



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 03:26 PM EDT

PDB ID : 3RI6  
Title : A Novel Mechanism of Sulfur Transfer Catalyzed by O-Acetylhomoserine  
Sulfhydrylase in Methionine Biosynthetic Pathway of Wolinella succinogenes  
Authors : Tran, T.H.; Krishnamoorthy, K.; Begley, T.P.; Ealick, S.E.  
Deposited on : unknown  
Resolution : 2.20 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

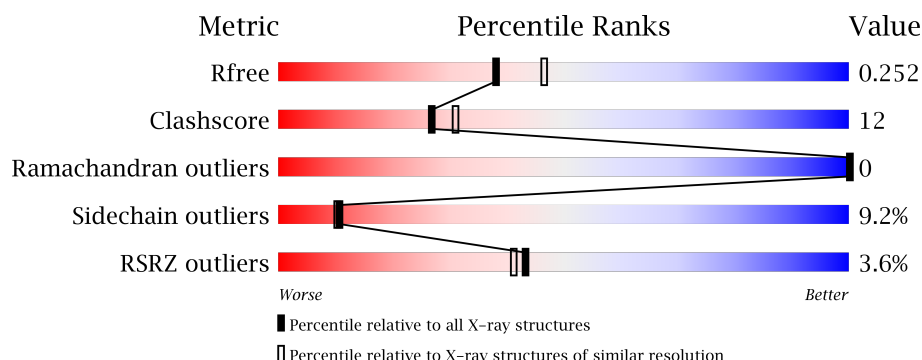
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	430	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>13%</div> <div>• •</div> <div>18%</div> </div> </div>
1	B	430	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>13%</div> <div>•</div> <div>21%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5448 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 O-ACETYLHOMOSERINE SULFHYDRYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2669	1708	449	500	12			
1	B	341	Total	C	N	O	S	0	0	0
			2596	1665	437	483	11			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP Q7M9C8
A	-21	GLY	-	EXPRESSION TAG	UNP Q7M9C8
A	-20	SER	-	EXPRESSION TAG	UNP Q7M9C8
A	-19	ASP	-	EXPRESSION TAG	UNP Q7M9C8
A	-18	LYS	-	EXPRESSION TAG	UNP Q7M9C8
A	-17	ILE	-	EXPRESSION TAG	UNP Q7M9C8
A	-16	HIS	-	EXPRESSION TAG	UNP Q7M9C8
A	-15	HIS	-	EXPRESSION TAG	UNP Q7M9C8
A	-14	HIS	-	EXPRESSION TAG	UNP Q7M9C8
A	-13	HIS	-	EXPRESSION TAG	UNP Q7M9C8
A	-12	HIS	-	EXPRESSION TAG	UNP Q7M9C8
A	-11	HIS	-	EXPRESSION TAG	UNP Q7M9C8
A	-10	SER	-	EXPRESSION TAG	UNP Q7M9C8
A	-9	SER	-	EXPRESSION TAG	UNP Q7M9C8
A	-8	GLY	-	EXPRESSION TAG	UNP Q7M9C8
A	-7	GLU	-	EXPRESSION TAG	UNP Q7M9C8
A	-6	ASN	-	EXPRESSION TAG	UNP Q7M9C8
A	-5	LEU	-	EXPRESSION TAG	UNP Q7M9C8
A	-4	TYR	-	EXPRESSION TAG	UNP Q7M9C8
A	-3	PHE	-	EXPRESSION TAG	UNP Q7M9C8
A	-2	GLN	-	EXPRESSION TAG	UNP Q7M9C8
A	-1	GLY	-	EXPRESSION TAG	UNP Q7M9C8
A	0	HIS	-	EXPRESSION TAG	UNP Q7M9C8
B	-22	MET	-	EXPRESSION TAG	UNP Q7M9C8
B	-21	GLY	-	EXPRESSION TAG	UNP Q7M9C8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	EXPRESSION TAG	UNP Q7M9C8
B	-19	ASP	-	EXPRESSION TAG	UNP Q7M9C8
B	-18	LYS	-	EXPRESSION TAG	UNP Q7M9C8
B	-17	ILE	-	EXPRESSION TAG	UNP Q7M9C8
B	-16	HIS	-	EXPRESSION TAG	UNP Q7M9C8
B	-15	HIS	-	EXPRESSION TAG	UNP Q7M9C8
B	-14	HIS	-	EXPRESSION TAG	UNP Q7M9C8
B	-13	HIS	-	EXPRESSION TAG	UNP Q7M9C8
B	-12	HIS	-	EXPRESSION TAG	UNP Q7M9C8
B	-11	HIS	-	EXPRESSION TAG	UNP Q7M9C8
B	-10	SER	-	EXPRESSION TAG	UNP Q7M9C8
B	-9	SER	-	EXPRESSION TAG	UNP Q7M9C8
B	-8	GLY	-	EXPRESSION TAG	UNP Q7M9C8
B	-7	GLU	-	EXPRESSION TAG	UNP Q7M9C8
B	-6	ASN	-	EXPRESSION TAG	UNP Q7M9C8
B	-5	LEU	-	EXPRESSION TAG	UNP Q7M9C8
B	-4	TYR	-	EXPRESSION TAG	UNP Q7M9C8
B	-3	PHE	-	EXPRESSION TAG	UNP Q7M9C8
B	-2	GLN	-	EXPRESSION TAG	UNP Q7M9C8
B	-1	GLY	-	EXPRESSION TAG	UNP Q7M9C8
B	0	HIS	-	EXPRESSION TAG	UNP Q7M9C8

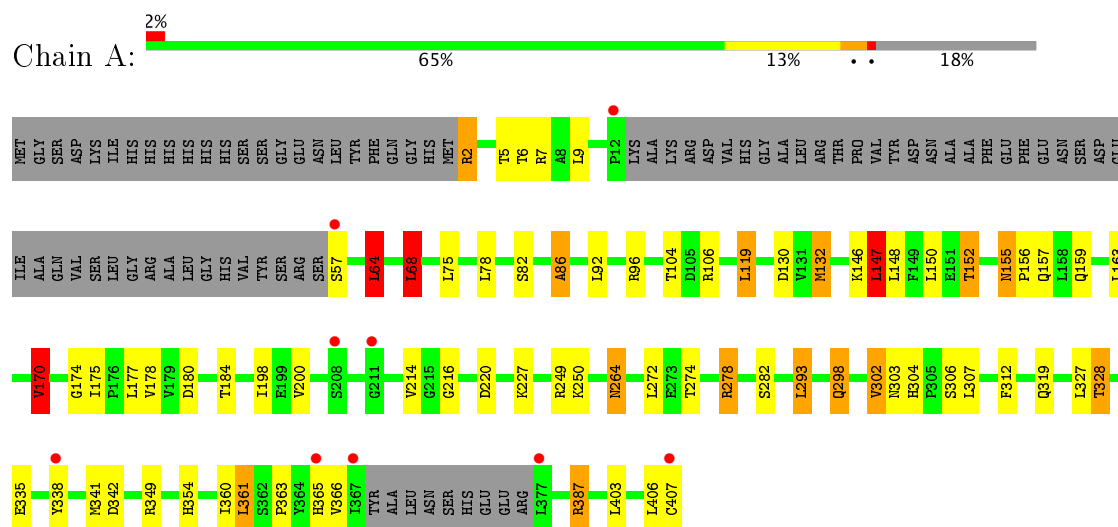
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	115	Total	O	0	0
			115	115		
2	B	68	Total	O	0	0
			68	68		

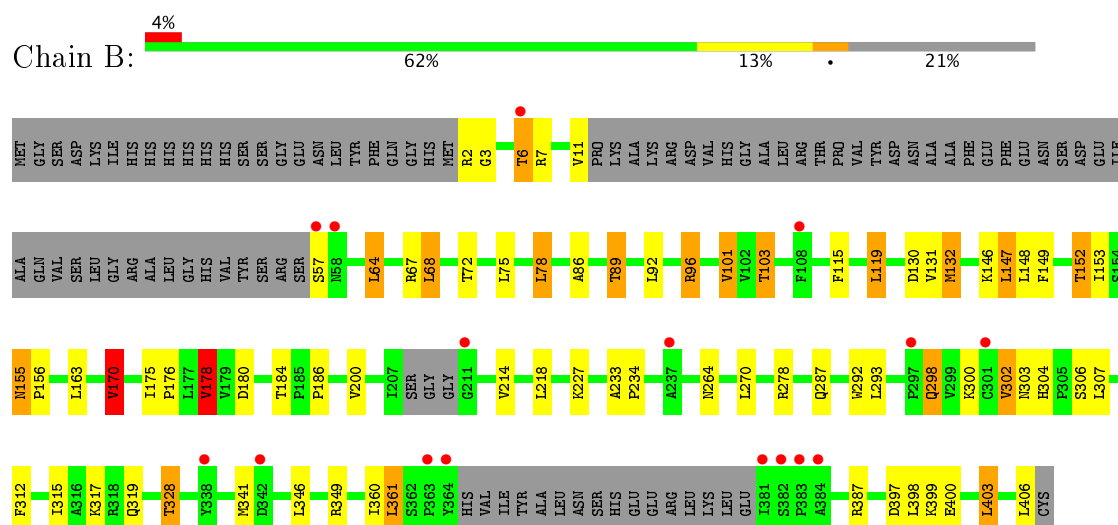
### 3 Residue-property plots [i](#)

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.

#### • Molecule 1: O-ACETHOMOSERINE SULFHYDRYLASE



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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.80 Å   62.50 Å   91.60 Å 90.00°   120.50°   90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.69 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.20) 98.9 (29.69-2.19)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.18 (at 2.20 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.225   ,   0.251 0.226   ,   0.252	Depositor DCC
$R_{free}$ test set	2015 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5448	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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

### 5.1 Standard geometry

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	1.05	3/2718 (0.1%)	0.95	10/3691 (0.3%)
1	B	1.07	5/2644 (0.2%)	0.99	11/3590 (0.3%)
All	All	1.06	8/5362 (0.1%)	0.97	21/7281 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	VAL	CB-CG1	-8.35	1.35	1.52
1	B	178	VAL	CB-CG1	-8.29	1.35	1.52
1	B	103	THR	CB-CG2	-6.33	1.31	1.52
1	A	282	SER	CB-OG	-6.28	1.34	1.42
1	A	170	VAL	CB-CG2	-5.56	1.41	1.52
1	B	131	VAL	CB-CG2	-5.30	1.41	1.52
1	B	170	VAL	CB-CG2	-5.05	1.42	1.52
1	A	86	ALA	CA-CB	5.01	1.62	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	VAL	CG1-CB-CG2	-10.03	94.85	110.90
1	B	278	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	B	278	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	A	96	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	89	THR	OG1-CB-CG2	-6.32	95.45	110.00
1	A	278	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	119	LEU	CB-CG-CD1	6.28	121.67	111.00
1	A	147	LEU	CA-CB-CG	6.22	129.61	115.30
1	A	180	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	101	VAL	CG1-CB-CG2	-6.01	101.28	110.90
1	A	278	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	96	ARG	CG-CD-NE	-5.97	99.26	111.80
1	A	387	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	400	GLU	OE1-CD-OE2	-5.96	116.14	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	LEU	CB-CG-CD1	5.89	121.01	111.00
1	B	96	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	220	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	68	LEU	CA-CB-CG	5.61	128.21	115.30
1	B	387	ARG	CG-CD-NE	5.53	123.41	111.80
1	B	78	LEU	CB-CG-CD2	5.02	119.53	111.00
1	A	64	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	2669	0	2680	62	0
1	B	2596	0	2627	60	0
2	A	115	0	0	8	0
2	B	68	0	0	1	0
All	All	5448	0	5307	122	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 12.

All (122) 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:132:MET:CE	1:B:312:PHE:CE1	2.30	1.14
1:A:104:THR:HG22	1:A:106:ARG:H	0.99	1.12
1:B:132:MET:CE	1:B:312:PHE:HE1	1.65	1.04
1:B:132:MET:HE3	1:B:312:PHE:HE1	1.19	1.02
1:A:132:MET:HE1	1:A:159:GLN:HB3	1.39	1.01
1:A:132:MET:HE3	1:A:312:PHE:CE1	2.01	0.95
1:B:101:VAL:HG13	1:B:147:LEU:HD22	1.48	0.95
1:A:104:THR:HG22	1:A:106:ARG:N	1.84	0.93
1:A:132:MET:CE	1:A:312:PHE:CE1	2.57	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:O	1:B:72:THR:HG22	1.74	0.87
1:A:104:THR:CG2	1:A:106:ARG:H	1.85	0.86
1:B:132:MET:HE1	1:B:312:PHE:CE1	2.14	0.81
1:A:298:GLN:HG3	1:A:406:LEU:HD22	1.65	0.79
1:A:328:THR:CG2	2:A:428:HOH:O	2.31	0.79
1:B:101:VAL:CG1	1:B:147:LEU:HD22	2.11	0.79
1:B:64:LEU:HD22	1:B:68:LEU:CD2	2.13	0.78
1:A:387:ARG:HD2	2:A:519:HOH:O	1.85	0.76
1:B:298:GLN:HG3	1:B:406:LEU:HD22	1.66	0.76
1:A:152:THR:HG21	1:A:184:THR:OG1	1.86	0.75
1:A:406:LEU:O	1:A:407:CYS:CB	2.34	0.74
1:A:406:LEU:O	1:A:407:CYS:HB2	1.88	0.73
1:A:132:MET:HE3	1:A:312:PHE:HE1	1.55	0.71
1:B:303:ASN:HB3	1:B:328:THR:HG22	1.72	0.71
1:B:163:LEU:H	1:B:319:GLN:HE22	1.40	0.69
1:A:341:MET:HE3	1:A:361:LEU:HA	1.76	0.68
1:A:132:MET:CE	1:A:312:PHE:HE1	2.04	0.67
1:A:302:VAL:HG22	1:A:307:LEU:HD11	1.77	0.67
1:B:103:THR:HG22	1:B:149:PHE:HB3	1.77	0.66
1:B:103:THR:HG21	1:B:115:PHE:CE2	2.31	0.66
1:A:328:THR:HG22	2:A:428:HOH:O	1.95	0.65
1:B:132:MET:HE2	1:B:312:PHE:CE1	2.31	0.64
1:B:341:MET:HE2	1:B:360:ILE:HG23	1.79	0.64
1:B:146:LYS:O	1:B:147:LEU:HB3	1.97	0.64
1:B:170:VAL:HG22	1:B:175:ILE:HB	1.80	0.63
1:A:130:ASP:OD1	1:A:132:MET:HB2	1.99	0.62
1:A:132:MET:HE2	1:A:312:PHE:CE1	2.34	0.62
1:A:341:MET:CE	1:A:361:LEU:HA	2.29	0.61
1:B:3:GLY:O	1:B:6:THR:HG23	1.99	0.61
1:B:302:VAL:HG22	1:B:307:LEU:HD11	1.83	0.61
1:A:406:LEU:O	1:A:407:CYS:SG	2.59	0.60
1:A:163:LEU:H	1:A:319:GLN:HE22	1.48	0.59
1:A:328:THR:HG23	2:A:428:HOH:O	1.99	0.58
1:B:130:ASP:OD1	1:B:132:MET:HB2	2.02	0.58
1:A:64:LEU:HD22	1:A:68:LEU:HD22	1.85	0.58
1:B:101:VAL:CG1	1:B:147:LEU:CD2	2.82	0.56
1:A:354:HIS:HE1	2:A:424:HOH:O	1.90	0.55
1:B:132:MET:HE3	1:B:312:PHE:CE1	2.09	0.55
1:B:302:VAL:CG2	1:B:307:LEU:HD11	2.37	0.55
1:A:341:MET:HE2	1:A:349:ARG:HG2	1.88	0.54
1:B:155:ASN:HD22	1:B:156:PRO:CA	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:VAL:HG22	1:A:198:ILE:HB	1.88	0.54
1:B:64:LEU:HD22	1:B:68:LEU:HD21	1.91	0.53
1:A:170:VAL:HG22	1:A:175:ILE:HB	1.89	0.53
1:B:341:MET:CE	1:B:360:ILE:HG23	2.38	0.53
1:A:68:LEU:HD13	1:A:272:LEU:HD11	1.91	0.52
1:A:298:GLN:HE21	1:A:298:GLN:H	1.57	0.52
1:A:264:ASN:HD22	1:A:264:ASN:N	2.08	0.52
1:B:341:MET:HE3	1:B:361:LEU:HA	1.92	0.52
1:B:103:THR:CG2	1:B:115:PHE:CE2	2.92	0.51
1:B:341:MET:CE	1:B:361:LEU:HA	2.40	0.51
1:A:249:ARG:HD2	1:A:250:LYS:HE3	1.92	0.51
1:B:302:VAL:HG22	1:B:307:LEU:CD1	2.40	0.51
1:A:146:LYS:O	1:A:147:LEU:HB3	2.10	0.51
1:B:103:THR:HG21	1:B:115:PHE:CZ	2.46	0.51
1:B:292:TRP:CG	1:B:399:LYS:HE2	2.47	0.50
1:A:155:ASN:HD22	1:A:156:PRO:CA	2.25	0.50
1:A:303:ASN:HB3	1:A:328:THR:HG22	1.93	0.50
1:B:155:ASN:HD22	1:B:156:PRO:HA	1.76	0.49
1:B:163:LEU:H	1:B:319:GLN:NE2	2.09	0.49
1:B:132:MET:HE2	1:B:312:PHE:CZ	2.48	0.49
1:B:152:THR:HG23	1:B:153:ILE:HG13	1.94	0.48
1:B:89:THR:HG23	1:B:218:LEU:CD1	2.43	0.48
1:B:349:ARG:HA	1:B:360:ILE:O	2.14	0.48
1:A:366:VAL:HG12	1:A:366:VAL:O	2.14	0.48
1:A:341:MET:CE	1:A:349:ARG:HG2	2.43	0.48
1:B:64:LEU:HD22	1:B:68:LEU:HD22	1.92	0.48
1:B:11:VAL:HG21	1:B:67:ARG:HG2	1.96	0.48
1:A:174:GLY:HA2	2:A:451:HOH:O	2.15	0.47
1:A:5:THR:O	1:A:9:LEU:HD13	2.14	0.47
1:B:233:ALA:N	1:B:234:PRO:CD	2.78	0.47
1:A:298:GLN:H	1:A:298:GLN:NE2	2.12	0.47
1:A:304:HIS:CD2	1:A:306:SER:H	2.33	0.47
1:A:342:ASP:OD2	1:A:349:ARG:NH1	2.48	0.47
1:A:227:LYS:HG2	2:A:439:HOH:O	2.14	0.46
1:A:2:ARG:HH11	1:A:7:ARG:HG2	1.81	0.46
1:B:149:PHE:HD2	1:B:178:VAL:HG13	1.79	0.46
1:A:106:ARG:HH21	1:A:157:GLN:CD	2.17	0.46
1:A:155:ASN:HD22	1:A:156:PRO:HA	1.80	0.46
1:A:304:HIS:HD2	1:A:306:SER:OG	1.99	0.46
1:A:341:MET:HE3	1:A:361:LEU:CA	2.44	0.46
1:B:152:THR:HG21	1:B:184:THR:OG1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ARG:HA	1:A:360:ILE:O	2.16	0.45
1:B:403:LEU:HD12	1:B:403:LEU:HA	1.83	0.45
1:B:101:VAL:HG13	1:B:147:LEU:CD2	2.32	0.45
1:B:170:VAL:HG22	1:B:175:ILE:CG2	2.47	0.45
1:A:82:SER:O	1:A:216:GLY:HA3	2.17	0.44
1:B:304:HIS:HD2	1:B:306:SER:OG	2.00	0.44
1:A:132:MET:HE2	1:A:312:PHE:CZ	2.52	0.44
1:B:303:ASN:HB3	1:B:328:THR:CG2	2.45	0.44
1:A:338:TYR:OH	1:A:365:HIS:CB	2.66	0.43
1:B:304:HIS:CD2	1:B:306:SER:H	2.36	0.43
1:B:86:ALA:O	1:B:89:THR:HG22	2.18	0.43
1:A:363:PRO:HD2	2:A:489:HOH:O	2.19	0.43
1:A:274:THR:OG1	1:A:278:ARG:HD3	2.19	0.43
1:B:180:ASP:HA	1:B:200:VAL:O	2.20	0.42
1:B:3:GLY:C	1:B:6:THR:HG23	2.39	0.42
1:B:398:LEU:HA	1:B:398:LEU:HD23	1.89	0.41
1:A:341:MET:CE	1:A:360:ILE:HG23	2.50	0.41
1:B:170:VAL:HG22	1:B:175:ILE:CB	2.50	0.41
1:B:175:ILE:HA	1:B:176:PRO:HD3	1.93	0.41
1:A:132:MET:CE	1:A:312:PHE:CZ	3.03	0.41
1:A:106:ARG:NH2	1:A:157:GLN:OE1	2.35	0.41
1:A:327:LEU:C	1:A:327:LEU:HD12	2.40	0.41
1:B:2:ARG:HH11	1:B:7:ARG:HG2	1.85	0.41
1:A:335:GLU:H	1:A:335:GLU:CD	2.24	0.41
1:B:214:VAL:HG13	2:B:410:HOH:O	2.21	0.41
1:B:346:LEU:HD11	1:B:397:ASP:HB3	2.03	0.41
1:A:150:LEU:HD21	1:A:177:LEU:HD11	2.02	0.41
1:A:293:LEU:HA	1:A:293:LEU:HD12	1.95	0.41
1:B:315:ILE:O	1:B:319:GLN:HG3	2.21	0.40
1:A:86:ALA:CB	1:A:200:VAL:HG13	2.52	0.40
1:B:178:VAL:O	1:B:178:VAL:CG1	2.68	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	347/430 (81%)	339 (98%)	8 (2%)	0	100	100
1	B	333/430 (77%)	330 (99%)	3 (1%)	0	100	100
All	All	680/860 (79%)	669 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	286/365 (78%)	263 (92%)	23 (8%)	14	14
1	B	281/365 (77%)	252 (90%)	29 (10%)	8	7
All	All	567/730 (78%)	515 (91%)	52 (9%)	11	10

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	6	THR
1	A	57	SER
1	A	64	LEU
1	A	68	LEU
1	A	75	LEU
1	A	78	LEU
1	A	92	LEU
1	A	119	LEU
1	A	132	MET
1	A	147	LEU
1	A	148	LEU
1	A	152	THR
1	A	155	ASN
1	A	170	VAL

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Mol	Chain	Res	Type
1	A	214	VAL
1	A	264	ASN
1	A	293	LEU
1	A	298	GLN
1	A	302	VAL
1	A	328	THR
1	A	361	LEU
1	A	403	LEU
1	B	6	THR
1	B	57	SER
1	B	64	LEU
1	B	68	LEU
1	B	75	LEU
1	B	78	LEU
1	B	92	LEU
1	B	96	ARG
1	B	119	LEU
1	B	132	MET
1	B	147	LEU
1	B	148	LEU
1	B	152	THR
1	B	155	ASN
1	B	170	VAL
1	B	178	VAL
1	B	186	PRO
1	B	227	LYS
1	B	264	ASN
1	B	270	LEU
1	B	287	GLN
1	B	293	LEU
1	B	298	GLN
1	B	300	LYS
1	B	302	VAL
1	B	317	LYS
1	B	328	THR
1	B	361	LEU
1	B	403	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN

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Mol	Chain	Res	Type
1	A	264	ASN
1	A	298	GLN
1	A	303	ASN
1	A	304	HIS
1	A	319	GLN
1	A	354	HIS
1	B	155	ASN
1	B	264	ASN
1	B	298	GLN
1	B	303	ASN
1	B	304	HIS
1	B	319	GLN

### 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](#)

There are no ligands in this entry.

### 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	353/430 (82%)	-0.25	9 (2%) 58 55	13, 22, 40, 54	0
1	B	341/430 (79%)	-0.11	16 (4%) 32 31	14, 22, 36, 45	0
All	All	694/860 (80%)	-0.18	25 (3%) 43 41	13, 22, 38, 54	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	CYS	4.5
1	B	57	SER	3.9
1	B	338	TYR	3.9
1	B	381	ILE	3.2
1	A	338	TYR	2.7
1	A	57	SER	2.7
1	B	108	PHE	2.7
1	B	383	PRO	2.7
1	A	12	PRO	2.7
1	A	208	SER	2.6
1	B	297	PRO	2.6
1	B	363	PRO	2.6
1	B	384	ALA	2.5
1	A	407	CYS	2.5
1	B	382	SER	2.4
1	B	342	ASP	2.4
1	B	6	THR	2.4
1	A	377	LEU	2.3
1	A	367	ILE	2.2
1	A	365	HIS	2.2
1	B	211	GLY	2.2
1	B	58	ASN	2.1
1	B	237	ALA	2.1
1	B	364	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	211	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.