



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:09 am GMT

PDB ID : 5CB5  
Title : Structural Insights into the Mechanism of Escherichia coli Ymdb  
Authors : Zhang, W.; Wang, C.; Song, Y.; Shao, C.; Zhang, X.; Zang, J.  
Deposited on : 2015-06-30  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

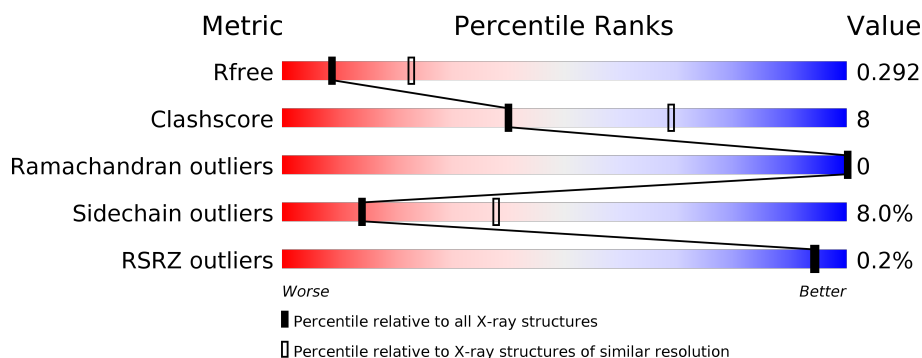
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.



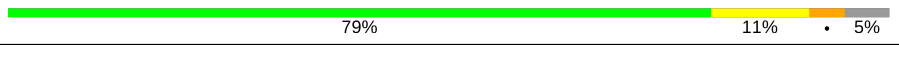
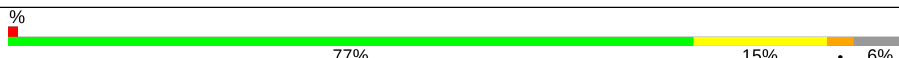
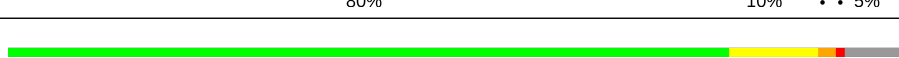

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	183	
1	B	183	
1	C	183	
1	D	183	
1	E	183	
1	F	183	

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Mol	Chain	Length	Quality of chain
1	G	183	
1	H	183	
1	I	183	
1	J	183	
1	K	183	
1	L	183	
1	M	183	
1	N	183	
1	O	183	
1	P	183	
1	Q	183	
1	R	183	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	C	202	-	-	X	-
3	SO4	D	202	-	-	X	-
3	SO4	J	202	-	-	X	-
3	SO4	K	202	-	-	X	-
3	SO4	M	202	-	-	X	-
3	SO4	O	202	-	-	X	-
3	SO4	Q	403	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23896 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 O-acetyl-ADP-ribose deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	173	Total	C	N	O	S	0	0	0
			1281	810	229	238	4			
1	A	173	Total	C	N	O	S	0	0	0
			1259	798	222	235	4			
1	B	172	Total	C	N	O	S	0	0	0
			1280	809	228	239	4			
1	C	173	Total	C	N	O	S	0	0	0
			1283	811	226	242	4			
1	D	170	Total	C	N	O	S	0	0	0
			1236	781	220	231	4			
1	E	173	Total	C	N	O	S	0	0	0
			1293	816	230	243	4			
1	F	173	Total	C	N	O	S	0	0	0
			1283	810	226	243	4			
1	G	173	Total	C	N	O	S	0	0	0
			1280	810	226	240	4			
1	H	173	Total	C	N	O	S	0	0	0
			1293	816	230	243	4			
1	I	173	Total	C	N	O	S	0	0	0
			1272	805	226	237	4			
1	J	172	Total	C	N	O	S	0	0	0
			1280	808	228	240	4			
1	K	172	Total	C	N	O	S	0	0	0
			1256	796	219	237	4			
1	L	172	Total	C	N	O	S	0	0	0
			1259	797	222	236	4			
1	M	173	Total	C	N	O	S	0	0	0
			1279	809	226	240	4			
1	N	173	Total	C	N	O	S	0	0	0
			1255	794	221	236	4			
1	O	171	Total	C	N	O	S	0	0	0
			1271	803	226	238	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	173	Total	C	N	O	S	0	0	0
			1277	807	227	239	4			
1	Q	173	Total	C	N	O	S	0	0	0
			1289	814	229	242	4			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-5	HIS	-	expression tag	UNP P0A8D6
R	-4	HIS	-	expression tag	UNP P0A8D6
R	-3	HIS	-	expression tag	UNP P0A8D6
R	-2	HIS	-	expression tag	UNP P0A8D6
R	-1	HIS	-	expression tag	UNP P0A8D6
R	0	HIS	-	expression tag	UNP P0A8D6
R	25	ALA	ASN	engineered mutation	UNP P0A8D6
R	35	ALA	ASP	engineered mutation	UNP P0A8D6
A	-5	HIS	-	expression tag	UNP P0A8D6
A	-4	HIS	-	expression tag	UNP P0A8D6
A	-3	HIS	-	expression tag	UNP P0A8D6
A	-2	HIS	-	expression tag	UNP P0A8D6
A	-1	HIS	-	expression tag	UNP P0A8D6
A	0	HIS	-	expression tag	UNP P0A8D6
A	25	ALA	ASN	engineered mutation	UNP P0A8D6
A	35	ALA	ASP	engineered mutation	UNP P0A8D6
B	-5	HIS	-	expression tag	UNP P0A8D6
B	-4	HIS	-	expression tag	UNP P0A8D6
B	-3	HIS	-	expression tag	UNP P0A8D6
B	-2	HIS	-	expression tag	UNP P0A8D6
B	-1	HIS	-	expression tag	UNP P0A8D6
B	0	HIS	-	expression tag	UNP P0A8D6
B	25	ALA	ASN	engineered mutation	UNP P0A8D6
B	35	ALA	ASP	engineered mutation	UNP P0A8D6
C	-5	HIS	-	expression tag	UNP P0A8D6
C	-4	HIS	-	expression tag	UNP P0A8D6
C	-3	HIS	-	expression tag	UNP P0A8D6
C	-2	HIS	-	expression tag	UNP P0A8D6
C	-1	HIS	-	expression tag	UNP P0A8D6
C	0	HIS	-	expression tag	UNP P0A8D6
C	25	ALA	ASN	engineered mutation	UNP P0A8D6
C	35	ALA	ASP	engineered mutation	UNP P0A8D6
D	-5	HIS	-	expression tag	UNP P0A8D6
D	-4	HIS	-	expression tag	UNP P0A8D6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	HIS	-	expression tag	UNP P0A8D6
D	-2	HIS	-	expression tag	UNP P0A8D6
D	-1	HIS	-	expression tag	UNP P0A8D6
D	0	HIS	-	expression tag	UNP P0A8D6
D	25	ALA	ASN	engineered mutation	UNP P0A8D6
D	35	ALA	ASP	engineered mutation	UNP P0A8D6
E	-5	HIS	-	expression tag	UNP P0A8D6
E	-4	HIS	-	expression tag	UNP P0A8D6
E	-3	HIS	-	expression tag	UNP P0A8D6
E	-2	HIS	-	expression tag	UNP P0A8D6
E	-1	HIS	-	expression tag	UNP P0A8D6
E	0	HIS	-	expression tag	UNP P0A8D6
E	25	ALA	ASN	engineered mutation	UNP P0A8D6
E	35	ALA	ASP	engineered mutation	UNP P0A8D6
F	-5	HIS	-	expression tag	UNP P0A8D6
F	-4	HIS	-	expression tag	UNP P0A8D6
F	-3	HIS	-	expression tag	UNP P0A8D6
F	-2	HIS	-	expression tag	UNP P0A8D6
F	-1	HIS	-	expression tag	UNP P0A8D6
F	0	HIS	-	expression tag	UNP P0A8D6
F	25	ALA	ASN	engineered mutation	UNP P0A8D6
F	35	ALA	ASP	engineered mutation	UNP P0A8D6
G	-5	HIS	-	expression tag	UNP P0A8D6
G	-4	HIS	-	expression tag	UNP P0A8D6
G	-3	HIS	-	expression tag	UNP P0A8D6
G	-2	HIS	-	expression tag	UNP P0A8D6
G	-1	HIS	-	expression tag	UNP P0A8D6
G	0	HIS	-	expression tag	UNP P0A8D6
G	25	ALA	ASN	engineered mutation	UNP P0A8D6
G	35	ALA	ASP	engineered mutation	UNP P0A8D6
H	-5	HIS	-	expression tag	UNP P0A8D6
H	-4	HIS	-	expression tag	UNP P0A8D6
H	-3	HIS	-	expression tag	UNP P0A8D6
H	-2	HIS	-	expression tag	UNP P0A8D6
H	-1	HIS	-	expression tag	UNP P0A8D6
H	0	HIS	-	expression tag	UNP P0A8D6
H	25	ALA	ASN	engineered mutation	UNP P0A8D6
H	35	ALA	ASP	engineered mutation	UNP P0A8D6
I	-5	HIS	-	expression tag	UNP P0A8D6
I	-4	HIS	-	expression tag	UNP P0A8D6
I	-3	HIS	-	expression tag	UNP P0A8D6
I	-2	HIS	-	expression tag	UNP P0A8D6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	HIS	-	expression tag	UNP P0A8D6
I	0	HIS	-	expression tag	UNP P0A8D6
I	25	ALA	ASN	engineered mutation	UNP P0A8D6
I	35	ALA	ASP	engineered mutation	UNP P0A8D6
J	-5	HIS	-	expression tag	UNP P0A8D6
J	-4	HIS	-	expression tag	UNP P0A8D6
J	-3	HIS	-	expression tag	UNP P0A8D6
J	-2	HIS	-	expression tag	UNP P0A8D6
J	-1	HIS	-	expression tag	UNP P0A8D6
J	0	HIS	-	expression tag	UNP P0A8D6
J	25	ALA	ASN	engineered mutation	UNP P0A8D6
J	35	ALA	ASP	engineered mutation	UNP P0A8D6
K	-5	HIS	-	expression tag	UNP P0A8D6
K	-4	HIS	-	expression tag	UNP P0A8D6
K	-3	HIS	-	expression tag	UNP P0A8D6
K	-2	HIS	-	expression tag	UNP P0A8D6
K	-1	HIS	-	expression tag	UNP P0A8D6
K	0	HIS	-	expression tag	UNP P0A8D6
K	25	ALA	ASN	engineered mutation	UNP P0A8D6
K	35	ALA	ASP	engineered mutation	UNP P0A8D6
L	-5	HIS	-	expression tag	UNP P0A8D6
L	-4	HIS	-	expression tag	UNP P0A8D6
L	-3	HIS	-	expression tag	UNP P0A8D6
L	-2	HIS	-	expression tag	UNP P0A8D6
L	-1	HIS	-	expression tag	UNP P0A8D6
L	0	HIS	-	expression tag	UNP P0A8D6
L	25	ALA	ASN	engineered mutation	UNP P0A8D6
L	35	ALA	ASP	engineered mutation	UNP P0A8D6
M	-5	HIS	-	expression tag	UNP P0A8D6
M	-4	HIS	-	expression tag	UNP P0A8D6
M	-3	HIS	-	expression tag	UNP P0A8D6
M	-2	HIS	-	expression tag	UNP P0A8D6
M	-1	HIS	-	expression tag	UNP P0A8D6
M	0	HIS	-	expression tag	UNP P0A8D6
M	25	ALA	ASN	engineered mutation	UNP P0A8D6
M	35	ALA	ASP	engineered mutation	UNP P0A8D6
N	-5	HIS	-	expression tag	UNP P0A8D6
N	-4	HIS	-	expression tag	UNP P0A8D6
N	-3	HIS	-	expression tag	UNP P0A8D6
N	-2	HIS	-	expression tag	UNP P0A8D6
N	-1	HIS	-	expression tag	UNP P0A8D6
N	0	HIS	-	expression tag	UNP P0A8D6

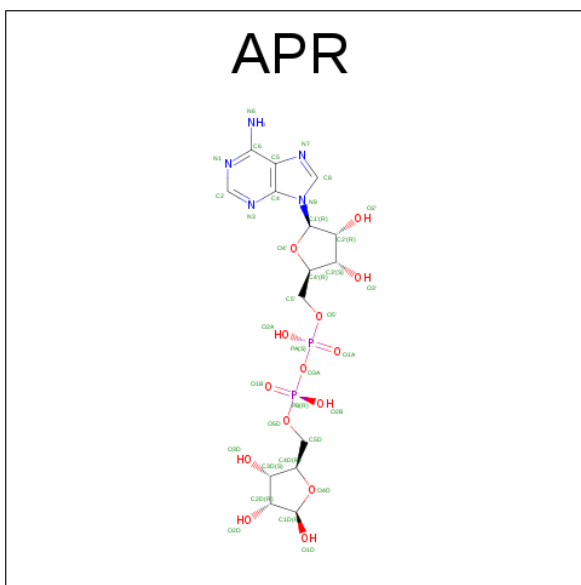
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Chain	Residue	Modelled	Actual	Comment	Reference
N	25	ALA	ASN	engineered mutation	UNP P0A8D6
N	35	ALA	ASP	engineered mutation	UNP P0A8D6
O	-5	HIS	-	expression tag	UNP P0A8D6
O	-4	HIS	-	expression tag	UNP P0A8D6
O	-3	HIS	-	expression tag	UNP P0A8D6
O	-2	HIS	-	expression tag	UNP P0A8D6
O	-1	HIS	-	expression tag	UNP P0A8D6
O	0	HIS	-	expression tag	UNP P0A8D6
O	25	ALA	ASN	engineered mutation	UNP P0A8D6
O	35	ALA	ASP	engineered mutation	UNP P0A8D6
P	-5	HIS	-	expression tag	UNP P0A8D6
P	-4	HIS	-	expression tag	UNP P0A8D6
P	-3	HIS	-	expression tag	UNP P0A8D6
P	-2	HIS	-	expression tag	UNP P0A8D6
P	-1	HIS	-	expression tag	UNP P0A8D6
P	0	HIS	-	expression tag	UNP P0A8D6
P	25	ALA	ASN	engineered mutation	UNP P0A8D6
P	35	ALA	ASP	engineered mutation	UNP P0A8D6
Q	-5	HIS	-	expression tag	UNP P0A8D6
Q	-4	HIS	-	expression tag	UNP P0A8D6
Q	-3	HIS	-	expression tag	UNP P0A8D6
Q	-2	HIS	-	expression tag	UNP P0A8D6
Q	-1	HIS	-	expression tag	UNP P0A8D6
Q	0	HIS	-	expression tag	UNP P0A8D6
Q	25	ALA	ASN	engineered mutation	UNP P0A8D6
Q	35	ALA	ASP	engineered mutation	UNP P0A8D6

- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula:  $C_{15}H_{23}N_5O_{14}P_2$ ).





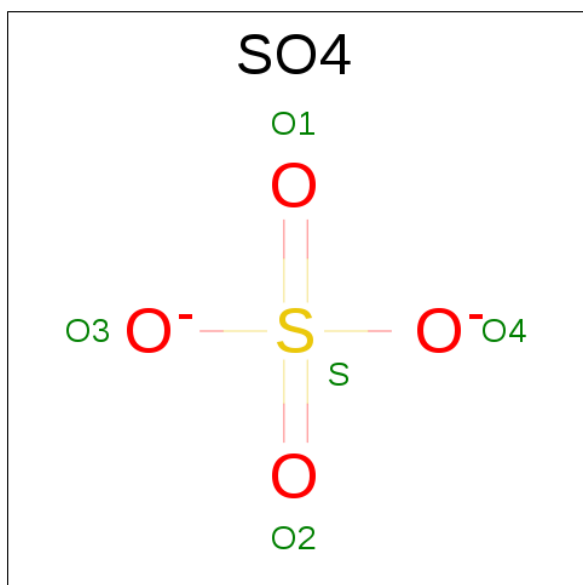
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	R	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	A	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	B	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	C	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	D	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	E	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	G	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	H	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	I	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	J	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	K	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	L	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	N	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	O	1	Total 36	C 15	N 5	O 14	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	P	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	Q	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



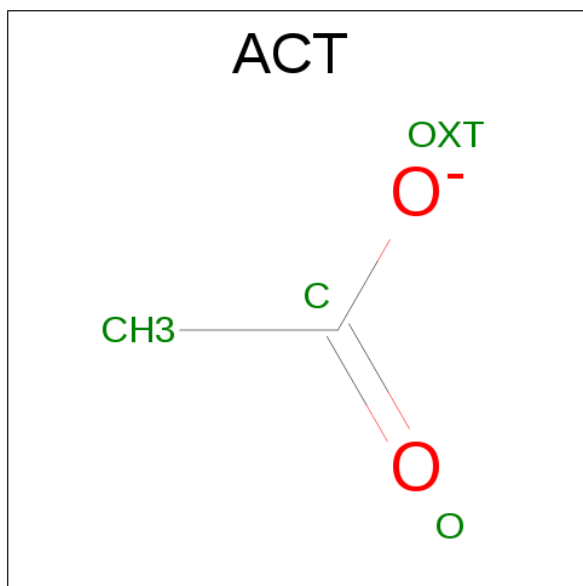
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	R	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total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

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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



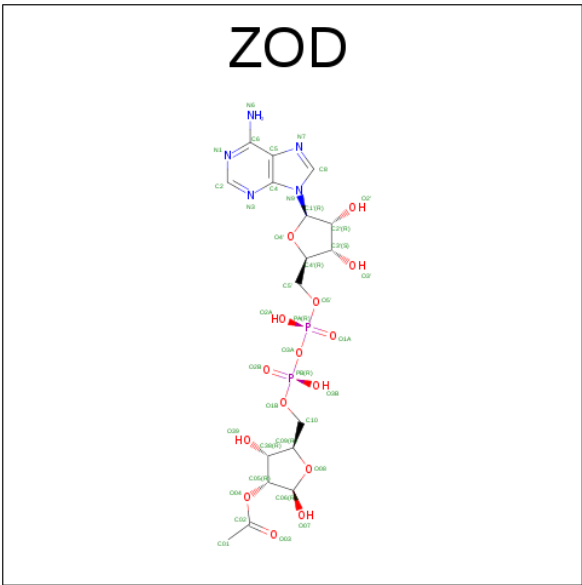
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	Q	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is [(2R,3R,4R,5R)-5-[[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxymethyl]-2,4-bis(oxidanyl)oxolan-3-yl] ethanoate (three-letter code: ZOD) (formula: C<sub>17</sub>H<sub>25</sub>N<sub>5</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	N	O	P	0	0
			39	17	5	15	2		
5	M	1	Total	C	N	O	P	0	0
			39	17	5	15	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	R	17	Total	O	0	0
			17	17		
6	A	11	Total	O	0	0
			11	11		
6	B	16	Total	O	0	0
			16	16		
6	C	10	Total	O	0	0
			10	10		
6	D	12	Total	O	0	0
			12	12		

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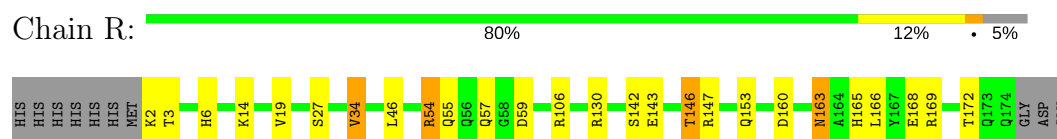
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	11	Total 11	O 11	0	0
6	F	10	Total 10	O 10	0	0
6	G	8	Total 8	O 8	0	0
6	H	12	Total 12	O 12	0	0
6	I	12	Total 12	O 12	0	0
6	J	12	Total 12	O 12	0	0
6	K	11	Total 11	O 11	0	0
6	L	11	Total 11	O 11	0	0
6	M	15	Total 15	O 15	0	0
6	N	12	Total 12	O 12	0	0
6	O	11	Total 11	O 11	0	0
6	P	14	Total 14	O 14	0	0
6	Q	9	Total 9	O 9	0	0

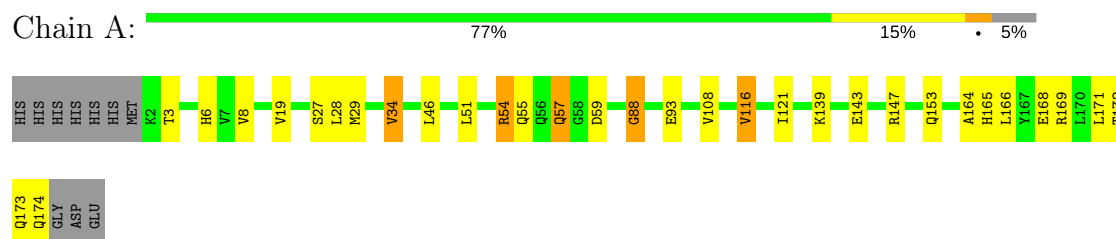
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

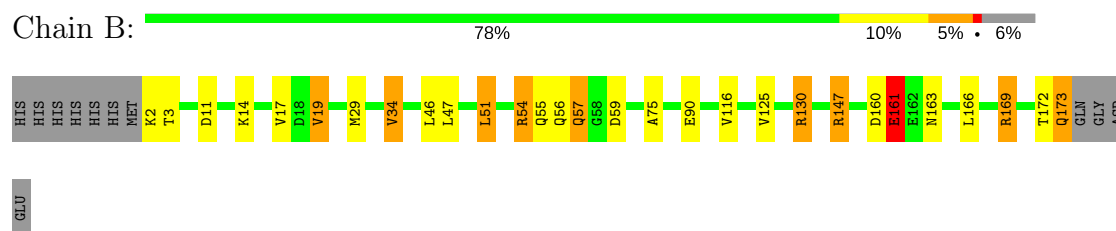
- Molecule 1: O-acetyl-ADP-ribose deacetylase



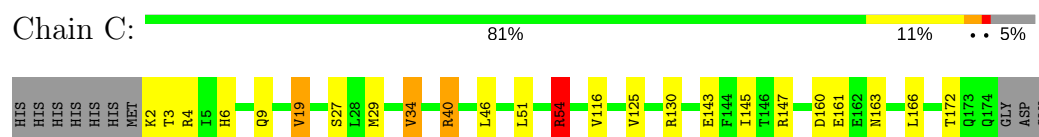
- Molecule 1: O-acetyl-ADP-ribose deacetylase



- Molecule 1: O-acetyl-ADP-ribose deacetylase

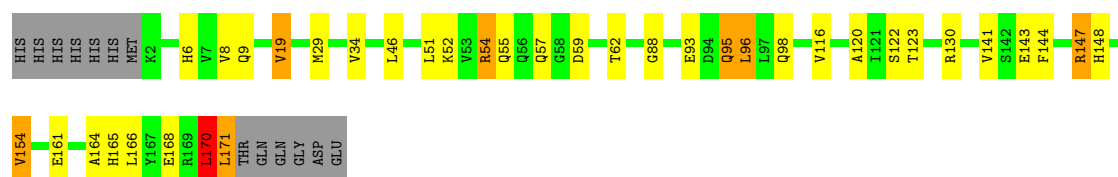


- Molecule 1: O-acetyl-ADP-ribose deacetylase



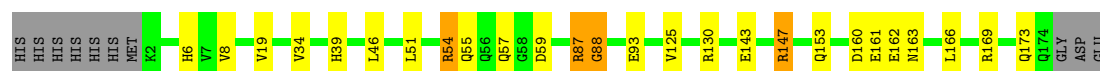
- Molecule 1: O-acetyl-ADP-ribose deacetylase





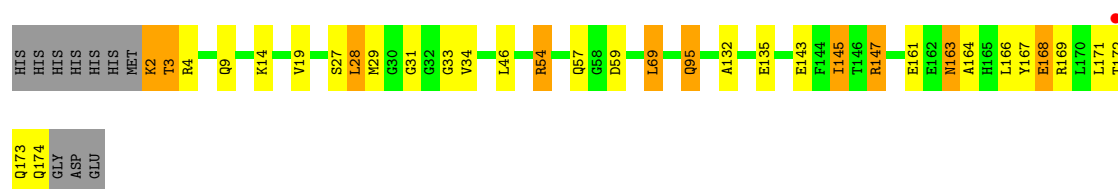
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain E: 80% 12% 5%



- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain F: 76% 13% 5% 5%



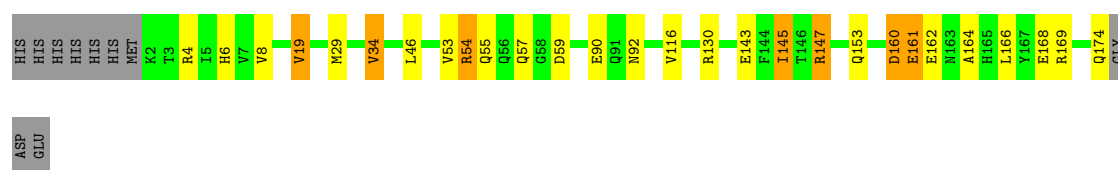
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain G: 83% 9% 5%



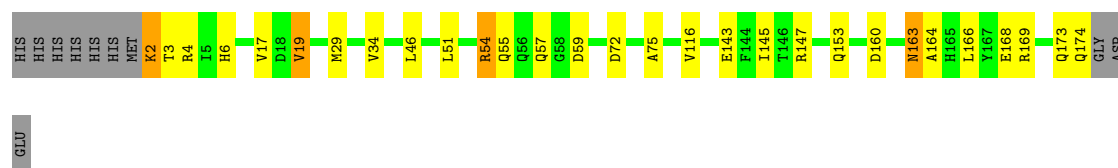
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain H: 79% 11% 5%

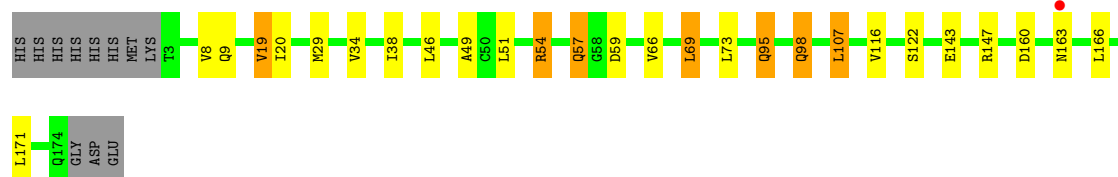
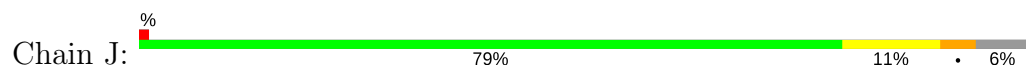


- Molecule 1: O-acetyl-ADP-ribose deacetylase

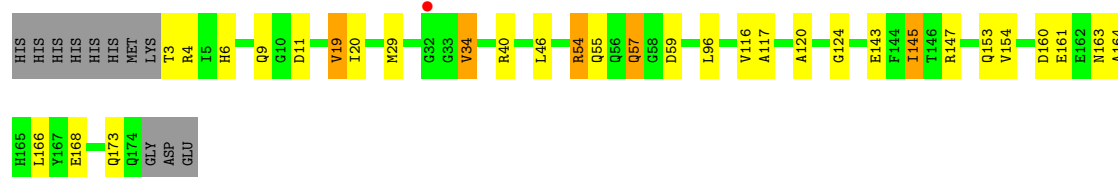
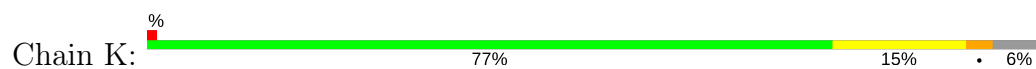
Chain I: 79% 14% 5%



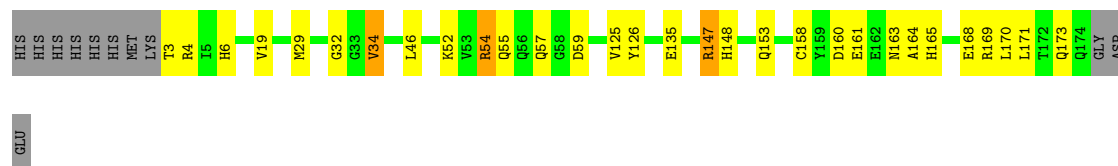
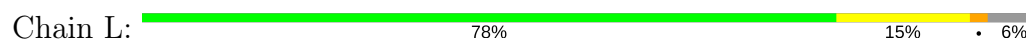
- Molecule 1: O-acetyl-ADP-ribose deacetylase



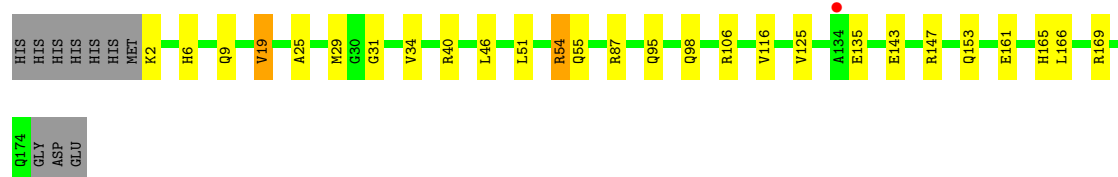
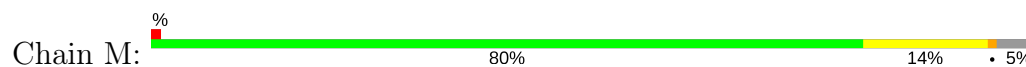
- Molecule 1: O-acetyl-ADP-ribose deacetylase



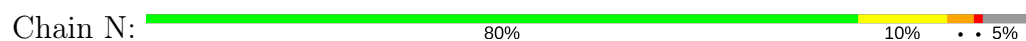
- Molecule 1: O-acetyl-ADP-ribose deacetylase



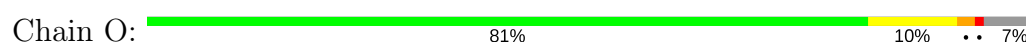
- Molecule 1: O-acetyl-ADP-ribose deacetylase



- Molecule 1: O-acetyl-ADP-ribose deacetylase



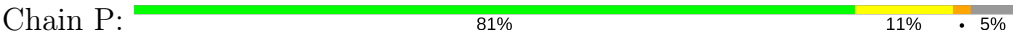
- Molecule 1: O-acetyl-ADP-ribose deacetylase



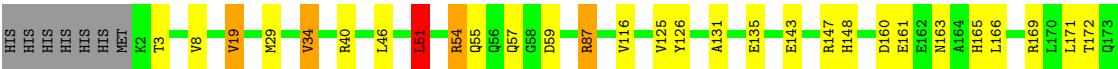
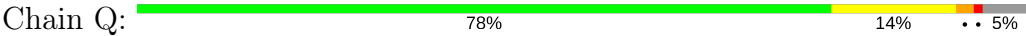




● Molecule 1: O-acetyl-ADP-ribose deacetylase



● Molecule 1: O-acetyl-ADP-ribose deacetylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	289.14Å 289.14Å 114.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.72 – 2.80 38.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.72-2.80) 98.9 (38.72-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.262 , 0.290 0.263 , 0.292	Depositor DCC
$R_{free}$ test set	6659 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 5.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.408 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.99 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.5839e-03.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: APR, ZOD, SO4, ACT

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	0.76	0/1284	0.98	4/1757 (0.2%)
1	B	0.79	0/1305	1.01	3/1782 (0.2%)
1	C	0.77	0/1308	0.97	1/1787 (0.1%)
1	D	0.79	0/1261	1.03	6/1727 (0.3%)
1	E	0.78	2/1318 (0.2%)	1.00	5/1799 (0.3%)
1	F	0.77	0/1308	1.01	5/1788 (0.3%)
1	G	0.77	0/1305	0.97	2/1783 (0.1%)
1	H	0.76	0/1318	0.95	2/1799 (0.1%)
1	I	0.74	0/1296	0.94	0/1771
1	J	0.79	0/1305	0.96	1/1783 (0.1%)
1	K	0.76	0/1280	0.92	0/1752
1	L	0.75	1/1284 (0.1%)	0.93	2/1758 (0.1%)
1	M	0.76	0/1304	0.93	0/1782
1	N	0.76	0/1279	0.98	4/1751 (0.2%)
1	O	0.77	0/1296	0.97	2/1771 (0.1%)
1	P	0.72	0/1302	0.94	2/1780 (0.1%)
1	Q	0.77	0/1314	0.97	2/1794 (0.1%)
1	R	0.78	0/1306	0.93	1/1784 (0.1%)
All	All	0.77	3/23373 (0.0%)	0.97	42/31948 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	162	GLU	CD-OE2	-5.87	1.19	1.25
1	E	161	GLU	CD-OE2	-5.22	1.20	1.25
1	L	161	GLU	CD-OE2	-5.13	1.20	1.25

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	69	LEU	CA-CB-CG	9.31	136.72	115.30
1	E	87	ARG	N-CA-C	-8.98	86.76	111.00
1	F	69	LEU	CB-CG-CD2	-8.64	96.31	111.00
1	B	147	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	C	54	ARG	CG-CD-NE	8.17	128.96	111.80
1	G	147	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	P	147	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	N	96	LEU	CA-CB-CG	7.26	132.00	115.30
1	D	96	LEU	CB-CG-CD1	-6.97	99.15	111.00
1	E	147	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	D	96	LEU	CB-CG-CD2	6.66	122.32	111.00
1	H	147	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	D	147	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	F	28	LEU	CA-CB-CG	6.43	130.09	115.30
1	H	29	MET	N-CA-C	-6.30	93.98	111.00
1	O	147	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	L	52	LYS	CD-CE-NZ	6.03	125.57	111.70
1	E	162	GLU	CG-CD-OE1	5.99	130.29	118.30
1	F	147	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	D	51	LEU	CB-CA-C	-5.85	99.09	110.20
1	F	19	VAL	CB-CA-C	-5.81	100.36	111.40
1	E	19	VAL	CB-CA-C	-5.64	100.68	111.40
1	O	54	ARG	CG-CD-NE	5.56	123.47	111.80
1	A	116	VAL	CA-CB-CG2	-5.54	102.59	110.90
1	J	107	LEU	CB-CG-CD1	-5.53	101.60	111.00
1	N	160	ASP	CB-CG-OD1	5.53	123.27	118.30
1	A	8	VAL	CA-CB-CG1	5.51	119.16	110.90
1	D	170	LEU	CB-CG-CD1	5.46	120.29	111.00
1	A	19	VAL	CB-CA-C	-5.32	101.30	111.40
1	N	29	MET	CG-SD-CE	5.29	108.66	100.20
1	Q	51	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	L	19	VAL	CB-CA-C	-5.26	101.41	111.40
1	P	19	VAL	CB-CA-C	-5.25	101.42	111.40
1	D	130	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	147	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	161	GLU	CG-CD-OE1	5.21	128.73	118.30
1	Q	87	ARG	CG-CD-NE	5.21	122.73	111.80
1	R	19	VAL	CB-CA-C	-5.18	101.56	111.40
1	E	88	GLY	N-CA-C	-5.17	100.17	113.10
1	N	170	LEU	CA-CB-CG	5.08	126.98	115.30
1	G	147	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	88	GLY	N-CA-C	-5.00	100.59	113.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1259	0	1237	29	0
1	B	1280	0	1278	29	0
1	C	1283	0	1273	22	0
1	D	1236	0	1204	34	1
1	E	1293	0	1290	15	0
1	F	1283	0	1268	50	0
1	G	1280	0	1267	12	0
1	H	1293	0	1290	14	0
1	I	1272	0	1265	21	0
1	J	1280	0	1273	23	0
1	K	1256	0	1238	23	0
1	L	1259	0	1237	26	0
1	M	1279	0	1269	21	0
1	N	1255	0	1228	31	0
1	O	1271	0	1265	16	0
1	P	1277	0	1263	19	0
1	Q	1289	0	1284	22	0
1	R	1281	0	1276	16	0
2	A	36	0	21	1	0
2	B	36	0	21	2	0
2	C	36	0	21	2	0
2	D	36	0	21	4	0
2	E	36	0	21	1	0
2	G	36	0	21	1	0
2	H	36	0	21	2	0
2	I	36	0	21	0	0
2	J	36	0	21	1	0
2	K	36	0	21	4	0
2	L	36	0	21	4	0
2	N	36	0	21	1	0
2	O	36	0	21	3	0
2	P	36	0	21	3	0
2	Q	36	0	21	3	0
2	R	36	0	21	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	2	0
3	D	5	0	0	3	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	1	0
3	I	5	0	0	0	0
3	J	5	0	0	3	0
3	K	5	0	0	2	0
3	L	5	0	0	1	0
3	M	5	0	0	3	0
3	N	5	0	0	0	0
3	O	5	0	0	3	0
3	P	5	0	0	1	0
3	Q	5	0	0	3	0
3	R	5	0	0	1	0
4	C	4	0	3	0	0
4	J	4	0	3	0	0
4	Q	4	0	3	0	0
5	F	39	0	23	4	0
5	M	39	0	23	6	0
6	A	11	0	0	0	0
6	B	16	0	0	1	0
6	C	10	0	0	0	0
6	D	12	0	0	0	0
6	E	11	0	0	1	0
6	F	10	0	0	0	0
6	G	8	0	0	0	0
6	H	12	0	0	1	0
6	I	12	0	0	0	0
6	J	12	0	0	0	0
6	K	11	0	0	0	0
6	L	11	0	0	2	0
6	M	15	0	0	0	0
6	N	12	0	0	1	0
6	O	11	0	0	0	0
6	P	14	0	0	2	0
6	Q	9	0	0	1	0
6	R	17	0	0	2	0
All	All	23896	0	23096	386	1

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 8.

All (386) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:GLN:OE1	1:F:161:GLU:CG	1.68	1.40
1:N:84:PRO:HB3	1:N:96:LEU:CD1	1.60	1.32
1:M:31:GLY:HA3	5:M:201:ZOD:O03	1.16	1.27
1:A:88:GLY:O	1:A:93:GLU:OE1	1.58	1.20
1:F:31:GLY:HA3	5:F:201:ZOD:O03	1.04	1.20
1:N:84:PRO:HB3	1:N:96:LEU:HD12	1.24	1.20
1:F:9:GLN:OE1	1:F:161:GLU:HG3	1.48	1.13
1:F:31:GLY:CA	5:F:201:ZOD:O03	1.99	1.09
1:M:31:GLY:CA	5:M:201:ZOD:O03	1.99	1.08
1:F:9:GLN:OE1	1:F:161:GLU:HG2	1.30	1.08
1:N:84:PRO:CB	1:N:96:LEU:HD12	1.82	1.08
1:C:2:LYS:O	1:C:3:THR:HG22	1.55	1.07
1:N:84:PRO:HB3	1:N:96:LEU:HD13	1.38	1.06
1:F:57:GLN:HB3	1:K:57:GLN:HE22	1.16	1.05
1:A:164:ALA:O	1:A:168:GLU:HG3	1.57	1.03
1:F:57:GLN:HB3	1:K:57:GLN:NE2	1.74	1.02
1:D:62:THR:CG2	1:D:96:LEU:HD23	1.89	1.02
1:B:2:LYS:HG3	1:B:3:THR:H	1.23	1.01
1:F:27:SER:O	1:F:29:MET:HE2	1.61	1.00
1:F:33:GLY:HA3	5:F:201:ZOD:O2A	1.62	0.98
1:Q:147:ARG:NH2	3:Q:403:SO4:O2	1.96	0.97
1:A:139:LYS:O	1:A:143:GLU:HG3	1.65	0.96
1:F:9:GLN:CD	1:F:161:GLU:HG2	1.84	0.96
1:B:29:MET:CE	1:B:51:LEU:HD11	1.94	0.96
1:K:147:ARG:NH2	3:K:202:SO4:O2	1.98	0.96
1:N:135:GLU:HA	1:N:170:LEU:HD21	1.46	0.95
1:O:147:ARG:NH2	3:O:202:SO4:O2	2.01	0.94
1:B:29:MET:HE1	1:B:51:LEU:HD11	1.49	0.92
1:D:62:THR:HG22	1:D:96:LEU:HD23	1.50	0.91
1:D:147:ARG:NH1	3:D:202:SO4:O4	2.03	0.91
1:F:27:SER:O	1:F:29:MET:CE	2.18	0.91
1:N:84:PRO:CB	1:N:96:LEU:CD1	2.43	0.91
1:J:147:ARG:NH2	3:J:202:SO4:O4	2.05	0.90
1:R:147:ARG:NH2	3:R:202:SO4:O2	2.05	0.89
1:R:142:SER:O	1:R:146:THR:CG2	2.20	0.89
1:D:57:GLN:OE1	1:I:57:GLN:CD	2.11	0.88
1:N:2:LYS:N	1:N:3:THR:HA	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:ARG:NH2	1:E:59:ASP:OD1	2.07	0.88
1:L:3:THR:HG23	1:L:4:ARG:H	1.38	0.87
1:A:54:ARG:NH2	1:A:59:ASP:OD1	2.08	0.87
1:D:54:ARG:NH2	1:D:59:ASP:OD1	2.08	0.87
1:B:54:ARG:NH2	1:B:59:ASP:OD1	2.07	0.87
1:G:54:ARG:NH2	1:G:59:ASP:OD1	2.07	0.87
1:R:54:ARG:NH2	1:R:59:ASP:OD1	2.08	0.87
1:R:165:HIS:O	1:R:169:ARG:HG2	1.75	0.86
1:H:54:ARG:NH2	1:H:59:ASP:OD1	2.08	0.86
1:M:106:ARG:NE	3:M:202:SO4:O4	2.07	0.86
1:K:54:ARG:NH2	1:K:59:ASP:OD1	2.08	0.86
1:I:54:ARG:NH2	1:I:59:ASP:OD1	2.08	0.86
1:P:54:ARG:NH2	1:P:59:ASP:OD1	2.08	0.86
1:H:130:ARG:NH2	1:H:160:ASP:OD2	2.08	0.86
1:N:29:MET:CE	1:N:47:LEU:CD1	2.53	0.85
1:Q:54:ARG:NH2	1:Q:59:ASP:OD1	2.08	0.85
1:N:54:ARG:NH2	1:N:59:ASP:OD1	2.09	0.85
1:A:168:GLU:O	1:A:172:THR:HG23	1.75	0.85
1:H:164:ALA:O	1:H:168:GLU:HG3	1.77	0.85
1:L:54:ARG:NH2	1:L:59:ASP:OD1	2.10	0.84
1:D:57:GLN:OE1	1:I:57:GLN:NE2	2.11	0.84
1:N:29:MET:CE	1:N:47:LEU:HD11	2.08	0.84
1:J:29:MET:HE1	1:J:51:LEU:HD23	1.61	0.81
1:M:31:GLY:HA3	5:M:201:ZOD:C02	2.10	0.81
1:R:142:SER:O	1:R:146:THR:HG23	1.80	0.80
1:B:29:MET:SD	1:B:51:LEU:CD1	2.70	0.80
1:D:164:ALA:O	1:D:168:GLU:HG3	1.81	0.80
1:Q:29:MET:HE3	1:Q:51:LEU:HD22	1.66	0.78
1:L:164:ALA:O	1:L:168:GLU:HG3	1.85	0.76
1:I:2:LYS:HB3	1:I:3:THR:HA	1.66	0.76
1:K:164:ALA:O	1:K:168:GLU:HG3	1.85	0.76
1:N:135:GLU:HA	1:N:170:LEU:CD2	2.16	0.75
1:J:147:ARG:NH2	3:J:202:SO4:O1	2.18	0.75
1:M:125:VAL:HG13	5:M:201:ZOD:O1A	1.85	0.75
1:A:108:VAL:HG21	1:A:116:VAL:HG11	1.69	0.75
1:B:2:LYS:HG3	1:B:3:THR:HG22	1.68	0.75
1:A:108:VAL:HG11	1:A:116:VAL:CG1	2.16	0.74
1:C:147:ARG:NH1	3:C:202:SO4:O4	2.21	0.74
1:I:29:MET:HE3	1:I:51:LEU:HD23	1.69	0.74
1:N:29:MET:CE	1:N:47:LEU:HD12	2.18	0.74
1:P:25:ALA:HB2	2:P:201:APR:O3D	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:GLY:O	1:E:93:GLU:OE1	2.06	0.74
1:A:108:VAL:HG11	1:A:116:VAL:HG12	1.70	0.73
1:I:6:HIS:HE1	1:I:153:GLN:OE1	1.72	0.73
1:F:57:GLN:CB	1:K:57:GLN:NE2	2.49	0.73
1:G:57:GLN:OE1	1:Q:57:GLN:OE1	2.07	0.73
1:N:29:MET:HE1	1:N:47:LEU:CD1	2.19	0.73
1:O:87:ARG:N	1:O:93:GLU:OE2	2.20	0.73
1:J:54:ARG:NH2	1:J:59:ASP:OD1	2.22	0.73
1:E:87:ARG:HG2	1:E:87:ARG:HH21	1.54	0.72
1:F:169:ARG:HH11	1:F:169:ARG:HG3	1.54	0.72
1:N:2:LYS:HG3	1:N:4:ARG:H	1.53	0.72
1:P:29:MET:HE3	1:P:51:LEU:HD23	1.70	0.72
1:F:29:MET:CE	1:F:54:ARG:HG3	2.20	0.71
1:P:130:ARG:HD3	1:P:130:ARG:H	1.54	0.71
1:D:62:THR:HG21	1:D:96:LEU:HD23	1.73	0.70
1:O:130:ARG:HD3	1:O:130:ARG:H	1.54	0.70
1:F:54:ARG:NH2	1:F:59:ASP:OD1	2.25	0.70
3:D:202:SO4:O2	1:M:40:ARG:HB3	1.91	0.70
1:B:130:ARG:H	1:B:130:ARG:HE	1.37	0.69
1:R:142:SER:O	1:R:146:THR:HG22	1.93	0.69
1:F:169:ARG:O	1:F:173:GLN:HG3	1.93	0.69
1:J:147:ARG:NH2	3:J:202:SO4:S	2.66	0.68
1:B:2:LYS:HE2	1:B:3:THR:HG22	1.75	0.68
1:F:2:LYS:HG2	1:F:4:ARG:HB2	1.75	0.68
1:R:6:HIS:HE1	1:R:153:GLN:OE1	1.77	0.68
1:M:165:HIS:O	1:M:169:ARG:HG3	1.94	0.67
1:N:2:LYS:HD2	1:N:2:LYS:O	1.94	0.67
1:B:29:MET:SD	1:B:51:LEU:HD11	2.32	0.67
1:K:40:ARG:HB3	3:Q:403:SO4:O4	1.94	0.67
1:F:9:GLN:NE2	1:F:161:GLU:HG2	2.08	0.67
1:N:29:MET:HE2	1:N:47:LEU:HD11	1.75	0.67
1:H:6:HIS:HE1	1:H:153:GLN:OE1	1.77	0.67
1:E:6:HIS:HE1	1:E:153:GLN:OE1	1.77	0.67
1:C:34:VAL:HG23	2:C:201:APR:O2A	1.95	0.66
1:F:29:MET:HG2	1:L:29:MET:HE3	1.76	0.66
1:N:29:MET:HE1	1:N:47:LEU:HD11	1.78	0.66
1:C:29:MET:HE2	1:C:54:ARG:HG3	1.77	0.66
1:O:29:MET:HE2	1:O:54:ARG:HG3	1.78	0.65
1:F:29:MET:HE3	1:F:54:ARG:HG3	1.78	0.65
1:A:6:HIS:HE1	1:A:153:GLN:OE1	1.80	0.65
1:A:168:GLU:OE2	1:D:168:GLU:OE2	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ARG:HG2	3:H:202:SO4:O1	1.95	0.65
1:A:172:THR:HG21	1:D:9:GLN:HB2	1.79	0.64
1:L:163:ASN:ND2	6:L:301:HOH:O	2.18	0.64
1:B:172:THR:C	1:B:173:GLN:HE21	2.01	0.64
1:M:6:HIS:HE1	1:M:153:GLN:OE1	1.78	0.64
1:L:6:HIS:HE1	1:L:153:GLN:OE1	1.81	0.64
1:D:164:ALA:O	1:D:168:GLU:CG	2.46	0.63
1:A:165:HIS:CE1	1:D:165:HIS:CD2	2.86	0.63
1:N:94:ASP:OD1	1:N:95:GLN:N	2.31	0.63
1:F:2:LYS:HG3	1:F:4:ARG:H	1.64	0.63
1:O:164:ALA:O	1:O:168:GLU:HG3	1.98	0.63
1:B:2:LYS:HE2	1:B:3:THR:CG2	2.29	0.62
1:B:125:VAL:HG13	2:B:201:APR:O1A	1.99	0.62
1:D:161:GLU:HG2	1:D:165:HIS:CE1	2.34	0.62
1:L:158:CYS:HA	6:L:301:HOH:O	2.00	0.62
1:L:3:THR:CG2	1:L:4:ARG:H	2.11	0.62
1:O:147:ARG:NH2	3:O:202:SO4:S	2.71	0.62
1:B:173:GLN:N	1:B:173:GLN:HE21	1.98	0.61
1:L:3:THR:HG23	1:L:4:ARG:N	2.13	0.61
1:C:54:ARG:HH21	1:C:54:ARG:HG3	1.65	0.61
1:O:124:GLY:HA3	2:O:201:APR:O1A	2.01	0.60
1:B:34:VAL:HG23	2:B:201:APR:O2A	2.01	0.60
1:F:163:ASN:ND2	1:F:167:TYR:CD1	2.70	0.60
1:F:29:MET:HG2	1:L:29:MET:CE	2.31	0.60
1:O:106:ARG:NE	3:O:202:SO4:O1	2.31	0.60
1:F:29:MET:HB3	1:L:29:MET:HB2	1.84	0.59
1:A:88:GLY:O	1:A:93:GLU:CD	2.38	0.59
1:F:164:ALA:O	1:F:168:GLU:HG3	2.02	0.59
1:L:147:ARG:HG3	1:L:148:HIS:CD2	2.37	0.59
1:R:130:ARG:NH1	6:R:302:HOH:O	2.34	0.59
1:K:6:HIS:HE1	1:K:153:GLN:OE1	1.86	0.59
1:K:11:ASP:OD1	2:K:201:APR:N6	2.34	0.58
1:N:126:TYR:CE1	2:N:201:APR:HR'4	2.38	0.58
1:D:57:GLN:OE1	1:I:57:GLN:CG	2.52	0.58
1:Q:29:MET:CE	1:Q:51:LEU:HD22	2.32	0.58
1:L:160:ASP:OD1	1:L:163:ASN:HB2	2.04	0.58
1:B:56:GLN:NE2	1:H:53:VAL:HG22	2.18	0.57
1:D:144:PHE:HE2	3:D:202:SO4:O3	1.87	0.57
1:M:29:MET:HE2	1:M:54:ARG:HG3	1.86	0.57
1:A:34:VAL:HG23	2:A:201:APR:O2A	2.04	0.57
1:C:29:MET:HE1	1:C:51:LEU:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:145:ILE:HD11	1:K:154:VAL:HG23	1.86	0.56
1:R:160:ASP:OD1	1:R:163:ASN:HB2	2.05	0.56
1:A:6:HIS:CD2	1:D:6:HIS:CD2	2.93	0.56
1:L:34:VAL:HG23	2:L:201:APR:O2A	2.05	0.56
1:C:29:MET:HE1	1:C:51:LEU:HD23	1.88	0.56
1:F:2:LYS:CG	1:F:4:ARG:H	2.17	0.56
1:C:125:VAL:HG13	2:C:201:APR:O1A	2.06	0.56
1:P:2:LYS:HE3	1:P:145:ILE:HD11	1.87	0.56
1:H:161:GLU:O	1:H:162:GLU:C	2.42	0.56
1:L:165:HIS:O	1:L:169:ARG:HG3	2.06	0.56
1:A:147:ARG:NH1	3:A:202:SO4:O1	2.35	0.56
1:L:147:ARG:NH2	3:L:202:SO4:O4	2.39	0.56
1:C:9:GLN:HB3	1:Q:172:THR:HG21	1.87	0.55
1:N:29:MET:CE	1:N:29:MET:HA	2.37	0.55
1:J:69:LEU:C	1:J:69:LEU:HD23	2.26	0.55
1:I:4:ARG:NH2	1:I:145:ILE:HB	2.21	0.55
1:E:147:ARG:NH1	3:E:202:SO4:O3	2.39	0.55
1:J:29:MET:CE	1:J:51:LEU:HD23	2.34	0.55
1:I:2:LYS:CB	1:I:3:THR:HA	2.34	0.55
1:B:2:LYS:HG3	1:B:3:THR:N	2.07	0.55
1:C:9:GLN:HE22	1:C:161:GLU:HG3	1.72	0.55
1:F:9:GLN:OE1	1:F:161:GLU:CB	2.51	0.55
1:F:29:MET:HE1	1:F:54:ARG:HG3	1.89	0.54
1:B:173:GLN:N	1:B:173:GLN:NE2	2.54	0.54
1:P:126:TYR:CD1	2:P:201:APR:H5R1	2.43	0.54
1:M:29:MET:HE3	1:M:51:LEU:HD23	1.88	0.54
1:P:130:ARG:H	1:P:130:ARG:CD	2.21	0.54
1:G:160:ASP:OD1	1:G:163:ASN:HB2	2.08	0.54
1:R:106:ARG:NH1	1:Q:40:ARG:HH21	2.05	0.54
1:F:132:ALA:O	1:F:135:GLU:HB3	2.07	0.54
1:M:25:ALA:CB	5:M:201:ZOD:H1	2.38	0.54
1:F:29:MET:HB3	1:L:29:MET:CB	2.37	0.53
1:F:9:GLN:OE1	1:F:161:GLU:CA	2.56	0.53
1:F:172:THR:HG22	1:F:172:THR:O	2.08	0.53
1:J:69:LEU:HD23	1:J:69:LEU:O	2.08	0.53
1:C:4:ARG:NH2	1:C:145:ILE:O	2.40	0.53
1:J:29:MET:CE	1:J:51:LEU:CD2	2.87	0.53
1:N:2:LYS:O	1:N:2:LYS:CD	2.57	0.53
1:I:29:MET:HE2	1:I:54:ARG:HG3	1.90	0.53
1:D:141:VAL:HG11	1:D:154:VAL:HG21	1.91	0.52
1:B:2:LYS:CG	1:B:3:THR:H	2.03	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:29:MET:HE3	1:N:29:MET:HA	1.92	0.52
1:F:163:ASN:C	1:F:163:ASN:HD22	2.12	0.52
1:L:135:GLU:HG3	1:L:170:LEU:HD22	1.92	0.52
1:Q:131:ALA:O	1:Q:135:GLU:HG3	2.09	0.52
1:O:29:MET:HE1	1:O:51:LEU:HA	1.92	0.52
1:I:164:ALA:O	1:I:168:GLU:HG3	2.10	0.52
1:P:29:MET:HE3	1:P:51:LEU:CD2	2.40	0.52
1:A:169:ARG:O	1:A:173:GLN:HB2	2.10	0.52
1:O:130:ARG:CD	1:O:130:ARG:H	2.21	0.52
1:P:143:GLU:O	1:P:147:ARG:HG3	2.10	0.52
1:P:173:GLN:O	1:P:173:GLN:HG2	2.10	0.51
1:P:6:HIS:CE1	6:P:307:HOH:O	2.63	0.51
1:C:27:SER:HB2	1:C:54:ARG:HH22	1.74	0.51
1:C:6:HIS:HB3	6:Q:501:HOH:O	2.09	0.51
1:C:27:SER:O	1:C:54:ARG:NH2	2.43	0.51
1:F:29:MET:HG2	1:L:29:MET:HB3	1.91	0.51
1:G:103:ASN:N	1:G:103:ASN:HD22	2.08	0.51
1:C:143:GLU:O	1:C:147:ARG:HG3	2.09	0.51
1:D:143:GLU:O	1:D:147:ARG:HG3	2.10	0.51
1:I:173:GLN:HA	1:I:174:GLN:HB2	1.92	0.51
1:F:2:LYS:HG3	1:F:3:THR:N	2.26	0.51
1:H:143:GLU:O	1:H:147:ARG:HG3	2.10	0.51
1:A:171:LEU:O	1:A:174:GLN:HG2	2.11	0.51
1:G:143:GLU:O	1:G:147:ARG:HG3	2.10	0.51
1:K:160:ASP:OD1	1:K:163:ASN:HB2	2.10	0.51
1:E:143:GLU:O	1:E:147:ARG:HG3	2.11	0.50
1:E:39:HIS:ND1	6:E:301:HOH:O	2.35	0.50
1:J:95:GLN:OE1	1:J:98:GLN:NE2	2.45	0.50
1:G:57:GLN:OE1	1:Q:57:GLN:HB3	2.11	0.50
1:M:106:ARG:NH2	3:M:202:SO4:O4	2.45	0.50
1:M:25:ALA:HB2	5:M:201:ZOD:H1	1.93	0.50
1:R:143:GLU:O	1:R:147:ARG:HG3	2.11	0.50
1:J:143:GLU:O	1:J:147:ARG:HG3	2.12	0.50
1:R:34:VAL:HG23	2:R:201:APR:O2A	2.12	0.50
1:Q:143:GLU:O	1:Q:147:ARG:HG3	2.12	0.50
1:A:139:LYS:HG2	1:A:143:GLU:OE1	2.11	0.49
1:D:95:GLN:NE2	1:D:98:GLN:NE2	2.61	0.49
1:D:95:GLN:HE22	1:D:98:GLN:NE2	2.10	0.49
1:F:29:MET:CG	1:L:29:MET:HE2	2.42	0.49
1:K:143:GLU:O	1:K:147:ARG:HG3	2.12	0.49
1:F:163:ASN:ND2	1:F:167:TYR:HD1	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:32:GLY:O	2:O:201:APR:O1D	2.30	0.49
1:A:165:HIS:ND1	1:D:165:HIS:CD2	2.81	0.49
1:B:161:GLU:HG3	6:B:314:HOH:O	2.10	0.49
1:R:27:SER:O	1:R:54:ARG:HD2	2.12	0.49
1:D:95:GLN:NE2	1:D:98:GLN:HE21	2.11	0.49
1:F:143:GLU:O	1:F:147:ARG:HG3	2.13	0.49
1:J:122:SER:HA	2:J:201:APR:O1B	2.12	0.49
1:A:29:MET:CE	1:A:51:LEU:HD23	2.43	0.49
1:H:161:GLU:HG3	1:H:162:GLU:N	2.26	0.49
1:K:4:ARG:NH2	1:K:145:ILE:HG23	2.27	0.49
1:M:143:GLU:O	1:M:147:ARG:HG3	2.13	0.49
1:N:143:GLU:O	1:N:147:ARG:HG3	2.12	0.49
1:P:8:VAL:HG23	6:P:314:HOH:O	2.13	0.49
1:F:169:ARG:HH11	1:F:169:ARG:CG	2.23	0.49
1:L:125:VAL:HG13	2:L:201:APR:O1A	2.12	0.49
1:P:29:MET:CE	1:P:51:LEU:HD23	2.40	0.49
1:N:29:MET:HE3	1:N:47:LEU:HD12	1.93	0.49
1:M:106:ARG:CZ	3:M:202:SO4:O4	2.60	0.48
1:F:29:MET:CG	1:L:29:MET:CE	2.91	0.48
1:J:95:GLN:HE22	1:J:98:GLN:HE21	1.59	0.48
1:C:2:LYS:C	1:C:3:THR:HG22	2.32	0.48
1:L:126:TYR:CE1	2:L:201:APR:HR'4	2.48	0.48
1:A:143:GLU:O	1:A:147:ARG:HG3	2.13	0.48
1:B:47:LEU:O	1:B:51:LEU:HD22	2.13	0.48
1:D:120:ALA:O	2:D:201:APR:H'4	2.13	0.48
1:E:51:LEU:HD11	1:Q:51:LEU:HD11	1.96	0.48
1:A:29:MET:HE1	1:A:51:LEU:HD23	1.96	0.48
1:E:125:VAL:HG13	2:E:201:APR:O1A	2.14	0.48
1:H:4:ARG:NH2	1:H:145:ILE:HG23	2.29	0.48
1:I:160:ASP:OD1	1:I:163:ASN:HB2	2.13	0.48
1:C:29:MET:CE	1:C:51:LEU:HD23	2.43	0.48
1:I:72:ASP:OD2	1:P:148:HIS:ND1	2.34	0.48
1:L:32:GLY:O	2:L:201:APR:O1D	2.27	0.47
1:O:29:MET:CE	1:O:51:LEU:HD23	2.44	0.47
1:Q:126:TYR:CE1	2:Q:402:APR:HR'4	2.50	0.47
1:G:34:VAL:HG23	2:G:201:APR:O2A	2.14	0.47
1:J:29:MET:HE1	1:J:51:LEU:CD2	2.37	0.47
1:M:29:MET:CE	1:M:51:LEU:HD23	2.45	0.47
1:O:126:TYR:CE1	2:O:201:APR:HR'4	2.50	0.47
1:K:20:ILE:HG22	1:K:117:ALA:HB3	1.96	0.47
1:D:122:SER:N	2:D:201:APR:O1B	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:SER:O	1:F:28:LEU:HB2	2.15	0.46
1:J:29:MET:HE3	1:J:51:LEU:HD21	1.98	0.46
1:M:19:VAL:HG22	1:M:116:VAL:HG23	1.98	0.46
1:F:4:ARG:NH2	1:F:145:ILE:HG23	2.31	0.46
1:Q:147:ARG:NH2	3:Q:403:SO4:S	2.86	0.46
1:Q:34:VAL:HG23	2:Q:402:APR:O2A	2.15	0.46
1:A:108:VAL:HG21	1:A:116:VAL:CG1	2.43	0.46
1:I:143:GLU:O	1:I:147:ARG:HG3	2.15	0.46
1:I:2:LYS:HB3	1:I:3:THR:CA	2.43	0.46
1:R:2:LYS:HG2	1:R:3:THR:H	1.79	0.46
1:J:19:VAL:HG22	1:J:116:VAL:HG23	1.97	0.46
1:N:2:LYS:HE2	1:N:4:ARG:HB2	1.98	0.46
1:I:72:ASP:HB3	1:P:147:ARG:O	2.16	0.46
1:E:87:ARG:HG2	1:E:87:ARG:NH2	2.27	0.46
1:D:123:THR:OG1	2:D:201:APR:O3'	2.27	0.46
1:F:169:ARG:NH1	1:F:169:ARG:HG3	2.28	0.46
1:C:2:LYS:O	1:C:3:THR:CG2	2.44	0.46
1:G:19:VAL:HG22	1:G:116:VAL:HG23	1.97	0.46
1:P:147:ARG:NH1	3:P:202:SO4:O1	2.49	0.46
1:F:163:ASN:HD21	1:F:167:TYR:HE1	1.58	0.45
1:D:122:SER:HA	2:D:201:APR:O1B	2.16	0.45
1:Q:125:VAL:HG13	2:Q:402:APR:O1A	2.17	0.45
1:E:160:ASP:OD1	1:E:163:ASN:HB2	2.16	0.45
1:B:19:VAL:HG22	1:B:116:VAL:HG23	1.99	0.45
1:E:87:ARG:CG	1:E:87:ARG:HH21	2.25	0.45
1:F:164:ALA:O	1:F:168:GLU:CG	2.64	0.45
1:K:120:ALA:O	2:K:201:APR:H5'1	2.16	0.45
1:K:34:VAL:HG23	2:K:201:APR:O2A	2.15	0.45
1:B:160:ASP:OD1	1:B:163:ASN:HB2	2.17	0.45
1:D:62:THR:HG21	1:D:96:LEU:CD2	2.45	0.45
1:N:135:GLU:CA	1:N:170:LEU:HD21	2.32	0.45
1:O:19:VAL:HG22	1:O:116:VAL:HG23	1.99	0.45
1:N:19:VAL:HG22	1:N:116:VAL:HG23	1.98	0.44
1:O:160:ASP:OD1	1:O:163:ASN:HB2	2.17	0.44
1:P:29:MET:HE2	1:P:54:ARG:HG3	1.99	0.44
1:D:19:VAL:HG22	1:D:116:VAL:HG23	1.99	0.44
1:J:34:VAL:HG22	1:J:38:ILE:CD1	2.48	0.44
1:Q:19:VAL:HG22	1:Q:116:VAL:HG23	1.99	0.44
1:C:147:ARG:NH1	3:C:202:SO4:S	2.90	0.44
1:K:9:GLN:HG3	1:K:164:ALA:HB2	1.99	0.44
1:P:2:LYS:HB3	1:P:4:ARG:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:160:ASP:OD1	1:Q:163:ASN:HB2	2.17	0.44
1:A:57:GLN:HB3	1:L:57:GLN:HE22	1.81	0.44
1:I:19:VAL:HG22	1:I:116:VAL:HG23	1.98	0.44
1:D:170:LEU:O	1:D:171:LEU:HB2	2.17	0.44
1:M:29:MET:HE1	1:M:51:LEU:HA	1.98	0.44
1:R:169:ARG:HB2	6:R:308:HOH:O	2.17	0.44
1:B:17:VAL:O	1:B:75:ALA:HA	2.18	0.43
1:F:147:ARG:O	1:G:72:ASP:HB3	2.18	0.43
1:B:130:ARG:H	1:B:130:ARG:NE	2.11	0.43
1:C:19:VAL:HG22	1:C:116:VAL:HG23	2.00	0.43
1:Q:161:GLU:HG2	1:Q:165:HIS:CE1	2.53	0.43
1:J:95:GLN:NE2	1:J:98:GLN:HE21	2.16	0.43
1:K:19:VAL:HG22	1:K:116:VAL:HG23	2.01	0.43
1:L:171:LEU:C	1:L:173:GLN:H	2.21	0.43
1:D:88:GLY:N	1:D:93:GLU:OE1	2.52	0.43
1:H:92:ASN:HA	6:H:304:HOH:O	2.18	0.43
1:A:29:MET:HE3	1:A:51:LEU:CD2	2.48	0.43
1:F:33:GLY:HA3	5:F:201:ZOD:PA	2.58	0.43
1:F:95:GLN:CA	1:F:95:GLN:HE21	2.32	0.43
1:I:17:VAL:O	1:I:75:ALA:HA	2.19	0.43
1:G:29:MET:HB3	1:K:29:MET:HG3	2.01	0.43
1:R:57:GLN:HE22	1:E:57:GLN:HB3	1.84	0.42
1:H:34:VAL:HG23	2:H:201:APR:O2A	2.19	0.42
1:N:147:ARG:HD2	6:N:310:HOH:O	2.19	0.42
1:B:147:ARG:NH2	3:B:202:SO4:O2	2.45	0.42
1:D:166:LEU:O	1:D:170:LEU:HD22	2.18	0.42
1:N:84:PRO:CG	1:N:96:LEU:HD12	2.47	0.42
1:J:57:GLN:OE1	1:J:66:VAL:HG11	2.19	0.42
1:F:171:LEU:C	1:F:173:GLN:H	2.21	0.42
1:N:57:GLN:O	1:N:57:GLN:HG3	2.20	0.42
1:A:29:MET:HE3	1:A:51:LEU:HD21	2.02	0.42
1:B:169:ARG:HB2	1:B:169:ARG:HE	1.70	0.42
1:H:19:VAL:HG22	1:H:116:VAL:HG23	2.00	0.42
1:Q:171:LEU:O	1:Q:174:GLN:HB3	2.20	0.42
1:D:148:HIS:CE1	1:M:40:ARG:O	2.73	0.42
1:E:87:ARG:CG	1:E:87:ARG:NH2	2.82	0.42
1:I:6:HIS:CE1	1:I:153:GLN:OE1	2.62	0.41
1:M:9:GLN:HE22	1:M:161:GLU:HB2	1.84	0.41
1:K:40:ARG:O	1:Q:148:HIS:HE1	2.03	0.41
1:A:27:SER:O	1:A:28:LEU:HB2	2.20	0.41
1:J:49:ALA:HB2	1:J:69:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:20:ILE:HD11	1:J:73:LEU:HD13	2.02	0.41
1:P:124:GLY:HA3	2:P:201:APR:O1A	2.20	0.41
1:B:51:LEU:HD12	1:B:51:LEU:HA	1.73	0.41
1:C:160:ASP:OD1	1:C:163:ASN:HB2	2.21	0.41
1:I:29:MET:HE3	1:I:51:LEU:CD2	2.44	0.41
1:B:11:ASP:HB3	1:B:14:LYS:CD	2.50	0.41
1:O:87:ARG:HB2	1:O:93:GLU:OE2	2.21	0.41
1:F:9:GLN:HE22	1:F:161:GLU:HG2	1.82	0.41
1:K:124:GLY:HA3	2:K:201:APR:O5'	2.21	0.41
1:D:148:HIS:HE1	1:M:40:ARG:O	2.02	0.41
1:N:92:ASN:O	1:N:96:LEU:HG	2.21	0.41
1:B:57:GLN:HB3	1:H:57:GLN:HE22	1.84	0.41
1:K:147:ARG:NH2	3:K:202:SO4:S	2.92	0.41
1:A:168:GLU:CD	1:D:168:GLU:OE2	2.59	0.40
1:J:160:ASP:OD1	1:J:163:ASN:HB2	2.19	0.40
1:J:171:LEU:HA	1:J:171:LEU:HD23	1.97	0.40
1:G:9:GLN:HE22	1:G:161:GLU:HB2	1.85	0.40
1:H:34:VAL:CG2	2:H:201:APR:H5'2	2.51	0.40
1:K:29:MET:CE	1:K:54:ARG:HG3	2.51	0.40
1:G:57:GLN:OE1	1:Q:57:GLN:CB	2.70	0.40
1:E:51:LEU:CD1	1:Q:51:LEU:HD11	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:MET:CE	1:D:29:MET:CE[6_554]	2.16	0.04

## 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	171/183 (93%)	166 (97%)	5 (3%)	0	100	100
1	B	170/183 (93%)	166 (98%)	4 (2%)	0	100	100
1	C	171/183 (93%)	168 (98%)	3 (2%)	0	100	100
1	D	168/183 (92%)	162 (96%)	6 (4%)	0	100	100
1	E	171/183 (93%)	167 (98%)	4 (2%)	0	100	100
1	F	171/183 (93%)	165 (96%)	6 (4%)	0	100	100
1	G	171/183 (93%)	166 (97%)	5 (3%)	0	100	100
1	H	171/183 (93%)	167 (98%)	4 (2%)	0	100	100
1	I	171/183 (93%)	165 (96%)	6 (4%)	0	100	100
1	J	170/183 (93%)	165 (97%)	5 (3%)	0	100	100
1	K	170/183 (93%)	168 (99%)	2 (1%)	0	100	100
1	L	170/183 (93%)	168 (99%)	2 (1%)	0	100	100
1	M	171/183 (93%)	167 (98%)	4 (2%)	0	100	100
1	N	171/183 (93%)	168 (98%)	3 (2%)	0	100	100
1	O	169/183 (92%)	166 (98%)	3 (2%)	0	100	100
1	P	171/183 (93%)	167 (98%)	4 (2%)	0	100	100
1	Q	171/183 (93%)	168 (98%)	3 (2%)	0	100	100
1	R	171/183 (93%)	168 (98%)	3 (2%)	0	100	100
All	All	3069/3294 (93%)	2997 (98%)	72 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	124/141 (88%)	116 (94%)	8 (6%)	20	49
1	B	130/141 (92%)	117 (90%)	13 (10%)	9	26
1	C	130/141 (92%)	122 (94%)	8 (6%)	21	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	121/141 (86%)	110 (91%)	11 (9%)	11	31
1	E	132/141 (94%)	123 (93%)	9 (7%)	18	47
1	F	130/141 (92%)	117 (90%)	13 (10%)	9	26
1	G	128/141 (91%)	117 (91%)	11 (9%)	12	34
1	H	132/141 (94%)	119 (90%)	13 (10%)	9	27
1	I	127/141 (90%)	118 (93%)	9 (7%)	17	44
1	J	130/141 (92%)	119 (92%)	11 (8%)	12	35
1	K	125/141 (89%)	113 (90%)	12 (10%)	10	28
1	L	125/141 (89%)	120 (96%)	5 (4%)	36	70
1	M	129/141 (92%)	118 (92%)	11 (8%)	12	35
1	N	123/141 (87%)	111 (90%)	12 (10%)	9	27
1	O	129/141 (92%)	120 (93%)	9 (7%)	18	45
1	P	128/141 (91%)	120 (94%)	8 (6%)	21	51
1	Q	131/141 (93%)	120 (92%)	11 (8%)	13	35
1	R	129/141 (92%)	119 (92%)	10 (8%)	15	39
All	All	2303/2538 (91%)	2119 (92%)	184 (8%)	14	38

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	14	LYS
1	R	34	VAL
1	R	46	LEU
1	R	54	ARG
1	R	55	GLN
1	R	146	THR
1	R	163	ASN
1	R	166	LEU
1	R	168	GLU
1	R	172	THR
1	A	3	THR
1	A	34	VAL
1	A	46	LEU
1	A	54	ARG
1	A	55	GLN
1	A	57	GLN
1	A	121	ILE

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Mol	Chain	Res	Type
1	A	166	LEU
1	B	19	VAL
1	B	34	VAL
1	B	46	LEU
1	B	51	LEU
1	B	54	ARG
1	B	55	GLN
1	B	57	GLN
1	B	90	GLU
1	B	130	ARG
1	B	161	GLU
1	B	166	LEU
1	B	169	ARG
1	B	173	GLN
1	C	19	VAL
1	C	34	VAL
1	C	40	ARG
1	C	46	LEU
1	C	54	ARG
1	C	130	ARG
1	C	166	LEU
1	C	172	THR
1	D	8	VAL
1	D	19	VAL
1	D	34	VAL
1	D	46	LEU
1	D	52	LYS
1	D	54	ARG
1	D	55	GLN
1	D	95	GLN
1	D	154	VAL
1	D	170	LEU
1	D	171	LEU
1	E	8	VAL
1	E	34	VAL
1	E	46	LEU
1	E	54	ARG
1	E	55	GLN
1	E	130	ARG
1	E	166	LEU
1	E	169	ARG
1	E	173	GLN

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Mol	Chain	Res	Type
1	F	2	LYS
1	F	3	THR
1	F	14	LYS
1	F	34	VAL
1	F	46	LEU
1	F	54	ARG
1	F	69	LEU
1	F	95	GLN
1	F	145	ILE
1	F	163	ASN
1	F	166	LEU
1	F	168	GLU
1	F	174	GLN
1	G	2	LYS
1	G	8	VAL
1	G	15	LEU
1	G	19	VAL
1	G	34	VAL
1	G	46	LEU
1	G	54	ARG
1	G	55	GLN
1	G	147	ARG
1	G	161	GLU
1	G	166	LEU
1	H	8	VAL
1	H	19	VAL
1	H	34	VAL
1	H	46	LEU
1	H	54	ARG
1	H	55	GLN
1	H	90	GLU
1	H	145	ILE
1	H	160	ASP
1	H	161	GLU
1	H	166	LEU
1	H	169	ARG
1	H	174	GLN
1	I	2	LYS
1	I	19	VAL
1	I	34	VAL
1	I	46	LEU
1	I	54	ARG

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Mol	Chain	Res	Type
1	I	55	GLN
1	I	163	ASN
1	I	166	LEU
1	I	169	ARG
1	J	8	VAL
1	J	9	GLN
1	J	19	VAL
1	J	46	LEU
1	J	54	ARG
1	J	57	GLN
1	J	69	LEU
1	J	95	GLN
1	J	98	GLN
1	J	107	LEU
1	J	166	LEU
1	K	3	THR
1	K	19	VAL
1	K	34	VAL
1	K	46	LEU
1	K	54	ARG
1	K	55	GLN
1	K	57	GLN
1	K	96	LEU
1	K	145	ILE
1	K	161	GLU
1	K	166	LEU
1	K	173	GLN
1	L	34	VAL
1	L	46	LEU
1	L	54	ARG
1	L	55	GLN
1	L	147	ARG
1	M	2	LYS
1	M	19	VAL
1	M	34	VAL
1	M	46	LEU
1	M	54	ARG
1	M	55	GLN
1	M	87	ARG
1	M	95	GLN
1	M	98	GLN
1	M	135	GLU

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Mol	Chain	Res	Type
1	M	166	LEU
1	N	2	LYS
1	N	19	VAL
1	N	34	VAL
1	N	46	LEU
1	N	54	ARG
1	N	95	GLN
1	N	96	LEU
1	N	135	GLU
1	N	166	LEU
1	N	169	ARG
1	N	170	LEU
1	N	173	GLN
1	O	19	VAL
1	O	34	VAL
1	O	46	LEU
1	O	54	ARG
1	O	55	GLN
1	O	95	GLN
1	O	130	ARG
1	O	166	LEU
1	O	173	GLN
1	P	34	VAL
1	P	46	LEU
1	P	54	ARG
1	P	87	ARG
1	P	130	ARG
1	P	160	ASP
1	P	166	LEU
1	P	174	GLN
1	Q	3	THR
1	Q	8	VAL
1	Q	19	VAL
1	Q	34	VAL
1	Q	46	LEU
1	Q	51	LEU
1	Q	54	ARG
1	Q	55	GLN
1	Q	87	ARG
1	Q	166	LEU
1	Q	169	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such

sidechains are listed below:

Mol	Chain	Res	Type
1	R	6	HIS
1	R	9	GLN
1	R	56	GLN
1	R	57	GLN
1	R	92	ASN
1	R	103	ASN
1	A	6	HIS
1	A	56	GLN
1	A	103	ASN
1	B	56	GLN
1	B	57	GLN
1	B	103	ASN
1	B	173	GLN
1	C	9	GLN
1	C	92	ASN
1	C	103	ASN
1	C	163	ASN
1	C	174	GLN
1	D	6	HIS
1	D	92	ASN
1	D	95	GLN
1	D	98	GLN
1	D	103	ASN
1	D	148	HIS
1	D	165	HIS
1	E	6	HIS
1	E	92	ASN
1	E	103	ASN
1	F	92	ASN
1	F	95	GLN
1	F	103	ASN
1	F	174	GLN
1	G	9	GLN
1	G	103	ASN
1	H	6	HIS
1	H	9	GLN
1	H	57	GLN
1	H	92	ASN
1	H	103	ASN
1	H	163	ASN
1	H	174	GLN
1	I	6	HIS

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Mol	Chain	Res	Type
1	I	57	GLN
1	I	103	ASN
1	I	163	ASN
1	J	95	GLN
1	J	98	GLN
1	J	103	ASN
1	J	163	ASN
1	J	174	GLN
1	K	6	HIS
1	K	57	GLN
1	K	91	GLN
1	K	95	GLN
1	K	103	ASN
1	K	174	GLN
1	L	6	HIS
1	L	56	GLN
1	L	57	GLN
1	L	92	ASN
1	L	103	ASN
1	L	174	GLN
1	M	6	HIS
1	M	9	GLN
1	M	39	HIS
1	M	57	GLN
1	M	92	ASN
1	M	103	ASN
1	M	174	GLN
1	N	103	ASN
1	N	173	GLN
1	O	98	GLN
1	O	103	ASN
1	P	39	HIS
1	P	92	ASN
1	P	98	GLN
1	P	103	ASN
1	P	163	ASN
1	P	174	GLN
1	Q	56	GLN
1	Q	92	ASN
1	Q	103	ASN
1	Q	173	GLN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

39 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	APR	A	201	-	34,39,39	1.18	4 (11%)	36,60,60	1.72	3 (8%)
3	SO4	A	202	-	4,4,4	0.58	0	6,6,6	0.48	0
2	APR	B	201	-	34,39,39	1.17	3 (8%)	36,60,60	1.64	7 (19%)
3	SO4	B	202	-	4,4,4	0.54	0	6,6,6	0.40	0
2	APR	C	201	-	34,39,39	0.91	1 (2%)	36,60,60	1.84	7 (19%)
3	SO4	C	202	-	4,4,4	0.62	0	6,6,6	1.03	0
4	ACT	C	203	-	1,3,3	2.59	1 (100%)	0,3,3	0.00	-
2	APR	D	201	-	34,39,39	1.49	4 (11%)	36,60,60	2.22	9 (25%)
3	SO4	D	202	-	4,4,4	0.44	0	6,6,6	0.53	0
2	APR	E	201	-	34,39,39	0.97	3 (8%)	36,60,60	2.20	9 (25%)
3	SO4	E	202	-	4,4,4	0.37	0	6,6,6	0.68	0
5	ZOD	F	201	-	36,42,42	1.46	8 (22%)	38,64,64	2.24	9 (23%)
3	SO4	F	202	-	4,4,4	0.58	0	6,6,6	0.35	0
2	APR	G	201	-	34,39,39	1.21	3 (8%)	36,60,60	2.01	8 (22%)
3	SO4	G	202	-	4,4,4	0.72	0	6,6,6	0.65	0
2	APR	H	201	-	34,39,39	1.20	4 (11%)	36,60,60	1.98	8 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	H	202	-	4,4,4	0.35	0	6,6,6	0.94	0
2	APR	I	201	-	34,39,39	1.23	4 (11%)	36,60,60	1.73	3 (8%)
3	SO4	I	202	-	4,4,4	0.50	0	6,6,6	0.55	0
2	APR	J	201	-	34,39,39	1.04	2 (5%)	36,60,60	2.13	8 (22%)
3	SO4	J	202	-	4,4,4	0.54	0	6,6,6	0.69	0
4	ACT	J	203	-	1,3,3	3.31	1 (100%)	0,3,3	0.00	-
2	APR	K	201	-	34,39,39	1.25	4 (11%)	36,60,60	2.31	7 (19%)
3	SO4	K	202	-	4,4,4	0.45	0	6,6,6	0.41	0
2	APR	L	201	-	34,39,39	1.31	4 (11%)	36,60,60	2.48	9 (25%)
3	SO4	L	202	-	4,4,4	0.67	0	6,6,6	0.57	0
5	ZOD	M	201	-	36,42,42	1.35	5 (13%)	38,64,64	1.97	8 (21%)
3	SO4	M	202	-	4,4,4	0.52	0	6,6,6	0.42	0
2	APR	N	201	-	34,39,39	1.18	4 (11%)	36,60,60	1.70	8 (22%)
3	SO4	N	202	-	4,4,4	0.43	0	6,6,6	0.95	0
2	APR	O	201	-	34,39,39	0.98	1 (2%)	36,60,60	1.51	3 (8%)
3	SO4	O	202	-	4,4,4	0.63	0	6,6,6	0.94	0
2	APR	P	201	-	34,39,39	1.20	3 (8%)	36,60,60	1.88	7 (19%)
3	SO4	P	202	-	4,4,4	0.50	0	6,6,6	0.32	0
4	ACT	Q	401	-	1,3,3	1.54	0	0,3,3	0.00	-
2	APR	Q	402	-	34,39,39	1.19	3 (8%)	36,60,60	1.82	7 (19%)
3	SO4	Q	403	-	4,4,4	0.37	0	6,6,6	0.75	0
2	APR	R	201	-	34,39,39	1.03	2 (5%)	36,60,60	2.07	8 (22%)
3	SO4	R	202	-	4,4,4	0.34	0	6,6,6	0.78	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
2	APR	A	201	-	-	0/18/54/54	0/4/4/4
3	SO4	A	202	-	-	0/0/0/0	0/0/0/0
2	APR	B	201	-	-	0/18/54/54	0/4/4/4
3	SO4	B	202	-	-	0/0/0/0	0/0/0/0
2	APR	C	201	-	-	0/18/54/54	0/4/4/4
3	SO4	C	202	-	-	0/0/0/0	0/0/0/0
4	ACT	C	203	-	-	0/0/0/0	0/0/0/0
2	APR	D	201	-	-	0/18/54/54	0/4/4/4
3	SO4	D	202	-	-	0/0/0/0	0/0/0/0
2	APR	E	201	-	-	0/18/54/54	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	E	202	-	-	0/0/0/0	0/0/0/0
5	ZOD	F	201	-	-	0/22/58/58	0/4/4/4
3	SO4	F	202	-	-	0/0/0/0	0/0/0/0
2	APR	G	201	-	-	0/18/54/54	0/4/4/4
3	SO4	G	202	-	-	0/0/0/0	0/0/0/0
2	APR	H	201	-	-	0/18/54/54	0/4/4/4
3	SO4	H	202	-	-	0/0/0/0	0/0/0/0
2	APR	I	201	-	-	0/18/54/54	0/4/4/4
3	SO4	I	202	-	-	0/0/0/0	0/0/0/0
2	APR	J	201	-	-	0/18/54/54	0/4/4/4
3	SO4	J	202	-	-	0/0/0/0	0/0/0/0
4	ACT	J	203	-	-	0/0/0/0	0/0/0/0
2	APR	K	201	-	-	0/18/54/54	0/4/4/4
3	SO4	K	202	-	-	0/0/0/0	0/0/0/0
2	APR	L	201	-	-	0/18/54/54	0/4/4/4
3	SO4	L	202	-	-	0/0/0/0	0/0/0/0
5	ZOD	M	201	-	-	0/22/58/58	0/4/4/4
3	SO4	M	202	-	-	0/0/0/0	0/0/0/0
2	APR	N	201	-	-	0/18/54/54	0/4/4/4
3	SO4	N	202	-	-	0/0/0/0	0/0/0/0
2	APR	O	201	-	-	0/18/54/54	0/4/4/4
3	SO4	O	202	-	-	0/0/0/0	0/0/0/0
2	APR	P	201	-	-	0/18/54/54	0/4/4/4
3	SO4	P	202	-	-	0/0/0/0	0/0/0/0
4	ACT	Q	401	-	-	0/0/0/0	0/0/0/0
2	APR	Q	402	-	-	0/18/54/54	0/4/4/4
3	SO4	Q	403	-	-	0/0/0/0	0/0/0/0
2	APR	R	201	-	-	0/18/54/54	0/4/4/4
3	SO4	R	202	-	-	0/0/0/0	0/0/0/0

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	402	APR	C1D-C2D	-3.69	1.48	1.52
2	H	201	APR	C2'-C1'	-3.41	1.48	1.53
2	E	201	APR	C2'-C1'	-2.89	1.49	1.53
5	F	201	ZOD	C2'-C1'	-2.71	1.49	1.53
2	R	201	APR	C2'-C1'	-2.68	1.49	1.53
2	L	201	APR	C2'-C1'	-2.66	1.49	1.53
5	M	201	ZOD	O04-C05	-2.46	1.41	1.44
2	E	201	APR	O4'-C4'	-2.45	1.39	1.45
2	B	201	APR	C2'-C1'	-2.42	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	201	APR	C1D-C2D	-2.31	1.50	1.52
2	D	201	APR	C5-N7	-2.28	1.31	1.39
2	N	201	APR	O4'-C4'	-2.08	1.40	1.45
5	F	201	ZOD	C38-C05	-2.05	1.48	1.53
5	F	201	ZOD	O04-C05	-2.05	1.41	1.44
2	H	201	APR	C5-N7	-2.01	1.32	1.39
2	G	201	APR	C1D-C2D	2.02	1.55	1.52
2	Q	402	APR	O4D-C1D	2.07	1.45	1.43
5	F	201	ZOD	C4-N3	2.08	1.38	1.35
2	K	201	APR	C8-N7	2.09	1.38	1.34
2	L	201	APR	C2-N3	2.10	1.35	1.32
2	K	201	APR	C2-N3	2.14	1.35	1.32
2	A	201	APR	C2-N3	2.14	1.35	1.32
2	P	201	APR	C8-N7	2.18	1.38	1.34
2	N	201	APR	O4'-C1'	2.22	1.44	1.41
2	A	201	APR	C8-N7	2.22	1.38	1.34
2	R	201	APR	C5-C4	2.25	1.45	1.40
2	B	201	APR	O4D-C1D	2.25	1.46	1.43
2	D	201	APR	C5-C4	2.26	1.45	1.40
2	H	201	APR	C2-N3	2.27	1.36	1.32
5	M	201	ZOD	C4-N3	2.32	1.39	1.35
2	N	201	APR	C2-N3	2.33	1.36	1.32
2	I	201	APR	O4'-C1'	2.36	1.44	1.41
2	G	201	APR	O4'-C1'	2.37	1.44	1.41
5	M	201	ZOD	O4'-C1'	2.37	1.44	1.41
2	I	201	APR	O4D-C1D	2.44	1.46	1.43
2	C	201	APR	C5-C4	2.47	1.46	1.40
2	E	201	APR	C5-C4	2.56	1.46	1.40
4	C	203	ACT	CH3-C	2.59	1.52	1.48
2	I	201	APR	C5-C4	2.63	1.46	1.40
5	F	201	ZOD	O4'-C1'	2.64	1.44	1.41
2	H	201	APR	C5-C4	2.65	1.46	1.40
2	A	201	APR	O4'-C1'	2.65	1.44	1.41
2	Q	402	APR	C5-C4	2.67	1.46	1.40
2	G	201	APR	C5-C4	2.74	1.46	1.40
5	F	201	ZOD	C6-N6	2.77	1.45	1.34
2	J	201	APR	C5-C4	2.85	1.46	1.40
2	L	201	APR	O4'-C1'	2.96	1.45	1.41
2	P	201	APR	C2-N3	3.00	1.37	1.32
2	I	201	APR	C2-N3	3.12	1.37	1.32
2	O	201	APR	C5-C4	3.12	1.47	1.40
5	F	201	ZOD	O08-C06	3.16	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	201	APR	C5-C4	3.16	1.47	1.40
5	M	201	ZOD	C2-N3	3.17	1.37	1.32
5	M	201	ZOD	C6-N6	3.24	1.47	1.34
4	J	203	ACT	CH3-C	3.31	1.53	1.48
2	K	201	APR	C5-C4	3.55	1.48	1.40
2	L	201	APR	C5-C4	3.57	1.48	1.40
2	P	201	APR	C5-C4	3.62	1.48	1.40
5	F	201	ZOD	C2-N3	3.63	1.38	1.32
2	B	201	APR	C5-C4	3.67	1.48	1.40
2	A	201	APR	C5-C4	3.82	1.49	1.40
2	K	201	APR	O4'-C1'	3.90	1.46	1.41
2	D	201	APR	O4D-C1D	4.03	1.48	1.43
2	D	201	APR	O4'-C1'	5.12	1.48	1.41

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	201	APR	N3-C2-N1	-8.59	121.37	128.86
2	J	201	APR	N3-C2-N1	-7.77	122.09	128.86
2	K	201	APR	C4'-O4'-C1'	-7.73	101.54	109.77
5	F	201	ZOD	N3-C2-N1	-7.53	122.30	128.86
2	L	201	APR	N3-C2-N1	-7.16	122.62	128.86
2	L	201	APR	C4'-O4'-C1'	-7.10	102.21	109.77
2	C	201	APR	N3-C2-N1	-6.94	122.82	128.86
2	H	201	APR	N3-C2-N1	-6.93	122.83	128.86
2	E	201	APR	C1'-N9-C4	-6.74	115.00	126.64
2	G	201	APR	N3-C2-N1	-6.65	123.06	128.86
2	D	201	APR	N3-C2-N1	-6.29	123.38	128.86
5	F	201	ZOD	C4'-O4'-C1'	-6.29	103.08	109.77
5	M	201	ZOD	N3-C2-N1	-6.21	123.45	128.86
2	A	201	APR	N3-C2-N1	-6.18	123.48	128.86
2	E	201	APR	N3-C2-N1	-6.10	123.54	128.86
2	I	201	APR	N3-C2-N1	-5.85	123.76	128.86
2	O	201	APR	N3-C2-N1	-5.72	123.88	128.86
2	K	201	APR	C1'-N9-C4	-5.62	116.92	126.64
2	I	201	APR	C4-C5-N7	-5.50	104.10	109.41
2	P	201	APR	N3-C2-N1	-5.49	124.07	128.86
5	M	201	ZOD	C4'-O4'-C1'	-5.40	104.02	109.77
2	Q	402	APR	N3-C2-N1	-5.36	124.19	128.86
2	Q	402	APR	C4'-O4'-C1'	-5.36	104.06	109.77
2	N	201	APR	N3-C2-N1	-5.30	124.24	128.86
2	K	201	APR	N3-C2-N1	-5.27	124.27	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	APR	O2'-C2'-C3'	-4.90	96.12	111.83
5	F	201	ZOD	O04-C02-O03	-4.87	113.08	122.94
2	A	201	APR	O3'-C3'-C4'	-4.65	97.51	111.09
2	L	201	APR	C1'-N9-C4	-4.61	118.67	126.64
2	G	201	APR	C4'-O4'-C1'	-4.58	104.89	109.77
2	P	201	APR	C4-C5-N7	-4.43	105.13	109.41
2	J	201	APR	C1'-N9-C4	-4.36	119.10	126.64
2	G	201	APR	C1'-N9-C4	-4.33	119.16	126.64
2	J	201	APR	O1D-C1D-O4D	-4.20	105.50	111.14
5	M	201	ZOD	C1'-N9-C4	-4.20	119.39	126.64
2	H	201	APR	C1'-N9-C4	-4.14	119.49	126.64
2	B	201	APR	C1'-N9-C4	-4.13	119.49	126.64
2	E	201	APR	O3'-C3'-C2'	-4.07	98.79	111.83
2	R	201	APR	C1'-N9-C4	-4.06	119.61	126.64
2	H	201	APR	O3'-C3'-C2'	-4.03	98.93	111.83
2	I	201	APR	C1'-N9-C4	-4.00	119.72	126.64
2	D	201	APR	O3'-C3'-C2'	-3.92	99.27	111.83
2	B	201	APR	N3-C2-N1	-3.91	125.45	128.86
2	L	201	APR	C4-C5-N7	-3.85	105.69	109.41
2	D	201	APR	C4-C5-N7	-3.83	105.71	109.41
2	J	201	APR	C4'-O4'-C1'	-3.67	105.86	109.77
2	E	201	APR	C4-C5-N7	-3.64	105.89	109.41
2	N	201	APR	O1D-C1D-O4D	-3.58	106.33	111.14
2	O	201	APR	C1'-N9-C4	-3.54	120.51	126.64
2	R	201	APR	O1D-C1D-O4D	-3.47	106.48	111.14
2	Q	402	APR	C1'-N9-C4	-3.46	120.66	126.64
5	M	201	ZOD	O04-C02-O03	-3.32	116.21	122.94
2	L	201	APR	O2D-C2D-C3D	-3.22	101.50	111.83
2	H	201	APR	C4-C5-N7	-3.16	106.35	109.41
2	C	201	APR	O3'-C3'-C4'	-3.13	101.95	111.09
2	D	201	APR	C1'-N9-C4	-3.12	121.25	126.64
2	L	201	APR	O3D-C3D-C4D	-3.12	101.98	111.09
2	K	201	APR	C4-C5-N7	-3.11	106.41	109.41
2	P	201	APR	O3'-C3'-C4'	-3.11	102.01	111.09
2	N	201	APR	C4'-O4'-C1'	-3.09	106.48	109.77
2	C	201	APR	C1'-N9-C4	-3.03	121.41	126.64
2	H	201	APR	O2'-C2'-C3'	-3.00	102.21	111.83
2	B	201	APR	O2'-C2'-C3'	-2.86	102.67	111.83
2	G	201	APR	O3D-C3D-C4D	-2.77	102.99	111.09
2	A	201	APR	C1'-N9-C4	-2.67	122.02	126.64
2	N	201	APR	C1'-N9-C4	-2.65	122.05	126.64
2	D	201	APR	O3'-C3'-C4'	-2.65	103.35	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	201	APR	C4'-O4'-C1'	-2.61	107.00	109.77
2	R	201	APR	C5D-C4D-C3D	-2.61	105.36	115.29
2	N	201	APR	C4-C5-N7	-2.59	106.91	109.41
2	B	201	APR	C4-C5-N7	-2.58	106.91	109.41
5	M	201	ZOD	C5'-C4'-C3'	-2.58	105.46	115.29
2	N	201	APR	C5'-C4'-C3'	-2.54	105.59	115.29
2	E	201	APR	O5'-PA-O1A	-2.51	99.11	109.25
2	N	201	APR	O3'-C3'-C4'	-2.45	103.94	111.09
2	B	201	APR	O3'-C3'-C4'	-2.42	104.03	111.09
2	E	201	APR	O1D-C1D-O4D	-2.39	107.92	111.14
5	F	201	ZOD	O1B-C10-C09	-2.39	100.53	109.00
2	J	201	APR	O3D-C3D-C4D	-2.35	104.21	111.09
2	C	201	APR	C4-C5-N7	-2.31	107.18	109.41
2	R	201	APR	C4-C5-N7	-2.31	107.18	109.41
5	F	201	ZOD	C10-C09-C38	-2.30	106.50	115.29
2	P	201	APR	C1'-N9-C4	-2.29	122.68	126.64
2	K	201	APR	O3D-C3D-C4D	-2.29	104.41	111.09
2	E	201	APR	O2'-C2'-C3'	-2.27	104.56	111.83
5	F	201	ZOD	C05-O04-C02	-2.22	114.24	117.72
2	C	201	APR	O3D-C3D-C2D	-2.18	104.86	111.83
5	M	201	ZOD	C4-C5-N7	-2.16	107.33	109.41
2	Q	402	APR	O5D-C5D-C4D	-2.15	101.39	109.00
2	C	201	APR	C1D-C2D-C3D	-2.12	99.61	102.30
2	L	201	APR	O2'-C2'-C1'	-2.10	105.04	111.61
5	F	201	ZOD	C4-C5-N7	-2.10	107.38	109.41
2	H	201	APR	O2'-C2'-C1'	-2.10	105.05	111.61
2	J	201	APR	C4-C5-N7	-2.08	107.40	109.41
2	H	201	APR	O3D-C3D-C4D	-2.07	105.03	111.09
2	P	201	APR	O2D-C2D-C3D	-2.06	105.22	111.83
2	R	201	APR	O2'-C2'-C1'	-2.02	105.31	111.61
2	Q	402	APR	C4-C5-N7	-2.01	107.47	109.41
2	O	201	APR	C4-C5-N7	-2.00	107.47	109.41
2	G	201	APR	C2-N1-C6	2.03	122.33	118.77
2	G	201	APR	N6-C6-N1	2.03	122.80	118.77
2	G	201	APR	O4D-C1D-C2D	2.03	107.03	104.46
2	P	201	APR	O3'-C3'-C2'	2.04	118.35	111.83
5	M	201	ZOD	C2'-C3'-C4'	2.06	106.63	102.62
2	D	201	APR	C5-C6-N6	2.07	124.69	120.47
5	F	201	ZOD	O07-C06-O08	2.08	113.93	111.14
2	K	201	APR	C2'-C3'-C4'	2.13	106.76	102.62
2	B	201	APR	C2-N1-C6	2.13	122.50	118.77
2	Q	402	APR	O2B-PB-O1B	2.23	123.85	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	201	APR	C2'-C3'-C4'	2.40	107.29	102.62
2	Q	402	APR	O1D-C1D-O4D	2.52	114.52	111.14
2	E	201	APR	C2-N1-C6	2.52	123.19	118.77
2	G	201	APR	C2D-C3D-C4D	2.60	107.68	102.62
2	L	201	APR	C2-N1-C6	2.92	123.88	118.77
2	J	201	APR	C2-N1-C6	2.93	123.90	118.77
2	J	201	APR	C2D-C3D-C4D	2.94	108.34	102.62
2	B	201	APR	O4D-C1D-C2D	3.03	108.28	104.46
2	R	201	APR	C2-N1-C6	3.03	124.08	118.77
5	M	201	ZOD	O04-C05-C06	3.19	117.83	108.52
2	D	201	APR	C2'-C3'-C4'	3.31	109.07	102.62
2	E	201	APR	C2'-C3'-C4'	3.42	109.27	102.62
2	H	201	APR	C2'-C3'-C4'	3.45	109.33	102.62
2	C	201	APR	C2'-C3'-C4'	3.53	109.48	102.62
2	P	201	APR	C1D-C2D-C3D	3.68	106.96	102.30
5	F	201	ZOD	O04-C02-C01	3.78	118.19	111.10
2	L	201	APR	C1D-C2D-C3D	4.19	107.61	102.30
2	D	201	APR	O1D-C1D-O4D	4.22	116.80	111.14
2	K	201	APR	C1D-C2D-C3D	4.32	107.78	102.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

31 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	APR	1	0
3	A	202	SO4	1	0
2	B	201	APR	2	0
3	B	202	SO4	1	0
2	C	201	APR	2	0
3	C	202	SO4	2	0
2	D	201	APR	4	0
3	D	202	SO4	3	0
2	E	201	APR	1	0
3	E	202	SO4	1	0
5	F	201	ZOD	4	0
2	G	201	APR	1	0
2	H	201	APR	2	0
3	H	202	SO4	1	0
2	J	201	APR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	202	SO4	3	0
2	K	201	APR	4	0
3	K	202	SO4	2	0
2	L	201	APR	4	0
3	L	202	SO4	1	0
5	M	201	ZOD	6	0
3	M	202	SO4	3	0
2	N	201	APR	1	0
2	O	201	APR	3	0
3	O	202	SO4	3	0
2	P	201	APR	3	0
3	P	202	SO4	1	0
2	Q	402	APR	3	0
3	Q	403	SO4	3	0
2	R	201	APR	1	0
3	R	202	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	173/183 (94%)	0.11	0 100 100	25, 42, 64, 74	0
1	B	172/183 (93%)	-0.01	0 100 100	19, 34, 53, 71	0
1	C	173/183 (94%)	-0.00	0 100 100	14, 33, 57, 69	0
1	D	170/183 (92%)	0.14	0 100 100	23, 45, 64, 71	0
1	E	173/183 (94%)	-0.01	0 100 100	15, 29, 53, 68	0
1	F	173/183 (94%)	0.22	1 (0%) 89 86	29, 46, 66, 76	0
1	G	173/183 (94%)	0.09	1 (0%) 89 86	21, 39, 65, 73	0
1	H	173/183 (94%)	-0.02	0 100 100	15, 29, 54, 61	0
1	I	173/183 (94%)	0.15	0 100 100	23, 42, 62, 72	0
1	J	172/183 (93%)	0.04	1 (0%) 89 86	15, 32, 57, 71	0
1	K	172/183 (93%)	0.10	1 (0%) 89 86	23, 42, 68, 82	0
1	L	172/183 (93%)	0.19	0 100 100	26, 45, 65, 77	0
1	M	173/183 (94%)	0.21	1 (0%) 89 86	27, 43, 66, 76	0
1	N	173/183 (94%)	0.11	0 100 100	18, 41, 68, 78	0
1	O	171/183 (93%)	0.07	0 100 100	15, 32, 60, 71	0
1	P	173/183 (94%)	0.14	0 100 100	22, 41, 68, 75	0
1	Q	173/183 (94%)	-0.01	0 100 100	16, 31, 52, 64	0
1	R	173/183 (94%)	-0.03	0 100 100	13, 32, 60, 75	0
All	All	3105/3294 (94%)	0.08	5 (0%) 94 94	13, 38, 64, 82	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	169	ARG	2.3
1	K	32	GLY	2.2
1	F	172	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	163	ASN	2.1
1	M	134	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	D	202	5/5	0.94	0.33	1.51	57,61,62,68	0
3	SO4	M	202	5/5	0.80	0.26	1.42	69,74,80,83	0
3	SO4	F	202	5/5	0.96	0.23	0.76	55,59,62,63	0
3	SO4	P	202	5/5	0.91	0.24	0.37	47,47,52,53	0
5	ZOD	F	201	39/39	0.94	0.20	0.14	38,47,56,59	0
4	ACT	Q	401	4/4	0.92	0.19	-0.04	27,29,29,29	0
3	SO4	E	202	5/5	0.99	0.22	-0.06	25,26,28,29	0
3	SO4	H	202	5/5	0.98	0.20	-0.16	27,28,29,30	0
5	ZOD	M	201	39/39	0.95	0.20	-0.27	33,41,51,51	0
3	SO4	K	202	5/5	0.92	0.21	-0.32	66,68,71,74	0
2	APR	Q	402	36/36	0.97	0.17	-0.41	20,24,27,29	0
3	SO4	I	202	5/5	0.97	0.19	-0.43	46,50,56,58	0
4	ACT	C	203	4/4	0.94	0.17	-0.56	37,39,41,44	0
2	APR	B	201	36/36	0.97	0.17	-0.72	21,24,26,34	0
2	APR	N	201	36/36	0.96	0.17	-0.74	24,26,29,29	0
2	APR	J	201	36/36	0.97	0.16	-0.75	23,25,28,32	0
2	APR	R	201	36/36	0.97	0.16	-0.81	21,24,26,26	0
2	APR	P	201	36/36	0.96	0.17	-0.84	24,26,29,32	0
3	SO4	B	202	5/5	0.98	0.19	-0.88	31,32,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	APR	I	201	36/36	0.97	0.17	-0.89	23,24,26,30	0
2	APR	K	201	36/36	0.97	0.16	-0.90	23,26,28,31	0
2	APR	O	201	36/36	0.97	0.15	-0.91	21,24,27,28	0
2	APR	D	201	36/36	0.97	0.17	-1.01	23,24,28,29	0
2	APR	H	201	36/36	0.97	0.15	-1.02	22,24,27,28	0
2	APR	G	201	36/36	0.97	0.16	-1.10	24,27,29,32	0
3	SO4	Q	403	5/5	0.97	0.19	-1.25	31,32,34,37	0
2	APR	C	201	36/36	0.97	0.15	-1.29	20,24,26,32	0
2	APR	A	201	36/36	0.98	0.15	-1.32	22,25,28,28	0
2	APR	L	201	36/36	0.97	0.14	-1.54	25,28,32,34	0
2	APR	E	201	36/36	0.97	0.15	-1.58	19,21,25,32	0
3	SO4	G	202	5/5	0.98	0.19	-1.60	30,34,35,36	0
3	SO4	C	202	5/5	0.96	0.18	-1.67	25,28,30,30	0
3	SO4	J	202	5/5	0.98	0.16	-1.79	33,35,35,35	0
3	SO4	O	202	5/5	0.98	0.15	-1.79	30,31,33,34	0
4	ACT	J	203	4/4	0.96	0.14	-1.89	33,34,34,37	0
3	SO4	N	202	5/5	0.98	0.16	-1.95	27,31,33,36	0
3	SO4	R	202	5/5	0.98	0.16	-2.41	25,26,30,33	0
3	SO4	L	202	5/5	0.99	0.17	-2.44	31,32,34,36	0
3	SO4	A	202	5/5	0.98	0.14	-4.89	47,50,56,62	0

## 6.5 Other polymers

There are no such residues in this entry.