



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:52 AM GMT

PDB ID : 2J3L  
Title : PROLYL-TRNA SYNTHETASE FROM ENTEROCOCCUS FAECALIS  
COMPLEXED WITH A PROLYL-ADENYLATE ANALOGUE ('5'-O-(N-(L-PROLYL)-SULFAMOYL)ADENOSINE)  
Authors : Crepin, T.; Yaremchuk, A.; Tukalo, M.; Cusack, S.  
Deposited on : 2006-08-22  
Resolution : 2.30 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (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

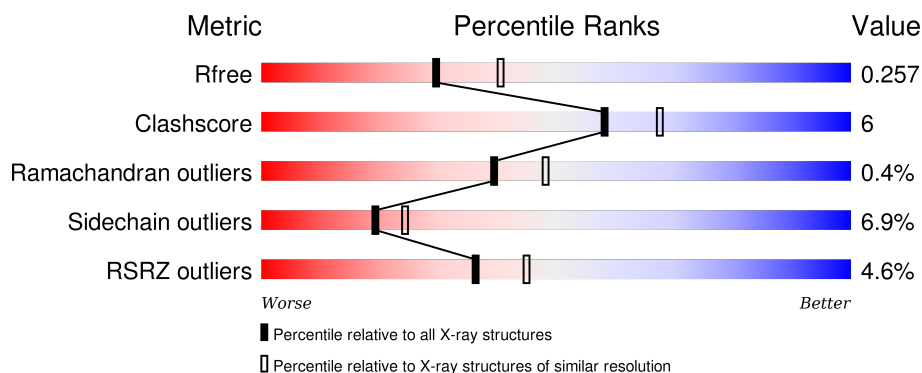
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	572	<div> <div>4%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
1	B	572	<div> <div>5%</div> <div>81%</div> <div>17%</div> <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	1569	-	-	X	-
2	SO4	B	1575	-	-	-	X
2	SO4	B	1578	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9327 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 PROLYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	0	0
			4461	2807	756	877	21			
1	B	570	Total	C	N	O	S	0	0	0
			4498	2827	762	888	21			

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



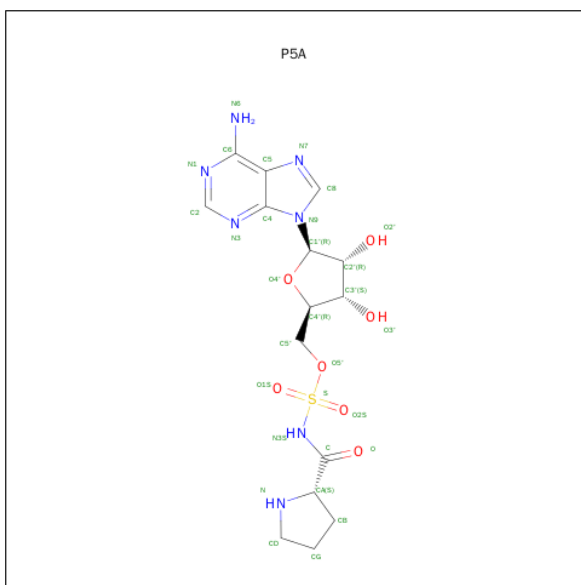
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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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		
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		
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 '5'-O-(N-(L-PROLYL)-SULFAMOYL)ADENOSINE (three-letter code: P5A) (formula: C<sub>15</sub>H<sub>21</sub>N<sub>7</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 30	C 15	N 7	O 7	S 1	0	0
3	B	1	Total 30	C 15	N 7	O 7	S 1	0	0

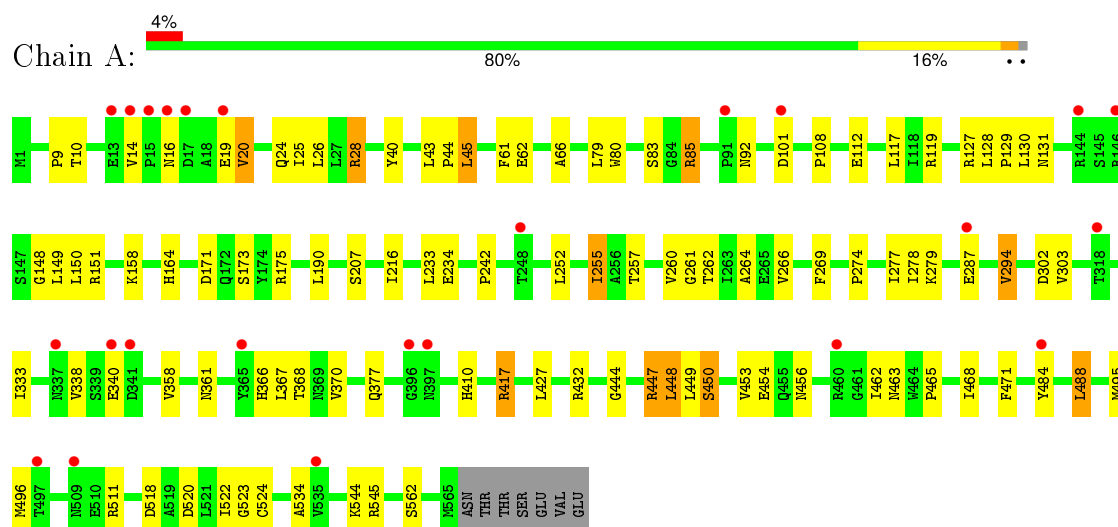
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	84	Total O 84 84	0	0
4	B	119	Total O 119 119	0	0

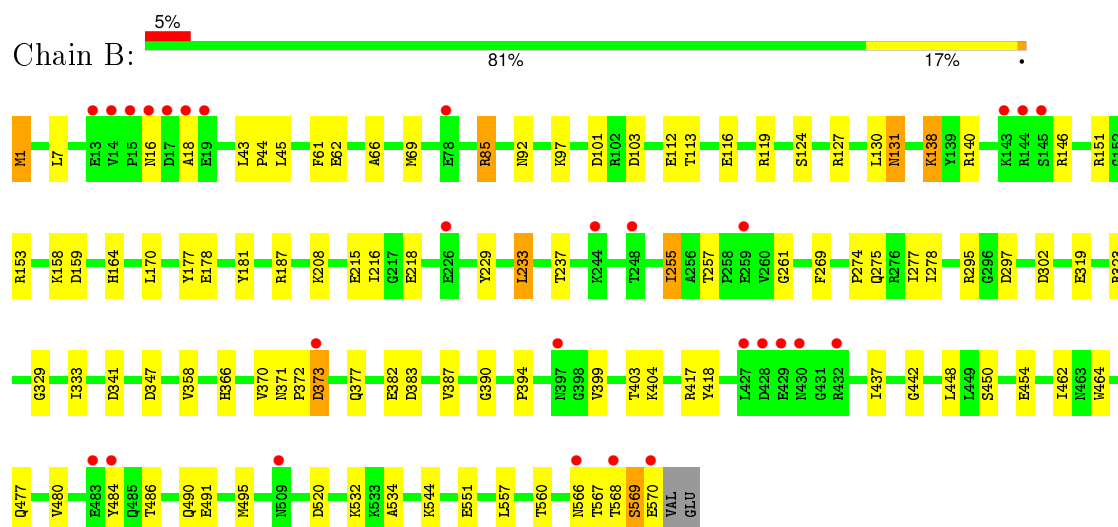
### 3 Residue-property plots

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: PROLYL-TRNA SYNTHETASE



#### • Molecule 1: PROLYL-TRNA SYNTHETASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.44Å 121.44Å 178.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.50 – 2.30 29.45 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (100.50-2.30) 97.8 (29.45-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.206 , 0.268 0.202 , 0.257	Depositor DCC
$R_{free}$ test set	2037 reflections (3.60%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 58612 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9327	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: P5A, 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	0.59	0/4535	0.72	3/6121 (0.0%)
1	B	0.62	0/4572	0.74	3/6172 (0.0%)
All	All	0.60	0/9107	0.73	6/12293 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	85	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	85	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	432	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	557	LEU	CA-CB-CG	5.15	127.14	115.30
1	B	233	LEU	CA-CB-CG	5.02	126.84	115.30

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	4461	0	4414	56	0
1	B	4498	0	4445	53	0
2	A	50	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	55	0	0	0	0
3	A	30	0	21	1	0
3	B	30	0	21	0	0
4	A	84	0	0	0	0
4	B	119	0	0	4	0
All	All	9327	0	8901	107	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 6.

All (107) 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:28:ARG:HG2	1:A:28:ARG:HH11	1.32	0.93
1:B:187:ARG:HE	1:B:569:SER:HB2	1.48	0.79
1:B:85:ARG:HD3	1:B:112:GLU:OE2	1.82	0.79
1:B:215:GLU:HG3	4:B:2053:HOH:O	1.84	0.78
1:B:486:THR:O	1:B:490:GLN:HG2	1.89	0.73
1:A:262:THR:O	1:A:266:VAL:HG23	1.95	0.67
1:A:85:ARG:HD3	1:A:112:GLU:OE2	1.93	0.67
1:B:1:MET:HE2	4:B:2001:HOH:O	1.95	0.66
1:A:25:ILE:HD11	1:A:453:VAL:CG1	2.25	0.66
1:B:295:ARG:HD2	1:B:297:ASP:OD1	1.95	0.66
1:A:417:ARG:NH1	2:A:1569:SO4:O1	2.31	0.63
1:A:417:ARG:NH1	2:A:1569:SO4:S	2.72	0.62
1:A:465:PRO:HB2	1:A:468:ILE:HD12	1.80	0.62
1:B:138:LYS:NZ	1:B:159:ASP:OD1	2.26	0.60
1:A:25:ILE:HD11	1:A:453:VAL:HG13	1.84	0.60
1:A:28:ARG:CG	1:A:28:ARG:HH11	2.10	0.59
1:B:319:GLU:O	1:B:323:ARG:HG3	2.02	0.59
1:B:85:ARG:HD2	1:B:418:TYR:HE1	1.68	0.59
1:B:358:VAL:HG22	1:B:370:VAL:HG21	1.85	0.58
1:B:275:GLN:HG3	1:B:295:ARG:HD3	1.86	0.56
1:B:16:ASN:C	1:B:18:ALA:H	2.09	0.56
1:A:255:ILE:HD11	1:A:269:PHE:HE2	1.70	0.56
1:B:278:ILE:HB	1:B:358:VAL:HG12	1.87	0.56
1:B:520:ASP:O	1:B:544:LYS:HE2	2.06	0.55
1:A:279:LYS:HB3	1:A:294:VAL:HG12	1.88	0.55
1:A:257:THR:OG1	1:A:366:HIS:HD2	1.90	0.54
1:B:484:TYR:CE1	1:B:534:ALA:HB3	2.42	0.54
1:B:484:TYR:CD1	1:B:534:ALA:HB3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ILE:HD11	1:B:269:PHE:HE2	1.74	0.53
1:B:116:GLU:OE1	1:B:119:ARG:CZ	2.57	0.52
1:A:25:ILE:HA	1:A:28:ARG:HB2	1.91	0.52
1:A:358:VAL:HG22	1:A:370:VAL:HG21	1.91	0.52
1:A:252:LEU:HD11	1:A:367:LEU:HB3	1.91	0.51
1:A:164:HIS:HE1	1:A:173:SER:OG	1.93	0.51
1:A:14:VAL:HG22	1:A:28:ARG:HD2	1.92	0.51
1:B:237:THR:HG22	1:B:383:ASP:OD2	2.09	0.51
1:A:150:LEU:CD2	1:A:450:SER:HB3	2.41	0.50
1:A:471:PHE:HB2	1:A:524:CYS:SG	2.52	0.50
1:A:257:THR:HB	1:A:260:VAL:HB	1.94	0.49
1:A:216:ILE:HD11	1:A:454:GLU:HG3	1.93	0.49
1:B:131:ASN:ND2	1:B:177:TYR:OH	2.39	0.48
1:B:43:LEU:HB3	1:B:44:PRO:CD	2.43	0.48
1:B:164:HIS:HB2	1:B:437:ILE:HB	1.96	0.48
1:A:20:VAL:O	1:A:24:GLN:HG3	2.14	0.48
1:A:10:THR:HG21	1:A:518:ASP:OD1	2.14	0.47
1:A:117:LEU:HD21	1:B:7:LEU:CD2	2.43	0.47
1:A:444:GLY:O	1:A:448:LEU:HB2	2.14	0.47
1:A:252:LEU:CD1	1:A:370:VAL:HG22	2.44	0.47
1:B:216:ILE:HD11	1:B:454:GLU:HG3	1.96	0.47
1:B:477:GLN:NE2	1:B:480:VAL:HA	2.30	0.47
1:B:404:LYS:HE3	4:B:2054:HOH:O	2.14	0.47
1:A:28:ARG:HG2	1:A:28:ARG:NH1	2.12	0.46
1:A:278:ILE:HB	1:A:358:VAL:HG12	1.97	0.46
1:A:25:ILE:HD11	1:A:453:VAL:HG11	1.97	0.46
1:B:85:ARG:CD	1:B:112:GLU:OE2	2.59	0.46
1:B:274:PRO:HA	1:B:277:ILE:HD12	1.97	0.46
1:A:488:LEU:HD12	1:A:534:ALA:HA	1.98	0.46
1:A:447:ARG:NH2	3:A:1576:P5A:H2'	2.31	0.45
1:A:520:ASP:HA	1:A:544:LYS:HE2	1.98	0.45
1:B:372:PRO:O	1:B:373:ASP:HB2	2.15	0.45
1:A:171:ASP:O	1:A:175:ARG:HG3	2.16	0.45
1:A:83:SER:O	1:A:417:ARG:NH2	2.49	0.45
1:B:371:ASN:HA	1:B:372:PRO:HD3	1.90	0.45
1:B:257:THR:OG1	1:B:366:HIS:HD2	2.00	0.45
1:A:234:GLU:HB3	1:A:303:VAL:HG21	1.99	0.45
1:B:140:ARG:O	1:B:153:ARG:HA	2.17	0.44
1:B:158:LYS:NZ	1:B:181:TYR:OH	2.50	0.44
1:A:449:LEU:C	1:A:449:LEU:HD23	2.38	0.44
1:A:20:VAL:HG13	1:A:454:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:PHE:CE2	1:B:158:LYS:HD2	2.53	0.43
1:B:178:GLU:OE2	1:B:208:LYS:NZ	2.47	0.43
1:B:1:MET:CE	1:B:1:MET:HA	2.48	0.43
1:B:43:LEU:HB3	1:B:44:PRO:HD2	2.00	0.43
1:A:150:LEU:O	1:A:447:ARG:HD3	2.19	0.43
1:B:390:GLY:HA2	1:B:399:VAL:HG13	2.00	0.43
1:A:80:TRP:CH2	1:A:108:PRO:HG2	2.54	0.43
1:A:61:PHE:HB3	1:A:66:ALA:HB3	1.99	0.43
1:B:347:ASP:HA	1:B:382:GLU:O	2.19	0.42
1:B:462:ILE:HG21	1:B:464:TRP:CE2	2.54	0.42
1:B:532:LYS:HB2	4:B:2115:HOH:O	2.19	0.42
1:B:229:TYR:CZ	1:B:394:PRO:HG3	2.55	0.42
1:A:252:LEU:HD12	1:A:370:VAL:HG22	2.01	0.42
1:A:523:GLY:HA2	1:A:544:LYS:HE3	2.02	0.42
1:A:128:LEU:HB3	1:A:129:PRO:HA	2.02	0.42
1:B:61:PHE:HB3	1:B:66:ALA:HB3	2.02	0.42
1:A:274:PRO:HA	1:A:277:ILE:HD12	2.01	0.42
1:A:495:MET:SD	1:A:496:MET:HE1	2.59	0.42
1:A:207:SER:HG	1:A:410:HIS:HE2	1.68	0.41
1:B:170:LEU:HD22	1:B:437:ILE:HG22	2.01	0.41
1:B:158:LYS:O	1:B:442:GLY:HA2	2.20	0.41
1:A:262:THR:HG22	1:A:264:ALA:N	2.36	0.41
1:B:1:MET:HA	1:B:1:MET:HE2	2.03	0.41
1:A:45:LEU:HD21	1:A:522:ILE:HG12	2.01	0.41
1:A:40:TYR:CZ	1:A:148:GLY:HA2	2.55	0.41
1:A:9:PRO:HD2	1:A:43:LEU:HD23	2.02	0.41
1:A:44:PRO:HD3	1:B:69:MET:CG	2.51	0.41
1:B:295:ARG:CD	1:B:297:ASP:OD1	2.66	0.41
1:B:16:ASN:C	1:B:18:ALA:N	2.74	0.41
1:A:333:ILE:HA	1:A:361:ASN:OD1	2.20	0.41
1:A:25:ILE:HD13	1:A:462:ILE:HG12	2.01	0.41
1:B:372:PRO:O	1:B:373:ASP:CB	2.69	0.40
1:A:207:SER:OG	1:A:410:HIS:NE2	2.52	0.40
1:B:491:GLU:O	1:B:495:MET:HB2	2.22	0.40
1:B:97:LYS:HE2	1:B:103:ASP:OD1	2.21	0.40
1:A:456:ASN:HB3	1:A:463:ASN:O	2.22	0.40
1:B:329:GLY:O	1:B:333:ILE:HG23	2.21	0.40
1:A:158:LYS:HD3	1:A:158:LYS:O	2.20	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	563/572 (98%)	550 (98%)	10 (2%)	3 (0%)	34	41
1	B	568/572 (99%)	557 (98%)	10 (2%)	1 (0%)	52	64
All	All	1131/1144 (99%)	1107 (98%)	20 (2%)	4 (0%)	39	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	ASP
1	A	261	GLY
1	B	261	GLY
1	A	242	PRO

### 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	480/487 (99%)	445 (93%)	35 (7%)	17	22
1	B	485/487 (100%)	453 (93%)	32 (7%)	21	27
All	All	965/974 (99%)	898 (93%)	67 (7%)	19	24

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	19	GLU

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Mol	Chain	Res	Type
1	A	20	VAL
1	A	26	LEU
1	A	28	ARG
1	A	45	LEU
1	A	62	GLU
1	A	79	LEU
1	A	92	ASN
1	A	101	ASP
1	A	119	ARG
1	A	127	ARG
1	A	130	LEU
1	A	131	ASN
1	A	149	LEU
1	A	151	ARG
1	A	190	LEU
1	A	233	LEU
1	A	255	ILE
1	A	287	GLU
1	A	294	VAL
1	A	338	VAL
1	A	340	GLU
1	A	368	THR
1	A	377	GLN
1	A	417	ARG
1	A	427	LEU
1	A	447	ARG
1	A	448	LEU
1	A	450	SER
1	A	484	TYR
1	A	488	LEU
1	A	511	ARG
1	A	545	ARG
1	A	562	SER
1	B	1	MET
1	B	45	LEU
1	B	62	GLU
1	B	92	ASN
1	B	101	ASP
1	B	113	THR
1	B	124	SER
1	B	127	ARG
1	B	130	LEU

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Mol	Chain	Res	Type
1	B	131	ASN
1	B	138	LYS
1	B	146	ARG
1	B	151	ARG
1	B	218	GLU
1	B	233	LEU
1	B	255	ILE
1	B	302	ASP
1	B	341	ASP
1	B	373	ASP
1	B	377	GLN
1	B	387	VAL
1	B	403	THR
1	B	417	ARG
1	B	448	LEU
1	B	450	SER
1	B	551	GLU
1	B	560	THR
1	B	566	ASN
1	B	567	THR
1	B	568	THR
1	B	569	SER
1	B	570	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	337	ASN
1	A	366	HIS
1	A	377	GLN
1	A	388	GLN
1	B	16	ASN
1	B	92	ASN
1	B	131	ASN
1	B	366	HIS
1	B	456	ASN
1	B	566	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 ⓘ

23 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	1566	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	A	1567	-	4,4,4	0.27	0	6,6,6	0.25	0
2	SO4	A	1568	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	A	1569	-	4,4,4	0.29	0	6,6,6	0.25	0
2	SO4	A	1570	-	4,4,4	0.18	0	6,6,6	0.25	0
2	SO4	A	1571	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	1572	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	A	1573	-	4,4,4	0.08	0	6,6,6	0.17	0
2	SO4	A	1574	-	4,4,4	0.19	0	6,6,6	0.16	0
2	SO4	A	1575	-	4,4,4	0.15	0	6,6,6	0.13	0
3	P5A	A	1576	-	26,33,33	2.12	3 (11%)	32,49,49	2.98	7 (21%)
2	SO4	B	1571	-	4,4,4	0.12	0	6,6,6	0.25	0
2	SO4	B	1572	-	4,4,4	0.30	0	6,6,6	0.34	0
2	SO4	B	1573	-	4,4,4	0.21	0	6,6,6	0.21	0
2	SO4	B	1574	-	4,4,4	0.21	0	6,6,6	0.31	0
2	SO4	B	1575	-	4,4,4	0.38	0	6,6,6	0.49	0
2	SO4	B	1576	-	4,4,4	0.31	0	6,6,6	0.38	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	1577	-	4,4,4	0.18	0	6,6,6	0.48	0
2	SO4	B	1578	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	B	1579	-	4,4,4	0.10	0	6,6,6	0.30	0
2	SO4	B	1580	-	4,4,4	0.18	0	6,6,6	0.21	0
2	SO4	B	1581	-	4,4,4	0.19	0	6,6,6	0.14	0
3	P5A	B	1582	-	26,33,33	2.16	3 (11%)	32,49,49	2.43	9 (28%)

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	1566	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1567	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1568	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1569	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1570	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1571	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1572	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1573	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1574	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1575	-	-	0/0/0/0	0/0/0/0
3	P5A	A	1576	-	-	0/13/42/42	0/4/4/4
2	SO4	B	1571	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1572	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1573	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1574	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1575	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1576	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1577	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1578	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1579	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1580	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1581	-	-	0/0/0/0	0/0/0/0
3	P5A	B	1582	-	-	0/13/42/42	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1582	P5A	C-N3S	-2.97	1.33	1.37
3	A	1576	P5A	C-N3S	-2.05	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1576	P5A	O1S-S	5.93	1.47	1.42
3	B	1582	P5A	O2S-S	5.99	1.47	1.42
3	B	1582	P5A	O1S-S	8.04	1.49	1.42
3	A	1576	P5A	O2S-S	8.07	1.49	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1576	P5A	N3-C2-N1	-11.48	120.10	128.89
3	B	1582	P5A	N3-C2-N1	-10.35	120.97	128.89
3	A	1576	P5A	O2S-S-O1S	-8.26	110.88	120.77
3	B	1582	P5A	O2S-S-O1S	-4.15	115.80	120.77
3	A	1576	P5A	C4-C5-N7	-3.43	106.32	109.48
3	A	1576	P5A	C2'-C1'-N9	-3.39	109.12	114.29
3	A	1576	P5A	C1'-N9-C4	-3.21	122.10	126.94
3	B	1582	P5A	C2'-C1'-N9	-3.00	109.70	114.29
3	B	1582	P5A	O1S-S-N3S	-2.84	104.70	108.50
3	B	1582	P5A	C4-C5-N7	-2.58	107.11	109.48
3	B	1582	P5A	O2S-S-N3S	2.05	111.23	108.50
3	B	1582	P5A	CD-N-CA	2.22	112.75	107.22
3	B	1582	P5A	O-C-N3S	2.27	125.60	121.62
3	B	1582	P5A	O4'-C1'-N9	2.53	113.39	108.10
3	A	1576	P5A	CD-N-CA	2.68	113.88	107.22
3	A	1576	P5A	O2S-S-N3S	5.25	115.50	108.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1569	SO4	2	0
3	A	1576	P5A	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, 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	565/572 (98%)	0.27	24 (4%)	40 49	10, 25, 37, 47	0
1	B	570/572 (99%)	0.15	28 (4%)	33 42	8, 19, 34, 45	0
All	All	1135/1144 (99%)	0.21	52 (4%)	36 45	8, 22, 37, 47	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	ASN	7.6
1	A	13	GLU	6.3
1	B	144	ARG	4.7
1	B	14	VAL	4.4
1	A	287	GLU	4.3
1	B	143	LYS	4.0
1	B	430	ASN	3.9
1	B	484	TYR	3.9
1	B	145	SER	3.8
1	B	19	GLU	3.7
1	B	17	ASP	3.7
1	A	14	VAL	3.6
1	B	428	ASP	3.6
1	A	318	THR	3.5
1	B	226	GLU	3.5
1	A	17	ASP	3.4
1	A	460	ARG	3.4
1	B	570	GLU	3.4
1	A	484	TYR	3.3
1	A	397	ASN	3.2
1	B	18	ALA	3.2
1	B	13	GLU	3.2
1	B	432	ARG	3.2
1	B	259	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	16	ASN	3.1
1	B	568	THR	3.1
1	A	248	THR	2.9
1	B	509	ASN	2.8
1	A	497	THR	2.7
1	A	146	ARG	2.7
1	A	19	GLU	2.7
1	B	15	PRO	2.7
1	A	144	ARG	2.7
1	B	429	GLU	2.7
1	B	248	THR	2.6
1	A	365	TYR	2.6
1	B	483	GLU	2.6
1	A	341	ASP	2.5
1	A	340	GLU	2.5
1	B	244	LYS	2.5
1	A	15	PRO	2.4
1	B	397	ASN	2.3
1	A	535	VAL	2.3
1	A	396	GLY	2.3
1	B	78	GLU	2.3
1	A	509	ASN	2.2
1	A	101	ASP	2.1
1	B	373	ASP	2.1
1	A	337	ASN	2.1
1	B	427	LEU	2.0
1	B	566	ASN	2.0
1	A	91	PRO	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 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	1578	5/5	0.89	0.28	3.63	92,93,93,94	0
2	SO4	B	1575	5/5	0.94	0.18	2.84	50,51,53,54	0
2	SO4	A	1574	5/5	0.89	0.18	0.99	88,88,89,89	0
2	SO4	A	1572	5/5	0.93	0.24	0.50	83,83,83,83	0
2	SO4	B	1572	5/5	0.99	0.12	-0.57	39,39,41,41	0
3	P5A	B	1582	30/30	0.97	0.13	-0.72	15,18,22,25	0
3	P5A	A	1576	30/30	0.98	0.13	-0.88	17,19,21,22	0
2	SO4	B	1574	5/5	0.96	0.12	-1.00	50,50,52,52	0
2	SO4	A	1569	5/5	0.97	0.12	-1.02	45,45,49,50	0
2	SO4	A	1567	5/5	0.97	0.10	-1.75	44,45,46,46	0
2	SO4	B	1576	5/5	0.97	0.14	-1.87	50,50,51,51	0
2	SO4	A	1573	5/5	0.92	0.25	-	75,75,76,76	0
2	SO4	B	1580	5/5	0.89	0.28	-	91,91,92,92	0
2	SO4	B	1573	5/5	0.98	0.13	-	46,46,48,50	0
2	SO4	A	1575	5/5	0.85	0.26	-	88,88,89,89	0
2	SO4	A	1571	5/5	0.96	0.07	-	75,75,76,76	0
2	SO4	B	1579	5/5	0.94	0.21	-	65,65,65,66	0
2	SO4	A	1568	5/5	0.98	0.09	-	42,43,44,44	0
2	SO4	B	1571	5/5	0.98	0.08	-	46,47,48,48	0
2	SO4	B	1577	5/5	0.92	0.16	-	56,58,59,60	0
2	SO4	B	1581	5/5	0.91	0.14	-	98,98,99,99	0
2	SO4	A	1570	5/5	0.95	0.13	-	49,49,51,51	0
2	SO4	A	1566	5/5	0.94	0.13	-	50,51,53,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.