



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:51 AM GMT

PDB ID : 3N70
Title : The Crystal Structure of the P-loop NTPase domain of the Sigma-54 transport activator from E. coli to 2.8Å
Authors : Stein, A.J.; Mulligan, R.; Volkart, L.; Freeman, L.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2010-05-26
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

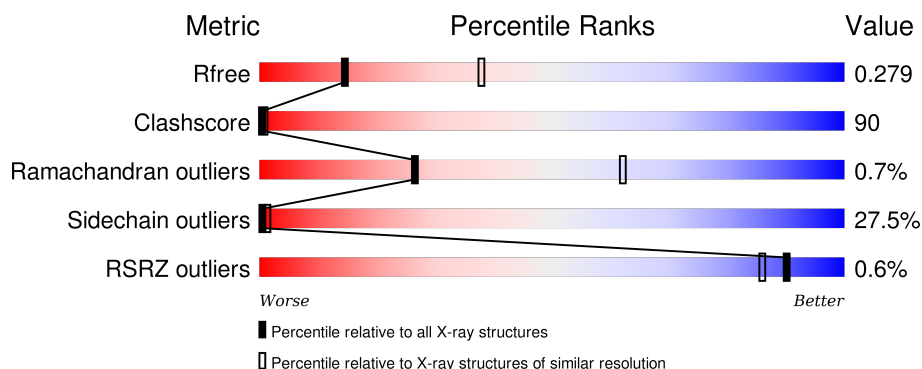
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.




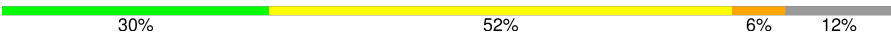

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 ≥ 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	145	<div> <div></div> <div> <div></div> <div>32%</div> <div>53%</div> <div>13%</div> <div>.</div> </div> </div>
1	B	145	<div> <div></div> <div> <div></div> <div>19%</div> <div>46%</div> <div>10%</div> <div>26%</div> </div> </div>
1	C	145	<div> <div></div> <div> <div></div> <div>30%</div> <div>50%</div> <div>10%</div> <div>9%</div> </div> </div>
1	D	145	<div> <div></div> <div> <div></div> <div>30%</div> <div>39%</div> <div>11%</div> <div>20%</div> </div> </div>
1	E	145	<div> <div></div> <div> <div></div> <div>31%</div> <div>48%</div> <div>14%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	145	
1	G	145	
1	H	145	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	2	-	-	X	-
2	SO4	D	4	-	-	X	-
2	SO4	F	7	-	-	X	-
2	SO4	G	6	-	-	X	-
2	SO4	H	8	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7146 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 Transport activator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	Se	0	0	0
			1060	672	190	195	2	1			
1	B	108	Total	C	N	O	S	Se	0	0	0
			734	464	129	138	1	2			
1	C	132	Total	C	N	O	S	Se	0	0	0
			959	615	169	171	2	2			
1	D	116	Total	C	N	O	S	Se	0	0	0
			833	535	149	148	1				
1	E	137	Total	C	N	O	S	Se	0	0	0
			1026	659	183	180	2	2			
1	F	105	Total	C	N	O	S	Se	0	0	0
			719	455	128	133	2	1			
1	G	128	Total	C	N	O	S	Se	0	0	0
			936	591	170	171	2	2			
1	H	122	Total	C	N	O	S	Se	0	0	0
			834	526	154	152	1	1			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

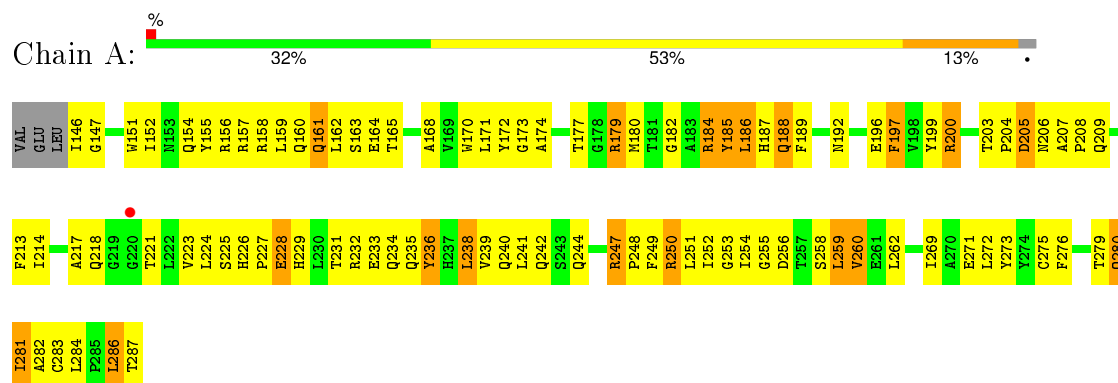
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	E	2	Total	O	0	0
			2	2		

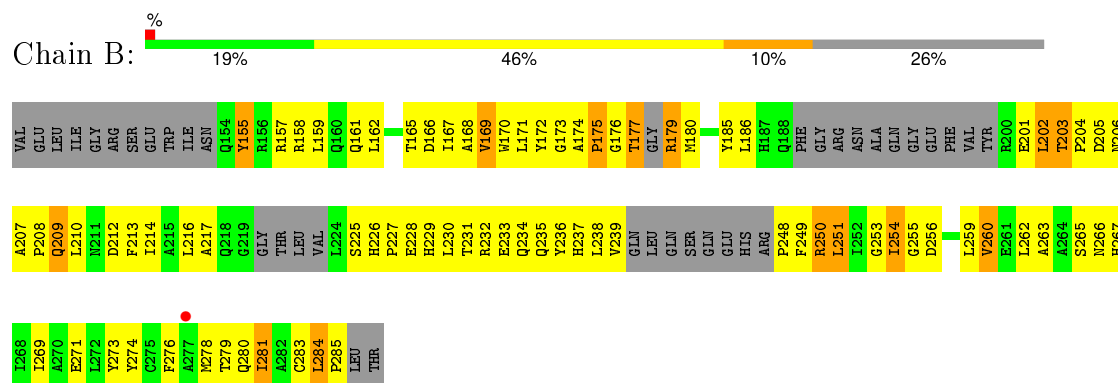
3 Residue-property plots

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 ($RSRZ > 2$). 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.

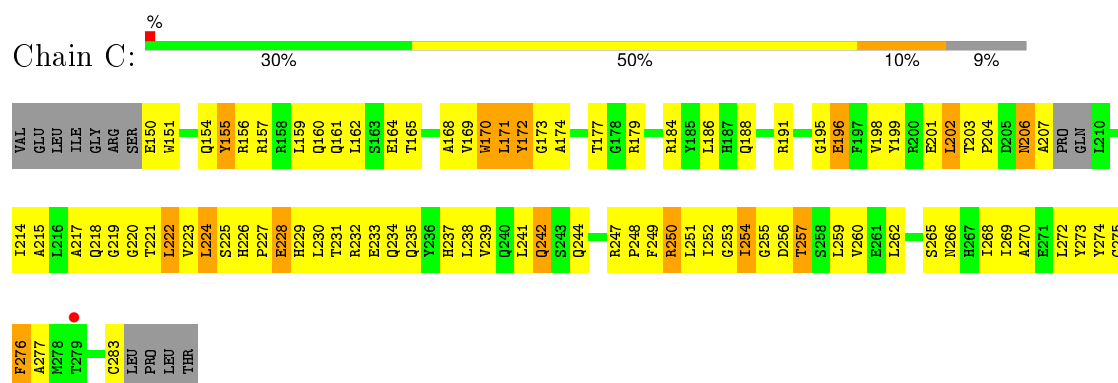
• Molecule 1: Transport activator



• Molecule 1: Transport activator



• Molecule 1: Transport activator



- [illegible]

A277	A278	A279	A280	A281	A282	A283	LEU	PRO	LEU	THR
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● Molecule 1: Transport activator

Chain H:

36%

38%

10%

16%

VAL	GLU	LEU	ILE	GLY	ARG	SER	GLU	TRP	ILE	ASN	Q154	Q160	T165	D166	I167	H170	L171	G178	R179	M180	T181	G182	R184	Y185	L186	H187	Q188	F189	G190	A193	Q194	G195	E196	F197	V198	L202	T203	P204	D205	N206	A207	P208	F213	I214	A217	Q218	G219	G220	T221	L222
V223	L224	S225	H226	P227	L230	T231	R232	E233	Q234	Q235	L238	L241	D242	S243	Q244	E245	H246	R247	P248	F249	R250	L251	I252	G255	E261	L262	A263	A264	S265	N266	H267	I268	I269	A270	E271	L272	C275	PHE	ALA	NSE	THR	GLN	ILE	ALA	CYS	LEU	PRO	LEU	THR	

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	77.61Å 77.61Å 215.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.80 48.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (48.88-2.80) 99.9 (48.88-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.229 , 0.280 0.261 , 0.279	Depositor DCC
R_{free} test set	1572 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.8	EDS
Estimated twinning fraction	0.496 for h,-k,-l 0.467 for h,-k,-l	Xtriage
Reported twinning fraction	0.496 for h,-k,-l	Depositor
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 31209 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7146	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: 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	0.50	0/1082	0.58	1/1474 (0.1%)
1	B	0.55	0/744	0.55	0/1014
1	C	0.47	0/978	0.57	0/1331
1	D	0.39	0/850	0.49	0/1158
1	E	0.47	0/1048	0.50	0/1426
1	F	0.55	0/731	0.54	0/998
1	G	0.49	0/953	0.49	0/1294
1	H	0.49	0/850	0.55	0/1162
All	All	0.49	0/7236	0.53	1/9857 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	238	LEU	CA-CB-CG	-5.17	103.41	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	250	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1060	0	975	124	1
1	B	734	0	611	166	0
1	C	959	0	861	161	4
1	D	833	0	740	152	3
1	E	1026	0	936	165	2
1	F	719	0	575	213	0
1	G	936	0	843	161	2
1	H	834	0	710	129	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	2	0
2	D	5	0	0	2	0
2	E	5	0	0	0	0
2	F	5	0	0	4	0
2	G	5	0	0	3	0
2	H	5	0	0	3	0
3	A	3	0	0	0	0
3	E	2	0	0	0	0
All	All	7146	0	6251	1203	6

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 90.

The worst 5 of 1203 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:199:TYR:HB2	1:F:223:VAL:CG1	1.31	1.55
1:F:187:HIS:CD2	1:F:197:PHE:HB2	1.54	1.42
1:F:278:MSE:HE1	1:G:263:ALA:CB	1.47	1.42
1:A:204:PRO:HD2	1:B:267:HIS:ND1	1.38	1.38
1:C:195:GLY:HA3	1:C:219:GLY:C	1.42	1.36

The worst 5 of 6 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:C:196:GLU:OE1	1:D:200:ARG:NH2[3_554]	0.86	1.34
1:A:160:GLN:NE2	1:C:164:GLU:OE2[4_555]	1.51	0.69
1:C:196:GLU:CD	1:D:200:ARG:NH2[3_554]	1.92	0.28
1:E:185:TYR:OH	1:G:160:GLN:CG[3_544]	1.95	0.25
1:C:196:GLU:OE1	1:D:200:ARG:CZ[3_554]	2.06	0.14

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	140/145 (97%)	134 (96%)	6 (4%)	0	100	100
1	B	98/145 (68%)	92 (94%)	5 (5%)	1 (1%)	19	52
1	C	128/145 (88%)	121 (94%)	6 (5%)	1 (1%)	24	58
1	D	112/145 (77%)	109 (97%)	2 (2%)	1 (1%)	21	55
1	E	131/145 (90%)	123 (94%)	6 (5%)	2 (2%)	13	40
1	F	95/145 (66%)	90 (95%)	3 (3%)	2 (2%)	9	29
1	G	124/145 (86%)	123 (99%)	1 (1%)	0	100	100
1	H	120/145 (83%)	118 (98%)	2 (2%)	0	100	100
All	All	948/1160 (82%)	910 (96%)	31 (3%)	7 (1%)	26	62

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	265	SER
1	E	273	TYR
1	F	177	THR
1	B	175	PRO
1	E	270	ALA

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	98/120 (82%)	67 (68%)	31 (32%)	0	1
1	B	57/120 (48%)	39 (68%)	18 (32%)	0	1
1	C	83/120 (69%)	67 (81%)	16 (19%)	2	5
1	D	70/120 (58%)	50 (71%)	20 (29%)	0	1
1	E	92/120 (77%)	65 (71%)	27 (29%)	0	1
1	F	55/120 (46%)	35 (64%)	20 (36%)	0	0
1	G	83/120 (69%)	69 (83%)	14 (17%)	2	7
1	H	65/120 (54%)	45 (69%)	20 (31%)	0	1
All	All	603/960 (63%)	437 (72%)	166 (28%)	0	1

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	214	ILE
1	E	201	GLU
1	H	203	THR
1	D	237	HIS
1	D	279	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	244	GLN
1	D	235	GLN
1	G	280	GLN
1	D	192	ASN
1	D	194	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 ⓘ

8 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	SO4	A	1	-	4,4,4	0.13	0	6,6,6	0.20	0
2	SO4	B	3	-	4,4,4	0.09	0	6,6,6	0.25	0
2	SO4	C	2	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	D	4	-	4,4,4	0.12	0	6,6,6	0.34	0
2	SO4	E	5	-	4,4,4	0.19	0	6,6,6	0.44	0
2	SO4	F	7	-	4,4,4	0.04	0	6,6,6	0.36	0
2	SO4	G	6	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	H	8	-	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
2	SO4	A	1	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2	-	-	0/0/0/0	0/0/0/0
2	SO4	D	4	-	-	0/0/0/0	0/0/0/0
2	SO4	E	5	-	-	0/0/0/0	0/0/0/0
2	SO4	F	7	-	-	0/0/0/0	0/0/0/0
2	SO4	G	6	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	H	8	-	-	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.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	SO4	1	0
2	C	2	SO4	2	0
2	D	4	SO4	2	0
2	F	7	SO4	4	0
2	G	6	SO4	3	0
2	H	8	SO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	140/145 (96%)	-0.06	1 (0%) 89 84	49, 59, 68, 76	0
1	B	106/145 (73%)	-0.36	1 (0%) 85 79	55, 68, 75, 78	0
1	C	130/145 (89%)	-0.12	1 (0%) 87 81	52, 65, 84, 89	0
1	D	114/145 (78%)	-0.03	2 (1%) 71 61	56, 66, 86, 95	0
1	E	135/145 (93%)	-0.17	1 (0%) 89 84	45, 59, 72, 83	0
1	F	103/145 (71%)	-0.29	0 100 100	60, 69, 99, 106	0
1	G	126/145 (86%)	-0.14	0 100 100	50, 60, 77, 86	0
1	H	121/145 (83%)	-0.17	0 100 100	52, 63, 83, 89	0
All	All	975/1160 (84%)	-0.16	6 (0%) 90 86	45, 64, 83, 106	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	GLY	2.5
1	D	165	THR	2.4
1	E	286	LEU	2.3
1	C	279	THR	2.2
1	D	163	SER	2.1

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

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

6.3 Carbohydrates ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	G	6	5/5	0.95	0.17	0.28	62,62,64,67	0
2	SO4	D	4	5/5	0.94	0.12	-0.35	70,73,75,77	0
2	SO4	H	8	5/5	0.94	0.14	-0.92	81,82,87,87	0
2	SO4	C	2	5/5	0.97	0.12	-1.16	80,80,83,86	0
2	SO4	F	7	5/5	0.90	0.12	-1.57	83,86,92,95	0
2	SO4	A	1	5/5	0.99	0.12	-1.63	56,57,60,61	0
2	SO4	E	5	5/5	0.99	0.11	-2.65	45,45,48,49	0
2	SO4	B	3	5/5	0.98	0.13	-	71,73,77,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.