



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 07:59 AM EDT

PDB ID : 5E6K  
Title : Ketosynthase from module 6 of the bacillaene synthase from *Bacillus subtilis* 168 (C167S mutant, crystal form 2)  
Authors : Wagner, D.T.; Gay, D.C.; Keatinge-Clay, A.T.  
Deposited on : 2015-10-10  
Resolution : 2.16 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 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	:	2.37.1
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)	:	2.37.1

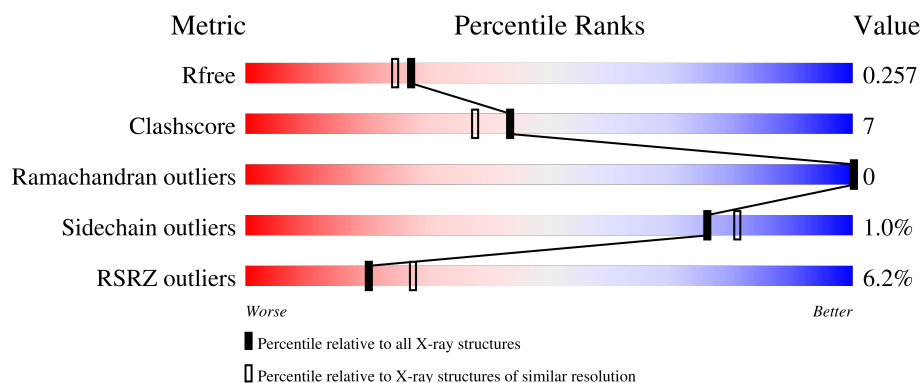
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	617	<div> <div>4%</div> <div>75%</div> <div>10%</div> <div>15%</div> </div>
1	B	617	<div> <div>7%</div> <div>75%</div> <div>10%</div> <div>14%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8408 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 Polyketide synthase PksL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4149	2637	698	790	24			
1	B	531	Total	C	N	O	S	0	0	0
			4171	2652	702	793	24			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q05470
A	-20	GLY	-	expression tag	UNP Q05470
A	-19	SER	-	expression tag	UNP Q05470
A	-18	SER	-	expression tag	UNP Q05470
A	-17	HIS	-	expression tag	UNP Q05470
A	-16	HIS	-	expression tag	UNP Q05470
A	-15	HIS	-	expression tag	UNP Q05470
A	-14	HIS	-	expression tag	UNP Q05470
A	-13	HIS	-	expression tag	UNP Q05470
A	-12	HIS	-	expression tag	UNP Q05470
A	-11	SER	-	expression tag	UNP Q05470
A	-10	SER	-	expression tag	UNP Q05470
A	-9	GLY	-	expression tag	UNP Q05470
A	-8	LEU	-	expression tag	UNP Q05470
A	-7	VAL	-	expression tag	UNP Q05470
A	-6	PRO	-	expression tag	UNP Q05470
A	-5	ARG	-	expression tag	UNP Q05470
A	-4	GLY	-	expression tag	UNP Q05470
A	-3	SER	-	expression tag	UNP Q05470
A	-2	SER	-	expression tag	UNP Q05470
A	169	SER	CYS	engineered mutation	UNP Q05470
B	-21	MET	-	initiating methionine	UNP Q05470
B	-20	GLY	-	expression tag	UNP Q05470
B	-19	SER	-	expression tag	UNP Q05470
B	-18	SER	-	expression tag	UNP Q05470

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	HIS	-	expression tag	UNP Q05470
B	-16	HIS	-	expression tag	UNP Q05470
B	-15	HIS	-	expression tag	UNP Q05470
B	-14	HIS	-	expression tag	UNP Q05470
B	-13	HIS	-	expression tag	UNP Q05470
B	-12	HIS	-	expression tag	UNP Q05470
B	-11	SER	-	expression tag	UNP Q05470
B	-10	SER	-	expression tag	UNP Q05470
B	-9	GLY	-	expression tag	UNP Q05470
B	-8	LEU	-	expression tag	UNP Q05470
B	-7	VAL	-	expression tag	UNP Q05470
B	-6	PRO	-	expression tag	UNP Q05470
B	-5	ARG	-	expression tag	UNP Q05470
B	-4	GLY	-	expression tag	UNP Q05470
B	-3	SER	-	expression tag	UNP Q05470
B	-2	SER	-	expression tag	UNP Q05470
B	169	SER	CYS	engineered mutation	UNP Q05470

- 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		

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

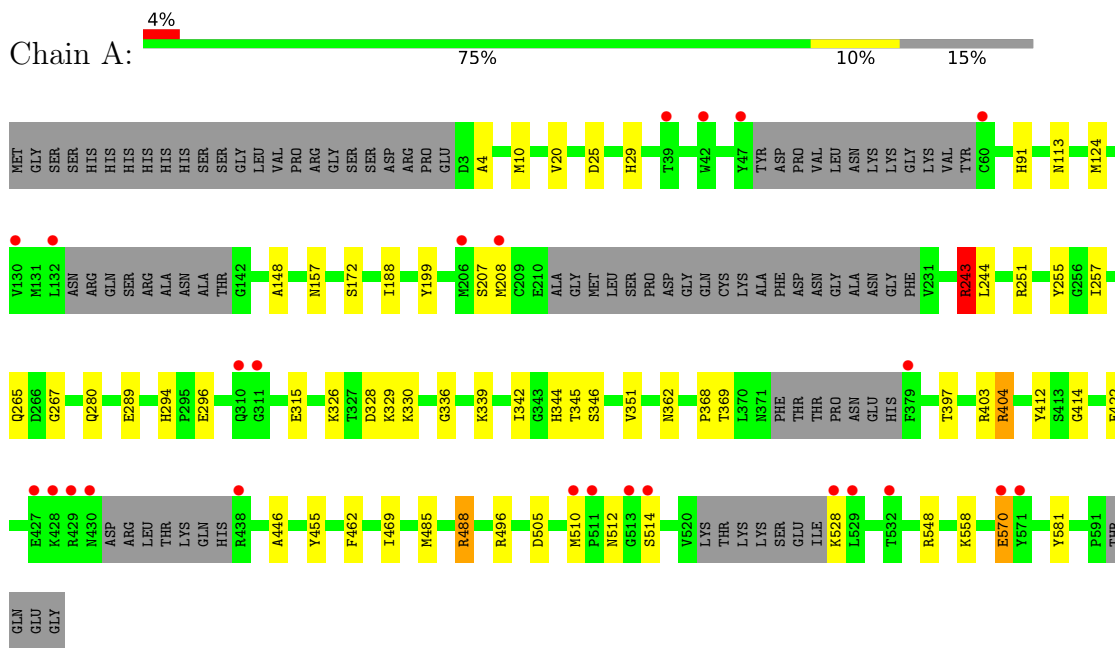
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	35	Total	O	0	0
			35	35		

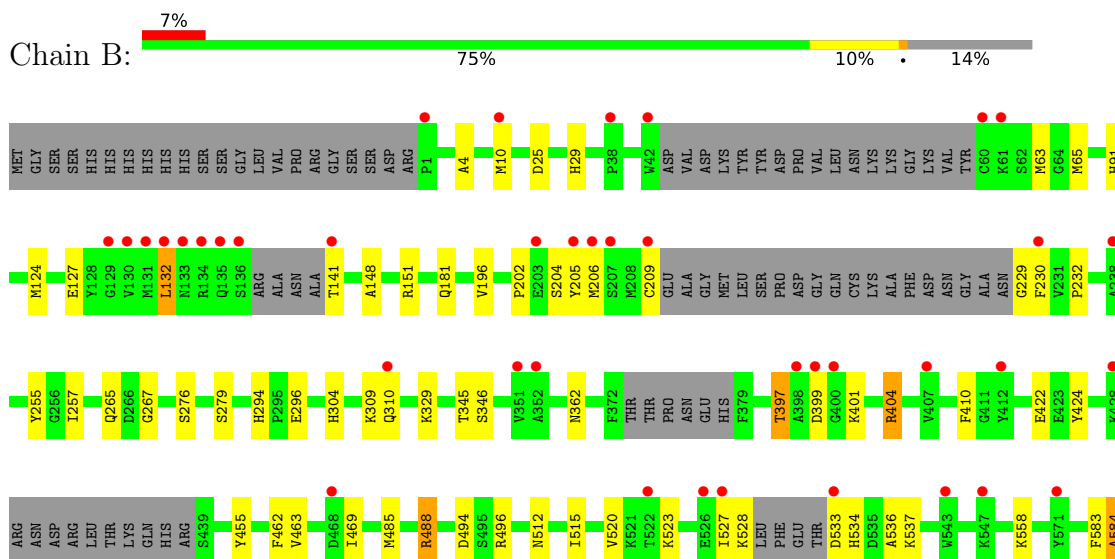
### 3 Residue-property plots

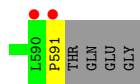
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Polyketide synthase PksL



#### • Molecule 1: Polyketide synthase PksL





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.61Å 105.45Å 89.33Å 90.00° 96.76° 90.00°	Depositor
Resolution (Å)	36.55 – 2.16 36.55 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.2 (36.55-2.16) 99.2 (36.55-2.16)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.221 , 0.254 0.225 , 0.257	Depositor DCC
$R_{free}$ test set	3769 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 32.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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

### 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	0.46	0/4237	0.73	7/5724 (0.1%)
1	B	0.45	0/4260	0.71	6/5752 (0.1%)
All	All	0.46	0/8497	0.72	13/11476 (0.1%)

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	2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	NE-CZ-NH1	-8.43	116.09	120.30
1	B	584	ALA	CB-CA-C	7.08	120.72	110.10
1	B	488	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	B	488	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	A	243	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	A	488	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	488	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	404	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	A	404	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	A	570	GLU	N-CA-CB	5.40	120.32	110.60
1	B	404	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	B	494	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	132	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	ARG	Sidechain
1	A	368	PRO	Peptide

## 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	4149	0	4071	53	0
1	B	4171	0	4105	60	0
2	A	15	0	0	1	0
2	B	5	0	0	0	0
3	A	33	0	0	0	0
3	B	35	0	0	1	0
All	All	8408	0	8176	111	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.

All (111) 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:B:63:MET:CE	1:B:65:MET:HG2	1.39	1.48
1:B:209:CYS:SG	1:B:230:PHE:O	2.03	1.17
1:B:63:MET:CE	1:B:65:MET:CG	2.21	1.17
1:B:63:MET:HE2	1:B:65:MET:CG	1.78	1.09
1:A:446:ALA:HA	1:A:485:MET:CE	1.81	1.08
1:A:512:ASN:ND2	1:A:514:SER:OG	1.87	1.07
1:A:446:ALA:HA	1:A:485:MET:HE2	1.38	1.05
1:B:63:MET:HE2	1:B:65:MET:HG2	1.07	1.03
1:B:533:ASP:O	1:B:537:LYS:HG3	1.63	0.99
1:B:63:MET:HE3	1:B:65:MET:HG2	1.44	0.97
1:B:527:ILE:HD13	1:B:536:ALA:HB1	1.45	0.96
1:B:63:MET:HE3	1:B:65:MET:CG	1.95	0.95
1:A:328:ASP:O	1:A:330:LYS:HE2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:THR:HG21	1:B:401:LYS:O	1.78	0.84
1:B:209:CYS:SG	1:B:230:PHE:N	2.55	0.80
1:A:446:ALA:CA	1:A:485:MET:CE	2.61	0.77
1:B:485:MET:O	1:B:488:ARG:HD2	1.85	0.76
1:A:485:MET:O	1:A:488:ARG:HD2	1.86	0.76
1:A:207:SER:OG	1:B:141:THR:HG23	1.85	0.76
1:A:294:HIS:HD2	1:A:296:GLU:H	1.32	0.74
1:A:512:ASN:O	1:A:512:ASN:OD1	2.07	0.72
1:B:294:HIS:HD2	1:B:296:GLU:H	1.38	0.71
1:B:512:ASN:HB3	1:B:515:ILE:HD12	1.73	0.69
1:B:209:CYS:SG	1:B:230:PHE:C	2.70	0.69
1:B:527:ILE:CD1	1:B:536:ALA:HB1	2.20	0.68
1:B:533:ASP:OD1	1:B:534:HIS:N	2.26	0.68
1:B:533:ASP:O	1:B:537:LYS:CG	2.40	0.67
1:A:446:ALA:C	1:A:485:MET:HE3	2.15	0.67
1:A:446:ALA:CA	1:A:485:MET:HE3	2.25	0.65
1:B:63:MET:HE3	1:B:65:MET:HG3	1.77	0.65
1:A:207:SER:OG	1:B:141:THR:CG2	2.46	0.63
1:B:205:TYR:O	1:B:206:MET:HB2	1.98	0.63
1:B:463:VAL:O	1:B:496:ARG:NH2	2.34	0.60
1:B:196:VAL:HG13	1:B:196:VAL:O	2.01	0.60
1:A:172:SER:HB2	1:A:351:VAL:HG23	1.84	0.59
1:A:404:ARG:HD2	1:A:422:GLU:OE2	2.02	0.59
1:A:244:LEU:HD13	1:A:257:ILE:HD11	1.84	0.59
1:B:404:ARG:HD2	1:B:422:GLU:OE2	2.01	0.59
1:B:202:PRO:O	1:B:205:TYR:O	2.23	0.57
1:B:230:PHE:O	1:B:232:PRO:HD3	2.06	0.56
1:B:255:TYR:HD1	1:B:362:ASN:HD21	1.53	0.56
1:A:339:LYS:HE2	1:A:344:HIS:CE1	2.40	0.56
1:A:113:ASN:ND2	1:A:157:ASN:HD22	2.03	0.55
1:B:63:MET:CE	1:B:65:MET:HG3	2.29	0.55
1:B:345:THR:HG23	3:B:702:HOH:O	2.06	0.55
1:B:209:CYS:SG	1:B:230:PHE:CA	2.95	0.55
1:A:265:GLN:HG3	1:A:267:GLY:H	1.72	0.54
1:B:10:MET:HE3	1:B:255:TYR:CE1	2.43	0.54
1:A:485:MET:CE	1:A:581:TYR:HE1	2.21	0.54
1:A:505:ASP:HA	1:A:510:MET:HG3	1.90	0.54
1:A:10:MET:SD	1:A:20:VAL:HG21	2.47	0.54
1:A:255:TYR:HD1	1:A:362:ASN:HD21	1.55	0.53
1:A:570:GLU:O	1:A:570:GLU:CG	2.57	0.53
1:B:265:GLN:HG3	1:B:267:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:HIS:HD2	1:A:346:SER:H	1.57	0.52
1:B:25:ASP:O	1:B:29:HIS:HD2	1.92	0.52
1:A:199:TYR:OH	1:A:346:SER:OG	2.27	0.52
1:A:289:GLU:OE2	1:A:326:LYS:NZ	2.31	0.52
1:A:113:ASN:HD21	1:A:157:ASN:HD22	1.57	0.52
1:A:485:MET:HE2	1:A:581:TYR:HE1	1.75	0.51
1:B:63:MET:HE1	1:B:65:MET:HG2	1.72	0.51
1:A:512:ASN:OD1	1:A:514:SER:HB3	2.10	0.51
1:A:25:ASP:O	1:A:29:HIS:HD2	1.94	0.50
1:B:304:HIS:CD2	1:B:410:PHE:H	2.28	0.50
1:A:485:MET:CE	1:A:581:TYR:CE1	2.94	0.50
1:A:512:ASN:ND2	1:A:514:SER:CB	2.72	0.50
1:B:527:ILE:O	1:B:528:LYS:C	2.50	0.50
1:A:485:MET:HE1	1:A:581:TYR:CE1	2.47	0.49
1:A:548:ARG:NE	1:A:548:ARG:HA	2.27	0.49
1:A:188:ILE:O	1:A:243:ARG:NH1	2.45	0.49
1:B:196:VAL:O	1:B:196:VAL:CG1	2.61	0.49
1:B:205:TYR:O	1:B:206:MET:CB	2.60	0.49
1:B:462:PHE:CE2	1:B:469:ILE:HD11	2.47	0.49
1:B:527:ILE:O	1:B:533:ASP:HA	2.13	0.48
1:A:462:PHE:CE2	1:A:469:ILE:HD11	2.48	0.48
1:A:570:GLU:O	1:A:570:GLU:HG2	2.13	0.48
1:B:181:GLN:HA	1:B:181:GLN:OE1	2.14	0.48
1:B:257:ILE:HD11	1:B:424:TYR:HD1	1.77	0.48
1:A:512:ASN:C	1:A:514:SER:H	2.17	0.47
1:B:10:MET:CE	1:B:255:TYR:CE1	2.97	0.47
1:A:342:ILE:HD12	1:A:345:THR:HG21	1.97	0.47
1:B:523:LYS:HG3	1:B:558:LYS:O	2.14	0.46
1:A:251:ARG:NH2	2:A:603:SO4:O2	2.47	0.46
1:B:209:CYS:SG	1:B:229:GLY:C	2.94	0.46
1:B:63:MET:HE2	1:B:65:MET:SD	2.55	0.46
1:B:276:SER:HB3	1:B:279:SER:HB2	1.98	0.45
1:B:4:ALA:HB1	1:B:257:ILE:CG2	2.47	0.45
1:A:512:ASN:OD1	1:A:512:ASN:C	2.55	0.45
1:A:199:TYR:OH	1:A:208:MET:HG2	2.17	0.44
1:B:124:MET:SD	1:B:346:SER:HB3	2.57	0.44
1:B:329:LYS:HB2	1:B:329:LYS:HE2	1.80	0.44
1:B:127:GLU:OE1	1:B:204:SER:CB	2.66	0.44
1:A:124:MET:HE1	1:A:412:TYR:HE2	1.82	0.44
1:B:294:HIS:CD2	1:B:296:GLU:HB2	2.53	0.44
1:B:10:MET:HE2	1:B:255:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:PHE:CD2	1:A:469:ILE:HD11	2.53	0.43
1:B:91:HIS:CE1	1:B:148:ALA:HB2	2.54	0.43
1:A:91:HIS:CE1	1:A:148:ALA:HB2	2.54	0.43
1:A:265:GLN:HA	1:A:414:GLY:O	2.18	0.43
1:B:462:PHE:CD2	1:B:469:ILE:HD11	2.54	0.43
1:B:520:VAL:O	1:B:523:LYS:HG2	2.19	0.43
1:A:265:GLN:HE21	1:A:267:GLY:H	1.66	0.42
1:A:397:THR:HG23	1:A:403:ARG:HG2	2.01	0.42
1:B:527:ILE:O	1:B:528:LYS:O	2.37	0.42
1:A:528:LYS:CE	1:A:558:LYS:O	2.68	0.42
1:A:4:ALA:HB1	1:A:257:ILE:CG2	2.49	0.42
1:A:336:GLY:HA3	1:A:369:THR:OG1	2.19	0.41
1:A:339:LYS:HE2	1:A:344:HIS:ND1	2.35	0.41
1:A:280:GLN:OE1	1:A:315:GLU:HA	2.21	0.41
1:B:583:PHE:C	1:B:584:ALA:O	2.58	0.40
1:B:309:LYS:HG3	1:B:310:GLN:N	2.37	0.40

There are no symmetry-related clashes.

## 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	513/617 (83%)	499 (97%)	14 (3%)	0	100	100
1	B	517/617 (84%)	497 (96%)	20 (4%)	0	100	100
All	All	1030/1234 (84%)	996 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	439/515 (85%)	436 (99%)	3 (1%)	84	89
1	B	442/515 (86%)	436 (99%)	6 (1%)	67	72
All	All	881/1030 (86%)	872 (99%)	9 (1%)	76	81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	LYS
1	A	455	TYR
1	A	496	ARG
1	B	132	LEU
1	B	151	ARG
1	B	397	THR
1	B	399	ASP
1	B	455	TYR
1	B	591	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	90	GLN
1	A	113	ASN
1	A	265	GLN
1	A	294	HIS
1	A	341	ASN
1	A	344	HIS
1	A	362	ASN
1	A	389	ASN
1	A	451	GLN
1	A	512	ASN
1	B	29	HIS
1	B	90	GLN

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Mol	Chain	Res	Type
1	B	96	GLN
1	B	265	GLN
1	B	294	HIS
1	B	304	HIS
1	B	341	ASN
1	B	355	GLN
1	B	362	ASN
1	B	363	HIS
1	B	389	ASN
1	B	451	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	603	-	4,4,4	0.33	0	6,6,6	0.11	0
2	SO4	B	601	-	4,4,4	0.36	0	6,6,6	0.11	0
2	SO4	A	602	-	4,4,4	0.38	0	6,6,6	0.16	0
2	SO4	A	601	-	4,4,4	0.31	0	6,6,6	0.32	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	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 ⓘ

### 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	527/617 (85%)	0.08	25 (4%) 31 41	22, 35, 72, 107	0
1	B	531/617 (86%)	0.15	41 (7%) 13 18	23, 36, 79, 118	0
All	All	1058/1234 (85%)	0.11	66 (6%) 20 27	22, 36, 77, 118	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	571	TYR	6.6
1	A	513	GLY	5.7
1	B	60	CYS	5.6
1	A	47	TYR	5.5
1	B	132	LEU	5.2
1	B	133	ASN	5.2
1	A	529	LEU	4.9
1	A	132	LEU	4.7
1	B	134	ARG	4.6
1	B	526	GLU	4.6
1	B	42	TRP	4.5
1	B	136	SER	4.3
1	A	379	PHE	4.1
1	B	398	ALA	4.1
1	B	135	GLN	4.0
1	B	533	ASP	3.8
1	B	209	CYS	3.8
1	B	522	THR	3.7
1	B	399	ASP	3.6
1	A	438	ARG	3.6
1	B	400	GLY	3.6
1	A	514	SER	3.5
1	B	527	ILE	3.3
1	B	130	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	571	TYR	3.2
1	B	61	LYS	3.2
1	B	206	MET	3.1
1	B	590	LEU	3.0
1	A	310	GLN	3.0
1	A	570	GLU	2.9
1	A	42	TRP	2.9
1	A	428	LYS	2.9
1	B	310	GLN	2.9
1	B	412	TYR	2.8
1	B	428	LYS	2.8
1	A	60	CYS	2.7
1	A	39	THR	2.6
1	B	351	VAL	2.6
1	A	430	ASN	2.6
1	A	130	VAL	2.6
1	B	129	GLY	2.5
1	A	511	PRO	2.5
1	B	141	THR	2.5
1	B	205	TYR	2.4
1	B	407	VAL	2.4
1	A	528	LYS	2.4
1	A	532	THR	2.3
1	B	1	PRO	2.3
1	B	207	SER	2.2
1	B	468	ASP	2.2
1	A	427	GLU	2.2
1	B	238	ALA	2.2
1	B	131	MET	2.2
1	B	203	GLU	2.2
1	B	352	ALA	2.2
1	A	206	MET	2.1
1	B	10	MET	2.1
1	B	547	LYS	2.1
1	B	591	PRO	2.1
1	B	38	PRO	2.0
1	A	311	GLY	2.0
1	A	429	ARG	2.0
1	B	230	PHE	2.0
1	A	208	MET	2.0
1	A	510	MET	2.0
1	B	543	TRP	2.0

## 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 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	602	5/5	0.90	0.22	72,80,90,90	0
2	SO4	A	603	5/5	0.92	0.21	80,90,93,101	0
2	SO4	A	601	5/5	0.95	0.22	61,63,64,68	0
2	SO4	B	601	5/5	0.96	0.23	64,65,70,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.