



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:21 PM GMT

PDB ID : 1JZS  
Title : Isoleucyl-tRNA synthetase Complexed with mupirocin  
Authors : Nakama, T.; Nureki, O.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2001-09-17  
Resolution : 2.50 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

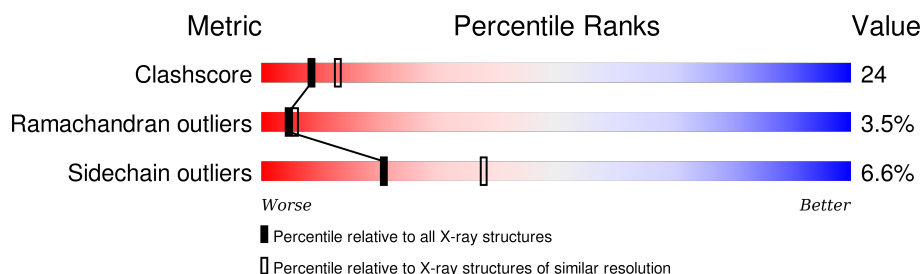
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	821	

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
3	MRC	A	1301	X	-	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6735 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.

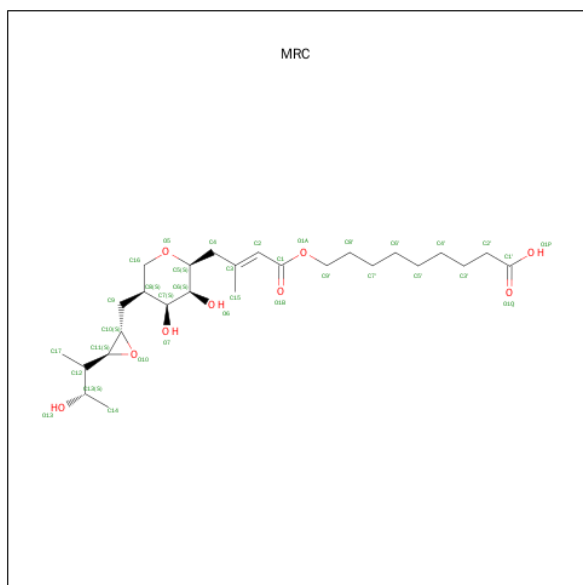
- Molecule 1 is a protein called Isoleucyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	821	Total	C	N	O	S	0	0	0
			6698	4334	1144	1200	20			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is MUPIROCIN (three-letter code: MRC) (formula: C<sub>26</sub>H<sub>44</sub>O<sub>9</sub>).



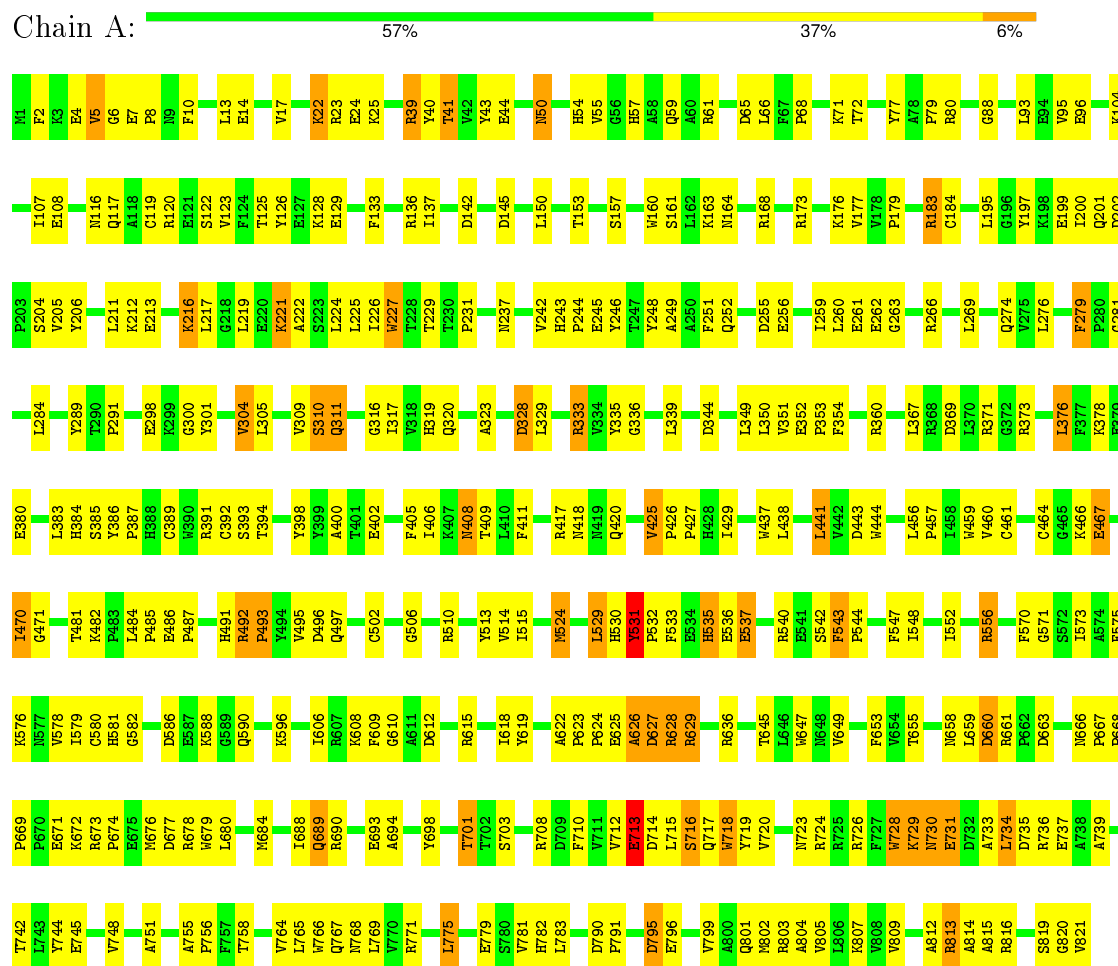
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	26	9		

### 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.

Note EDS was not executed.

- Molecule 1: Isoleucyl-tRNA synthetase



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.64Å 94.58Å 125.90Å 90.00° 126.30° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.249 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6735	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

## 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: ZN, MRC

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	0.39	0/6901	0.66	5/9386 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	88	GLY	N-CA-C	6.42	129.14	113.10
1	A	529	LEU	N-CA-C	-6.38	93.78	111.00
1	A	543	PHE	C-N-CD	5.55	140.05	128.40
1	A	531	TYR	N-CA-C	5.46	125.73	111.00
1	A	627	ASP	N-CA-C	-5.09	97.25	111.00

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	6698	0	6576	319	0
2	A	2	0	0	0	0
3	A	35	0	42	0	0
All	All	6735	0	6618	319	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 24.

All (319) 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:673:ARG:HH22	1:A:739:ALA:HA	0.95	1.06
1:A:676:MET:HG2	1:A:723:ASN:HD21	1.20	1.03
1:A:408:ASN:HD21	1:A:443:ASP:HA	1.25	0.97
1:A:486:GLU:HB2	1:A:487:PRO:HD3	1.47	0.96
1:A:673:ARG:NH2	1:A:739:ALA:HA	1.78	0.95
1:A:775:LEU:HD23	1:A:775:LEU:H	1.29	0.95
1:A:425:VAL:HG21	1:A:579:ILE:HG12	1.45	0.93
1:A:460:VAL:HG13	1:A:466:LYS:HB2	1.49	0.93
1:A:456:LEU:HD13	1:A:515:ILE:HD11	1.51	0.93
1:A:729:LYS:HG3	1:A:730:ASN:H	1.38	0.89
1:A:623:PRO:HA	1:A:701:THR:HG21	1.56	0.88
1:A:426:PRO:HB3	1:A:625:GLU:HG2	1.52	0.87
1:A:673:ARG:HH22	1:A:739:ALA:CA	1.84	0.85
1:A:408:ASN:ND2	1:A:443:ASP:HA	1.90	0.85
1:A:629:ARG:H	1:A:629:ARG:CZ	1.88	0.85
1:A:425:VAL:HG23	1:A:578:VAL:O	1.77	0.84
1:A:486:GLU:HB2	1:A:487:PRO:CD	2.09	0.83
1:A:389:CYS:HB3	1:A:392:CYS:O	1.78	0.83
1:A:608:LYS:HB3	1:A:608:LYS:NZ	1.93	0.82
1:A:333:ARG:HA	1:A:333:ARG:NE	1.96	0.81
1:A:5:VAL:HG23	1:A:6:GLY:H	1.46	0.80
1:A:619:TYR:O	1:A:701:THR:HB	1.82	0.80
1:A:116:ASN:ND2	1:A:493:PRO:HD3	1.98	0.78
1:A:801:GLN:O	1:A:805:VAL:HG23	1.84	0.76
1:A:2:PHE:H	1:A:658:ASN:HD21	1.31	0.75
1:A:694:ALA:HB3	1:A:703:SER:HB3	1.70	0.74
1:A:775:LEU:N	1:A:775:LEU:HD23	2.03	0.73
1:A:628:ARG:HA	1:A:629:ARG:HH21	1.52	0.73
1:A:775:LEU:CD2	1:A:775:LEU:H	2.03	0.72
1:A:676:MET:CG	1:A:723:ASN:HD21	1.99	0.71
1:A:221:LYS:HE3	1:A:222:ALA:N	2.06	0.71
1:A:715:LEU:HD22	1:A:720:VAL:HG11	1.72	0.70
1:A:622:ALA:O	1:A:628:ARG:NH2	2.25	0.70
1:A:804:ALA:HA	1:A:807:LYS:HD3	1.73	0.70
1:A:252:GLN:HG3	1:A:276:LEU:HD21	1.73	0.69
1:A:712:VAL:CG1	1:A:716:SER:HB2	2.22	0.69
1:A:676:MET:HG2	1:A:723:ASN:ND2	2.00	0.69
1:A:300:GLY:O	1:A:301:TYR:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:HD22	1:A:493:PRO:HD3	1.58	0.68
1:A:767:GLN:O	1:A:771:ARG:HB2	1.93	0.68
1:A:729:LYS:HG3	1:A:730:ASN:N	2.09	0.68
1:A:575:PHE:HE1	1:A:578:VAL:HG21	1.60	0.67
1:A:204:SER:HG	1:A:227:TRP:HZ3	1.43	0.67
1:A:263:GLY:HA2	1:A:266:ARG:HG2	1.76	0.66
1:A:279:PHE:N	1:A:279:PHE:CD2	2.63	0.66
1:A:608:LYS:HB3	1:A:608:LYS:HZ3	1.59	0.66
1:A:712:VAL:HG12	1:A:716:SER:HB2	1.79	0.65
1:A:544:PRO:HB2	1:A:576:LYS:NZ	2.11	0.65
1:A:369:ASP:O	1:A:373:ARG:HG3	1.96	0.64
1:A:54:HIS:HD2	1:A:55:VAL:O	1.80	0.64
1:A:128:LYS:HD2	1:A:128:LYS:N	2.11	0.64
1:A:459:TRP:CE2	1:A:510:ARG:HB3	2.33	0.64
1:A:408:ASN:N	1:A:408:ASN:HD22	1.94	0.64
1:A:531:TYR:O	1:A:532:PRO:C	2.33	0.64
1:A:765:LEU:O	1:A:769:LEU:HB2	1.99	0.63
1:A:437:TRP:HB2	1:A:556:ARG:HH21	1.63	0.63
1:A:744:TYR:O	1:A:748:VAL:HG23	1.97	0.63
1:A:426:PRO:HB3	1:A:625:GLU:CG	2.26	0.63
1:A:77:TYR:O	1:A:79:PRO:HD3	1.99	0.63
1:A:655:THR:O	1:A:659:LEU:HD23	1.99	0.62
1:A:96:GLU:OE1	1:A:183:ARG:NH2	2.32	0.62
1:A:814:ALA:C	1:A:816:ARG:H	2.02	0.62
1:A:645:THR:HG23	1:A:715:LEU:HD12	1.81	0.62
1:A:133:PHE:O	1:A:137:ILE:HG12	1.98	0.62
1:A:262:GLU:HG2	1:A:263:GLY:N	2.15	0.61
1:A:353:PRO:HG2	1:A:354:PHE:CD1	2.35	0.61
1:A:717:GLN:O	1:A:718:TRP:HE3	1.83	0.61
1:A:274:GLN:OE1	1:A:274:GLN:N	2.26	0.61
1:A:177:VAL:HG22	1:A:400:ALA:HB2	1.83	0.61
1:A:755:ALA:HB3	1:A:756:PRO:HD3	1.81	0.60
1:A:386:TYR:CD1	1:A:387:PRO:HD2	2.35	0.60
1:A:674:PRO:HD2	1:A:677:ASP:OD2	2.02	0.60
1:A:298:GLU:H	1:A:298:GLU:CD	2.05	0.60
1:A:24:GLU:OE1	1:A:779:GLU:OE1	2.20	0.60
1:A:726:ARG:HD2	1:A:736:ARG:HG2	1.83	0.60
1:A:715:LEU:HA	1:A:720:VAL:CG1	2.31	0.60
1:A:805:VAL:O	1:A:809:VAL:HG23	2.01	0.60
1:A:497:GLN:HE21	1:A:497:GLN:HA	1.67	0.60
1:A:284:LEU:N	1:A:284:LEU:HD12	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:TYR:HB3	1:A:524:MET:HE3	1.84	0.59
1:A:715:LEU:HD13	1:A:716:SER:N	2.17	0.59
1:A:710:PHE:O	1:A:713:GLU:HG3	2.03	0.59
1:A:205:VAL:HG11	1:A:367:LEU:HD11	1.85	0.58
1:A:543:PHE:HB3	1:A:544:PRO:HD3	1.85	0.58
1:A:392:CYS:SG	1:A:392:CYS:O	2.61	0.58
1:A:715:LEU:C	1:A:715:LEU:HD13	2.24	0.58
1:A:663:ASP:OD1	1:A:666:ASN:HB2	2.03	0.58
1:A:719:TYR:O	1:A:723:ASN:HB2	2.04	0.58
1:A:425:VAL:O	1:A:427:PRO:N	2.36	0.58
1:A:728:TRP:HA	1:A:728:TRP:CE3	2.39	0.58
1:A:211:LEU:HD23	1:A:222:ALA:O	2.03	0.58
1:A:243:HIS:HD2	1:A:245:GLU:H	1.51	0.58
1:A:729:LYS:O	1:A:731:GLU:N	2.37	0.58
1:A:575:PHE:CE1	1:A:578:VAL:HG21	2.39	0.58
1:A:728:TRP:HE3	1:A:728:TRP:HA	1.69	0.57
1:A:532:PRO:HG2	1:A:533:PHE:CD1	2.39	0.57
1:A:93:LEU:HG	1:A:183:ARG:HH21	1.69	0.57
1:A:65:ASP:CG	1:A:615:ARG:HH22	2.07	0.57
1:A:22:LYS:HB3	1:A:22:LYS:NZ	2.19	0.57
1:A:284:LEU:H	1:A:284:LEU:HD12	1.70	0.56
1:A:10:PHE:O	1:A:14:GLU:HG3	2.05	0.56
1:A:204:SER:OG	1:A:227:TRP:HZ3	1.88	0.56
1:A:536:GLU:O	1:A:540:ARG:HG3	2.06	0.56
1:A:41:THR:HG21	1:A:542:SER:HA	1.85	0.56
1:A:408:ASN:H	1:A:408:ASN:HD22	1.53	0.56
1:A:497:GLN:NE2	1:A:497:GLN:HA	2.21	0.56
1:A:351:VAL:HG12	1:A:353:PRO:HD2	1.88	0.56
1:A:536:GLU:OE1	1:A:540:ARG:HD3	2.04	0.56
1:A:717:GLN:HG2	1:A:717:GLN:O	2.06	0.55
1:A:333:ARG:HD3	1:A:333:ARG:O	2.06	0.55
1:A:535:HIS:HA	1:A:537:GLU:OE2	2.06	0.55
1:A:751:ALA:HB2	1:A:765:LEU:HD23	1.89	0.55
1:A:418:ASN:HB3	1:A:573:ILE:HG22	1.89	0.55
1:A:689:GLN:O	1:A:693:GLU:HB2	2.06	0.55
1:A:344:ASP:HB3	1:A:350:LEU:HD11	1.89	0.55
1:A:556:ARG:CG	1:A:556:ARG:HH11	2.19	0.54
1:A:176:LYS:HE2	1:A:405:PHE:CZ	2.43	0.54
1:A:408:ASN:OD1	1:A:441:LEU:HD11	2.07	0.54
1:A:514:VAL:CG1	1:A:515:ILE:N	2.70	0.54
1:A:645:THR:O	1:A:649:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ILE:HA	1:A:580:CYS:SG	2.47	0.54
1:A:217:LEU:N	1:A:217:LEU:HD22	2.23	0.54
1:A:311:GLN:O	1:A:311:GLN:HG2	2.07	0.54
1:A:586:ASP:HB2	1:A:590:GLN:O	2.08	0.54
1:A:371:ARG:HB2	1:A:376:LEU:HD12	1.90	0.54
1:A:715:LEU:CD2	1:A:720:VAL:HG11	2.38	0.53
1:A:249:ALA:HB3	1:A:251:PHE:CE1	2.44	0.53
1:A:39:ARG:HG3	1:A:40:TYR:N	2.23	0.53
1:A:514:VAL:HG12	1:A:515:ILE:N	2.22	0.53
1:A:809:VAL:HG12	1:A:813:ARG:HD2	1.91	0.53
1:A:669:PRO:HD2	1:A:672:LYS:HD3	1.89	0.53
1:A:126:TYR:O	1:A:129:GLU:HG2	2.09	0.53
1:A:219:LEU:HD22	1:A:276:LEU:HD12	1.90	0.53
1:A:608:LYS:HB3	1:A:608:LYS:HZ2	1.71	0.52
1:A:259:ILE:O	1:A:260:LEU:HB3	2.09	0.52
1:A:496:ASP:OD1	1:A:510:ARG:NH1	2.43	0.52
1:A:161:SER:O	1:A:164:ASN:HB3	2.10	0.52
1:A:629:ARG:H	1:A:629:ARG:NE	2.07	0.52
1:A:122:SER:O	1:A:125:THR:HG23	2.10	0.52
1:A:726:ARG:HH11	1:A:736:ARG:HG3	1.75	0.52
1:A:679:TRP:CE2	1:A:802:MET:HG2	2.45	0.51
1:A:629:ARG:H	1:A:629:ARG:NH2	2.08	0.51
1:A:251:PHE:CD2	1:A:269:LEU:HD12	2.45	0.51
1:A:544:PRO:HB2	1:A:576:LYS:HZ3	1.76	0.51
1:A:671:GLU:CD	1:A:671:GLU:H	2.13	0.51
1:A:524:MET:C	1:A:524:MET:SD	2.89	0.51
1:A:65:ASP:O	1:A:68:PRO:HD2	2.11	0.51
1:A:59:GLN:NE2	1:A:581:HIS:HD2	2.09	0.51
1:A:624:PRO:HD3	1:A:701:THR:CG2	2.41	0.51
1:A:812:ALA:HB1	1:A:813:ARG:HH21	1.75	0.51
1:A:677:ASP:CG	1:A:726:ARG:HH22	2.13	0.51
1:A:249:ALA:HB3	1:A:251:PHE:HE1	1.76	0.51
1:A:40:TYR:CE1	1:A:71:LYS:HE3	2.46	0.51
1:A:291:PRO:HG3	1:A:301:TYR:CE2	2.46	0.50
1:A:304:VAL:HG13	1:A:335:TYR:CE1	2.46	0.50
1:A:43:TYR:HB3	1:A:524:MET:CE	2.41	0.50
1:A:328:ASP:N	1:A:328:ASP:OD1	2.45	0.50
1:A:425:VAL:O	1:A:426:PRO:C	2.44	0.50
1:A:176:LYS:O	1:A:400:ALA:HA	2.11	0.50
1:A:481:THR:O	1:A:482:LYS:HG3	2.11	0.50
1:A:814:ALA:O	1:A:816:ARG:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:VAL:HG12	1:A:317:ILE:HG12	1.93	0.50
1:A:548:ILE:HG13	1:A:578:VAL:HG13	1.94	0.50
1:A:54:HIS:O	1:A:57:HIS:HB2	2.12	0.50
1:A:179:PRO:HG3	1:A:398:TYR:CE1	2.47	0.50
1:A:157:SER:O	1:A:160:TRP:HB3	2.12	0.49
1:A:248:TYR:HD2	1:A:261:GLU:N	2.10	0.49
1:A:50:ASN:HD22	1:A:50:ASN:C	2.15	0.49
1:A:737:GLU:C	1:A:739:ALA:H	2.15	0.49
1:A:93:LEU:HG	1:A:183:ARG:NH2	2.26	0.49
1:A:809:VAL:O	1:A:813:ARG:HD2	2.13	0.49
1:A:5:VAL:HG23	1:A:6:GLY:N	2.22	0.49
1:A:715:LEU:HA	1:A:720:VAL:HG11	1.93	0.49
1:A:795:ASP:O	1:A:799:VAL:HG23	2.13	0.49
1:A:213:GLU:HB3	1:A:216:LYS:HD3	1.94	0.49
1:A:221:LYS:HE3	1:A:222:ALA:H	1.75	0.49
1:A:66:LEU:C	1:A:66:LEU:HD23	2.33	0.49
1:A:243:HIS:O	1:A:281:GLY:HA3	2.13	0.48
1:A:179:PRO:HG3	1:A:398:TYR:HE1	1.77	0.48
1:A:606:ILE:O	1:A:610:GLY:HA2	2.12	0.48
1:A:425:VAL:HG21	1:A:579:ILE:CG1	2.31	0.48
1:A:386:TYR:CG	1:A:387:PRO:HD2	2.49	0.48
1:A:197:TYR:HE1	1:A:387:PRO:HD3	1.77	0.48
1:A:243:HIS:CD2	1:A:245:GLU:H	2.31	0.48
1:A:734:LEU:HG	1:A:735:ASP:N	2.28	0.48
1:A:183:ARG:HG3	1:A:184:CYS:N	2.25	0.48
1:A:50:ASN:C	1:A:50:ASN:ND2	2.66	0.48
1:A:537:GLU:CD	1:A:537:GLU:H	2.17	0.48
1:A:715:LEU:HA	1:A:720:VAL:HG12	1.96	0.48
1:A:708:ARG:C	1:A:708:ARG:HD3	2.34	0.48
1:A:212:LYS:HE3	1:A:289:TYR:O	2.13	0.48
1:A:224:LEU:HD22	1:A:317:ILE:HD13	1.96	0.48
1:A:120:ARG:O	1:A:123:VAL:HG22	2.13	0.48
1:A:104:LYS:O	1:A:108:GLU:HG2	2.13	0.48
1:A:645:THR:HG23	1:A:715:LEU:CD1	2.44	0.48
1:A:323:ALA:HB2	1:A:339:LEU:CD1	2.44	0.48
1:A:674:PRO:HG2	1:A:726:ARG:NH1	2.28	0.47
1:A:122:SER:HA	1:A:125:THR:CG2	2.44	0.47
1:A:628:ARG:HA	1:A:629:ARG:NH2	2.26	0.47
1:A:211:LEU:HD23	1:A:222:ALA:C	2.35	0.47
1:A:408:ASN:H	1:A:408:ASN:ND2	2.12	0.47
1:A:629:ARG:NE	1:A:629:ARG:N	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:CE1	1:A:387:PRO:HD3	2.50	0.47
1:A:40:TYR:CZ	1:A:71:LYS:HG3	2.50	0.47
1:A:199:GLU:CD	1:A:383:LEU:HD11	2.35	0.47
1:A:93:LEU:HD22	1:A:391:ARG:HB3	1.95	0.47
1:A:40:TYR:CE1	1:A:71:LYS:HG3	2.50	0.47
1:A:199:GLU:OE2	1:A:383:LEU:HD11	2.15	0.47
1:A:417:ARG:O	1:A:420:GLN:HB2	2.15	0.47
1:A:163:LYS:HD2	1:A:471:GLY:N	2.29	0.47
1:A:575:PHE:CE1	1:A:578:VAL:CG2	2.99	0.46
1:A:459:TRP:HA	1:A:510:ARG:HA	1.97	0.46
1:A:781:VAL:C	1:A:783:LEU:H	2.18	0.46
1:A:243:HIS:CG	1:A:244:PRO:HD2	2.51	0.46
1:A:246:TYR:CE1	1:A:311:GLN:HB2	2.51	0.46
1:A:409:THR:C	1:A:411:PHE:H	2.19	0.46
1:A:8:PRO:HG3	1:A:647:TRP:CD1	2.51	0.46
1:A:734:LEU:O	1:A:737:GLU:HB3	2.16	0.46
1:A:408:ASN:ND2	1:A:408:ASN:N	2.62	0.46
1:A:266:ARG:NH1	1:A:266:ARG:HB3	2.30	0.46
1:A:153:THR:HB	1:A:530:HIS:CD2	2.51	0.46
1:A:173:ARG:NH2	1:A:467:GLU:OE2	2.48	0.46
1:A:266:ARG:NH1	1:A:266:ARG:CB	2.79	0.46
1:A:514:VAL:CG1	1:A:515:ILE:H	2.29	0.46
1:A:814:ALA:C	1:A:816:ARG:N	2.69	0.46
1:A:243:HIS:CD2	1:A:244:PRO:HD2	2.51	0.46
1:A:713:GLU:OE1	1:A:713:GLU:O	2.34	0.46
1:A:582:GLY:HA3	1:A:626:ALA:O	2.15	0.45
1:A:252:GLN:CG	1:A:276:LEU:HD21	2.44	0.45
1:A:164:ASN:ND2	1:A:168:ARG:HH11	2.14	0.45
1:A:470:ILE:O	1:A:470:ILE:HG22	2.15	0.45
1:A:492:ARG:HD2	1:A:492:ARG:HA	1.88	0.45
1:A:690:ARG:HH21	1:A:803:ARG:HH21	1.63	0.45
1:A:556:ARG:CG	1:A:556:ARG:NH1	2.78	0.45
1:A:766:TRP:CB	1:A:781:VAL:HG22	2.45	0.45
1:A:612:ASP:HB3	1:A:758:THR:HG22	1.98	0.45
1:A:183:ARG:HG2	1:A:392:CYS:SG	2.56	0.45
1:A:244:PRO:HB3	1:A:305:LEU:HD22	1.98	0.45
1:A:676:MET:HA	1:A:676:MET:CE	2.47	0.45
1:A:510:ARG:NH2	1:A:513:TYR:O	2.49	0.45
1:A:408:ASN:HD21	1:A:443:ASP:CA	2.11	0.45
1:A:96:GLU:OE2	1:A:107:ILE:HD11	2.17	0.45
1:A:243:HIS:HB3	1:A:246:TYR:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:VAL:HG22	1:A:821:VAL:OXT	2.16	0.45
1:A:677:ASP:HB3	1:A:742:THR:HG21	1.98	0.45
1:A:221:LYS:HE3	1:A:221:LYS:HA	1.98	0.44
1:A:281:GLY:HA2	1:A:284:LEU:HD13	2.00	0.44
1:A:7:GLU:OE1	1:A:7:GLU:N	2.50	0.44
1:A:529:LEU:C	1:A:531:TYR:H	2.19	0.44
1:A:367:LEU:HA	1:A:367:LEU:HD12	1.81	0.44
1:A:461:CYS:CB	1:A:502:CYS:HG	2.30	0.44
1:A:266:ARG:HH11	1:A:266:ARG:CB	2.31	0.44
1:A:406:ILE:HB	1:A:444:TRP:HB3	1.99	0.44
1:A:491:HIS:O	1:A:495:VAL:HG22	2.18	0.44
1:A:392:CYS:O	1:A:394:THR:N	2.50	0.44
1:A:237:ASN:HB2	1:A:319:HIS:CE1	2.53	0.44
1:A:625:GLU:O	1:A:626:ALA:O	2.36	0.43
1:A:543:PHE:O	1:A:544:PRO:C	2.52	0.43
1:A:206:TYR:HA	1:A:226:ILE:O	2.18	0.43
1:A:333:ARG:NH1	1:A:336:GLY:HA2	2.32	0.43
1:A:261:GLU:HB2	1:A:316:GLY:HA3	2.00	0.43
1:A:4:GLU:CD	1:A:4:GLU:H	2.21	0.43
1:A:95:VAL:HG21	1:A:119:CYS:HA	2.01	0.43
1:A:733:ALA:O	1:A:734:LEU:C	2.55	0.43
1:A:13:LEU:O	1:A:17:VAL:HG23	2.19	0.43
1:A:728:TRP:O	1:A:731:GLU:HB2	2.19	0.43
1:A:575:PHE:CD1	1:A:578:VAL:HG22	2.53	0.43
1:A:310:SER:OG	1:A:311:GLN:N	2.51	0.43
1:A:136:ARG:HD2	1:A:136:ARG:HA	1.88	0.43
1:A:353:PRO:HG2	1:A:354:PHE:CE1	2.53	0.43
1:A:243:HIS:CD2	1:A:245:GLU:HG3	2.54	0.43
1:A:199:GLU:HA	1:A:385:SER:HA	2.01	0.43
1:A:425:VAL:HB	1:A:426:PRO:CD	2.49	0.43
1:A:667:PRO:HA	1:A:668:PRO:HD3	1.89	0.43
1:A:438:LEU:O	1:A:441:LEU:HB2	2.18	0.42
1:A:266:ARG:HB2	1:A:266:ARG:HH11	1.83	0.42
1:A:547:PHE:CD2	1:A:698:TYR:CE2	3.06	0.42
1:A:226:ILE:HG22	1:A:227:TRP:N	2.33	0.42
1:A:425:VAL:O	1:A:427:PRO:CD	2.67	0.42
1:A:68:PRO:O	1:A:72:THR:HG23	2.19	0.42
1:A:221:LYS:CA	1:A:221:LYS:HE3	2.48	0.42
1:A:653:PHE:CZ	1:A:744:TYR:HB2	2.55	0.42
1:A:59:GLN:CD	1:A:581:HIS:CD2	2.93	0.42
1:A:229:THR:C	1:A:231:PRO:HD3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ASP:O	1:A:661:ARG:C	2.57	0.42
1:A:333:ARG:CZ	1:A:333:ARG:HA	2.49	0.42
1:A:65:ASP:OD1	1:A:615:ARG:NH2	2.42	0.42
1:A:718:TRP:HA	1:A:718:TRP:CE3	2.54	0.42
1:A:378:LYS:HE2	1:A:380:GLU:OE2	2.20	0.42
1:A:466:LYS:HD3	1:A:467:GLU:HG3	2.02	0.42
1:A:173:ARG:HH22	1:A:466:LYS:CD	2.33	0.41
1:A:200:ILE:HG12	1:A:201:GLN:N	2.36	0.41
1:A:676:MET:HA	1:A:676:MET:HE2	2.01	0.41
1:A:133:PHE:CZ	1:A:137:ILE:HD13	2.55	0.41
1:A:782:HIS:N	1:A:782:HIS:CD2	2.86	0.41
1:A:429:ILE:O	1:A:429:ILE:HG22	2.21	0.41
1:A:59:GLN:NE2	1:A:581:HIS:CD2	2.88	0.41
1:A:790:ASP:HA	1:A:791:PRO:HD3	1.93	0.41
1:A:609:PHE:CZ	1:A:636:ARG:HB2	2.55	0.41
1:A:570:PHE:O	1:A:571:GLY:C	2.59	0.41
1:A:809:VAL:CG1	1:A:813:ARG:HD2	2.50	0.41
1:A:724:ARG:HB2	1:A:724:ARG:HH11	1.86	0.41
1:A:680:LEU:HD22	1:A:719:TYR:CD1	2.55	0.41
1:A:298:GLU:CD	1:A:298:GLU:N	2.74	0.41
1:A:543:PHE:C	1:A:543:PHE:CD1	2.93	0.41
1:A:678:ARG:HB3	1:A:678:ARG:HH11	1.86	0.41
1:A:408:ASN:CG	1:A:441:LEU:HD11	2.41	0.41
1:A:261:GLU:OE1	1:A:262:GLU:O	2.39	0.41
1:A:461:CYS:HB2	1:A:502:CYS:SG	2.61	0.41
1:A:57:HIS:O	1:A:61:ARG:HG3	2.19	0.40
1:A:142:ASP:HB3	1:A:145:ASP:OD1	2.21	0.40
1:A:221:LYS:O	1:A:256:GLU:HB2	2.21	0.40
1:A:150:LEU:HD12	1:A:150:LEU:C	2.42	0.40
1:A:402:GLU:OE1	1:A:513:TYR:OH	2.34	0.40
1:A:284:LEU:CD1	1:A:284:LEU:H	2.33	0.40
1:A:202:ASP:OD2	1:A:384:HIS:HE1	2.04	0.40
1:A:59:GLN:HG3	1:A:618:ILE:CG2	2.51	0.40
1:A:684:MET:O	1:A:688:ILE:HG13	2.21	0.40
1:A:484:LEU:HB3	1:A:485:PRO:HD2	2.03	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	819/821 (100%)	705 (86%)	85 (10%)	29 (4%)	<b>4</b> <b>6</b>

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	467	GLU
1	A	531	TYR
1	A	626	ALA
1	A	713	GLU
1	A	730	ASN
1	A	734	LEU
1	A	310	SER
1	A	393	SER
1	A	716	SER
1	A	815	ALA
1	A	25	LYS
1	A	352	GLU
1	A	596	LYS
1	A	819	SER
1	A	820	GLY
1	A	311	GLN
1	A	425	VAL
1	A	535	HIS
1	A	768	ASN
1	A	23	ARG
1	A	216	LYS
1	A	464	CYS
1	A	729	LYS
1	A	795	ASP
1	A	506	GLY
1	A	492	ARG
1	A	457	PRO

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Mol	Chain	Res	Type
1	A	493	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	698/698 (100%)	652 (93%)	46 (7%)	21	38

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	39	ARG
1	A	41	THR
1	A	44	GLU
1	A	50	ASN
1	A	80	ARG
1	A	117	GLN
1	A	183	ARG
1	A	195	LEU
1	A	221	LYS
1	A	225	LEU
1	A	227	TRP
1	A	255	ASP
1	A	279	PHE
1	A	304	VAL
1	A	309	VAL
1	A	320	GLN
1	A	328	ASP
1	A	329	LEU
1	A	333	ARG
1	A	349	LEU
1	A	360	ARG
1	A	376	LEU
1	A	408	ASN
1	A	441	LEU

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Mol	Chain	Res	Type
1	A	470	ILE
1	A	524	MET
1	A	537	GLU
1	A	556	ARG
1	A	588	LYS
1	A	627	ASP
1	A	628	ARG
1	A	629	ARG
1	A	660	ASP
1	A	689	GLN
1	A	701	THR
1	A	713	GLU
1	A	714	ASP
1	A	718	TRP
1	A	728	TRP
1	A	731	GLU
1	A	745	GLU
1	A	764	VAL
1	A	775	LEU
1	A	796	GLU
1	A	813	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	54	HIS
1	A	59	GLN
1	A	116	ASN
1	A	164	ASN
1	A	191	HIS
1	A	237	ASN
1	A	243	HIS
1	A	295	GLN
1	A	311	GLN
1	A	384	HIS
1	A	408	ASN
1	A	418	ASN
1	A	419	ASN
1	A	462	GLN
1	A	497	GLN
1	A	560	ASN

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Mol	Chain	Res	Type
1	A	577	ASN
1	A	581	HIS
1	A	590	GLN
1	A	658	ASN
1	A	717	GLN
1	A	723	ASN
1	A	801	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	MRC	A	1301	-	33,36,36	1.66	3 (9%)	35,48,48	2.81	9 (25%)

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
3	MRC	A	1301	-	2/2/11/12	0/30/54/54	0/1/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1301	MRC	C2-C1	-2.93	1.39	1.47
3	A	1301	MRC	O1A-C1	4.07	1.44	1.34
3	A	1301	MRC	C11-C10	5.96	1.54	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1301	MRC	C17-C12-C13	-8.19	96.16	112.82
3	A	1301	MRC	C9-C10-C11	-6.16	111.21	124.52
3	A	1301	MRC	C17-C12-C11	-5.58	100.94	111.38
3	A	1301	MRC	C4-C5-C6	-3.77	109.81	113.12
3	A	1301	MRC	O10-C11-C10	-2.14	57.41	59.86
3	A	1301	MRC	C16-O5-C5	3.28	116.41	112.25
3	A	1301	MRC	C9'-O1A-C1	4.29	124.19	116.66
3	A	1301	MRC	C11-O10-C10	5.18	63.53	60.59
3	A	1301	MRC	C11-C12-C13	6.28	122.57	110.78

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1301	MRC	C6
3	A	1301	MRC	C7

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 ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.