



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 04:47 AM EDT

PDB ID : 4TWA  
Title : Crystal Structure of Prolyl-tRNA Synthetase (PRS) from Plasmodium falciparum  
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Deposited on : 2014-06-30  
Resolution : 3.00 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 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 : 2.35.1  
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) : 2.35.1

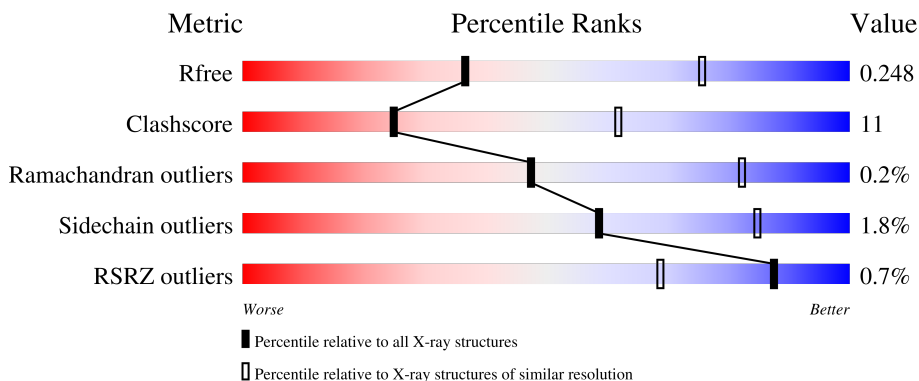
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	497	76% 21% ..
1	B	497	% 72% 23% ..

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7948 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 Proline-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	488	3980	2575	657	727	21	0	4	0
1	B	480	3850	2490	641	697	22	0	3	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	GLY	-	expression tag	UNP Q8I5R7
A	251	ALA	-	expression tag	UNP Q8I5R7
A	252	MET	-	expression tag	UNP Q8I5R7
A	253	ALA	-	expression tag	UNP Q8I5R7
B	250	GLY	-	expression tag	UNP Q8I5R7
B	251	ALA	-	expression tag	UNP Q8I5R7
B	252	MET	-	expression tag	UNP Q8I5R7
B	253	ALA	-	expression tag	UNP Q8I5R7

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	B	22	Total	O	0	0
			22	22		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.24Å 104.11Å 111.42Å 90.00° 92.30° 90.00°	Depositor
Resolution (Å)	38.79 – 3.00 47.15 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.79-3.00) 99.9 (47.15-2.99)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.172 , 0.249 0.174 , 0.248	Depositor DCC
$R_{free}$ test set	1548 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.6	Xtrriage
Anisotropy	0.120	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0/4094	0.60	0/5544
1	B	0.46	0/3959	0.62	0/5371
All	All	0.46	0/8053	0.61	0/10915

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3980	0	3914	90	0
1	B	3850	0	3729	89	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	30	0	0	1	0
3	B	25	0	0	1	0
4	A	35	0	0	0	0
4	B	22	0	0	2	0
All	All	7948	0	7643	167	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 11.



All (167) 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:279:TYR:HB3	1:B:342:VAL:HG12	1.41	0.99
1:B:512:THR:HG22	1:B:514:ARG:H	1.30	0.92
1:B:670:ASN:N	1:B:670:ASN:HD22	1.70	0.89
1:B:670:ASN:HD22	1:B:670:ASN:H	1.27	0.82
1:A:279:TYR:HB3	1:B:342:VAL:CG1	2.16	0.75
1:B:342:VAL:HG12	1:B:342:VAL:O	1.87	0.74
1:A:387:THR:HB	1:A:406:LEU:CD1	2.21	0.70
1:A:674:MET:HE2	1:A:741:LEU:HD22	1.73	0.70
1:A:389:VAL:HG22	1:A:404:GLU:HG3	1.73	0.70
1:B:303:ASN:O	1:B:307:LYS:HG2	1.93	0.69
1:B:729:CYS:SG	1:B:730:PHE:N	2.67	0.67
1:A:589:HIS:O	1:A:593[A]:ARG:HG3	1.95	0.67
1:A:319:PHE:HE1	1:A:345:TYR:HD2	1.42	0.67
1:B:670:ASN:N	1:B:670:ASN:ND2	2.43	0.66
1:A:381:LYS:HA	1:A:412:THR:HG22	1.77	0.65
1:A:387:THR:HB	1:A:406:LEU:HD11	1.76	0.65
1:A:525:ASP:HB3	1:A:527:LYS:H	1.62	0.64
1:B:361:GLU:HG2	1:B:411:HIS:NE2	2.13	0.64
1:A:406:LEU:O	1:A:513:THR:HG23	1.98	0.64
1:A:667:ASN:OD1	1:A:671:LYS:NZ	2.32	0.62
1:A:686:GLU:HG2	1:A:713:PRO:HG3	1.81	0.62
1:B:484:THR:HG23	1:B:505:HIS:CE1	2.34	0.61
1:A:631:LEU:O	1:A:635:GLN:HG3	2.02	0.60
1:B:448:LYS:HE2	1:B:452:GLU:HB3	1.83	0.60
1:A:316:PHE:HB2	1:A:360:SER:HB2	1.83	0.59
1:A:431:TYR:O	1:A:434:TRP:HB3	2.03	0.59
1:A:390:ARG:NH2	3:A:804:SO4:O2	2.34	0.59
1:B:427:ILE:HG21	1:B:509:TRP:CG	2.37	0.59
1:B:450:GLU:OE2	1:B:453:LYS:NZ	2.27	0.59
1:A:279:TYR:CD2	1:B:342:VAL:HG11	2.38	0.58
1:B:435:TYR:CZ	1:B:476:ALA:HB1	2.38	0.58
1:B:674:MET:HE3	1:B:714:LEU:HD12	1.86	0.58
1:A:408:GLN:HE22	1:A:509:TRP:HD1	1.52	0.58
1:A:496:ASP:OD1	1:A:500:VAL:N	2.30	0.58
1:B:399:PHE:O	1:B:514:ARG:HA	2.04	0.58
1:A:279:TYR:CB	1:B:342:VAL:CG1	2.82	0.57
1:A:431:TYR:HH	1:A:509:TRP:HD1	1.52	0.57
1:A:279:TYR:CB	1:B:342:VAL:HG12	2.27	0.57
1:B:449:SER:OG	1:B:686:GLU:OE2	2.22	0.57
1:B:304:LYS:NZ	4:B:909:HOH:O	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:VAL:CG1	1:B:342:VAL:O	2.53	0.56
1:B:357:ARG:HH11	1:B:357:ARG:HG2	1.70	0.56
1:B:385:TRP:CE3	1:B:408:GLN:HB2	2.41	0.56
1:B:412:THR:HG23	1:B:509:TRP:CH2	2.41	0.56
1:A:709:GLY:HA2	1:A:744:ARG:HD3	1.88	0.55
1:B:357:ARG:HG2	1:B:357:ARG:NH1	2.22	0.55
1:A:335:PHE:CZ	1:A:343:THR:HG21	2.42	0.54
1:A:319:PHE:HE1	1:A:345:TYR:CD2	2.24	0.54
1:A:525:ASP:OD2	1:A:616:ARG:NH1	2.37	0.54
1:A:589:HIS:O	1:A:593[B]:ARG:HG3	2.08	0.54
1:A:589:HIS:CE1	1:A:593[A]:ARG:HE	2.26	0.54
1:A:443:ILE:HD13	1:A:463:ALA:HB1	1.89	0.53
1:B:655:SER:HA	1:B:673:LYS:HD3	1.90	0.53
1:A:328:GLU:HG2	1:B:319:PHE:HE1	1.74	0.53
1:A:303:ASN:O	1:A:307[B]:LYS:HD3	2.08	0.53
1:A:675:VAL:HG22	1:A:711:MET:HE1	1.91	0.53
1:B:319:PHE:H	1:B:339:VAL:HG13	1.74	0.53
1:A:289:PRO:HB3	1:B:312:GLU:HB3	1.92	0.52
1:B:690:LYS:HG2	1:B:711:MET:O	2.08	0.52
1:B:417:GLU:N	1:B:505:HIS:HD2	2.08	0.52
1:A:387:THR:HB	1:A:406:LEU:HD12	1.91	0.52
1:A:431:TYR:OH	1:A:509:TRP:HD1	1.92	0.52
1:B:341:TRP:CH2	1:B:362:THR:HG22	2.45	0.52
1:A:405:PHE:CD1	1:A:512:THR:HG21	2.45	0.51
1:A:662:PHE:HA	1:A:665:VAL:HG23	1.91	0.51
1:A:679:TRP:CD2	1:A:681:GLU:HA	2.46	0.51
1:A:636:MET:O	1:A:640:ILE:HG13	2.10	0.51
1:A:495:GLU:HG3	1:A:501:LYS:HG3	1.93	0.51
1:A:435:TYR:CZ	1:A:476:ALA:HB1	2.45	0.51
1:A:512:THR:HG22	1:A:513:THR:N	2.25	0.50
1:B:383:ASN:OD1	1:B:408:GLN:HG2	2.12	0.50
1:A:432:ARG:O	1:A:436[A]:GLU:HG3	2.10	0.50
1:B:385:TRP:CZ3	1:B:408:GLN:HB2	2.47	0.50
1:A:279:TYR:CG	1:B:342:VAL:HG11	2.47	0.49
1:A:359:THR:HG22	1:A:409:GLU:OE1	2.13	0.49
1:A:709:GLY:O	1:A:744:ARG:NH1	2.44	0.49
1:B:525:ASP:HB3	1:B:527:LYS:H	1.76	0.49
1:A:516:ILE:O	1:A:520:ILE:HG13	2.13	0.49
1:A:519:MET:HE2	1:A:520:ILE:HG12	1.95	0.49
1:A:319:PHE:CE1	1:A:345:TYR:CD2	3.01	0.49
1:B:274:GLU:HG2	1:B:288:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:PHE:HD1	1:B:473:ALA:HB2	1.77	0.48
1:B:431:TYR:O	1:B:434:TRP:HB3	2.12	0.48
1:B:716:ILE:HG23	1:B:739:TRP:O	2.14	0.48
1:B:431:TYR:OH	1:B:509:TRP:HD1	1.95	0.48
1:A:259:ILE:H	1:A:259:ILE:HD12	1.77	0.48
1:B:427:ILE:HG21	1:B:509:TRP:CD1	2.49	0.48
1:B:590:TRP:CE3	1:B:593:ARG:HD2	2.49	0.48
1:B:417:GLU:N	1:B:505:HIS:CD2	2.82	0.47
1:B:432:ARG:NH2	1:B:433:ARG:HG2	2.28	0.47
1:B:657:VAL:HG21	1:B:668:ALA:HB1	1.96	0.47
1:B:412:THR:HG23	1:B:509:TRP:HH2	1.76	0.47
1:B:470:ASN:OD1	1:B:472:ARG:HB2	2.14	0.47
1:A:267:THR:O	1:A:271:VAL:HG23	2.14	0.47
1:A:453:LYS:HG3	1:A:454:PHE:O	2.15	0.47
1:B:295:TRP:CD1	1:B:406:LEU:HD23	2.49	0.47
1:B:428:LEU:HD22	1:B:461:SER:HB2	1.97	0.47
1:B:680:CYS:HG	1:B:729:CYS:HG	1.62	0.47
1:B:484:THR:CG2	1:B:505:HIS:CE1	2.97	0.47
1:B:453:LYS:HD2	1:B:457:ALA:O	2.15	0.46
1:A:599:ILE:HG12	1:A:613:ILE:HG13	1.97	0.46
1:B:405:PHE:HB2	1:B:513:THR:HG22	1.96	0.46
1:B:322:LYS:HA	1:B:323:ASN:HA	1.51	0.45
1:B:541:VAL:HG21	1:B:590:TRP:CD1	2.50	0.45
1:B:560:LYS:HA	1:B:560:LYS:HE2	1.98	0.45
1:A:385:TRP:CE3	1:A:408:GLN:HB2	2.52	0.45
1:A:427:ILE:HG21	1:A:509:TRP:CG	2.51	0.45
1:A:649:LYS:NZ	1:A:653:ASP:OD2	2.41	0.45
1:A:389:VAL:HG21	1:B:317:PRO:HB3	1.98	0.45
1:A:575:TYR:CE2	1:A:577:ASP:HB3	2.52	0.45
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.87	0.45
1:A:691:LYS:HE3	1:A:695:ARG:NE	2.32	0.45
1:B:355:ALA:O	1:B:358:PRO:HD3	2.17	0.45
1:A:525:ASP:HB2	1:A:616:ARG:HH22	1.82	0.45
1:A:711:MET:HG3	1:A:742:PHE:HB3	1.98	0.45
1:B:599:ILE:HG12	1:B:613:ILE:HG13	1.99	0.44
1:B:562:ILE:HA	1:B:565:ILE:HD12	1.99	0.44
1:B:589:HIS:CE1	1:B:593:ARG:HE	2.36	0.44
1:B:682:ASP:HB2	1:B:685:THR:HG23	2.00	0.44
1:A:364:MET:HE3	1:A:364:MET:HB3	1.85	0.44
1:A:408:GLN:NE2	1:A:509:TRP:CD1	2.85	0.44
1:A:669:LEU:HD23	1:A:669:LEU:HA	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ASP:O	1:A:433:ARG:HG3	2.17	0.44
1:A:431:TYR:CE1	1:A:511:CYS:HB2	2.53	0.44
1:A:296:GLU:OE2	1:B:313:ASN:HB2	2.17	0.43
1:A:439:LEU:O	1:A:441:VAL:HG23	2.18	0.43
1:A:393:PHE:HB2	1:A:396:PRO:HB3	1.99	0.43
1:B:532:PRO:HA	1:B:533:PRO:HD3	1.90	0.43
1:A:389:VAL:HG22	1:A:404:GLU:CG	2.43	0.43
1:A:294:ILE:O	1:A:298:VAL:HG22	2.19	0.43
1:B:529:LEU:HD21	1:B:531:LEU:HD21	2.01	0.43
1:B:416[B]:ASN:ND2	1:B:418:GLU:HG2	2.34	0.43
1:B:263:SER:O	1:B:267:THR:HG23	2.19	0.43
1:A:316:PHE:HB2	1:A:360:SER:CB	2.48	0.43
1:A:349:ASN:HA	1:A:350:LEU:HA	1.74	0.43
1:A:630:LEU:O	1:A:634:GLN:HG3	2.19	0.43
1:B:429:ASP:O	1:B:433:ARG:HG3	2.18	0.43
1:A:316:PHE:CD2	1:A:316:PHE:N	2.87	0.42
1:B:294:ILE:HG12	1:B:535:VAL:HB	2.01	0.42
1:A:674:MET:CE	1:A:714:LEU:HD12	2.49	0.42
1:B:605:ASP:HB3	1:B:610:SER:O	2.19	0.42
1:A:324:LYS:HA	1:A:324:LYS:HD2	1.88	0.42
1:B:341:TRP:CG	1:B:345:TYR:CE1	3.07	0.42
1:B:430:LEU:HD23	1:B:430:LEU:HA	1.77	0.42
1:B:533:PRO:HB3	1:B:637:LEU:HD22	2.00	0.42
1:B:575:TYR:CZ	1:B:577:ASP:HB3	2.53	0.42
1:B:336:SER:HA	1:B:337:PRO:HD3	1.80	0.42
1:B:341:TRP:CD1	1:B:358:PRO:HG3	2.55	0.42
1:A:286:ILE:HD13	1:B:316:PHE:CE1	2.55	0.42
1:A:679:TRP:CE2	1:A:681:GLU:HA	2.55	0.42
1:A:467:ILE:HG22	1:A:470:ASN:H	1.85	0.41
1:B:339:VAL:HG12	1:B:340:ALA:O	2.20	0.41
1:A:359:THR:HB	1:A:361:GLU:H	1.84	0.41
1:A:674:MET:HE3	1:A:714:LEU:HD12	2.02	0.41
1:B:305:GLU:O	1:B:308:LYS:HB2	2.21	0.41
1:B:445:LYS:NZ	4:B:907:HOH:O	2.47	0.41
1:A:328:GLU:HG3	1:A:391:TRP:HB2	2.03	0.41
1:A:279:TYR:CG	1:B:342:VAL:CG1	3.04	0.41
1:A:410:GLY:HA3	1:A:509:TRP:CE2	2.56	0.41
1:B:386:ASN:HB3	1:B:407:TRP:CH2	2.56	0.41
1:A:593[B]:ARG:HE	1:A:593[B]:ARG:HB3	1.52	0.41
1:B:650:LYS:HA	1:B:650:LYS:HD2	1.83	0.41
1:B:481:TYR:CZ	1:B:483:GLY:HA2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:VAL:HG23	1:A:574:VAL:HG13	2.03	0.40
1:A:364:MET:HE3	1:A:368:PHE:CZ	2.56	0.40
1:B:618:ASN:HB3	3:B:805:SO4:O4	2.22	0.40
1:B:644:LEU:HA	1:B:644:LEU:HD23	1.84	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	488/497 (98%)	455 (93%)	32 (7%)	1 (0%)	47 82
1	B	477/497 (96%)	435 (91%)	41 (9%)	1 (0%)	47 82
All	All	965/994 (97%)	890 (92%)	73 (8%)	2 (0%)	47 82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	354	ILE
1	A	350	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/450 (95%)	423 (99%)	6 (1%)	67	88
1	B	405/450 (90%)	395 (98%)	10 (2%)	47	79
All	All	834/900 (93%)	818 (98%)	16 (2%)	59	84

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	SER
1	A	316	PHE
1	A	345	TYR
1	A	408	GLN
1	A	663	SER
1	A	727	MET
1	B	252	MET
1	B	416[A]	ASN
1	B	416[B]	ASN
1	B	505	HIS
1	B	555	ILE
1	B	556	HIS
1	B	632	GLU
1	B	670	ASN
1	B	671	LYS
1	B	729	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	505	HIS
1	B	589	HIS
1	B	670	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	$\# Z  > 2$
3	SO4	A	804	-	4,4,4	0.08	0	6,6,6	0.16	0
3	SO4	A	808	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	B	805	-	4,4,4	0.14	0	6,6,6	0.14	0
3	SO4	B	807	-	4,4,4	0.16	0	6,6,6	0.21	0
3	SO4	A	806	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	A	809	-	4,4,4	0.20	0	6,6,6	0.08	0
3	SO4	B	808	-	4,4,4	0.14	0	6,6,6	0.13	0
3	SO4	B	806	-	4,4,4	0.14	0	6,6,6	0.11	0
3	SO4	A	805	-	4,4,4	0.19	0	6,6,6	0.08	0
3	SO4	B	804	-	4,4,4	0.18	0	6,6,6	0.15	0
3	SO4	A	807	-	4,4,4	0.12	0	6,6,6	0.12	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	SO4	1	0
3	B	805	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	488/497 (98%)	-0.65	2 (0%) 92 79	18, 42, 80, 135	0
1	B	480/497 (96%)	-0.39	5 (1%) 82 59	26, 57, 100, 168	0
All	All	968/994 (97%)	-0.52	7 (0%) 87 69	18, 48, 92, 168	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	GLU	3.8
1	A	346	GLY	3.1
1	B	698	LEU	2.7
1	B	347	ASP	2.7
1	B	346	GLY	2.5
1	B	351	PRO	2.3
1	A	347	ASP	2.1

### 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	CL	B	801	1/1	0.76	0.23	58,58,58,58	1
3	SO4	B	808	5/5	0.79	0.40	123,125,127,129	5
2	CL	B	802	1/1	0.86	0.12	66,66,66,66	0
2	CL	A	803	1/1	0.87	0.17	44,44,44,44	1
3	SO4	A	809	5/5	0.88	0.18	73,75,78,78	5
3	SO4	A	807	5/5	0.88	0.19	125,126,127,127	0
3	SO4	B	806	5/5	0.90	0.18	115,121,123,124	0
3	SO4	A	806	5/5	0.90	0.24	84,88,89,90	5
3	SO4	B	807	5/5	0.92	0.17	90,96,98,102	0
2	CL	B	803	1/1	0.92	0.07	45,45,45,45	0
3	SO4	B	805	5/5	0.93	0.19	106,107,111,114	0
3	SO4	A	808	5/5	0.93	0.18	100,101,105,109	0
2	CL	A	801	1/1	0.96	0.10	44,44,44,44	0
3	SO4	A	804	5/5	0.96	0.13	71,72,78,79	0
2	CL	A	802	1/1	0.97	0.08	53,53,53,53	0
3	SO4	A	805	5/5	0.98	0.14	61,64,66,67	0
3	SO4	B	804	5/5	0.98	0.10	28,36,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.