1	P	363	SER
1	P	386	SER
1	P	444	LEU
1	P	458	GLU
1	P	462	GLU
2	O	4	LEU
2	O	5	SER
2	O	18	THR
2	O	44	MET
2	O	76	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	72	ASN
1	D	170	HIS
1	F	69	HIS
1	F	150	ASN
1	F	390	GLN
1	H	72	ASN
1	H	170	HIS
1	J	34	HIS
1	J	60	HIS
1	J	69	HIS
1	J	72	ASN
1	L	69	HIS
1	L	72	ASN
1	L	200	GLN
1	P	150	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

11 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	$\#\|Z\|>2$
4	PNS	M	101	2	13,20,21	1.25	2 (15%)	18,26,29	3.88	10 (55%)
4	PNS	K	101	2	13,20,21	0.80	0	18,26,29	4.71	9 (50%)
3	GOL	D	501	-	5,5,5	0.77	0	5,5,5	0.49	0
4	PNS	A	101	2	13,20,21	1.53	2 (15%)	18,26,29	5.73	9 (50%)
4	PNS	E	101	2	13,20,21	0.93	1 (7%)	18,26,29	5.04	10 (55%)
4	PNS	O	101	2	13,20,21	0.99	0	18,26,29	2.32	7 (38%)
4	PNS	I	101	2	13,20,21	0.79	0	18,26,29	1.67	3 (16%)
4	PNS	C	101	2	13,20,21	0.77	0	18,26,29	2.24	6 (33%)
3	GOL	B	501	-	5,5,5	0.68	0	5,5,5	0.64	0
4	PNS	G	101	2	13,20,21	1.09	1 (7%)	18,26,29	3.28	7 (38%)
3	GOL	P	501	-	5,5,5	1.07	0	5,5,5	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PNS	M	101	2	-	5/24/26/27	-
4	PNS	K	101	2	-	11/24/26/27	-
3	GOL	D	501	-	-	3/4/4/4	-
4	PNS	A	101	2	-	6/24/26/27	-
4	PNS	E	101	2	-	12/24/26/27	-
4	PNS	O	101	2	-	3/24/26/27	-
4	PNS	I	101	2	-	3/24/26/27	-
4	PNS	C	101	2	-	2/24/26/27	-
3	GOL	B	501	-	-	0/4/4/4	-
4	PNS	G	101	2	-	4/24/26/27	-
3	GOL	P	501	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	101	PNS	O33-C32	3.47	1.48	1.42
4	M	101	PNS	C30-C29	-3.05	1.47	1.53
4	A	101	PNS	C37-N36	-2.83	1.39	1.46
4	G	101	PNS	C38-C39	-2.35	1.46	1.51
4	M	101	PNS	C31-C29	-2.24	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	101	PNS	O40-C39	-2.10	1.19	1.23

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	101	PNS	C30-C29-C28	-14.92	83.89	108.23
4	K	101	PNS	C30-C29-C28	-12.54	87.77	108.23
4	A	101	PNS	C31-C29-C28	-11.68	89.18	108.23
4	A	101	PNS	C30-C29-C28	-10.23	91.54	108.23
4	E	101	PNS	C30-C29-C32	10.14	126.40	108.82
4	A	101	PNS	C32-C34-N36	9.65	135.79	116.58
4	A	101	PNS	O35-C34-N36	-9.20	103.25	122.99
4	K	101	PNS	C31-C29-C30	9.18	127.88	109.17
4	K	101	PNS	C30-C29-C32	8.97	124.37	108.82
4	M	101	PNS	C31-C29-C32	8.43	123.43	108.82
4	E	101	PNS	C31-C29-C30	7.52	124.50	109.17
4	A	101	PNS	C37-N36-C34	7.30	135.61	122.59
4	M	101	PNS	C30-C29-C28	-7.04	96.74	108.23
4	M	101	PNS	C31-C29-C28	-6.84	97.07	108.23
4	G	101	PNS	C37-N36-C34	-6.47	111.04	122.59
4	G	101	PNS	C37-C38-C39	-6.12	102.17	112.36
4	A	101	PNS	C31-C29-C32	6.09	119.38	108.82
4	M	101	PNS	C37-C38-C39	-5.93	102.48	112.36
4	A	101	PNS	C30-C29-C32	5.61	118.55	108.82
4	G	101	PNS	C38-C37-N36	5.55	123.11	111.90
4	A	101	PNS	C31-C29-C30	5.43	120.24	109.17
4	K	101	PNS	C31-C29-C28	-5.36	99.49	108.23
4	G	101	PNS	C32-C34-N36	5.32	127.17	116.58
4	G	101	PNS	O40-C39-C38	-5.02	112.84	122.02
4	M	101	PNS	C30-C29-C32	4.77	117.09	108.82
4	E	101	PNS	O35-C34-N36	4.69	133.07	122.99
4	O	101	PNS	C38-C39-N41	4.50	124.00	116.42
4	I	101	PNS	C42-N41-C39	-4.21	115.03	122.84
4	C	101	PNS	C37-C38-C39	-4.16	105.42	112.36
4	O	101	PNS	C38-C37-N36	4.05	120.08	111.90
4	O	101	PNS	O40-C39-N41	-4.00	115.47	123.01
4	C	101	PNS	C30-C29-C32	3.95	115.68	108.82
4	C	101	PNS	C38-C37-N36	3.77	119.50	111.90
4	A	101	PNS	C37-C38-C39	3.68	118.49	112.36
4	C	101	PNS	C42-N41-C39	-3.66	116.04	122.84
4	G	101	PNS	C38-C39-N41	3.65	122.56	116.42
4	E	101	PNS	O33-C32-C34	-3.48	92.67	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	101	PNS	C37-C38-C39	-3.46	106.59	112.36
4	I	101	PNS	C37-C38-C39	-3.44	106.62	112.36
4	O	101	PNS	C42-N41-C39	3.30	128.96	122.84
4	K	101	PNS	C42-N41-C39	-3.27	116.77	122.84
4	M	101	PNS	C38-C39-N41	3.12	121.67	116.42
4	E	101	PNS	C38-C39-N41	2.99	121.46	116.42
4	C	101	PNS	C38-C39-N41	2.97	121.42	116.42
4	K	101	PNS	C37-C38-C39	-2.96	107.44	112.36
4	C	101	PNS	C30-C29-C28	-2.89	103.52	108.23
4	K	101	PNS	C32-C34-N36	-2.69	111.22	116.58
4	K	101	PNS	C31-C29-C32	-2.68	104.17	108.82
4	M	101	PNS	C42-N41-C39	-2.67	117.88	122.84
4	I	101	PNS	O40-C39-N41	-2.60	118.11	123.01
4	E	101	PNS	O40-C39-C38	-2.54	117.36	122.02
4	M	101	PNS	C31-C29-C30	2.52	114.31	109.17
4	K	101	PNS	O35-C34-N36	2.42	128.18	122.99
4	M	101	PNS	C38-C37-N36	2.39	116.72	111.90
4	G	101	PNS	O35-C34-C32	-2.38	113.79	121.06
4	E	101	PNS	C43-C42-N41	2.27	117.49	112.31
4	E	101	PNS	O35-C34-C32	-2.22	114.31	121.06
4	M	101	PNS	C32-C34-N36	-2.18	112.24	116.58
4	O	101	PNS	C31-C29-C28	2.16	111.75	108.23
4	O	101	PNS	C30-C29-C28	-2.05	104.88	108.23
4	E	101	PNS	C32-C34-N36	-2.01	112.58	116.58

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	GOL	O1-C1-C2-C3
3	P	501	GOL	O1-C1-C2-C3
4	A	101	PNS	C30-C29-C32-C34
4	A	101	PNS	C32-C34-N36-C37
4	A	101	PNS	N41-C42-C43-S44
4	C	101	PNS	N41-C42-C43-S44
4	E	101	PNS	O27-C28-C29-C32
4	E	101	PNS	C31-C29-C32-O33
4	E	101	PNS	O33-C32-C34-O35
4	E	101	PNS	N36-C37-C38-C39
4	E	101	PNS	N41-C42-C43-S44
4	G	101	PNS	N41-C42-C43-S44
4	I	101	PNS	N41-C42-C43-S44

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Mol	Chain	Res	Type	Atoms
4	K	101	PNS	C29-C32-C34-O35
4	K	101	PNS	C29-C32-C34-N36
4	K	101	PNS	O33-C32-C34-O35
4	K	101	PNS	O33-C32-C34-N36
4	K	101	PNS	N36-C37-C38-C39
4	K	101	PNS	N41-C42-C43-S44
4	M	101	PNS	C30-C29-C32-C34
4	M	101	PNS	N41-C42-C43-S44
4	O	101	PNS	N36-C37-C38-C39
4	G	101	PNS	C38-C39-N41-C42
4	O	101	PNS	C38-C39-N41-C42
4	A	101	PNS	O35-C34-N36-C37
4	G	101	PNS	O40-C39-N41-C42
4	O	101	PNS	O40-C39-N41-C42
4	E	101	PNS	O27-C28-C29-C30
4	E	101	PNS	O27-C28-C29-C31
3	D	501	GOL	O1-C1-C2-O2
3	P	501	GOL	O1-C1-C2-O2
4	M	101	PNS	N36-C37-C38-C39
4	A	101	PNS	C30-C29-C32-O33
4	M	101	PNS	C30-C29-C32-O33
4	E	101	PNS	C29-C32-C34-O35
4	E	101	PNS	C29-C32-C34-N36
4	E	101	PNS	O33-C32-C34-N36
4	G	101	PNS	O33-C32-C34-N36
4	I	101	PNS	O33-C32-C34-N36
4	M	101	PNS	O33-C32-C34-N36
4	E	101	PNS	C30-C29-C32-C34
4	K	101	PNS	C37-C38-C39-O40
3	D	501	GOL	C1-C2-C3-O3
4	E	101	PNS	C28-C29-C32-O33
4	K	101	PNS	O27-C28-C29-C32
4	K	101	PNS	C31-C29-C32-O33
4	C	101	PNS	N36-C37-C38-C39
4	I	101	PNS	N36-C37-C38-C39
4	K	101	PNS	C37-C38-C39-N41
4	A	101	PNS	O33-C32-C34-N36
4	K	101	PNS	C30-C29-C32-C34

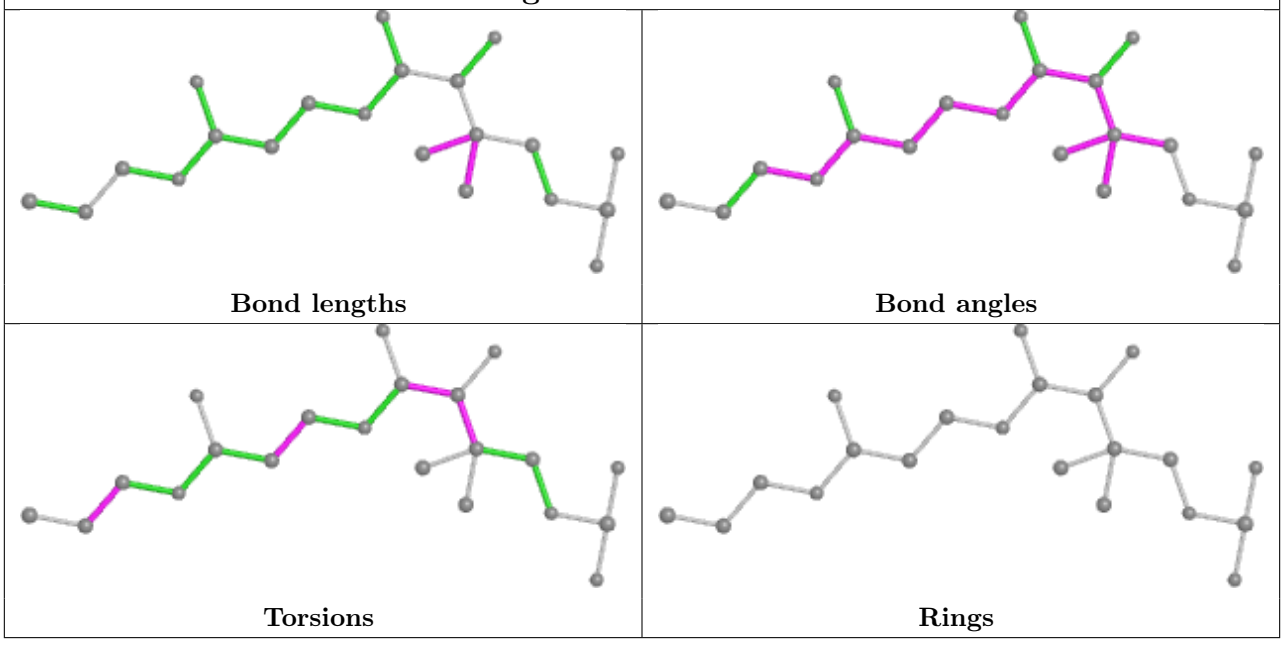
There are no ring outliers.

6 monomers are involved in 13 short contacts:

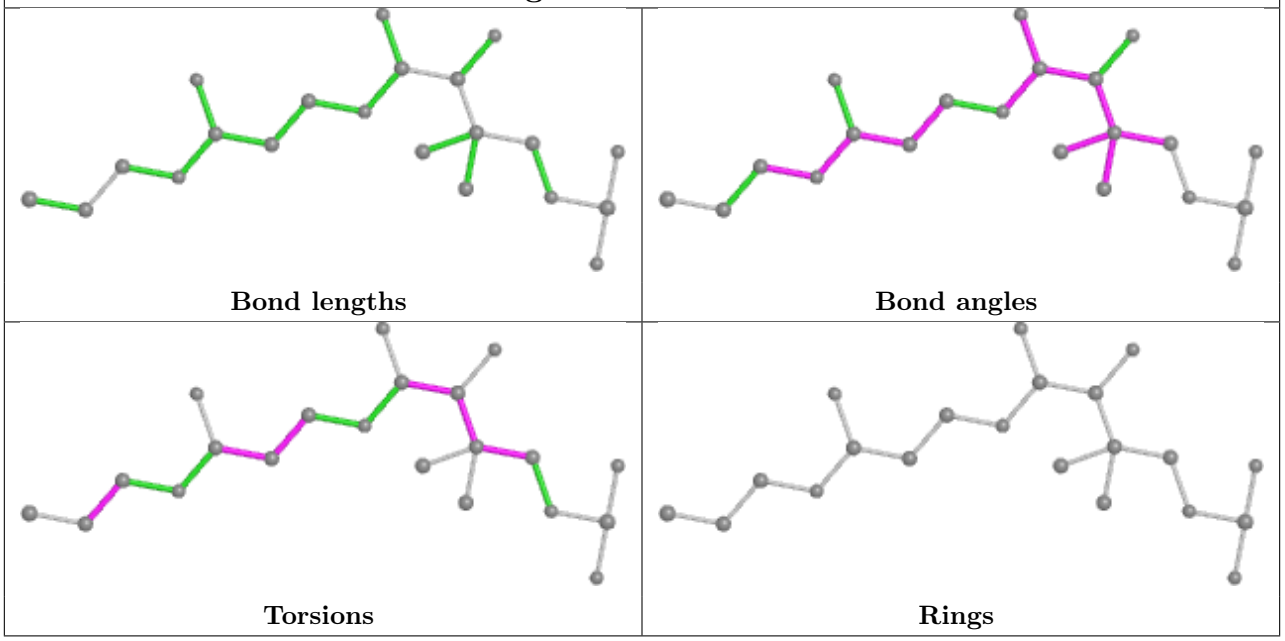
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	101	PNS	1	0
4	K	101	PNS	5	0
4	A	101	PNS	1	0
4	E	101	PNS	3	0
4	O	101	PNS	2	0
4	C	101	PNS	1	0

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

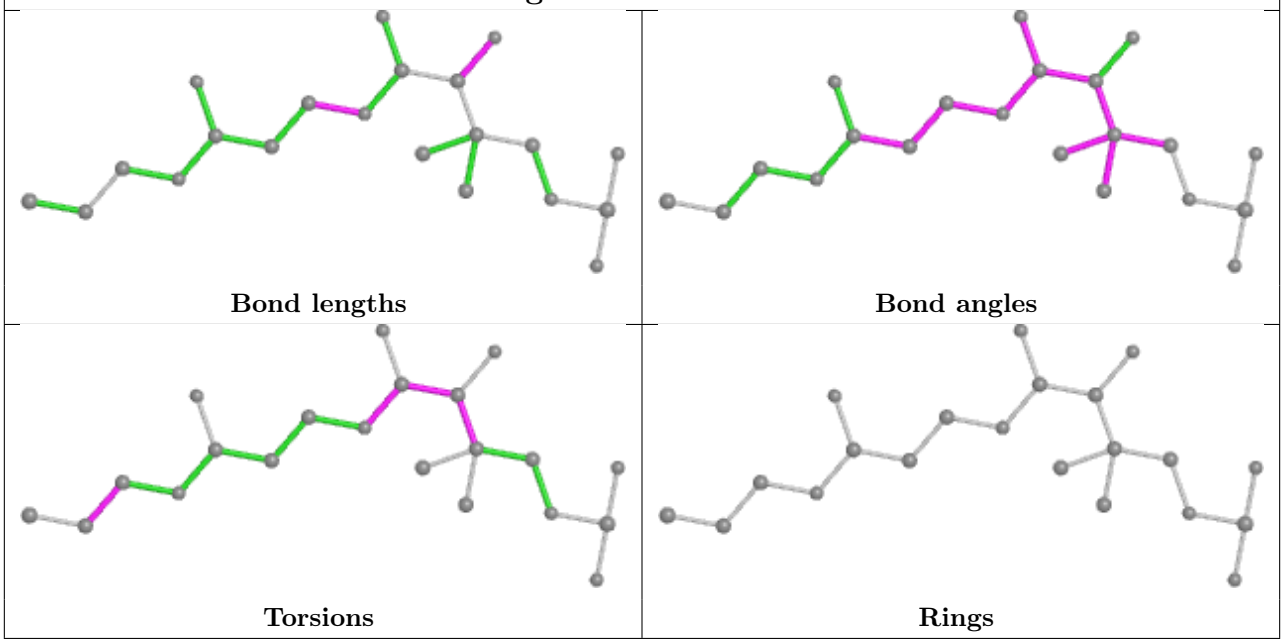
Ligand PNS M 101



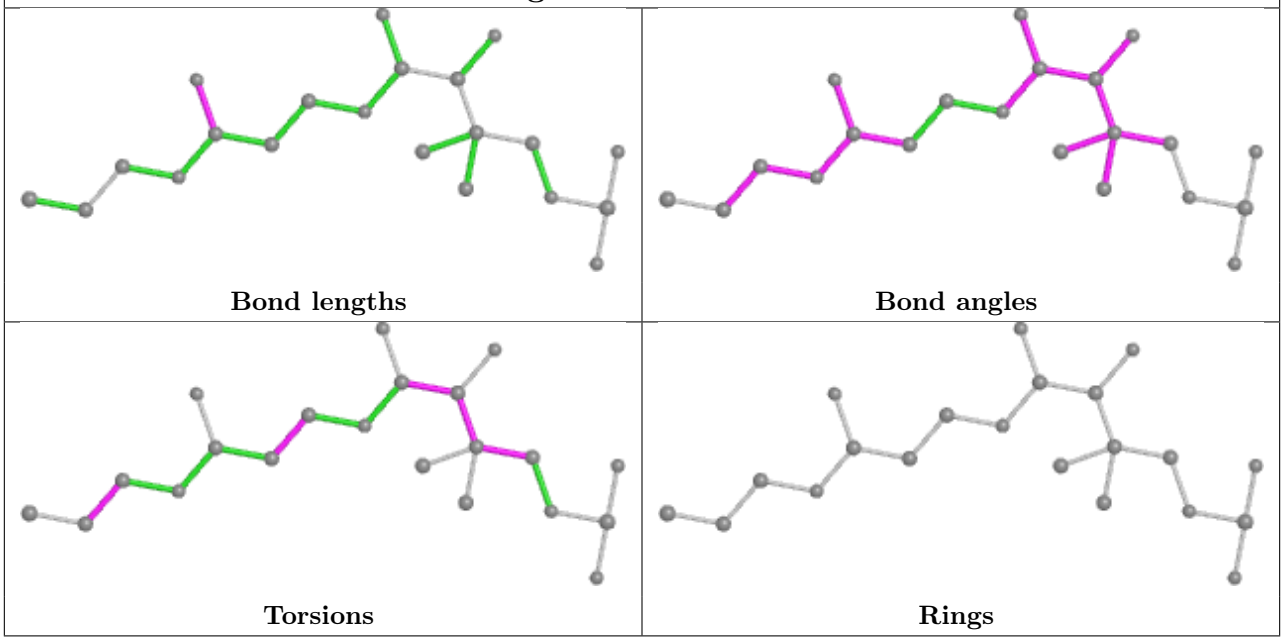
Ligand PNS K 101



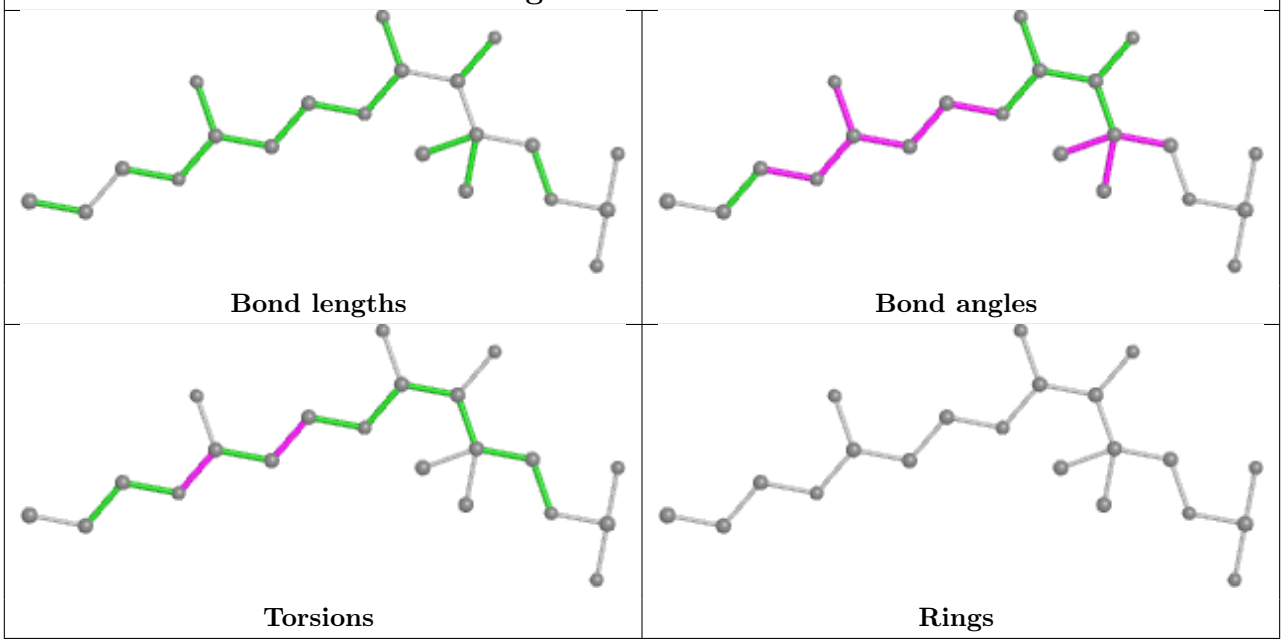
Ligand PNS A 101



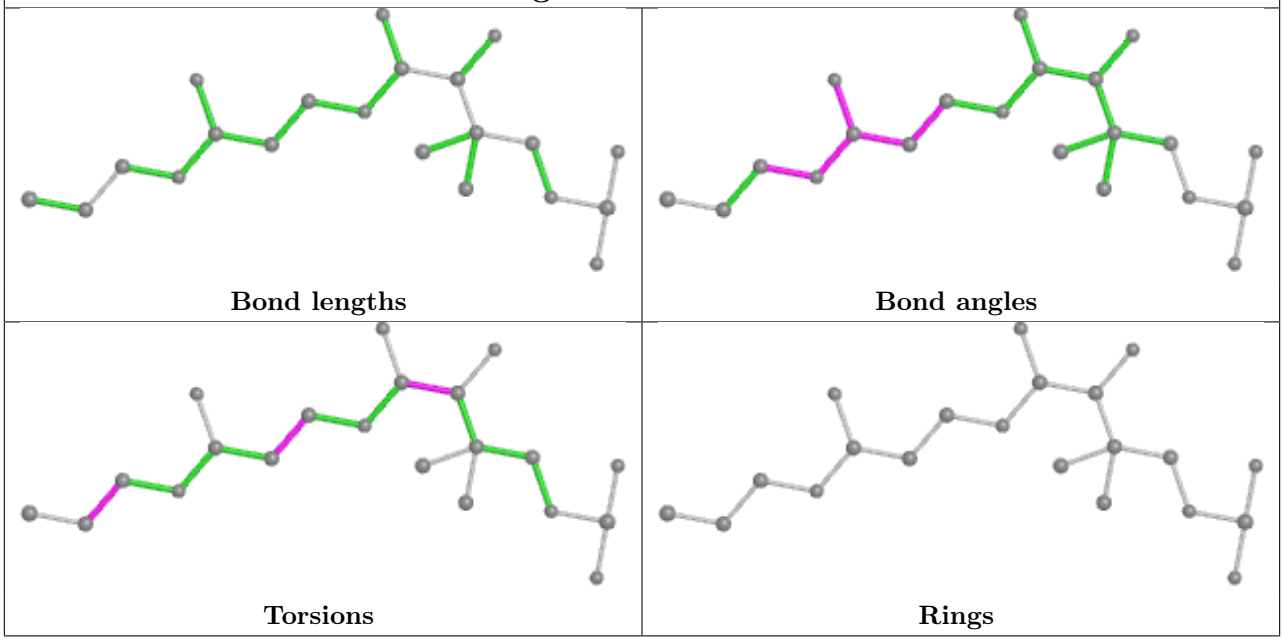
Ligand PNS E 101



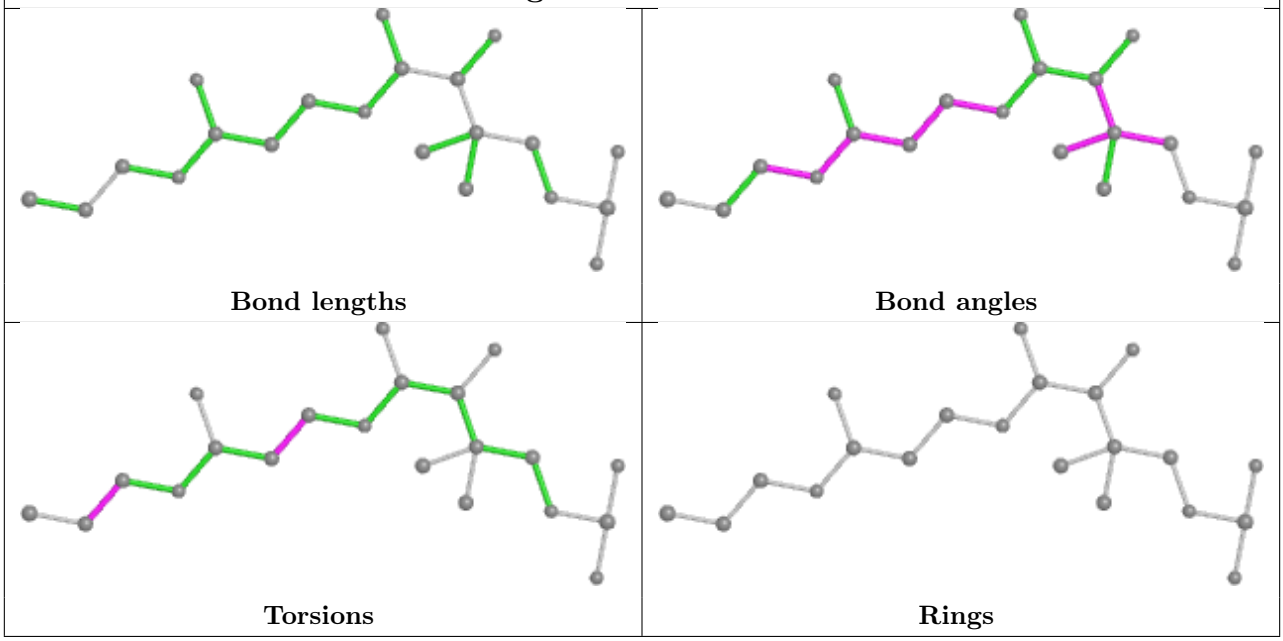
Ligand PNS O 101



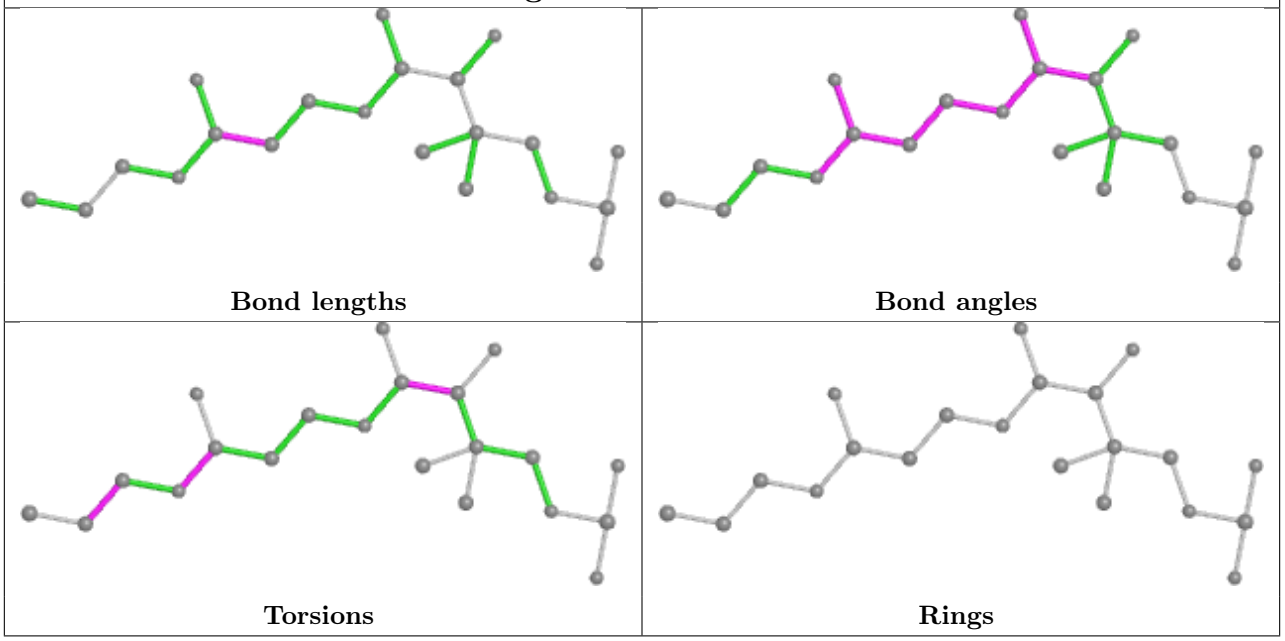
Ligand PNS I 101



Ligand PNS C 101



Ligand PNS G 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	B	436/477 (91%)	-0.04	5 (1%) 80 82	20, 35, 62, 80	0
1	D	437/477 (91%)	-0.09	3 (0%) 87 89	20, 34, 63, 81	0
1	F	435/477 (91%)	-0.04	11 (2%) 57 61	22, 41, 72, 115	0
1	H	435/477 (91%)	0.05	18 (4%) 37 40	25, 43, 75, 114	0
1	J	436/477 (91%)	0.11	13 (2%) 50 53	25, 43, 76, 116	0
1	L	435/477 (91%)	0.24	23 (5%) 26 28	24, 47, 86, 116	0
1	N	435/477 (91%)	0.11	17 (3%) 39 42	25, 45, 76, 129	0
1	P	436/477 (91%)	0.01	10 (2%) 60 63	23, 41, 70, 103	0
2	A	75/77 (97%)	-0.13	0 100 100	23, 37, 61, 81	0
2	C	74/77 (96%)	-0.07	1 (1%) 75 77	23, 38, 61, 81	0
2	E	72/77 (93%)	-0.20	0 100 100	26, 42, 64, 80	0
2	G	75/77 (97%)	-0.14	0 100 100	28, 41, 67, 76	0
2	I	72/77 (93%)	0.03	1 (1%) 75 77	25, 39, 57, 86	0
2	K	73/77 (94%)	0.52	7 (9%) 8 7	34, 58, 89, 105	0
2	M	70/77 (90%)	0.34	3 (4%) 35 38	31, 56, 87, 105	0
2	O	74/77 (96%)	0.17	4 (5%) 25 27	28, 47, 75, 85	0
All	All	4070/4432 (91%)	0.05	116 (2%) 51 55	20, 41, 74, 129	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	342	SER	5.2
1	P	342	SER	5.0
1	L	340	GLU	4.6
1	H	341	ASP	4.0
1	N	342	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	29	ASP	3.9
1	J	78	ARG	3.8
1	N	341	ASP	3.7
1	L	442	ASP	3.7
1	N	482	LEU	3.6
1	N	416	SER	3.6
1	H	78	ARG	3.5
1	H	298	TYR	3.5
1	N	298	TYR	3.4
1	L	226	GLN	3.4
1	J	484	ASP	3.4
1	L	343	THR	3.4
1	H	222	GLU	3.3
1	N	340	GLU	3.3
1	N	442	ASP	3.3
1	L	416	SER	3.3
1	J	344	ASP	3.2
1	P	416	SER	3.2
1	N	343	THR	3.2
2	M	5	SER	3.2
1	N	345	TRP	3.1
1	H	343	THR	3.1
2	I	3	GLN	3.1
1	H	416	SER	3.1
1	F	343	THR	3.0
1	H	223	ASP	3.0
1	L	265	GLN	3.0
2	K	5	SER	2.9
1	F	298	TYR	2.9
1	L	441	ALA	2.9
1	H	45	VAL	2.9
1	L	78	ARG	2.9
1	J	218	SER	2.9
1	L	238	ASP	2.9
1	J	311	VAL	2.8
1	P	202	PRO	2.8
1	L	225	GLN	2.8
1	N	274	VAL	2.8
1	L	481	ARG	2.8
1	L	389	VAL	2.7
1	F	342	SER	2.7
1	L	267	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	226	GLN	2.7
1	N	265	GLN	2.7
1	B	310	THR	2.6
1	J	298	TYR	2.6
1	F	200	GLN	2.6
1	H	441	ALA	2.6
1	P	222	GLU	2.6
1	J	327	CYS	2.6
2	M	29	ALA	2.6
1	L	239	GLY	2.6
1	N	39	SER	2.6
2	O	5	SER	2.6
1	N	344	ASP	2.5
1	J	310	THR	2.5
2	O	3	GLN	2.5
1	L	458	GLU	2.5
1	H	476	THR	2.5
1	D	182	TRP	2.5
1	F	224	VAL	2.4
2	O	35	PHE	2.4
2	K	6	THR	2.4
1	B	329	LEU	2.4
1	N	453	ARG	2.4
1	P	78	ARG	2.4
1	H	274	VAL	2.4
1	H	344	ASP	2.4
1	N	78	ARG	2.4
1	L	339	PRO	2.4
1	P	340	GLU	2.4
1	F	310	THR	2.4
1	J	220	ALA	2.4
2	K	35	PHE	2.4
1	F	340	GLU	2.4
1	H	340	GLU	2.3
2	K	70	GLU	2.3
1	P	483	LEU	2.3
1	B	311	VAL	2.3
1	P	378	ASN	2.3
1	D	78	ARG	2.3
1	H	226	GLN	2.3
1	L	379	TRP	2.3
2	M	28	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	481	ARG	2.3
1	L	341	ASP	2.3
1	N	483	LEU	2.3
2	O	74	VAL	2.2
2	C	55	MET	2.2
1	L	274	VAL	2.2
1	H	477	ASP	2.2
1	L	483	LEU	2.2
1	H	481	ARG	2.2
1	P	177	ILE	2.2
1	P	453	ARG	2.2
1	F	416	SER	2.2
1	D	329	LEU	2.1
1	J	329	LEU	2.1
1	J	222	GLU	2.1
1	L	378	ASN	2.1
1	H	442	ASP	2.1
1	J	341	ASP	2.1
2	K	76	VAL	2.1
1	B	298	TYR	2.1
2	K	56	SER	2.1
2	K	73	SER	2.1
1	J	224	VAL	2.0
1	H	311	VAL	2.0
1	N	311	VAL	2.0
1	F	311	VAL	2.0
1	L	329	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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,

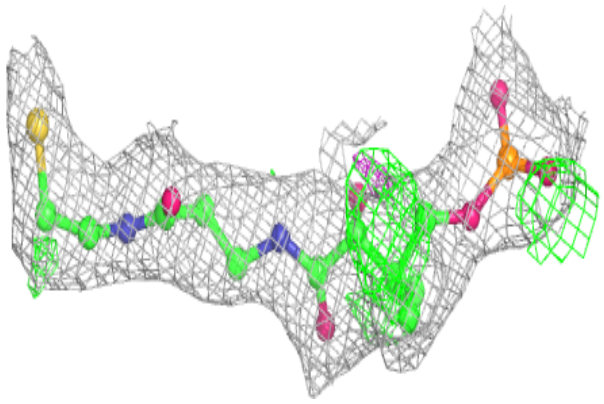
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

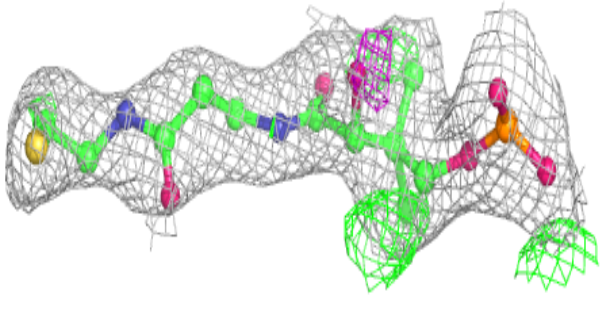
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	P	501	6/6	0.77	0.44	63,66,75,77	0
3	GOL	D	501	6/6	0.84	0.53	58,63,67,70	0
3	GOL	B	501	6/6	0.86	0.28	51,53,56,61	0
4	PNS	E	101	21/22	0.94	0.34	28,38,61,74	0
4	PNS	K	101	21/22	0.94	0.26	37,50,65,89	0
4	PNS	G	101	21/22	0.97	0.22	27,34,59,63	0
4	PNS	M	101	21/22	0.97	0.24	34,44,62,71	0
4	PNS	I	101	21/22	0.98	0.29	28,32,60,64	0
4	PNS	A	101	21/22	0.98	0.26	19,24,49,56	0
4	PNS	C	101	21/22	0.98	0.24	21,24,53,63	0
4	PNS	O	101	21/22	0.98	0.22	25,32,53,64	0

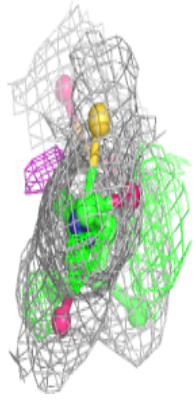
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PNS E 101:

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

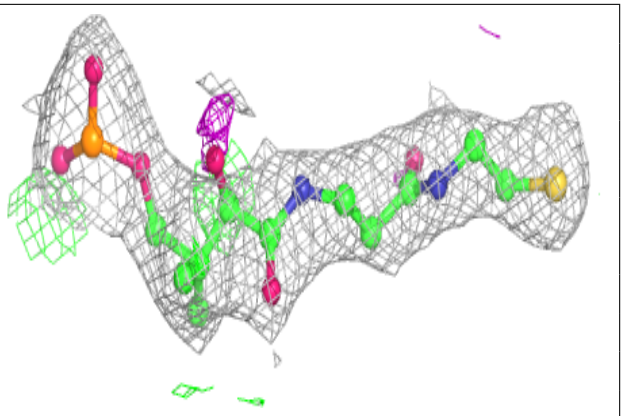


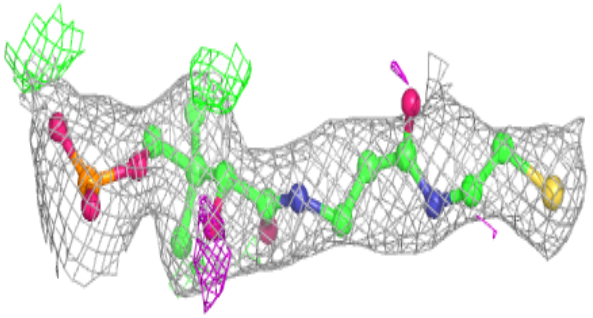


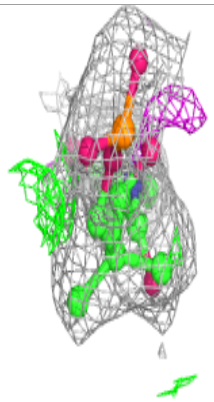


Electron density around PNS K 101:

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

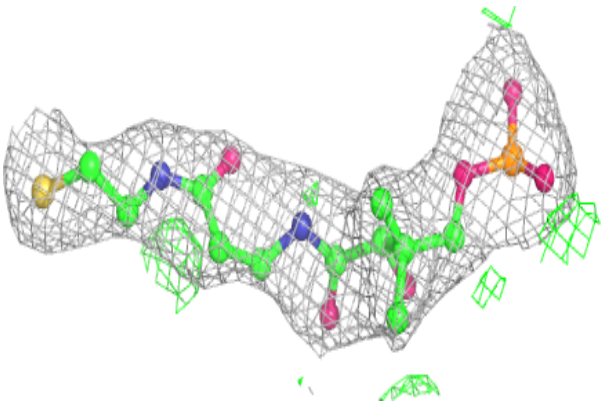


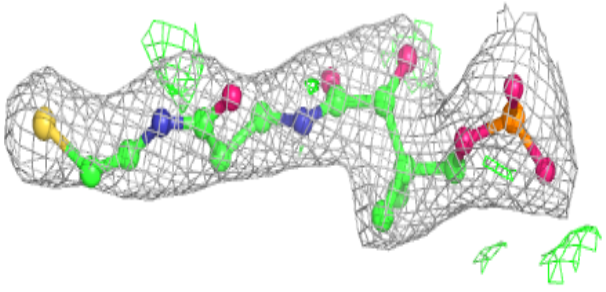


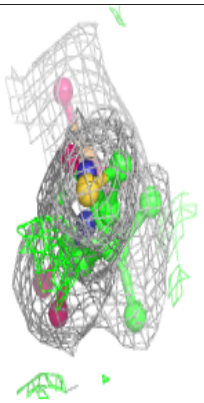


Electron density around PNS G 101:

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

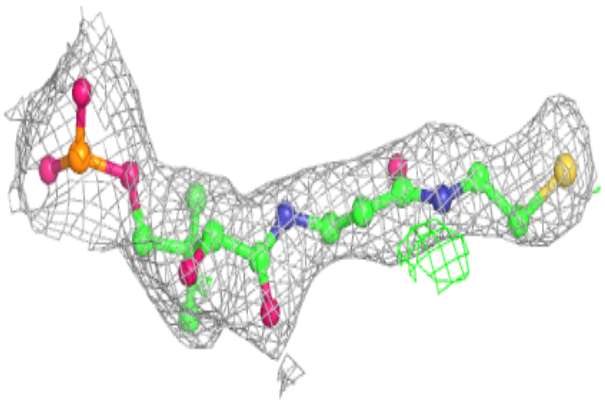


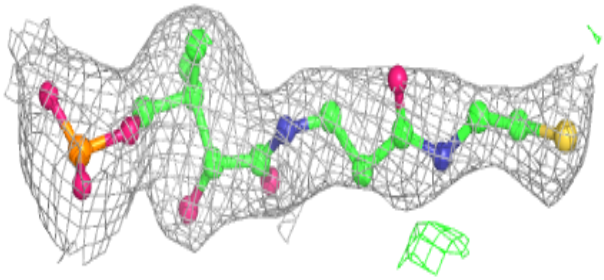


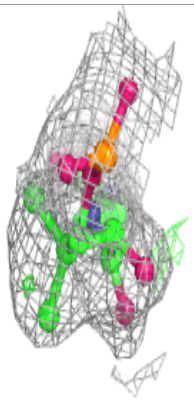


Electron density around PNS M 101:

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

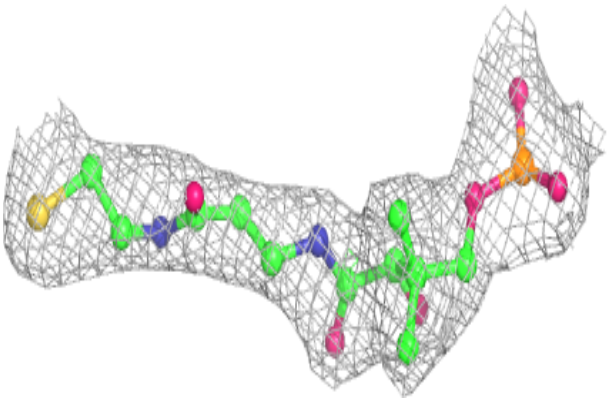


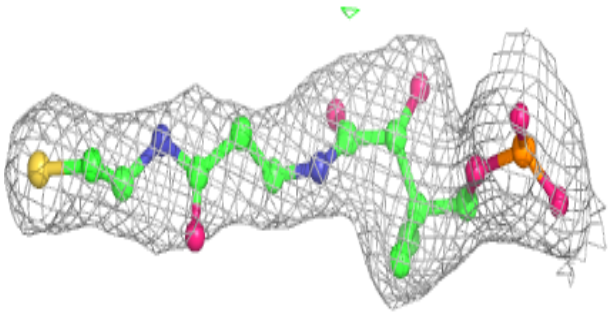


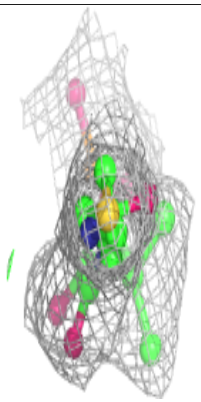


Electron density around PNS I 101:

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

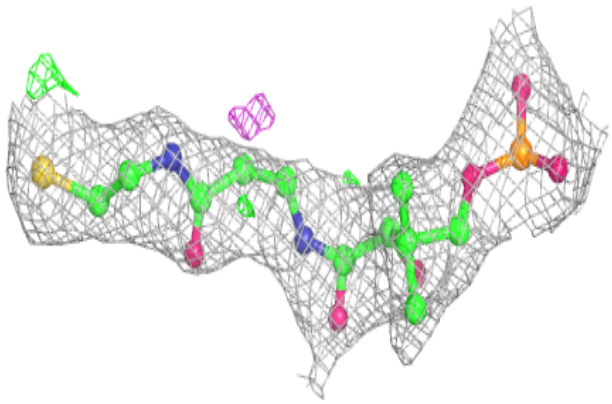


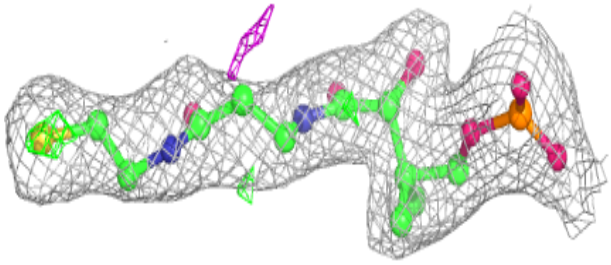


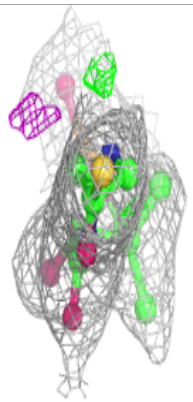


Electron density around PNS A 101:

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

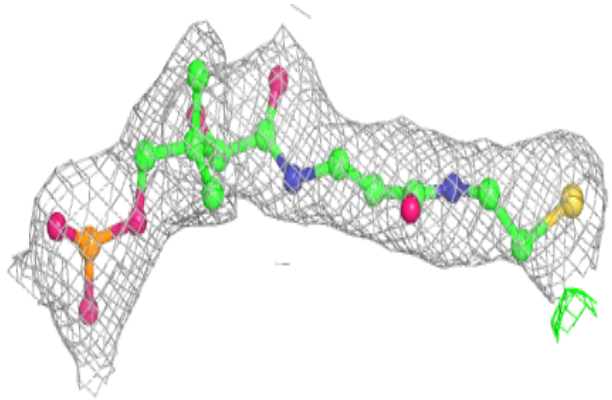


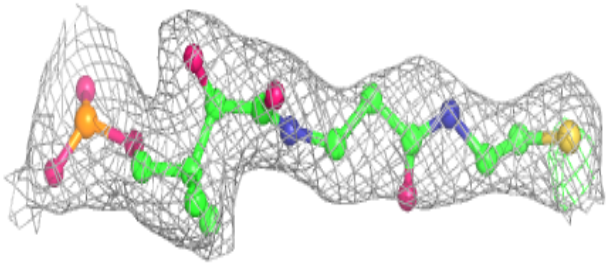


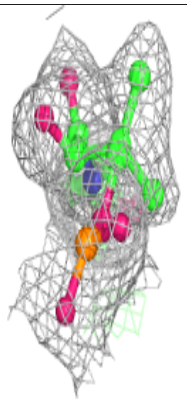


Electron density around PNS C 101:

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

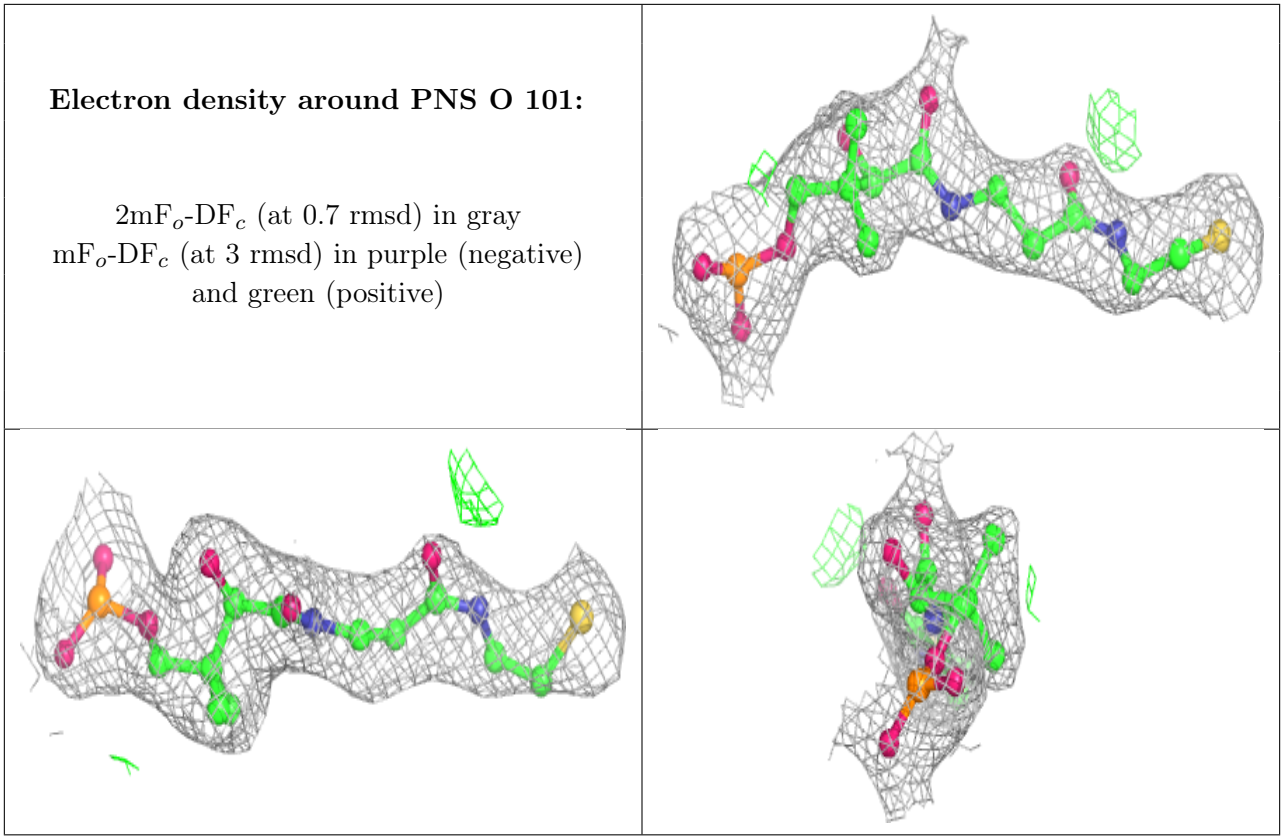






Electron density around PNS O 101:

$2mF_o$-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.