



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 02:46 am BST

PDB ID : 3U4Y  
Title : The crystal structure of a functionally unknown protein (Dtox\_1751) from Desulfotomaculum acetoxidans DSM 771.  
Authors : Tan, K.; Bigelow, L.; Bearden, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2011-10-10  
Resolution : 2.99 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 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 : 2.11  
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) : 2.11

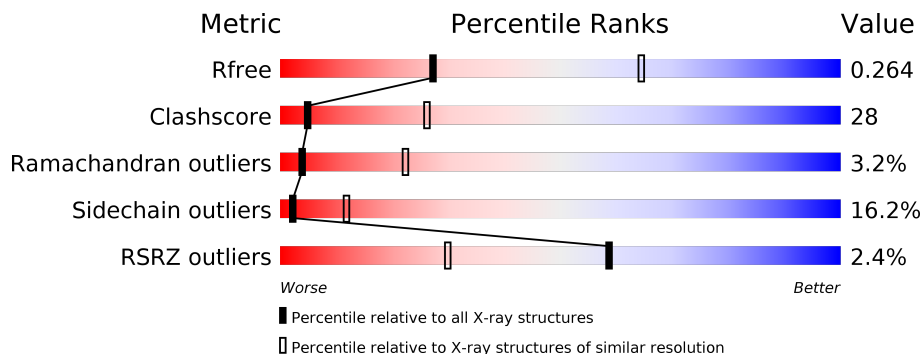
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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 on 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	331	
1	B	331	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4862 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.

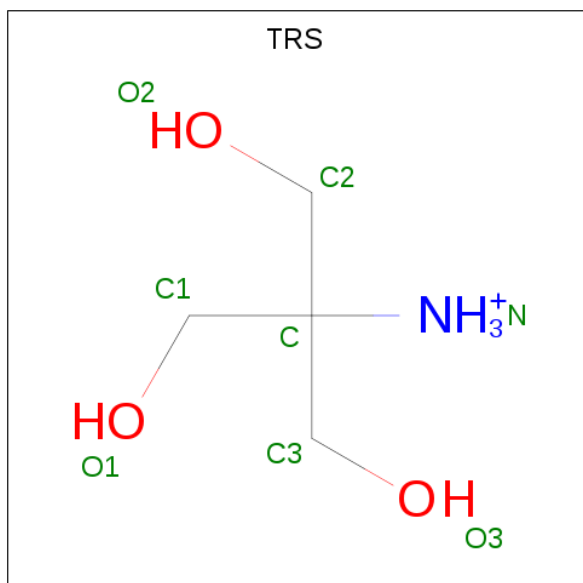
- Molecule 1 is a protein called uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
1	A	319	Total 2425	C 1542	N 400	O 477	S 3	Se 3	0	0	0
1	B	317	Total 2413	C 1535	N 398	O 474	S 3	Se 3	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP C8VX32
A	-1	ASN	-	EXPRESSION TAG	UNP C8VX32
A	0	ALA	-	EXPRESSION TAG	UNP C8VX32
B	-2	SER	-	EXPRESSION TAG	UNP C8VX32
B	-1	ASN	-	EXPRESSION TAG	UNP C8VX32
B	0	ALA	-	EXPRESSION TAG	UNP C8VX32

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	A	1	Total	C	N	O	0	0
			8	4	1	3		

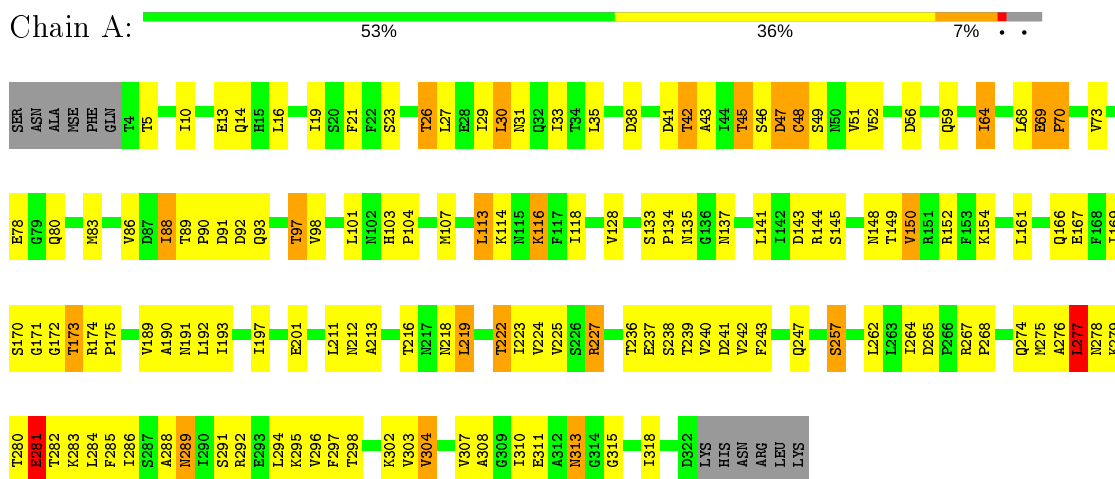
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	1	Total	O	0	0
			1	1		

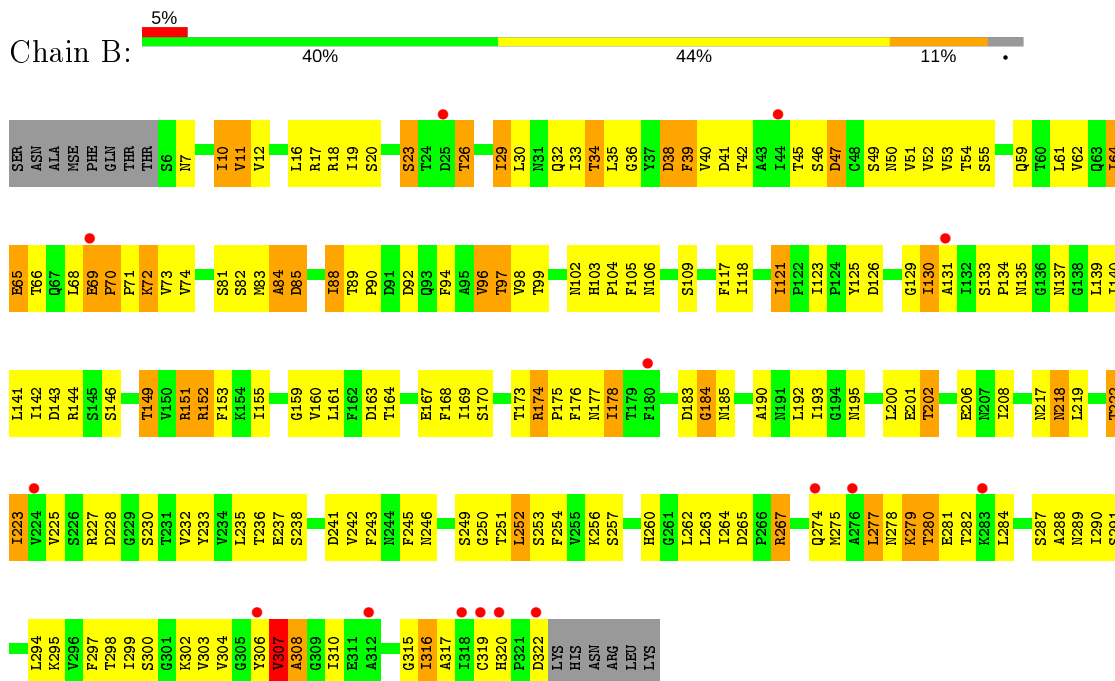
### 3 Residue-property plots

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.

- Molecule 1: uncharacterized protein



- Molecule 1: uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.64Å 66.66Å 80.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.21 – 2.99 48.21 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.21-2.99) 98.6 (48.21-2.99)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.176 , 0.268 0.176 , 0.264	Depositor DCC
$R_{free}$ test set	776 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.4	Xtrriage
Anisotropy	0.592	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: TRS

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	0.49	0/2467	0.70	1/3357 (0.0%)
1	B	0.38	0/2455	0.62	0/3340
All	All	0.44	0/4922	0.66	1/6697 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	LEU	CA-CB-CG	6.16	129.46	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2425	0	2397	110	0
1	B	2413	0	2388	157	0
2	A	16	0	24	3	0
3	A	7	0	0	0	0
3	B	1	0	0	0	0
All	All	4862	0	4809	266	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 (266) 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:280:THR:O	1:A:282:THR:HG23	1.55	1.05
1:B:99:THR:HG21	1:B:105:PHE:HA	1.41	1.01
1:A:29:ILE:HD11	1:A:308:ALA:O	1.60	0.99
1:A:227:ARG:HG2	1:A:281:GLU:OE1	1.73	0.89
1:B:190:ALA:HB2	1:B:223:ILE:HD11	1.56	0.87
1:B:109:SER:O	1:B:117:PHE:HD1	1.60	0.84
1:A:45:THR:CG2	1:A:47:ASP:HB3	2.07	0.84
1:B:222:THR:HG21	1:B:274:GLN:H	1.40	0.84
1:B:235:LEU:HB2	1:B:275:MSE:HE3	1.60	0.83
1:A:45:THR:HG23	1:A:47:ASP:HB3	1.62	0.81
1:A:240:VAL:HG22	1:A:275:MSE:HE1	1.61	0.81
1:A:236:THR:HG22	1:A:238:SER:H	1.46	0.80
1:A:29:ILE:H	1:A:29:ILE:HD12	1.44	0.80
1:B:41:ASP:OD2	1:B:42:THR:N	2.15	0.79
1:B:42:THR:HG22	1:B:53:VAL:HG22	1.64	0.78
1:B:298:THR:HG22	1:B:300:SER:H	1.46	0.78
1:B:225:VAL:HG12	1:B:232:VAL:HG22	1.67	0.77
1:B:192:LEU:HD22	1:B:219:LEU:HD12	1.68	0.76
1:B:279:LYS:H	1:B:279:LYS:CD	1.98	0.76
1:A:294:LEU:HB3	1:A:307:VAL:HG22	1.70	0.74
1:B:98:VAL:HG21	1:B:130:ILE:HB	1.70	0.72
1:B:265:ASP:O	1:B:289:ASN:ND2	2.23	0.72
1:A:69:GLU:CB	1:A:70:PRO:HD3	2.20	0.72
1:A:277:LEU:HD13	1:A:284:LEU:CD2	2.21	0.70
1:B:279:LYS:HE3	1:B:319:CYS:O	1.91	0.70
1:A:222:THR:HG21	1:A:274:GLN:H	1.55	0.70
1:B:135:ASN:HB2	1:B:137:ASN:HD22	1.57	0.70
1:B:277:LEU:HD13	1:B:284:LEU:HD23	1.73	0.69
1:A:114:LYS:HD3	1:A:116:LYS:NZ	2.08	0.69
1:A:218:ASN:O	1:A:236:THR:HG23	1.92	0.69
1:B:144:ARG:HB2	1:B:149:THR:HG22	1.75	0.69
1:A:167:GLU:H	2:A:330:TRS:C1	2.07	0.68
1:A:240:VAL:CG2	1:A:275:MSE:HE1	2.24	0.67
1:A:236:THR:HB	1:A:239:THR:O	1.94	0.67
1:A:29:ILE:N	1:A:29:ILE:HD12	2.09	0.67
1:A:103:HIS:HB2	1:A:104:PRO:HA	1.76	0.66
1:A:107:MSE:HG2	1:A:161:LEU:HD13	1.78	0.66
1:A:265:ASP:O	1:A:289:ASN:ND2	2.29	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ASP:HB3	1:B:55:SER:HB2	1.78	0.65
1:A:10:ILE:HD13	1:A:42:THR:HG21	1.78	0.65
1:A:277:LEU:HD13	1:A:284:LEU:HD23	1.79	0.64
1:A:21:PHE:CZ	1:A:64:ILE:HD11	2.33	0.64
1:B:265:ASP:OD1	1:B:267:ARG:HD2	1.97	0.64
1:B:69:GLU:HB3	1:B:70:PRO:HD3	1.80	0.64
1:B:245:PHE:CZ	1:B:250:GLY:HA2	2.33	0.63
1:A:69:GLU:HB3	1:A:70:PRO:HD3	1.81	0.63
1:B:90:PRO:HG3	1:B:134:PRO:HA	1.81	0.63
1:B:135:ASN:HB2	1:B:137:ASN:ND2	2.13	0.63
1:B:45:THR:CG2	1:B:50:ASN:H	2.12	0.63
1:B:69:GLU:HG2	1:B:70:PRO:HD3	1.80	0.63
1:A:197:ILE:CD1	1:A:216:THR:HG21	2.29	0.62
1:B:18:ARG:HD3	1:B:32:GLN:HB3	1.82	0.62
1:B:99:THR:CG2	1:B:106:ASN:H	2.13	0.61
1:B:183:ASP:O	1:B:185:ASN:N	2.29	0.61
1:B:135:ASN:HD21	1:B:184:GLY:H	1.47	0.61
1:A:114:LYS:O	1:A:116:LYS:HG3	2.00	0.61
1:A:262:LEU:HD13	1:A:288:ALA:HB2	1.83	0.61
1:B:260:HIS:ND1	1:B:262:LEU:HB2	2.16	0.60
1:B:135:ASN:CB	1:B:137:ASN:HD22	2.13	0.60
1:B:135:ASN:ND2	1:B:184:GLY:H	1.99	0.60
1:A:292:ARG:HG3	1:B:125:TYR:HB3	1.84	0.60
1:B:294:LEU:HD23	1:B:307:VAL:HG11	1.83	0.60
1:B:233:TYR:CD1	1:B:242:VAL:HG12	2.37	0.59
1:B:281:GLU:O	1:B:299:ILE:HD13	2.02	0.59
1:B:83:MSE:CG	1:B:97:THR:OG1	2.51	0.59
1:B:201:GLU:O	1:B:208:ILE:HG23	2.03	0.59
1:A:167:GLU:H	2:A:330:TRS:H12	1.67	0.59
1:B:263:LEU:HB3	1:B:290:ILE:HB	1.83	0.58
1:B:242:VAL:CG2	1:B:256:LYS:HB3	2.33	0.58
1:B:69:GLU:CB	1:B:70:PRO:HD3	2.33	0.58
1:A:172:GLY:H	1:A:191:ASN:ND2	2.02	0.57
1:B:262:LEU:HD22	1:B:288:ALA:HB2	1.87	0.57
1:B:29:ILE:HD11	1:B:32:GLN:OE1	2.04	0.57
1:B:47:ASP:OD2	1:B:47:ASP:N	2.36	0.57
1:A:145:SER:HA	1:A:175:PRO:HD2	1.87	0.57
1:B:277:LEU:HD13	1:B:284:LEU:CD2	2.34	0.57
1:B:81:SER:HB3	1:B:104:PRO:HG2	1.87	0.57
1:A:295:LYS:HD3	1:A:297:PHE:CZ	2.40	0.56
1:B:228:ASP:OD1	1:B:230:SER:HB3	2.06	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:NH1	1:B:32:GLN:OE1	2.38	0.56
1:B:246:ASN:ND2	1:B:249:SER:OG	2.39	0.56
1:A:201:GLU:HG3	1:A:211:LEU:HD21	1.88	0.56
1:B:233:TYR:HD1	1:B:242:VAL:HG12	1.71	0.56
1:B:39:PHE:HA	1:B:54:THR:O	2.06	0.55
1:B:83:MSE:HG3	1:B:97:THR:OG1	2.05	0.55
1:A:149:THR:HG21	1:A:167:GLU:OE1	2.06	0.55
1:B:19:ILE:HD12	1:B:19:ILE:C	2.27	0.55
1:A:46:SER:HB2	1:A:92:ASP:OD2	2.06	0.55
1:A:29:ILE:HG22	1:A:30:LEU:N	2.21	0.55
1:A:169:ILE:HG22	1:A:171:GLY:H	1.72	0.55
1:B:135:ASN:OD1	1:B:184:GLY:HA3	2.07	0.54
1:B:295:LYS:HD2	1:B:297:PHE:CE2	2.43	0.54
1:B:217:ASN:ND2	1:B:241:ASP:OD1	2.41	0.54
1:B:89:THR:O	1:B:92:ASP:N	2.33	0.54
1:A:148:ASN:HA	1:A:175:PRO:HD3	1.89	0.54
1:B:88:ILE:HD13	1:B:88:ILE:H	1.72	0.54
1:B:23:SER:OG	1:B:26:THR:HG23	2.08	0.54
1:A:265:ASP:O	1:A:268:PRO:HD2	2.08	0.53
1:B:279:LYS:N	1:B:279:LYS:CD	2.69	0.53
1:B:151:ARG:NH1	1:B:163:ASP:OD2	2.41	0.53
1:B:42:THR:CG2	1:B:53:VAL:HG22	2.38	0.53
1:A:277:LEU:HD13	1:A:284:LEU:HD21	1.90	0.53
1:A:166:GLN:HA	2:A:330:TRS:H11	1.91	0.53
1:B:96:VAL:HB	1:B:130:ILE:CD1	2.38	0.53
1:B:279:LYS:O	1:B:281:GLU:HG2	2.08	0.53
1:B:121:ILE:CD1	1:B:161:LEU:HB3	2.38	0.53
1:A:38:ASP:OD2	1:A:56:ASP:HB3	2.09	0.53
1:A:47:ASP:O	1:A:48:CYS:HB2	2.07	0.53
1:B:316:ILE:HG13	1:B:317:ALA:N	2.24	0.53
1:A:91:ASP:O	1:A:92:ASP:HB2	2.08	0.53
1:B:195:ASN:OD1	1:B:218:ASN:HA	2.08	0.53
1:B:288:ALA:HB1	1:B:291:SER:HB2	1.91	0.52
1:B:185:ASN:O	1:B:202:THR:N	2.40	0.52
1:A:223:ILE:HD13	1:A:223:ILE:N	2.24	0.52
1:A:280:THR:O	1:A:281:GLU:C	2.47	0.52
1:A:267:ARG:N	1:A:268:PRO:HD2	2.26	0.51
1:B:69:GLU:HB3	1:B:70:PRO:CD	2.40	0.51
1:B:69:GLU:CG	1:B:70:PRO:HD3	2.40	0.51
1:A:241:ASP:OD1	1:A:257:SER:HB3	2.10	0.51
1:A:298:THR:OG1	1:A:302:LYS:HB3	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:SER:N	1:B:30:LEU:HD13	2.24	0.51
1:A:307:VAL:HG21	1:A:310:ILE:HD12	1.91	0.51
1:B:307:VAL:HG23	1:B:308:ALA:H	1.76	0.51
1:A:21:PHE:HZ	1:A:64:ILE:HD11	1.72	0.51
1:B:142:ILE:HA	1:B:178:ILE:HD11	1.93	0.51
1:B:262:LEU:HD22	1:B:288:ALA:CB	2.40	0.51
1:A:43:ALA:HB3	1:A:88:ILE:HD11	1.93	0.51
1:B:243:PHE:HB3	1:B:252:LEU:HD22	1.93	0.51
1:A:69:GLU:CB	1:A:70:PRO:CD	2.89	0.51
1:A:69:GLU:HB2	1:A:70:PRO:HD3	1.92	0.51
1:A:43:ALA:CB	1:A:88:ILE:HD11	2.40	0.51
1:B:227:ARG:NH1	1:B:320:HIS:HD2	2.08	0.51
1:B:45:THR:HG22	1:B:50:ASN:H	1.75	0.51
1:A:114:LYS:HB2	1:A:116:LYS:HE2	1.93	0.51
1:B:219:LEU:HB2	1:B:237:GLU:HB2	1.93	0.51
1:B:238:SER:HA	1:B:260:HIS:CE1	2.46	0.51
1:B:262:LEU:O	1:B:263:LEU:HD23	2.11	0.51
1:B:279:LYS:H	1:B:279:LYS:HD2	1.75	0.51
1:A:280:THR:O	1:A:282:THR:CG2	2.45	0.50
1:A:29:ILE:H	1:A:29:ILE:CD1	2.19	0.50
1:A:114:LYS:HD3	1:A:116:LYS:HZ3	1.74	0.50
1:B:279:LYS:CE	1:B:319:CYS:O	2.59	0.50
1:A:128:VAL:O	1:A:143:ASP:HB2	2.12	0.50
1:B:139:LEU:HD12	1:B:140:ILE:H	1.77	0.50
1:B:51:VAL:CG1	1:B:52:VAL:N	2.75	0.50
1:A:222:THR:C	1:A:223:ILE:HD13	2.31	0.49
1:B:195:ASN:OD1	1:B:219:LEU:N	2.43	0.49
1:A:16:LEU:HD23	1:A:16:LEU:N	2.28	0.49
1:B:279:LYS:N	1:B:279:LYS:HD2	2.28	0.49
1:A:280:THR:O	1:A:282:THR:N	2.46	0.49
1:B:98:VAL:CG2	1:B:130:ILE:HB	2.39	0.49
1:B:61:LEU:HD23	1:B:61:LEU:C	2.33	0.49
1:B:46:SER:HB3	1:B:92:ASP:OD1	2.12	0.49
1:A:33:ILE:HG22	1:A:35:LEU:HD12	1.95	0.49
1:A:41:ASP:OD2	1:A:315:GLY:HA3	2.14	0.48
1:B:68:LEU:HD11	1:B:72:LYS:HG3	1.95	0.48
1:A:114:LYS:CB	1:A:116:LYS:HE2	2.44	0.48
1:B:302:LYS:HB2	1:B:302:LYS:NZ	2.29	0.48
1:A:26:THR:O	1:A:27:LEU:HB2	2.13	0.48
1:B:10:ILE:HD12	1:B:11:VAL:H	1.79	0.48
1:A:173:THR:OG1	1:A:193:ILE:HD11	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ASN:O	1:B:281:GLU:N	2.46	0.48
1:A:14:GLN:H	1:A:313:ASN:HB3	1.79	0.48
1:A:83:MSE:HB3	1:A:97:THR:HG21	1.96	0.48
1:B:121:ILE:HD11	1:B:161:LEU:HB3	1.96	0.48
1:A:33:ILE:HG22	1:A:35:LEU:CD1	2.45	0.47
1:B:84:ALA:O	1:B:85:ASP:HB2	2.12	0.47
1:A:174:ARG:HB2	1:A:193:ILE:HG12	1.97	0.47
1:A:148:ASN:HA	1:A:175:PRO:CD	2.45	0.47
1:A:51:VAL:CG1	1:A:52:VAL:N	2.78	0.47
1:A:83:MSE:HG2	1:A:97:THR:HG21	1.97	0.47
1:A:45:THR:HG22	1:A:48:CYS:H	1.80	0.47
1:B:45:THR:OG1	1:B:46:SER:N	2.48	0.47
1:B:130:ILE:HG12	1:B:131:ALA:N	2.29	0.47
1:B:217:ASN:O	1:B:218:ASN:HB2	2.14	0.47
1:B:242:VAL:HG22	1:B:256:LYS:O	2.14	0.47
1:B:33:ILE:HG22	1:B:35:LEU:HD21	1.97	0.47
1:B:139:LEU:HD12	1:B:140:ILE:N	2.30	0.46
1:B:83:MSE:HG3	1:B:97:THR:CG2	2.45	0.46
1:B:235:LEU:HB2	1:B:275:MSE:CE	2.37	0.46
1:B:64:ILE:HD12	1:B:65:GLU:O	2.15	0.46
1:A:170:SER:OG	1:A:175:PRO:HG3	2.16	0.46
1:B:222:THR:HG21	1:B:274:GLN:N	2.21	0.46
1:B:310:ILE:O	1:B:310:ILE:HG22	2.16	0.46
1:B:152:ARG:HG2	1:B:164:THR:HG21	1.98	0.46
1:B:83:MSE:HE3	1:B:83:MSE:HB2	1.91	0.46
1:B:254:PHE:HZ	1:B:257:SER:OG	2.00	0.45
1:A:277:LEU:HG	1:A:281:GLU:HA	1.97	0.45
1:A:278:ASN:ND2	1:A:280:THR:OG1	2.49	0.45
1:A:243:PHE:N	1:A:243:PHE:CD1	2.84	0.45
1:A:296:VAL:HB	1:A:304:VAL:HG22	1.99	0.45
1:B:99:THR:HG21	1:B:105:PHE:CA	2.29	0.45
1:B:109:SER:O	1:B:117:PHE:CD1	2.52	0.45
1:B:135:ASN:HD21	1:B:184:GLY:N	2.12	0.45
1:B:126:ASP:OD2	1:B:146:SER:HB2	2.17	0.45
1:B:149:THR:HG21	1:B:167:GLU:OE1	2.17	0.45
1:B:33:ILE:HG22	1:B:35:LEU:CD2	2.47	0.45
1:B:45:THR:HG21	1:B:50:ASN:H	1.80	0.45
1:B:10:ILE:HD12	1:B:11:VAL:N	2.33	0.44
1:B:170:SER:OG	1:B:175:PRO:HG3	2.17	0.44
1:B:12:VAL:CG2	1:B:42:THR:HG23	2.47	0.44
1:B:315:GLY:C	1:B:316:ILE:HG22	2.38	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:HG11	1:A:189:VAL:HG21	2.00	0.44
1:B:155:ILE:HA	1:B:160:VAL:O	2.17	0.44
1:A:89:THR:HB	1:A:90:PRO:CD	2.48	0.44
1:B:218:ASN:O	1:B:236:THR:HB	2.17	0.44
1:A:30:LEU:HB3	1:A:31:ASN:ND2	2.32	0.44
1:B:143:ASP:HB3	1:B:175:PRO:HB2	1.99	0.44
1:B:99:THR:HG21	1:B:106:ASN:H	1.83	0.43
1:B:17:ARG:HG3	1:B:36:GLY:HA2	1.99	0.43
1:B:29:ILE:HG22	1:B:308:ALA:CB	2.47	0.43
1:A:236:THR:CG2	1:A:237:GLU:N	2.80	0.43
1:B:49:SER:O	1:B:66:THR:OG1	2.35	0.43
1:B:29:ILE:HG22	1:B:308:ALA:HB3	2.00	0.43
1:A:13:GLU:HG2	1:A:311:GLU:O	2.19	0.43
1:B:82:SER:HB3	1:B:102:ASN:CB	2.48	0.43
1:A:93:GLN:HG3	1:A:113:LEU:HD11	2.00	0.43
1:A:174:ARG:CB	1:A:193:ILE:HG12	2.48	0.43
1:B:306:TYR:HB3	1:B:307:VAL:H	1.66	0.43
1:B:40:VAL:HG12	1:B:41:ASP:N	2.32	0.43
1:B:18:ARG:HG3	1:B:34:THR:HB	2.01	0.43
1:B:287:SER:HB2	1:B:316:ILE:HG21	2.01	0.43
1:B:288:ALA:CB	1:B:291:SER:HB2	2.49	0.42
1:B:69:GLU:CB	1:B:70:PRO:CD	2.95	0.42
1:A:93:GLN:HE21	1:A:113:LEU:HD11	1.85	0.42
1:B:96:VAL:HB	1:B:130:ILE:HD11	1.99	0.42
1:A:192:LEU:HD11	1:A:219:LEU:HG	2.01	0.42
1:A:10:ILE:CD1	1:A:42:THR:HG21	2.47	0.42
1:B:174:ARG:HB2	1:B:193:ILE:HG12	2.01	0.42
1:B:19:ILE:HD12	1:B:20:SER:N	2.35	0.42
1:A:286:ILE:O	1:A:294:LEU:HD12	2.20	0.42
1:A:45:THR:HG22	1:A:48:CYS:N	2.35	0.42
1:B:278:ASN:O	1:B:279:LYS:C	2.58	0.42
1:A:224:VAL:HG11	1:A:277:LEU:HD22	2.01	0.42
1:A:294:LEU:HB3	1:A:307:VAL:CG2	2.46	0.42
1:B:280:THR:OG1	1:B:282:THR:OG1	2.37	0.42
1:B:94:PHE:CZ	1:B:159:GLY:HA3	2.55	0.42
1:B:29:ILE:HD11	1:B:32:GLN:CD	2.40	0.42
1:A:285:PHE:CD1	1:A:296:VAL:HG22	2.55	0.42
1:A:29:ILE:CG2	1:A:30:LEU:N	2.83	0.42
1:B:252:LEU:HD23	1:B:252:LEU:HA	1.68	0.41
1:A:280:THR:HB	1:A:282:THR:HG23	2.01	0.41
1:B:82:SER:HB3	1:B:102:ASN:HB2	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:MSE:HG3	1:B:97:THR:HG21	2.02	0.41
1:B:85:ASP:OD1	1:B:129:GLY:HA2	2.20	0.41
1:A:144:ARG:HB3	1:A:144:ARG:HE	1.70	0.41
1:A:276:ALA:HB3	1:A:318:ILE:HG13	2.02	0.41
1:B:217:ASN:HB2	1:B:236:THR:HG21	2.03	0.41
1:B:243:PHE:CD2	1:B:254:PHE:HA	2.56	0.41
1:B:52:VAL:HG13	1:B:61:LEU:HD21	2.01	0.41
1:A:276:ALA:CB	1:A:318:ILE:HG13	2.50	0.41
1:B:152:ARG:C	1:B:153:PHE:CD2	2.94	0.41
1:A:133:SER:HA	1:A:134:PRO:HD3	1.79	0.41
1:A:135:ASN:HB2	1:A:137:ASN:H	1.86	0.41
1:A:197:ILE:O	1:A:213:ALA:HA	2.20	0.41
1:A:212:ASN:HB2	1:A:213:ALA:H	1.70	0.41
1:B:103:HIS:CD2	1:B:104:PRO:HA	2.55	0.41
1:A:152:ARG:HG2	1:A:152:ARG:O	2.21	0.40
1:A:27:LEU:HA	1:A:27:LEU:HD23	1.77	0.40
1:B:121:ILE:HG12	1:B:121:ILE:H	1.59	0.40
1:B:133:SER:HA	1:B:134:PRO:HD3	1.78	0.40
1:A:45:THR:HG22	1:A:49:SER:H	1.87	0.40
1:A:190:ALA:HB2	1:A:223:ILE:HD11	2.02	0.40
1:B:206:GLU:OE2	1:B:206:GLU:HA	2.22	0.40
1:B:265:ASP:H	1:B:289:ASN:HB3	1.87	0.40
1:B:263:LEU:CB	1:B:290:ILE:HB	2.51	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	317/331 (96%)	283 (89%)	27 (8%)	7 (2%)	6   31
1	B	315/331 (95%)	267 (85%)	35 (11%)	13 (4%)	3   16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	632/662 (96%)	550 (87%)	62 (10%)	20 (3%)	4	22

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	281	GLU
1	A	289	ASN
1	B	59	GLN
1	B	118	ILE
1	B	184	GLY
1	A	70	PRO
1	B	38	ASP
1	B	39	PHE
1	B	70	PRO
1	B	84	ALA
1	A	59	GLN
1	B	69	GLU
1	B	85	ASP
1	A	313	ASN
1	B	218	ASN
1	B	308	ALA
1	B	71	PRO
1	A	69	GLU
1	B	307	VAL

### 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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/283 (97%)	235 (86%)	40 (14%)	3	15
1	B	274/283 (97%)	225 (82%)	49 (18%)	2	9
All	All	549/566 (97%)	460 (84%)	89 (16%)	2	12

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	19	ILE
1	A	23	SER
1	A	26	THR
1	A	30	LEU
1	A	42	THR
1	A	45	THR
1	A	48	CYS
1	A	64	ILE
1	A	68	LEU
1	A	73	VAL
1	A	78	GLU
1	A	80	GLN
1	A	86	VAL
1	A	88	ILE
1	A	97	THR
1	A	98	VAL
1	A	101	LEU
1	A	113	LEU
1	A	116	LYS
1	A	118	ILE
1	A	141	LEU
1	A	150	VAL
1	A	154	LYS
1	A	173	THR
1	A	219	LEU
1	A	222	THR
1	A	225	VAL
1	A	227	ARG
1	A	242	VAL
1	A	247	GLN
1	A	257	SER
1	A	264	ILE
1	A	277	LEU
1	A	279	LYS
1	A	281	GLU
1	A	283	LYS
1	A	291	SER
1	A	303	VAL
1	A	304	VAL
1	B	7	ASN
1	B	10	ILE
1	B	11	VAL

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	16	LEU
1	B	23	SER
1	B	26	THR
1	B	29	ILE
1	B	34	THR
1	B	47	ASP
1	B	62	VAL
1	B	64	ILE
1	B	65	GLU
1	B	72	LYS
1	B	73	VAL
1	B	74	VAL
1	B	88	ILE
1	B	96	VAL
1	B	97	THR
1	B	121	ILE
1	B	123	ILE
1	B	130	ILE
1	B	141	LEU
1	B	149	THR
1	B	151	ARG
1	B	152	ARG
1	B	168	PHE
1	B	169	ILE
1	B	173	THR
1	B	174	ARG
1	B	176	PHE
1	B	177	ASN
1	B	178	ILE
1	B	200	LEU
1	B	202	THR
1	B	222	THR
1	B	223	ILE
1	B	251	THR
1	B	252	LEU
1	B	253	SER
1	B	264	ILE
1	B	267	ARG
1	B	277	LEU
1	B	279	LYS
1	B	280	THR
1	B	303	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	304	VAL
1	B	307	VAL
1	B	316	ILE
1	B	322	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	B	135	ASN
1	B	137	ASN
1	B	246	ASN
1	B	313	ASN
1	B	320	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TRS	A	330	-	7,7,7	0.36	0	9,9,9	0.37	0
2	TRS	A	329	-	7,7,7	0.27	0	9,9,9	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	A	330	-	-	3/9/9/9	-
2	TRS	A	329	-	-	9/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	329	TRS	C2-C-C1-O1
2	A	329	TRS	C1-C-C2-O2
2	A	329	TRS	C3-C-C2-O2
2	A	329	TRS	N-C-C2-O2
2	A	329	TRS	C1-C-C3-O3
2	A	329	TRS	C2-C-C3-O3
2	A	329	TRS	N-C-C3-O3
2	A	330	TRS	C1-C-C2-O2
2	A	329	TRS	C3-C-C1-O1
2	A	330	TRS	C3-C-C2-O2
2	A	330	TRS	N-C-C2-O2
2	A	329	TRS	N-C-C1-O1

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	330	TRS	3	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	316/331 (95%)	-0.45	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	17, 38, 63, 98	0
1	B	314/331 (94%)	0.26	15 (4%) <span style="border: 1px solid red; padding: 2px;">30</span> <span style="border: 1px solid red; padding: 2px;">11</span>	22, 67, 108, 153	0
All	All	630/662 (95%)	-0.10	15 (2%) <span style="border: 1px solid blue; padding: 2px;">59</span> <span style="border: 1px solid red; padding: 2px;">30</span>	17, 49, 100, 153	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	69	GLU	3.9
1	B	318	ILE	2.9
1	B	322	ASP	2.9
1	B	276	ALA	2.7
1	B	320	HIS	2.7
1	B	44	ILE	2.6
1	B	274	GLN	2.5
1	B	283	LYS	2.5
1	B	306	TYR	2.5
1	B	131	ALA	2.4
1	B	319	CYS	2.3
1	B	180	PHE	2.3
1	B	224	VAL	2.3
1	B	25	ASP	2.0
1	B	312	ALA	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](#)

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(Å <sup>2</sup> )	Q<0.9
2	TRS	A	330	8/8	0.89	0.23	65,74,76,81	0
2	TRS	A	329	8/8	0.93	0.19	75,81,83,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.