



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:32 AM GMT

PDB ID : 3ITE  
Title : The third adenylation domain of the fungal SidN non-ribosomal peptide synthetase  
Authors : Lee, T.V.; Lott, J.S.; Johnson, R.D.; Johnson, L.J.; Arcus, V.L.  
Deposited on : 2009-08-28  
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  
<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 : trunk26765  
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

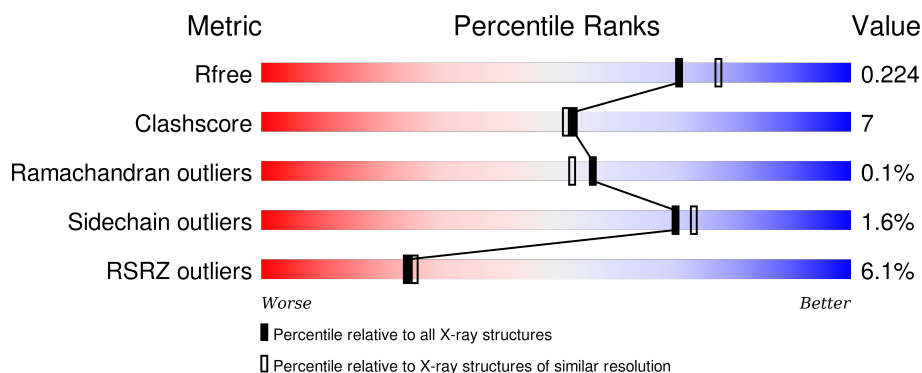
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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	562	<div> <div></div> <div>65% 6% • 28%</div> </div>
1	B	562	<div> <div>9%</div> <div>75% 13% • 10%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7397 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 SidN siderophore synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	Se	0	1	1
			3075	1944	536	580	6	9			
1	B	503	Total	C	N	O	S	Se	0	0	1
			3855	2437	668	733	7	10			

- 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		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cl 1	0	0
3	A	1	Total 1	Cl 1	0	0

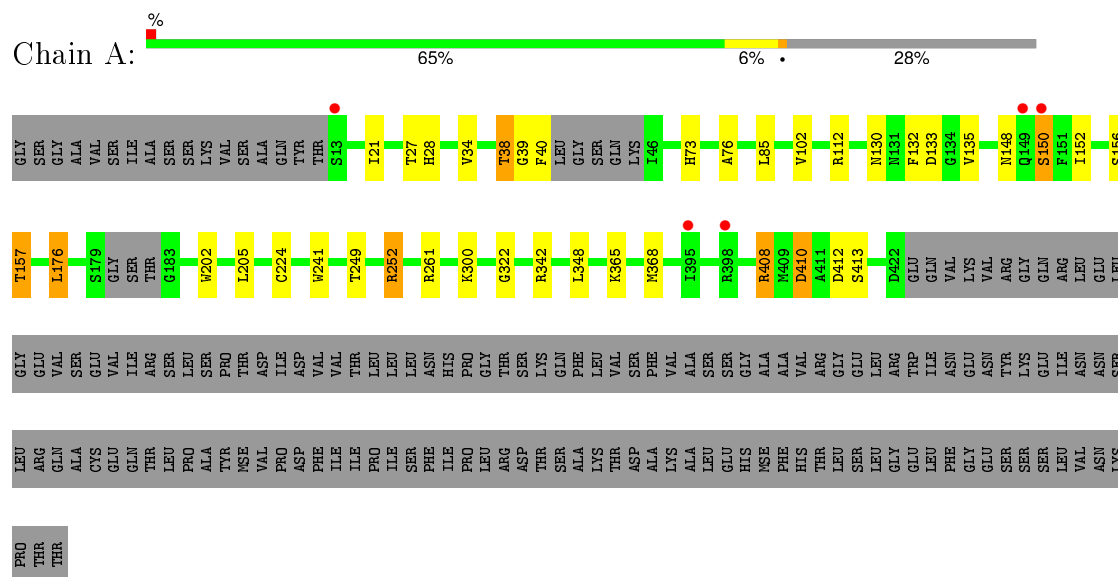
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	230	Total 230	O 230	0	0
4	B	225	Total 225	O 225	0	0

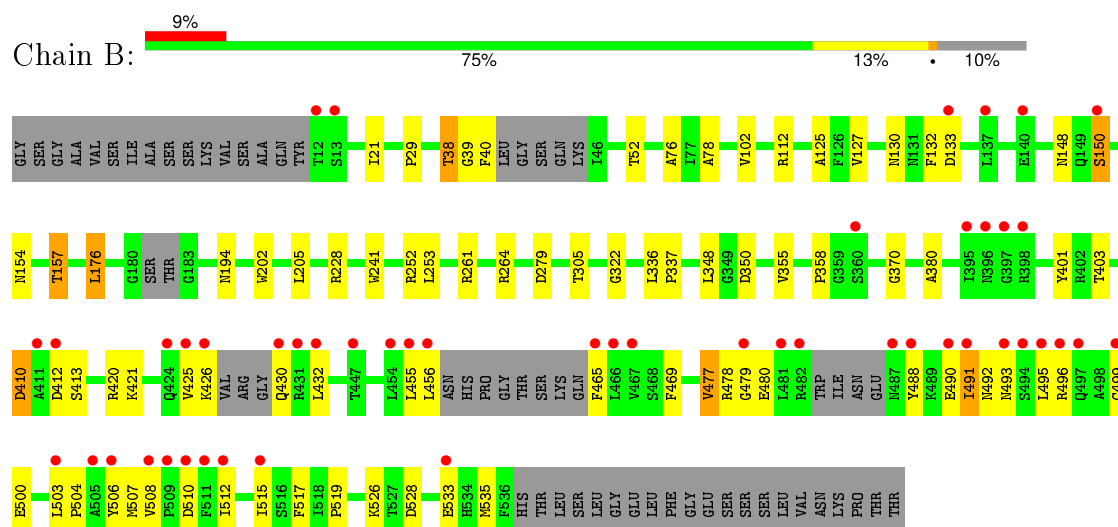
### 3 Residue-property plots

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: SidN siderophore synthetase



- Molecule 1: SidN siderophore synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.60Å 75.28Å 84.14Å 114.85° 94.78° 90.18°	Depositor
Resolution (Å)	42.62 – 2.00 42.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (42.62-2.00) 82.0 (42.62-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.194 , 0.228 0.192 , 0.224	Depositor DCC
$R_{free}$ test set	3690 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.6	EDS
Estimated twinning fraction	0.159 for -h,k,-k-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 72881 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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: SO4, CL

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	0.90	0/3135	0.87	3/4243 (0.1%)
1	B	0.82	0/3918	0.82	3/5299 (0.1%)
All	All	0.85	0/7053	0.84	6/9542 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ARG	NE-CZ-NH2	-12.62	113.99	120.30
1	B	252	ARG	NE-CZ-NH2	-10.95	114.83	120.30
1	A	252	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	B	252	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	A	176	LEU	CA-CB-CG	-7.14	98.89	115.30
1	B	176	LEU	CA-CB-CG	-6.86	99.52	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	3075	0	3059	30	0
1	B	3855	0	3851	68	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	230	0	0	7	0
4	B	225	0	0	4	0
All	All	7397	0	6910	92	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 (92) 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:492:ASN:OD1	1:B:496:ARG:HG3	1.77	0.84
1:A:156:SER:CB	1:B:479:GLY:HA2	2.20	0.72
1:B:425:VAL:HG13	1:B:455:LEU:HD22	1.75	0.68
1:B:432:LEU:HD13	1:B:507:MSE:HG2	1.76	0.68
1:B:432:LEU:HD12	1:B:507:MSE:HE2	1.81	0.63
1:B:477:VAL:HG13	1:B:517:PHE:CD2	2.36	0.60
1:A:156:SER:HB3	1:B:479:GLY:HA2	1.82	0.60
1:A:152:ILE:HG21	1:B:480:GLU:HB3	1.84	0.60
1:B:491:ILE:HD12	1:B:491:ILE:C	2.22	0.59
1:A:28:HIS:ND1	4:A:826:HOH:O	2.33	0.57
1:B:425:VAL:HG11	1:B:455:LEU:HB2	1.86	0.57
1:B:205:LEU:HD13	1:B:348:LEU:HD21	1.86	0.57
1:A:365:LYS:HB2	1:A:368[A]:MSE:SE	2.54	0.57
1:A:27:THR:HG21	1:B:253:LEU:HD23	1.87	0.56
1:B:322:GLY:HA2	4:B:959:HOH:O	2.05	0.56
1:B:130:ASN:HB3	1:B:133:ASP:CG	2.27	0.55
1:A:39:GLY:O	1:A:40:PHE:HB2	2.07	0.54
1:B:358:PRO:HB3	1:B:421:LYS:HD2	1.90	0.54
1:B:38:THR:HG22	1:B:39:GLY:H	1.73	0.54
1:B:420:ARG:HG2	1:B:526:LYS:HG2	1.89	0.54
1:B:425:VAL:HG12	1:B:425:VAL:O	2.07	0.53
1:B:21:ILE:HD11	1:B:241:TRP:CE3	2.44	0.53
1:A:38:THR:HG22	1:A:39:GLY:H	1.74	0.53
1:B:112:ARG:HB3	4:B:979:HOH:O	2.09	0.53
1:A:156:SER:HB2	1:B:479:GLY:HA2	1.92	0.52
1:B:504:PRO:HB2	1:B:506:TYR:CE1	2.44	0.52
1:B:490:GLU:O	1:B:493:ASN:HB2	2.09	0.52
1:B:519:PRO:HB2	1:B:528:ASP:HB3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:LYS:HA	1:B:430:GLN:O	2.10	0.51
1:A:130:ASN:HB3	1:A:133:ASP:CG	2.31	0.51
1:B:425:VAL:O	1:B:432:LEU:HB3	2.10	0.51
1:A:21:ILE:HD11	1:A:241:TRP:CE3	2.46	0.51
1:B:492:ASN:ND2	1:B:512:ILE:H	2.09	0.49
1:A:202:TRP:CE2	1:A:348:LEU:HD13	2.48	0.49
1:B:469:PHE:HB3	1:B:515:ILE:HD13	1.94	0.49
1:A:322:GLY:HA2	4:A:829:HOH:O	2.12	0.49
1:A:205:LEU:HD13	1:A:348:LEU:HD21	1.95	0.48
1:B:425:VAL:CG1	1:B:455:LEU:HD22	2.43	0.48
1:B:495:LEU:O	1:B:499:CYS:CB	2.62	0.48
1:B:420:ARG:CG	1:B:526:LYS:HG2	2.43	0.48
1:A:252:ARG:NH2	4:A:909:HOH:O	2.47	0.47
1:B:504:PRO:HB2	1:B:506:TYR:CD1	2.50	0.47
1:A:76:ALA:HB1	1:A:102:VAL:HG21	1.96	0.47
1:A:408:ARG:NH1	4:A:843:HOH:O	2.48	0.46
1:B:412:ASP:O	1:B:413:SER:HB2	2.16	0.46
1:A:148:ASN:OD1	1:A:150:SER:HB3	2.16	0.46
1:A:40:PHE:HA	1:A:261:ARG:NH1	2.30	0.46
1:B:39:GLY:O	1:B:40:PHE:HB2	2.15	0.46
1:A:130:ASN:HA	4:A:928:HOH:O	2.16	0.45
1:B:355:VAL:HG12	1:B:370:GLY:HA3	1.97	0.45
1:B:148:ASN:OD1	1:B:150:SER:HB3	2.17	0.45
1:B:503:LEU:HD23	1:B:504:PRO:HD2	1.98	0.45
1:B:154:ASN:O	1:B:157:THR:HB	2.17	0.45
1:B:465:PHE:HB3	1:B:510:ASP:OD2	2.17	0.45
1:B:228:ARG:NH2	4:B:750:HOH:O	2.50	0.44
1:B:40:PHE:HA	1:B:261:ARG:NH1	2.33	0.44
1:B:76:ALA:HB1	1:B:102:VAL:HG21	1.99	0.44
1:B:488:TYR:HB3	1:B:491:ILE:HG23	1.99	0.44
1:B:455:LEU:HD12	1:B:465:PHE:O	2.18	0.43
1:B:432:LEU:CD1	1:B:507:MSE:HG2	2.46	0.43
1:A:34:VAL:HG23	1:A:85:LEU:HD22	2.00	0.43
1:B:506:TYR:OH	1:B:507:MSE:HE3	2.19	0.43
1:B:495:LEU:O	1:B:499:CYS:HB2	2.19	0.43
1:B:495:LEU:O	1:B:499:CYS:HB3	2.18	0.43
1:A:300:LYS:HE2	1:A:342:ARG:HG2	2.01	0.43
1:B:336:LEU:HB3	1:B:337:PRO:HD2	2.01	0.43
1:B:500:GLU:HG3	1:B:508:VAL:HG11	2.00	0.43
1:B:456:LEU:HD21	1:B:533:GLU:HG2	2.01	0.43
1:B:264:ARG:HD3	4:B:951:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:HA	1:B:478:ARG:HD3	2.00	0.42
1:B:350:ASP:OD1	1:B:350:ASP:C	2.58	0.42
1:A:410:ASP:HB3	1:A:412:ASP:OD1	2.20	0.42
1:A:73:HIS:CE1	4:A:732:HOH:O	2.73	0.42
1:B:477:VAL:HG13	1:B:517:PHE:CE2	2.54	0.42
1:B:401:TYR:CE2	1:B:403:THR:HA	2.55	0.42
1:A:412:ASP:O	1:A:413:SER:HB2	2.19	0.41
1:B:78:ALA:O	1:B:125:ALA:HA	2.20	0.41
1:A:224:CYS:HB2	1:A:249:THR:HB	2.03	0.41
1:B:500:GLU:HG3	1:B:508:VAL:HG21	2.03	0.41
1:B:490:GLU:O	1:B:493:ASN:N	2.54	0.41
1:B:127:VAL:HG11	1:B:132:PHE:CD2	2.55	0.41
1:A:202:TRP:CZ2	1:A:348:LEU:CD1	3.03	0.41
1:B:456:LEU:CD2	1:B:533:GLU:HG2	2.50	0.41
1:B:279:ASP:OD1	1:B:305:THR:OG1	2.36	0.41
1:B:410:ASP:HB3	1:B:412:ASP:OD1	2.20	0.41
1:B:535:MSE:HE2	1:B:535:MSE:HB3	2.03	0.41
1:B:492:ASN:C	1:B:492:ASN:OD1	2.59	0.40
1:B:202:TRP:CE2	1:B:348:LEU:HD13	2.56	0.40
1:A:132:PHE:HA	1:A:135:VAL:HG21	2.04	0.40
1:B:194:ASN:OD1	1:B:380:ALA:HA	2.22	0.40
1:A:112:ARG:HB3	4:A:907:HOH:O	2.21	0.40
1:B:29:PRO:O	1:B:52:THR:HB	2.22	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	397/562 (71%)	388 (98%)	9 (2%)	0	100	100
1	B	491/562 (87%)	464 (94%)	26 (5%)	1 (0%)	52	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	888/1124 (79%)	852 (96%)	35 (4%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	477	VAL

### 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	335/463 (72%)	329 (98%)	6 (2%)	66	69
1	B	423/463 (91%)	417 (99%)	6 (1%)	74	77
All	All	758/926 (82%)	746 (98%)	12 (2%)	70	73

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	150	SER
1	A	157	THR
1	A	176	LEU
1	A	408	ARG
1	A	410	ASP
1	B	38	THR
1	B	150	SER
1	B	157	THR
1	B	176	LEU
1	B	410	ASP
1	B	491	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	B	208	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	558	-	4,4,4	0.60	0	6,6,6	0.67	0
2	SO4	B	558	-	4,4,4	0.38	0	6,6,6	0.86	0

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	558	-	-	0/0/0/0	0/0/0/0
2	SO4	B	558	-	-	0/0/0/0	0/0/0/0

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	394/562 (70%)	-0.25	5 (1%) 79 80	14, 26, 60, 83	0
1	B	493/562 (87%)	0.25	49 (9%) 9 10	15, 33, 92, 126	0
All	All	887/1124 (78%)	0.03	54 (6%) 25 26	14, 29, 81, 126	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	425	VAL	10.8
1	B	465	PHE	8.7
1	B	488	TYR	8.3
1	B	431	ARG	7.6
1	B	511	PHE	6.7
1	B	455	LEU	6.1
1	B	491	ILE	5.9
1	B	395	ILE	5.7
1	B	432	LEU	5.7
1	B	466	LEU	5.5
1	B	456	LEU	5.4
1	B	509	PRO	5.2
1	B	430	GLN	5.0
1	B	426	LYS	4.8
1	B	454	LEU	4.7
1	B	506	TYR	4.5
1	B	505	ALA	4.2
1	B	512	ILE	4.0
1	B	12	THR	3.6
1	B	487	ASN	3.6
1	B	150	SER	3.6
1	B	496	ARG	3.5
1	B	467	VAL	3.4
1	B	499	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	424	GLN	3.3
1	B	508	VAL	3.2
1	B	398	ARG	3.1
1	B	494	SER	3.0
1	B	482	ARG	3.0
1	B	510	ASP	3.0
1	B	397	GLY	3.0
1	B	493	ASN	2.9
1	B	140	GLU	2.9
1	B	481	LEU	2.9
1	B	497	GLN	2.6
1	B	396	ASN	2.6
1	B	137	LEU	2.6
1	B	495	LEU	2.6
1	B	503	LEU	2.6
1	A	13	SER	2.5
1	A	395	ILE	2.5
1	B	13	SER	2.5
1	B	515	ILE	2.4
1	B	411	ALA	2.4
1	A	150	SER	2.3
1	B	133	ASP	2.3
1	B	490	GLU	2.2
1	B	412	ASP	2.2
1	B	447	THR	2.2
1	A	149	GLN	2.2
1	B	479	GLY	2.1
1	B	360	SER	2.1
1	A	398	ARG	2.0
1	B	533	GLU	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 [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	A	558	5/5	0.99	0.11	-0.16	27,40,46,46	0
3	CL	A	559	1/1	0.99	0.08	-0.55	24,24,24,24	0
2	SO4	B	558	5/5	0.98	0.10	-0.62	30,46,48,54	0
3	CL	B	559	1/1	0.99	0.07	-1.14	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.