W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 12, 2024 – 12:37 PM EST

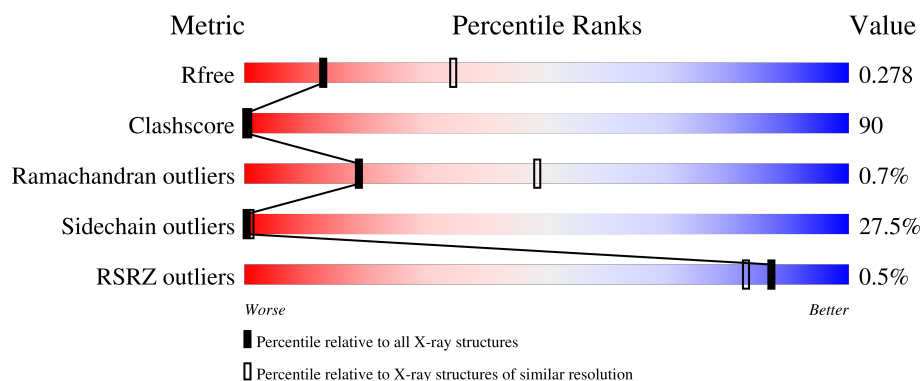|		
PDB ID	:	3N70
Title	:	The Crystal Structure of the P-loop NTPase domain of the Sigma-54 transport activator from E. coli to 2.8A
Authors	:	Stein, A.J.; Mulligan, R.; Volkart, L.; Freeman, L.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2010-05-26
Resolution	:	2.80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

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	Percentile Ranks	Value
Rfree		0.278
Clashscore		90
Ramachandran outliers		0.7%
Sidechain outliers		27.5%
RSRZ outliers		0.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	32% 53% 13% •
1	B	145	19% 46% 10% 26%
1	C	145	30% 50% 10% 9%
1	D	145	30% 39% 11% 20%
1	E	145	31% 48% 14% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	145	% 12%　　46%　　14%　　28%
1	G	145	% 30%　　52%　　6%　12%
1	H	145	36%　　38%　　10%　·　16%

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		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: O_4S).

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

- Molecule 3 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Transport activator

• Molecule 1: Transport activator

• Molecule 1: Transport activator

F276 A277 M278 T279 C283 LEU PRO LEU THR

• Molecule 1: Transport activator

Chain D:

30%   39%   11%   20%

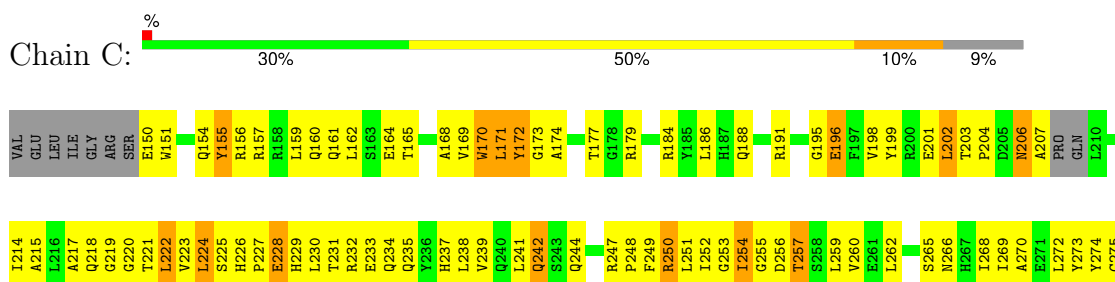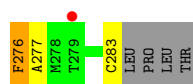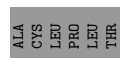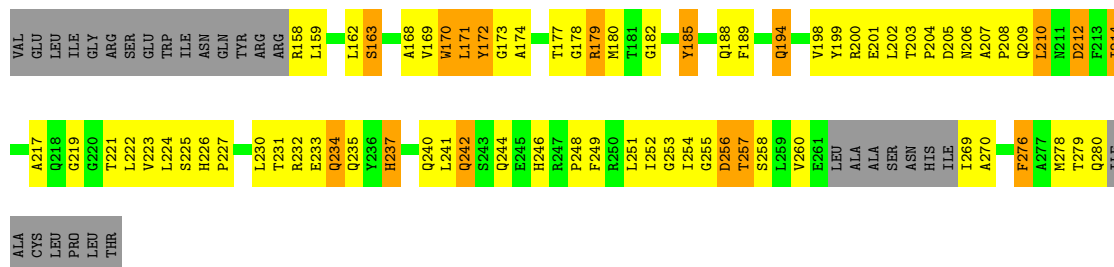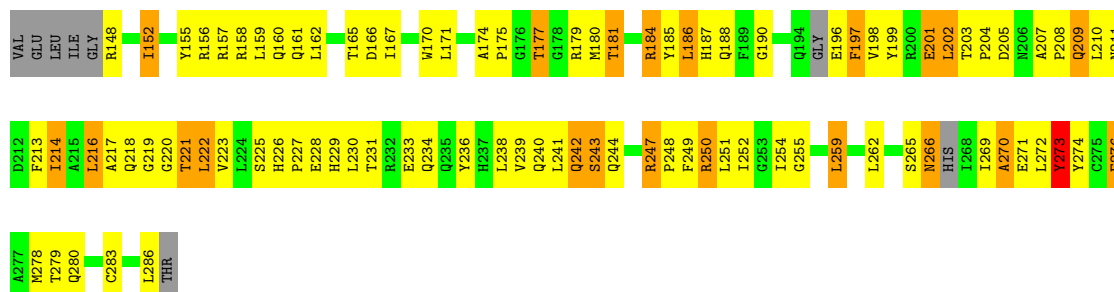VAL GLU LEU ILE GLY ARG SER GLU TRP ILE ASN GLN TYR ARG ARG R158 L159 L162 S163 A168 V169 W170 L171 Y172 G173 A174 T177 G178 R179 M180 T181 G182 Y185 Q188 F189 Q194 V198 Y199 R200 E201 L202 T203 P204 D205 N206 A207 P208 Q209 L210 N211 D212 F213 I214

A217 Q218 G219 G220 T221 L222 V223 L224 S225 H226 P227 L230 T231 R232 E233 Q234 Q235 Y236 H237 Q240 L241 Q242 S243 Q244 E245 H246 R247 P248 F249 R250 L251 I252 G253 I254 G255 D256 T257 S258 L259 V260 E261 LEU ALA ALA SER ASN HIS ILE I268 I269 A270 F276 A277 M278 T279 Q280 ILE

ALA CYS LEU PRO LEU THR

• Molecule 1: Transport activator

Chain E:

31%   48%   14%   • 6%

VAL GLU LEU ILE GLY R148 I152 Y155 R156 R157 R158 L159 Q160 Q161 L162 T165 D166 I167 W170 L171 A174 P175 G176 T177 G178 R179 M180 T181 R184 Y185 L186 H187 Q188 F189 G190 Q194 GLY E196 F197 V198 Y199 R200 E201 L202 T203 P204 D205 N206 A207 P208 Q209 L210 N211

D212 F213 I214 A215 L216 A217 Q218 G219 G220 T221 L222 V223 L224 S225 H226 P227 E228 H229 L230 T231 R232 E233 Q234 Q235 Y236 H237 L238 V239 Q240 L241 Q242 S243 Q244 R247 P248 F249 R250 L251 I252 G253 I254 G255 L259 L262 S265 N266 HIS I268 I269 A270 E271 L272 Y273 Y274 C275 F276

A277 M278 T279 Q280 C283 L286 THR

• Molecule 1: Transport activator

Chain F:

%

12%   46%   14%   28%

VAL GLU LEU ILE GLY ARG SER S149 E150 W151 I152 N153 Q154 Y155 R156 R157 Q160 Q161 L162 SER GLU THR ASP ILE ALA VAL W170 L171 Y172 G173 A174 P175 G176 T177 G178 R179 G182 A183 R184 Y185 L186 H187 GLN PHE GLY ARG ASN ALA GLN GLY GLU F197 V198 Y199 R200 E201 L202 T203 P204

D205 N206 A207 P208 Q209 L210 N211 D212 F213 I214 A215 L216 ALA GLN GLY GLY T221 L222 V223 L224 S225 H226 P227 E228 H229 L230 T231 R232 E233 Q234 Q235 Y236 H237 L238 V239 Q240 L241 Q242 S243 GLU GLU HIS ARG PRO PHE ARG LEU ILE GLY ILE GLY D256 T257 S258 L259 V260 E261 L262 A263 A264

S265 N266 H267 I268 I269 A270 E271 L272 Y273 Y274 C275 F276 A277 M278 T279 Q280 I281 A282 C283 L284 P285 LEU THR

• Molecule 1: Transport activator

Chain G:

%

30%   52%   6%   12%

VAL GLU LEU ILE GLY ARG SER GLU TRP ILE ASN Q154 Y155 R156 R157 R158 L159 Q160 Q161 L162 T165 D166 I167 A168 V169 W170 L171 Y172 G173 A174 T177 G178 R179 M180 T181 R184 Y185 L186 H187 Q188 F189 G190 R191 N192 G195 E196 Y199 R200 E201 L202 D205 N206 A207 P208

Q209 L210 F213 A217 Q218 G219 G220 T221 L222 V223 L224 S225 H226 P227 E228 H229 L230 T231 R232 E233 Q234 Q235 Y236 H237 L238 V239 Q240 L241 Q242 S243 Q244 R247 P248 F249 R250 L251 I252 G253 I254 G255 D256 T257 S258 L259 A263 A264 S265 ASN HIS I268 I269 A270 Y273 F276

A277 M278 T279 Q280 I281 A282 C283 LEU PRO THR

• **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 W170 L171 G178 R179 M180 T181 G182 A183 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 Q242 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 MSE THR GLN ILE ALA CYS LEU PRO LEU THR

4   Data and refinement statistics   (i)

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
$< I/\sigma(I) >$ [1]	2.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.229 , 0.280 0.260 , 0.278	Depositor DCC
R_{free} test set	1572 reflections (4.98%)	wwPDB-VP
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 , 88.2	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
Reported twinning fraction	0.496 for h,-k,-l	Depositor
Outliers	0 of 31209 reflections	Xtriage
F_o,F_c correlation	0.95	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 $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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　ⓘ

5.3.1　Protein backbone　ⓘ

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%)	13	39
1	C	128/145 (88%)	121 (94%)	6 (5%)	1 (1%)	16	44
1	D	112/145 (77%)	109 (97%)	2 (2%)	1 (1%)	14	42
1	E	131/145 (90%)	123 (94%)	6 (5%)	2 (2%)	8	29
1	F	95/145 (66%)	90 (95%)	3 (3%)	2 (2%)	5	20
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%)	19	48

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 (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	98/120 (82%)	67 (68%)	31 (32%)	0	0	
1	B	57/120 (48%)	39 (68%)	18 (32%)	0	0	
1	C	83/120 (69%)	67 (81%)	16 (19%)	1	4	
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%)	1	5	
1	H	65/120 (54%)	45 (69%)	20 (31%)	0	0	
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	F	187	HIS
1	G	254	ILE
1	F	212	ASP
1	F	279	THR
1	H	194	GLN

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

Mol	Chain	Res	Type
1	F	211	ASN
1	H	237	HIS
1	F	242	GLN
1	G	209	GLN
1	C	226	HIS

5.3.3 RNA (i)

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 oligosaccharides 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	F	7	-	4,4,4	0.26	0	6,6,6	0.24	0
2	SO4	E	5	-	4,4,4	0.34	0	6,6,6	0.42	0
2	SO4	G	6	-	4,4,4	0.27	0	6,6,6	0.07	0
2	SO4	D	4	-	4,4,4	0.22	0	6,6,6	0.31	0
2	SO4	C	2	-	4,4,4	0.26	0	6,6,6	0.14	0
2	SO4	H	8	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	B	3	-	4,4,4	0.30	0	6,6,6	0.20	0
2	SO4	A	1	-	4,4,4	0.24	0	6,6,6	0.26	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	F	7	SO4	4	0
2	G	6	SO4	3	0

Continued on next page...

Continued from previous page...

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

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	140/145 (96%)	-0.74	1 (0%)	84	79	49, 59, 68, 76	0
1	B	106/145 (73%)	-0.93	0	100	100	55, 68, 75, 78	0
1	C	130/145 (89%)	-0.73	1 (0%)	82	77	52, 65, 84, 89	0
1	D	114/145 (78%)	-0.68	0	100	100	56, 66, 86, 95	0
1	E	135/145 (93%)	-0.84	0	100	100	45, 59, 72, 83	0
1	F	103/145 (71%)	-0.77	1 (0%)	79	73	60, 69, 99, 106	0
1	G	126/145 (86%)	-0.83	2 (1%)	70	63	50, 60, 77, 86	0
1	H	121/145 (83%)	-0.91	0	100	100	52, 63, 83, 89	0
All	All	975/1160 (84%)	-0.80	5 (0%)	87	83	45, 64, 83, 106	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	279	THR	4.3
1	A	271	GLU	2.5
1	G	282	ALA	2.5
1	G	233	GLU	2.3
1	F	260	VAL	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 monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	3	5/5	0.98	0.04	71,73,77,78	0
2	SO4	C	2	5/5	0.98	0.05	80,80,83,86	0
2	SO4	F	7	5/5	0.98	0.03	83,86,92,95	0
2	SO4	D	4	5/5	0.99	0.03	70,73,75,77	0
2	SO4	E	5	5/5	0.99	0.04	45,45,48,49	0
2	SO4	A	1	5/5	0.99	0.04	56,57,60,61	0
2	SO4	G	6	5/5	0.99	0.03	62,62,64,67	0
2	SO4	H	8	5/5	0.99	0.04	81,82,87,87	0

6.5 Other polymers ⓘ

There are no such residues in this entry.