



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:20 PM GMT

PDB ID : 4XDS  
Title : Deoxyguanosinetriphosphate Triphosphohydrolase from Escherichia coli with Nickel  
Authors : Singh, D.; Gawel, D.; Itsko, M.; Krahn, J.M.; London, R.E.; Schaaper, R.M.  
Deposited on : 2014-12-19  
Resolution : 3.35 Å(reported)

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<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
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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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

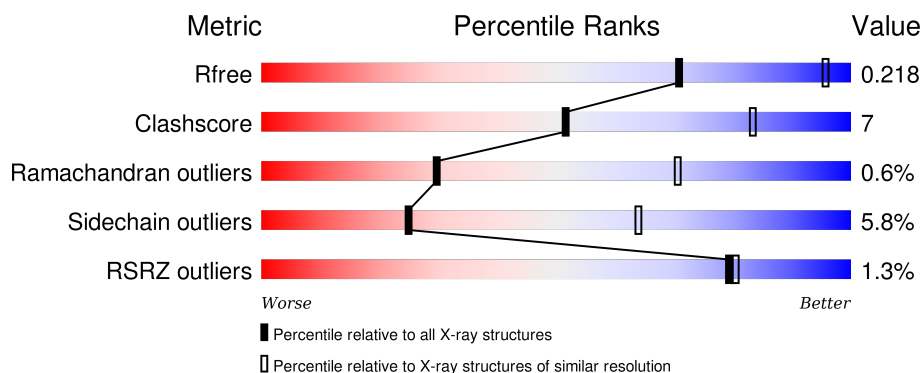
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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))
$R_{free}$	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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	505	<div> <div>3%</div> <div>78% 18% ..</div> </div>
1	B	505	<div> <div>2%</div> <div>81% 16% ..</div> </div>
1	C	505	<div> <div>%</div> <div>79% 19% .</div> </div>
1	D	505	<div> <div></div> <div>76% 20% ..</div> </div>
1	E	505	<div> <div>%</div> <div>76% 21% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	505	

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	A	602	-	-	-	X
3	SO4	B	607	-	-	-	X
3	SO4	C	606	-	-	-	X
3	SO4	D	607	-	-	-	X
3	SO4	E	605	-	-	-	X
3	SO4	F	603	-	-	-	X
3	SO4	F	609	-	-	-	X
3	SO4	F	610	-	-	-	X
3	SO4	F	612	-	-	-	X
3	SO4	F	615	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24538 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 Deoxyguanosinetriphosphate triphosphohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3952	2533	692	712	15			
1	B	494	Total	C	N	O	S	0	0	0
			3981	2554	698	713	16			
1	C	503	Total	C	N	O	S	0	0	0
			4062	2598	720	727	17			
1	D	494	Total	C	N	O	S	0	0	0
			4010	2571	704	719	16			
1	E	503	Total	C	N	O	S	0	0	0
			4086	2614	720	736	16			
1	F	494	Total	C	N	O	S	0	0	0
			4028	2582	713	717	16			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Ni	0	0
			1	1		
2	E	1	Total	Ni	0	0
			1	1		
2	B	1	Total	Ni	0	0
			1	1		
2	C	1	Total	Ni	0	0
			1	1		
2	A	1	Total	Ni	0	0
			1	1		
2	F	1	Total	Ni	0	0
			1	1		

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



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

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

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

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

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

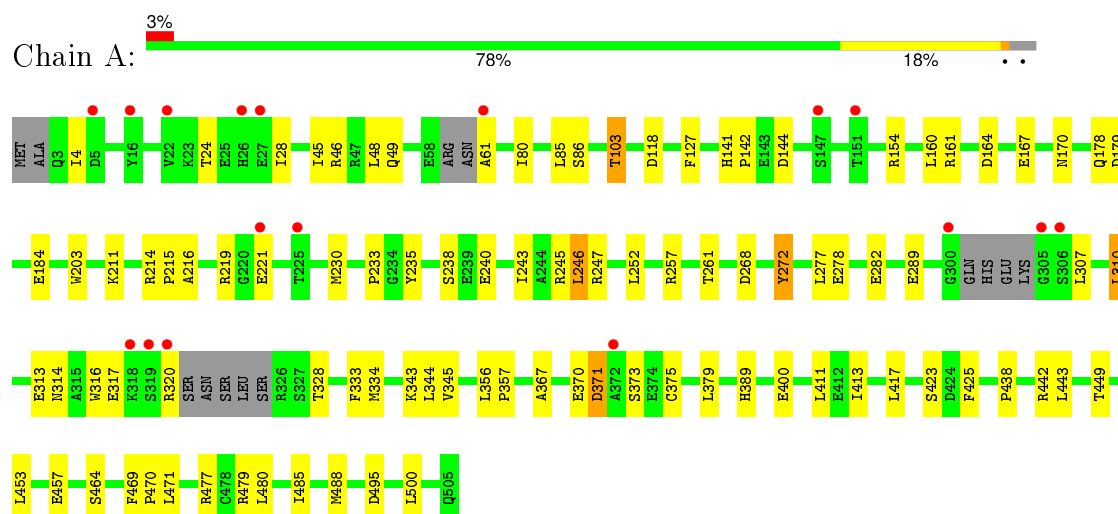
- Molecule 4 is water.

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

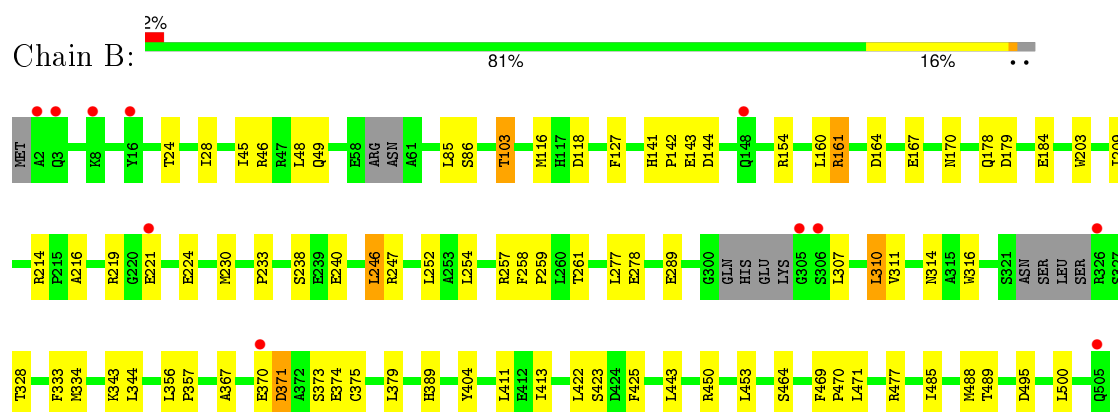
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

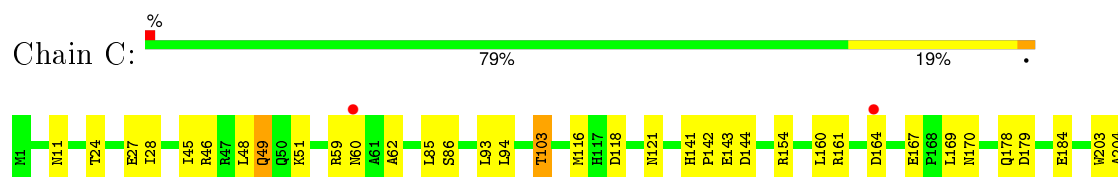
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase



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L381	C273	R163	E400	K283	H170	F425	E184	L410	V288	K175	D424	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
V385	V274	D164	E400	E278	N170	F425	E184	L410	E289	K175	D424	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
H389	E278	D164	E400	E278	N170	F425	E184	L410	E289	K175	D424	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
R389	E278	D164	E400	E278	N170	F425	E184	L410	E289	K175	D424	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
E400	K283	D164	E400	K283	H170	F425	E184	L410	V288	K175	D424	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
L410	V288	D164	E400	V288	H170	F425	E184	L410	V288	K175	D424	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
I413	H294	D164	E400	H294	L295	F425	E184	L410	H294	L295	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
S423	L295	D164	E400	L295	L295	F425	E184	L410	L295	L295	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
D424	W299	D164	E400	W299	W299	F425	E184	L410	W299	W299	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
F425	G300	D164	E400	G300	G300	F425	E184	L410	G300	G300	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
R431	GLN	D164	E400	GLN	GLN	F425	E184	L410	GLN	GLN	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
V434	HIS	D164	E400	HIS	HIS	F425	E184	L410	HIS	HIS	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
F437	GLU	D164	E400	GLU	GLU	F425	E184	L410	GLU	GLU	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
P438	LYS	D164	E400	LYS	LYS	F425	E184	L410	LYS	LYS	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
I439	GLY	D164	E400	GLY	GLY	F425	E184	L410	GLY	GLY	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
E440	S306	D164	E400	S306	S306	F425	E184	L410	S306	S306	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
S441	L307	D164	E400	L307	L307	F425	E184	L410	L307	L307	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
R450	L310	D164	E400	L310	L310	F425	E184	L410	L310	L310	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
H451	N314	D164	E400	N314	N314	F425	E184	L410	N314	N314	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
R452	A315	D164	E400	A315	A315	F425	E184	L410	A315	A315	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
L453	W316	D164	E400	W316	W316	F425	E184	L410	W316	W316	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
V456	S321	D164	E400	S321	S321	F425	E184	L410	S321	S321	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
S464	ASN	D164	E400	ASN	ASN	F425	E184	L410	ASN	ASN	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
L471	SER	D164	E400	SER	SER	F425	E184	L410	SER	SER	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
R477	LEU	D164	E400	LEU	LEU	F425	E184	L410	LEU	LEU	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
C478	S325	D164	E400	S325	S325	F425	E184	L410	S325	S325	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
R479	R326	D164	E400	R326	R326	F425	E184	L410	R326	R326	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
I485	S327	D164	E400	S327	S327	F425	E184	L410	S327	S327	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
W488	T328	D164	E400	T328	T328	F425	E184	L410	T328	T328	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
D495	E329	D164	E400	E329	E329	F425	E184	L410	E329	E329	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
L500	D330	D164	E400	D330	D330	F425	E184	L410	D330	D330	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
M501	F333	D164	E400	F333	F333	F425	E184	L410	F333	F333	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
Q505	M334	D164	E400	M334	M334	F425	E184	L410	M334	M334	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248	E249	L254	R257	F258	P259	L260	T261	I270	S271	Y272
	K343	D164	E400	K343	K343	F425	E184	L410	K343	K343	D178	L196	E166	E167	W203	A204	I209	R214	P215	A216	R219	W230	P233	G234	Y235	S238	E239	E240	I243	A244	R245	L246	R247	K248										

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.80Å 189.80Å 296.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.35 20.02 – 3.35	Depositor EDS
% Data completeness (in resolution range)	85.2 (19.99-3.35) 97.5 (20.02-3.35)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 3.36Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.172 , 0.209 0.185 , 0.218	Depositor DCC
$R_{free}$ test set	3888 reflections (5.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.4	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 39.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	1 of 75820 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24538	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: NI, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.44	0/4051	0.55	0/5499
1	B	0.47	0/4079	0.57	0/5529
1	C	0.55	0/4162	0.62	0/5642
1	D	0.56	0/4109	0.63	0/5568
1	E	0.56	1/4187 (0.0%)	0.62	1/5673 (0.0%)
1	F	0.57	0/4127	0.64	0/5587
All	All	0.53	1/24715 (0.0%)	0.61	1/33498 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	478	CYS	CB-SG	-6.08	1.72	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	324	LEU	CA-CB-CG	5.11	127.06	115.30

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	3952	0	3785	51	0
1	B	3981	0	3844	42	0
1	C	4062	0	3946	52	0
1	D	4010	0	3890	62	0
1	E	4086	0	3974	57	0
1	F	4028	0	3938	68	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	50	0	0	3	0
3	B	40	0	0	1	0
3	C	70	0	0	2	0
3	D	65	0	0	2	0
3	E	75	0	0	3	0
3	F	95	0	0	5	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
All	All	24538	0	23377	324	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 7.

The worst 5 of 324 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:247:ARG:NH1	3:F:609:SO4:O3	2.14	0.78
1:C:247:ARG:NH1	3:C:610:SO4:O4	2.17	0.77
1:C:485:ILE:HD13	1:C:488:MET:HE3	1.67	0.76
1:F:485:ILE:HD13	1:F:488:MET:HE3	1.66	0.76
1:A:371:ASP:HB3	1:A:373:SER:H	1.51	0.75

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	484/505 (96%)	457 (94%)	26 (5%)	1 (0%)	52	86
1	B	486/505 (96%)	460 (95%)	24 (5%)	2 (0%)	39	78
1	C	499/505 (99%)	467 (94%)	26 (5%)	6 (1%)	16	56
1	D	486/505 (96%)	459 (94%)	26 (5%)	1 (0%)	52	86
1	E	499/505 (99%)	465 (93%)	27 (5%)	7 (1%)	14	52
1	F	486/505 (96%)	461 (95%)	24 (5%)	1 (0%)	52	86
All	All	2940/3030 (97%)	2769 (94%)	153 (5%)	18 (1%)	30	70

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	301	GLN
1	C	304	LYS
1	E	301	GLN
1	E	304	LYS
1	A	310	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/450 (90%)	382 (95%)	22 (5%)	27	66
1	B	407/450 (90%)	385 (95%)	22 (5%)	27	66
1	C	420/450 (93%)	399 (95%)	21 (5%)	30	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	415/450 (92%)	390 (94%)	25 (6%)	24	62
1	E	425/450 (94%)	394 (93%)	31 (7%)	17	54
1	F	419/450 (93%)	395 (94%)	24 (6%)	25	64
All	All	2490/2700 (92%)	2345 (94%)	145 (6%)	25	64

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	49	GLN
1	D	374	GLU
1	F	328	THR
1	D	103	THR
1	D	238	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	121	ASN
1	D	290	GLN
1	F	290	GLN
1	D	126	HIS
1	D	294	HIS

### 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 ⓘ

Of 85 ligands modelled in this entry, 6 are monoatomic - leaving 79 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	A	602	-	4,4,4	0.20	0	6,6,6	0.20	0
3	SO4	A	603	-	4,4,4	0.23	0	6,6,6	0.17	0
3	SO4	A	604	-	4,4,4	0.18	0	6,6,6	0.17	0
3	SO4	A	605	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	A	606	-	4,4,4	0.19	0	6,6,6	0.15	0
3	SO4	A	607	-	4,4,4	0.20	0	6,6,6	0.12	0
3	SO4	A	608	-	4,4,4	0.17	0	6,6,6	0.10	0
3	SO4	A	609	-	4,4,4	0.28	0	6,6,6	0.16	0
3	SO4	A	610	-	4,4,4	0.19	0	6,6,6	0.07	0
3	SO4	A	611	-	4,4,4	0.17	0	6,6,6	0.30	0
3	SO4	B	602	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	B	603	-	4,4,4	0.19	0	6,6,6	0.15	0
3	SO4	B	604	-	4,4,4	0.22	0	6,6,6	0.31	0
3	SO4	B	605	-	4,4,4	0.19	0	6,6,6	0.17	0
3	SO4	B	606	-	4,4,4	0.26	0	6,6,6	0.15	0
3	SO4	B	607	-	4,4,4	0.16	0	6,6,6	0.27	0
3	SO4	B	608	-	4,4,4	0.17	0	6,6,6	0.15	0
3	SO4	B	609	-	4,4,4	0.22	0	6,6,6	0.17	0
3	SO4	C	602	-	4,4,4	0.16	0	6,6,6	0.14	0
3	SO4	C	603	-	4,4,4	0.23	0	6,6,6	0.15	0
3	SO4	C	604	-	4,4,4	0.14	0	6,6,6	0.21	0
3	SO4	C	605	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	C	606	-	4,4,4	0.16	0	6,6,6	0.11	0
3	SO4	C	607	-	4,4,4	0.55	0	6,6,6	0.25	0
3	SO4	C	608	-	4,4,4	0.12	0	6,6,6	0.19	0
3	SO4	C	609	-	4,4,4	0.23	0	6,6,6	0.27	0
3	SO4	C	610	-	4,4,4	0.27	0	6,6,6	0.38	0
3	SO4	C	611	-	4,4,4	0.16	0	6,6,6	0.21	0
3	SO4	C	612	-	4,4,4	0.18	0	6,6,6	0.25	0
3	SO4	C	613	-	4,4,4	0.12	0	6,6,6	0.13	0
3	SO4	C	614	-	4,4,4	0.20	0	6,6,6	0.20	0
3	SO4	C	615	-	4,4,4	0.23	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	D	601	-	4,4,4	0.24	0	6,6,6	0.25	0
3	SO4	D	603	-	4,4,4	0.21	0	6,6,6	0.12	0
3	SO4	D	604	-	4,4,4	0.16	0	6,6,6	0.33	0
3	SO4	D	605	-	4,4,4	0.22	0	6,6,6	0.18	0
3	SO4	D	606	-	4,4,4	0.28	0	6,6,6	0.29	0
3	SO4	D	607	-	4,4,4	0.17	0	6,6,6	0.30	0
3	SO4	D	608	-	4,4,4	0.17	0	6,6,6	0.20	0
3	SO4	D	609	-	4,4,4	0.12	0	6,6,6	0.20	0
3	SO4	D	610	-	4,4,4	0.18	0	6,6,6	0.20	0
3	SO4	D	611	-	4,4,4	0.19	0	6,6,6	0.28	0
3	SO4	D	612	-	4,4,4	0.20	0	6,6,6	0.19	0
3	SO4	D	613	-	4,4,4	0.10	0	6,6,6	0.20	0
3	SO4	D	614	-	4,4,4	0.30	0	6,6,6	0.31	0
3	SO4	E	602	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	E	603	-	4,4,4	0.22	0	6,6,6	0.14	0
3	SO4	E	604	-	4,4,4	0.14	0	6,6,6	0.17	0
3	SO4	E	605	-	4,4,4	0.27	0	6,6,6	0.12	0
3	SO4	E	606	-	4,4,4	0.18	0	6,6,6	0.19	0
3	SO4	E	607	-	4,4,4	0.18	0	6,6,6	0.15	0
3	SO4	E	608	-	4,4,4	0.38	0	6,6,6	0.17	0
3	SO4	E	609	-	4,4,4	0.24	0	6,6,6	0.17	0
3	SO4	E	610	-	4,4,4	0.21	0	6,6,6	0.11	0
3	SO4	E	611	-	4,4,4	0.13	0	6,6,6	0.29	0
3	SO4	E	612	-	4,4,4	0.22	0	6,6,6	0.19	0
3	SO4	E	613	-	4,4,4	0.19	0	6,6,6	0.14	0
3	SO4	E	614	-	4,4,4	0.12	0	6,6,6	0.10	0
3	SO4	E	615	-	4,4,4	0.18	0	6,6,6	0.21	0
3	SO4	E	616	-	4,4,4	0.21	0	6,6,6	0.40	0
3	SO4	F	601	-	4,4,4	0.56	0	6,6,6	0.20	0
3	SO4	F	603	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	F	604	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	F	605	-	4,4,4	0.13	0	6,6,6	0.22	0
3	SO4	F	606	-	4,4,4	0.19	0	6,6,6	0.25	0
3	SO4	F	607	-	4,4,4	0.11	0	6,6,6	0.19	0
3	SO4	F	608	-	4,4,4	0.18	0	6,6,6	0.20	0
3	SO4	F	609	-	4,4,4	0.30	0	6,6,6	0.27	0
3	SO4	F	610	-	4,4,4	0.16	0	6,6,6	0.17	0
3	SO4	F	611	-	4,4,4	0.14	0	6,6,6	0.21	0
3	SO4	F	612	-	4,4,4	0.21	0	6,6,6	0.15	0
3	SO4	F	613	-	4,4,4	0.19	0	6,6,6	0.10	0
3	SO4	F	614	-	4,4,4	0.23	0	6,6,6	0.30	0
3	SO4	F	615	-	4,4,4	0.19	0	6,6,6	0.35	0
3	SO4	F	616	-	4,4,4	0.11	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	F	617	-	4,4,4	0.11	0	6,6,6	0.19	0
3	SO4	F	618	-	4,4,4	0.11	0	6,6,6	0.30	0
3	SO4	F	619	-	4,4,4	0.21	0	6,6,6	0.48	0
3	SO4	F	620	-	4,4,4	0.15	0	6,6,6	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	A	604	-	-	0/0/0/0	0/0/0/0
3	SO4	A	605	-	-	0/0/0/0	0/0/0/0
3	SO4	A	606	-	-	0/0/0/0	0/0/0/0
3	SO4	A	607	-	-	0/0/0/0	0/0/0/0
3	SO4	A	608	-	-	0/0/0/0	0/0/0/0
3	SO4	A	609	-	-	0/0/0/0	0/0/0/0
3	SO4	A	610	-	-	0/0/0/0	0/0/0/0
3	SO4	A	611	-	-	0/0/0/0	0/0/0/0
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	SO4	B	603	-	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0
3	SO4	B	605	-	-	0/0/0/0	0/0/0/0
3	SO4	B	606	-	-	0/0/0/0	0/0/0/0
3	SO4	B	607	-	-	0/0/0/0	0/0/0/0
3	SO4	B	608	-	-	0/0/0/0	0/0/0/0
3	SO4	B	609	-	-	0/0/0/0	0/0/0/0
3	SO4	C	602	-	-	0/0/0/0	0/0/0/0
3	SO4	C	603	-	-	0/0/0/0	0/0/0/0
3	SO4	C	604	-	-	0/0/0/0	0/0/0/0
3	SO4	C	605	-	-	0/0/0/0	0/0/0/0
3	SO4	C	606	-	-	0/0/0/0	0/0/0/0
3	SO4	C	607	-	-	0/0/0/0	0/0/0/0
3	SO4	C	608	-	-	0/0/0/0	0/0/0/0
3	SO4	C	609	-	-	0/0/0/0	0/0/0/0
3	SO4	C	610	-	-	0/0/0/0	0/0/0/0
3	SO4	C	611	-	-	0/0/0/0	0/0/0/0
3	SO4	C	612	-	-	0/0/0/0	0/0/0/0
3	SO4	C	613	-	-	0/0/0/0	0/0/0/0
3	SO4	C	614	-	-	0/0/0/0	0/0/0/0
3	SO4	C	615	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	D	601	-	-	0/0/0/0	0/0/0/0
3	SO4	D	603	-	-	0/0/0/0	0/0/0/0
3	SO4	D	604	-	-	0/0/0/0	0/0/0/0
3	SO4	D	605	-	-	0/0/0/0	0/0/0/0
3	SO4	D	606	-	-	0/0/0/0	0/0/0/0
3	SO4	D	607	-	-	0/0/0/0	0/0/0/0
3	SO4	D	608	-	-	0/0/0/0	0/0/0/0
3	SO4	D	609	-	-	0/0/0/0	0/0/0/0
3	SO4	D	610	-	-	0/0/0/0	0/0/0/0
3	SO4	D	611	-	-	0/0/0/0	0/0/0/0
3	SO4	D	612	-	-	0/0/0/0	0/0/0/0
3	SO4	D	613	-	-	0/0/0/0	0/0/0/0
3	SO4	D	614	-	-	0/0/0/0	0/0/0/0
3	SO4	E	602	-	-	0/0/0/0	0/0/0/0
3	SO4	E	603	-	-	0/0/0/0	0/0/0/0
3	SO4	E	604	-	-	0/0/0/0	0/0/0/0
3	SO4	E	605	-	-	0/0/0/0	0/0/0/0
3	SO4	E	606	-	-	0/0/0/0	0/0/0/0
3	SO4	E	607	-	-	0/0/0/0	0/0/0/0
3	SO4	E	608	-	-	0/0/0/0	0/0/0/0
3	SO4	E	609	-	-	0/0/0/0	0/0/0/0
3	SO4	E	610	-	-	0/0/0/0	0/0/0/0
3	SO4	E	611	-	-	0/0/0/0	0/0/0/0
3	SO4	E	612	-	-	0/0/0/0	0/0/0/0
3	SO4	E	613	-	-	0/0/0/0	0/0/0/0
3	SO4	E	614	-	-	0/0/0/0	0/0/0/0
3	SO4	E	615	-	-	0/0/0/0	0/0/0/0
3	SO4	E	616	-	-	0/0/0/0	0/0/0/0
3	SO4	F	601	-	-	0/0/0/0	0/0/0/0
3	SO4	F	603	-	-	0/0/0/0	0/0/0/0
3	SO4	F	604	-	-	0/0/0/0	0/0/0/0
3	SO4	F	605	-	-	0/0/0/0	0/0/0/0
3	SO4	F	606	-	-	0/0/0/0	0/0/0/0
3	SO4	F	607	-	-	0/0/0/0	0/0/0/0
3	SO4	F	608	-	-	0/0/0/0	0/0/0/0
3	SO4	F	609	-	-	0/0/0/0	0/0/0/0
3	SO4	F	610	-	-	0/0/0/0	0/0/0/0
3	SO4	F	611	-	-	0/0/0/0	0/0/0/0
3	SO4	F	612	-	-	0/0/0/0	0/0/0/0
3	SO4	F	613	-	-	0/0/0/0	0/0/0/0
3	SO4	F	614	-	-	0/0/0/0	0/0/0/0
3	SO4	F	615	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	F	616	-	-	0/0/0/0	0/0/0/0
3	SO4	F	617	-	-	0/0/0/0	0/0/0/0
3	SO4	F	618	-	-	0/0/0/0	0/0/0/0
3	SO4	F	619	-	-	0/0/0/0	0/0/0/0
3	SO4	F	620	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	SO4	1	0
3	A	606	SO4	1	0
3	A	611	SO4	1	0
3	B	609	SO4	1	0
3	C	605	SO4	1	0
3	C	610	SO4	1	0
3	D	606	SO4	1	0
3	D	612	SO4	1	0
3	E	605	SO4	1	0
3	E	609	SO4	1	0
3	E	616	SO4	1	0
3	F	606	SO4	1	0
3	F	609	SO4	1	0
3	F	613	SO4	1	0
3	F	614	SO4	1	0
3	F	616	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	492/505 (97%)	-0.10	17 (3%) 48 47	68, 133, 179, 210	0
1	B	494/505 (97%)	-0.18	11 (2%) 65 65	56, 120, 170, 202	0
1	C	503/505 (99%)	-0.48	4 (0%) 87 88	44, 79, 129, 180	0
1	D	494/505 (97%)	-0.50	2 (0%) 93 94	46, 75, 118, 163	0
1	E	503/505 (99%)	-0.44	4 (0%) 87 88	45, 79, 129, 174	0
1	F	494/505 (97%)	-0.50	2 (0%) 93 94	43, 71, 117, 151	0
All	All	2980/3030 (98%)	-0.37	40 (1%) 79 80	43, 89, 160, 210	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	4.5
1	F	2	ALA	3.8
1	D	2	ALA	3.8
1	B	505	GLN	3.4
1	B	16	TYR	3.4

### 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 ⓘ

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	F	615	5/5	0.66	0.50	7.74	154,162,163,167	0
3	SO4	D	607	5/5	0.74	0.46	7.34	117,124,129,132	5
3	SO4	C	606	5/5	0.89	0.36	4.94	136,139,147,150	0
3	SO4	F	603	5/5	0.98	0.31	3.10	119,124,125,129	0
3	SO4	F	610	5/5	0.73	0.48	2.78	177,177,177,178	0
3	SO4	E	605	5/5	0.93	0.34	2.41	137,137,138,142	0
3	SO4	F	609	5/5	0.95	0.30	2.40	105,110,111,111	5
3	SO4	B	607	5/5	0.86	0.33	2.39	200,201,205,215	0
3	SO4	F	612	5/5	0.75	0.42	2.33	167,167,170,170	0
3	SO4	E	616	5/5	0.89	0.27	1.77	111,114,114,116	5
3	SO4	F	605	5/5	0.89	0.36	1.48	145,146,150,153	0
3	SO4	A	602	5/5	0.81	0.42	1.46	120,129,132,133	5
3	SO4	A	608	5/5	0.89	0.31	1.35	219,222,227,229	0
3	SO4	C	610	5/5	0.95	0.19	1.27	90,93,94,96	5
3	SO4	E	607	5/5	0.86	0.27	1.25	110,112,117,123	5
3	SO4	A	607	5/5	0.89	0.22	0.88	141,142,144,145	5
3	SO4	D	608	5/5	0.96	0.18	0.74	87,91,93,96	5
3	SO4	D	606	5/5	0.88	0.25	0.61	132,134,137,138	0
3	SO4	D	614	5/5	0.93	0.20	0.56	94,96,99,100	5
3	SO4	D	603	5/5	0.95	0.25	0.50	114,115,117,121	0
3	SO4	F	608	5/5	0.94	0.22	0.50	118,119,122,126	0
3	SO4	B	602	5/5	0.95	0.24	0.14	124,127,128,130	0
3	SO4	E	615	5/5	0.82	0.23	0.13	161,162,163,163	0
3	SO4	C	605	5/5	0.95	0.21	0.11	113,115,117,118	0
3	SO4	E	606	5/5	0.88	0.20	-0.33	166,174,176,179	0
3	SO4	B	605	5/5	0.91	0.28	-0.34	173,175,177,182	0
3	SO4	E	602	5/5	0.97	0.21	-0.35	132,133,135,135	0
3	SO4	A	605	5/5	0.94	0.22	-0.49	118,125,129,129	5
3	SO4	F	601	5/5	0.98	0.16	-0.63	76,83,90,95	0
3	SO4	B	604	5/5	0.93	0.22	-0.66	137,142,144,146	0
3	SO4	A	609	5/5	0.93	0.21	-0.79	130,133,136,138	5
3	SO4	A	606	5/5	0.88	0.22	-0.80	168,173,173,176	0
3	SO4	D	601	5/5	0.98	0.11	-1.03	69,73,75,80	0
3	SO4	C	607	5/5	0.97	0.11	-1.22	84,86,87,93	0
3	SO4	E	608	5/5	0.99	0.07	-1.38	51,62,67,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	F	606	5/5	0.95	0.13	-1.73	104,107,109,112	0
3	SO4	C	602	5/5	0.96	0.14	-1.82	110,118,119,121	0
2	NI	F	602	1/1	0.99	0.05	-2.51	85,85,85,85	0
3	SO4	F	617	5/5	0.70	0.63	-	133,134,136,136	5
3	SO4	A	604	5/5	0.90	0.34	-	150,151,152,154	0
3	SO4	C	615	5/5	0.74	0.35	-	139,139,141,143	5
3	SO4	C	613	5/5	0.92	0.42	-	113,115,116,116	5
3	SO4	D	609	5/5	0.88	0.29	-	133,135,137,139	0
3	SO4	C	614	5/5	0.65	0.45	-	149,156,158,159	5
3	SO4	B	609	5/5	0.50	0.57	-	190,191,192,194	5
3	SO4	E	614	5/5	0.93	0.32	-	106,106,108,110	5
3	SO4	D	605	5/5	0.85	0.26	-	154,155,155,156	0
3	SO4	B	606	5/5	0.78	0.38	-	119,120,123,128	5
3	SO4	F	616	5/5	0.81	0.49	-	140,140,142,144	5
3	SO4	D	611	5/5	0.86	0.34	-	139,140,141,145	5
3	SO4	D	604	5/5	0.94	0.23	-	110,111,115,118	5
3	SO4	F	611	5/5	0.83	0.34	-	115,116,118,118	5
3	SO4	E	603	5/5	0.93	0.27	-	102,109,112,113	5
3	SO4	E	604	5/5	0.80	0.34	-	166,169,171,174	0
3	SO4	A	610	5/5	0.62	0.53	-	197,198,199,200	0
3	SO4	A	611	5/5	0.84	0.37	-	171,172,173,175	0
2	NI	D	602	1/1	0.99	0.04	-	88,88,88,88	0
3	SO4	C	612	5/5	0.95	0.39	-	172,173,174,174	0
3	SO4	B	603	5/5	0.96	0.21	-	105,108,110,111	0
3	SO4	C	611	5/5	0.89	0.38	-	170,171,172,173	0
3	SO4	B	608	5/5	0.83	0.44	-	178,178,180,181	0
3	SO4	E	611	5/5	0.92	0.33	-	131,134,136,137	0
3	SO4	D	613	5/5	0.85	0.41	-	134,138,139,139	5
3	SO4	E	613	5/5	0.52	0.44	-	216,216,217,217	0
2	NI	A	601	1/1	0.99	0.03	-	114,114,114,114	0
2	NI	B	601	1/1	0.99	0.04	-	124,124,124,124	0
3	SO4	E	612	5/5	0.70	0.40	-	204,205,205,206	0
3	SO4	F	619	5/5	0.84	0.45	-	99,101,102,103	5
3	SO4	C	604	5/5	0.92	0.31	-	152,155,156,156	0
3	SO4	A	603	5/5	0.92	0.31	-	109,111,114,116	5
2	NI	E	601	1/1	0.99	0.04	-	73,73,73,73	0
3	SO4	C	603	5/5	0.97	0.20	-	113,122,126,127	0
3	SO4	F	604	5/5	0.96	0.24	-	114,117,119,120	0
2	NI	C	601	1/1	0.97	0.04	-	91,91,91,91	0
3	SO4	F	618	5/5	0.89	0.30	-	128,131,132,134	5
3	SO4	F	620	5/5	0.73	0.44	-	154,157,158,159	0
3	SO4	C	609	5/5	0.53	0.35	-	163,164,167,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	F	614	5/5	0.88	0.21	-	140,140,143,148	0
3	SO4	D	612	5/5	0.82	0.42	-	85,90,94,94	5
3	SO4	D	610	5/5	0.89	0.24	-	103,107,109,116	5
3	SO4	F	607	5/5	0.84	0.25	-	119,126,129,133	5
3	SO4	E	609	5/5	0.89	0.59	-	178,179,181,181	0
3	SO4	C	608	5/5	0.95	0.28	-	145,145,147,147	0
3	SO4	F	613	5/5	0.66	0.44	-	204,204,205,206	0
3	SO4	E	610	5/5	0.76	0.50	-	173,173,174,175	0

## 6.5 Other polymers

There are no such residues in this entry.