



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 09:44 PM EDT

PDB ID : 7LJ1
Title : Human Prx1-Srx Decameric Complex
Authors : Forshaw, T.E.; Reisz, J.A.; Nelson, K.J.; Gumpena, R.; Lawson, J.R.; Jonsson, T.; Wu, H.; Clodfelter, J.E.; Johnson, L.; Furdui, C.M.; Lowther, W.T.
Deposited on : 2021-01-28
Resolution : 2.97 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

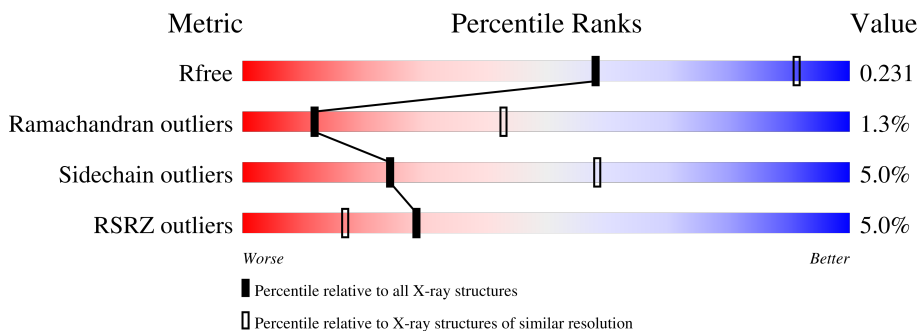
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	2754 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	199	
1	B	199	
1	C	199	
1	D	199	
1	E	199	
1	F	199	

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Mol	Chain	Length	Quality of chain
1	G	199	88% 9%
1	H	199	89% 8%
1	I	199	91% 5%
1	J	199	90% 8%
1	K	199	89% 8%
1	L	199	88% 9%
1	M	199	86% 11%
1	N	199	89% 7%
1	O	199	91% 6%
1	P	199	89% 8%
1	Q	199	90% 8%
1	R	199	90% 7%
1	S	199	89% 7%
1	T	199	90% 7%
2	a	109	93% 5%
2	b	109	90% 8%
2	c	109	85% 13%
2	d	109	90% 9%
2	e	109	89% 9%
2	f	109	88% 9%
2	g	109	84% 9% 6%
2	h	109	88% 11%
2	i	109	86% 8% 6%
2	j	109	87% 11%
2	k	109	81% 8% 11%

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Mol	Chain	Length	Quality of chain
2	l	109	<p>24% 87% 6% • 6%</p>
2	m	109	<p>3% 91% 7% •</p>
2	n	109	<p>28% 76% 9% • 14%</p>
2	o	109	<p>6% 88% 10% •</p>
2	p	109	<p>6% 90% 9% •</p>
2	q	109	<p>7% 87% 11% •</p>
2	r	109	<p>5% 83% 8% 9%</p>
2	s	109	<p>21% 90% 8% •</p>
2	t	109	<p>8% 91% 7% •</p>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 44942 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 Peroxiredoxin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	185	1434	926	240	265	3	0	0	0
1	B	185	1422	918	237	264	3	0	0	0
1	C	187	1448	933	242	270	3	0	0	0
1	D	181	1404	906	235	259	4	0	0	0
1	E	185	1430	923	239	265	3	0	0	0
1	F	185	1435	925	239	268	3	0	0	0
1	G	182	1414	912	237	262	3	0	0	0
1	H	183	1419	915	237	264	3	0	0	0
1	I	191	1487	958	250	276	3	0	0	0
1	J	184	1419	917	237	262	3	0	0	0
1	K	183	1419	915	237	264	3	0	0	0
1	L	181	1401	904	233	261	3	0	0	0
1	M	178	1386	896	232	255	3	0	0	0
1	N	185	1418	915	236	264	3	0	0	0
1	O	187	1446	932	241	270	3	0	0	0
1	P	183	1415	912	236	264	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	184	1426	921	239	263	3	0	0	0
1	R	186	1443	930	241	269	3	0	0	0
1	S	185	1431	924	239	265	3	0	0	0
1	T	185	1430	923	239	265	3	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	SER	CYS	engineered mutation	UNP Q06830
A	83	VAL	CYS	engineered mutation	UNP Q06830
A	173	SER	CYS	engineered mutation	UNP Q06830
B	71	SER	CYS	engineered mutation	UNP Q06830
B	83	VAL	CYS	engineered mutation	UNP Q06830
B	173	SER	CYS	engineered mutation	UNP Q06830
C	71	SER	CYS	engineered mutation	UNP Q06830
C	83	VAL	CYS	engineered mutation	UNP Q06830
C	173	SER	CYS	engineered mutation	UNP Q06830
D	71	SER	CYS	engineered mutation	UNP Q06830
D	83	VAL	CYS	engineered mutation	UNP Q06830
D	173	SER	CYS	engineered mutation	UNP Q06830
E	71	SER	CYS	engineered mutation	UNP Q06830
E	83	VAL	CYS	engineered mutation	UNP Q06830
E	173	SER	CYS	engineered mutation	UNP Q06830
F	71	SER	CYS	engineered mutation	UNP Q06830
F	83	VAL	CYS	engineered mutation	UNP Q06830
F	173	SER	CYS	engineered mutation	UNP Q06830
G	71	SER	CYS	engineered mutation	UNP Q06830
G	83	VAL	CYS	engineered mutation	UNP Q06830
G	173	SER	CYS	engineered mutation	UNP Q06830
H	71	SER	CYS	engineered mutation	UNP Q06830
H	83	VAL	CYS	engineered mutation	UNP Q06830
H	173	SER	CYS	engineered mutation	UNP Q06830
I	71	SER	CYS	engineered mutation	UNP Q06830
I	83	VAL	CYS	engineered mutation	UNP Q06830
I	173	SER	CYS	engineered mutation	UNP Q06830
J	71	SER	CYS	engineered mutation	UNP Q06830
J	83	VAL	CYS	engineered mutation	UNP Q06830
J	173	SER	CYS	engineered mutation	UNP Q06830
K	71	SER	CYS	engineered mutation	UNP Q06830

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Chain	Residue	Modelled	Actual	Comment	Reference
K	83	VAL	CYS	engineered mutation	UNP Q06830
K	173	SER	CYS	engineered mutation	UNP Q06830
L	71	SER	CYS	engineered mutation	UNP Q06830
L	83	VAL	CYS	engineered mutation	UNP Q06830
L	173	SER	CYS	engineered mutation	UNP Q06830
M	71	SER	CYS	engineered mutation	UNP Q06830
M	83	VAL	CYS	engineered mutation	UNP Q06830
M	173	SER	CYS	engineered mutation	UNP Q06830
N	71	SER	CYS	engineered mutation	UNP Q06830
N	83	VAL	CYS	engineered mutation	UNP Q06830
N	173	SER	CYS	engineered mutation	UNP Q06830
O	71	SER	CYS	engineered mutation	UNP Q06830
O	83	VAL	CYS	engineered mutation	UNP Q06830
O	173	SER	CYS	engineered mutation	UNP Q06830
P	71	SER	CYS	engineered mutation	UNP Q06830
P	83	VAL	CYS	engineered mutation	UNP Q06830
P	173	SER	CYS	engineered mutation	UNP Q06830
Q	71	SER	CYS	engineered mutation	UNP Q06830
Q	83	VAL	CYS	engineered mutation	UNP Q06830
Q	173	SER	CYS	engineered mutation	UNP Q06830
R	71	SER	CYS	engineered mutation	UNP Q06830
R	83	VAL	CYS	engineered mutation	UNP Q06830
R	173	SER	CYS	engineered mutation	UNP Q06830
S	71	SER	CYS	engineered mutation	UNP Q06830
S	83	VAL	CYS	engineered mutation	UNP Q06830
S	173	SER	CYS	engineered mutation	UNP Q06830
T	71	SER	CYS	engineered mutation	UNP Q06830
T	83	VAL	CYS	engineered mutation	UNP Q06830
T	173	SER	CYS	engineered mutation	UNP Q06830

- Molecule 2 is a protein called Sulfiredoxin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	a	106	804	514	137	152	1	0	0	0
2	b	107	817	522	139	154	2	0	0	0
2	c	107	822	525	140	155	2	0	0	0
2	d	108	835	533	144	156	2	0	0	0
2	e	107	809	518	136	154	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	f	106	804	515	138	150	1	0	0	0
2	g	102	786	503	134	148	1	0	0	0
2	h	108	825	528	141	154	2	0	0	0
2	i	103	775	494	132	148	1	0	0	0
2	j	107	816	522	137	155	2	0	0	0
2	k	97	741	474	126	140	1	0	0	0
2	l	103	764	488	129	146	1	0	0	0
2	m	107	828	528	143	155	2	0	0	0
2	n	94	708	455	117	135	1	0	0	0
2	o	107	804	514	138	150	2	0	0	0
2	p	108	817	521	138	156	2	0	0	0
2	q	107	828	528	143	155	2	0	0	0
2	r	99	763	489	130	143	1	0	0	0
2	s	107	798	508	137	152	1	0	0	0
2	t	107	816	521	140	153	2	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	29	GLY	-	expression tag	UNP Q9BYN0
a	30	PRO	-	expression tag	UNP Q9BYN0
a	31	MET	-	expression tag	UNP Q9BYN0
b	29	GLY	-	expression tag	UNP Q9BYN0
b	30	PRO	-	expression tag	UNP Q9BYN0
b	31	MET	-	expression tag	UNP Q9BYN0
c	29	GLY	-	expression tag	UNP Q9BYN0
c	30	PRO	-	expression tag	UNP Q9BYN0
c	31	MET	-	expression tag	UNP Q9BYN0

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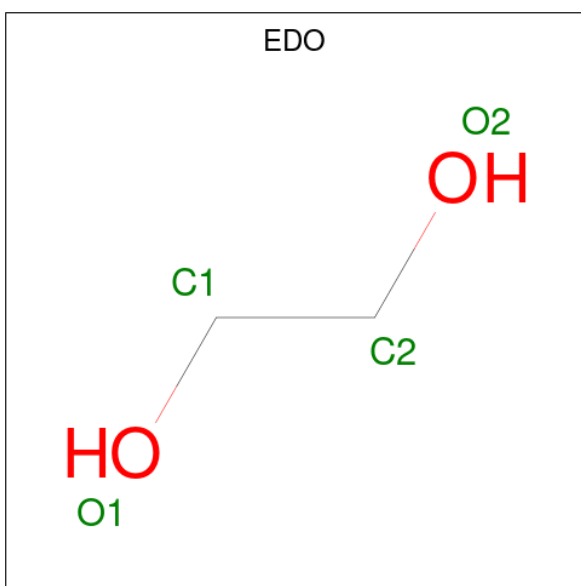
Chain	Residue	Modelled	Actual	Comment	Reference
d	29	GLY	-	expression tag	UNP Q9BYN0
d	30	PRO	-	expression tag	UNP Q9BYN0
d	31	MET	-	expression tag	UNP Q9BYN0
e	29	GLY	-	expression tag	UNP Q9BYN0
e	30	PRO	-	expression tag	UNP Q9BYN0
e	31	MET	-	expression tag	UNP Q9BYN0
f	29	GLY	-	expression tag	UNP Q9BYN0
f	30	PRO	-	expression tag	UNP Q9BYN0
f	31	MET	-	expression tag	UNP Q9BYN0
g	29	GLY	-	expression tag	UNP Q9BYN0
g	30	PRO	-	expression tag	UNP Q9BYN0
g	31	MET	-	expression tag	UNP Q9BYN0
h	29	GLY	-	expression tag	UNP Q9BYN0
h	30	PRO	-	expression tag	UNP Q9BYN0
h	31	MET	-	expression tag	UNP Q9BYN0
i	29	GLY	-	expression tag	UNP Q9BYN0
i	30	PRO	-	expression tag	UNP Q9BYN0
i	31	MET	-	expression tag	UNP Q9BYN0
j	29	GLY	-	expression tag	UNP Q9BYN0
j	30	PRO	-	expression tag	UNP Q9BYN0
j	31	MET	-	expression tag	UNP Q9BYN0
k	29	GLY	-	expression tag	UNP Q9BYN0
k	30	PRO	-	expression tag	UNP Q9BYN0
k	31	MET	-	expression tag	UNP Q9BYN0
l	29	GLY	-	expression tag	UNP Q9BYN0
l	30	PRO	-	expression tag	UNP Q9BYN0
l	31	MET	-	expression tag	UNP Q9BYN0
m	29	GLY	-	expression tag	UNP Q9BYN0
m	30	PRO	-	expression tag	UNP Q9BYN0
m	31	MET	-	expression tag	UNP Q9BYN0
n	29	GLY	-	expression tag	UNP Q9BYN0
n	30	PRO	-	expression tag	UNP Q9BYN0
n	31	MET	-	expression tag	UNP Q9BYN0
o	29	GLY	-	expression tag	UNP Q9BYN0
o	30	PRO	-	expression tag	UNP Q9BYN0
o	31	MET	-	expression tag	UNP Q9BYN0
p	29	GLY	-	expression tag	UNP Q9BYN0
p	30	PRO	-	expression tag	UNP Q9BYN0
p	31	MET	-	expression tag	UNP Q9BYN0
q	29	GLY	-	expression tag	UNP Q9BYN0
q	30	PRO	-	expression tag	UNP Q9BYN0
q	31	MET	-	expression tag	UNP Q9BYN0

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Chain	Residue	Modelled	Actual	Comment	Reference
r	29	GLY	-	expression tag	UNP Q9BYN0
r	30	PRO	-	expression tag	UNP Q9BYN0
r	31	MET	-	expression tag	UNP Q9BYN0
s	29	GLY	-	expression tag	UNP Q9BYN0
s	30	PRO	-	expression tag	UNP Q9BYN0
s	31	MET	-	expression tag	UNP Q9BYN0
t	29	GLY	-	expression tag	UNP Q9BYN0
t	30	PRO	-	expression tag	UNP Q9BYN0
t	31	MET	-	expression tag	UNP Q9BYN0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



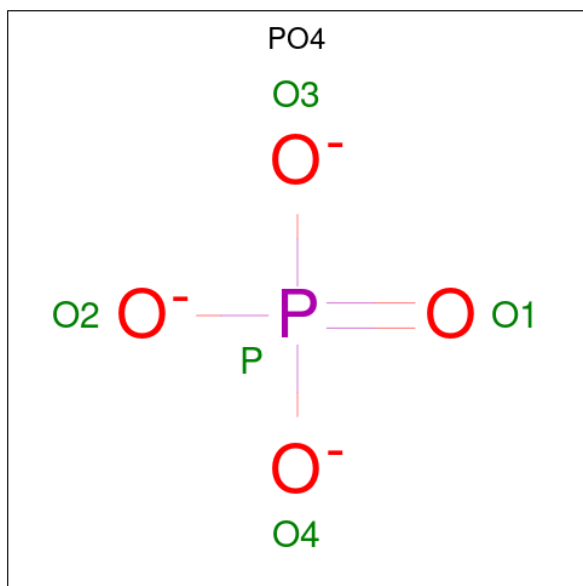
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	O	1	Total C O 4 2 2	0	0
3	P	1	Total C O 4 2 2	0	0
3	Q	1	Total C O 4 2 2	0	0
3	R	1	Total C O 4 2 2	0	0
3	R	1	Total C O 4 2 2	0	0
3	S	1	Total C O 4 2 2	0	0
3	S	1	Total C O 4 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	a	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	b	1	Total	O	P	0	0
			5	4	1		
4	d	1	Total	O	P	0	0
			5	4	1		
4	e	1	Total	O	P	0	0
			5	4	1		
4	f	1	Total	O	P	0	0
			5	4	1		
4	h	1	Total	O	P	0	0
			5	4	1		
4	i	1	Total	O	P	0	0
			5	4	1		
4	j	1	Total	O	P	0	0
			5	4	1		
4	k	1	Total	O	P	0	0
			5	4	1		
4	l	1	Total	O	P	0	0
			5	4	1		
4	m	1	Total	O	P	0	0
			5	4	1		
4	n	1	Total	O	P	0	0
			5	4	1		
4	o	1	Total	O	P	0	0
			5	4	1		
4	p	1	Total	O	P	0	0
			5	4	1		
4	q	1	Total	O	P	0	0
			5	4	1		
4	r	1	Total	O	P	0	0
			5	4	1		
4	s	1	Total	O	P	0	0
			5	4	1		
4	t	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



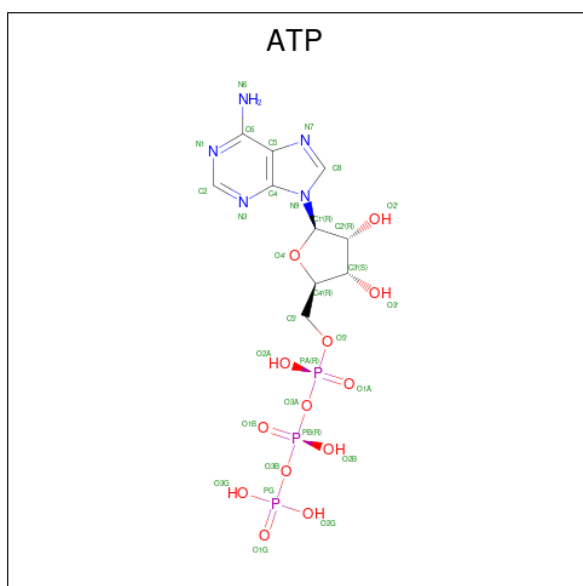
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 7 4 3	0	0
5	G	1	Total C O 7 4 3	0	0
5	K	1	Total C O 7 4 3	0	0
5	N	1	Total C O 7 4 3	0	0
5	O	1	Total C O 7 4 3	0	0
5	P	1	Total C O 7 4 3	0	0
5	Q	1	Total C O 7 4 3	0	0
5	R	1	Total C O 7 4 3	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf		
6	H	1	Total	C	O	0	0
			6	3	3		
6	O	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf		
7	c	1	Total	O	P	0	0
			13	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	g	1	Total	C	O	P	0	0
			15	2	10	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	9	Total	O	0	0
			9	9		
8	B	5	Total	O	0	0
			5	5		
8	C	14	Total	O	0	0
			14	14		
8	D	10	Total	O	0	0
			10	10		
8	E	10	Total	O	0	0
			10	10		
8	F	7	Total	O	0	0
			7	7		
8	G	17	Total	O	0	0
			17	17		
8	H	18	Total	O	0	0
			18	18		
8	I	13	Total	O	0	0
			13	13		
8	J	9	Total	O	0	0
			9	9		
8	K	5	Total	O	0	0
			5	5		
8	L	1	Total	O	0	0
			1	1		
8	M	8	Total	O	0	0
			8	8		
8	N	6	Total	O	0	0
			6	6		
8	O	4	Total	O	0	0
			4	4		
8	P	5	Total	O	0	0
			5	5		
8	Q	6	Total	O	0	0
			6	6		
8	R	10	Total	O	0	0
			10	10		

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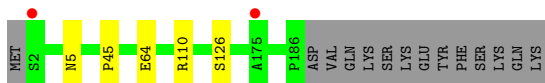
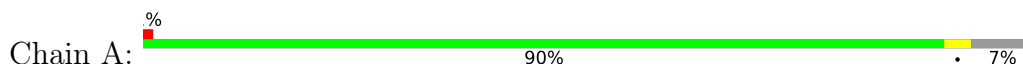
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	S	4	Total O 4 4	0	0
8	T	8	Total O 8 8	0	0
8	b	2	Total O 2 2	0	0
8	c	4	Total O 4 4	0	0
8	d	2	Total O 2 2	0	0
8	e	1	Total O 1 1	0	0
8	f	1	Total O 1 1	0	0
8	g	1	Total O 1 1	0	0
8	h	4	Total O 4 4	0	0
8	j	3	Total O 3 3	0	0
8	l	1	Total O 1 1	0	0
8	m	2	Total O 2 2	0	0
8	n	1	Total O 1 1	0	0
8	o	2	Total O 2 2	0	0
8	p	1	Total O 1 1	0	0
8	q	2	Total O 2 2	0	0
8	r	3	Total O 3 3	0	0
8	t	1	Total O 1 1	0	0

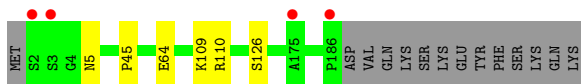
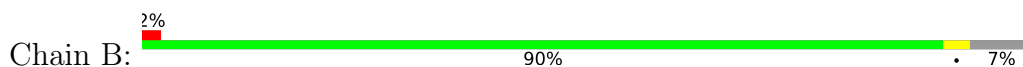
3 Residue-property plots [i](#)

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.

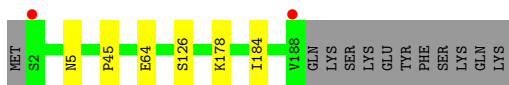
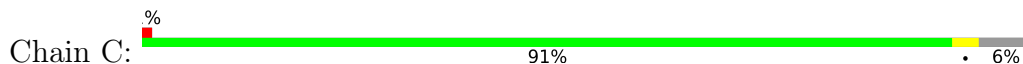
- Molecule 1: Peroxiredoxin-1



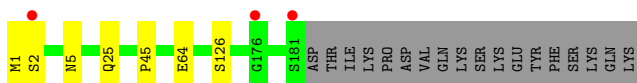
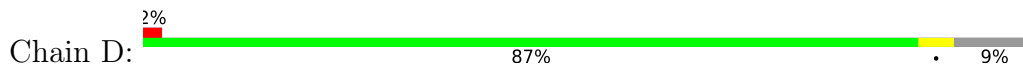
- Molecule 1: Peroxiredoxin-1



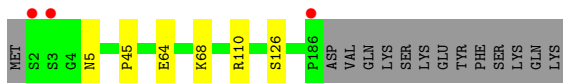
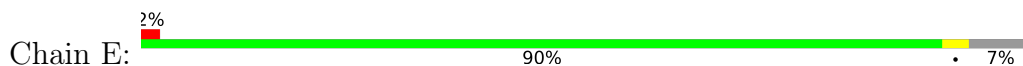
- Molecule 1: Peroxiredoxin-1



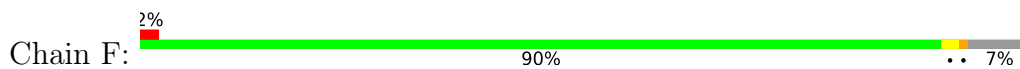
- Molecule 1: Peroxiredoxin-1



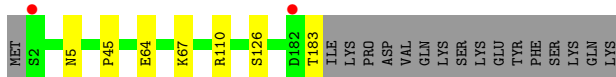
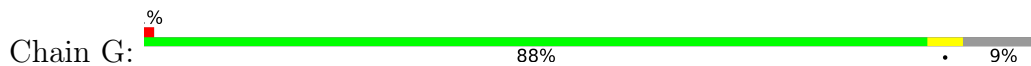
- Molecule 1: Peroxiredoxin-1



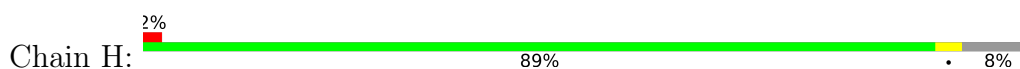
- Molecule 1: Peroxiredoxin-1



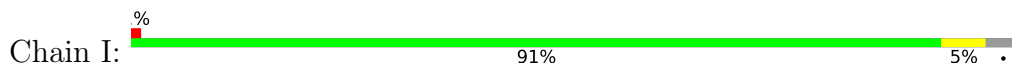
- Molecule 1: Peroxiredoxin-1



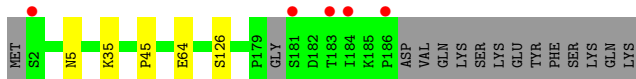
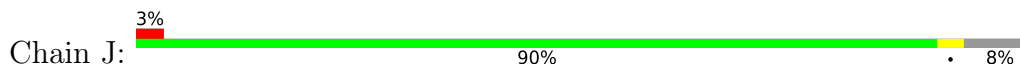
- Molecule 1: Peroxiredoxin-1



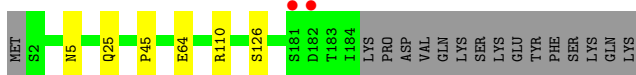
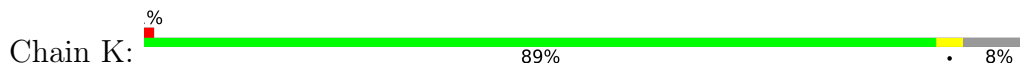
- Molecule 1: Peroxiredoxin-1



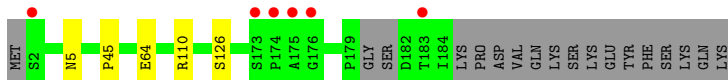
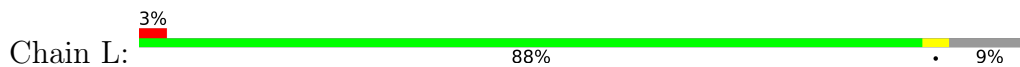
- Molecule 1: Peroxiredoxin-1



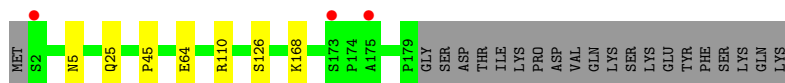
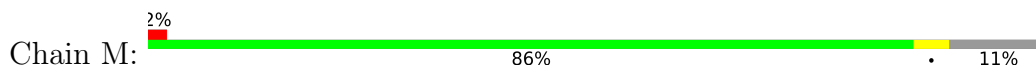
- Molecule 1: Peroxiredoxin-1



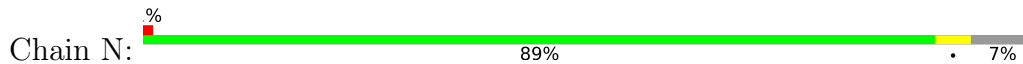
- Molecule 1: Peroxiredoxin-1



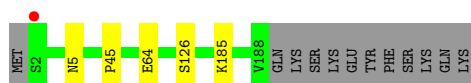
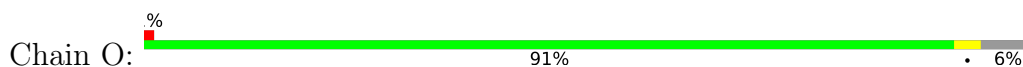
- Molecule 1: Peroxiredoxin-1



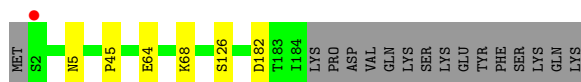
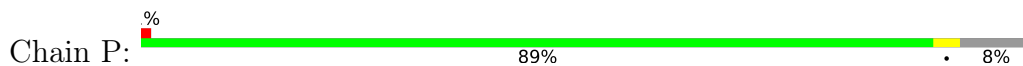
● Molecule 1: Peroxiredoxin-1



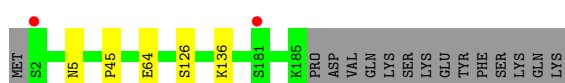
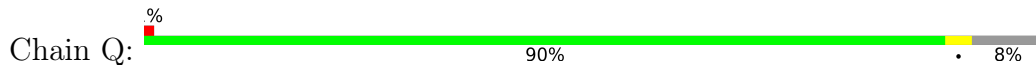
● Molecule 1: Peroxiredoxin-1



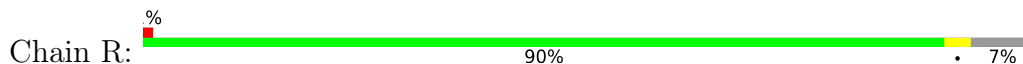
● Molecule 1: Peroxiredoxin-1



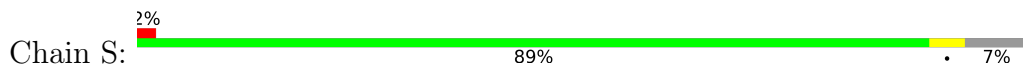
● Molecule 1: Peroxiredoxin-1



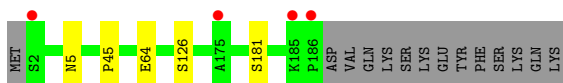
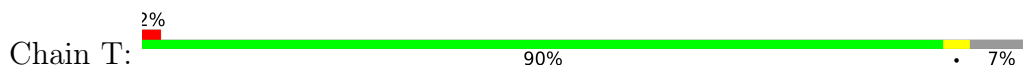
● Molecule 1: Peroxiredoxin-1



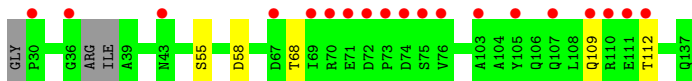
● Molecule 1: Peroxiredoxin-1



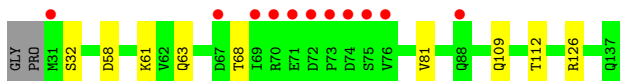
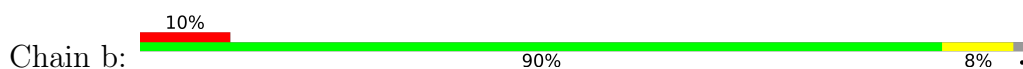
● Molecule 1: Peroxiredoxin-1



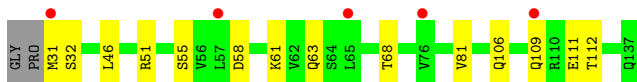
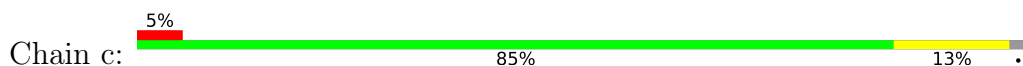
- Molecule 2: Sulfiredoxin-1



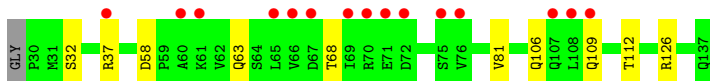
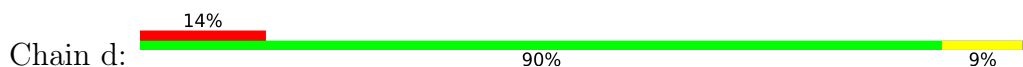
- Molecule 2: Sulfiredoxin-1



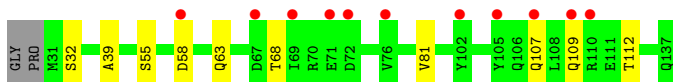
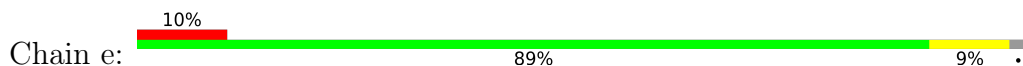
- Molecule 2: Sulfiredoxin-1



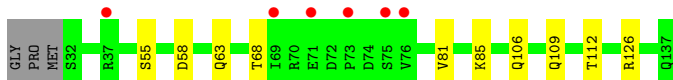
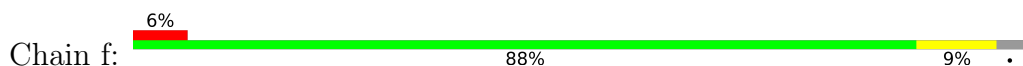
- Molecule 2: Sulfiredoxin-1



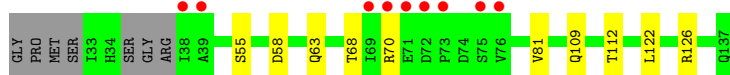
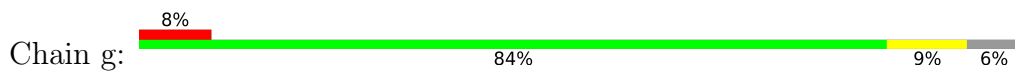
- Molecule 2: Sulfiredoxin-1



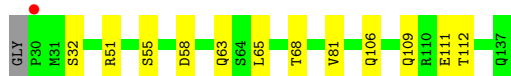
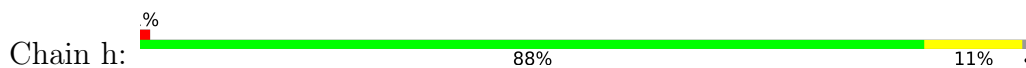
- Molecule 2: Sulfiredoxin-1



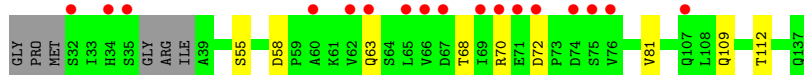
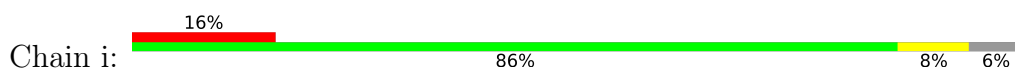
- Molecule 2: Sulfiredoxin-1



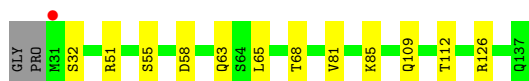
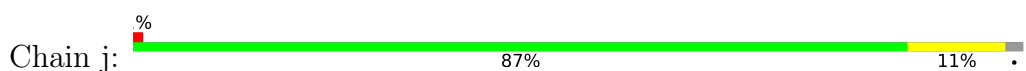
- Molecule 2: Sulfiredoxin-1



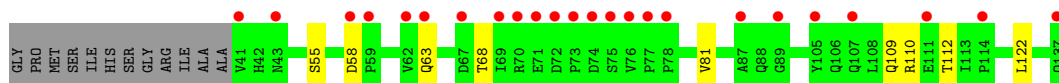
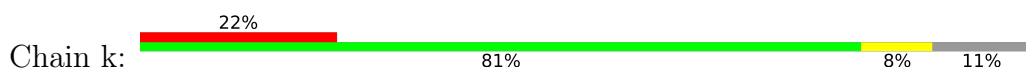
- Molecule 2: Sulfiredoxin-1



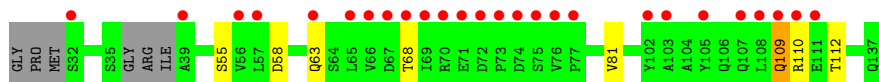
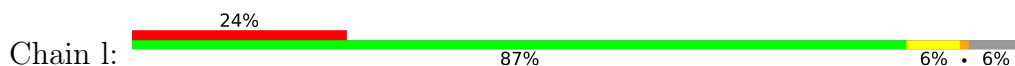
- Molecule 2: Sulfiredoxin-1



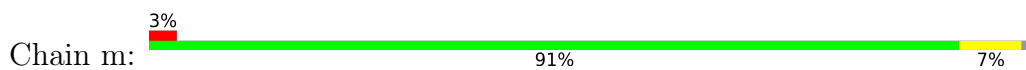
- Molecule 2: Sulfiredoxin-1



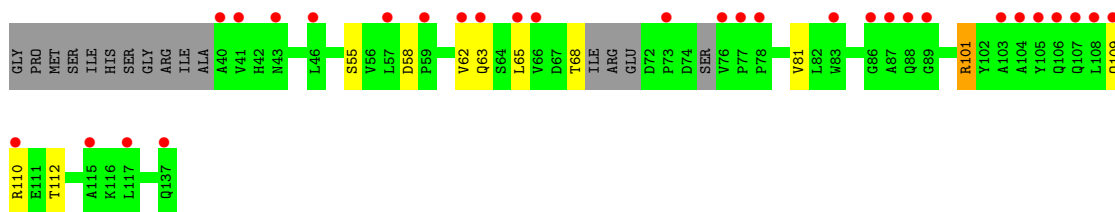
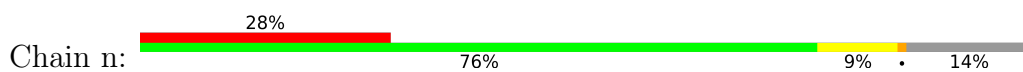
- Molecule 2: Sulfiredoxin-1



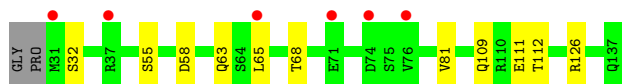
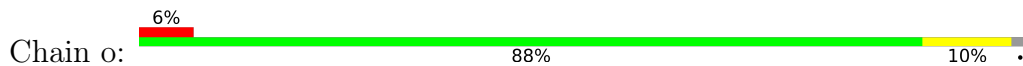
- Molecule 2: Sulfiredoxin-1



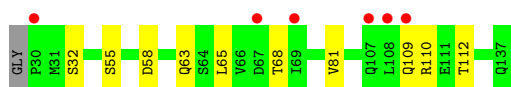
- Molecule 2: Sulfiredoxin-1



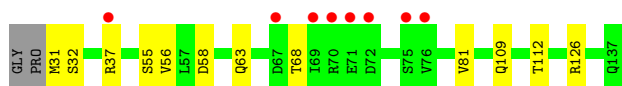
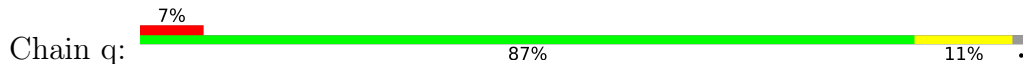
- Molecule 2: Sulfiredoxin-1



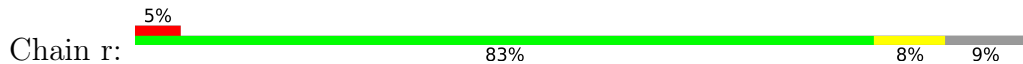
- Molecule 2: Sulfiredoxin-1



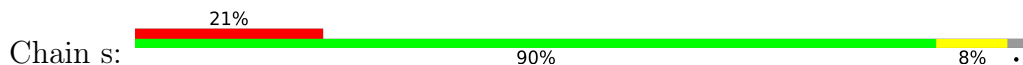
- Molecule 2: Sulfiredoxin-1



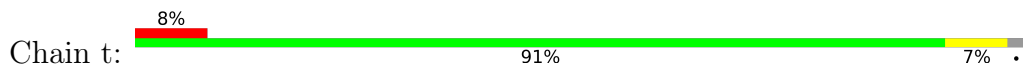
- Molecule 2: Sulfiredoxin-1

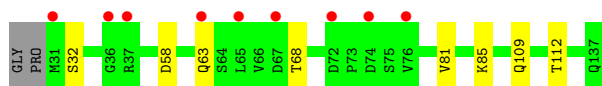


- Molecule 2: Sulfiredoxin-1



- Molecule 2: Sulfiredoxin-1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	330.83Å 109.94Å 260.14Å 90.00° 122.34° 90.00°	Depositor
Resolution (Å)	38.97 – 2.97 38.93 – 2.97	Depositor EDS
% Data completeness (in resolution range)	91.8 (38.97-2.97) 91.8 (38.93-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.95Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.192 , 0.230 0.194 , 0.231	Depositor DCC
R_{free} test set	7475 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtrriage
Anisotropy	0.098	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	44942	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, EDO, GOL, PEG, ATP

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	0.64	0/1472	0.79	0/1997
1	B	0.63	0/1460	0.78	0/1984
1	C	0.68	0/1486	0.81	0/2016
1	D	0.66	0/1441	0.81	0/1953
1	E	0.63	0/1468	0.79	0/1993
1	F	0.66	0/1472	0.81	1/1997 (0.1%)
1	G	0.66	0/1451	0.82	0/1967
1	H	0.66	0/1456	0.81	0/1975
1	I	0.66	0/1525	0.81	0/2065
1	J	0.64	0/1456	0.80	0/1977
1	K	0.62	0/1456	0.79	0/1975
1	L	0.63	0/1437	0.79	0/1951
1	M	0.64	0/1423	0.79	0/1930
1	N	0.67	0/1456	0.83	0/1980
1	O	0.66	0/1484	0.80	0/2015
1	P	0.65	0/1452	0.80	0/1971
1	Q	0.65	0/1463	0.78	0/1984
1	R	0.64	0/1481	0.81	0/2009
1	S	0.64	0/1469	0.80	0/1993
1	T	0.63	0/1468	0.77	0/1993
2	a	0.69	0/824	0.84	0/1127
2	b	0.69	0/837	0.83	0/1145
2	c	0.79	0/842	0.95	1/1150 (0.1%)
2	d	0.69	0/856	0.88	0/1168
2	e	0.69	0/829	0.89	0/1135
2	f	0.67	0/824	0.83	0/1128
2	g	0.67	0/805	0.88	1/1101 (0.1%)
2	h	0.74	0/846	0.91	1/1156 (0.1%)
2	i	0.69	0/794	0.85	1/1088 (0.1%)
2	j	0.72	0/836	0.89	1/1143 (0.1%)
2	k	0.66	0/760	0.83	0/1043
2	l	0.68	0/783	0.82	0/1073

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	m	0.70	0/848	0.84	0/1157
2	n	0.69	0/725	0.87	1/993 (0.1%)
2	o	0.68	0/824	0.84	0/1128
2	p	0.70	0/838	0.85	0/1149
2	q	0.69	0/848	0.88	0/1157
2	r	0.70	0/782	0.85	0/1070
2	s	0.68	0/818	0.81	0/1122
2	t	0.70	0/836	0.84	0/1142
All	All	0.67	0/45631	0.82	7/62100 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	110	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	j	51	ARG	NE-CZ-NH1	-6.01	117.30	120.30
2	c	51	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	n	101	ARG	NE-CZ-NH2	5.29	122.95	120.30
2	h	51	ARG	NE-CZ-NH1	5.15	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	A	183/199 (92%)	176 (96%)	5 (3%)	2 (1%)	14 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	183/199 (92%)	176 (96%)	5 (3%)	2 (1%)	14	47
1	C	185/199 (93%)	178 (96%)	5 (3%)	2 (1%)	14	47
1	D	179/199 (90%)	171 (96%)	5 (3%)	3 (2%)	9	36
1	E	183/199 (92%)	176 (96%)	5 (3%)	2 (1%)	14	47
1	F	181/199 (91%)	173 (96%)	6 (3%)	2 (1%)	14	47
1	G	180/199 (90%)	172 (96%)	6 (3%)	2 (1%)	14	47
1	H	181/199 (91%)	173 (96%)	6 (3%)	2 (1%)	14	47
1	I	189/199 (95%)	180 (95%)	7 (4%)	2 (1%)	14	47
1	J	180/199 (90%)	173 (96%)	5 (3%)	2 (1%)	14	47
1	K	181/199 (91%)	175 (97%)	4 (2%)	2 (1%)	14	47
1	L	177/199 (89%)	169 (96%)	6 (3%)	2 (1%)	14	47
1	M	176/199 (88%)	168 (96%)	6 (3%)	2 (1%)	14	47
1	N	183/199 (92%)	176 (96%)	5 (3%)	2 (1%)	14	47
1	O	185/199 (93%)	177 (96%)	6 (3%)	2 (1%)	14	47
1	P	181/199 (91%)	175 (97%)	4 (2%)	2 (1%)	14	47
1	Q	182/199 (92%)	174 (96%)	6 (3%)	2 (1%)	14	47
1	R	184/199 (92%)	176 (96%)	6 (3%)	2 (1%)	14	47
1	S	183/199 (92%)	176 (96%)	5 (3%)	2 (1%)	14	47
1	T	183/199 (92%)	175 (96%)	6 (3%)	2 (1%)	14	47
2	a	102/109 (94%)	95 (93%)	6 (6%)	1 (1%)	15	50
2	b	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	8	33
2	c	105/109 (96%)	97 (92%)	6 (6%)	2 (2%)	8	33
2	d	106/109 (97%)	99 (93%)	5 (5%)	2 (2%)	8	33
2	e	105/109 (96%)	97 (92%)	5 (5%)	3 (3%)	4	22
2	f	104/109 (95%)	98 (94%)	5 (5%)	1 (1%)	15	50
2	g	98/109 (90%)	95 (97%)	2 (2%)	1 (1%)	15	50
2	h	106/109 (97%)	99 (93%)	5 (5%)	2 (2%)	8	33
2	i	99/109 (91%)	95 (96%)	3 (3%)	1 (1%)	15	50
2	j	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	8	33
2	k	95/109 (87%)	92 (97%)	2 (2%)	1 (1%)	14	47
2	l	99/109 (91%)	95 (96%)	3 (3%)	1 (1%)	15	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	m	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	8	33
2	n	88/109 (81%)	85 (97%)	2 (2%)	1 (1%)	14	47
2	o	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	8	33
2	p	106/109 (97%)	99 (93%)	5 (5%)	2 (2%)	8	33
2	q	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	8	33
2	r	97/109 (89%)	94 (97%)	2 (2%)	1 (1%)	15	50
2	s	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	8	33
2	t	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	8	33
All	All	5684/6160 (92%)	5415 (95%)	195 (3%)	74 (1%)	12	43

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	B	5	ASN
1	C	5	ASN
1	D	5	ASN
1	E	5	ASN

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	A	155/171 (91%)	152 (98%)	3 (2%)	57	82
1	B	152/171 (89%)	148 (97%)	4 (3%)	46	76
1	C	157/171 (92%)	153 (98%)	4 (2%)	47	77
1	D	152/171 (89%)	148 (97%)	4 (3%)	46	76
1	E	154/171 (90%)	150 (97%)	4 (3%)	46	76
1	F	156/171 (91%)	153 (98%)	3 (2%)	57	82
1	G	153/171 (90%)	148 (97%)	5 (3%)	38	71
1	H	154/171 (90%)	151 (98%)	3 (2%)	57	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	163/171 (95%)	156 (96%)	7 (4%)	29	64
1	J	152/171 (89%)	149 (98%)	3 (2%)	55	81
1	K	154/171 (90%)	150 (97%)	4 (3%)	46	76
1	L	151/171 (88%)	148 (98%)	3 (2%)	55	81
1	M	150/171 (88%)	145 (97%)	5 (3%)	38	71
1	N	151/171 (88%)	145 (96%)	6 (4%)	31	66
1	O	157/171 (92%)	154 (98%)	3 (2%)	57	82
1	P	153/171 (90%)	149 (97%)	4 (3%)	46	76
1	Q	153/171 (90%)	150 (98%)	3 (2%)	55	81
1	R	157/171 (92%)	153 (98%)	4 (2%)	47	77
1	S	155/171 (91%)	150 (97%)	5 (3%)	39	72
1	T	154/171 (90%)	151 (98%)	3 (2%)	57	82
2	a	87/93 (94%)	83 (95%)	4 (5%)	27	61
2	b	89/93 (96%)	82 (92%)	7 (8%)	12	39
2	c	91/93 (98%)	80 (88%)	11 (12%)	5	20
2	d	93/93 (100%)	85 (91%)	8 (9%)	10	35
2	e	88/93 (95%)	81 (92%)	7 (8%)	12	38
2	f	87/93 (94%)	78 (90%)	9 (10%)	7	26
2	g	86/93 (92%)	78 (91%)	8 (9%)	9	31
2	h	91/93 (98%)	82 (90%)	9 (10%)	8	28
2	i	82/93 (88%)	75 (92%)	7 (8%)	10	36
2	j	90/93 (97%)	81 (90%)	9 (10%)	7	27
2	k	80/93 (86%)	72 (90%)	8 (10%)	7	27
2	l	80/93 (86%)	72 (90%)	8 (10%)	7	27
2	m	92/93 (99%)	86 (94%)	6 (6%)	17	48
2	n	75/93 (81%)	65 (87%)	10 (13%)	4	16
2	o	86/93 (92%)	77 (90%)	9 (10%)	7	25
2	p	89/93 (96%)	81 (91%)	8 (9%)	9	33
2	q	92/93 (99%)	82 (89%)	10 (11%)	6	24
2	r	84/93 (90%)	76 (90%)	8 (10%)	8	30
2	s	84/93 (90%)	77 (92%)	7 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	t	89/93 (96%)	83 (93%)	6 (7%)	16	47
All	All	4818/5280 (91%)	4579 (95%)	239 (5%)	24	58

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	e	107	GLN
2	r	68	THR
2	i	55	SER
2	r	61	LYS
2	t	81	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

47 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	EDO	S	201	-	3,3,3	0.35	0	2,2,2	0.53	0
4	PO4	j	201	-	4,4,4	0.77	0	6,6,6	0.58	0
4	PO4	n	201	-	4,4,4	0.89	0	6,6,6	0.44	0
4	PO4	s	201	-	4,4,4	1.34	1 (25%)	6,6,6	0.27	0
5	PEG	Q	202	-	6,6,6	0.27	0	5,5,5	0.12	0
3	EDO	A	201	-	3,3,3	0.07	0	2,2,2	0.23	0
5	PEG	G	203	-	6,6,6	0.26	0	5,5,5	0.16	0
4	PO4	l	201	-	4,4,4	1.22	1 (25%)	6,6,6	0.28	0
5	PEG	K	201	-	6,6,6	0.26	0	5,5,5	0.23	0
5	PEG	P	202	-	6,6,6	0.18	0	5,5,5	0.11	0
7	ATP	c	201	-	8,12,33	0.89	0	15,20,52	1.05	0
4	PO4	o	201	-	4,4,4	0.43	0	6,6,6	0.62	0
4	PO4	d	201	-	4,4,4	1.16	1 (25%)	6,6,6	0.62	0
4	PO4	a	201	-	4,4,4	0.59	0	6,6,6	0.54	0
4	PO4	f	201	-	4,4,4	0.57	0	6,6,6	0.62	0
3	EDO	H	204	-	3,3,3	0.18	0	2,2,2	0.27	0
3	EDO	H	202	-	3,3,3	0.21	0	2,2,2	0.27	0
4	PO4	e	201	-	4,4,4	0.43	0	6,6,6	0.72	0
4	PO4	k	201	-	4,4,4	0.66	0	6,6,6	0.64	0
6	GOL	H	201	-	5,5,5	0.21	0	5,5,5	0.43	0
3	EDO	J	201	-	3,3,3	0.33	0	2,2,2	0.45	0
4	PO4	t	201	-	4,4,4	0.55	0	6,6,6	0.63	0
4	PO4	m	201	-	4,4,4	1.09	1 (25%)	6,6,6	0.54	0
4	PO4	E	201	-	4,4,4	0.80	0	6,6,6	0.39	0
3	EDO	O	202	-	3,3,3	0.22	0	2,2,2	0.37	0
4	PO4	b	201	-	4,4,4	1.09	1 (25%)	6,6,6	0.38	0
3	EDO	C	201	-	3,3,3	0.13	0	2,2,2	0.32	0
6	GOL	O	203	-	5,5,5	0.10	0	5,5,5	0.28	0
3	EDO	H	203	-	3,3,3	0.31	0	2,2,2	0.53	0
5	PEG	D	201	-	6,6,6	0.34	0	5,5,5	0.20	0
3	EDO	G	202	-	3,3,3	0.48	0	2,2,2	0.61	0
5	PEG	N	201	-	6,6,6	0.42	0	5,5,5	0.29	0
3	EDO	P	201	-	3,3,3	0.29	0	2,2,2	0.30	0
3	EDO	Q	201	-	3,3,3	0.28	0	2,2,2	0.36	0
5	PEG	O	201	-	6,6,6	0.31	0	5,5,5	0.16	0
7	ATP	g	201	-	10,14,33	0.82	0	14,22,52	1.18	2 (14%)
5	PEG	R	203	-	6,6,6	0.24	0	5,5,5	0.15	0
3	EDO	C	202	-	3,3,3	0.41	0	2,2,2	0.66	0
4	PO4	r	201	-	4,4,4	0.90	0	6,6,6	0.63	0
3	EDO	G	201	-	3,3,3	0.31	0	2,2,2	0.41	0
3	EDO	S	202	-	3,3,3	0.33	0	2,2,2	0.51	0
3	EDO	R	201	-	3,3,3	0.17	0	2,2,2	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	q	201	-	4,4,4	0.62	0	6,6,6	0.70	0
4	PO4	i	201	-	4,4,4	1.33	1 (25%)	6,6,6	0.37	0
4	PO4	h	201	-	4,4,4	0.73	0	6,6,6	0.58	0
3	EDO	R	202	-	3,3,3	0.37	0	2,2,2	0.42	0
4	PO4	p	201	-	4,4,4	0.62	0	6,6,6	0.76	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
3	EDO	S	201	-	-	0/1/1/1	-
5	PEG	Q	202	-	-	2/4/4/4	-
5	PEG	G	203	-	-	2/4/4/4	-
3	EDO	A	201	-	-	1/1/1/1	-
5	PEG	P	202	-	-	3/4/4/4	-
5	PEG	K	201	-	-	3/4/4/4	-
7	ATP	c	201	-	-	2/12/12/38	-
3	EDO	H	204	-	-	1/1/1/1	-
3	EDO	H	202	-	-	1/1/1/1	-
6	GOL	H	201	-	-	4/4/4/4	-
3	EDO	J	201	-	-	1/1/1/1	-
3	EDO	O	202	-	-	1/1/1/1	-
3	EDO	C	201	-	-	1/1/1/1	-
6	GOL	O	203	-	-	2/4/4/4	-
3	EDO	H	203	-	-	0/1/1/1	-
5	PEG	D	201	-	-	2/4/4/4	-
3	EDO	G	202	-	-	1/1/1/1	-
5	PEG	N	201	-	-	3/4/4/4	-
3	EDO	P	201	-	-	0/1/1/1	-
3	EDO	Q	201	-	-	1/1/1/1	-
5	PEG	O	201	-	-	0/4/4/4	-
7	ATP	g	201	-	-	0/16/16/38	-
5	PEG	R	203	-	-	1/4/4/4	-
3	EDO	C	202	-	-	1/1/1/1	-
3	EDO	G	201	-	-	1/1/1/1	-
3	EDO	S	202	-	-	1/1/1/1	-
3	EDO	R	201	-	-	1/1/1/1	-
3	EDO	R	202	-	-	1/1/1/1	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	s	201	PO4	P-O1	2.60	1.56	1.50
4	i	201	PO4	P-O1	2.39	1.56	1.50
4	l	201	PO4	P-O1	2.27	1.56	1.50
4	d	201	PO4	P-O1	2.23	1.56	1.50
4	b	201	PO4	P-O1	2.04	1.55	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	201	ATP	PB-O3B-PG	3.17	143.71	132.83
7	g	201	ATP	PA-O3A-PB	2.12	140.09	132.83

There are no chirality outliers.

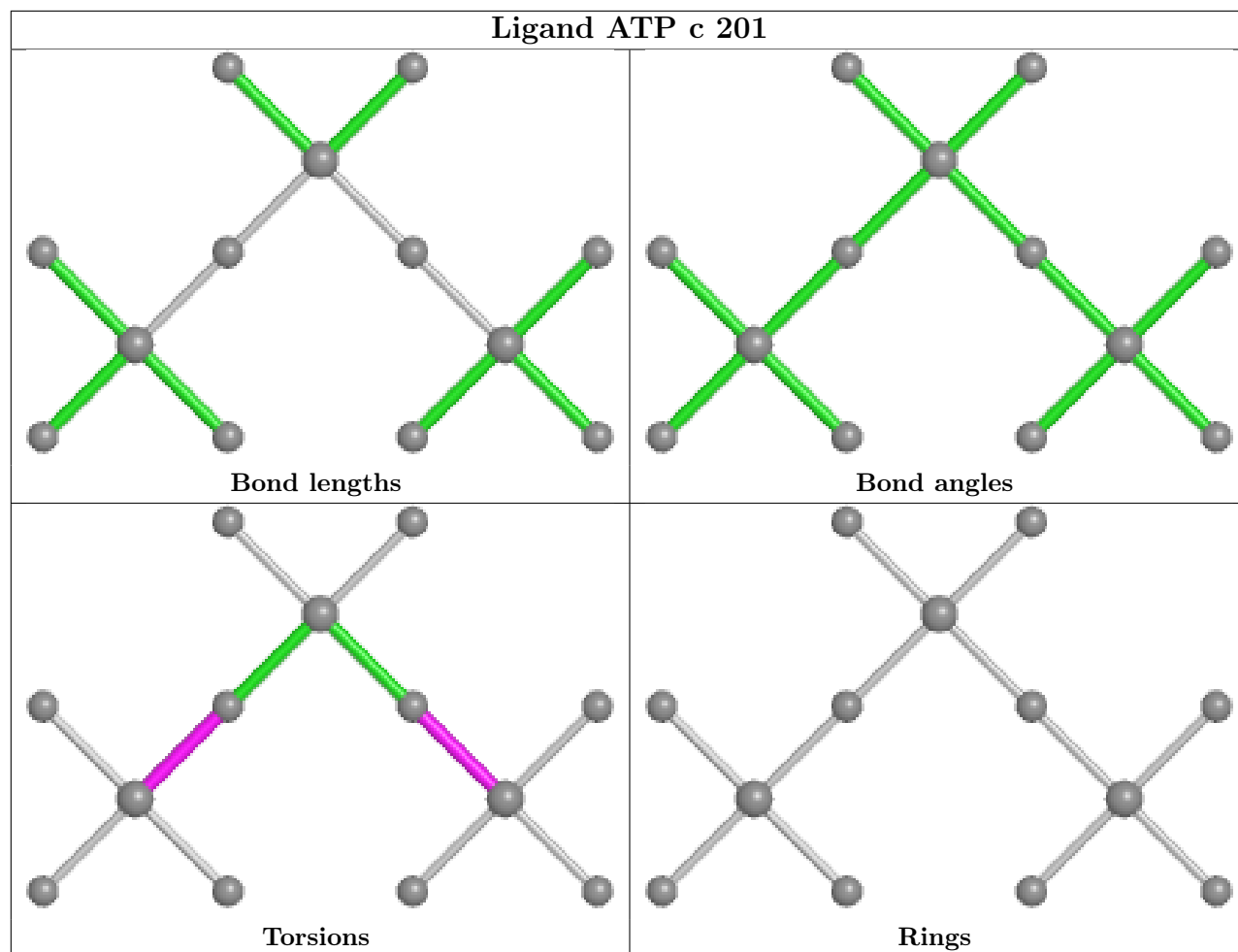
5 of 37 torsion outliers are listed below:

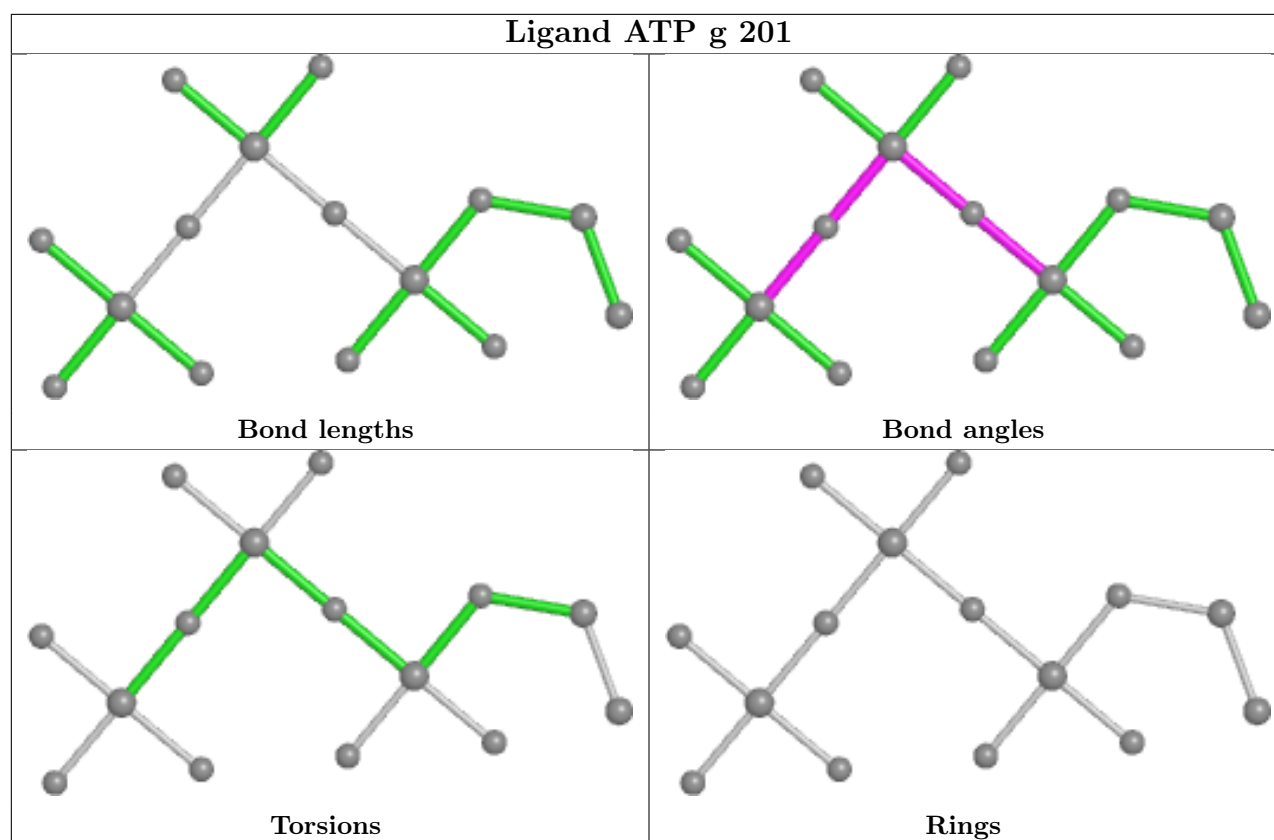
Mol	Chain	Res	Type	Atoms
6	H	201	GOL	O1-C1-C2-C3
6	H	201	GOL	C1-C2-C3-O3
6	O	203	GOL	C1-C2-C3-O3
7	c	201	ATP	PB-O3B-PG-O3G
7	c	201	ATP	PB-O3A-PA-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	185/199 (92%)	-0.14	2 (1%) 80 63	47, 65, 92, 111	0
1	B	185/199 (92%)	-0.19	4 (2%) 62 42	47, 63, 98, 123	0
1	C	187/199 (93%)	-0.31	2 (1%) 80 63	33, 49, 85, 123	0
1	D	181/199 (90%)	-0.30	3 (1%) 70 50	33, 54, 89, 123	0
1	E	185/199 (92%)	-0.22	3 (1%) 72 52	41, 57, 94, 128	0
1	F	185/199 (92%)	-0.36	3 (1%) 72 52	39, 55, 87, 111	0
1	G	182/199 (91%)	-0.25	2 (1%) 80 63	29, 47, 83, 144	0
1	H	183/199 (91%)	-0.27	4 (2%) 62 42	27, 45, 90, 144	0
1	I	191/199 (95%)	-0.33	1 (0%) 91 80	36, 55, 86, 116	0
1	J	184/199 (92%)	-0.19	5 (2%) 54 35	34, 52, 101, 156	0
1	K	183/199 (91%)	-0.15	2 (1%) 80 63	47, 69, 102, 145	0
1	L	181/199 (90%)	-0.10	6 (3%) 46 28	45, 64, 100, 158	0
1	M	178/199 (89%)	-0.33	3 (1%) 70 50	36, 56, 102, 127	0
1	N	185/199 (92%)	-0.22	2 (1%) 80 63	38, 61, 95, 113	0
1	O	187/199 (93%)	-0.41	1 (0%) 91 80	36, 56, 83, 120	0
1	P	183/199 (91%)	-0.30	1 (0%) 91 80	36, 51, 92, 132	0
1	Q	184/199 (92%)	-0.19	2 (1%) 80 63	30, 51, 88, 138	0
1	R	186/199 (93%)	-0.36	1 (0%) 91 80	31, 47, 82, 110	0
1	S	185/199 (92%)	-0.13	3 (1%) 72 52	43, 61, 98, 115	0
1	T	185/199 (92%)	-0.24	4 (2%) 62 42	38, 59, 98, 128	0
2	a	106/109 (97%)	0.83	19 (17%) 1 1	45, 86, 138, 152	0
2	b	107/109 (98%)	0.43	11 (10%) 6 3	52, 81, 119, 162	0
2	c	107/109 (98%)	0.18	5 (4%) 31 18	38, 67, 104, 118	0
2	d	108/109 (99%)	0.55	15 (13%) 2 1	46, 77, 116, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	e	107/109 (98%)	0.51	11 (10%) 6 3	45, 79, 119, 131	0
2	f	106/109 (97%)	0.25	6 (5%) 23 13	47, 78, 133, 156	0
2	g	102/109 (93%)	0.41	9 (8%) 10 5	44, 74, 115, 140	0
2	h	108/109 (99%)	-0.16	1 (0%) 84 69	35, 58, 92, 142	0
2	i	103/109 (94%)	0.65	17 (16%) 1 1	52, 90, 141, 165	0
2	j	107/109 (98%)	0.00	1 (0%) 84 69	37, 63, 101, 118	0
2	k	97/109 (88%)	1.17	24 (24%) 0 0	59, 91, 137, 145	0
2	l	103/109 (94%)	0.90	26 (25%) 0 0	45, 95, 141, 154	0
2	m	107/109 (98%)	-0.06	3 (2%) 53 34	32, 59, 102, 150	0
2	n	94/109 (86%)	1.15	30 (31%) 0 0	67, 105, 143, 174	0
2	o	107/109 (98%)	0.40	6 (5%) 24 13	45, 83, 133, 152	0
2	p	108/109 (99%)	0.36	6 (5%) 24 13	46, 74, 120, 155	0
2	q	107/109 (98%)	0.29	8 (7%) 14 7	47, 76, 109, 157	0
2	r	99/109 (90%)	0.07	5 (5%) 28 16	42, 68, 102, 119	0
2	s	107/109 (98%)	0.78	23 (21%) 0 0	49, 84, 131, 144	0
2	t	107/109 (98%)	0.50	9 (8%) 11 5	49, 84, 127, 154	0
All	All	5782/6160 (93%)	0.00	289 (4%) 28 17	27, 62, 116, 174	0

The worst 5 of 289 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	186	PRO	5.9
1	C	188	VAL	5.7
2	f	71	GLU	5.4
1	J	186	PRO	5.1
2	k	75	SER	5.0

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, 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.

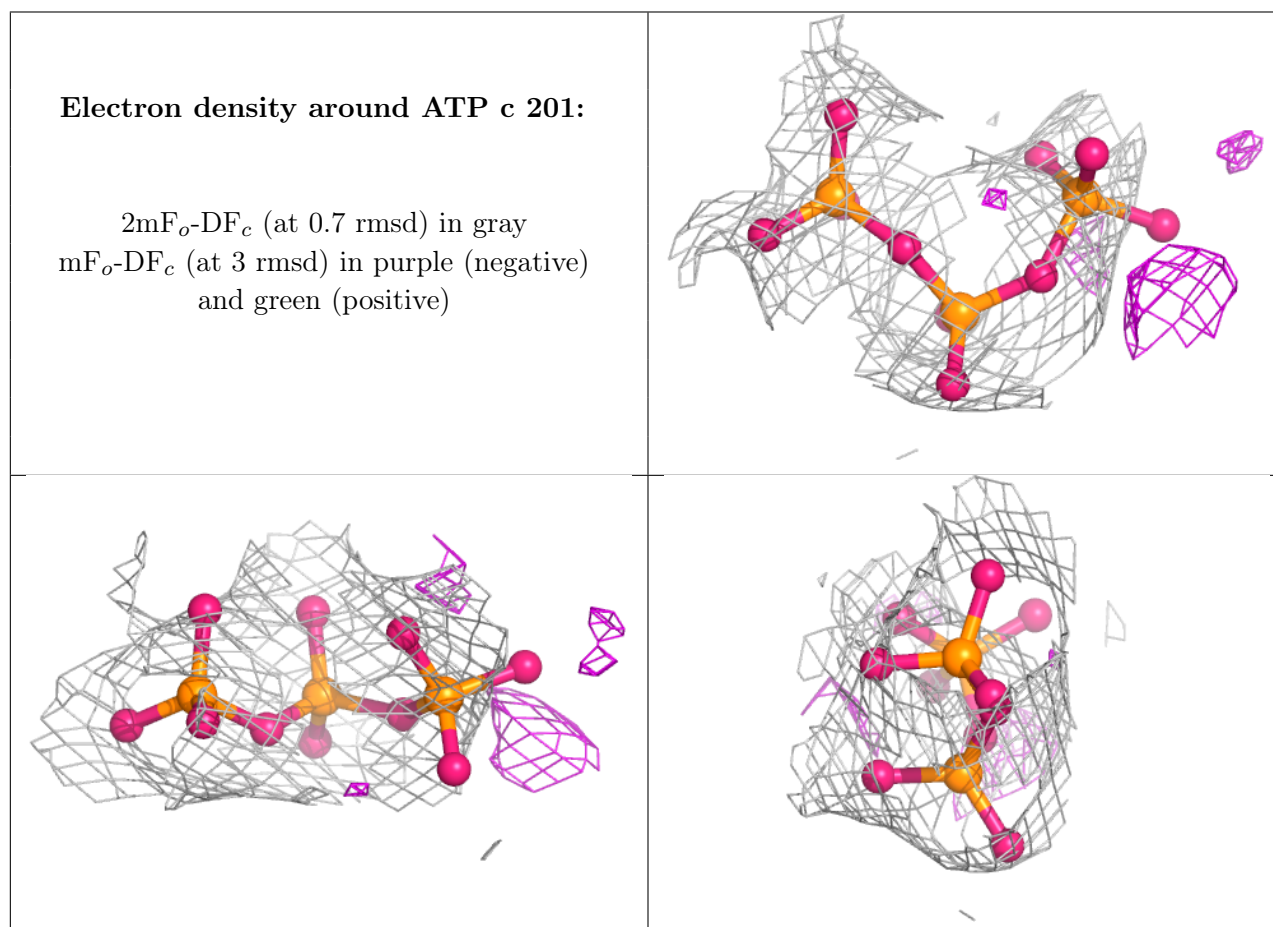
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	t	201	5/5	0.52	0.26	90,111,122,134	0
6	GOL	O	203	6/6	0.66	0.22	92,97,105,111	0
4	PO4	n	201	5/5	0.70	0.19	97,124,136,137	0
3	EDO	R	202	4/4	0.72	0.26	68,72,74,79	0
3	EDO	H	202	4/4	0.73	0.30	72,74,79,80	0
4	PO4	o	201	5/5	0.73	0.21	103,104,127,135	0
4	PO4	d	201	5/5	0.74	0.22	84,90,115,120	0
4	PO4	p	201	5/5	0.75	0.27	90,90,112,117	0
4	PO4	b	201	5/5	0.75	0.20	94,97,118,127	0
4	PO4	i	201	5/5	0.75	0.23	81,88,111,116	0
6	GOL	H	201	6/6	0.76	0.24	86,95,107,113	0
4	PO4	e	201	5/5	0.77	0.19	90,94,122,125	0
5	PEG	O	201	7/7	0.78	0.28	78,92,106,115	0
3	EDO	A	201	4/4	0.78	0.23	72,73,82,83	0
3	EDO	S	201	4/4	0.78	0.27	74,83,83,86	0
4	PO4	l	201	5/5	0.79	0.23	96,126,129,132	0
4	PO4	E	201	5/5	0.79	0.26	112,118,126,133	0
4	PO4	r	201	5/5	0.80	0.23	73,81,100,102	0
5	PEG	Q	202	7/7	0.80	0.23	63,78,94,101	0
4	PO4	a	201	5/5	0.81	0.14	87,94,113,116	0
3	EDO	G	202	4/4	0.81	0.26	53,65,65,68	0
3	EDO	H	204	4/4	0.81	0.50	66,81,83,83	0
5	PEG	D	201	7/7	0.81	0.25	69,82,95,98	0
5	PEG	P	202	7/7	0.82	0.22	77,81,98,102	0
4	PO4	j	201	5/5	0.82	0.24	80,109,124,125	0
4	PO4	k	201	5/5	0.83	0.20	95,100,124,130	0
4	PO4	s	201	5/5	0.84	0.17	82,96,118,121	0
5	PEG	R	203	7/7	0.84	0.26	67,72,83,89	0
3	EDO	Q	201	4/4	0.85	0.18	67,68,69,72	0
4	PO4	q	201	5/5	0.85	0.21	82,96,107,112	0
3	EDO	H	203	4/4	0.85	0.20	65,77,79,81	0
7	ATP	c	201	13/31	0.85	0.21	112,145,174,185	0
4	PO4	m	201	5/5	0.86	0.14	69,88,98,107	0
5	PEG	G	203	7/7	0.86	0.19	72,83,91,93	0
3	EDO	J	201	4/4	0.86	0.24	65,73,75,79	0
4	PO4	h	201	5/5	0.88	0.14	85,102,110,113	0
3	EDO	P	201	4/4	0.89	0.19	62,63,69,70	0

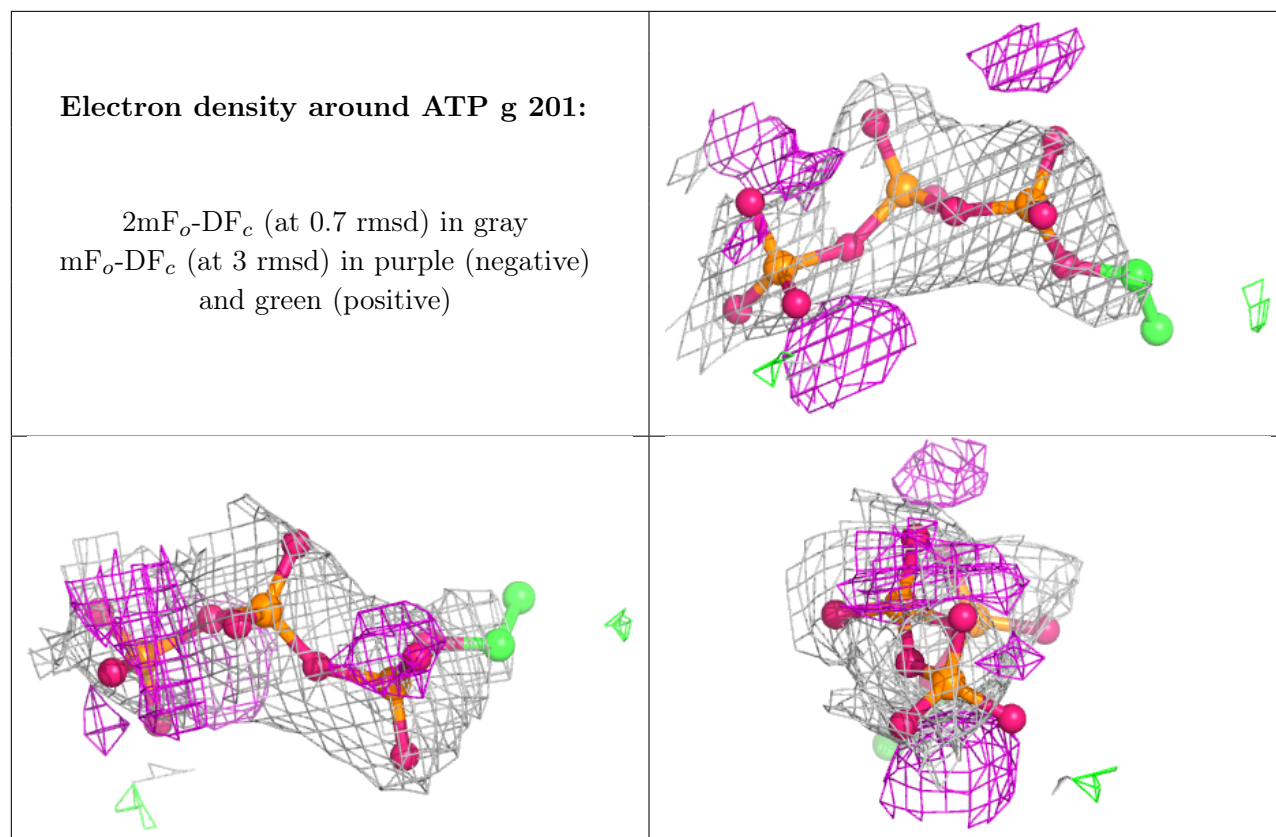
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	S	202	4/4	0.89	0.22	68,71,76,77	0
5	PEG	K	201	7/7	0.89	0.20	73,85,98,100	0
3	EDO	C	201	4/4	0.89	0.19	63,64,65,66	0
3	EDO	O	202	4/4	0.89	0.17	70,75,78,79	0
3	EDO	C	202	4/4	0.90	0.18	52,60,64,64	0
7	ATP	g	201	15/31	0.90	0.28	94,115,155,157	0
3	EDO	R	201	4/4	0.92	0.11	52,52,53,55	0
4	PO4	f	201	5/5	0.93	0.12	75,96,107,109	0
3	EDO	G	201	4/4	0.94	0.30	58,64,67,67	0
5	PEG	N	201	7/7	0.94	0.18	74,81,90,96	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.