



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 8, 2025 – 02:32 PM EDT

PDB ID : 9NCU / pdb_00009ncu
Title : NitrOFF1 "OFF" State
Authors : Smailys, J.; Zhang, Y.
Deposited on : 2025-02-17
Resolution : 3.17 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

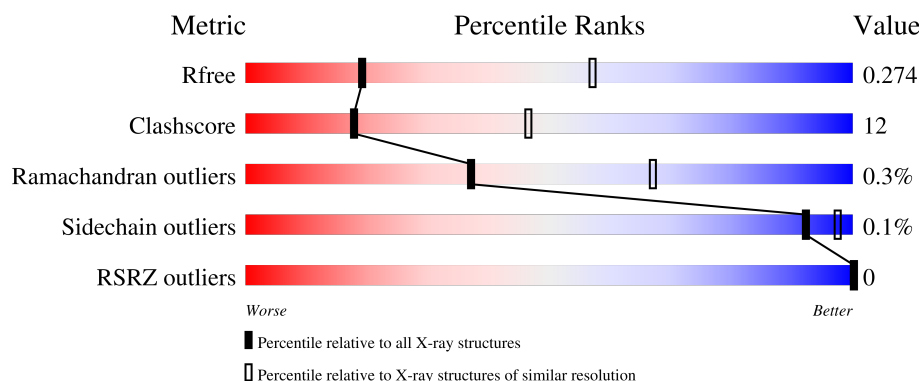
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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.










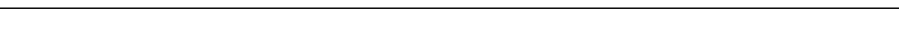
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1851 (3.20-3.16)
Clashscore	180529	1999 (3.20-3.16)
Ramachandran outliers	177936	1961 (3.20-3.16)
Sidechain outliers	177891	1960 (3.20-3.16)
RSRZ outliers	164620	1852 (3.20-3.16)

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	379	<div> <div style="width: 71%; background-color: green;"></div> <div style="width: 29%; background-color: yellow;"></div> <div style="width: 0%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>71% 29% .</div>
1	B	379	<div> <div style="width: 75%; background-color: green;"></div> <div style="width: 25%; background-color: yellow;"></div> <div style="width: 0%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>75% 25%</div>
1	C	379	<div> <div style="width: 73%; background-color: green;"></div> <div style="width: 26%; background-color: yellow;"></div> <div style="width: 0%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>73% 26% .</div>
1	D	379	<div> <div style="width: 75%; background-color: green;"></div> <div style="width: 24%; background-color: yellow;"></div> <div style="width: 0%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>75% 24% ..</div>
1	E	379	<div> <div style="width: 72%; background-color: green;"></div> <div style="width: 28%; background-color: yellow;"></div> <div style="width: 0%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>72% 28%</div>

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Mol	Chain	Length	Quality of chain
1	F	379	
1	G	379	
1	H	379	
1	I	379	
1	J	379	
1	K	379	
1	L	379	
1	M	379	
1	N	379	
1	O	379	
1	P	379	
1	Q	379	
1	R	379	

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
2	NO3	E	402	-	-	X	-
2	NO3	M	401	-	-	X	-
3	SO4	N	404	-	-	X	-
3	SO4	P	402	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 54506 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 Engineered fluorescent biosensor NitrOFF1 in the "OFF" State.

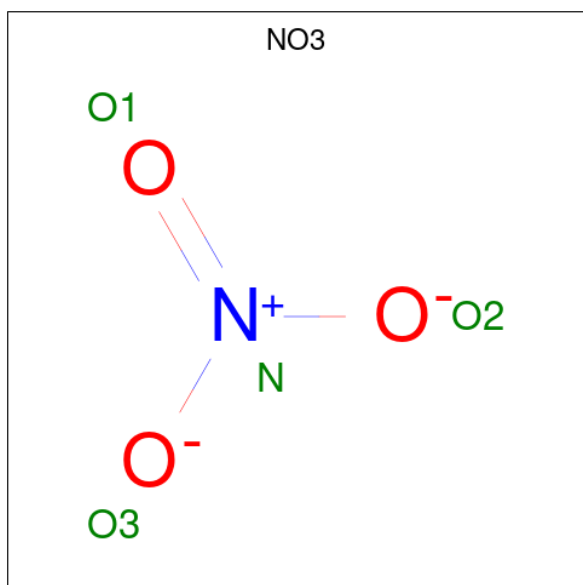
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	B	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	C	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	D	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	E	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	F	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	G	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	H	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	I	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	J	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	K	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	L	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	M	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	N	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	O	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	P	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			
1	R	379	Total	C	N	O	S	0	0	0
			3008	1915	510	576	7			

- Molecule 2 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



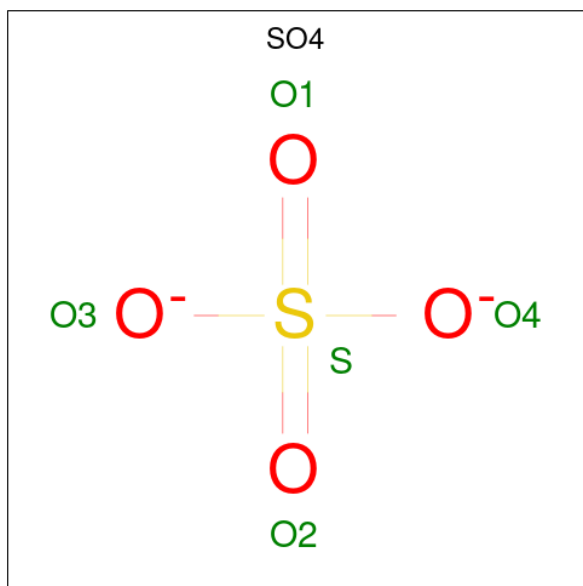
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	C	1	Total	N	O	0	0
			4	1	3		
2	D	1	Total	N	O	0	0
			4	1	3		
2	E	1	Total	N	O	0	0
			4	1	3		
2	F	1	Total	N	O	0	0
			4	1	3		
2	G	1	Total	N	O	0	0
			4	1	3		
2	H	1	Total	N	O	0	0
			4	1	3		
2	I	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	J	1	Total	N	O	0	0
			4	1	3		
2	K	1	Total	N	O	0	0
			4	1	3		
2	L	1	Total	N	O	0	0
			4	1	3		
2	M	1	Total	N	O	0	0
			4	1	3		
2	N	1	Total	N	O	0	0
			4	1	3		
2	O	1	Total	N	O	0	0
			4	1	3		
2	P	1	Total	N	O	0	0
			4	1	3		
2	Q	1	Total	N	O	0	0
			4	1	3		
2	R	1	Total	N	O	0	0
			4	1	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		

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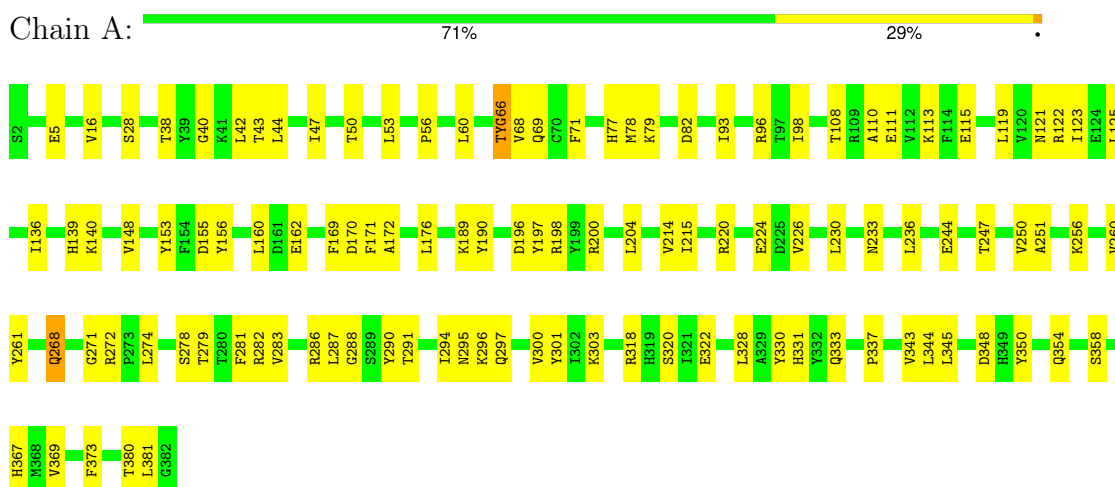
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		

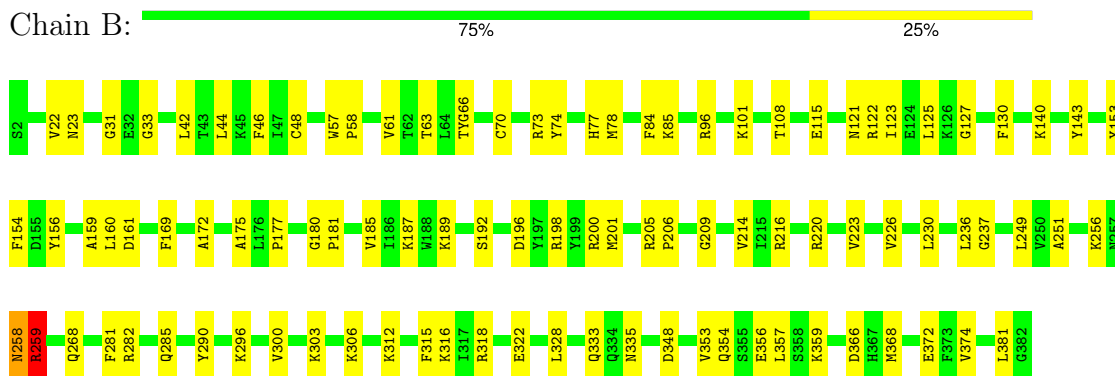
3 Residue-property plots

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

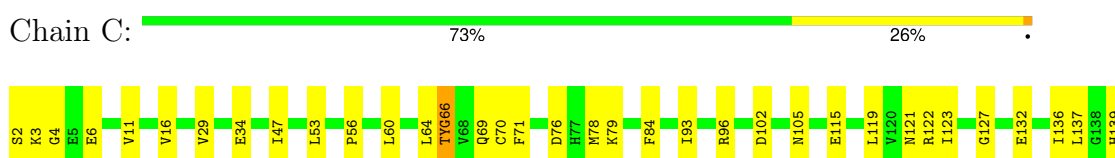
- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

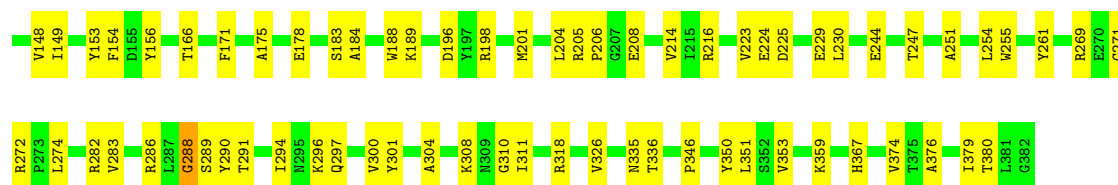


- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State



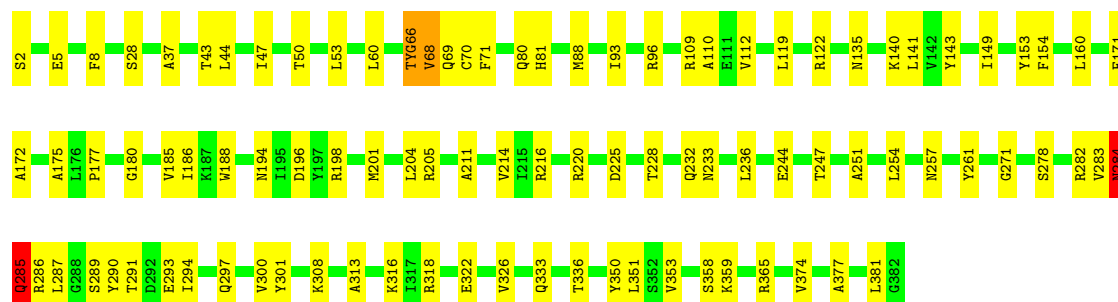
- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State





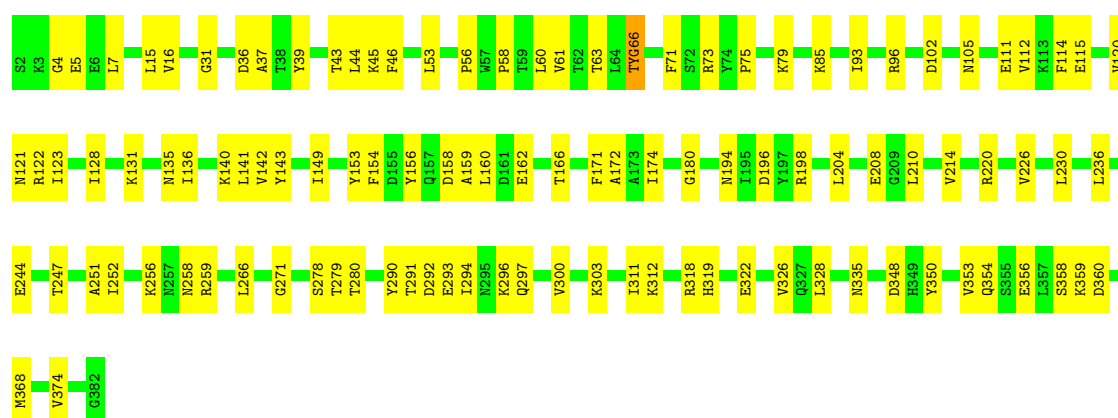
- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

Chain D: 75% 24% ..



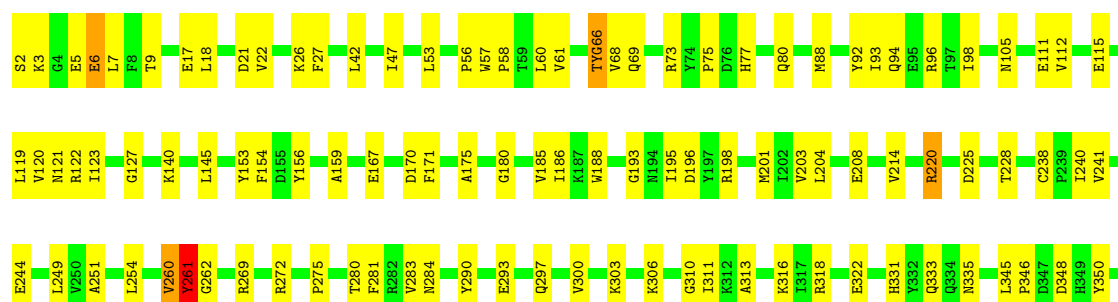
- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

Chain E: 72% 28%



- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

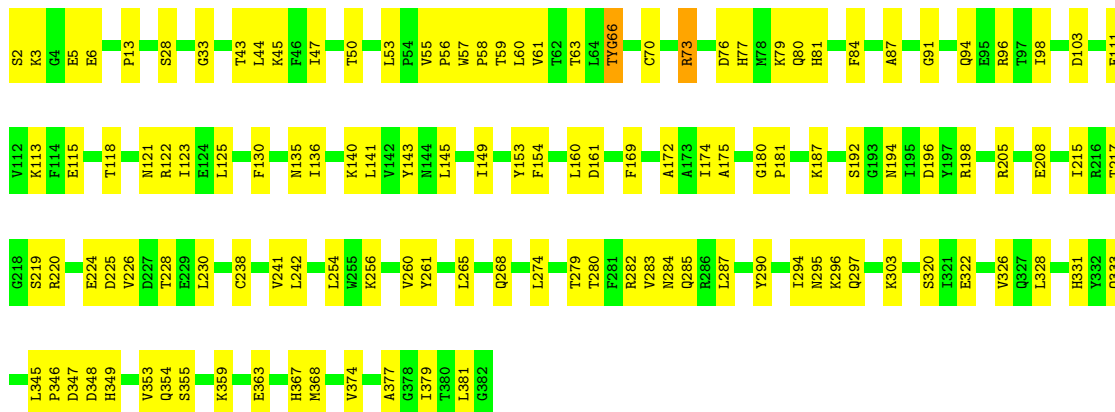
Chain F: 70% 29%





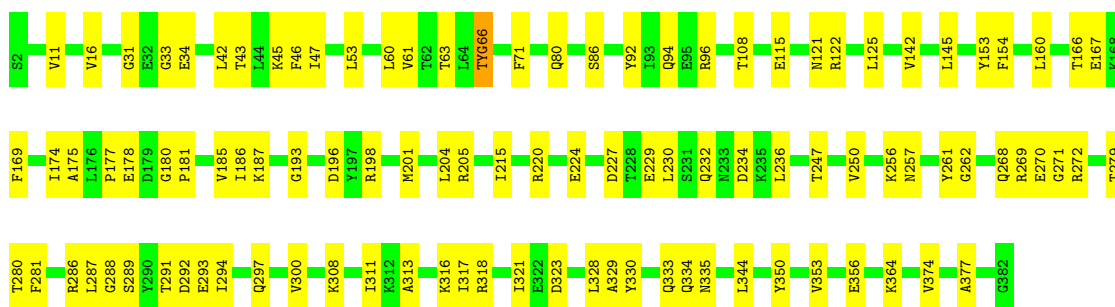
- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

Chain G: 68% 32% .



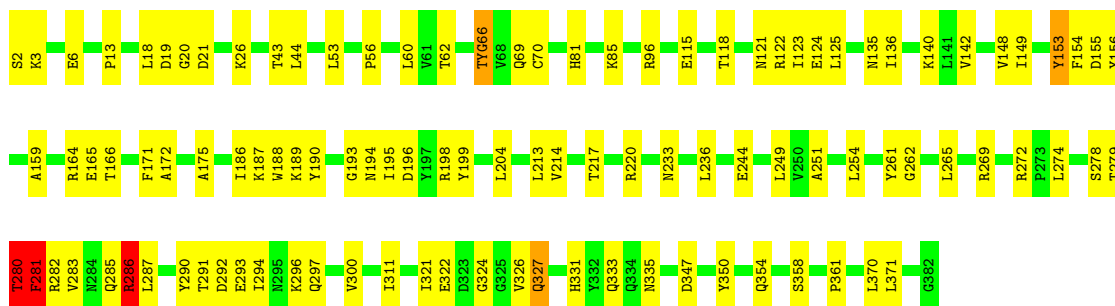
- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

Chain H: 73% 27%



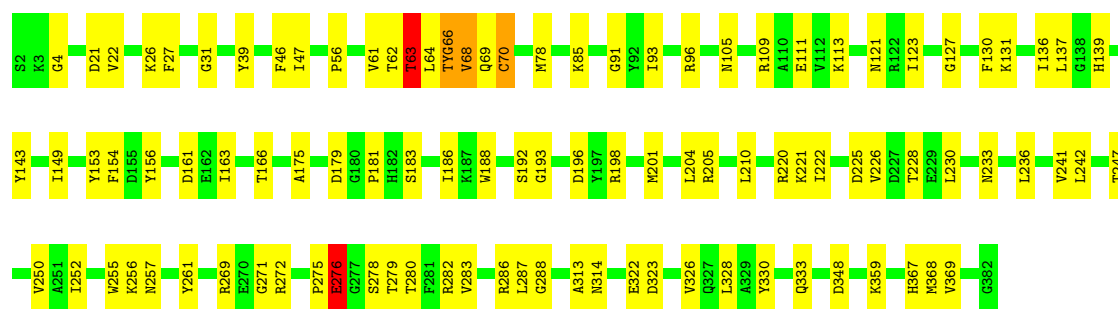
- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

Chain I: 72% 26% ..



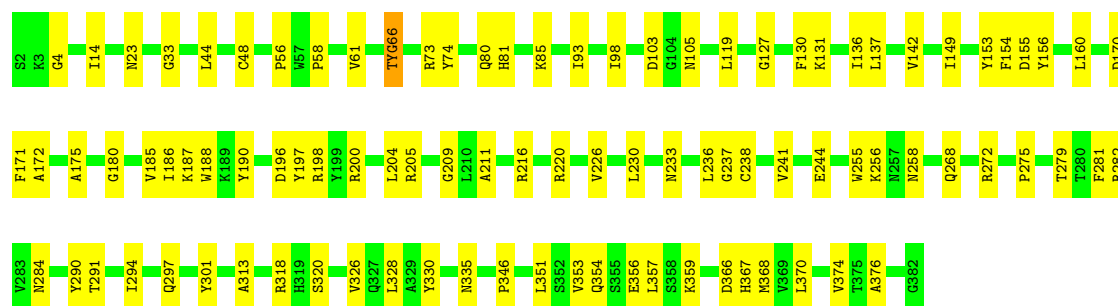
- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

Chain J: 73% 25% ..



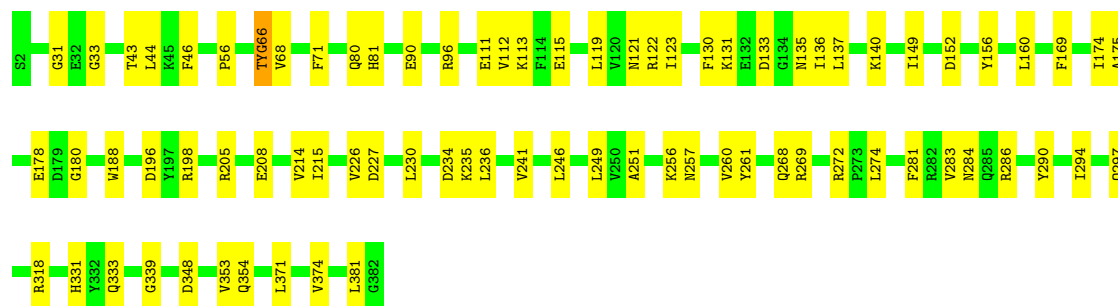
- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

Chain K: 75% 25%



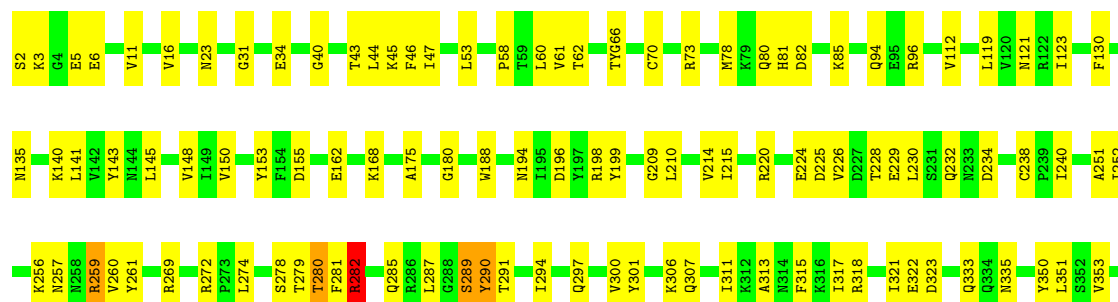
- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

Chain L: 79% 21%



- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

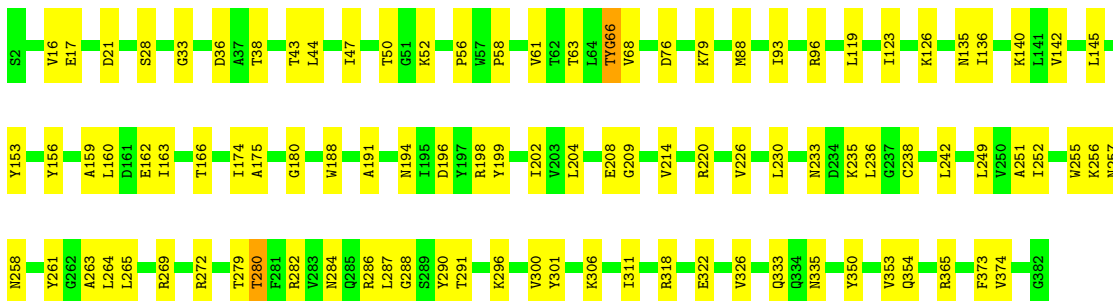
Chain M: 70% 28%





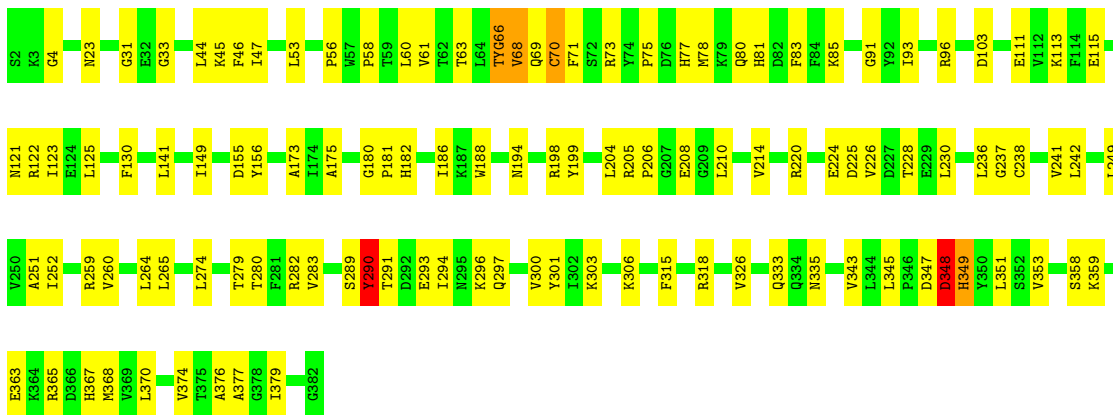
- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

Chain N: 74% 25% .



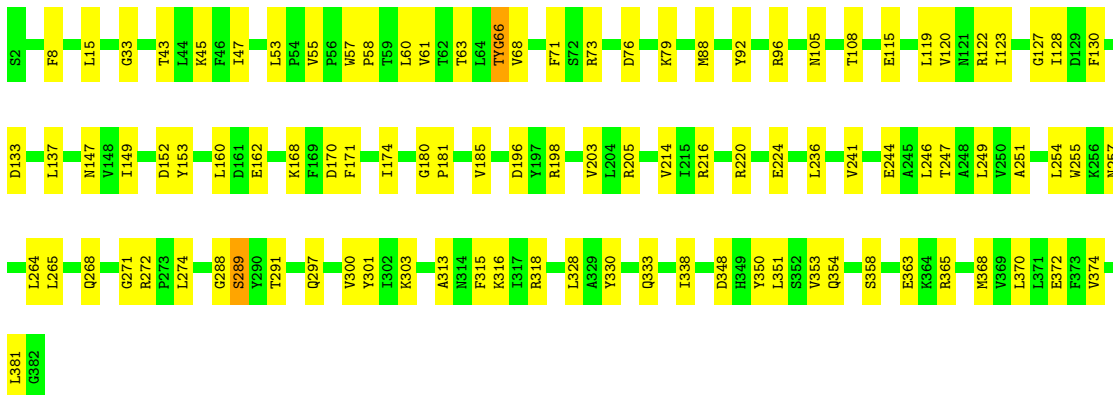
- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

Chain O: 69% 29% ..



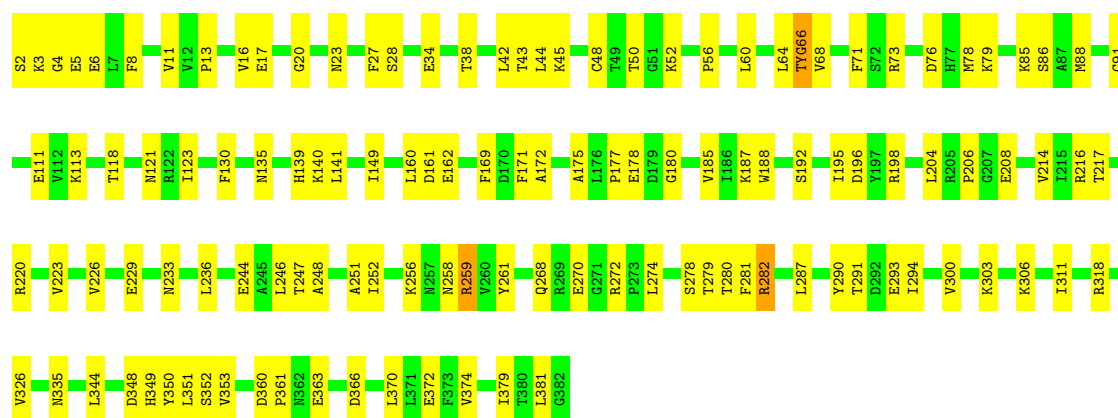
- Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

Chain P: 74% 26% .



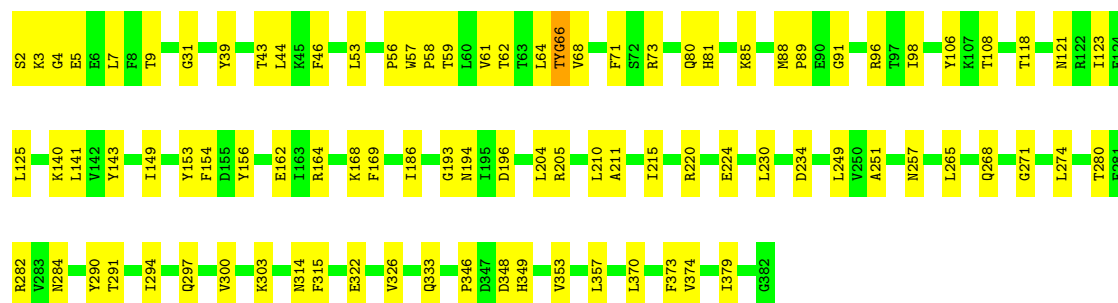
• Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

Chain Q:  67% 32%



• Molecule 1: Engineered fluorescent biosensor NitrOFF1 in the "OFF" State

Chain R:  76% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	275.60Å 275.60Å 438.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.83 – 3.17 49.83 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.83-3.17) 99.3 (49.83-3.17)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.228 , 0.272 0.229 , 0.274	Depositor DCC
R_{free} test set	2008 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 13.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.288 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	54506	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 1.81% 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: NO3, CRO, SO4

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	0.30	1/3048 (0.0%)	0.64	2/4124 (0.0%)
1	B	0.58	5/3048 (0.2%)	0.74	4/4124 (0.1%)
1	C	0.25	0/3048	0.80	4/4124 (0.1%)
1	D	0.34	1/3048 (0.0%)	0.96	12/4124 (0.3%)
1	E	0.25	0/3048	0.64	0/4124
1	F	0.28	0/3048	0.72	5/4124 (0.1%)
1	G	0.24	0/3048	0.63	2/4124 (0.0%)
1	H	0.24	0/3048	0.63	0/4124
1	I	0.28	0/3048	0.77	12/4124 (0.3%)
1	J	0.43	5/3048 (0.2%)	0.76	7/4124 (0.2%)
1	K	0.25	0/3048	0.63	0/4124
1	L	0.23	0/3048	0.61	0/4124
1	M	0.27	0/3048	0.71	3/4124 (0.1%)
1	N	0.24	0/3048	0.67	1/4124 (0.0%)
1	O	0.27	0/3048	0.73	5/4124 (0.1%)
1	P	0.22	0/3048	0.59	0/4124
1	Q	0.28	0/3048	0.70	3/4124 (0.1%)
1	R	0.27	0/3048	0.69	2/4124 (0.0%)
All	All	0.30	12/54864 (0.0%)	0.71	62/74232 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	3
1	I	0	3
1	J	0	3
1	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
1	M	0	2
All	All	0	14

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259	ARG	CZ-NH1	21.94	1.63	1.32
1	B	259	ARG	CZ-NH2	-11.50	1.18	1.33
1	J	276	GLU	CA-CB	10.37	1.70	1.53
1	B	259	ARG	CG-CD	-8.12	1.28	1.52
1	B	259	ARG	NE-CZ	-7.80	1.24	1.33

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	285	GLN	N-CA-C	-33.83	70.12	111.40
1	C	102	ASP	OD1-CG-OD2	-18.46	78.59	122.90
1	B	259	ARG	CG-CD-NE	17.23	149.92	112.00
1	C	102	ASP	CB-CG-OD2	-17.15	78.95	118.40
1	C	102	ASP	CB-CG-OD1	16.27	155.82	118.40

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	259	ARG	Sidechain
1	D	284	ASN	Peptide
1	D	285	GLN	Sidechain,Peptide
1	I	280	THR	Peptide
1	I	281	PHE	Sidechain

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	3008	0	2968	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3008	0	2968	77	0
1	C	3008	0	2968	78	0
1	D	3008	0	2966	77	0
1	E	3008	0	2968	77	0
1	F	3008	0	2968	109	0
1	G	3008	0	2968	81	0
1	H	3008	0	2968	80	0
1	I	3008	0	2968	87	0
1	J	3008	0	2967	70	0
1	K	3008	0	2968	69	0
1	L	3008	0	2968	60	0
1	M	3008	0	2968	82	0
1	N	3008	0	2968	84	0
1	O	3008	0	2967	91	0
1	P	3008	0	2968	73	0
1	Q	3008	0	2968	90	0
1	R	3008	0	2968	59	0
2	A	4	0	0	1	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	2	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	1	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0
2	M	4	0	0	2	0
2	N	4	0	0	0	0
2	O	4	0	0	0	0
2	P	4	0	0	0	0
2	Q	4	0	0	0	0
2	R	4	0	0	1	0
3	A	20	0	0	0	0
3	B	15	0	0	1	0
3	C	15	0	0	0	0
3	D	15	0	0	1	0
3	E	20	0	0	1	0
3	F	15	0	0	1	0
3	G	15	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	15	0	0	0	0
3	I	20	0	0	0	0
3	J	15	0	0	0	0
3	K	15	0	0	2	0
3	L	20	0	0	1	0
3	M	15	0	0	0	0
3	N	25	0	0	2	0
3	O	10	0	0	1	0
3	P	10	0	0	2	0
3	Q	10	0	0	1	0
3	R	20	0	0	1	0
All	All	54506	0	53420	1302	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 12.

The worst 5 of 1302 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:Q:220:ARG:NH2	1:Q:278:SER:O	1.88	1.04
1:J:220:ARG:NH2	1:J:278:SER:O	1.94	1.00
1:H:94:GLN:HG2	1:H:335:ASN:HD21	1.28	0.98
1:O:348:ASP:O	1:O:349:HIS:ND1	1.98	0.96
1:E:220:ARG:NH2	1:E:278:SER:O	2.02	0.92

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	374/379 (99%)	360 (96%)	14 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	374/379 (99%)	364 (97%)	10 (3%)	0	100	100
1	C	374/379 (99%)	360 (96%)	14 (4%)	0	100	100
1	D	374/379 (99%)	359 (96%)	14 (4%)	1 (0%)	37	67
1	E	374/379 (99%)	360 (96%)	14 (4%)	0	100	100
1	F	374/379 (99%)	356 (95%)	16 (4%)	2 (0%)	25	58
1	G	374/379 (99%)	364 (97%)	10 (3%)	0	100	100
1	H	374/379 (99%)	363 (97%)	11 (3%)	0	100	100
1	I	374/379 (99%)	359 (96%)	13 (4%)	2 (0%)	25	58
1	J	374/379 (99%)	359 (96%)	14 (4%)	1 (0%)	37	67
1	K	374/379 (99%)	359 (96%)	15 (4%)	0	100	100
1	L	374/379 (99%)	360 (96%)	13 (4%)	1 (0%)	37	67
1	M	374/379 (99%)	358 (96%)	12 (3%)	4 (1%)	12	42
1	N	374/379 (99%)	360 (96%)	13 (4%)	1 (0%)	37	67
1	O	374/379 (99%)	359 (96%)	11 (3%)	4 (1%)	12	42
1	P	374/379 (99%)	361 (96%)	12 (3%)	1 (0%)	37	67
1	Q	374/379 (99%)	361 (96%)	12 (3%)	1 (0%)	37	67
1	R	374/379 (99%)	362 (97%)	11 (3%)	1 (0%)	37	67
All	All	6732/6822 (99%)	6484 (96%)	229 (3%)	19 (0%)	37	67

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	290	TYR
1	O	348	ASP
1	D	70	CYS
1	F	6	GLU
1	F	261	TYR

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	324/324 (100%)	324 (100%)	0	100	100
1	B	324/324 (100%)	324 (100%)	0	100	100
1	C	324/324 (100%)	324 (100%)	0	100	100
1	D	324/324 (100%)	324 (100%)	0	100	100
1	E	324/324 (100%)	324 (100%)	0	100	100
1	F	324/324 (100%)	324 (100%)	0	100	100
1	G	324/324 (100%)	324 (100%)	0	100	100
1	H	324/324 (100%)	324 (100%)	0	100	100
1	I	324/324 (100%)	324 (100%)	0	100	100
1	J	324/324 (100%)	322 (99%)	2 (1%)	84	92
1	K	324/324 (100%)	324 (100%)	0	100	100
1	L	324/324 (100%)	324 (100%)	0	100	100
1	M	324/324 (100%)	324 (100%)	0	100	100
1	N	324/324 (100%)	324 (100%)	0	100	100
1	O	324/324 (100%)	324 (100%)	0	100	100
1	P	324/324 (100%)	324 (100%)	0	100	100
1	Q	324/324 (100%)	323 (100%)	1 (0%)	91	95
1	R	324/324 (100%)	324 (100%)	0	100	100
All	All	5832/5832 (100%)	5829 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	63	THR
1	J	70	CYS
1	Q	17	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	268	GLN
1	Q	297	GLN
1	J	314	ASN
1	Q	285	GLN
1	P	257	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues 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$
1	CRO	P	66	1	22,23,24	0.59	0	30,32,34	1.06	1 (3%)
1	CRO	D	66	1	22,23,24	0.62	0	30,32,34	2.22	7 (23%)
1	CRO	J	66	1	22,23,24	0.71	0	30,32,34	3.49	11 (36%)
1	CRO	I	66	1	22,23,24	0.58	0	30,32,34	0.92	2 (6%)
1	CRO	L	66	1	22,23,24	0.60	0	30,32,34	1.11	2 (6%)
1	CRO	M	66	1	22,23,24	0.57	0	30,32,34	0.81	1 (3%)
1	CRO	O	66	1	22,23,24	0.62	0	30,32,34	2.07	6 (20%)
1	CRO	Q	66	1	22,23,24	0.58	0	30,32,34	0.86	1 (3%)
1	CRO	C	66	1	22,23,24	0.52	0	30,32,34	0.84	1 (3%)
1	CRO	G	66	1	22,23,24	0.54	0	30,32,34	0.88	1 (3%)
1	CRO	R	66	1	22,23,24	0.58	0	30,32,34	0.91	2 (6%)
1	CRO	A	66	1	22,23,24	0.54	0	30,32,34	0.97	2 (6%)
1	CRO	B	66	1	22,23,24	0.54	0	30,32,34	0.79	0
1	CRO	H	66	1	22,23,24	0.54	0	30,32,34	0.99	2 (6%)
1	CRO	F	66	1	22,23,24	0.57	0	30,32,34	0.91	2 (6%)
1	CRO	N	66	1	22,23,24	0.62	0	30,32,34	1.32	4 (13%)
1	CRO	E	66	1	22,23,24	0.54	0	30,32,34	0.95	2 (6%)
1	CRO	K	66	1	22,23,24	0.54	0	30,32,34	0.94	2 (6%)

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
1	CRO	P	66	1	-	0/12/31/32	0/2/2/2
1	CRO	D	66	1	-	3/12/31/32	0/2/2/2
1	CRO	J	66	1	-	6/12/31/32	0/2/2/2
1	CRO	I	66	1	-	5/12/31/32	0/2/2/2
1	CRO	L	66	1	-	2/12/31/32	0/2/2/2
1	CRO	M	66	1	-	1/12/31/32	0/2/2/2
1	CRO	O	66	1	-	2/12/31/32	0/2/2/2
1	CRO	Q	66	1	-	4/12/31/32	0/2/2/2
1	CRO	C	66	1	-	4/12/31/32	0/2/2/2
1	CRO	G	66	1	-	4/12/31/32	0/2/2/2
1	CRO	R	66	1	-	1/12/31/32	0/2/2/2
1	CRO	A	66	1	-	1/12/31/32	0/2/2/2
1	CRO	B	66	1	-	0/12/31/32	0/2/2/2
1	CRO	H	66	1	-	0/12/31/32	0/2/2/2
1	CRO	F	66	1	-	2/12/31/32	0/2/2/2
1	CRO	N	66	1	-	0/12/31/32	0/2/2/2
1	CRO	E	66	1	-	1/12/31/32	0/2/2/2
1	CRO	K	66	1	-	1/12/31/32	0/2/2/2

There are no bond length outliers.

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	66	CRO	C1-CA1-N1	11.69	130.69	109.78
1	J	66	CRO	C2-N3-C1	-9.99	103.44	108.07
1	D	66	CRO	C2-N3-C1	-8.43	104.17	108.07
1	O	66	CRO	C2-N3-C1	-7.97	104.38	108.07
1	J	66	CRO	CA1-C1-N3	4.85	130.43	124.69

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRO	C2-CA2-CB2-CG2
1	C	66	CRO	N1-CA1-CB1-CG1
1	C	66	CRO	C1-CA1-CB1-CG1
1	C	66	CRO	C1-CA1-CB1-OG1
1	E	66	CRO	C2-CA2-CB2-CG2

There are no ring outliers.

17 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	66	CRO	2	0
1	D	66	CRO	5	0
1	J	66	CRO	4	0
1	I	66	CRO	2	0
1	L	66	CRO	2	0
1	O	66	CRO	2	0
1	Q	66	CRO	2	0
1	C	66	CRO	2	0
1	G	66	CRO	1	0
1	R	66	CRO	1	0
1	A	66	CRO	2	0
1	B	66	CRO	1	0
1	H	66	CRO	3	0
1	F	66	CRO	2	0
1	N	66	CRO	2	0
1	E	66	CRO	1	0
1	K	66	CRO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

76 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	405	-	4,4,4	0.25	0	6,6,6	0.16	0
3	SO4	O	403	-	4,4,4	0.23	0	6,6,6	0.13	0
2	NO3	N	401	-	1,3,3	0.48	0	0,3,3	-	-
3	SO4	G	403	-	4,4,4	0.24	0	6,6,6	0.17	0
3	SO4	H	404	-	4,4,4	0.26	0	6,6,6	0.08	0
3	SO4	M	402	-	4,4,4	0.23	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	402	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	H	401	-	4,4,4	0.24	0	6,6,6	0.17	0
3	SO4	K	401	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	G	402	-	4,4,4	0.23	0	6,6,6	0.15	0
3	SO4	P	403	-	4,4,4	0.22	0	6,6,6	0.10	0
2	NO3	B	401	-	1,3,3	0.52	0	0,3,3	-	-
2	NO3	L	401	-	1,3,3	0.51	0	0,3,3	-	-
2	NO3	P	401	-	1,3,3	0.51	0	0,3,3	-	-
3	SO4	F	402	-	4,4,4	0.24	0	6,6,6	0.11	0
2	NO3	Q	401	-	1,3,3	0.45	0	0,3,3	-	-
3	SO4	I	405	-	4,4,4	0.24	0	6,6,6	0.16	0
3	SO4	R	403	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	N	402	-	4,4,4	0.22	0	6,6,6	0.15	0
2	NO3	I	402	-	1,3,3	0.49	0	0,3,3	-	-
3	SO4	A	403	-	4,4,4	0.24	0	6,6,6	0.18	0
3	SO4	L	403	-	4,4,4	0.23	0	6,6,6	0.16	0
2	NO3	D	401	-	1,3,3	0.47	0	0,3,3	-	-
2	NO3	J	402	-	1,3,3	0.48	0	0,3,3	-	-
3	SO4	D	402	-	4,4,4	0.23	0	6,6,6	0.20	0
3	SO4	L	402	-	4,4,4	0.26	0	6,6,6	0.19	0
3	SO4	Q	402	-	4,4,4	0.22	0	6,6,6	0.16	0
3	SO4	R	401	-	4,4,4	0.25	0	6,6,6	0.15	0
3	SO4	E	403	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	O	402	-	4,4,4	0.23	0	6,6,6	0.21	0
2	NO3	M	401	-	1,3,3	0.39	0	0,3,3	-	-
3	SO4	D	403	-	4,4,4	0.22	0	6,6,6	0.13	0
2	NO3	C	401	-	1,3,3	0.50	0	0,3,3	-	-
3	SO4	Q	403	-	4,4,4	0.25	0	6,6,6	0.19	0
3	SO4	J	403	-	4,4,4	0.26	0	6,6,6	0.14	0
2	NO3	A	401	-	1,3,3	0.56	0	0,3,3	-	-
3	SO4	A	404	-	4,4,4	0.26	0	6,6,6	0.12	0
3	SO4	I	401	-	4,4,4	0.24	0	6,6,6	0.16	0
3	SO4	P	402	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	L	404	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	K	404	-	4,4,4	0.22	0	6,6,6	0.16	0
3	SO4	E	404	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	J	401	-	4,4,4	0.26	0	6,6,6	0.31	0
3	SO4	R	404	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	B	402	-	4,4,4	0.23	0	6,6,6	0.09	0
2	NO3	F	401	-	1,3,3	0.42	0	0,3,3	-	-
3	SO4	B	404	-	4,4,4	0.23	0	6,6,6	0.18	0
3	SO4	F	404	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	402	-	4,4,4	0.24	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NO3	K	402	-	1,3,3	0.61	0	0,3,3	-	-
3	SO4	I	404	-	4,4,4	0.25	0	6,6,6	0.13	0
2	NO3	E	402	-	1,3,3	0.32	0	0,3,3	-	-
3	SO4	B	403	-	4,4,4	0.23	0	6,6,6	0.27	0
2	NO3	O	401	-	1,3,3	0.45	0	0,3,3	-	-
3	SO4	H	402	-	4,4,4	0.23	0	6,6,6	0.26	0
3	SO4	E	405	-	4,4,4	0.26	0	6,6,6	0.15	0
3	SO4	M	403	-	4,4,4	0.25	0	6,6,6	0.16	0
2	NO3	G	401	-	1,3,3	0.50	0	0,3,3	-	-
3	SO4	C	403	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	J	404	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	I	403	-	4,4,4	0.26	0	6,6,6	0.11	0
3	SO4	D	404	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	C	404	-	4,4,4	0.23	0	6,6,6	0.15	0
3	SO4	N	404	-	4,4,4	0.23	0	6,6,6	0.20	0
3	SO4	N	405	-	4,4,4	0.25	0	6,6,6	0.17	0
3	SO4	K	403	-	4,4,4	0.23	0	6,6,6	0.10	0
2	NO3	R	402	-	1,3,3	0.39	0	0,3,3	-	-
3	SO4	N	403	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	M	404	-	4,4,4	0.24	0	6,6,6	0.05	0
3	SO4	E	401	-	4,4,4	0.23	0	6,6,6	0.18	0
3	SO4	N	406	-	4,4,4	0.25	0	6,6,6	0.23	0
3	SO4	R	405	-	4,4,4	0.24	0	6,6,6	0.17	0
3	SO4	F	403	-	4,4,4	0.25	0	6,6,6	0.17	0
3	SO4	G	404	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	L	405	-	4,4,4	0.23	0	6,6,6	0.18	0
2	NO3	H	403	-	1,3,3	0.40	0	0,3,3	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	401	SO4	1	0
3	G	402	SO4	1	0
3	R	403	SO4	1	0
2	J	402	NO3	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	402	SO4	1	0
2	M	401	NO3	2	0
3	Q	403	SO4	1	0
2	A	401	NO3	1	0
3	P	402	SO4	2	0
3	L	404	SO4	1	0
3	K	404	SO4	1	0
3	E	404	SO4	1	0
3	B	402	SO4	1	0
2	E	402	NO3	2	0
3	D	404	SO4	1	0
3	N	404	SO4	2	0
2	R	402	NO3	1	0
3	F	403	SO4	1	0
3	G	404	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	378/379 (99%)	-1.98	0 100 100	15, 36, 59, 85	0
1	B	378/379 (99%)	-1.99	0 100 100	12, 33, 51, 79	0
1	C	378/379 (99%)	-1.99	0 100 100	16, 37, 57, 88	0
1	D	378/379 (99%)	-1.96	0 100 100	16, 38, 60, 80	0
1	E	378/379 (99%)	-1.95	0 100 100	13, 38, 60, 74	0
1	F	378/379 (99%)	-2.01	0 100 100	14, 27, 47, 73	0
1	G	378/379 (99%)	-1.97	0 100 100	17, 41, 60, 89	0
1	H	378/379 (99%)	-1.97	0 100 100	17, 37, 56, 89	0
1	I	378/379 (99%)	-1.96	0 100 100	19, 41, 62, 83	0
1	J	378/379 (99%)	-2.02	0 100 100	15, 28, 48, 78	0
1	K	378/379 (99%)	-1.97	0 100 100	19, 37, 58, 81	0
1	L	378/379 (99%)	-1.98	0 100 100	20, 38, 59, 80	0
1	M	378/379 (99%)	-2.03	0 100 100	12, 25, 48, 65	0
1	N	378/379 (99%)	-2.01	0 100 100	13, 26, 47, 73	0
1	O	378/379 (99%)	-1.96	0 100 100	21, 37, 56, 73	0
1	P	378/379 (99%)	-1.95	0 100 100	22, 43, 64, 80	0
1	Q	378/379 (99%)	-1.99	0 100 100	11, 34, 53, 73	0
1	R	378/379 (99%)	-1.96	0 100 100	22, 44, 62, 85	0
All	All	6804/6822 (99%)	-1.98	0 100 100	11, 36, 58, 89	0

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CRO	G	66	22/23	0.99	0.04	35,50,66,70	0
1	CRO	B	66	22/23	1.00	0.02	14,31,39,43	0
1	CRO	C	66	22/23	1.00	0.03	26,41,57,84	0
1	CRO	D	66	22/23	1.00	0.03	27,41,52,55	0
1	CRO	E	66	22/23	1.00	0.02	27,36,53,71	0
1	CRO	F	66	22/23	1.00	0.03	18,32,46,52	0
1	CRO	A	66	22/23	1.00	0.02	21,32,41,62	0
1	CRO	H	66	22/23	1.00	0.03	26,39,55,64	0
1	CRO	I	66	22/23	1.00	0.03	32,44,59,65	0
1	CRO	J	66	22/23	1.00	0.03	20,30,47,67	0
1	CRO	K	66	22/23	1.00	0.03	33,43,53,67	0
1	CRO	L	66	22/23	1.00	0.02	22,43,52,77	0
1	CRO	M	66	22/23	1.00	0.02	12,20,28,40	0
1	CRO	N	66	22/23	1.00	0.02	14,24,34,36	0
1	CRO	O	66	22/23	1.00	0.03	25,44,53,62	0
1	CRO	P	66	22/23	1.00	0.03	35,46,58,60	0
1	CRO	Q	66	22/23	1.00	0.02	19,35,42,66	0
1	CRO	R	66	22/23	1.00	0.03	29,49,57,68	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	403	5/5	0.99	0.06	48,56,75,91	0
3	SO4	D	403	5/5	0.99	0.03	30,51,70,71	0
3	SO4	E	405	5/5	0.99	0.05	45,62,65,92	0
3	SO4	F	404	5/5	0.99	0.05	30,32,58,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	H	404	5/5	0.99	0.03	41,56,82,99	0
3	SO4	I	405	5/5	0.99	0.04	52,60,73,100	0
3	SO4	L	405	5/5	0.99	0.04	36,39,90,92	0
3	SO4	M	404	5/5	0.99	0.03	44,47,65,67	0
3	SO4	N	404	5/5	0.99	0.04	47,55,71,88	0
3	SO4	N	406	5/5	0.99	0.05	41,47,86,92	0
3	SO4	O	403	5/5	0.99	0.02	42,50,81,85	0
3	SO4	P	403	5/5	0.99	0.02	46,58,75,79	0
3	SO4	R	401	5/5	0.99	0.04	50,57,64,90	0
3	SO4	R	405	5/5	0.99	0.02	40,64,76,103	0
2	NO3	O	401	4/4	1.00	0.03	26,28,28,40	0
2	NO3	P	401	4/4	1.00	0.02	28,33,36,40	0
2	NO3	Q	401	4/4	1.00	0.02	21,25,34,41	0
2	NO3	R	402	4/4	1.00	0.03	24,27,29,39	0
3	SO4	A	402	5/5	1.00	0.01	29,31,57,60	0
2	NO3	A	401	4/4	1.00	0.02	32,35,37,38	0
3	SO4	A	404	5/5	1.00	0.02	37,45,75,80	0
3	SO4	A	405	5/5	1.00	0.03	42,47,73,78	0
3	SO4	B	402	5/5	1.00	0.02	20,23,40,48	0
3	SO4	B	403	5/5	1.00	0.04	29,37,59,62	0
3	SO4	B	404	5/5	1.00	0.05	34,37,71,72	0
3	SO4	C	402	5/5	1.00	0.02	34,41,48,59	0
3	SO4	C	403	5/5	1.00	0.02	37,43,82,87	0
3	SO4	C	404	5/5	1.00	0.04	38,50,54,74	0
3	SO4	D	402	5/5	1.00	0.02	26,41,57,59	0
2	NO3	B	401	4/4	1.00	0.02	21,22,28,34	0
3	SO4	D	404	5/5	1.00	0.04	48,51,79,90	0
3	SO4	E	401	5/5	1.00	0.03	25,26,43,45	0
3	SO4	E	403	5/5	1.00	0.04	34,56,72,85	0
3	SO4	E	404	5/5	1.00	0.02	48,50,67,68	0
2	NO3	C	401	4/4	1.00	0.02	27,28,35,35	0
3	SO4	F	402	5/5	1.00	0.02	33,43,62,65	0
3	SO4	F	403	5/5	1.00	0.02	43,50,72,81	0
2	NO3	D	401	4/4	1.00	0.02	27,31,36,38	0
3	SO4	G	402	5/5	1.00	0.03	37,43,44,48	0
3	SO4	G	403	5/5	1.00	0.02	41,49,84,90	0
3	SO4	G	404	5/5	1.00	0.03	53,60,64,84	0
3	SO4	H	401	5/5	1.00	0.02	20,24,45,63	0
3	SO4	H	402	5/5	1.00	0.02	36,48,59,74	0
2	NO3	E	402	4/4	1.00	0.01	33,33,38,42	0
3	SO4	I	401	5/5	1.00	0.02	19,35,49,50	0
3	SO4	I	403	5/5	1.00	0.02	38,47,54,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	I	404	5/5	1.00	0.03	57,72,81,104	0
2	NO3	F	401	4/4	1.00	0.02	13,18,27,33	0
3	SO4	J	401	5/5	1.00	0.03	22,45,48,48	0
3	SO4	J	403	5/5	1.00	0.01	21,28,56,70	0
3	SO4	J	404	5/5	1.00	0.04	40,44,74,78	0
3	SO4	K	401	5/5	1.00	0.01	30,32,59,61	0
3	SO4	K	403	5/5	1.00	0.04	42,49,67,67	0
3	SO4	K	404	5/5	1.00	0.03	50,54,64,64	0
3	SO4	L	402	5/5	1.00	0.02	17,22,40,62	0
3	SO4	L	403	5/5	1.00	0.04	43,46,62,69	0
3	SO4	L	404	5/5	1.00	0.02	50,54,59,76	0
2	NO3	G	401	4/4	1.00	0.02	25,28,28,30	0
3	SO4	M	402	5/5	1.00	0.02	33,33,54,61	0
3	SO4	M	403	5/5	1.00	0.02	18,39,43,50	0
2	NO3	H	403	4/4	1.00	0.02	29,31,34,42	0
3	SO4	N	402	5/5	1.00	0.02	20,33,39,57	0
3	SO4	N	403	5/5	1.00	0.05	41,43,61,65	0
2	NO3	I	402	4/4	1.00	0.04	32,32,33,39	0
3	SO4	N	405	5/5	1.00	0.03	42,46,55,92	0
2	NO3	J	402	4/4	1.00	0.02	20,20,26,26	0
3	SO4	O	402	5/5	1.00	0.04	24,43,50,54	0
2	NO3	K	402	4/4	1.00	0.02	23,28,42,44	0
3	SO4	P	402	5/5	1.00	0.03	20,36,52,60	0
2	NO3	L	401	4/4	1.00	0.02	32,35,37,41	0
3	SO4	Q	402	5/5	1.00	0.02	26,39,56,67	0
3	SO4	Q	403	5/5	1.00	0.02	49,52,58,78	0
2	NO3	M	401	4/4	1.00	0.01	13,14,18,29	0
3	SO4	R	403	5/5	1.00	0.01	25,39,46,49	0
3	SO4	R	404	5/5	1.00	0.02	36,40,60,64	0
2	NO3	N	401	4/4	1.00	0.02	21,26,27,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.