



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:49 pm BST

PDB ID : 1TWS  
Title : Dihydropteroate Synthetase From Bacillus anthracis  
Authors : Babaoglu, K.; Qi, J.; Lee, R.E.; White, S.W.  
Deposited on : 2004-07-01  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

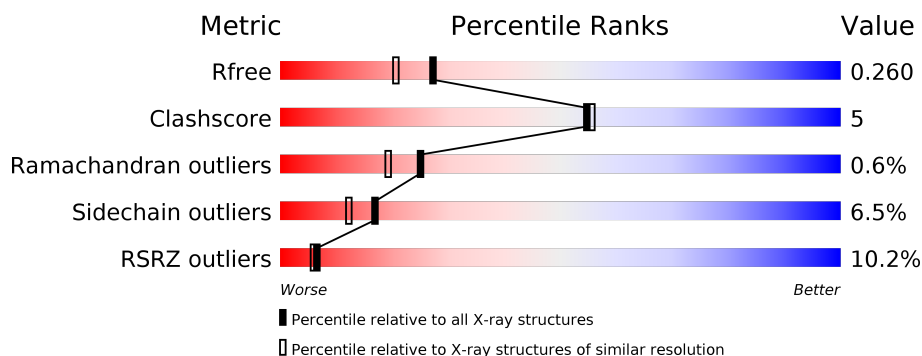
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	297	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	297	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>•</div> <div>10%</div> </div> </div>

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	A	336	-	-	-	X
2	SO4	B	341	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4571 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 DHPS, Dihydropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	38	0	0
			2116	1330	364	406	16			
1	B	267	Total	C	N	O	S	13	0	0
			2070	1300	358	396	16			

There are 40 discrepancies between the modelled and reference sequences:

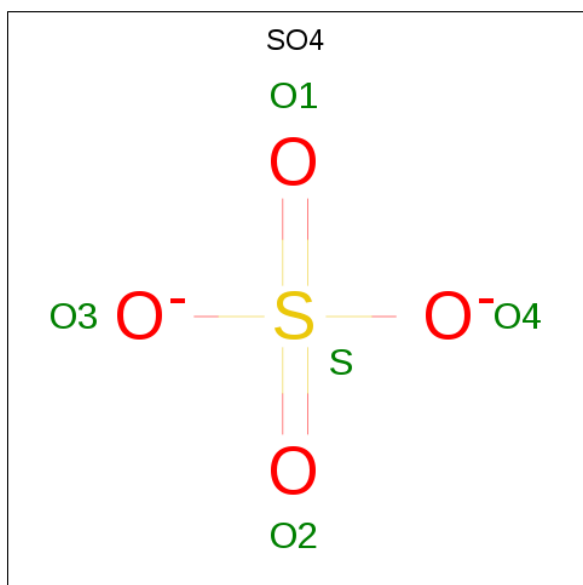
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q81VW8
A	-18	GLY	-	EXPRESSION TAG	UNP Q81VW8
A	-17	SER	-	EXPRESSION TAG	UNP Q81VW8
A	-16	SER	-	EXPRESSION TAG	UNP Q81VW8
A	-15	HIS	-	EXPRESSION TAG	UNP Q81VW8
A	-14	HIS	-	EXPRESSION TAG	UNP Q81VW8
A	-13	HIS	-	EXPRESSION TAG	UNP Q81VW8
A	-12	HIS	-	EXPRESSION TAG	UNP Q81VW8
A	-11	HIS	-	EXPRESSION TAG	UNP Q81VW8
A	-10	HIS	-	EXPRESSION TAG	UNP Q81VW8
A	-9	SER	-	EXPRESSION TAG	UNP Q81VW8
A	-8	SER	-	EXPRESSION TAG	UNP Q81VW8
A	-7	GLY	-	EXPRESSION TAG	UNP Q81VW8
A	-6	LEU	-	EXPRESSION TAG	UNP Q81VW8
A	-5	VAL	-	EXPRESSION TAG	UNP Q81VW8
A	-4	PRO	-	EXPRESSION TAG	UNP Q81VW8
A	-3	ARG	-	EXPRESSION TAG	UNP Q81VW8
A	-2	GLY	-	EXPRESSION TAG	UNP Q81VW8
A	-1	SER	-	EXPRESSION TAG	UNP Q81VW8
A	0	HIS	-	EXPRESSION TAG	UNP Q81VW8
B	-19	MET	-	EXPRESSION TAG	UNP Q81VW8
B	-18	GLY	-	EXPRESSION TAG	UNP Q81VW8
B	-17	SER	-	EXPRESSION TAG	UNP Q81VW8
B	-16	SER	-	EXPRESSION TAG	UNP Q81VW8
B	-15	HIS	-	EXPRESSION TAG	UNP Q81VW8

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q81VW8
B	-13	HIS	-	EXPRESSION TAG	UNP Q81VW8
B	-12	HIS	-	EXPRESSION TAG	UNP Q81VW8
B	-11	HIS	-	EXPRESSION TAG	UNP Q81VW8
B	-10	HIS	-	EXPRESSION TAG	UNP Q81VW8
B	-9	SER	-	EXPRESSION TAG	UNP Q81VW8
B	-8	SER	-	EXPRESSION TAG	UNP Q81VW8
B	-7	GLY	-	EXPRESSION TAG	UNP Q81VW8
B	-6	LEU	-	EXPRESSION TAG	UNP Q81VW8
B	-5	VAL	-	EXPRESSION TAG	UNP Q81VW8
B	-4	PRO	-	EXPRESSION TAG	UNP Q81VW8
B	-3	ARG	-	EXPRESSION TAG	UNP Q81VW8
B	-2	GLY	-	EXPRESSION TAG	UNP Q81VW8
B	-1	SER	-	EXPRESSION TAG	UNP Q81VW8
B	0	HIS	-	EXPRESSION TAG	UNP Q81VW8

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

Continued on next page...

*Continued from previous page...*

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

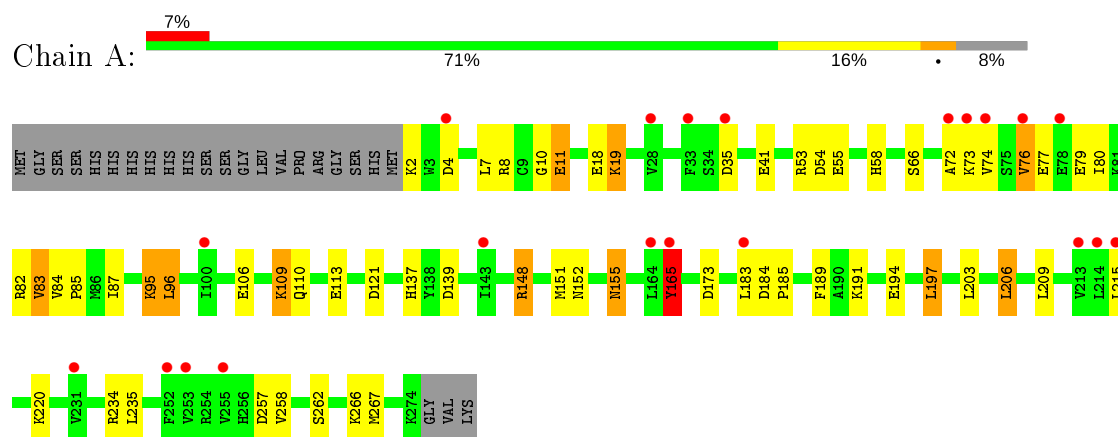
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total	O	0	0
			164	164		
3	B	161	Total	O	0	0
			161	161		

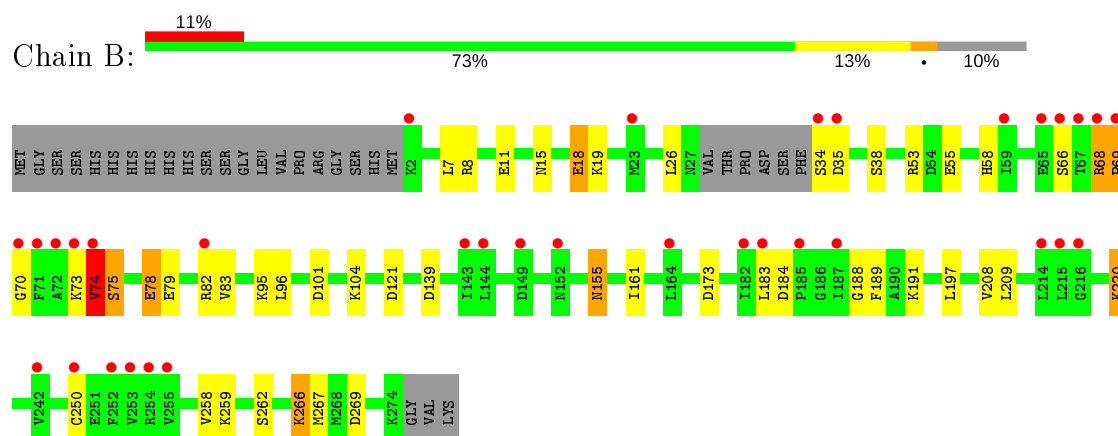
### 3 Residue-property plots [i](#)

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

- Molecule 1: DHPS, Dihydropteroate synthase



- Molecule 1: DHPS, Dihydropteroate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6 <sub>2</sub> 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.44 Å 97.44 Å 263.62 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.9 (30.00-2.00) 92.9 (29.80-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.212 , 0.255 0.227 , 0.260	Depositor DCC
$R_{free}$ test set	2422 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4571	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1207e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.15	10/2149 (0.5%)	1.30	26/2899 (0.9%)
1	B	2.47	7/2100 (0.3%)	1.40	16/2829 (0.6%)
All	All	1.92	17/4249 (0.4%)	1.35	42/5728 (0.7%)

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	A	0	1
1	B	0	5
All	All	0	6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	18	GLU	CB-CG	75.50	2.95	1.52
1	B	18	GLU	CG-CD	-68.20	0.49	1.51
1	B	78	GLU	CG-CD	29.08	1.95	1.51
1	A	11	GLU	CG-CD	-21.98	1.19	1.51
1	A	194	GLU	CB-CG	-12.20	1.28	1.52
1	A	55	GLU	CG-CD	-11.63	1.34	1.51
1	A	77	GLU	CB-CG	-11.23	1.30	1.52
1	A	137	HIS	CB-CG	-10.58	1.31	1.50
1	A	266	LYS	CD-CE	-9.39	1.27	1.51
1	B	267	MET	SD-CE	-8.23	1.31	1.77
1	B	266	LYS	CD-CE	7.21	1.69	1.51
1	A	267	MET	SD-CE	-7.20	1.37	1.77
1	B	55	GLU	CG-CD	-7.00	1.41	1.51
1	A	18	GLU	CA-CB	-6.65	1.39	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	TYR	CB-CG	-6.46	1.42	1.51
1	A	109	LYS	CB-CG	6.04	1.68	1.52
1	B	208	VAL	CB-CG2	-5.17	1.42	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	GLU	CG-CD-OE2	-38.91	40.47	118.30
1	A	11	GLU	CG-CD-OE2	-32.26	53.77	118.30
1	B	18	GLU	CB-CG-CD	-26.86	41.69	114.20
1	B	78	GLU	CG-CD-OE2	-22.41	73.48	118.30
1	A	11	GLU	CG-CD-OE1	17.35	152.99	118.30
1	A	11	GLU	CB-CG-CD	-11.25	83.82	114.20
1	B	18	GLU	CB-CA-C	10.21	130.82	110.40
1	A	2	LYS	N-CA-CB	10.10	128.77	110.60
1	A	137	HIS	CA-CB-CG	9.38	129.54	113.60
1	A	184	ASP	CB-CG-OD2	8.86	126.27	118.30
1	B	18	GLU	CA-CB-CG	8.78	132.71	113.40
1	A	121	ASP	CB-CG-OD2	7.96	125.47	118.30
1	B	184	ASP	CB-CG-OD2	7.71	125.23	118.30
1	A	11	GLU	CA-C-N	7.53	133.78	117.20
1	A	11	GLU	CA-C-O	-7.24	104.89	120.10
1	B	78	GLU	CB-CG-CD	7.20	133.65	114.20
1	A	4	ASP	CB-CG-OD2	6.43	124.08	118.30
1	A	53	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	101	ASP	CB-CG-OD2	6.34	124.01	118.30
1	B	78	GLU	CG-CD-OE1	-6.32	105.66	118.30
1	A	18	GLU	N-CA-CB	6.08	121.54	110.60
1	B	173	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	269	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	54	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	10	GLY	C-N-CA	-5.75	107.33	121.70
1	A	197	LEU	CA-CB-CG	5.75	128.51	115.30
1	B	53	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	121	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	165	TYR	CB-CG-CD1	-5.68	117.59	121.00
1	B	139	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	173	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	11	GLU	N-CA-CB	-5.62	100.48	110.60
1	A	18	GLU	CB-CA-C	5.55	121.50	110.40
1	A	234	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	206	LEU	CA-CB-CG	5.47	127.89	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	148	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	35	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	257	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	35	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	96	LEU	CA-CB-CG	5.02	126.84	115.30
1	B	250	CYS	CA-CB-SG	-5.02	104.97	114.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	GLU	Sidechain
1	B	18	GLU	Sidechain
1	B	68	ARG	Peptide
1	B	73	LYS	Peptide
1	B	74	VAL	Peptide
1	B	78	GLU	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	2116	0	2127	23	1
1	B	2070	0	2085	20	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0
3	A	164	0	0	2	1
3	B	161	0	0	3	1
All	All	4571	0	4212	43	2

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 5.

All (43) 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:165:TYR:CE1	1:A:209:LEU:CD2	2.51	0.92
1:A:165:TYR:CE1	1:A:209:LEU:HD22	2.09	0.87
1:B:266:LYS:NZ	3:B:460:HOH:O	2.09	0.85
1:B:19:LYS:HE3	1:B:58:HIS:HE2	1.47	0.78
1:B:19:LYS:HE3	1:B:58:HIS:NE2	2.05	0.71
1:B:66:SER:HB3	1:B:79:GLU:OE1	1.92	0.69
1:A:19:LYS:HE3	1:A:58:HIS:HE2	1.58	0.69
1:B:74:VAL:HG11	1:B:104:LYS:NZ	2.08	0.68
1:A:155:ASN:HD22	1:A:155:ASN:C	1.97	0.68
1:B:11:GLU:OE1	1:B:95:LYS:NZ	2.28	0.67
1:A:165:TYR:HE1	1:A:209:LEU:CD2	2.06	0.66
1:A:19:LYS:HE3	1:A:58:HIS:NE2	2.12	0.65
1:B:74:VAL:HG11	1:B:104:LYS:HZ1	1.62	0.65
1:A:165:TYR:CE1	1:A:209:LEU:HD21	2.30	0.64
1:B:69:PRO:HD2	1:B:70:GLY:H	1.65	0.61
1:B:155:ASN:HD22	1:B:155:ASN:C	2.04	0.60
1:A:106:GLU:OE2	1:A:110:GLN:NE2	2.37	0.57
1:B:189:PHE:O	1:B:191:LYS:HG3	2.05	0.56
1:B:15:ASN:O	3:B:351:HOH:O	2.18	0.56
1:B:161:ILE:HG23	1:B:209:LEU:HD21	1.88	0.55
1:A:41:GLU:OE2	1:A:82:ARG:HD3	2.10	0.52
1:B:74:VAL:HG23	1:B:75:SER:H	1.76	0.50
1:B:19:LYS:CE	1:B:58:HIS:NE2	2.74	0.49
1:B:258:VAL:O	1:B:262:SER:HB2	2.11	0.49
1:B:68:ARG:O	1:B:68:ARG:HG3	2.13	0.48
1:A:185:PRO:HG3	1:A:203:LEU:HD21	1.95	0.48
1:B:259:LYS:NZ	3:B:461:HOH:O	2.47	0.48
1:A:109:LYS:O	1:A:113:GLU:HG3	2.15	0.47
1:A:83:VAL:HG13	1:A:87:ILE:HD12	1.98	0.46
1:B:188:GLY:HA3	1:B:220:LYS:HD3	1.97	0.46
1:B:66:SER:HB2	1:B:74:VAL:HG12	1.97	0.46
1:A:19:LYS:CE	1:A:58:HIS:NE2	2.80	0.45
1:A:258:VAL:O	1:A:262:SER:HB3	2.17	0.45
1:A:95:LYS:HE2	3:A:485:HOH:O	2.18	0.44
1:A:66:SER:HB3	1:A:79:GLU:CD	2.38	0.43
1:A:76:VAL:HG23	1:A:80:ILE:HD12	2.00	0.42
1:A:189:PHE:O	1:A:191:LYS:HG3	2.20	0.41
1:A:72:ALA:O	1:A:74:VAL:HG12	2.20	0.41
1:A:165:TYR:OH	3:A:354:HOH:O	2.18	0.41
1:A:155:ASN:ND2	1:A:155:ASN:C	2.70	0.41
1:B:74:VAL:CG1	1:B:104:LYS:NZ	2.82	0.41
1:A:84:VAL:HB	1:A:85:PRO:HD3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD11	1:A:215:LEU:HD13	2.02	0.40

All (2) 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)
3:A:380:HOH:O	3:B:382:HOH:O[5_454]	1.83	0.37
1:A:151:MET:SD	1:A:151:MET:SD[10_665]	2.19	0.01

## 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	271/297 (91%)	265 (98%)	6 (2%)	0	100	100
1	B	263/297 (89%)	257 (98%)	3 (1%)	3 (1%)	14	8
All	All	534/594 (90%)	522 (98%)	9 (2%)	3 (1%)	25	19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	69	PRO
1	B	75	SER
1	B	74	VAL

### 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	227/247 (92%)	210 (92%)	17 (8%)	13	9
1	B	221/247 (90%)	209 (95%)	12 (5%)	22	18
All	All	448/494 (91%)	419 (94%)	29 (6%)	17	12

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	8	ARG
1	A	19	LYS
1	A	73	LYS
1	A	76	VAL
1	A	83	VAL
1	A	95	LYS
1	A	96	LEU
1	A	148	ARG
1	A	152	ASN
1	A	155	ASN
1	A	165	TYR
1	A	183	LEU
1	A	197	LEU
1	A	206	LEU
1	A	220	LYS
1	A	235	LEU
1	B	7	LEU
1	B	8	ARG
1	B	26	LEU
1	B	34	SER
1	B	38	SER
1	B	82	ARG
1	B	83	VAL
1	B	96	LEU
1	B	155	ASN
1	B	183	LEU
1	B	197	LEU
1	B	220	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	88	GLN
1	A	155	ASN
1	A	180	ASN
1	B	88	GLN
1	B	155	ASN
1	B	180	ASN

### 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 ⓘ

12 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	334	-	4,4,4	0.19	0	6,6,6	1.04	0
2	SO4	B	338	-	4,4,4	0.13	0	6,6,6	0.21	0
2	SO4	B	332	-	4,4,4	0.32	0	6,6,6	0.49	0
2	SO4	A	339	-	4,4,4	0.13	0	6,6,6	0.75	0
2	SO4	A	342	-	4,4,4	0.12	0	6,6,6	0.27	0
2	SO4	A	335	-	4,4,4	0.20	0	6,6,6	0.16	0
2	SO4	B	337	-	4,4,4	0.16	0	6,6,6	0.22	0
2	SO4	A	331	-	4,4,4	0.41	0	6,6,6	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	336	-	4,4,4	0.21	0	6,6,6	0.20	0
2	SO4	B	341	-	4,4,4	0.13	0	6,6,6	0.33	0
2	SO4	B	333	-	4,4,4	0.19	0	6,6,6	1.20	0
2	SO4	B	340	-	4,4,4	0.26	0	6,6,6	0.75	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	273/297 (91%)	0.25	21 (7%) 13 12	16, 24, 44, 61	10 (3%)
1	B	267/297 (89%)	0.50	34 (12%) 3 3	16, 24, 49, 61	5 (1%)
All	All	540/594 (90%)	0.37	55 (10%) 6 6	16, 24, 46, 61	15 (2%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	VAL	7.4
1	B	71	PHE	6.7
1	B	73	LYS	6.2
1	B	35	ASP	6.1
1	B	70	GLY	5.6
1	A	165	TYR	5.4
1	B	143	ILE	5.4
1	B	66	SER	5.3
1	B	214	LEU	5.1
1	B	72	ALA	5.0
1	A	74	VAL	4.5
1	A	183	LEU	4.4
1	A	35	ASP	4.2
1	A	143	ILE	3.9
1	A	214	LEU	3.7
1	B	215	LEU	3.7
1	A	72	ALA	3.7
1	B	67	THR	3.6
1	B	183	LEU	3.5
1	A	73	LYS	3.5
1	B	65	GLU	3.3
1	B	34	SER	3.2
1	B	182	ILE	3.1
1	A	252	PHE	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	255	VAL	2.9
1	A	215	LEU	2.9
1	B	144	LEU	2.8
1	B	82	ARG	2.7
1	B	59	ILE	2.6
1	B	149	ASP	2.6
1	A	4	ASP	2.5
1	B	69	PRO	2.5
1	B	164	LEU	2.5
1	B	216	GLY	2.5
1	A	28	VAL	2.5
1	B	250	CYS	2.5
1	B	185	PRO	2.4
1	A	76	VAL	2.4
1	B	252	PHE	2.4
1	B	254	ARG	2.4
1	A	164	LEU	2.4
1	B	68	ARG	2.4
1	A	33	PHE	2.4
1	A	100	ILE	2.3
1	B	152	ASN	2.3
1	B	253	VAL	2.3
1	B	187	ILE	2.3
1	A	78	GLU	2.2
1	A	253	VAL	2.2
1	A	213	VAL	2.2
1	B	242	VAL	2.2
1	A	231	VAL	2.1
1	A	255	VAL	2.1
1	B	23	MET	2.1
1	B	2	LYS	2.0

## 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 ⓘ

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	B	341	5/5	0.65	0.52	92,93,94,95	0
2	SO4	A	336	5/5	0.73	0.49	132,132,133,134	0
2	SO4	A	342	5/5	0.84	0.49	77,77,79,81	0
2	SO4	A	335	5/5	0.85	0.41	81,81,82,82	0
2	SO4	B	337	5/5	0.87	0.39	87,88,89,89	0
2	SO4	B	340	5/5	0.90	0.27	58,59,62,63	0
2	SO4	B	338	5/5	0.92	0.27	118,119,119,119	0
2	SO4	A	339	5/5	0.94	0.29	59,60,60,62	0
2	SO4	B	333	5/5	0.95	0.24	50,51,53,54	0
2	SO4	A	334	5/5	0.96	0.20	55,56,57,57	0
2	SO4	B	332	5/5	0.97	0.10	42,43,44,45	0
2	SO4	A	331	5/5	0.99	0.07	24,25,27,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.