



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:33 AM UTC

PDB ID : 7LJ1 / pdb_00007lj1
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

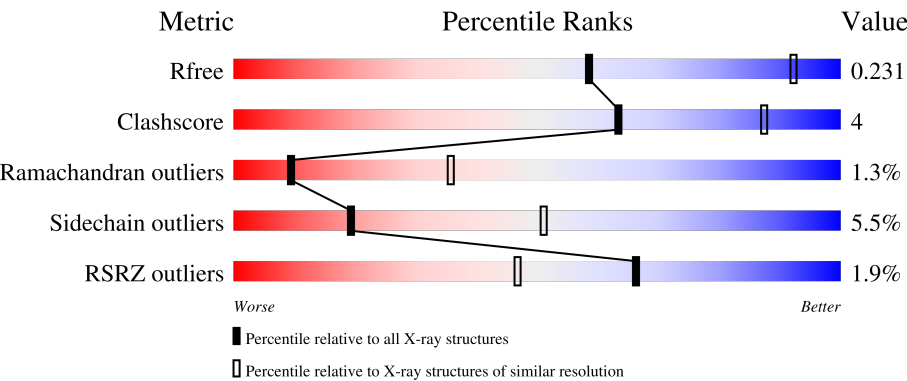
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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.



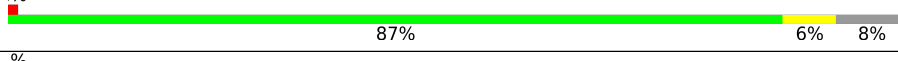
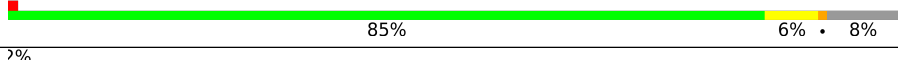
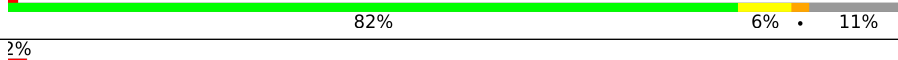
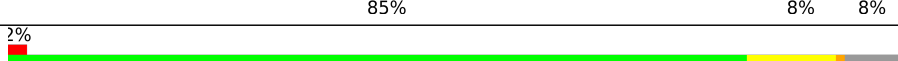
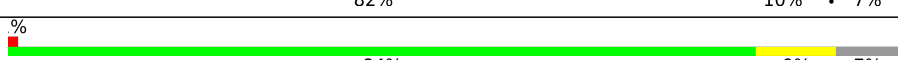
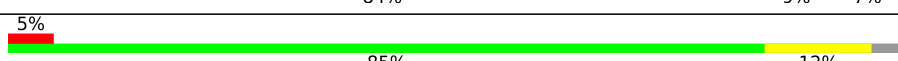
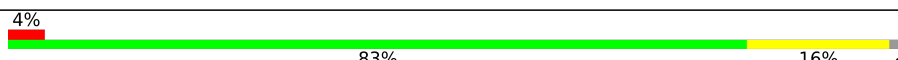
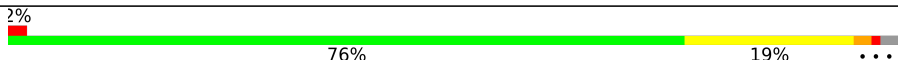
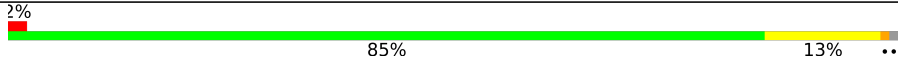
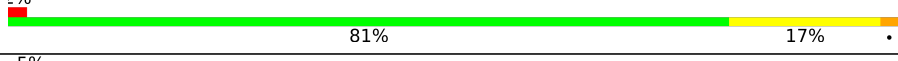
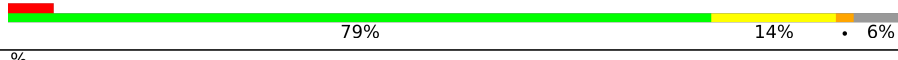
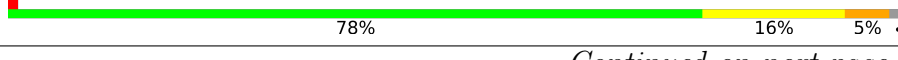
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	

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Mol	Chain	Length	Quality of chain
1	F	199	
1	G	199	
1	H	199	
1	I	199	
1	J	199	
1	K	199	
1	L	199	
1	M	199	
1	N	199	
1	O	199	
1	P	199	
1	Q	199	
1	R	199	
1	S	199	
1	T	199	
2	a	109	
2	b	109	
2	c	109	
2	d	109	
2	e	109	
2	f	109	
2	g	109	
2	h	109	
2	i	109	
2	j	109	

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Mol	Chain	Length	Quality of chain
2	k	109	
2	l	109	
2	m	109	
2	n	109	
2	o	109	
2	p	109	
2	q	109	
2	r	109	
2	s	109	
2	t	109	

2 Entry composition

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

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

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

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

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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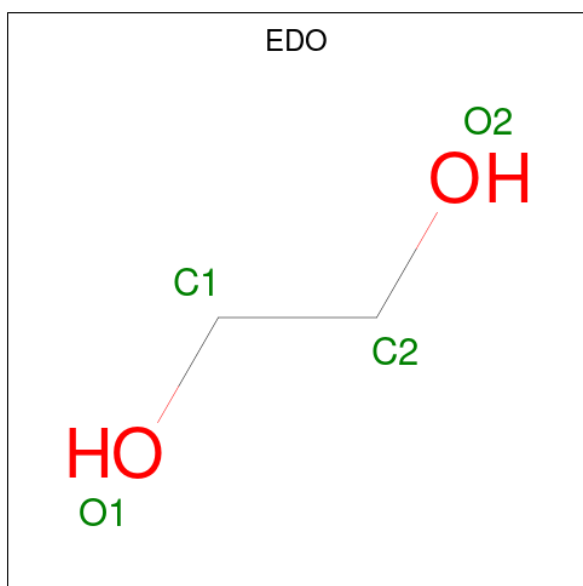
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d	29	GLY	-	expression tag	UNP Q9BYN0
d	30	PRO	-	expression tag	UNP Q9BYN0
d	31	MET	-	expression tag	UNP Q9BYN0
e	29	GLY	-	expression tag	UNP Q9BYN0
e	30	PRO	-	expression tag	UNP Q9BYN0
e	31	MET	-	expression tag	UNP Q9BYN0
f	29	GLY	-	expression tag	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 (CCD ID: EDO) (formula: C₂H₆O₂).



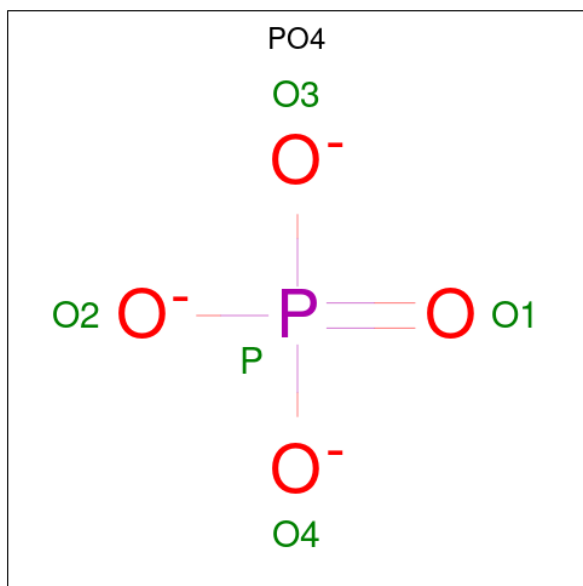
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

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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 (CCD ID: PO4) (formula: O₄P).



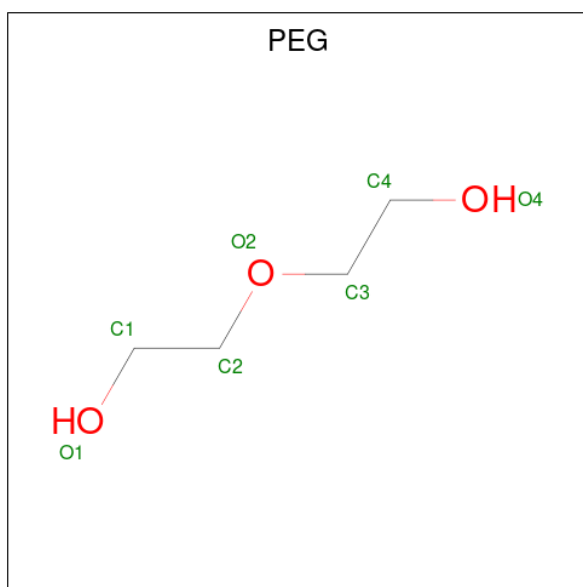
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	a	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0

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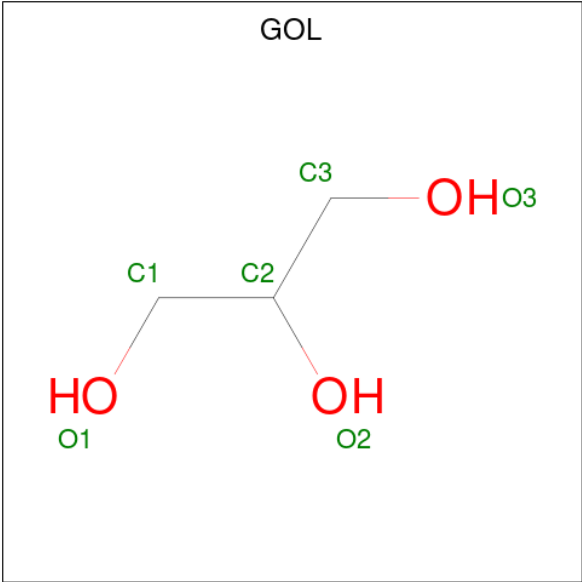
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	b	1	Total	O	P	0	0
			5	4	1		
4	d	1	Total	O	P	0	0
			5	4	1		
4	e	1	Total	O	P	0	0
			5	4	1		
4	f	1	Total	O	P	0	0
			5	4	1		
4	h	1	Total	O	P	0	0
			5	4	1		
4	i	1	Total	O	P	0	0
			5	4	1		
4	j	1	Total	O	P	0	0
			5	4	1		
4	k	1	Total	O	P	0	0
			5	4	1		
4	l	1	Total	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 (CCD ID: PEG) (formula: C₄H₁₀O₃).



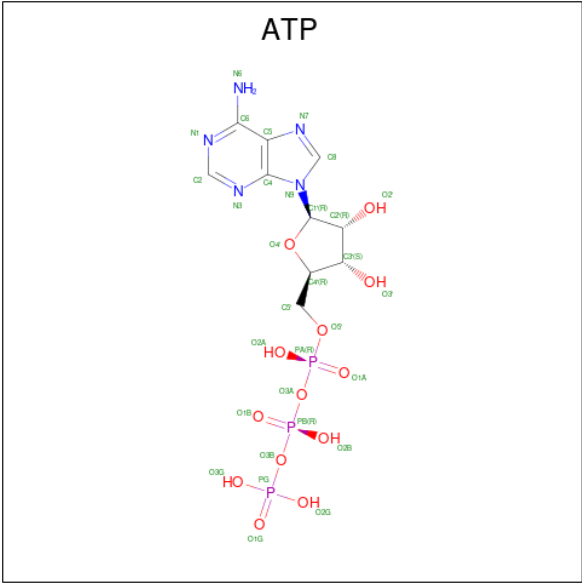
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	K	1	Total	C	O	0	0
			7	4	3		
5	N	1	Total	C	O	0	0
			7	4	3		
5	O	1	Total	C	O	0	0
			7	4	3		
5	P	1	Total	C	O	0	0
			7	4	3		
5	Q	1	Total	C	O	0	0
			7	4	3		
5	R	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is GLYCEROL (CCD ID: 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 (CCD ID: 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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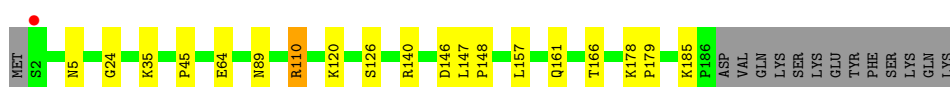
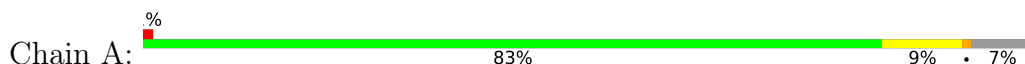
Continued from previous page...

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

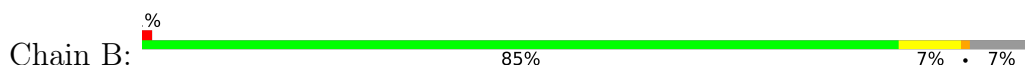
3 Residue-property plots [i](#)

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.

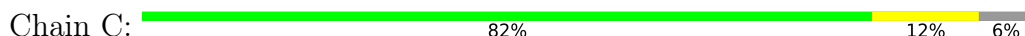
• Molecule 1: Peroxiredoxin-1



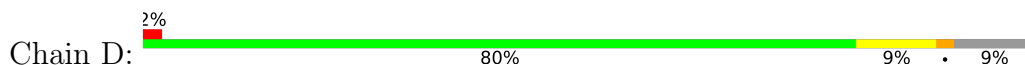
• Molecule 1: Peroxiredoxin-1



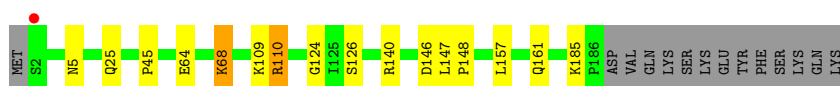
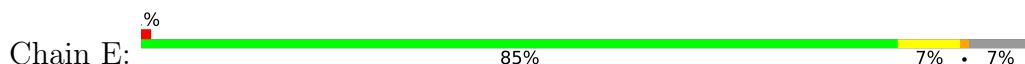
• Molecule 1: Peroxiredoxin-1



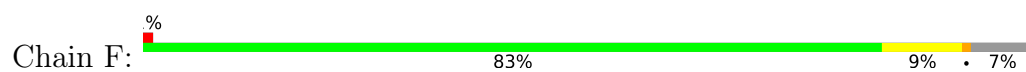
• Molecule 1: Peroxiredoxin-1



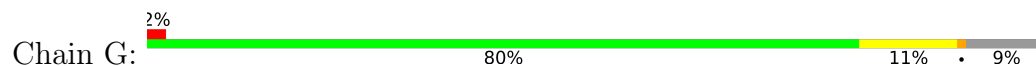
• Molecule 1: Peroxiredoxin-1



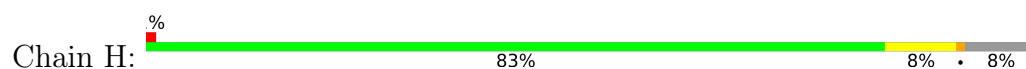
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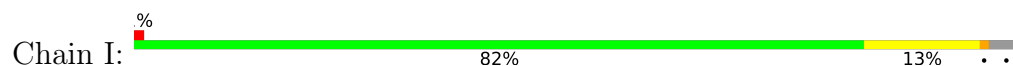
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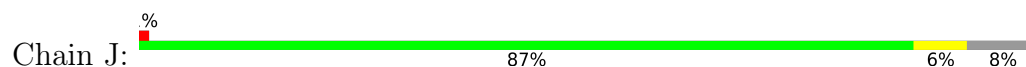
• Molecule 1: Peroxiredoxin-1



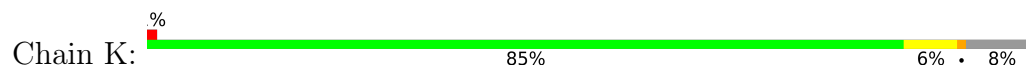
• Molecule 1: Peroxiredoxin-1



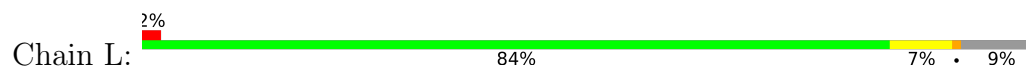
• Molecule 1: Peroxiredoxin-1



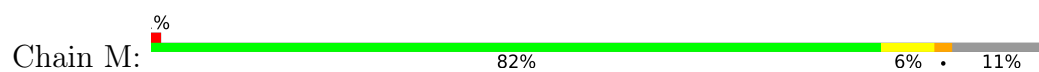
• Molecule 1: Peroxiredoxin-1



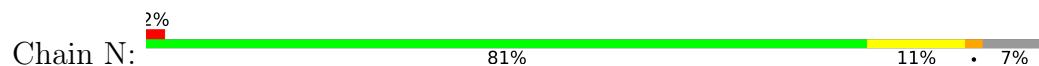
• Molecule 1: Peroxiredoxin-1



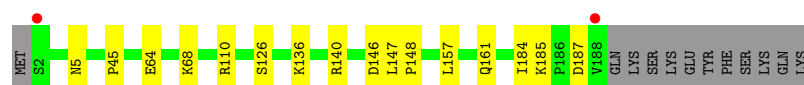
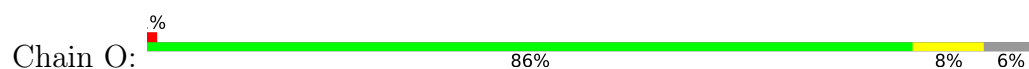
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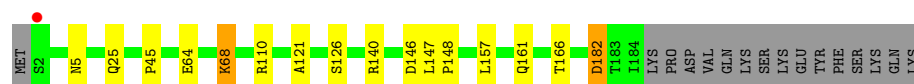
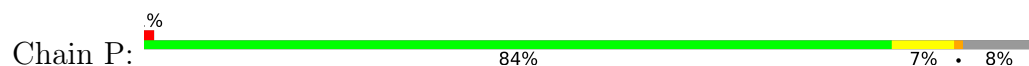
• Molecule 1: Peroxiredoxin-1



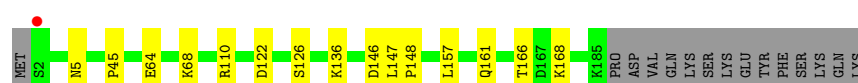
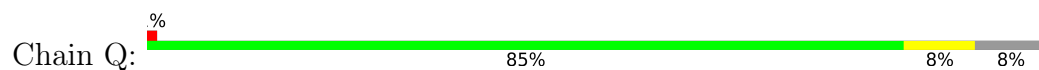
• Molecule 1: Peroxiredoxin-1



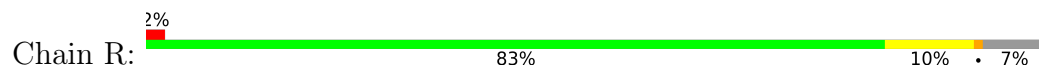
• Molecule 1: Peroxiredoxin-1



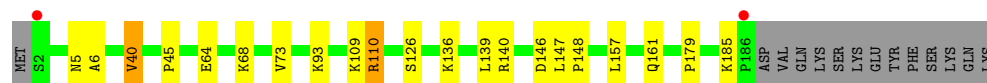
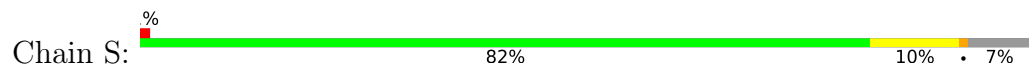
• Molecule 1: Peroxiredoxin-1



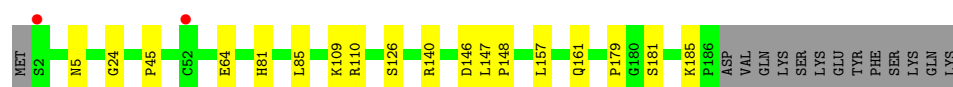
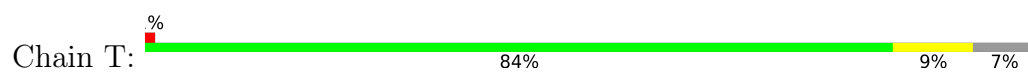
• Molecule 1: Peroxiredoxin-1



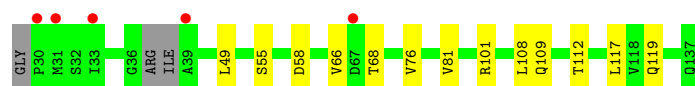
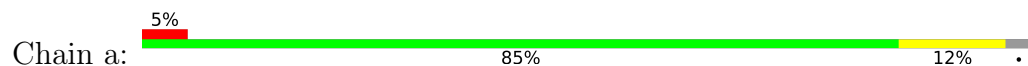
• Molecule 1: Peroxiredoxin-1



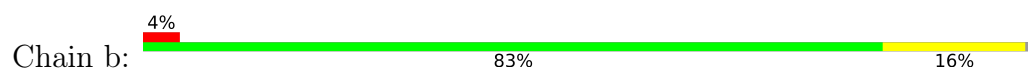
• Molecule 1: Peroxiredoxin-1



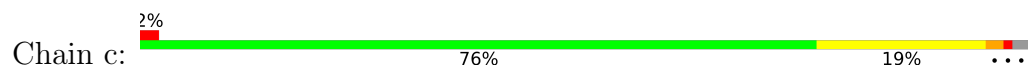
- Molecule 2: Sulfiredoxin-1



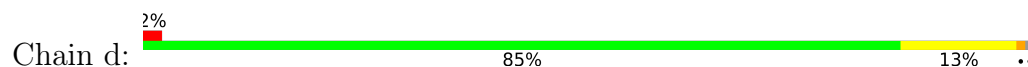
- Molecule 2: Sulfiredoxin-1



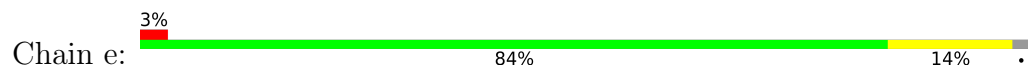
- Molecule 2: Sulfiredoxin-1



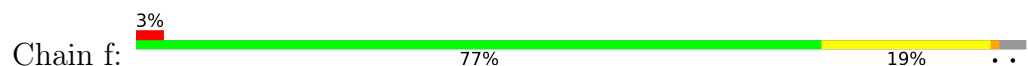
- Molecule 2: Sulfiredoxin-1



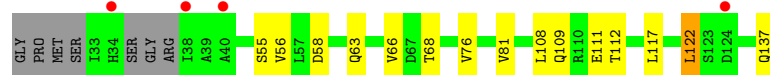
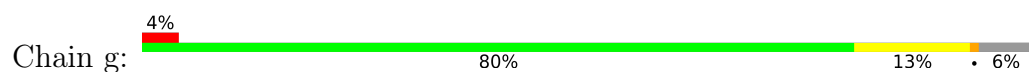
- Molecule 2: Sulfiredoxin-1



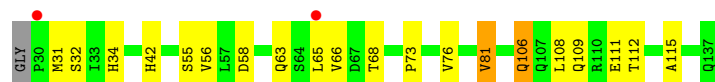
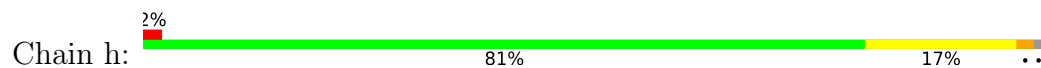
- Molecule 2: Sulfiredoxin-1



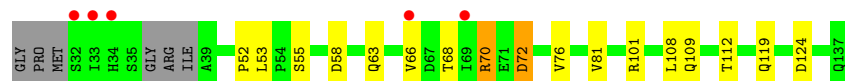
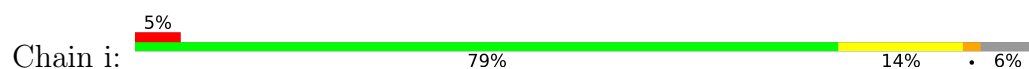
- Molecule 2: Sulfiredoxin-1



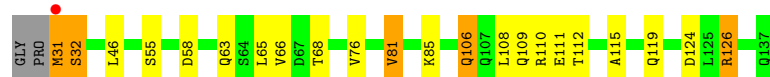
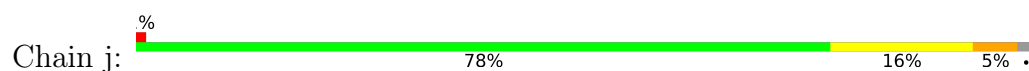
- Molecule 2: Sulfiredoxin-1



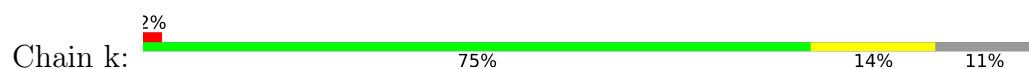
- Molecule 2: Sulfiredoxin-1



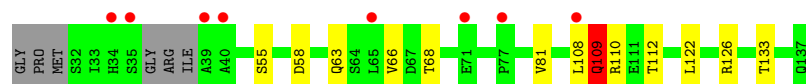
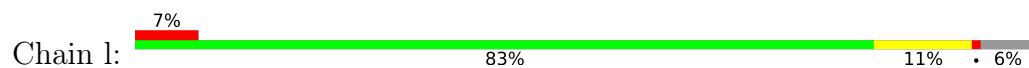
- Molecule 2: Sulfiredoxin-1



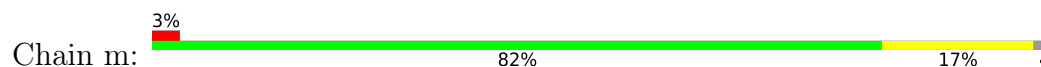
- Molecule 2: Sulfiredoxin-1



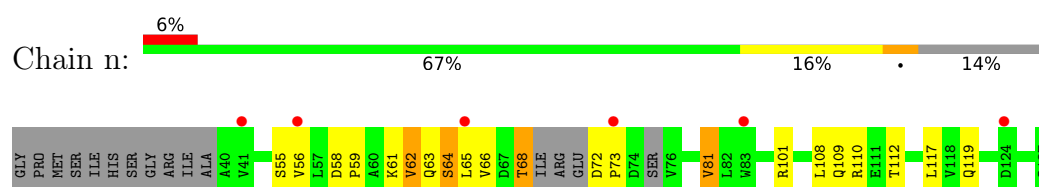
- Molecule 2: Sulfiredoxin-1



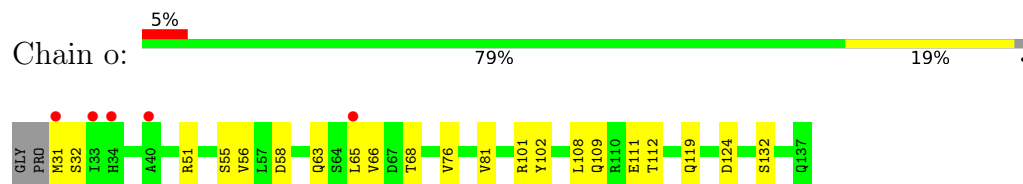
- Molecule 2: Sulfiredoxin-1



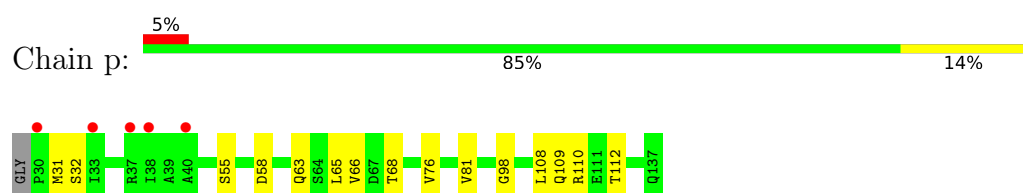
- Molecule 2: Sulfiredoxin-1



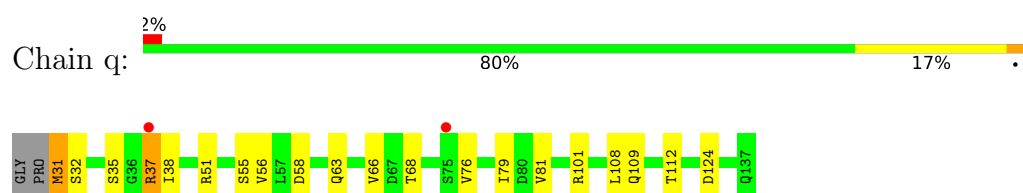
• Molecule 2: Sulfiredoxin-1



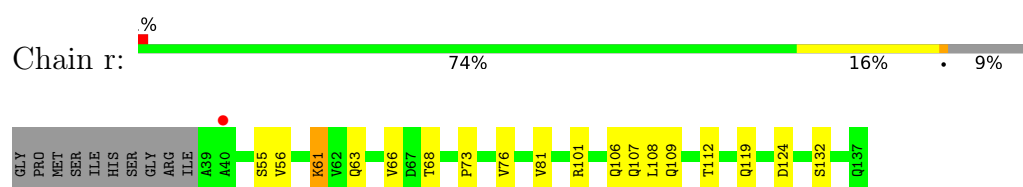
• Molecule 2: Sulfiredoxin-1



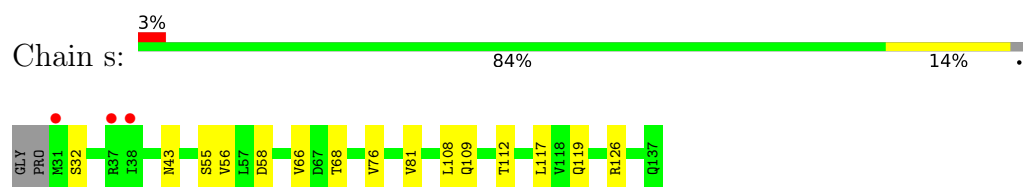
• Molecule 2: Sulfiredoxin-1



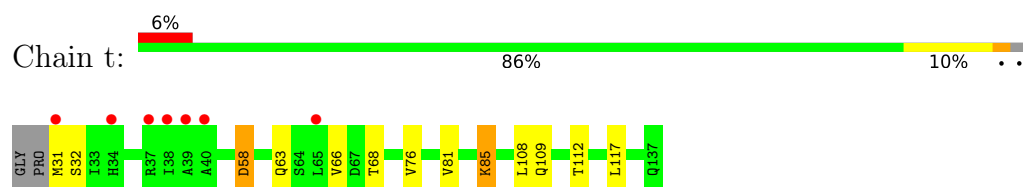
• Molecule 2: Sulfiredoxin-1



• 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 38.97 – 2.97	Depositor EDS
% Data completeness (in resolution range)	91.8 (38.97-2.97) 91.8 (38.97-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.95Å)	Xtriage
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 (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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: ATP, PO4, PEG, EDO, GOL

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	0.97	0/1472	1.36	0/1997
1	B	0.96	0/1460	1.36	1/1984 (0.1%)
1	C	1.01	0/1486	1.38	0/2016
1	D	0.99	0/1441	1.38	1/1953 (0.1%)
1	E	0.96	0/1468	1.36	1/1993 (0.1%)
1	F	0.98	1/1472 (0.1%)	1.36	0/1997
1	G	0.98	0/1451	1.38	0/1967
1	H	0.99	0/1456	1.37	0/1975
1	I	0.98	0/1525	1.38	1/2065 (0.0%)
1	J	0.98	0/1456	1.37	1/1977 (0.1%)
1	K	0.96	0/1456	1.36	0/1975
1	L	0.96	0/1437	1.35	0/1951
1	M	0.96	0/1423	1.35	0/1930
1	N	1.01	3/1456 (0.2%)	1.39	1/1980 (0.1%)
1	O	0.99	0/1484	1.37	0/2015
1	P	0.98	0/1452	1.37	1/1971 (0.1%)
1	Q	0.99	0/1463	1.37	0/1984
1	R	0.97	1/1481 (0.1%)	1.37	1/2009 (0.0%)
1	S	0.98	0/1469	1.37	0/1993
1	T	0.96	0/1468	1.36	0/1993
2	a	1.06	0/824	1.40	0/1127
2	b	1.07	0/837	1.41	0/1145
2	c	1.18	0/842	1.52	2/1150 (0.2%)
2	d	1.06	0/856	1.44	2/1168 (0.2%)
2	e	1.08	0/829	1.53	4/1135 (0.4%)
2	f	1.03	0/824	1.43	1/1128 (0.1%)
2	g	1.01	0/805	1.43	1/1101 (0.1%)
2	h	1.11	0/846	1.49	3/1156 (0.3%)
2	i	1.05	0/794	1.41	1/1088 (0.1%)
2	j	1.09	0/836	1.47	2/1143 (0.2%)
2	k	1.02	0/760	1.39	0/1043
2	l	1.05	0/783	1.41	0/1073

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	m	1.06	0/848	1.42	0/1157
2	n	1.06	1/725 (0.1%)	1.41	0/993
2	o	1.04	0/824	1.42	2/1128 (0.2%)
2	p	1.06	0/838	1.43	2/1149 (0.2%)
2	q	1.05	0/848	1.45	2/1157 (0.2%)
2	r	1.06	0/782	1.41	0/1070
2	s	1.05	0/818	1.43	0/1122
2	t	1.08	0/836	1.45	3/1142 (0.3%)
All	All	1.01	6/45631 (0.0%)	1.39	33/62100 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	172	VAL	C-O	6.12	1.30	1.24
1	N	172	VAL	C-O	-5.88	1.18	1.24
1	N	171	GLU	C-O	5.52	1.30	1.23
2	n	73	PRO	C-O	-5.51	1.16	1.24
1	N	96	GLY	C-O	5.18	1.28	1.23
1	R	96	GLY	C-O	5.01	1.28	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	38	ILE	CA-C-O	-12.86	109.77	120.70
2	e	38	ILE	N-CA-C	10.33	121.19	111.48
2	g	111	GLU	CB-CG-CD	8.48	127.02	112.60
2	f	111	GLU	CB-CG-CD	6.42	123.52	112.60
2	h	106	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	P	182	ASP	CA-CB-CG	6.20	118.80	112.60
2	q	31	MET	CA-C-N	6.10	133.19	121.54
2	q	31	MET	C-N-CA	6.10	133.19	121.54
2	i	70	ARG	CB-CG-CD	5.87	124.80	111.30
1	B	109	LYS	CG-CD-CE	5.87	124.79	111.30
2	h	31	MET	CA-C-N	5.77	132.55	121.54
2	h	31	MET	C-N-CA	5.77	132.55	121.54
2	j	31	MET	CA-C-N	5.71	132.45	121.54
2	j	31	MET	C-N-CA	5.71	132.45	121.54
1	E	68	LYS	CG-CD-CE	5.66	124.31	111.30
2	t	85	LYS	CG-CD-CE	5.64	124.26	111.30
2	d	31	MET	CA-C-N	5.54	132.11	121.54
2	d	31	MET	C-N-CA	5.54	132.11	121.54
2	t	31	MET	CA-C-N	5.44	131.92	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	t	31	MET	C-N-CA	5.44	131.92	121.54
2	p	31	MET	CA-C-N	5.41	131.87	121.54
2	p	31	MET	C-N-CA	5.41	131.87	121.54
1	I	171	GLU	CA-C-O	-5.34	116.22	122.37
1	D	181	SER	CA-C-O	5.29	129.79	120.80
1	R	136	LYS	CB-CG-CD	5.21	123.28	111.30
1	J	27	LYS	CB-CG-CD	5.11	123.06	111.30
1	N	171	GLU	CA-C-O	-5.10	116.51	122.37
2	e	31	MET	CA-C-N	5.09	131.27	121.54
2	e	31	MET	C-N-CA	5.09	131.27	121.54
2	c	31	MET	CA-C-N	5.09	131.26	121.54
2	c	31	MET	C-N-CA	5.09	131.26	121.54
2	o	31	MET	CA-C-N	5.03	131.15	121.54
2	o	31	MET	C-N-CA	5.03	131.15	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1434	0	1415	26	0
1	B	1422	0	1387	14	0
1	C	1448	0	1424	14	0
1	D	1404	0	1388	19	0
1	E	1430	0	1404	14	0
1	F	1435	0	1407	15	0
1	G	1414	0	1395	14	0
1	H	1419	0	1398	14	0
1	I	1487	0	1481	18	0
1	J	1419	0	1388	6	0
1	K	1419	0	1398	13	0
1	L	1401	0	1367	10	0
1	M	1386	0	1368	12	0
1	N	1418	0	1376	22	0
1	O	1446	0	1420	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1415	0	1387	11	0
1	Q	1426	0	1405	10	0
1	R	1443	0	1422	13	0
1	S	1431	0	1412	18	0
1	T	1430	0	1404	21	0
2	a	804	0	786	7	0
2	b	817	0	805	10	0
2	c	822	0	819	12	0
2	d	835	0	838	10	0
2	e	809	0	795	3	0
2	f	804	0	795	12	0
2	g	786	0	774	9	0
2	h	825	0	823	5	0
2	i	775	0	740	9	0
2	j	816	0	809	11	0
2	k	741	0	718	8	0
2	l	764	0	725	4	0
2	m	828	0	830	14	0
2	n	708	0	677	15	0
2	o	804	0	787	8	0
2	p	817	0	794	4	0
2	q	828	0	830	13	0
2	r	763	0	762	9	0
2	s	798	0	764	11	0
2	t	816	0	808	7	0
3	A	4	0	6	0	0
3	C	8	0	12	0	0
3	G	8	0	12	0	0
3	H	12	0	18	0	0
3	J	4	0	6	0	0
3	O	4	0	6	0	0
3	P	4	0	6	0	0
3	Q	4	0	6	0	0
3	R	8	0	12	0	0
3	S	8	0	12	0	0
4	E	5	0	0	0	0
4	a	5	0	0	1	0
4	b	5	0	0	0	0
4	d	5	0	0	0	0
4	e	5	0	0	0	0
4	f	5	0	0	1	0
4	h	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	i	5	0	0	1	0
4	j	5	0	0	0	0
4	k	5	0	0	0	0
4	l	5	0	0	0	0
4	m	5	0	0	0	0
4	n	5	0	0	0	0
4	o	5	0	0	1	0
4	p	5	0	0	1	0
4	q	5	0	0	0	0
4	r	5	0	0	1	0
4	s	5	0	0	0	0
4	t	5	0	0	0	0
5	D	7	0	10	2	0
5	G	7	0	10	0	0
5	K	7	0	10	0	0
5	N	7	0	10	3	0
5	O	7	0	10	1	0
5	P	7	0	10	0	0
5	Q	7	0	10	0	0
5	R	7	0	10	0	0
6	H	6	0	8	0	0
6	O	6	0	8	0	0
7	c	13	0	0	1	0
7	g	15	0	2	1	0
8	A	9	0	0	0	0
8	B	5	0	0	1	0
8	C	14	0	0	1	0
8	D	10	0	0	3	0
8	E	10	0	0	0	0
8	F	7	0	0	0	0
8	G	17	0	0	1	0
8	H	18	0	0	2	0
8	I	13	0	0	2	0
8	J	9	0	0	1	0
8	K	5	0	0	0	0
8	L	1	0	0	0	0
8	M	8	0	0	1	0
8	N	6	0	0	0	0
8	O	4	0	0	2	0
8	P	5	0	0	0	0
8	Q	6	0	0	1	0
8	R	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	S	4	0	0	2	0
8	T	8	0	0	0	0
8	b	2	0	0	0	0
8	c	4	0	0	2	0
8	d	2	0	0	0	0
8	e	1	0	0	0	0
8	f	1	0	0	1	0
8	g	1	0	0	0	0
8	h	4	0	0	1	0
8	j	3	0	0	1	0
8	l	1	0	0	0	0
8	m	2	0	0	0	0
8	n	1	0	0	0	0
8	o	2	0	0	0	0
8	p	1	0	0	0	0
8	q	2	0	0	0	0
8	r	3	0	0	1	0
8	t	1	0	0	0	0
All	All	44942	0	43919	354	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 4.

All (354) 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)
2:n:59:PRO:HA	2:n:62:VAL:CG1	1.80	1.12
1:A:110:ARG:HD3	8:D:302:HOH:O	1.54	1.08
1:C:4:GLY:HA2	1:D:1:MET:HA	1.37	1.04
1:K:110:ARG:HD2	1:N:110:ARG:CZ	1.93	0.98
1:F:110:ARG:NH1	1:I:110:ARG:HD2	1.81	0.96
1:L:110:ARG:HD3	8:O:301:HOH:O	1.66	0.95
2:n:59:PRO:HA	2:n:62:VAL:HG13	1.53	0.90
1:S:110:ARG:HD3	8:S:302:HOH:O	1.75	0.86
2:n:68:THR:C	2:n:72:ASP:HB3	2.00	0.85
1:B:110:ARG:HD3	8:B:201:HOH:O	1.78	0.83
8:Q:301:HOH:O	1:T:110:ARG:HD2	1.79	0.83
1:M:25:GLN:HG3	2:r:119:GLN:HB2	1.60	0.83
8:C:303:HOH:O	1:H:110:ARG:HD3	1.81	0.81
1:M:110:ARG:HD3	8:M:205:HOH:O	1.80	0.80
1:K:110:ARG:HD2	1:N:110:ARG:NH2	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:122:LEU:HD12	2:k:123:SER:N	1.98	0.79
1:A:110:ARG:NH1	1:D:110:ARG:HD3	1.98	0.78
2:j:126:ARG:HD3	8:j:301:HOH:O	1.83	0.78
1:I:181:SER:HB2	2:m:110:ARG:O	1.83	0.77
1:F:110:ARG:NH1	1:I:110:ARG:CD	2.48	0.77
1:Q:110:ARG:HD3	1:T:110:ARG:NH1	2.03	0.74
1:L:110:ARG:NH1	1:O:110:ARG:HD3	2.02	0.74
1:T:85:LEU:HD11	2:q:37:ARG:NH1	2.03	0.74
1:B:110:ARG:NH1	1:E:110:ARG:HD2	2.02	0.73
1:B:110:ARG:CZ	1:E:110:ARG:HD2	2.18	0.73
1:A:24:GLY:HA3	2:d:37:ARG:HE	1.54	0.73
1:C:110:ARG:HD3	1:H:110:ARG:NH2	2.04	0.73
1:N:136:LYS:HE3	5:N:201:PEG:H31	1.72	0.72
1:N:171:GLU:O	2:j:111:GLU:HB2	1.91	0.71
1:A:89:ASN:HD21	2:d:37:ARG:NH1	1.87	0.71
1:M:109:LYS:HE3	1:R:122:ASP:O	1.91	0.71
1:T:185:LYS:HD3	2:s:43:ASN:HD21	1.56	0.70
2:n:59:PRO:CA	2:n:62:VAL:HG13	2.23	0.69
1:P:110:ARG:HD3	1:S:110:ARG:NH2	2.08	0.68
2:c:71:GLU:HG3	8:c:302:HOH:O	1.93	0.68
2:c:102:TYR:CE1	2:c:106:GLN:HG3	2.29	0.68
1:Q:122:ASP:O	1:T:109:LYS:HD3	1.95	0.67
2:c:71:GLU:CG	8:c:302:HOH:O	2.43	0.66
1:A:185:LYS:HD3	2:b:43:ASN:OD1	1.96	0.66
1:I:128:ARG:HD2	1:I:151:ARG:NH2	2.11	0.66
1:C:4:GLY:CA	1:D:1:MET:HA	2.21	0.65
2:g:117:LEU:N	2:g:117:LEU:HD12	2.12	0.64
1:I:182:ASP:O	2:m:47:SER:HA	1.97	0.64
2:n:59:PRO:O	2:n:62:VAL:HG13	1.97	0.64
1:S:40:VAL:CG1	1:S:73:VAL:HG22	2.28	0.63
2:a:49:LEU:HD21	2:a:81:VAL:HG21	1.79	0.63
1:K:110:ARG:NH1	1:N:108:PRO:O	2.31	0.63
2:o:101:ARG:HD3	4:o:201:PO4:O1	1.97	0.63
1:N:136:LYS:HE3	5:N:201:PEG:C3	2.28	0.63
1:G:140:ARG:NH1	1:H:146:ASP:OD2	2.32	0.62
2:q:35:SER:HA	2:q:37:ARG:NH2	2.15	0.62
2:g:56:VAL:O	2:g:56:VAL:HG23	2.00	0.62
1:A:24:GLY:HA3	2:d:37:ARG:NE	2.14	0.61
1:O:136:LYS:HE3	5:O:201:PEG:O2	2.01	0.61
1:H:170:GLY:HA2	8:H:304:HOH:O	2.00	0.61
2:f:56:VAL:HG23	2:f:56:VAL:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:56:VAL:HG23	2:n:56:VAL:O	2.01	0.60
2:t:58:ASP:OD1	2:t:58:ASP:O	2.19	0.60
2:s:56:VAL:HG23	2:s:56:VAL:O	2.00	0.60
2:n:59:PRO:C	2:n:62:VAL:HG13	2.27	0.60
2:r:56:VAL:HG23	2:r:56:VAL:O	2.02	0.60
2:c:98:GLY:HA2	7:c:201:ATP:O1G	2.01	0.60
1:D:50:PHE:CD2	2:d:82:LEU:HD11	2.37	0.60
2:f:51:ARG:HD3	8:f:301:HOH:O	2.02	0.59
1:K:110:ARG:CD	1:N:110:ARG:NH2	2.65	0.59
1:G:110:ARG:NH2	1:J:110:ARG:HD3	2.17	0.59
2:j:46:LEU:HD23	2:j:106:GLN:HG2	1.85	0.59
1:F:25:GLN:HB2	2:i:119:GLN:HB2	1.85	0.58
2:g:117:LEU:N	2:g:117:LEU:CD1	2.66	0.58
1:R:99:PRO:HB3	2:m:37:ARG:HG2	1.85	0.58
2:i:72:ASP:N	2:i:72:ASP:OD1	2.36	0.58
2:q:35:SER:HA	2:q:37:ARG:HH21	1.69	0.58
1:C:146:ASP:OD2	1:D:140:ARG:NH1	2.37	0.58
2:m:31:MET:HG2	2:m:31:MET:O	2.03	0.58
2:p:98:GLY:HA2	4:p:201:PO4:O1	2.04	0.58
1:N:136:LYS:HE3	5:N:201:PEG:C4	2.34	0.57
1:S:157:LEU:O	1:S:161:GLN:HG3	2.05	0.57
1:O:140:ARG:NH1	1:P:146:ASP:OD2	2.38	0.56
1:S:40:VAL:HG13	1:S:73:VAL:HA	1.86	0.56
1:M:110:ARG:NH2	1:R:110:ARG:HD2	2.20	0.56
1:D:128:ARG:NH2	8:D:301:HOH:O	2.32	0.56
1:E:146:ASP:OD2	1:F:140:ARG:NH1	2.39	0.56
1:M:109:LYS:CE	1:R:122:ASP:O	2.53	0.56
2:g:122:LEU:HD12	2:g:122:LEU:O	2.06	0.56
2:l:126:ARG:HG2	2:l:133:THR:HG21	1.88	0.56
2:r:101:ARG:HD3	4:r:201:PO4:O2	2.06	0.56
2:d:37:ARG:O	2:d:37:ARG:HG2	2.06	0.56
1:A:157:LEU:O	1:A:161:GLN:HG3	2.06	0.56
1:O:157:LEU:O	1:O:161:GLN:HG3	2.06	0.56
1:T:24:GLY:CA	2:q:37:ARG:NH1	2.69	0.56
2:n:59:PRO:CA	2:n:62:VAL:CG1	2.71	0.56
1:L:157:LEU:O	1:L:161:GLN:HG3	2.06	0.55
1:N:173:SER:OG	2:j:110:ARG:HD2	2.06	0.55
1:B:157:LEU:O	1:B:161:GLN:HG3	2.07	0.55
2:n:61:LYS:HA	2:n:64:SER:OG	2.07	0.55
1:F:186:PRO:O	1:F:187:ASP:HB3	2.06	0.55
1:K:157:LEU:O	1:K:161:GLN:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:LEU:O	1:F:161:GLN:HG3	2.06	0.55
1:I:157:LEU:O	1:I:161:GLN:HG3	2.06	0.55
1:N:157:LEU:O	1:N:161:GLN:HG3	2.06	0.55
2:i:101:ARG:HD3	4:i:201:PO4:O2	2.06	0.55
1:M:157:LEU:O	1:M:161:GLN:HG3	2.07	0.55
1:D:136:LYS:HE2	5:D:201:PEG:H41	1.89	0.55
1:I:181:SER:CB	2:m:110:ARG:O	2.55	0.55
1:J:157:LEU:O	1:J:161:GLN:HG3	2.07	0.55
1:D:157:LEU:O	1:D:161:GLN:HG3	2.07	0.54
1:S:40:VAL:HG13	1:S:73:VAL:HG22	1.89	0.54
1:T:24:GLY:HA3	2:q:37:ARG:NH1	2.21	0.54
1:T:157:LEU:O	1:T:161:GLN:HG3	2.08	0.54
1:Q:157:LEU:O	1:Q:161:GLN:HG3	2.08	0.54
1:D:136:LYS:HE2	5:D:201:PEG:C4	2.36	0.54
1:A:89:ASN:OD1	2:d:37:ARG:HD3	2.08	0.54
1:G:157:LEU:O	1:G:161:GLN:HG3	2.07	0.54
1:T:85:LEU:HD11	2:q:37:ARG:HH12	1.71	0.54
2:t:76:VAL:HG23	2:t:76:VAL:O	2.08	0.54
1:H:157:LEU:O	1:H:161:GLN:HG3	2.07	0.53
1:K:140:ARG:NH1	1:L:146:ASP:OD2	2.41	0.53
1:P:157:LEU:O	1:P:161:GLN:HG3	2.08	0.53
1:E:157:LEU:O	1:E:161:GLN:HG3	2.08	0.53
1:P:25:GLN:HB2	2:s:119:GLN:HB2	1.90	0.53
1:R:157:LEU:O	1:R:161:GLN:HG3	2.08	0.53
2:q:76:VAL:HG23	2:q:76:VAL:O	2.08	0.53
1:F:2:SER:OG	1:F:3:SER:N	2.38	0.53
1:K:25:GLN:HG3	2:n:119:GLN:HB2	1.90	0.53
2:p:76:VAL:HG23	2:p:76:VAL:O	2.09	0.53
1:N:25:GLN:HB2	2:k:119:GLN:HB2	1.91	0.53
2:k:76:VAL:O	2:k:76:VAL:HG23	2.09	0.53
2:l:109:GLN:CG	2:l:109:GLN:O	2.56	0.53
2:n:59:PRO:HA	2:n:62:VAL:HG11	1.83	0.53
1:C:157:LEU:O	1:C:161:GLN:HG3	2.09	0.52
2:m:76:VAL:HG23	2:m:76:VAL:O	2.08	0.52
2:g:76:VAL:HG23	2:g:76:VAL:O	2.09	0.52
2:i:76:VAL:HG23	2:i:76:VAL:O	2.09	0.52
1:C:122:ASP:O	1:H:109:LYS:HD3	2.10	0.52
1:A:89:ASN:ND2	2:d:37:ARG:NH1	2.55	0.52
2:q:79:ILE:HG22	2:q:101:ARG:HH21	1.75	0.52
1:F:110:ARG:CZ	1:I:110:ARG:HD2	2.40	0.52
1:R:25:GLN:HB2	2:m:119:GLN:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:76:VAL:HG23	2:e:76:VAL:O	2.09	0.52
2:f:76:VAL:O	2:f:76:VAL:HG23	2.09	0.52
1:F:147:LEU:N	1:F:148:PRO:HD2	2.25	0.52
1:C:16:LYS:HD3	1:C:30:SER:OG	2.10	0.52
2:c:51:ARG:NH2	2:c:99:CYS:HA	2.25	0.52
1:Q:110:ARG:CD	1:T:110:ARG:NH1	2.72	0.52
2:o:76:VAL:HG23	2:o:76:VAL:O	2.09	0.52
1:M:25:GLN:CG	2:r:119:GLN:HB2	2.35	0.51
1:A:178:LYS:HE2	2:b:91:ASP:OD2	2.10	0.51
2:k:122:LEU:HD12	2:k:122:LEU:C	2.34	0.51
1:I:25:GLN:HB2	2:f:119:GLN:HB2	1.92	0.51
1:S:179:PRO:HG3	2:t:117:LEU:CD1	2.41	0.51
1:G:147:LEU:N	1:G:148:PRO:HD2	2.26	0.51
1:H:81:HIS:NE2	2:c:124:ASP:OD1	2.33	0.51
1:E:185:LYS:HD3	2:f:43:ASN:HD21	1.75	0.51
2:s:76:VAL:HG23	2:s:76:VAL:O	2.09	0.51
1:P:147:LEU:N	1:P:148:PRO:HD2	2.26	0.51
2:n:59:PRO:HA	2:n:62:VAL:HG12	1.85	0.51
1:I:82:PHE:CZ	2:f:124:ASP:OD1	2.64	0.51
2:r:73:PRO:HG3	8:r:301:HOH:O	2.10	0.51
1:D:147:LEU:N	1:D:148:PRO:HD2	2.27	0.50
1:F:110:ARG:HD2	8:I:207:HOH:O	2.11	0.50
1:O:147:LEU:N	1:O:148:PRO:HD2	2.26	0.50
1:T:185:LYS:HD3	2:s:43:ASN:ND2	2.23	0.50
1:A:147:LEU:N	1:A:148:PRO:HD2	2.27	0.50
1:G:25:GLN:HB2	2:j:119:GLN:HB2	1.94	0.50
1:M:147:LEU:N	1:M:148:PRO:HD2	2.27	0.50
1:R:99:PRO:HB3	2:m:37:ARG:CG	2.41	0.50
2:a:49:LEU:CD2	2:a:81:VAL:HG21	2.42	0.49
1:B:147:LEU:N	1:B:148:PRO:HD2	2.27	0.49
1:G:46:LEU:HD22	8:J:301:HOH:O	2.12	0.49
1:G:146:ASP:OD2	1:H:140:ARG:NH1	2.45	0.49
1:E:25:GLN:HB2	2:b:119:GLN:HB2	1.93	0.49
1:N:147:LEU:N	1:N:148:PRO:HD2	2.26	0.49
1:B:110:ARG:NH1	1:E:110:ARG:CD	2.75	0.49
1:J:147:LEU:N	1:J:148:PRO:HD2	2.28	0.49
1:A:140:ARG:NH1	1:B:146:ASP:OD2	2.46	0.49
1:A:185:LYS:HG3	2:b:43:ASN:HD21	1.77	0.49
1:C:147:LEU:N	1:C:148:PRO:HD2	2.27	0.49
1:R:147:LEU:N	1:R:148:PRO:HD2	2.28	0.49
1:T:85:LEU:CD1	2:q:37:ARG:NH1	2.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:66:VAL:HG13	2:e:108:LEU:HD21	1.95	0.49
1:G:52:CYS:SG	7:g:201:ATP:O2G	2.71	0.49
1:I:147:LEU:N	1:I:148:PRO:HD2	2.28	0.49
1:K:147:LEU:N	1:K:148:PRO:HD2	2.28	0.49
2:a:119:GLN:HB2	1:D:25:GLN:HB2	1.94	0.49
1:H:147:LEU:N	1:H:148:PRO:HD2	2.28	0.49
1:L:147:LEU:N	1:L:148:PRO:HD2	2.27	0.48
1:S:147:LEU:N	1:S:148:PRO:HD2	2.28	0.48
1:H:136:LYS:HE2	8:H:308:HOH:O	2.13	0.48
1:K:146:ASP:OD2	1:L:140:ARG:NH1	2.46	0.48
1:S:136:LYS:HE2	8:S:303:HOH:O	2.12	0.48
2:q:66:VAL:HG13	2:q:108:LEU:HD21	1.96	0.48
2:s:76:VAL:O	2:s:76:VAL:CG2	2.62	0.48
1:H:82:PHE:CZ	2:c:124:ASP:OD1	2.67	0.48
1:I:184:ILE:O	2:m:47:SER:CB	2.62	0.48
1:I:184:ILE:O	2:m:47:SER:OG	2.25	0.48
1:E:147:LEU:N	1:E:148:PRO:HD2	2.27	0.48
2:f:76:VAL:O	2:f:76:VAL:CG2	2.62	0.48
1:Q:147:LEU:N	1:Q:148:PRO:HD2	2.29	0.48
1:T:147:LEU:N	1:T:148:PRO:HD2	2.29	0.48
1:A:185:LYS:CG	2:b:43:ASN:HD21	2.27	0.47
2:t:76:VAL:O	2:t:76:VAL:CG2	2.62	0.47
2:m:76:VAL:O	2:m:76:VAL:CG2	2.62	0.47
2:p:76:VAL:O	2:p:76:VAL:CG2	2.62	0.47
1:G:81:HIS:NE2	2:j:124:ASP:OD1	2.33	0.47
1:Q:146:ASP:OD2	1:R:140:ARG:NH1	2.47	0.47
2:b:66:VAL:HG13	2:b:108:LEU:HD21	1.96	0.47
2:e:76:VAL:O	2:e:76:VAL:CG2	2.62	0.47
2:q:76:VAL:O	2:q:76:VAL:CG2	2.62	0.47
1:B:121:ALA:O	1:E:109:LYS:HE3	2.14	0.47
1:D:110:ARG:NH1	8:D:302:HOH:O	2.46	0.47
1:S:40:VAL:HG11	1:S:73:VAL:HG22	1.95	0.47
2:g:76:VAL:O	2:g:76:VAL:CG2	2.62	0.47
1:E:140:ARG:NH1	1:F:146:ASP:OD2	2.46	0.47
1:S:140:ARG:NH1	1:T:146:ASP:OD2	2.47	0.47
2:i:76:VAL:O	2:i:76:VAL:CG2	2.62	0.47
2:a:66:VAL:HG13	2:a:108:LEU:HD21	1.97	0.47
2:o:66:VAL:HG13	2:o:108:LEU:HD21	1.97	0.47
2:p:66:VAL:HG13	2:p:108:LEU:HD21	1.96	0.47
1:L:25:GLN:HB2	2:o:119:GLN:HB2	1.97	0.47
2:h:66:VAL:HG13	2:h:108:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:117:LEU:CD1	1:B:179:PRO:HG3	2.45	0.46
1:N:171:GLU:HB2	2:j:111:GLU:HB2	1.96	0.46
2:f:66:VAL:HG13	2:f:108:LEU:HD21	1.97	0.46
2:k:76:VAL:O	2:k:76:VAL:CG2	2.62	0.46
2:l:122:LEU:O	2:l:126:ARG:HG3	2.15	0.46
1:T:81:HIS:NE2	2:q:124:ASP:OD1	2.35	0.46
2:c:31:MET:HG3	2:c:36:GLY:HA2	1.96	0.46
1:G:179:PRO:HB3	2:h:42:HIS:ND1	2.31	0.46
2:d:66:VAL:HG13	2:d:108:LEU:HD21	1.98	0.46
1:N:81:HIS:NE2	2:k:124:ASP:OD1	2.33	0.46
2:o:76:VAL:O	2:o:76:VAL:CG2	2.62	0.46
1:N:171:GLU:O	2:j:111:GLU:CB	2.61	0.46
2:k:66:VAL:HG13	2:k:108:LEU:HD21	1.97	0.46
2:s:66:VAL:HG13	2:s:108:LEU:HD21	1.98	0.46
1:A:166:THR:HG22	2:b:132:SER:CB	2.46	0.46
1:O:146:ASP:OD2	1:P:140:ARG:NH1	2.48	0.46
1:S:179:PRO:HG3	2:t:117:LEU:HD11	1.98	0.46
1:K:110:ARG:CD	1:N:110:ARG:CZ	2.81	0.45
1:S:146:ASP:OD2	1:T:140:ARG:NH1	2.49	0.45
1:A:166:THR:HG22	2:b:132:SER:HB3	1.97	0.45
1:N:170:GLY:O	2:m:134:PRO:HB3	2.16	0.45
2:l:66:VAL:HG13	2:l:108:LEU:HD21	1.99	0.45
1:P:68:LYS:HA	1:P:68:LYS:HD3	1.73	0.45
1:S:179:PRO:CG	2:t:117:LEU:CD1	2.94	0.45
1:M:82:PHE:CZ	2:r:124:ASP:OD1	2.70	0.45
1:A:120:LYS:HE2	1:A:147:LEU:HD11	1.99	0.44
1:I:110:ARG:NH1	1:I:124:GLY:O	2.50	0.44
2:r:66:VAL:HG13	2:r:108:LEU:HD21	1.99	0.44
1:A:89:ASN:CG	2:d:37:ARG:HH11	2.25	0.44
1:P:147:LEU:N	1:P:148:PRO:CD	2.81	0.44
2:c:102:TYR:CE1	2:c:106:GLN:CG	3.00	0.44
1:R:110:ARG:NH1	1:R:124:GLY:O	2.51	0.44
1:S:147:LEU:N	1:S:148:PRO:CD	2.81	0.44
2:c:66:VAL:HG13	2:c:108:LEU:HD21	2.00	0.44
1:E:110:ARG:NH1	1:E:124:GLY:O	2.50	0.44
1:L:81:HIS:NE2	2:o:124:ASP:OD1	2.31	0.44
1:N:147:LEU:N	1:N:148:PRO:CD	2.81	0.44
1:Q:147:LEU:N	1:Q:148:PRO:CD	2.81	0.44
1:A:147:LEU:N	1:A:148:PRO:CD	2.81	0.44
2:j:66:VAL:HG13	2:j:108:LEU:HD21	2.00	0.44
1:C:140:ARG:NH1	1:D:146:ASP:OD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:LEU:N	1:F:148:PRO:CD	2.81	0.43
1:D:147:LEU:N	1:D:148:PRO:CD	2.81	0.43
1:M:147:LEU:N	1:M:148:PRO:CD	2.81	0.43
2:f:101:ARG:HD3	4:f:201:PO4:O1	2.18	0.43
1:A:179:PRO:HG3	2:b:117:LEU:CD1	2.48	0.43
1:K:147:LEU:N	1:K:148:PRO:CD	2.82	0.43
1:C:147:LEU:N	1:C:148:PRO:CD	2.81	0.43
1:J:147:LEU:N	1:J:148:PRO:CD	2.82	0.43
1:L:146:ASP:C	1:L:148:PRO:HD2	2.44	0.43
1:M:146:ASP:OD2	1:N:140:ARG:NH1	2.52	0.43
1:P:121:ALA:O	1:S:109:LYS:HE3	2.19	0.43
1:T:147:LEU:N	1:T:148:PRO:CD	2.81	0.43
1:R:147:LEU:N	1:R:148:PRO:CD	2.81	0.43
2:g:137:GLN:HA	2:g:137:GLN:OE1	2.18	0.43
1:F:146:ASP:C	1:F:148:PRO:HD2	2.43	0.43
1:I:147:LEU:N	1:I:148:PRO:CD	2.81	0.43
1:L:147:LEU:N	1:L:148:PRO:CD	2.81	0.43
1:N:140:ARG:NH2	2:m:132:SER:OG	2.52	0.43
1:Q:148:PRO:CB	1:R:166:THR:HG21	2.49	0.43
1:B:147:LEU:N	1:B:148:PRO:CD	2.82	0.43
1:D:146:ASP:C	1:D:148:PRO:HD2	2.43	0.43
1:I:136:LYS:HE2	8:I:210:HOH:O	2.17	0.43
1:M:146:ASP:C	1:M:148:PRO:HD2	2.44	0.43
1:G:147:LEU:N	1:G:148:PRO:CD	2.81	0.43
1:I:146:ASP:C	1:I:148:PRO:HD2	2.44	0.43
1:P:146:ASP:C	1:P:148:PRO:HD2	2.44	0.43
2:a:101:ARG:HD3	4:a:201:PO4:O2	2.19	0.43
1:E:146:ASP:C	1:E:148:PRO:HD2	2.44	0.43
1:G:146:ASP:C	1:G:148:PRO:HD2	2.44	0.43
2:n:56:VAL:O	2:n:56:VAL:CG2	2.67	0.43
1:O:146:ASP:C	1:O:148:PRO:HD2	2.43	0.42
1:B:146:ASP:C	1:B:148:PRO:HD2	2.44	0.42
1:H:147:LEU:N	1:H:148:PRO:CD	2.81	0.42
1:N:146:ASP:C	1:N:148:PRO:HD2	2.43	0.42
1:O:147:LEU:N	1:O:148:PRO:CD	2.81	0.42
1:Q:146:ASP:C	1:Q:148:PRO:HD2	2.44	0.42
1:O:110:ARG:NH1	8:O:301:HOH:O	2.52	0.42
1:R:146:ASP:C	1:R:148:PRO:HD2	2.43	0.42
2:n:66:VAL:HG13	2:n:108:LEU:HD21	2.00	0.42
1:E:147:LEU:N	1:E:148:PRO:CD	2.82	0.42
1:S:146:ASP:C	1:S:148:PRO:HD2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:73:PRO:HG3	8:h:301:HOH:O	2.20	0.42
1:C:146:ASP:C	1:C:148:PRO:HD2	2.44	0.42
1:F:50:PHE:CZ	2:f:34:HIS:HB3	2.54	0.42
2:r:61:LYS:HD3	2:r:61:LYS:HA	1.77	0.42
1:A:89:ASN:ND2	2:d:37:ARG:HH11	2.18	0.42
1:A:110:ARG:HH11	1:D:110:ARG:HD3	1.83	0.42
1:T:179:PRO:CG	2:s:117:LEU:CD1	2.98	0.42
2:i:66:VAL:HG13	2:i:108:LEU:HD21	2.01	0.42
1:K:146:ASP:C	1:K:148:PRO:HD2	2.45	0.42
1:K:110:ARG:NH1	1:K:124:GLY:O	2.52	0.42
1:T:146:ASP:C	1:T:148:PRO:HD2	2.45	0.42
1:T:185:LYS:CD	2:s:43:ASN:HD21	2.27	0.42
1:G:114:GLN:HG2	8:G:310:HOH:O	2.20	0.42
2:i:52:PRO:HG2	2:i:53:LEU:HD13	2.01	0.42
2:i:53:LEU:CD1	2:i:53:LEU:N	2.82	0.42
2:n:81:VAL:HG22	2:n:117:LEU:HD22	2.02	0.42
1:P:166:THR:HG22	2:o:132:SER:HB3	2.02	0.41
1:C:94:GLN:O	2:c:33:ILE:HG13	2.20	0.41
1:H:50:PHE:CZ	2:h:34:HIS:HB3	2.55	0.41
1:I:140:ARG:NH1	1:J:146:ASP:OD2	2.53	0.41
1:J:146:ASP:C	1:J:148:PRO:HD2	2.44	0.41
2:t:66:VAL:HG13	2:t:108:LEU:HD21	2.01	0.41
1:A:146:ASP:C	1:A:148:PRO:HD2	2.44	0.41
1:A:146:ASP:OD2	1:B:140:ARG:NH1	2.54	0.41
1:D:180:GLY:O	1:D:181:SER:CB	2.67	0.41
1:F:82:PHE:CZ	2:i:124:ASP:OD1	2.74	0.41
2:g:66:VAL:HG13	2:g:108:LEU:HD21	2.02	0.41
1:B:108:PRO:O	1:E:110:ARG:NH1	2.52	0.41
1:A:185:LYS:HE2	2:b:114:PRO:HB3	2.01	0.41
2:g:56:VAL:O	2:g:56:VAL:CG2	2.66	0.41
2:k:122:LEU:C	2:k:122:LEU:CD1	2.93	0.41
1:A:110:ARG:NH1	1:D:110:ARG:CD	2.77	0.41
2:a:117:LEU:HD11	1:B:179:PRO:HG3	2.03	0.41
1:H:146:ASP:C	1:H:148:PRO:HD2	2.45	0.41
1:Q:166:THR:HG22	2:r:132:SER:HB3	2.03	0.41
1:T:179:PRO:HG3	2:s:117:LEU:CD1	2.50	0.41
2:c:81:VAL:HG13	2:c:115:ALA:HB1	2.03	0.41
2:q:37:ARG:NH2	2:q:38:ILE:HG13	2.36	0.41
1:C:34:TYR:CE2	1:C:72:GLN:HG2	2.57	0.41
1:G:15:PHE:O	1:G:30:SER:HA	2.22	0.41
2:m:66:VAL:HG13	2:m:108:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:PHE:O	1:C:30:SER:HA	2.21	0.40
1:D:47:ASP:OD2	1:D:84:HIS:ND1	2.50	0.40
2:j:81:VAL:HG13	2:j:115:ALA:HB1	2.03	0.40
1:S:6:ALA:HB1	1:S:139:LEU:HD22	2.04	0.40
1:N:6:ALA:HB1	1:N:139:LEU:HD22	2.04	0.40
2:f:56:VAL:O	2:f:56:VAL:CG2	2.68	0.40
2:f:81:VAL:HG22	2:f:117:LEU:HD22	2.04	0.40
2:j:31:MET:O	2:j:32:SER:O	2.39	0.40
2:h:81:VAL:HG13	2:h:115:ALA:HB1	2.03	0.40
2:o:51:ARG:NH1	2:o:102:TYR:CZ	2.89	0.40
2:s:56:VAL:O	2:s:56:VAL:CG2	2.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	183/199 (92%)	176 (96%)	5 (3%)	2 (1%)	11	40
1	B	183/199 (92%)	176 (96%)	5 (3%)	2 (1%)	11	40
1	C	185/199 (93%)	178 (96%)	5 (3%)	2 (1%)	11	40
1	D	179/199 (90%)	171 (96%)	5 (3%)	3 (2%)	7	30
1	E	183/199 (92%)	176 (96%)	5 (3%)	2 (1%)	11	40
1	F	181/199 (91%)	173 (96%)	6 (3%)	2 (1%)	11	40
1	G	180/199 (90%)	172 (96%)	6 (3%)	2 (1%)	11	40
1	H	181/199 (91%)	173 (96%)	6 (3%)	2 (1%)	11	40
1	I	189/199 (95%)	180 (95%)	7 (4%)	2 (1%)	11	40
1	J	180/199 (90%)	173 (96%)	5 (3%)	2 (1%)	11	40
1	K	181/199 (91%)	175 (97%)	4 (2%)	2 (1%)	11	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	177/199 (89%)	169 (96%)	6 (3%)	2 (1%)	11	40
1	M	176/199 (88%)	168 (96%)	6 (3%)	2 (1%)	11	40
1	N	183/199 (92%)	176 (96%)	5 (3%)	2 (1%)	11	40
1	O	185/199 (93%)	177 (96%)	6 (3%)	2 (1%)	11	40
1	P	181/199 (91%)	175 (97%)	4 (2%)	2 (1%)	11	40
1	Q	182/199 (92%)	174 (96%)	6 (3%)	2 (1%)	11	40
1	R	184/199 (92%)	176 (96%)	6 (3%)	2 (1%)	11	40
1	S	183/199 (92%)	176 (96%)	5 (3%)	2 (1%)	11	40
1	T	183/199 (92%)	175 (96%)	6 (3%)	2 (1%)	11	40
2	a	102/109 (94%)	95 (93%)	6 (6%)	1 (1%)	12	42
2	b	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	6	27
2	c	105/109 (96%)	97 (92%)	6 (6%)	2 (2%)	6	27
2	d	106/109 (97%)	99 (93%)	5 (5%)	2 (2%)	6	27
2	e	105/109 (96%)	97 (92%)	5 (5%)	3 (3%)	3	18
2	f	104/109 (95%)	98 (94%)	5 (5%)	1 (1%)	12	42
2	g	98/109 (90%)	95 (97%)	2 (2%)	1 (1%)	12	42
2	h	106/109 (97%)	99 (93%)	5 (5%)	2 (2%)	6	27
2	i	99/109 (91%)	95 (96%)	3 (3%)	1 (1%)	12	42
2	j	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	6	27
2	k	95/109 (87%)	92 (97%)	2 (2%)	1 (1%)	11	40
2	l	99/109 (91%)	95 (96%)	3 (3%)	1 (1%)	12	42
2	m	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	6	27
2	n	88/109 (81%)	85 (97%)	2 (2%)	1 (1%)	11	40
2	o	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	6	27
2	p	106/109 (97%)	99 (93%)	5 (5%)	2 (2%)	6	27
2	q	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	6	27
2	r	97/109 (89%)	94 (97%)	2 (2%)	1 (1%)	12	42
2	s	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	6	27
2	t	105/109 (96%)	98 (93%)	5 (5%)	2 (2%)	6	27
All	All	5684/6160 (92%)	5415 (95%)	195 (3%)	74 (1%)	9	36

All (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
1	F	5	ASN
1	G	5	ASN
1	H	5	ASN
1	I	5	ASN
1	J	5	ASN
1	K	5	ASN
1	L	5	ASN
1	M	5	ASN
1	N	5	ASN
1	O	5	ASN
1	P	5	ASN
1	Q	5	ASN
1	R	5	ASN
1	S	5	ASN
1	T	5	ASN
2	b	32	SER
2	c	32	SER
2	d	32	SER
2	e	32	SER
2	e	39	ALA
2	h	32	SER
2	j	32	SER
2	m	32	SER
2	o	32	SER
2	p	32	SER
2	q	32	SER
2	s	32	SER
2	t	32	SER
2	a	109	GLN
1	D	2	SER
2	b	109	GLN
2	c	109	GLN
2	d	109	GLN
2	e	109	GLN
2	f	109	GLN
2	g	109	GLN
2	h	109	GLN
2	i	109	GLN

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Mol	Chain	Res	Type
2	j	109	GLN
2	k	109	GLN
2	l	109	GLN
2	n	109	GLN
2	o	109	GLN
2	p	109	GLN
2	q	109	GLN
2	r	109	GLN
2	s	109	GLN
2	t	109	GLN
2	m	109	GLN
1	C	45	PRO
1	E	45	PRO
1	F	45	PRO
1	H	45	PRO
1	J	45	PRO
1	M	45	PRO
1	Q	45	PRO
1	A	45	PRO
1	B	45	PRO
1	D	45	PRO
1	G	45	PRO
1	I	45	PRO
1	K	45	PRO
1	L	45	PRO
1	N	45	PRO
1	O	45	PRO
1	P	45	PRO
1	R	45	PRO
1	S	45	PRO
1	T	45	PRO

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	155/171 (91%)	151 (97%)	4 (3%)	40	70
1	B	152/171 (89%)	147 (97%)	5 (3%)	33	65
1	C	157/171 (92%)	151 (96%)	6 (4%)	29	61
1	D	152/171 (89%)	148 (97%)	4 (3%)	40	70
1	E	154/171 (90%)	150 (97%)	4 (3%)	40	70
1	F	156/171 (91%)	153 (98%)	3 (2%)	50	75
1	G	153/171 (90%)	147 (96%)	6 (4%)	28	60
1	H	154/171 (90%)	151 (98%)	3 (2%)	50	75
1	I	163/171 (95%)	154 (94%)	9 (6%)	19	51
1	J	152/171 (89%)	150 (99%)	2 (1%)	61	81
1	K	154/171 (90%)	150 (97%)	4 (3%)	40	70
1	L	151/171 (88%)	147 (97%)	4 (3%)	40	70
1	M	150/171 (88%)	143 (95%)	7 (5%)	23	56
1	N	151/171 (88%)	145 (96%)	6 (4%)	28	60
1	O	157/171 (92%)	151 (96%)	6 (4%)	29	61
1	P	153/171 (90%)	149 (97%)	4 (3%)	40	70
1	Q	153/171 (90%)	148 (97%)	5 (3%)	33	65
1	R	157/171 (92%)	151 (96%)	6 (4%)	29	61
1	S	155/171 (91%)	148 (96%)	7 (4%)	24	57
1	T	154/171 (90%)	151 (98%)	3 (2%)	50	75
2	a	87/93 (94%)	82 (94%)	5 (6%)	18	50
2	b	89/93 (96%)	82 (92%)	7 (8%)	11	37
2	c	91/93 (98%)	80 (88%)	11 (12%)	5	20
2	d	93/93 (100%)	84 (90%)	9 (10%)	8	29
2	e	88/93 (95%)	81 (92%)	7 (8%)	11	36
2	f	87/93 (94%)	78 (90%)	9 (10%)	7	26
2	g	86/93 (92%)	79 (92%)	7 (8%)	11	36
2	h	91/93 (98%)	80 (88%)	11 (12%)	5	20
2	i	82/93 (88%)	74 (90%)	8 (10%)	7	28
2	j	90/93 (97%)	79 (88%)	11 (12%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	k	80/93 (86%)	73 (91%)	7 (9%)	9	33
2	l	80/93 (86%)	72 (90%)	8 (10%)	7	27
2	m	92/93 (99%)	86 (94%)	6 (6%)	15	45
2	n	75/93 (81%)	64 (85%)	11 (15%)	3	14
2	o	86/93 (92%)	77 (90%)	9 (10%)	6	26
2	p	89/93 (96%)	81 (91%)	8 (9%)	9	32
2	q	92/93 (99%)	82 (89%)	10 (11%)	6	24
2	r	84/93 (90%)	75 (89%)	9 (11%)	6	25
2	s	84/93 (90%)	78 (93%)	6 (7%)	13	41
2	t	89/93 (96%)	83 (93%)	6 (7%)	15	44
All	All	4818/5280 (91%)	4555 (94%)	263 (6%)	19	51

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	64	GLU
1	A	110	ARG
1	A	126	SER
2	a	55	SER
2	a	58	ASP
2	a	68	THR
2	a	76	VAL
2	a	112	THR
1	B	64	GLU
1	B	68	LYS
1	B	109	LYS
1	B	110	ARG
1	B	126	SER
1	C	37	LYS
1	C	64	GLU
1	C	68	LYS
1	C	126	SER
1	C	178	LYS
1	C	184	ILE
1	D	1	MET
1	D	25	GLN
1	D	64	GLU

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Mol	Chain	Res	Type
1	D	126	SER
1	E	64	GLU
1	E	68	LYS
1	E	110	ARG
1	E	126	SER
1	F	64	GLU
1	F	110	ARG
1	F	126	SER
1	G	64	GLU
1	G	67	LYS
1	G	68	LYS
1	G	110	ARG
1	G	126	SER
1	G	183	THR
1	H	64	GLU
1	H	110	ARG
1	H	126	SER
1	I	35	LYS
1	I	37	LYS
1	I	64	GLU
1	I	68	LYS
1	I	110	ARG
1	I	126	SER
1	I	185	LYS
1	I	191	SER
1	I	192	LYS
1	J	64	GLU
1	J	126	SER
1	K	25	GLN
1	K	64	GLU
1	K	110	ARG
1	K	126	SER
1	L	64	GLU
1	L	68	LYS
1	L	110	ARG
1	L	126	SER
1	M	25	GLN
1	M	64	GLU
1	M	68	LYS
1	M	109	LYS
1	M	110	ARG
1	M	126	SER

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Mol	Chain	Res	Type
1	M	168	LYS
1	N	64	GLU
1	N	92	LYS
1	N	110	ARG
1	N	126	SER
1	N	173	SER
1	N	181	SER
1	O	64	GLU
1	O	68	LYS
1	O	126	SER
1	O	184	ILE
1	O	185	LYS
1	O	187	ASP
1	P	64	GLU
1	P	68	LYS
1	P	126	SER
1	P	182	ASP
1	Q	64	GLU
1	Q	68	LYS
1	Q	126	SER
1	Q	136	LYS
1	Q	168	LYS
1	R	64	GLU
1	R	110	ARG
1	R	126	SER
1	R	168	LYS
1	R	184	ILE
1	R	185	LYS
1	S	40	VAL
1	S	64	GLU
1	S	68	LYS
1	S	93	LYS
1	S	110	ARG
1	S	126	SER
1	S	185	LYS
1	T	64	GLU
1	T	126	SER
1	T	181	SER
2	b	58	ASP
2	b	61	LYS
2	b	63	GLN
2	b	68	THR

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Mol	Chain	Res	Type
2	b	76	VAL
2	b	81	VAL
2	b	112	THR
2	c	31	MET
2	c	46	LEU
2	c	55	SER
2	c	58	ASP
2	c	61	LYS
2	c	63	GLN
2	c	68	THR
2	c	81	VAL
2	c	106	GLN
2	c	111	GLU
2	c	112	THR
2	d	37	ARG
2	d	58	ASP
2	d	63	GLN
2	d	68	THR
2	d	76	VAL
2	d	81	VAL
2	d	106	GLN
2	d	112	THR
2	d	126	ARG
2	e	55	SER
2	e	58	ASP
2	e	63	GLN
2	e	68	THR
2	e	81	VAL
2	e	107	GLN
2	e	112	THR
2	f	55	SER
2	f	58	ASP
2	f	63	GLN
2	f	68	THR
2	f	81	VAL
2	f	85	LYS
2	f	106	GLN
2	f	112	THR
2	f	126	ARG
2	g	55	SER
2	g	58	ASP
2	g	63	GLN

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Mol	Chain	Res	Type
2	g	68	THR
2	g	81	VAL
2	g	112	THR
2	g	122	LEU
2	h	55	SER
2	h	56	VAL
2	h	58	ASP
2	h	63	GLN
2	h	65	LEU
2	h	68	THR
2	h	76	VAL
2	h	81	VAL
2	h	106	GLN
2	h	111	GLU
2	h	112	THR
2	i	55	SER
2	i	58	ASP
2	i	63	GLN
2	i	68	THR
2	i	70	ARG
2	i	72	ASP
2	i	81	VAL
2	i	112	THR
2	j	55	SER
2	j	58	ASP
2	j	63	GLN
2	j	65	LEU
2	j	68	THR
2	j	76	VAL
2	j	81	VAL
2	j	85	LYS
2	j	106	GLN
2	j	112	THR
2	j	126	ARG
2	k	55	SER
2	k	58	ASP
2	k	63	GLN
2	k	68	THR
2	k	81	VAL
2	k	110	ARG
2	k	112	THR
2	l	55	SER

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Mol	Chain	Res	Type
2	l	58	ASP
2	l	63	GLN
2	l	68	THR
2	l	81	VAL
2	l	109	GLN
2	l	110	ARG
2	l	112	THR
2	m	58	ASP
2	m	63	GLN
2	m	68	THR
2	m	81	VAL
2	m	106	GLN
2	m	112	THR
2	n	55	SER
2	n	58	ASP
2	n	62	VAL
2	n	63	GLN
2	n	64	SER
2	n	65	LEU
2	n	68	THR
2	n	81	VAL
2	n	101	ARG
2	n	110	ARG
2	n	112	THR
2	o	55	SER
2	o	56	VAL
2	o	58	ASP
2	o	63	GLN
2	o	65	LEU
2	o	68	THR
2	o	81	VAL
2	o	111	GLU
2	o	112	THR
2	p	55	SER
2	p	58	ASP
2	p	63	GLN
2	p	65	LEU
2	p	68	THR
2	p	81	VAL
2	p	110	ARG
2	p	112	THR
2	q	31	MET

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Mol	Chain	Res	Type
2	q	37	ARG
2	q	51	ARG
2	q	55	SER
2	q	56	VAL
2	q	58	ASP
2	q	63	GLN
2	q	68	THR
2	q	81	VAL
2	q	112	THR
2	r	55	SER
2	r	61	LYS
2	r	63	GLN
2	r	68	THR
2	r	76	VAL
2	r	81	VAL
2	r	106	GLN
2	r	107	GLN
2	r	112	THR
2	s	55	SER
2	s	58	ASP
2	s	68	THR
2	s	81	VAL
2	s	112	THR
2	s	126	ARG
2	t	58	ASP
2	t	63	GLN
2	t	68	THR
2	t	81	VAL
2	t	85	LYS
2	t	112	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
2	a	119	GLN
1	B	94	GLN
1	C	25	GLN
1	E	25	GLN
1	G	25	GLN
1	G	94	GLN
1	G	114	GLN

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Mol	Chain	Res	Type
1	H	25	GLN
1	H	94	GLN
1	J	25	GLN
1	J	94	GLN
1	K	94	GLN
1	L	94	GLN
1	M	94	GLN
1	N	25	GLN
1	P	94	GLN
1	Q	25	GLN
1	Q	94	GLN
1	R	94	GLN
1	T	94	GLN
2	c	34	HIS
2	e	63	GLN
2	i	63	GLN
2	l	63	GLN
2	m	34	HIS
2	n	42	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
7	ATP	g	201	-	13,14,33	1.49	3 (23%)	18,22,52	0.77	0
4	PO4	r	201	-	4,4,4	0.95	0	6,6,6	0.67	0
4	PO4	p	201	-	4,4,4	0.66	0	6,6,6	0.80	0
6	GOL	H	201	-	5,5,5	0.21	0	5,5,5	0.43	0
4	PO4	b	201	-	4,4,4	1.15	1 (25%)	6,6,6	0.41	0
3	EDO	R	201	-	3,3,3	0.17	0	2,2,2	0.04	0
4	PO4	n	201	-	4,4,4	0.95	0	6,6,6	0.47	0
5	PEG	P	202	-	6,6,6	0.18	0	5,5,5	0.11	0
3	EDO	Q	201	-	3,3,3	0.27	0	2,2,2	0.28	0
3	EDO	C	201	-	3,3,3	0.13	0	2,2,2	0.26	0
4	PO4	a	201	-	4,4,4	0.63	0	6,6,6	0.57	0
4	PO4	l	201	-	4,4,4	1.28	1 (25%)	6,6,6	0.31	0
4	PO4	d	201	-	4,4,4	1.22	1 (25%)	6,6,6	0.65	0
3	EDO	J	201	-	3,3,3	0.31	0	2,2,2	0.37	0
4	PO4	f	201	-	4,4,4	0.61	0	6,6,6	0.66	0
4	PO4	q	201	-	4,4,4	0.67	0	6,6,6	0.74	0
3	EDO	S	202	-	3,3,3	0.32	0	2,2,2	0.44	0
6	GOL	O	203	-	5,5,5	0.09	0	5,5,5	0.27	0
4	PO4	s	201	-	4,4,4	1.40	1 (25%)	6,6,6	0.29	0
3	EDO	P	201	-	3,3,3	0.27	0	2,2,2	0.22	0
3	EDO	G	202	-	3,3,3	0.46	0	2,2,2	0.52	0
4	PO4	e	201	-	4,4,4	0.47	0	6,6,6	0.76	0
5	PEG	G	203	-	6,6,6	0.26	0	5,5,5	0.15	0
4	PO4	E	201	-	4,4,4	0.85	0	6,6,6	0.42	0
3	EDO	S	201	-	3,3,3	0.33	0	2,2,2	0.43	0
5	PEG	D	201	-	6,6,6	0.34	0	5,5,5	0.19	0
4	PO4	i	201	-	4,4,4	1.39	1 (25%)	6,6,6	0.39	0
5	PEG	K	201	-	6,6,6	0.26	0	5,5,5	0.23	0
4	PO4	o	201	-	4,4,4	0.46	0	6,6,6	0.66	0
5	PEG	R	203	-	6,6,6	0.24	0	5,5,5	0.15	0
3	EDO	R	202	-	3,3,3	0.36	0	2,2,2	0.34	0
5	PEG	O	201	-	6,6,6	0.32	0	5,5,5	0.16	0
4	PO4	h	201	-	4,4,4	0.78	0	6,6,6	0.61	0
3	EDO	H	202	-	3,3,3	0.20	0	2,2,2	0.20	0
3	EDO	O	202	-	3,3,3	0.22	0	2,2,2	0.29	0
3	EDO	G	201	-	3,3,3	0.30	0	2,2,2	0.33	0
4	PO4	k	201	-	4,4,4	0.70	0	6,6,6	0.68	0
3	EDO	H	203	-	3,3,3	0.30	0	2,2,2	0.44	0
3	EDO	A	201	-	3,3,3	0.07	0	2,2,2	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	H	204	-	3,3,3	0.18	0	2,2,2	0.21	0
3	EDO	C	202	-	3,3,3	0.40	0	2,2,2	0.56	0
4	PO4	j	201	-	4,4,4	0.82	0	6,6,6	0.62	0
4	PO4	m	201	-	4,4,4	1.15	1 (25%)	6,6,6	0.57	0
5	PEG	N	201	-	6,6,6	0.43	0	5,5,5	0.29	0
4	PO4	t	201	-	4,4,4	0.59	0	6,6,6	0.67	0
7	ATP	c	201	-	10,12,33	1.11	0	17,20,52	1.04	0
5	PEG	Q	202	-	6,6,6	0.27	0	5,5,5	0.11	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
7	ATP	g	201	-	-	0/16/16/38	-
6	GOL	H	201	-	-	4/4/4/4	-
3	EDO	R	201	-	-	1/1/1/1	-
5	PEG	P	202	-	-	3/4/4/4	-
3	EDO	Q	201	-	-	1/1/1/1	-
3	EDO	C	201	-	-	1/1/1/1	-
3	EDO	J	201	-	-	1/1/1/1	-
3	EDO	S	202	-	-	1/1/1/1	-
6	GOL	O	203	-	-	2/4/4/4	-
3	EDO	P	201	-	-	0/1/1/1	-
3	EDO	G	202	-	-	1/1/1/1	-
5	PEG	G	203	-	-	2/4/4/4	-
3	EDO	S	201	-	-	0/1/1/1	-
5	PEG	K	201	-	-	3/4/4/4	-
5	PEG	R	203	-	-	2/4/4/4	-
3	EDO	R	202	-	-	1/1/1/1	-
5	PEG	O	201	-	-	0/4/4/4	-
3	EDO	H	202	-	-	1/1/1/1	-
3	EDO	O	202	-	-	1/1/1/1	-
3	EDO	G	201	-	-	1/1/1/1	-
3	EDO	H	203	-	-	0/1/1/1	-
3	EDO	A	201	-	-	1/1/1/1	-
3	EDO	H	204	-	-	1/1/1/1	-
3	EDO	C	202	-	-	1/1/1/1	-
7	ATP	c	201	-	-	3/12/12/38	-
5	PEG	N	201	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	D	201	-	-	2/4/4/4	-
5	PEG	Q	202	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	201	ATP	PB-O3B	2.97	1.62	1.59
7	g	201	ATP	PA-O3A	2.91	1.62	1.59
4	s	201	PO4	P-O1	2.72	1.56	1.50
4	i	201	PO4	P-O1	2.51	1.56	1.50
4	l	201	PO4	P-O1	2.38	1.56	1.50
4	d	201	PO4	P-O1	2.34	1.56	1.50
7	g	201	ATP	PB-O3A	2.16	1.61	1.59
4	b	201	PO4	P-O1	2.15	1.55	1.50
4	m	201	PO4	P-O1	2.12	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (39) 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'
5	Q	202	PEG	O1-C1-C2-O2
5	K	201	PEG	O2-C3-C4-O4
5	P	202	PEG	O2-C3-C4-O4
5	D	201	PEG	O1-C1-C2-O2
5	R	203	PEG	O1-C1-C2-O2
6	H	201	GOL	O1-C1-C2-O2
6	H	201	GOL	O2-C2-C3-O3
5	K	201	PEG	O1-C1-C2-O2
5	P	202	PEG	O1-C1-C2-O2
3	C	202	EDO	O1-C1-C2-O2
5	D	201	PEG	O2-C3-C4-O4
5	Q	202	PEG	O2-C3-C4-O4
6	O	203	GOL	O2-C2-C3-O3
5	N	201	PEG	O2-C3-C4-O4
3	A	201	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	G	202	EDO	O1-C1-C2-O2
3	H	202	EDO	O1-C1-C2-O2
3	Q	201	EDO	O1-C1-C2-O2
3	R	202	EDO	O1-C1-C2-O2
3	S	202	EDO	O1-C1-C2-O2
5	G	203	PEG	O2-C3-C4-O4
3	J	201	EDO	O1-C1-C2-O2
3	R	201	EDO	O1-C1-C2-O2
5	N	201	PEG	C1-C2-O2-C3
5	G	203	PEG	O1-C1-C2-O2
3	C	201	EDO	O1-C1-C2-O2
5	K	201	PEG	C4-C3-O2-C2
5	P	202	PEG	C1-C2-O2-C3
3	O	202	EDO	O1-C1-C2-O2
5	N	201	PEG	C4-C3-O2-C2
3	G	201	EDO	O1-C1-C2-O2
3	H	204	EDO	O1-C1-C2-O2
5	R	203	PEG	C1-C2-O2-C3
7	c	201	ATP	PG-O3B-PB-O2B

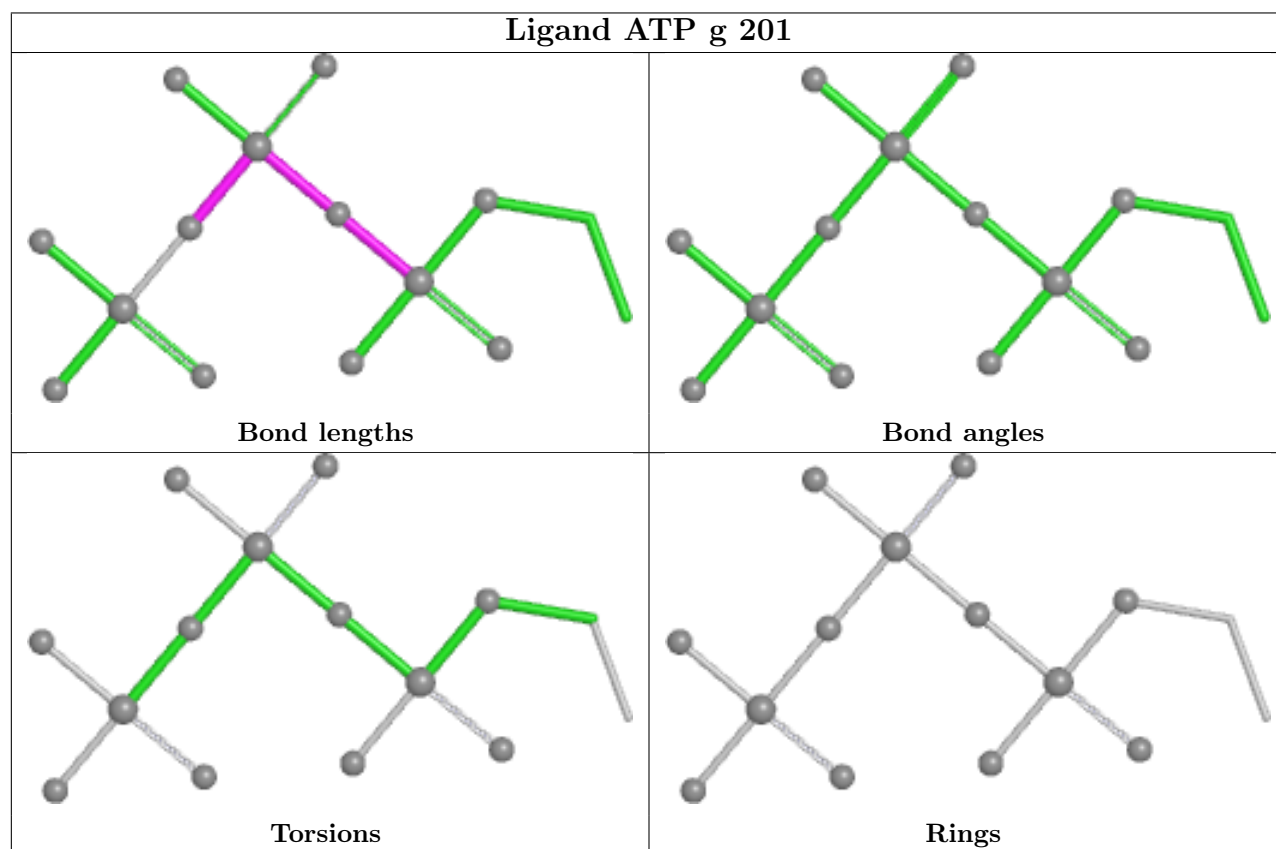
There are no ring outliers.

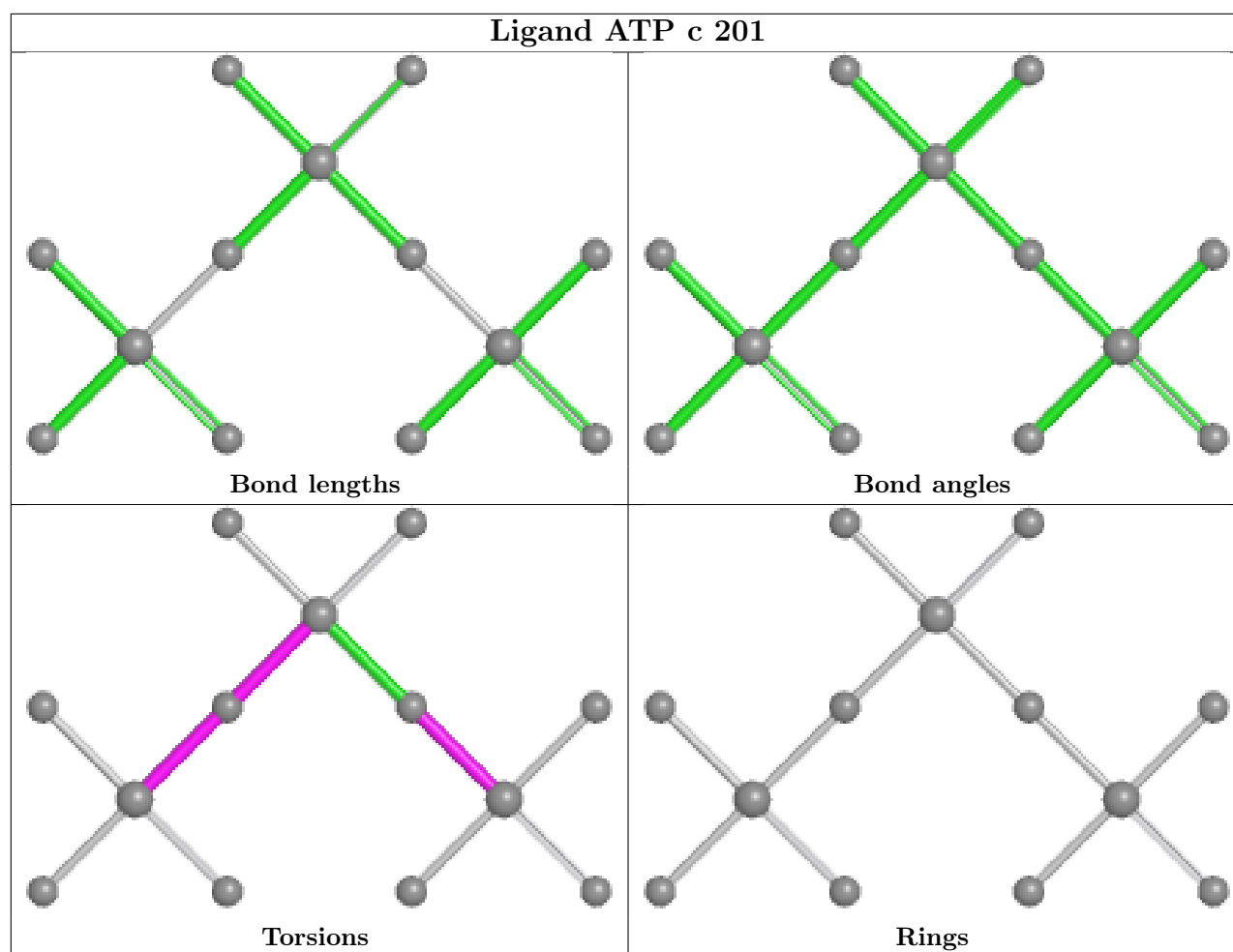
11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	g	201	ATP	1	0
4	r	201	PO4	1	0
4	p	201	PO4	1	0
4	a	201	PO4	1	0
4	f	201	PO4	1	0
5	D	201	PEG	2	0
4	i	201	PO4	1	0
4	o	201	PO4	1	0
5	O	201	PEG	1	0
5	N	201	PEG	3	0
7	c	201	ATP	1	0

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

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	185/199 (92%)	-0.12	1 (0%) 87 75	47, 65, 92, 111	0
1	B	185/199 (92%)	-0.15	1 (0%) 87 75	47, 63, 98, 123	0
1	C	187/199 (93%)	-0.29	0 100 100	33, 49, 85, 123	0
1	D	181/199 (90%)	-0.20	3 (1%) 69 50	33, 54, 89, 123	0
1	E	185/199 (92%)	-0.21	1 (0%) 87 75	41, 57, 94, 128	0
1	F	185/199 (92%)	-0.13	2 (1%) 78 61	39, 55, 87, 111	0
1	G	182/199 (91%)	-0.29	4 (2%) 62 43	29, 47, 83, 144	0
1	H	183/199 (91%)	-0.33	1 (0%) 87 75	27, 45, 90, 144	0
1	I	191/199 (95%)	-0.21	2 (1%) 79 63	36, 55, 86, 116	0
1	J	184/199 (92%)	-0.16	1 (0%) 87 75	34, 52, 101, 156	0
1	K	183/199 (91%)	0.04	1 (0%) 87 75	47, 69, 102, 145	0
1	L	181/199 (90%)	0.07	4 (2%) 62 43	45, 64, 100, 158	0
1	M	178/199 (89%)	-0.24	1 (0%) 85 72	36, 56, 102, 127	0
1	N	185/199 (92%)	-0.06	4 (2%) 62 43	38, 61, 95, 113	0
1	O	187/199 (93%)	-0.25	2 (1%) 78 61	36, 56, 83, 120	0
1	P	183/199 (91%)	-0.27	1 (0%) 87 75	36, 51, 92, 132	0
1	Q	184/199 (92%)	-0.30	1 (0%) 87 75	30, 51, 88, 138	0
1	R	186/199 (93%)	-0.32	3 (1%) 70 51	31, 47, 82, 110	0
1	S	185/199 (92%)	-0.17	2 (1%) 78 61	43, 61, 98, 115	0
1	T	185/199 (92%)	-0.16	2 (1%) 78 61	38, 59, 98, 128	0
2	a	106/109 (97%)	0.47	5 (4%) 36 22	45, 86, 138, 152	0
2	b	107/109 (98%)	0.27	4 (3%) 45 28	52, 81, 119, 162	0
2	c	107/109 (98%)	0.32	2 (1%) 66 47	38, 67, 104, 118	0
2	d	108/109 (99%)	0.14	2 (1%) 66 47	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%)	0.39	3 (2%) 55 36	45, 79, 119, 131	0
2	f	106/109 (97%)	0.31	3 (2%) 55 36	47, 78, 133, 156	0
2	g	102/109 (93%)	0.23	4 (3%) 43 27	44, 74, 115, 140	0
2	h	108/109 (99%)	-0.11	2 (1%) 66 47	35, 58, 92, 142	0
2	i	103/109 (94%)	0.33	5 (4%) 35 21	52, 90, 141, 165	0
2	j	107/109 (98%)	0.02	1 (0%) 81 65	37, 63, 101, 118	0
2	k	97/109 (88%)	0.30	2 (2%) 63 44	59, 91, 137, 145	0
2	l	103/109 (94%)	0.61	8 (7%) 19 12	45, 95, 141, 154	0
2	m	107/109 (98%)	-0.03	3 (2%) 55 36	32, 59, 102, 150	0
2	n	94/109 (86%)	0.61	6 (6%) 25 15	67, 105, 143, 174	0
2	o	107/109 (98%)	0.44	5 (4%) 36 22	45, 83, 133, 152	0
2	p	108/109 (99%)	0.19	5 (4%) 37 23	46, 74, 120, 155	0
2	q	107/109 (98%)	0.06	2 (1%) 66 47	47, 76, 109, 157	0
2	r	99/109 (90%)	0.12	1 (1%) 79 63	42, 68, 102, 119	0
2	s	107/109 (98%)	0.30	3 (2%) 55 36	49, 84, 131, 144	0
2	t	107/109 (98%)	0.39	7 (6%) 25 15	49, 84, 127, 154	0
All	All	5782/6160 (93%)	-0.02	110 (1%) 66 47	27, 62, 116, 174	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	188	VAL	4.6
2	f	37	ARG	4.1
2	b	38	ILE	4.0
2	p	30	PRO	3.8
2	g	34	HIS	3.6
2	p	40	ALA	3.5
2	a	30	PRO	3.5
1	F	175	ALA	3.4
2	t	38	ILE	3.4
2	p	37	ARG	3.4
1	B	2	SER	3.3
2	f	38	ILE	3.2
2	b	37	ARG	3.1
2	l	34	HIS	3.0
2	d	37	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	q	37	ARG	2.9
2	p	38	ILE	2.9
2	a	31	MET	2.9
2	i	34	HIS	2.9
2	a	39	ALA	2.8
1	T	2	SER	2.8
2	s	31	MET	2.8
1	D	181	SER	2.8
1	H	184	ILE	2.8
2	r	40	ALA	2.8
1	A	2	SER	2.7
2	e	37	ARG	2.7
2	m	37	ARG	2.7
2	t	31	MET	2.7
2	n	73	PRO	2.7
1	D	52	CYS	2.7
2	g	38	ILE	2.6
2	q	75	SER	2.6
2	t	40	ALA	2.6
1	R	176	GLY	2.6
2	c	37	ARG	2.6
1	E	2	SER	2.5
1	J	2	SER	2.5
2	b	55	SER	2.5
1	L	4	GLY	2.5
2	h	30	PRO	2.5
2	i	33	ILE	2.5
1	L	184	ILE	2.5
2	t	37	ARG	2.5
2	o	65	LEU	2.5
2	l	40	ALA	2.5
2	t	34	HIS	2.5
2	l	35	SER	2.4
2	o	40	ALA	2.4
2	o	34	HIS	2.4
2	d	30	PRO	2.4
2	c	56	VAL	2.4
2	m	31	MET	2.4
2	l	77	PRO	2.4
2	a	67	ASP	2.4
2	n	124	ASP	2.4
2	m	38	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	S	186	PRO	2.4
2	s	37	ARG	2.4
2	k	122	LEU	2.4
2	a	33	ILE	2.4
2	l	71	GLU	2.3
2	g	124	ASP	2.3
2	t	39	ALA	2.3
1	G	52	CYS	2.3
1	T	52	CYS	2.3
1	P	2	SER	2.3
1	L	175	ALA	2.3
2	g	40	ALA	2.3
2	o	31	MET	2.3
2	o	33	ILE	2.3
2	l	108	LEU	2.2
2	t	65	LEU	2.2
2	p	33	ILE	2.2
1	G	183	THR	2.2
1	D	2	SER	2.2
1	S	2	SER	2.2
2	i	32	SER	2.2
2	n	41	VAL	2.2
1	F	24	GLY	2.2
2	j	31	MET	2.2
2	s	38	ILE	2.2
1	N	186	PRO	2.2
2	n	56	VAL	2.2
1	I	2	SER	2.2
2	f	35	SER	2.2
2	l	65	LEU	2.2
2	e	56	VAL	2.2
2	i	66	VAL	2.2
1	G	93	LYS	2.2
1	L	2	SER	2.2
1	N	2	SER	2.2
1	K	2	SER	2.1
1	O	2	SER	2.1
1	R	52	CYS	2.1
2	l	39	ALA	2.1
1	I	93	LYS	2.1
2	k	71	GLU	2.1
2	b	31	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	R	95	GLY	2.1
2	i	69	ILE	2.1
1	G	2	SER	2.1
1	M	2	SER	2.1
1	N	3	SER	2.0
1	Q	2	SER	2.0
2	h	65	LEU	2.0
1	N	170	GLY	2.0
2	n	65	LEU	2.0
2	e	31	MET	2.0
2	n	83	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
4	PO4	d	201	5/5	0.63	0.15	84,90,115,120	0
4	PO4	l	201	5/5	0.64	0.12	96,126,129,132	0
4	PO4	s	201	5/5	0.71	0.10	82,96,118,121	0
4	PO4	t	201	5/5	0.71	0.11	90,111,122,134	0
4	PO4	e	201	5/5	0.72	0.10	90,94,122,125	0
4	PO4	p	201	5/5	0.72	0.14	90,90,112,117	0
4	PO4	b	201	5/5	0.73	0.11	94,97,118,127	0
4	PO4	i	201	5/5	0.73	0.11	81,88,111,116	0
6	GOL	H	201	6/6	0.73	0.24	86,95,107,113	0
4	PO4	n	201	5/5	0.74	0.11	97,124,136,137	0
7	ATP	c	201	13/31	0.75	0.10	112,145,174,185	0
4	PO4	a	201	5/5	0.76	0.10	87,94,113,116	0

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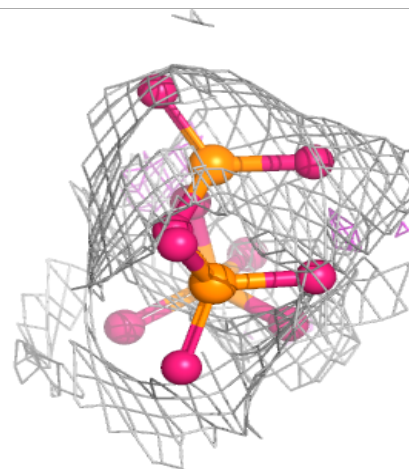
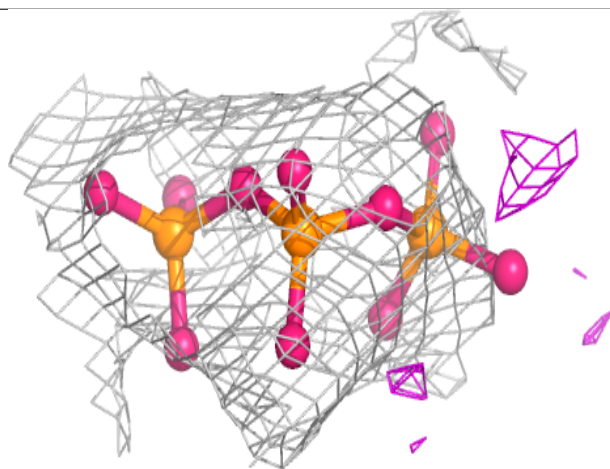
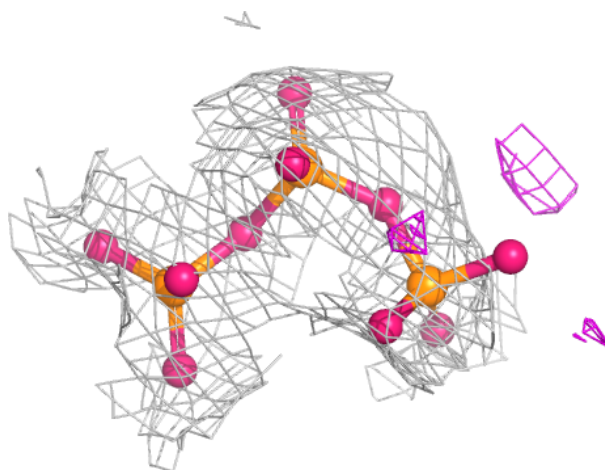
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	o	201	5/5	0.77	0.10	103,104,127,135	0
4	PO4	k	201	5/5	0.78	0.10	95,100,124,130	0
3	EDO	O	202	4/4	0.79	0.23	70,75,78,79	0
5	PEG	P	202	7/7	0.79	0.17	77,81,98,102	0
4	PO4	q	201	5/5	0.80	0.11	82,96,107,112	0
7	ATP	g	201	15/31	0.80	0.14	94,115,155,157	0
4	PO4	m	201	5/5	0.81	0.10	69,88,98,107	0
4	PO4	r	201	5/5	0.81	0.12	73,81,100,102	0
3	EDO	R	202	4/4	0.82	0.16	68,72,74,79	0
4	PO4	j	201	5/5	0.82	0.12	80,109,124,125	0
3	EDO	S	201	4/4	0.82	0.14	74,83,83,86	0
3	EDO	J	201	4/4	0.82	0.18	65,73,75,79	0
5	PEG	R	203	7/7	0.83	0.17	67,72,83,89	0
5	PEG	O	201	7/7	0.84	0.19	78,92,106,115	0
4	PO4	h	201	5/5	0.85	0.11	85,102,110,113	0
6	GOL	O	203	6/6	0.86	0.19	92,97,105,111	0
5	PEG	D	201	7/7	0.86	0.17	69,82,95,98	0
5	PEG	G	203	7/7	0.86	0.20	72,83,91,93	0
3	EDO	A	201	4/4	0.87	0.10	72,73,82,83	0
4	PO4	f	201	5/5	0.87	0.09	75,96,107,109	0
3	EDO	C	201	4/4	0.87	0.09	63,64,65,66	0
4	PO4	E	201	5/5	0.87	0.10	112,118,126,133	0
3	EDO	Q	201	4/4	0.87	0.17	67,68,69,72	0
3	EDO	H	204	4/4	0.87	0.19	66,81,83,83	0
3	EDO	H	202	4/4	0.88	0.14	72,74,79,80	0
5	PEG	N	201	7/7	0.88	0.17	74,81,90,96	0
3	EDO	H	203	4/4	0.88	0.17	65,77,79,81	0
5	PEG	Q	202	7/7	0.89	0.19	63,78,94,101	0
3	EDO	P	201	4/4	0.89	0.12	62,63,69,70	0
3	EDO	S	202	4/4	0.89	0.12	68,71,76,77	0
5	PEG	K	201	7/7	0.91	0.13	73,85,98,100	0
3	EDO	G	201	4/4	0.93	0.08	58,64,67,67	0
3	EDO	C	202	4/4	0.94	0.10	52,60,64,64	0
3	EDO	G	202	4/4	0.95	0.09	53,65,65,68	0
3	EDO	R	201	4/4	0.95	0.08	52,52,53,55	0

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

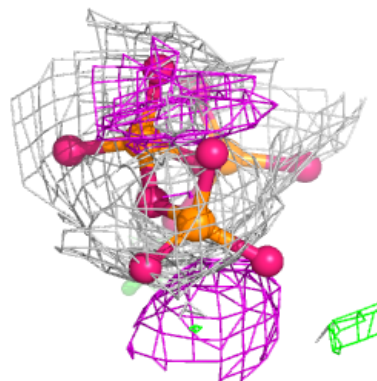
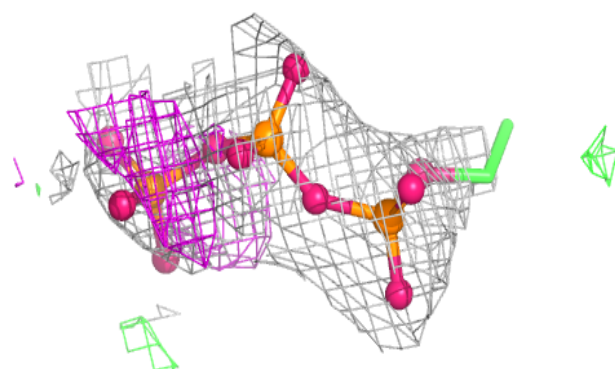
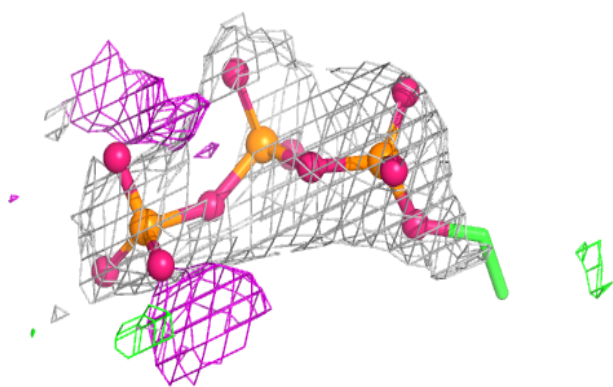
Electron density around ATP c 201:

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



Electron density around ATP g 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.