



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:15 am GMT

PDB ID : 2HI7  
Title : Crystal structure of DsbA-DsbB-ubiquinone complex  
Authors : Inaba, K.; Murakami, S.; Suzuki, M.; Nakagawa, A.; Yamashita, E.; Okada, K.; Ito, K.  
Deposited on : 2006-06-29  
Resolution : 3.70 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

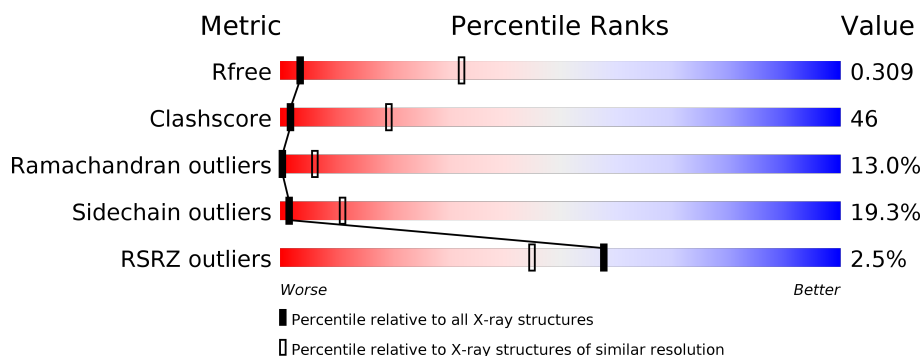
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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	1234 (3.90-3.50)
Clashscore	112137	1377 (3.90-3.50)
Ramachandran outliers	110173	1323 (3.90-3.50)
Sidechain outliers	110143	1320 (3.90-3.50)
RSRZ outliers	101464	1262 (3.90-3.50)

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.

Mol	Chain	Length	Quality of chain
1	A	189	<div> <div>2%</div> <div>40%</div> <div>47%</div> <div>12%</div> <div>..</div> </div>
2	B	176	<div> <div>2%</div> <div>16%</div> <div>39%</div> <div>19%</div> <div>•</div> <div>24%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2575 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 Thiol:disulfide interchange protein dsbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1477	946	242	282	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	ALA	CYS	ENGINEERED	UNP P0AEG4

- Molecule 2 is a protein called Disulfide bond formation protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	0	0	0
			1079	741	164	165	9			

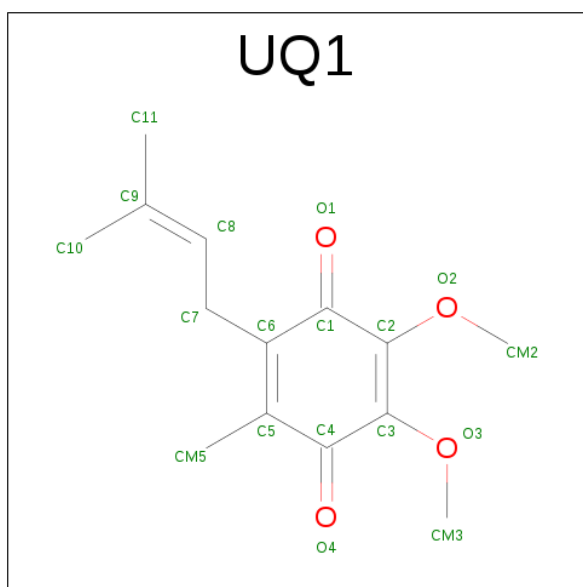
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	ALA	CYS	ENGINEERED	UNP P0A6M2
B	49	VAL	CYS	ENGINEERED	UNP P0A6M2
B	130	SER	CYS	ENGINEERED	UNP P0A6M2

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is UBIQUINONE-1 (three-letter code: UQ1) (formula: C<sub>14</sub>H<sub>18</sub>O<sub>4</sub>).

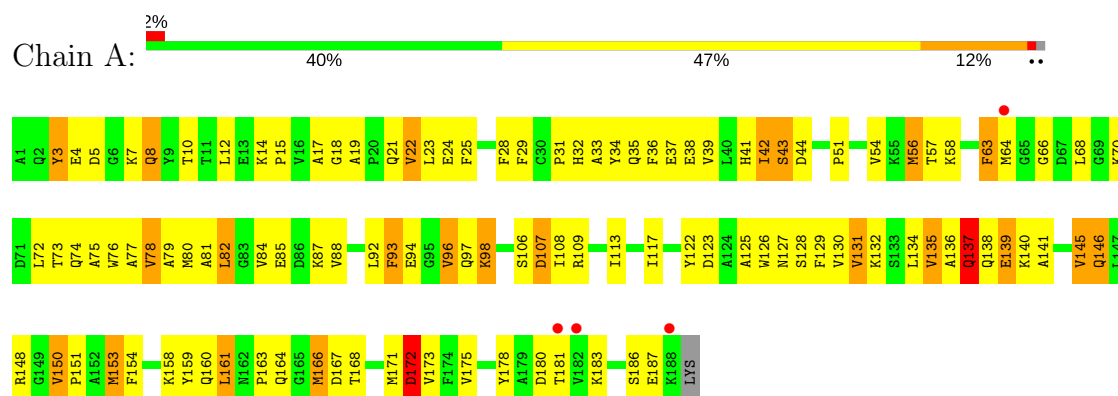


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			18	14	4		

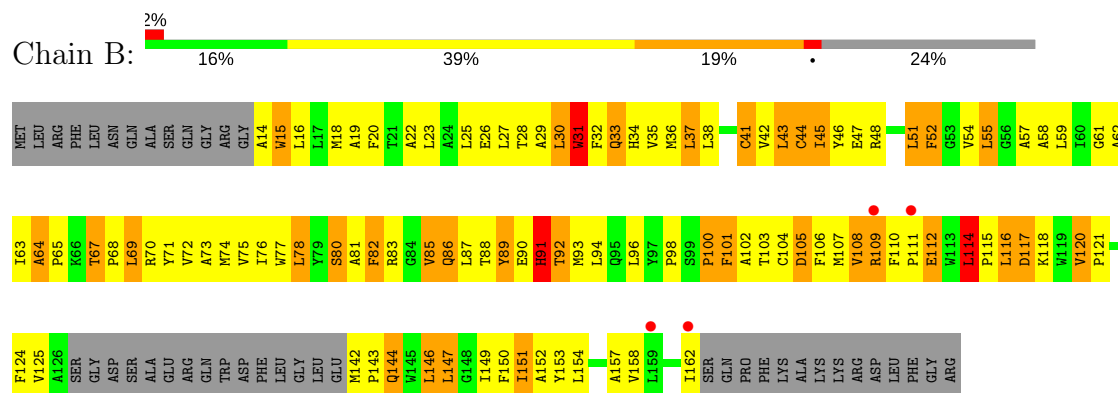
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: Thiol:disulfide interchange protein dsbA



- Molecule 2: Disulfide bond formation protein B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.50Å 165.50Å 65.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 57.43 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-3.70) 99.1 (57.43-3.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.341 , 0.362 0.340 , 0.309	Depositor DCC
$R_{free}$ test set	519 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	162.9	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 137.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	2575	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	185.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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

Bond lengths and bond angles in the following residue types are not validated in this section: UQ1, 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	0.69	0/1509	0.73	0/2041
2	B	0.66	0/1115	0.75	1/1529 (0.1%)
All	All	0.68	0/2624	0.74	1/3570 (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
2	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	51	LEU	CA-CB-CG	5.27	127.41	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	114	LEU	Peptide

### 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	1477	0	1450	120	0
2	B	1079	0	1122	130	0
3	A	1	0	0	0	0
4	B	18	0	18	5	0
All	All	2575	0	2590	239	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 46.

All (239) 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:32:HIS:HD2	2:B:102:ALA:HB3	0.99	1.14
2:B:86:GLN:HA	2:B:89:TYR:HB3	1.26	1.14
1:A:32:HIS:CD2	2:B:102:ALA:HB3	1.90	1.07
1:A:82:LEU:HB2	1:A:84:VAL:HG23	1.39	1.05
2:B:86:GLN:HA	2:B:89:TYR:CB	1.89	1.00
1:A:32:HIS:HD2	2:B:102:ALA:CB	1.74	0.99
2:B:27:LEU:HA	2:B:30:LEU:HB2	1.50	0.91
1:A:134:LEU:HA	1:A:137:GLN:HG3	1.53	0.91
2:B:58:ALA:HB1	2:B:77:TRP:HE1	1.37	0.90
2:B:62:ALA:HB2	2:B:72:VAL:HB	1.55	0.89
1:A:127:ASN:HA	1:A:132:LYS:HZ3	1.36	0.88
2:B:143:PRO:HA	2:B:146:LEU:HD12	1.53	0.88
1:A:106:SER:HA	1:A:109:ARG:HB2	1.56	0.88
1:A:29:PHE:O	1:A:31:PRO:HD3	1.76	0.86
1:A:109:ARG:HG3	1:A:122:TYR:HE2	1.39	0.85
1:A:163:PRO:HD2	1:A:164:GLN:HE21	1.42	0.83
1:A:160:GLN:HG2	1:A:161:LEU:H	1.43	0.82
2:B:121:PRO:O	2:B:125:VAL:HG23	1.80	0.81
1:A:148:ARG:HD3	2:B:107:MET:HB3	1.65	0.77
2:B:86:GLN:CA	2:B:89:TYR:HB3	2.14	0.76
1:A:31:PRO:O	1:A:35:GLN:HG2	1.85	0.76
1:A:135:VAL:HA	1:A:138:GLN:NE2	2.02	0.74
2:B:54:VAL:HG11	2:B:80:SER:HB2	1.69	0.74
2:B:110:PHE:CZ	2:B:117:ASP:HB2	2.23	0.73
2:B:73:ALA:O	2:B:77:TRP:N	2.21	0.73
1:A:32:HIS:CD2	2:B:102:ALA:CB	2.62	0.73
1:A:78:VAL:O	1:A:81:ALA:N	2.21	0.73
1:A:160:GLN:HG2	1:A:161:LEU:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:PRO:O	2:B:147:LEU:HG	1.90	0.71
2:B:18:MET:O	2:B:22:ALA:N	2.15	0.71
2:B:67:THR:HB	2:B:70:ARG:HE	1.56	0.70
1:A:135:VAL:HA	1:A:138:GLN:HE21	1.58	0.68
1:A:21:GLN:OE1	1:A:54:VAL:HG13	1.94	0.68
1:A:167:ASP:OD1	1:A:168:THR:N	2.26	0.68
1:A:153:MET:HB3	1:A:161:LEU:HG	1.74	0.68
2:B:100:PRO:O	2:B:102:ALA:N	2.25	0.67
2:B:35:VAL:C	2:B:37:LEU:H	1.98	0.67
1:A:125:ALA:HA	1:A:128:SER:HB3	1.77	0.67
2:B:108:VAL:HG13	2:B:118:LYS:HB2	1.77	0.67
1:A:127:ASN:HA	1:A:132:LYS:NZ	2.09	0.66
1:A:23:LEU:CD2	1:A:25:PHE:CE2	2.78	0.66
1:A:23:LEU:HD21	1:A:25:PHE:CE2	2.31	0.66
1:A:34:TYR:O	1:A:38:GLU:HB2	1.96	0.66
2:B:64:ALA:HB1	2:B:65:PRO:HD2	1.77	0.66
1:A:70:LYS:O	1:A:73:THR:HB	1.97	0.65
2:B:27:LEU:O	2:B:31:TRP:N	2.29	0.65
2:B:108:VAL:O	2:B:109:ARG:HG2	1.98	0.64
2:B:62:ALA:HB3	2:B:73:ALA:H	1.62	0.64
1:A:38:GLU:O	1:A:41:HIS:CE1	2.51	0.64
2:B:81:ALA:O	2:B:85:VAL:N	2.26	0.64
2:B:77:TRP:CE3	2:B:157:ALA:HB1	2.33	0.64
2:B:81:ALA:O	2:B:85:VAL:HG23	1.99	0.63
1:A:163:PRO:HD2	1:A:164:GLN:NE2	2.14	0.62
1:A:78:VAL:O	1:A:80:MET:N	2.32	0.62
2:B:76:ILE:O	2:B:80:SER:HB3	2.00	0.62
1:A:36:PHE:CE1	1:A:42:ILE:HD12	2.35	0.62
2:B:14:ALA:HB3	2:B:63:ILE:HG21	1.79	0.62
1:A:106:SER:HA	1:A:109:ARG:CB	2.28	0.62
1:A:109:ARG:HG3	1:A:122:TYR:CE2	2.29	0.61
1:A:37:GLU:OE1	1:A:43:SER:OG	2.16	0.61
1:A:7:LYS:HB3	1:A:8:GLN:OE1	2.00	0.61
2:B:30:LEU:HA	2:B:33:GLN:CD	2.21	0.61
2:B:120:VAL:O	2:B:124:PHE:N	2.28	0.61
1:A:35:GLN:HB3	2:B:100:PRO:HG3	1.83	0.60
2:B:58:ALA:HB1	2:B:77:TRP:NE1	2.12	0.60
2:B:147:LEU:O	2:B:151:ILE:HG23	2.01	0.60
1:A:84:VAL:HG13	1:A:87:LYS:HZ2	1.68	0.59
2:B:77:TRP:CZ3	2:B:157:ALA:HB1	2.37	0.59
2:B:75:VAL:HA	2:B:78:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:CG2	1:A:122:TYR:HB2	2.32	0.59
2:B:69:LEU:HG	2:B:71:TYR:CE2	2.38	0.58
1:A:153:MET:C	1:A:154:PHE:CD1	2.78	0.57
2:B:64:ALA:HB1	2:B:65:PRO:CD	2.34	0.57
1:A:23:LEU:HD23	1:A:24:GLU:N	2.19	0.57
1:A:24:GLU:HB2	1:A:153:MET:HE1	1.87	0.57
2:B:110:PHE:CZ	2:B:117:ASP:CB	2.88	0.57
2:B:67:THR:N	2:B:68:PRO:HD3	2.19	0.57
1:A:82:LEU:HD12	1:A:84:VAL:HG21	1.86	0.56
1:A:24:GLU:HB2	1:A:153:MET:CE	2.35	0.56
1:A:92:LEU:O	1:A:96:VAL:HG23	2.05	0.56
2:B:48:ARG:HA	2:B:51:LEU:HD12	1.87	0.56
1:A:158:LYS:HD2	1:A:159:TYR:CZ	2.40	0.56
1:A:22:VAL:CG1	1:A:56:MET:HG2	2.36	0.56
2:B:149:ILE:HA	2:B:152:ALA:HB3	1.88	0.56
2:B:30:LEU:O	2:B:32:PHE:N	2.39	0.55
2:B:43:LEU:HD13	2:B:91:HIS:CE1	2.40	0.55
2:B:92:THR:HB	2:B:147:LEU:HD22	1.88	0.55
2:B:74:MET:SD	2:B:162:ILE:HG22	2.46	0.55
2:B:91:HIS:CD2	2:B:91:HIS:C	2.79	0.55
2:B:90:GLU:O	2:B:91:HIS:C	2.44	0.55
1:A:75:ALA:O	1:A:78:VAL:HB	2.06	0.55
2:B:30:LEU:HD23	2:B:33:GLN:OE1	2.07	0.55
2:B:25:LEU:HA	2:B:28:THR:HB	1.89	0.55
2:B:90:GLU:O	2:B:93:MET:N	2.40	0.55
2:B:86:GLN:HA	2:B:89:TYR:HB2	1.80	0.55
2:B:15:TRP:NE1	2:B:59:LEU:O	2.41	0.54
1:A:82:LEU:HB2	1:A:84:VAL:CG2	2.28	0.54
2:B:120:VAL:HB	2:B:121:PRO:HD3	1.90	0.54
2:B:108:VAL:C	2:B:109:ARG:HG2	2.28	0.53
1:A:84:VAL:HG11	1:A:117:ILE:HD11	1.89	0.53
1:A:131:VAL:HG12	1:A:132:LYS:N	2.24	0.53
1:A:87:LYS:HZ2	1:A:87:LYS:HB2	1.74	0.53
2:B:52:PHE:HD1	2:B:52:PHE:N	2.07	0.53
1:A:34:TYR:CD1	1:A:34:TYR:C	2.82	0.53
1:A:84:VAL:O	1:A:85:GLU:C	2.47	0.53
1:A:12:LEU:HD12	1:A:158:LYS:C	2.29	0.52
1:A:23:LEU:HD22	1:A:25:PHE:HE2	1.75	0.52
2:B:112:GLU:OE1	2:B:114:LEU:HD23	2.10	0.52
2:B:27:LEU:O	2:B:31:TRP:HB2	2.10	0.52
2:B:52:PHE:CD1	2:B:52:PHE:N	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ARG:HA	2:B:86:GLN:OE1	2.09	0.52
2:B:75:VAL:O	2:B:78:LEU:HB2	2.10	0.51
2:B:120:VAL:HB	2:B:121:PRO:CD	2.41	0.51
2:B:29:ALA:O	2:B:33:GLN:HG3	2.10	0.51
2:B:54:VAL:O	2:B:58:ALA:N	2.43	0.51
1:A:117:ILE:HG22	1:A:122:TYR:HB2	1.92	0.51
2:B:117:ASP:O	2:B:121:PRO:HD2	2.10	0.51
1:A:34:TYR:HB2	1:A:97:GLN:NE2	2.26	0.51
1:A:138:GLN:O	1:A:141:ALA:N	2.43	0.50
2:B:117:ASP:O	2:B:121:PRO:HG2	2.10	0.50
2:B:47:GLU:HG2	2:B:87:LEU:HB3	1.92	0.50
1:A:161:LEU:O	1:A:163:PRO:HD3	2.10	0.50
2:B:48:ARG:NH1	4:B:501:UQ1:H72	2.27	0.50
1:A:23:LEU:CD2	1:A:25:PHE:HE2	2.25	0.50
2:B:142:MET:N	2:B:143:PRO:HD2	2.25	0.50
2:B:146:LEU:O	2:B:150:PHE:HD1	1.95	0.50
1:A:3:TYR:HA	1:A:8:GLN:HE22	1.77	0.50
2:B:15:TRP:HE1	2:B:64:ALA:N	2.10	0.50
1:A:109:ARG:CG	1:A:122:TYR:HE2	2.18	0.49
1:A:145:VAL:O	1:A:146:GLN:C	2.50	0.49
1:A:106:SER:O	1:A:107:ASP:C	2.51	0.49
1:A:23:LEU:HD22	1:A:25:PHE:CE2	2.47	0.49
1:A:23:LEU:HD23	1:A:23:LEU:C	2.32	0.49
2:B:35:VAL:C	2:B:37:LEU:N	2.66	0.49
2:B:51:LEU:O	2:B:55:LEU:HG	2.11	0.49
1:A:76:TRP:O	1:A:79:ALA:N	2.45	0.49
2:B:41:CYS:C	2:B:44:CYS:HB2	2.32	0.49
2:B:73:ALA:HA	2:B:76:ILE:HB	1.95	0.49
1:A:148:ARG:HD3	2:B:107:MET:CB	2.38	0.49
1:A:33:ALA:HB2	1:A:151:PRO:HD3	1.95	0.49
2:B:110:PHE:CZ	2:B:118:LYS:HD2	2.48	0.49
2:B:96:LEU:O	2:B:98:PRO:HD3	2.12	0.49
2:B:117:ASP:O	2:B:121:PRO:CG	2.61	0.48
1:A:76:TRP:NE1	1:A:80:MET:HG3	2.28	0.48
2:B:105:ASP:OD1	2:B:105:ASP:N	2.46	0.48
2:B:54:VAL:HG11	2:B:80:SER:CB	2.41	0.48
1:A:78:VAL:HG23	1:A:131:VAL:HG21	1.95	0.48
2:B:149:ILE:O	2:B:153:TYR:CD1	2.67	0.48
2:B:29:ALA:HB2	4:B:501:UQ1:H113	1.96	0.48
2:B:54:VAL:O	2:B:58:ALA:CB	2.62	0.48
1:A:33:ALA:HA	1:A:151:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:HD2	2:B:109:ARG:CZ	2.44	0.47
1:A:108:ILE:O	1:A:109:ARG:C	2.52	0.47
1:A:171:MET:O	1:A:173:VAL:N	2.47	0.47
2:B:51:LEU:HB3	2:B:52:PHE:HD1	1.79	0.47
1:A:150:VAL:O	2:B:103:THR:HA	2.14	0.47
1:A:74:GLN:O	1:A:77:ALA:HB3	2.14	0.47
2:B:88:THR:HB	2:B:147:LEU:HA	1.96	0.47
2:B:147:LEU:HG	2:B:147:LEU:H	1.49	0.47
2:B:91:HIS:HE1	4:B:501:UQ1:HM32	1.79	0.47
1:A:117:ILE:HG21	1:A:122:TYR:HB2	1.95	0.47
1:A:36:PHE:CD1	1:A:42:ILE:HD12	2.50	0.46
1:A:43:SER:O	1:A:44:ASP:C	2.54	0.46
2:B:32:PHE:O	2:B:33:GLN:C	2.54	0.46
2:B:80:SER:OG	2:B:81:ALA:N	2.45	0.46
2:B:58:ALA:CB	2:B:77:TRP:HE1	2.20	0.46
1:A:21:GLN:CD	1:A:54:VAL:HG13	2.34	0.46
1:A:5:ASP:C	1:A:7:LYS:H	2.18	0.46
1:A:94:GLU:OE1	1:A:98:LYS:HD3	2.15	0.46
2:B:54:VAL:O	2:B:58:ALA:HB2	2.16	0.46
2:B:77:TRP:HA	2:B:80:SER:HB3	1.98	0.46
1:A:171:MET:O	1:A:172:ASP:C	2.54	0.46
2:B:57:ALA:O	2:B:76:ILE:HG21	2.16	0.46
2:B:44:CYS:HB3	2:B:45:ILE:H	1.44	0.46
2:B:62:ALA:CB	2:B:73:ALA:H	2.27	0.46
2:B:43:LEU:O	2:B:44:CYS:C	2.54	0.46
2:B:83:ARG:HA	2:B:86:GLN:CD	2.36	0.46
1:A:129:PHE:CD1	1:A:129:PHE:N	2.84	0.46
2:B:108:VAL:HG22	2:B:118:LYS:HB3	1.98	0.46
1:A:154:PHE:CE2	1:A:160:GLN:HG3	2.52	0.45
1:A:175:VAL:O	1:A:178:TYR:HB3	2.16	0.45
2:B:149:ILE:HB	2:B:153:TYR:CE1	2.51	0.45
2:B:28:THR:O	2:B:32:PHE:HD1	1.99	0.45
1:A:14:LYS:HA	1:A:15:PRO:HD3	1.72	0.45
2:B:82:PHE:O	2:B:85:VAL:HB	2.17	0.45
1:A:136:ALA:HA	1:A:139:GLU:HB2	1.99	0.44
1:A:84:VAL:HG13	1:A:87:LYS:NZ	2.31	0.44
2:B:42:VAL:O	2:B:46:TYR:CD1	2.70	0.44
2:B:47:GLU:HB2	4:B:501:UQ1:HM53	1.98	0.44
1:A:109:ARG:CG	1:A:122:TYR:CE2	2.97	0.44
2:B:62:ALA:HB3	2:B:73:ALA:N	2.30	0.44
1:A:12:LEU:HB2	1:A:158:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:THR:HG22	1:A:58:LYS:N	2.33	0.44
2:B:41:CYS:HB2	2:B:44:CYS:HB2	1.75	0.44
2:B:86:GLN:O	2:B:87:LEU:C	2.54	0.44
1:A:107:ASP:OD1	1:A:107:ASP:N	2.51	0.44
2:B:14:ALA:O	2:B:15:TRP:C	2.56	0.44
1:A:77:ALA:O	1:A:80:MET:HB2	2.17	0.44
2:B:121:PRO:O	2:B:125:VAL:CG2	2.60	0.44
1:A:154:PHE:HA	1:A:159:TYR:O	2.17	0.43
1:A:28:PHE:CD1	1:A:93:PHE:CD1	3.06	0.43
1:A:129:PHE:N	1:A:129:PHE:HD1	2.16	0.43
1:A:34:TYR:CE2	1:A:38:GLU:HG3	2.54	0.43
1:A:37:GLU:HB3	1:A:93:PHE:HE2	1.83	0.43
2:B:67:THR:N	2:B:68:PRO:CD	2.82	0.43
1:A:136:ALA:O	1:A:138:GLN:N	2.52	0.43
1:A:78:VAL:C	1:A:80:MET:N	2.69	0.43
2:B:22:ALA:O	2:B:26:GLU:HG3	2.18	0.43
1:A:148:ARG:HA	2:B:107:MET:HG3	2.01	0.43
1:A:84:VAL:HG12	1:A:84:VAL:O	2.17	0.43
2:B:45:ILE:O	2:B:46:TYR:C	2.56	0.43
1:A:154:PHE:CD1	1:A:154:PHE:N	2.86	0.43
2:B:33:GLN:HB3	2:B:125:VAL:HG13	2.01	0.42
1:A:148:ARG:HH12	2:B:108:VAL:HB	1.83	0.42
2:B:23:LEU:HA	2:B:26:GLU:OE1	2.19	0.42
2:B:16:LEU:O	2:B:20:PHE:N	2.41	0.42
2:B:88:THR:CB	2:B:147:LEU:HA	2.49	0.42
1:A:148:ARG:HB3	2:B:107:MET:HB2	2.00	0.42
1:A:164:GLN:C	1:A:166:MET:H	2.23	0.42
2:B:32:PHE:O	2:B:35:VAL:N	2.53	0.42
1:A:78:VAL:O	1:A:79:ALA:C	2.57	0.42
2:B:83:ARG:HA	2:B:86:GLN:NE2	2.35	0.42
1:A:126:TRP:CD1	1:A:126:TRP:C	2.93	0.42
2:B:26:GLU:O	2:B:29:ALA:HB3	2.20	0.42
1:A:35:GLN:HA	1:A:39:VAL:HG23	2.01	0.41
1:A:37:GLU:HB3	1:A:93:PHE:CE2	2.54	0.41
2:B:55:LEU:O	2:B:59:LEU:HG	2.20	0.41
1:A:109:ARG:NH2	1:A:123:ASP:OD2	2.53	0.41
2:B:19:ALA:HA	2:B:22:ALA:HB3	2.03	0.41
4:B:501:UQ1:HM51	4:B:501:UQ1:H71	1.71	0.41
1:A:63:PHE:HD1	1:A:64:MET:HG3	1.86	0.41
1:A:17:ALA:O	1:A:19:ALA:N	2.54	0.41
1:A:73:THR:O	1:A:76:TRP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:THR:O	2:B:32:PHE:CD1	2.73	0.41
1:A:109:ARG:HA	1:A:122:TYR:CE2	2.55	0.41
1:A:126:TRP:HD1	1:A:127:ASN:ND2	2.18	0.40
1:A:12:LEU:HD12	1:A:158:LYS:CA	2.51	0.40
2:B:143:PRO:O	2:B:144:GLN:C	2.59	0.40
1:A:17:ALA:C	1:A:19:ALA:N	2.75	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	186/189 (98%)	124 (67%)	47 (25%)	15 (8%)	1	16
2	B	130/176 (74%)	75 (58%)	29 (22%)	26 (20%)	0	2
All	All	316/365 (87%)	199 (63%)	76 (24%)	41 (13%)	0	6

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	31	TRP
2	B	44	CYS
2	B	80	SER
2	B	101	PHE
2	B	144	GLN
1	A	66	GLY
1	A	139	GLU
1	A	146	GLN
1	A	172	ASP
2	B	15	TRP
2	B	36	MET
2	B	61	GLY

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Mol	Chain	Res	Type
2	B	64	ALA
2	B	108	VAL
2	B	116	LEU
2	B	120	VAL
2	B	33	GLN
2	B	37	LEU
2	B	78	LEU
2	B	146	LEU
1	A	137	GLN
2	B	30	LEU
2	B	91	HIS
2	B	104	CYS
2	B	115	PRO
1	A	42	ILE
1	A	43	SER
2	B	111	PRO
2	B	38	LEU
2	B	41	CYS
1	A	78	VAL
1	A	135	VAL
1	A	145	VAL
2	B	67	THR
1	A	18	GLY
1	A	51	PRO
1	A	96	VAL
1	A	113	ILE
2	B	85	VAL
2	B	100	PRO
1	A	130	VAL

### 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	157/158 (99%)	130 (83%)	27 (17%)	2	16
2	B	113/147 (77%)	88 (78%)	25 (22%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	270/305 (88%)	218 (81%)	52 (19%)	<b>1</b> <b>11</b>

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

Mol	Chain	Res	Type
1	A	3	TYR
1	A	4	GLU
1	A	8	GLN
1	A	10	THR
1	A	22	VAL
1	A	56	MET
1	A	63	PHE
1	A	68	LEU
1	A	72	LEU
1	A	82	LEU
1	A	88	VAL
1	A	93	PHE
1	A	98	LYS
1	A	107	ASP
1	A	131	VAL
1	A	137	GLN
1	A	140	LYS
1	A	150	VAL
1	A	153	MET
1	A	161	LEU
1	A	166	MET
1	A	172	ASP
1	A	180	ASP
1	A	181	THR
1	A	183	LYS
1	A	186	SER
1	A	187	GLU
2	B	31	TRP
2	B	34	HIS
2	B	43	LEU
2	B	45	ILE
2	B	52	PHE
2	B	55	LEU
2	B	69	LEU
2	B	82	PHE
2	B	86	GLN
2	B	89	TYR

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Mol	Chain	Res	Type
2	B	91	HIS
2	B	92	THR
2	B	94	LEU
2	B	101	PHE
2	B	105	ASP
2	B	106	PHE
2	B	109	ARG
2	B	112	GLU
2	B	114	LEU
2	B	116	LEU
2	B	117	ASP
2	B	147	LEU
2	B	151	ILE
2	B	154	LEU
2	B	158	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	74	GLN
1	A	97	GLN
1	A	100	GLN
1	A	127	ASN
1	A	137	GLN
1	A	138	GLN
1	A	146	GLN
1	A	160	GLN
1	A	164	GLN
2	B	91	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
4	UQ1	B	501	-	18,18,18	1.88	2 (11%)	22,25,25	1.23	3 (13%)

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
4	UQ1	B	501	-	-	0/9/33/33	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	UQ1	C3-C2	3.49	1.50	1.35
4	B	501	UQ1	C6-C5	6.59	1.49	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	UQ1	CM5-C5-C6	-2.54	119.04	124.20
4	B	501	UQ1	C11-C9-C10	2.13	119.56	114.60
4	B	501	UQ1	C7-C6-C1	2.44	121.59	118.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	UQ1	5	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	188/189 (99%)	-0.06	4 (2%) 64 51	113, 156, 191, 202	0
2	B	134/176 (76%)	-0.12	4 (2%) 51 38	166, 229, 258, 260	0
All	All	322/365 (88%)	-0.09	8 (2%) 58 45	113, 176, 256, 260	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	109	ARG	3.3
1	A	181	THR	3.1
1	A	188	LYS	3.1
1	A	64	MET	2.5
2	B	159	LEU	2.5
2	B	111	PRO	2.5
2	B	162	ILE	2.4
1	A	182	VAL	2.2

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	UQ1	B	501	18/18	0.86	0.29	0.13	200,201,201,201	0
3	ZN	A	190	1/1	0.95	0.44	-	168,168,168,168	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.