



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 12:03 AM JST

PDB ID : 7E2Q  
Title : Crystal structure of Mycoplasma pneumoniae Enolase  
Authors : Chen, R.; Zhang, S.; Gan, R.; Wang, W.; Ran, T.; Xiong, Q.; Shao, G.; Feng, Z.  
Deposited on : 2021-02-07  
Resolution : 1.80 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

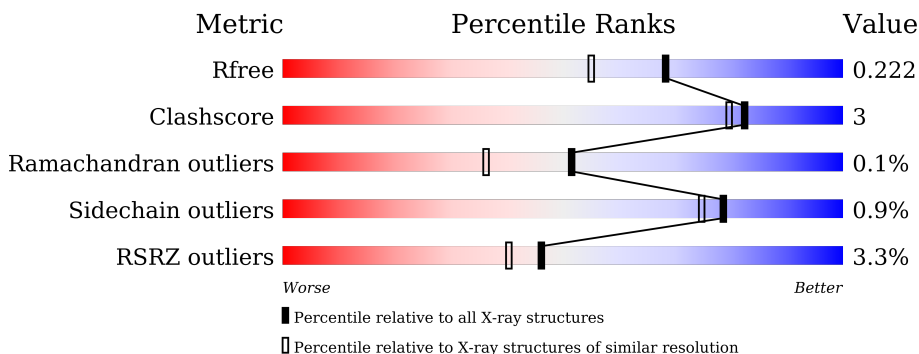
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	464	
1	B	464	
1	C	464	
1	D	464	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 14599 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 Enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	Total 3423	C 2166	N 581	O 661	S 15	0	0	0
1	B	447	Total 3406	C 2158	N 578	O 655	S 15	0	0	0
1	C	450	Total 3424	C 2168	N 581	O 660	S 15	0	0	0
1	D	454	Total 3454	C 2185	N 587	O 667	S 15	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

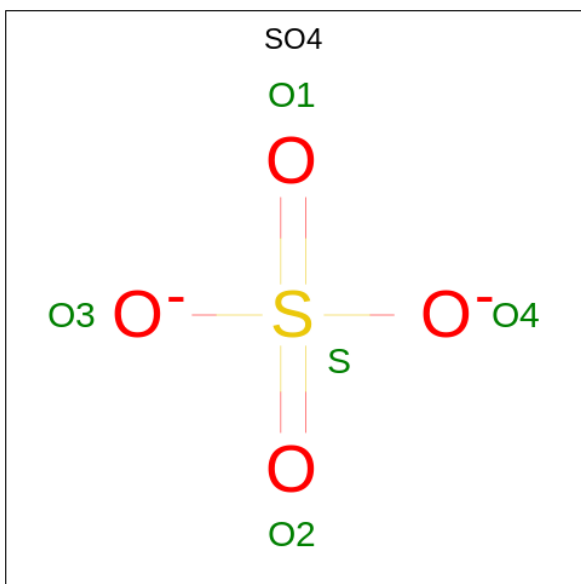
Chain	Residue	Modelled	Actual	Comment	Reference
A	457	LEU	-	expression tag	UNP A0A449A037
A	458	GLU	-	expression tag	UNP A0A449A037
A	459	HIS	-	expression tag	UNP A0A449A037
A	460	HIS	-	expression tag	UNP A0A449A037
A	461	HIS	-	expression tag	UNP A0A449A037
A	462	HIS	-	expression tag	UNP A0A449A037
A	463	HIS	-	expression tag	UNP A0A449A037
A	464	HIS	-	expression tag	UNP A0A449A037
B	457	LEU	-	expression tag	UNP A0A449A037
B	458	GLU	-	expression tag	UNP A0A449A037
B	459	HIS	-	expression tag	UNP A0A449A037
B	460	HIS	-	expression tag	UNP A0A449A037
B	461	HIS	-	expression tag	UNP A0A449A037
B	462	HIS	-	expression tag	UNP A0A449A037
B	463	HIS	-	expression tag	UNP A0A449A037
B	464	HIS	-	expression tag	UNP A0A449A037
C	457	LEU	-	expression tag	UNP A0A449A037
C	458	GLU	-	expression tag	UNP A0A449A037
C	459	HIS	-	expression tag	UNP A0A449A037
C	460	HIS	-	expression tag	UNP A0A449A037
C	461	HIS	-	expression tag	UNP A0A449A037

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Chain	Residue	Modelled	Actual	Comment	Reference
C	462	HIS	-	expression tag	UNP A0A449A037
C	463	HIS	-	expression tag	UNP A0A449A037
C	464	HIS	-	expression tag	UNP A0A449A037
D	457	LEU	-	expression tag	UNP A0A449A037
D	458	GLU	-	expression tag	UNP A0A449A037
D	459	HIS	-	expression tag	UNP A0A449A037
D	460	HIS	-	expression tag	UNP A0A449A037
D	461	HIS	-	expression tag	UNP A0A449A037
D	462	HIS	-	expression tag	UNP A0A449A037
D	463	HIS	-	expression tag	UNP A0A449A037
D	464	HIS	-	expression tag	UNP A0A449A037

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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		

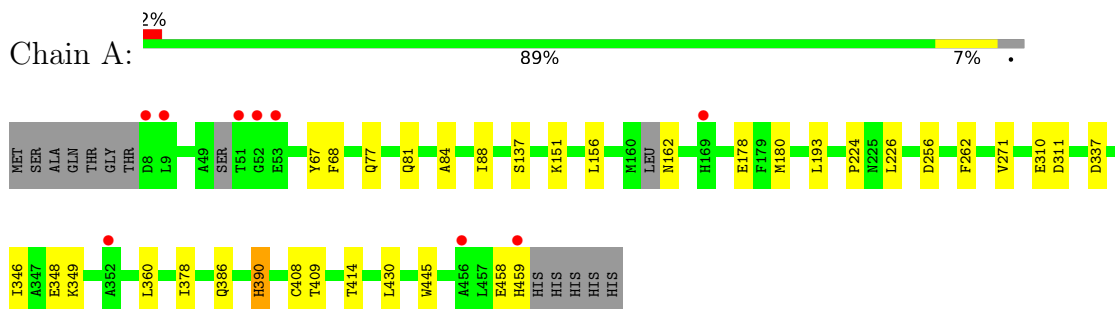
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	195	Total 195	O 195	0	0
3	B	265	Total 265	O 265	0	0
3	C	144	Total 144	O 144	0	0
3	D	268	Total 268	O 268	0	0

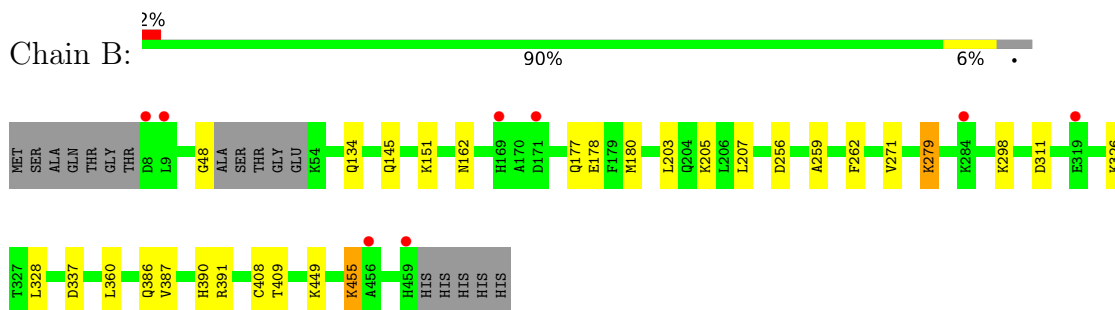
### 3 Residue-property plots [i](#)

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

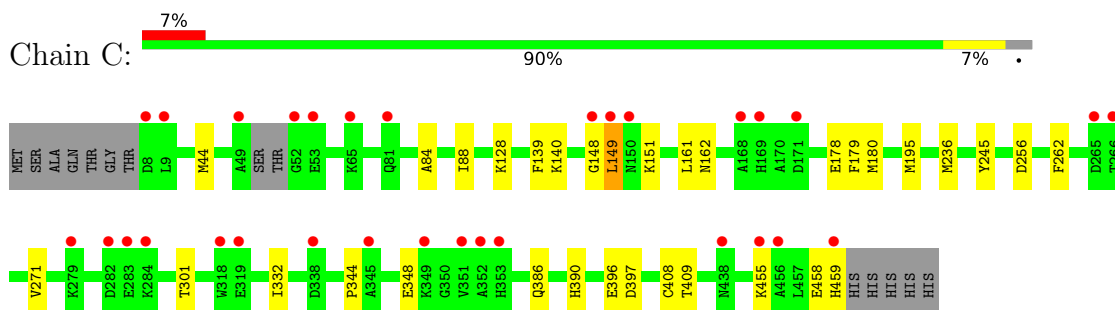
- Molecule 1: Enolase



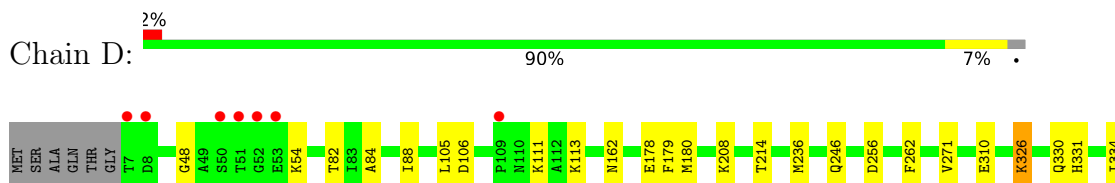
- Molecule 1: Enolase



- Molecule 1: Enolase



- Molecule 1: Enolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.07Å 106.55Å 128.59Å 90.00° 103.15° 90.00°	Depositor
Resolution (Å)	19.84 – 1.80 19.84 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.84-1.80) 98.7 (19.84-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.80Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.189 , 0.223 0.189 , 0.222	Depositor DCC
$R_{free}$ test set	9156 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtrriage
Anisotropy	0.390	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14599	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.36	0/3474	0.55	0/4693
1	B	0.34	0/3458	0.53	0/4673
1	C	0.33	0/3476	0.52	0/4697
1	D	0.33	0/3508	0.52	0/4743
All	All	0.34	0/13916	0.53	0/18806

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3423	0	3467	18	0
1	B	3406	0	3458	17	0
1	C	3424	0	3472	16	0
1	D	3454	0	3499	19	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	195	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	265	0	0	2	0
3	C	144	0	0	0	0
3	D	268	0	0	1	0
All	All	14599	0	13896	70	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 3.

All (70) 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:A:151:LYS:NZ	1:A:408:CYS:SG	2.42	0.93
1:C:151:LYS:NZ	1:C:408:CYS:SG	2.48	0.87
1:B:151:LYS:NZ	1:B:408:CYS:SG	2.55	0.73
1:D:178:GLU:HB2	1:D:256:ASP:HB3	1.73	0.70
1:B:134:GLN:HE22	1:B:145:GLN:HG2	1.59	0.68
1:A:178:GLU:HB2	1:A:256:ASP:HB3	1.81	0.62
1:C:178:GLU:HB2	1:C:256:ASP:HB3	1.83	0.61
1:C:149:LEU:HB3	1:C:151:LYS:HG3	1.84	0.60
1:A:162:ASN:HA	1:A:180:MET:HG2	1.85	0.58
1:B:455:LYS:NZ	3:B:603:HOH:O	2.37	0.57
1:C:162:ASN:HA	1:C:180:MET:HG2	1.89	0.55
1:D:326:LYS:NZ	1:D:354:LYS:O	2.40	0.54
1:B:178:GLU:HB2	1:B:256:ASP:HB3	1.91	0.52
1:A:346:ILE:HA	1:A:349:LYS:HE3	1.92	0.51
1:D:84:ALA:O	1:D:88:ILE:HG12	2.11	0.51
1:B:177:GLN:HG2	1:B:178:GLU:HG3	1.92	0.50
1:B:386:GLN:O	1:B:409:THR:HB	2.11	0.50
1:D:386:GLN:O	1:D:409:THR:HB	2.12	0.50
1:C:139:PHE:CE2	1:C:140:LYS:HG3	2.46	0.49
1:B:48:GLY:HA3	1:B:391:ARG:NH2	2.27	0.48
1:B:326:LYS:NZ	3:B:601:HOH:O	2.35	0.48
1:B:162:ASN:HA	1:B:180:MET:HG2	1.95	0.48
1:B:311:ASP:OD2	1:B:337:ASP:HB3	2.13	0.48
1:D:162:ASN:HA	1:D:180:MET:HG2	1.95	0.48
1:A:262:PHE:HB2	1:A:271:VAL:O	2.14	0.47
1:D:256:ASP:HA	1:D:310:GLU:HB3	1.96	0.47
1:D:54:LYS:HD2	1:D:346:ILE:HD13	1.97	0.47
1:C:386:GLN:O	1:C:409:THR:HB	2.14	0.46
1:C:84:ALA:O	1:C:88:ILE:HG12	2.15	0.46
1:A:193:LEU:HD12	1:A:430:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:GLN:NE2	3:D:608:HOH:O	2.45	0.46
1:B:298:LYS:HG3	1:B:328:LEU:HD21	1.98	0.46
1:C:301:THR:HG21	1:C:332:ILE:HD13	1.99	0.45
1:C:344:PRO:O	1:C:348:GLU:HG3	2.17	0.44
1:C:179:PHE:HB3	1:C:236:MET:SD	2.58	0.44
1:D:390:HIS:CG	1:D:414:THR:HA	2.52	0.44
1:A:386:GLN:O	1:A:409:THR:HB	2.17	0.44
1:A:445:TRP:CD2	1:A:458:GLU:HG2	2.53	0.44
1:A:458:GLU:O	1:A:459:HIS:HB2	2.18	0.44
1:A:390:HIS:CG	1:A:414:THR:HA	2.53	0.43
1:D:262:PHE:HB2	1:D:271:VAL:O	2.18	0.43
1:D:330:GLN:HG2	1:D:331:HIS:CE1	2.54	0.43
1:A:224:PRO:HG2	1:A:226:LEU:HG	2.00	0.43
1:B:360:LEU:HD12	1:B:387:VAL:HB	1.99	0.43
1:B:262:PHE:HB2	1:B:271:VAL:O	2.18	0.43
1:C:262:PHE:HB2	1:C:271:VAL:O	2.18	0.43
1:D:48:GLY:HA3	1:D:391:ARG:NH2	2.33	0.43
1:A:162:ASN:CA	1:A:180:MET:HG2	2.48	0.43
1:B:205:LYS:HB3	1:B:205:LYS:HE2	1.74	0.43
1:A:77:GLN:O	1:A:81:GLN:HG2	2.20	0.42
1:B:259:ALA:HA	1:B:262:PHE:CE1	2.54	0.42
1:B:279:LYS:HA	1:B:279:LYS:HD2	1.71	0.42
1:D:106:ASP:O	1:D:113:LYS:HE2	2.19	0.42
1:D:179:PHE:HB3	1:D:236:MET:SD	2.60	0.42
1:A:348:GLU:HG3	1:A:378:ILE:HD13	2.00	0.42
1:C:128:LYS:NZ	1:C:397:ASP:OD2	2.45	0.42
1:D:106:ASP:OD2	1:D:111:LYS:HA	2.20	0.42
1:A:310:GLU:OE2	1:A:360:LEU:HD22	2.20	0.41
1:C:195:MET:HG2	1:C:245:TYR:CE1	2.56	0.41
1:D:82:THR:HG22	1:D:105:LEU:HD21	2.02	0.41
1:C:44:MET:HE1	1:C:396:GLU:HG2	2.03	0.41
1:C:161:LEU:O	1:C:180:MET:HA	2.21	0.41
1:A:311:ASP:OD2	1:A:337:ASP:HB3	2.21	0.41
1:A:67:TYR:C	1:A:68:PHE:CG	2.94	0.40
1:D:334:ILE:O	1:D:356:THR:HB	2.21	0.40
1:C:458:GLU:O	1:C:459:HIS:HB2	2.21	0.40
1:D:441:LYS:HE2	1:D:441:LYS:HB2	1.80	0.40
1:A:84:ALA:O	1:A:88:ILE:HG12	2.22	0.40
1:B:203:LEU:O	1:B:207:LEU:HG	2.22	0.40
1:D:208:LYS:HG2	1:D:214:THR:HG21	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/464 (96%)	436 (98%)	8 (2%)	0	100	100
1	B	443/464 (96%)	436 (98%)	7 (2%)	0	100	100
1	C	446/464 (96%)	433 (97%)	11 (2%)	2 (0%)	34	21
1	D	452/464 (97%)	443 (98%)	9 (2%)	0	100	100
All	All	1785/1856 (96%)	1748 (98%)	35 (2%)	2 (0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	148	GLY
1	C	149	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	359/371 (97%)	356 (99%)	3 (1%)	81	78
1	B	358/371 (96%)	354 (99%)	4 (1%)	73	68
1	C	359/371 (97%)	357 (99%)	2 (1%)	86	84
1	D	363/371 (98%)	359 (99%)	4 (1%)	73	68
All	All	1439/1484 (97%)	1426 (99%)	13 (1%)	78	75

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	SER
1	A	156	LEU
1	A	390	HIS
1	B	279	LYS
1	B	390	HIS
1	B	449	LYS
1	B	455	LYS
1	C	390	HIS
1	C	455	LYS
1	D	326	LYS
1	D	364	ASN
1	D	390	HIS
1	D	455	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	501	-	4,4,4	0.11	0	6,6,6	0.21	0
2	SO4	D	501	-	4,4,4	0.15	0	6,6,6	0.21	0
2	SO4	B	501	-	4,4,4	0.21	0	6,6,6	0.19	0
2	SO4	C	501	-	4,4,4	0.16	0	6,6,6	0.31	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.

No monomer is involved in short contacts.

## 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	450/464 (96%)	-0.14	9 (2%) 65 61	15, 24, 44, 83	0
1	B	447/464 (96%)	-0.08	8 (1%) 68 64	16, 27, 45, 69	0
1	C	450/464 (96%)	0.07	31 (6%) 16 13	19, 31, 53, 91	0
1	D	454/464 (97%)	-0.10	11 (2%) 59 54	18, 28, 48, 97	0
All	All	1801/1856 (97%)	-0.06	59 (3%) 46 40	15, 28, 48, 97	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	460	HIS	7.1
1	A	52	GLY	6.3
1	A	51	THR	6.3
1	C	53	GLU	6.0
1	D	7	THR	5.6
1	C	171	ASP	4.5
1	B	459	HIS	4.5
1	D	50	SER	4.4
1	C	459	HIS	4.1
1	C	148	GLY	4.1
1	A	53	GLU	3.9
1	D	8	ASP	3.9
1	B	9	LEU	3.8
1	C	52	GLY	3.7
1	C	150	ASN	3.7
1	C	349	LYS	3.6
1	C	49	ALA	3.6
1	C	351	VAL	3.6
1	C	345	ALA	3.5
1	D	52	GLY	3.5
1	C	266	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	169	HIS	3.4
1	C	169	HIS	3.4
1	D	53	GLU	3.4
1	D	51	THR	3.3
1	C	338	ASP	3.3
1	A	459	HIS	3.3
1	C	9	LEU	3.2
1	C	353	HIS	3.1
1	D	456	ALA	3.0
1	B	284	LYS	2.9
1	B	171	ASP	2.9
1	D	459	HIS	2.8
1	A	9	LEU	2.8
1	D	109	PRO	2.7
1	C	168	ALA	2.7
1	C	265	ASP	2.6
1	D	455	LYS	2.6
1	A	8	ASP	2.6
1	C	149	LEU	2.6
1	A	456	ALA	2.6
1	C	279	LYS	2.6
1	C	283	GLU	2.6
1	C	284	LYS	2.6
1	C	438	ASN	2.6
1	C	8	ASP	2.5
1	B	8	ASP	2.4
1	A	352	ALA	2.3
1	C	456	ALA	2.3
1	C	282	ASP	2.3
1	B	319	GLU	2.3
1	A	169	HIS	2.3
1	C	65	LYS	2.3
1	B	456	ALA	2.2
1	C	81	GLN	2.2
1	C	455	LYS	2.1
1	C	318	TRP	2.1
1	C	352	ALA	2.1
1	C	319	GLU	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 [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	501	5/5	0.98	0.07	29,33,35,37	0
2	SO4	C	501	5/5	0.98	0.07	37,39,40,40	0
2	SO4	D	501	5/5	0.98	0.06	28,32,36,40	0
2	SO4	B	501	5/5	0.99	0.08	29,30,37,38	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.