



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:14 pm GMT

PDB ID : 1RQG  
Title : Methionyl-tRNA synthetase from *Pyrococcus abyssi*  
Authors : Crepin, T.; Schmitt, E.; Blanquet, S.; Mechulam, Y.  
Deposited on : 2003-12-05  
Resolution : 2.90 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.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

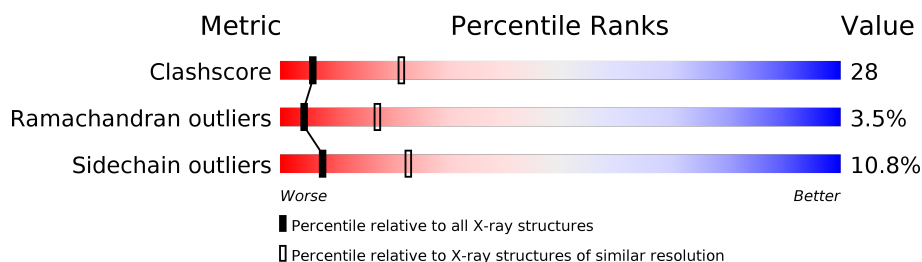
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)

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	722	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5026 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 Methionyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	0	0	0
			4973	3228	846	880	19			

- 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 water.

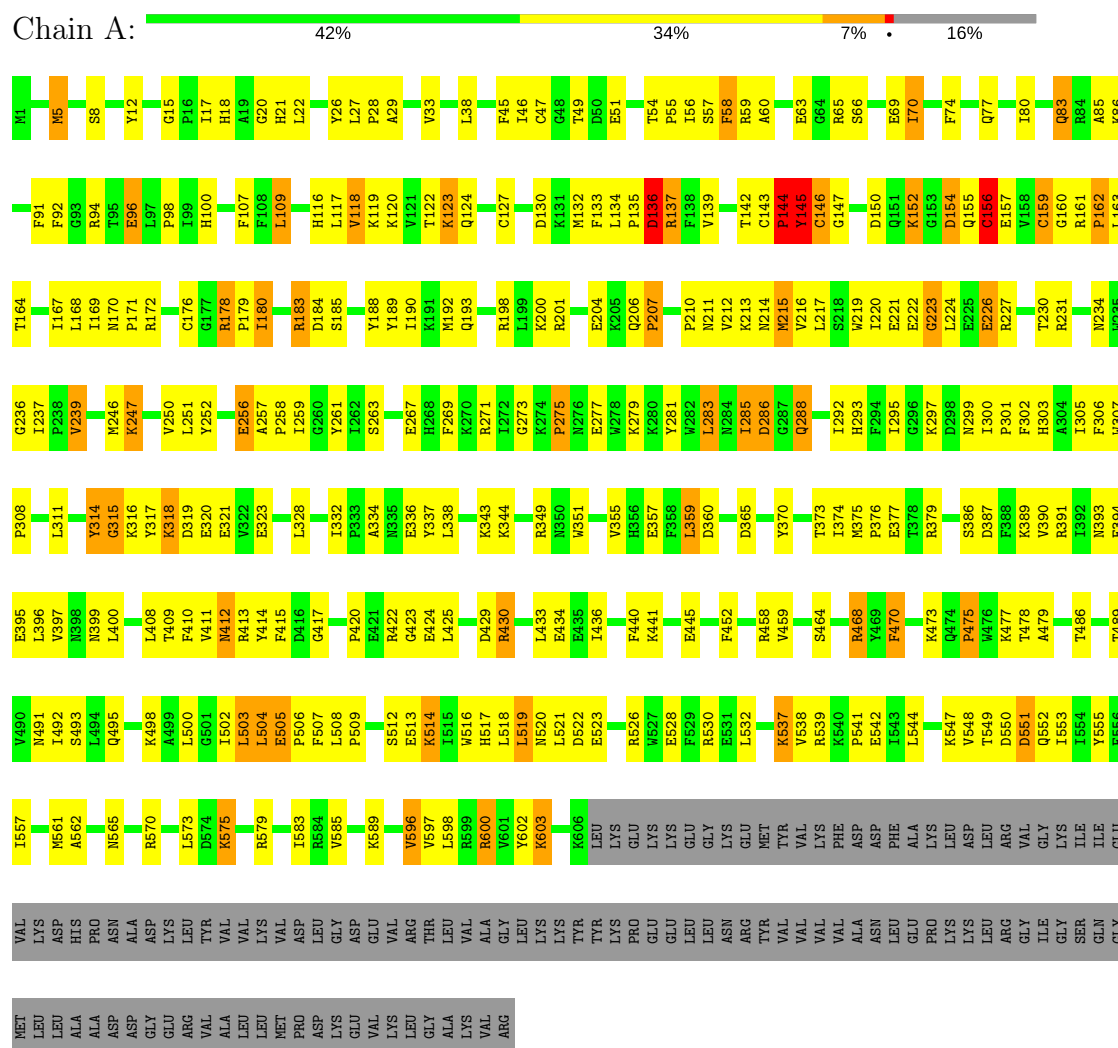
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		

### 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: Methionyl-tRNA synthetase



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.15Å 113.15Å 287.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.50 – 2.90	Depositor
% Data completeness (in resolution range)	94.7 (72.50-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.244 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5026	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	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

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	0.45	0/5111	0.70	3/6916 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	318	LYS	N-CA-C	5.60	126.13	111.00
1	A	144	PRO	N-CA-CB	5.44	109.83	103.30
1	A	161	ARG	N-CA-C	-5.04	97.38	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	TYR	Sidechain

### 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	4973	0	4858	274	0
2	A	2	0	0	0	0
3	A	51	0	0	2	0
All	All	5026	0	4858	274	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 28.

All (274) 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:400:LEU:HD21	1:A:504:LEU:HD21	1.37	1.04
1:A:183:ARG:HG3	1:A:183:ARG:HH11	1.17	1.02
1:A:549:THR:HG22	1:A:551:ASP:H	1.20	1.00
1:A:139:VAL:CG2	1:A:168:LEU:HD12	2.00	0.91
1:A:5:MET:HG2	1:A:281:TYR:HB3	1.54	0.90
1:A:478:THR:HG22	1:A:486:THR:OG1	1.72	0.89
1:A:393:ASN:HD21	1:A:548:VAL:H	0.97	0.89
1:A:156:CYS:HB2	1:A:160:GLY:O	1.75	0.87
1:A:139:VAL:HG21	1:A:168:LEU:HD12	1.58	0.86
1:A:236:GLY:HA3	1:A:250:VAL:HG21	1.58	0.86
1:A:373:THR:HG21	1:A:391:ARG:HD2	1.59	0.83
1:A:200:LYS:O	1:A:204:GLU:HG2	1.79	0.80
1:A:549:THR:HB	1:A:552:GLN:HG3	1.65	0.78
1:A:393:ASN:HD21	1:A:548:VAL:N	1.78	0.78
1:A:183:ARG:HH11	1:A:183:ARG:CG	1.97	0.76
1:A:300:ILE:HB	1:A:301:PRO:HD3	1.66	0.76
1:A:51:GLU:OE1	1:A:94:ARG:HB2	1.86	0.76
1:A:145:TYR:C	1:A:145:TYR:CD2	2.56	0.75
1:A:38:LEU:HD11	1:A:505:GLU:HG2	1.68	0.74
1:A:475:PRO:HG3	1:A:489:THR:HG21	1.70	0.73
1:A:314:TYR:HD2	1:A:314:TYR:O	1.70	0.73
1:A:549:THR:HG22	1:A:551:ASP:N	1.99	0.73
1:A:585:VAL:O	1:A:589:LYS:HB2	1.87	0.73
1:A:230:THR:HG21	1:A:246:MET:HE1	1.70	0.72
1:A:145:TYR:O	1:A:145:TYR:HD2	1.71	0.72
1:A:200:LYS:HE3	1:A:217:LEU:HD22	1.71	0.71
1:A:100:HIS:HE1	1:A:256:GLU:OE1	1.75	0.69
1:A:213:LYS:O	1:A:217:LEU:HG	1.93	0.69
1:A:336:GLU:HG3	1:A:379:ARG:CA	2.22	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ARG:HD2	1:A:414:TYR:CE1	2.27	0.69
1:A:349:ARG:O	1:A:349:ARG:HG2	1.93	0.68
1:A:430:ARG:O	1:A:434:GLU:HG3	1.94	0.68
1:A:159:CYS:SG	1:A:160:GLY:N	2.67	0.68
1:A:279:LYS:O	1:A:283:LEU:HB2	1.93	0.67
1:A:200:LYS:HD2	1:A:201:ARG:NH2	2.09	0.67
1:A:526:ARG:HH22	1:A:530:ARG:CD	2.07	0.67
1:A:412:ASN:HA	1:A:417:GLY:H	1.59	0.67
1:A:183:ARG:NH1	1:A:183:ARG:HG3	1.97	0.66
1:A:145:TYR:HD2	1:A:145:TYR:C	1.96	0.66
1:A:400:LEU:CD2	1:A:504:LEU:HD21	2.21	0.66
1:A:537:LYS:H	1:A:537:LYS:CD	2.09	0.66
1:A:370:TYR:O	1:A:373:THR:HB	1.95	0.65
1:A:256:GLU:HA	1:A:259:ILE:HD12	1.79	0.64
1:A:139:VAL:HG22	1:A:168:LEU:HD12	1.79	0.64
1:A:227:ARG:HG2	1:A:227:ARG:HH11	1.62	0.64
1:A:273:GLY:C	1:A:275:PRO:HD3	2.18	0.64
1:A:80:ILE:HA	1:A:83:GLN:HE21	1.62	0.64
1:A:343:LYS:HD2	1:A:349:ARG:HH12	1.63	0.64
1:A:22:LEU:HD12	1:A:26:TYR:HB2	1.80	0.64
1:A:314:TYR:O	1:A:314:TYR:CD2	2.51	0.64
1:A:38:LEU:HD11	1:A:505:GLU:CG	2.28	0.63
1:A:143:CYS:SG	1:A:144:PRO:N	2.73	0.62
1:A:258:PRO:HB2	1:A:307:TRP:CE3	2.34	0.62
1:A:283:LEU:HD21	1:A:317:TYR:CD2	2.35	0.62
1:A:285:ILE:HG22	1:A:286:ASP:N	2.15	0.61
1:A:393:ASN:ND2	1:A:548:VAL:H	1.83	0.61
1:A:237:ILE:N	1:A:250:VAL:HG23	2.16	0.61
1:A:498:LYS:HD3	1:A:532:LEU:HD13	1.82	0.60
1:A:237:ILE:O	1:A:250:VAL:HG23	2.01	0.60
1:A:318:LYS:CB	1:A:323:GLU:HB3	2.32	0.60
1:A:583:ILE:HG12	1:A:598:LEU:HD13	1.81	0.60
1:A:18:HIS:HD2	1:A:21:HIS:H	1.50	0.60
1:A:15:GLY:HA2	1:A:74:PHE:CZ	2.36	0.60
1:A:286:ASP:O	1:A:288:GLN:HG2	2.02	0.59
1:A:415:PHE:CD2	1:A:420:PRO:HG3	2.37	0.59
1:A:273:GLY:O	1:A:275:PRO:HD3	2.03	0.59
1:A:549:THR:HG22	1:A:550:ASP:N	2.17	0.59
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.17	0.59
1:A:29:ALA:O	1:A:33:VAL:HG23	2.03	0.58
1:A:183:ARG:NH1	1:A:183:ARG:CG	2.63	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:PRO:HG3	1:A:302:PHE:HE1	1.68	0.58
1:A:96:GLU:OE2	1:A:96:GLU:HA	2.04	0.58
1:A:373:THR:HG22	1:A:374:ILE:HG23	1.85	0.58
1:A:18:HIS:CD2	1:A:21:HIS:H	2.21	0.58
1:A:5:MET:CG	1:A:281:TYR:HB3	2.30	0.58
1:A:397:VAL:HG11	1:A:547:LYS:HG3	1.86	0.57
1:A:413:ARG:HD2	1:A:414:TYR:HE1	1.70	0.57
1:A:509:PRO:O	1:A:512:SER:HB3	2.05	0.57
1:A:468:ARG:HH11	1:A:468:ARG:HG3	1.70	0.57
1:A:80:ILE:HA	1:A:83:GLN:NE2	2.19	0.57
1:A:391:ARG:O	1:A:395:GLU:HB2	2.04	0.57
1:A:47:CYS:O	1:A:92:PHE:HA	2.05	0.57
1:A:144:PRO:CB	1:A:167:ILE:HG23	2.35	0.56
1:A:292:ILE:N	1:A:292:ILE:HD12	2.20	0.56
1:A:269:PHE:CD2	1:A:277:GLU:HB2	2.41	0.56
1:A:549:THR:HG23	3:A:1045:HOH:O	2.05	0.56
1:A:257:ALA:HB3	1:A:258:PRO:HD3	1.88	0.56
1:A:122:THR:HG22	1:A:124:GLN:HG3	1.87	0.55
1:A:117:LEU:HA	1:A:189:TYR:O	2.06	0.55
1:A:579:ARG:O	1:A:583:ILE:HG13	2.07	0.55
1:A:127:CYS:SG	1:A:130:ASP:HB2	2.46	0.55
1:A:336:GLU:HG3	1:A:379:ARG:C	2.27	0.55
1:A:258:PRO:HG3	1:A:302:PHE:CE1	2.42	0.55
1:A:343:LYS:CD	1:A:349:ARG:HH12	2.21	0.54
1:A:176:CYS:SG	1:A:178:ARG:HG3	2.47	0.54
1:A:365:ASP:HB3	1:A:508:LEU:HD13	1.90	0.54
1:A:60:ALA:HB1	1:A:65:ARG:O	2.07	0.53
1:A:137:ARG:HG3	1:A:152:LYS:HG3	1.90	0.53
1:A:119:LYS:HD3	1:A:188:TYR:CZ	2.43	0.53
1:A:293:HIS:HB2	1:A:332:ILE:HG22	1.88	0.53
1:A:387:ASP:O	1:A:391:ARG:HG3	2.09	0.53
1:A:200:LYS:HD3	1:A:200:LYS:O	2.09	0.53
1:A:250:VAL:HG22	1:A:251:LEU:N	2.24	0.53
1:A:55:PRO:HG3	1:A:137:ARG:HD3	1.91	0.53
1:A:142:THR:O	1:A:168:LEU:HD22	2.08	0.53
1:A:425:LEU:HB3	1:A:429:ASP:HB2	1.91	0.53
1:A:295:ILE:O	1:A:334:ALA:HA	2.09	0.53
1:A:336:GLU:HG3	1:A:379:ARG:HA	1.89	0.52
1:A:520:ASN:HD22	1:A:539:ARG:HE	1.56	0.52
1:A:132:MET:HE3	1:A:133:PHE:O	2.09	0.52
1:A:85:ALA:O	1:A:86:LYS:HB2	2.08	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:PHE:HA	1:A:306:PHE:HD2	1.74	0.52
1:A:143:CYS:HB3	1:A:147:GLY:H	1.75	0.52
1:A:192:MET:HB3	1:A:224:LEU:HB3	1.92	0.51
1:A:305:ILE:C	1:A:308:PRO:HD2	2.30	0.51
1:A:338:LEU:HD13	1:A:376:PRO:HG3	1.93	0.51
1:A:349:ARG:HD3	1:A:351:TRP:HB2	1.93	0.51
1:A:118:VAL:HG13	1:A:189:TYR:HB2	1.93	0.51
1:A:200:LYS:HE2	1:A:204:GLU:OE2	2.11	0.51
1:A:478:THR:HG22	1:A:486:THR:HG1	1.75	0.51
1:A:198:ARG:HH11	1:A:198:ARG:HG3	1.76	0.51
1:A:513:GLU:HG3	1:A:517:HIS:NE2	2.25	0.51
1:A:314:TYR:O	1:A:315:GLY:C	2.49	0.50
1:A:237:ILE:C	1:A:250:VAL:HG23	2.32	0.50
1:A:55:PRO:O	1:A:58:PHE:HB3	2.11	0.50
1:A:91:PHE:CE1	1:A:271:ARG:NH1	2.80	0.50
1:A:307:TRP:CH2	1:A:311:LEU:HD21	2.47	0.50
1:A:211:ASN:O	1:A:215:MET:HG3	2.12	0.50
1:A:27:LEU:HB3	1:A:28:PRO:HD3	1.94	0.50
1:A:526:ARG:HB2	1:A:528:GLU:OE2	2.12	0.50
1:A:237:ILE:N	1:A:250:VAL:CG2	2.75	0.50
1:A:459:VAL:HG11	1:A:504:LEU:CD1	2.42	0.49
1:A:410:PHE:CD1	1:A:470:PHE:CE1	3.00	0.49
1:A:600:ARG:HG2	1:A:600:ARG:O	2.10	0.49
1:A:267:GLU:O	1:A:271:ARG:HG2	2.11	0.49
1:A:409:THR:HA	1:A:541:PRO:HG2	1.94	0.49
1:A:597:VAL:O	1:A:600:ARG:N	2.45	0.49
1:A:349:ARG:HD3	1:A:351:TRP:CB	2.42	0.49
1:A:172:ARG:HA	1:A:179:PRO:HA	1.94	0.49
1:A:236:GLY:CA	1:A:250:VAL:HG21	2.38	0.49
1:A:297:LYS:HD2	1:A:336:GLU:HA	1.94	0.49
1:A:230:THR:HG22	1:A:231:ARG:N	2.28	0.49
1:A:295:ILE:HG21	1:A:303:HIS:CD2	2.48	0.48
1:A:375:MET:HE2	1:A:452:PHE:HB2	1.94	0.48
1:A:549:THR:HG21	1:A:551:ASP:HB2	1.95	0.48
1:A:122:THR:HG22	1:A:123:LYS:O	2.12	0.48
1:A:422:ARG:HD3	1:A:491:ASN:CG	2.34	0.48
1:A:54:THR:O	1:A:57:SER:HB2	2.13	0.48
1:A:212:VAL:O	1:A:216:VAL:HG23	2.13	0.48
1:A:459:VAL:HG11	1:A:504:LEU:HD12	1.95	0.48
1:A:549:THR:CG2	1:A:550:ASP:N	2.76	0.48
1:A:557:ILE:O	1:A:561:MET:HB2	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:TRP:O	1:A:222:GLU:OE2	2.33	0.47
1:A:424:GLU:OE2	1:A:424:GLU:HA	2.14	0.47
1:A:441:LYS:O	1:A:445:GLU:HG3	2.15	0.47
1:A:145:TYR:O	1:A:145:TYR:CD2	2.57	0.47
1:A:373:THR:HG21	1:A:391:ARG:CD	2.37	0.47
1:A:422:ARG:HD3	1:A:491:ASN:OD1	2.14	0.47
1:A:12:TYR:CE2	1:A:56:ILE:HG13	2.49	0.47
1:A:503:LEU:O	1:A:506:PRO:HD2	2.14	0.47
1:A:206:GLN:HA	1:A:207:PRO:HD3	1.58	0.47
1:A:498:LYS:HA	1:A:519:LEU:CD2	2.45	0.47
1:A:537:LYS:CD	1:A:537:LYS:N	2.75	0.47
1:A:58:PHE:HD2	1:A:137:ARG:HG2	1.80	0.47
1:A:58:PHE:CD1	1:A:58:PHE:C	2.88	0.47
1:A:557:ILE:HA	1:A:561:MET:HG3	1.96	0.47
1:A:12:TYR:HE2	1:A:55:PRO:HB2	1.78	0.47
1:A:500:LEU:O	1:A:504:LEU:HB2	2.14	0.47
1:A:146:CYS:HB3	1:A:159:CYS:SG	2.55	0.46
1:A:12:TYR:CZ	1:A:56:ILE:HG13	2.50	0.46
1:A:133:PHE:CE2	1:A:185:SER:HB2	2.50	0.46
1:A:314:TYR:O	1:A:316:LYS:N	2.48	0.46
1:A:122:THR:O	1:A:184:ASP:HA	2.16	0.46
1:A:357:GLU:O	1:A:360:ASP:HB2	2.15	0.46
1:A:602:TYR:O	1:A:603:LYS:C	2.53	0.46
1:A:239:VAL:HG11	1:A:246:MET:CE	2.46	0.46
1:A:247:LYS:HD2	1:A:247:LYS:C	2.36	0.46
1:A:256:GLU:O	1:A:259:ILE:HB	2.15	0.46
1:A:399:ASN:HD21	1:A:464:SER:HA	1.81	0.46
1:A:423:GLY:O	1:A:425:LEU:HD12	2.15	0.46
1:A:600:ARG:HG3	1:A:600:ARG:HH11	1.81	0.46
1:A:597:VAL:O	1:A:600:ARG:HB3	2.16	0.46
1:A:134:LEU:N	1:A:135:PRO:HD3	2.31	0.46
1:A:58:PHE:CD2	1:A:137:ARG:HG2	2.51	0.46
1:A:470:PHE:CE1	1:A:475:PRO:HG2	2.51	0.46
1:A:216:VAL:O	1:A:220:ILE:HG13	2.16	0.45
1:A:507:PHE:O	1:A:508:LEU:HD23	2.16	0.45
1:A:136:ASP:HB2	1:A:137:ARG:H	1.61	0.45
1:A:171:PRO:C	1:A:180:ILE:HG23	2.36	0.45
1:A:170:ASN:N	1:A:171:PRO:HD3	2.31	0.45
1:A:505:GLU:HB3	1:A:506:PRO:HD3	1.99	0.45
1:A:518:LEU:HD21	1:A:542:GLU:HB2	1.97	0.45
1:A:473:LYS:HG2	1:A:489:THR:HG23	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:TYR:O	1:A:374:ILE:HG12	2.17	0.45
1:A:12:TYR:CE2	1:A:55:PRO:HB2	2.51	0.45
1:A:123:LYS:HA	1:A:184:ASP:HA	1.99	0.45
1:A:430:ARG:HG3	1:A:430:ARG:HH11	1.81	0.45
1:A:320:GLU:O	1:A:321:GLU:HG2	2.16	0.45
1:A:514:LYS:HD2	1:A:544:LEU:HD23	1.99	0.45
1:A:54:THR:HB	1:A:55:PRO:HD3	1.99	0.45
1:A:549:THR:CG2	1:A:551:ASP:HB2	2.46	0.45
1:A:122:THR:CG2	1:A:123:LYS:N	2.80	0.44
1:A:118:VAL:HG22	1:A:120:LYS:HG3	2.00	0.44
1:A:297:LYS:O	1:A:300:ILE:HG13	2.16	0.44
1:A:498:LYS:HA	1:A:519:LEU:HD21	1.99	0.44
1:A:122:THR:HG22	1:A:123:LYS:N	2.32	0.44
1:A:557:ILE:HA	1:A:561:MET:CG	2.48	0.44
1:A:8:SER:HB3	1:A:26:TYR:CE2	2.52	0.44
1:A:83:GLN:HB2	1:A:83:GLN:HE21	1.49	0.44
1:A:389:LYS:HD2	1:A:553:ILE:CD1	2.48	0.44
1:A:410:PHE:CD1	1:A:470:PHE:HE1	2.36	0.44
1:A:414:TYR:CD2	1:A:479:ALA:HB1	2.53	0.44
1:A:210:PRO:C	1:A:212:VAL:N	2.71	0.44
1:A:349:ARG:HG2	1:A:565:ASN:ND2	2.32	0.44
1:A:573:LEU:C	1:A:575:LYS:H	2.20	0.44
1:A:109:LEU:HD21	3:A:1001:HOH:O	2.17	0.44
1:A:46:ILE:CG2	1:A:47:CYS:N	2.81	0.43
1:A:526:ARG:HH22	1:A:530:ARG:HD3	1.80	0.43
1:A:522:ASP:O	1:A:523:GLU:C	2.56	0.43
1:A:54:THR:N	1:A:55:PRO:CD	2.81	0.43
1:A:190:ILE:O	1:A:226:GLU:HA	2.18	0.43
1:A:390:VAL:O	1:A:394:GLU:HB2	2.19	0.43
1:A:297:LYS:HD3	1:A:337:TYR:CE1	2.53	0.43
1:A:491:ASN:O	1:A:495:GLN:HG2	2.19	0.43
1:A:59:ARG:HD3	1:A:70:ILE:CD1	2.49	0.43
1:A:222:GLU:O	1:A:222:GLU:HG2	2.18	0.43
1:A:436:ILE:O	1:A:440:PHE:HD1	2.01	0.43
1:A:395:GLU:O	1:A:399:ASN:HB3	2.19	0.42
1:A:226:GLU:H	1:A:226:GLU:HG3	1.63	0.42
1:A:477:LYS:C	1:A:477:LYS:HD3	2.39	0.42
1:A:154:ASP:CB	1:A:162:PRO:HA	2.49	0.42
1:A:386:SER:O	1:A:390:VAL:HB	2.19	0.42
1:A:532:LEU:HD12	1:A:532:LEU:HA	1.95	0.42
1:A:498:LYS:CD	1:A:532:LEU:HD13	2.49	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:CYS:SG	1:A:178:ARG:CG	3.08	0.42
1:A:198:ARG:HH11	1:A:198:ARG:CG	2.33	0.42
1:A:502:ILE:O	1:A:505:GLU:HB3	2.20	0.42
1:A:66:SER:OG	1:A:69:GLU:HG3	2.19	0.42
1:A:210:PRO:C	1:A:212:VAL:H	2.23	0.41
1:A:285:ILE:HG22	1:A:286:ASP:H	1.82	0.41
1:A:167:ILE:O	1:A:167:ILE:HG13	2.20	0.41
1:A:305:ILE:O	1:A:308:PRO:HD2	2.20	0.41
1:A:555:TYR:HD1	1:A:589:LYS:HG2	1.85	0.41
1:A:116:HIS:O	1:A:117:LEU:HD23	2.19	0.41
1:A:154:ASP:HB2	1:A:162:PRO:HA	2.02	0.41
1:A:210:PRO:O	1:A:212:VAL:N	2.54	0.41
1:A:239:VAL:CG2	1:A:239:VAL:O	2.69	0.41
1:A:142:THR:CB	1:A:169:ILE:HB	2.50	0.41
1:A:163:LEU:O	1:A:164:THR:C	2.57	0.41
1:A:258:PRO:HB2	1:A:307:TRP:CZ3	2.56	0.41
1:A:100:HIS:HD2	1:A:263:SER:OG	2.02	0.41
1:A:396:LEU:HA	1:A:396:LEU:HD12	1.93	0.41
1:A:408:LEU:HA	1:A:411:VAL:HG12	2.02	0.41
1:A:307:TRP:HB3	1:A:308:PRO:HD3	2.02	0.41
1:A:498:LYS:HD2	1:A:521:LEU:HD11	2.03	0.41
1:A:389:LYS:HD2	1:A:553:ILE:HD11	2.03	0.41
1:A:470:PHE:HE2	1:A:493:SER:HB2	1.85	0.41
1:A:498:LYS:HE3	1:A:530:ARG:O	2.21	0.41
1:A:156:CYS:SG	1:A:160:GLY:HA3	2.60	0.41
1:A:214:ASN:HA	1:A:217:LEU:HD12	2.03	0.41
1:A:18:HIS:HD2	1:A:20:GLY:N	2.19	0.41
1:A:250:VAL:CG2	1:A:251:LEU:N	2.84	0.40
1:A:261:TYR:CE1	1:A:303:HIS:HE1	2.39	0.40
1:A:192:MET:HE1	1:A:306:PHE:HA	2.02	0.40
1:A:433:LEU:HD21	1:A:492:ILE:CD1	2.51	0.40
1:A:596:VAL:HG12	1:A:596:VAL:O	2.21	0.40
1:A:33:VAL:HG11	1:A:45:PHE:HB2	2.02	0.40
1:A:505:GLU:HG3	1:A:506:PRO:N	2.36	0.40
1:A:409:THR:HA	1:A:541:PRO:CG	2.51	0.40
1:A:544:LEU:HD23	1:A:544:LEU:HA	1.76	0.40
1:A:355:VAL:O	1:A:359:LEU:HB2	2.21	0.40
1:A:414:TYR:CE2	1:A:479:ALA:CB	3.04	0.40
1:A:193:GLN:OE1	1:A:223:GLY:HA2	2.21	0.40
1:A:215:MET:HA	1:A:215:MET:HE3	2.04	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	604/722 (84%)	505 (84%)	78 (13%)	21 (4%)	4	17

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ASP
1	A	137	ARG
1	A	145	TYR
1	A	162	PRO
1	A	285	ILE
1	A	288	GLN
1	A	377	GLU
1	A	157	GLU
1	A	159	CYS
1	A	223	GLY
1	A	315	GLY
1	A	562	ALA
1	A	603	LYS
1	A	144	PRO
1	A	156	CYS
1	A	180	ILE
1	A	150	ASP
1	A	207	PRO
1	A	505	GLU
1	A	596	VAL
1	A	275	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	517/635 (81%)	461 (89%)	56 (11%)	7 23

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	17	ILE
1	A	49	THR
1	A	58	PHE
1	A	63	GLU
1	A	70	ILE
1	A	77	GLN
1	A	83	GLN
1	A	96	GLU
1	A	98	PRO
1	A	107	PHE
1	A	109	LEU
1	A	118	VAL
1	A	123	LYS
1	A	136	ASP
1	A	145	TYR
1	A	146	CYS
1	A	152	LYS
1	A	154	ASP
1	A	155	GLN
1	A	156	CYS
1	A	178	ARG
1	A	183	ARG
1	A	215	MET
1	A	221	GLU
1	A	226	GLU
1	A	234	ASN
1	A	239	VAL
1	A	247	LYS
1	A	252	TYR
1	A	256	GLU
1	A	283	LEU
1	A	286	ASP
1	A	299	ASN
1	A	314	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	319	ASP
1	A	328	LEU
1	A	344	LYS
1	A	359	LEU
1	A	412	ASN
1	A	430	ARG
1	A	458	ARG
1	A	468	ARG
1	A	470	PHE
1	A	475	PRO
1	A	503	LEU
1	A	504	LEU
1	A	514	LYS
1	A	516	TRP
1	A	519	LEU
1	A	537	LYS
1	A	538	VAL
1	A	551	ASP
1	A	570	ARG
1	A	575	LYS
1	A	600	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	75	HIS
1	A	77	GLN
1	A	83	GLN
1	A	100	HIS
1	A	105	GLN
1	A	114	ASN
1	A	155	GLN
1	A	170	ASN
1	A	187	HIS
1	A	211	ASN
1	A	276	ASN
1	A	303	HIS
1	A	335	ASN
1	A	393	ASN
1	A	399	ASN
1	A	520	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	536	HIS

### 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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.