



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6LSU  
Title : Crystal structure of Uso1-2  
Authors : Heo, Y.Y.; Lee, H.H.  
Deposited on : 2020-01-20  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)	:	1.13
EDS	:	2.29
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)	:	2.29

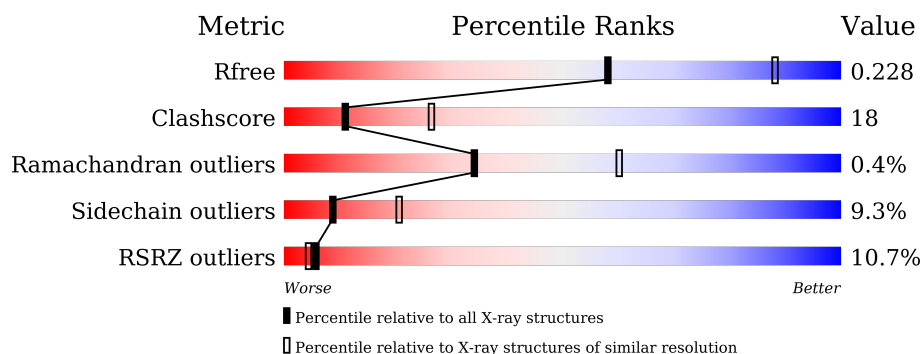
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of 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	731	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5573 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 Intracellular protein transport protein USO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	676	Total	C	N	O	S	0	0	0
			5449	3506	897	1028	18			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P25386
A	-3	ALA	-	expression tag	UNP P25386
A	-2	MET	-	expression tag	UNP P25386
A	-1	GLY	-	expression tag	UNP P25386
A	0	SER	-	expression tag	UNP P25386

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	124	Total	O	0	0
			124	124		

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

- [illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.38Å 104.38Å 231.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.79 – 2.70 48.79 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.79-2.70) 99.8 (48.79-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.65 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.198 , 0.230 0.201 , 0.228	Depositor DCC
$R_{free}$ test set	2058 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 70.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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	0.83	1/5558 (0.0%)	0.91	4/7541 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	GLU	CD-OE1	5.30	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	PRO	N-CA-CB	-6.42	95.54	102.60
1	A	126	ASP	CB-CA-C	-6.17	98.07	110.40
1	A	350	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	98	ARG	NE-CZ-NH1	-5.07	117.76	120.30

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	5449	0	5479	198	18
2	A	124	0	0	4	2
All	All	5573	0	5479	198	20

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 18.

All (198) 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:351:PRO:O	1:A:355:LEU:HD12	1.40	1.19
1:A:268:LEU:O	1:A:272:THR:HG23	1.43	1.15
1:A:36:ARG:CZ	1:A:68:ARG:NH2	2.09	1.15
1:A:36:ARG:NE	1:A:68:ARG:NH2	1.96	1.13
1:A:599:LYS:NZ	2:A:801:HOH:O	1.78	1.13
1:A:351:PRO:O	1:A:355:LEU:CD1	2.04	1.04
1:A:328:LEU:HD11	1:A:367:ALA:HA	1.36	1.02
1:A:184:PRO:O	1:A:185:THR:HG22	1.63	0.96
1:A:184:PRO:O	1:A:185:THR:CG2	2.17	0.92
1:A:48:ARG:NH1	1:A:95:ASP:OD2	2.04	0.90
1:A:212:VAL:HG12	1:A:219:VAL:HG11	1.55	0.89
1:A:520:MET:HE2	1:A:583:TYR:CG	2.08	0.89
1:A:88:ILE:O	2:A:802:HOH:O	1.92	0.87
1:A:155:PHE:CE1	1:A:198:HIS:HB3	2.10	0.86
1:A:36:ARG:CZ	1:A:68:ARG:CZ	2.53	0.86
1:A:36:ARG:HD2	1:A:68:ARG:HH21	1.41	0.84
1:A:268:LEU:O	1:A:272:THR:CG2	2.26	0.83
1:A:606:LEU:HD12	1:A:648:PHE:HE1	1.43	0.83
1:A:36:ARG:NH1	1:A:68:ARG:CZ	2.45	0.80
1:A:158:ARG:NH1	1:A:196:ASP:OD2	2.14	0.80
1:A:606:LEU:HD12	1:A:648:PHE:CE1	2.17	0.80
1:A:36:ARG:CD	1:A:68:ARG:HH21	1.94	0.79
1:A:51:ARG:NH1	1:A:126:ASP:OD2	2.12	0.79
1:A:37:ARG:NH1	1:A:72:ASP:OD2	2.16	0.78
1:A:27:VAL:O	1:A:36:ARG:HG2	1.84	0.78
1:A:33:ILE:CD1	1:A:69:ASP:OD2	2.32	0.78
1:A:36:ARG:CZ	1:A:68:ARG:HH22	1.97	0.78
1:A:155:PHE:HE1	1:A:198:HIS:HB3	1.45	0.77
1:A:18:GLU:O	1:A:22:THR:OG1	2.03	0.76
1:A:267:THR:HG23	1:A:323:HIS:NE2	2.02	0.75
1:A:37:ARG:O	1:A:41:LEU:CD1	2.35	0.73
1:A:520:MET:CE	1:A:583:TYR:CD1	2.72	0.72
1:A:36:ARG:CD	1:A:68:ARG:NH2	2.50	0.72
1:A:328:LEU:HD11	1:A:367:ALA:CA	2.17	0.72
1:A:52:GLU:OE2	1:A:89:ARG:NH1	2.21	0.72
1:A:573:ILE:HB	1:A:574:PRO:HD3	1.72	0.71
1:A:355:LEU:HD12	1:A:355:LEU:H	1.54	0.71
1:A:36:ARG:NE	1:A:68:ARG:HH22	1.86	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:MET:HE2	1:A:583:TYR:CD1	2.27	0.70
1:A:144:HIS:CE1	1:A:183:LEU:HB2	2.26	0.70
1:A:37:ARG:O	1:A:41:LEU:HD12	1.91	0.69
1:A:556:GLN:OE1	2:A:803:HOH:O	2.10	0.68
1:A:134:ASP:OD2	1:A:172:ARG:NH1	2.26	0.68
1:A:378:TYR:CD1	1:A:397:ILE:HD13	2.29	0.68
1:A:112:TYR:OH	1:A:250:ASP:OD2	2.09	0.67
1:A:675:ASP:HB2	1:A:677:ASN:HD22	1.59	0.67
1:A:52:GLU:OE1	1:A:52:GLU:N	2.27	0.66
1:A:195:ASP:OD2	1:A:231:ARG:NH1	2.27	0.66
1:A:606:LEU:CD1	1:A:648:PHE:CE1	2.79	0.66
1:A:184:PRO:C	1:A:185:THR:HG22	2.16	0.65
1:A:134:ASP:OD1	1:A:172:ARG:NH1	2.29	0.65
1:A:134:ASP:O	1:A:138:GLN:HG2	1.96	0.64
1:A:312:THR:O	1:A:323:HIS:ND1	2.30	0.64
1:A:113:PRO:HB2	1:A:116:LEU:HB2	1.78	0.63
1:A:566:LEU:HB3	1:A:608:PHE:CE2	2.33	0.62
1:A:355:LEU:HD12	1:A:355:LEU:N	2.16	0.61
1:A:655:LYS:H	1:A:655:LYS:HD2	1.66	0.61
1:A:134:ASP:CG	1:A:172:ARG:NH1	2.54	0.60
1:A:172:ARG:HD2	1:A:175:LYS:HE2	1.84	0.60
1:A:41:LEU:HD12	1:A:41:LEU:N	2.16	0.60
1:A:490:PHE:HD1	1:A:490:PHE:C	2.05	0.59
1:A:267:THR:CG2	1:A:323:HIS:NE2	2.64	0.59
1:A:137:THR:HG21	1:A:175:LYS:HE3	1.84	0.59
1:A:675:ASP:N	1:A:675:ASP:OD1	2.35	0.59
1:A:520:MET:CE	1:A:583:TYR:CG	2.82	0.58
1:A:37:ARG:NH1	1:A:72:ASP:CG	2.57	0.58
1:A:512:LEU:HD13	1:A:576:SER:HB2	1.85	0.58
1:A:32:LEU:HD23	1:A:32:LEU:H	1.68	0.58
1:A:137:THR:HG23	1:A:175:LYS:CB	2.34	0.57
1:A:501:TYR:H	1:A:544:ASN:HD21	1.51	0.56
1:A:490:PHE:C	1:A:490:PHE:CD1	2.78	0.56
1:A:602:ILE:HD12	1:A:602:ILE:N	2.20	0.56
1:A:137:THR:CG2	1:A:175:LYS:HB2	2.36	0.56
1:A:34:SER:O	1:A:38:SER:OG	2.24	0.56
1:A:104:GLN:HE21	1:A:108:GLN:HE21	1.54	0.56
1:A:490:PHE:HD1	1:A:490:PHE:O	1.90	0.55
1:A:137:THR:CG2	1:A:175:LYS:CB	2.85	0.55
1:A:681:ILE:HG12	1:A:681:ILE:O	2.06	0.55
1:A:221:LYS:HE3	1:A:265:ASN:OD1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:ILE:HG13	1:A:615:GLU:HG3	1.89	0.54
1:A:330:SER:OG	1:A:332:VAL:HG23	2.06	0.54
1:A:574:PRO:HB2	1:A:619:ILE:HD12	1.89	0.54
1:A:126:ASP:HB3	1:A:128:PHE:H	1.73	0.54
1:A:328:LEU:CD1	1:A:367:ALA:HA	2.25	0.54
1:A:33:ILE:CD1	1:A:69:ASP:CG	2.76	0.54
1:A:41:LEU:HD12	1:A:41:LEU:H	1.73	0.54
1:A:33:ILE:HD11	1:A:69:ASP:OD2	2.07	0.54
1:A:646:PHE:CZ	1:A:650:THR:HG21	2.42	0.54
1:A:137:THR:HG23	1:A:175:LYS:HB3	1.91	0.53
1:A:140:GLU:O	1:A:144:HIS:CD2	2.62	0.53
1:A:124:GLN:HE21	1:A:124:GLN:HA	1.74	0.53
1:A:270:LEU:HD12	1:A:323:HIS:CD2	2.44	0.53
1:A:249:ASN:O	1:A:253:SER:HB2	2.08	0.52
1:A:351:PRO:C	1:A:355:LEU:CD1	2.76	0.52
1:A:610:TYR:OH	1:A:652:THR:O	2.29	0.51
1:A:144:HIS:ND1	1:A:183:LEU:HB2	2.26	0.50
1:A:111:LYS:N	1:A:111:LYS:HD2	2.27	0.50
1:A:562:LEU:C	1:A:562:LEU:HD23	2.30	0.50
1:A:313:VAL:HG23	1:A:359:ASN:HB3	1.92	0.50
1:A:520:MET:HE3	1:A:583:TYR:HB2	1.94	0.50
1:A:242:LEU:HD13	1:A:281:LEU:CD1	2.42	0.49
1:A:33:ILE:HD13	1:A:69:ASP:CG	2.32	0.49
1:A:184:PRO:O	1:A:185:THR:HG23	2.05	0.49
1:A:20:ILE:N	1:A:21:PRO:CD	2.76	0.49
1:A:340:ALA:O	1:A:350:ARG:NH1	2.45	0.49
1:A:296:ASP:O	1:A:300:VAL:HG23	2.13	0.49
1:A:243:ARG:HG2	1:A:298:ARG:CZ	2.43	0.48
1:A:328:LEU:HD21	1:A:333:LEU:HD22	1.96	0.48
1:A:60:LYS:N	1:A:61:PRO:CD	2.77	0.48
1:A:562:LEU:C	1:A:562:LEU:CD2	2.82	0.48
1:A:675:ASP:HB2	1:A:677:ASN:ND2	2.29	0.48
1:A:588:ASP:OD2	2:A:804:HOH:O	2.20	0.48
1:A:60:LYS:N	1:A:61:PRO:HD2	2.29	0.47
1:A:199:GLU:N	1:A:200:PRO:CD	2.77	0.47
1:A:140:GLU:O	1:A:144:HIS:HD2	1.96	0.47
1:A:524:GLN:O	1:A:527:HIS:HB2	2.14	0.47
1:A:380:ASP:HA	1:A:381:PRO:HD3	1.75	0.47
1:A:602:ILE:HD12	1:A:602:ILE:H	1.80	0.47
1:A:406:TRP:O	1:A:410:ALA:HB3	2.15	0.47
1:A:564:THR:HG22	1:A:564:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:ASN:HB2	1:A:680:SER:OG	2.16	0.46
1:A:137:THR:HG23	1:A:175:LYS:HB2	1.95	0.46
1:A:155:PHE:CE1	1:A:198:HIS:CB	2.92	0.46
1:A:32:LEU:HD23	1:A:32:LEU:N	2.31	0.45
1:A:632:GLU:O	1:A:632:GLU:HG3	2.16	0.45
1:A:223:VAL:CG1	1:A:228:ILE:HD13	2.47	0.45
1:A:523:PHE:O	1:A:524:GLN:C	2.55	0.45
1:A:640:PHE:CE1	1:A:645:TYR:HA	2.52	0.45
1:A:7:LEU:H	1:A:7:LEU:HD23	1.82	0.45
1:A:20:ILE:HB	1:A:21:PRO:HD3	1.99	0.45
1:A:33:ILE:N	1:A:36:ARG:HH21	2.15	0.45
1:A:378:TYR:HB2	1:A:397:ILE:CD1	2.48	0.44
1:A:383:LEU:HD12	1:A:383:LEU:O	2.18	0.44
1:A:137:THR:HG21	1:A:175:LYS:HB2	1.99	0.44
1:A:112:TYR:OH	1:A:250:ASP:HA	2.18	0.44
1:A:242:LEU:HD13	1:A:281:LEU:HD11	2.00	0.44
1:A:213:VAL:HG12	1:A:223:VAL:HG21	2.00	0.44
1:A:647:GLU:OE1	1:A:651:LYS:HE2	2.17	0.44
1:A:81:GLU:O	1:A:85:ILE:HG13	2.17	0.44
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.82	0.44
1:A:506:ASN:HD22	1:A:507:LEU:HD23	1.83	0.44
1:A:718:ASP:N	1:A:718:ASP:OD1	2.51	0.43
1:A:381:PRO:HD2	1:A:384:PRO:HB3	2.01	0.43
1:A:182:SER:O	1:A:184:PRO:HD3	2.18	0.43
1:A:571:ILE:O	1:A:575:ILE:HG13	2.18	0.43
1:A:665:PHE:O	1:A:669:SER:OG	2.30	0.43
1:A:332:VAL:O	1:A:336:VAL:HG13	2.18	0.43
1:A:62:LEU:HD12	1:A:62:LEU:HA	1.89	0.43
1:A:376:VAL:HG11	1:A:402:ILE:HD12	2.01	0.43
1:A:518:ILE:O	1:A:521:PHE:HB3	2.19	0.43
1:A:37:ARG:HH12	1:A:72:ASP:CG	2.22	0.42
1:A:263:THR:HB	1:A:319:VAL:HG21	2.01	0.42
1:A:572:ARG:NH1	1:A:695:TYR:CE1	2.87	0.42
1:A:116:LEU:HD23	1:A:116:LEU:N	2.33	0.42
1:A:172:ARG:HD2	1:A:175:LYS:CE	2.49	0.42
1:A:378:TYR:HE1	1:A:402:ILE:HD11	1.84	0.42
1:A:675:ASP:O	1:A:677:ASN:ND2	2.52	0.42
1:A:556:GLN:NE2	1:A:594:ASP:O	2.41	0.42
1:A:573:ILE:HB	1:A:574:PRO:CD	2.46	0.42
1:A:37:ARG:NH1	1:A:72:ASP:OD1	2.52	0.42
1:A:331:SER:O	1:A:335:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ASN:OD1	1:A:362:ARG:NH2	2.53	0.42
1:A:673:LYS:CE	1:A:673:LYS:HA	2.48	0.42
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.88	0.42
1:A:506:ASN:ND2	1:A:507:LEU:CD2	2.83	0.42
1:A:274:ASN:O	1:A:277:LYS:HB2	2.20	0.42
1:A:574:PRO:HB2	1:A:619:ILE:CD1	2.49	0.42
1:A:628:GLY:HA3	1:A:658:TYR:CE1	2.55	0.42
1:A:52:GLU:HB3	1:A:128:PHE:CE1	2.55	0.42
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.86	0.42
1:A:38:SER:HA	1:A:41:LEU:HD13	2.02	0.41
1:A:666:LYS:O	1:A:666:LYS:HD2	2.20	0.41
1:A:262:ASN:HB3	1:A:265:ASN:HB2	2.03	0.41
1:A:114:SER:N	1:A:115:PRO:CD	2.83	0.41
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.92	0.41
1:A:499:LEU:HB3	1:A:542:THR:HG21	2.03	0.41
1:A:687:ASP:HB2	1:A:691:LEU:H	1.86	0.41
1:A:126:ASP:O	1:A:130:LEU:HG	2.21	0.41
1:A:155:PHE:CD1	1:A:198:HIS:CB	3.03	0.41
1:A:319:VAL:HB	1:A:323:HIS:CE1	2.56	0.41
1:A:150:TRP:HA	1:A:158:ARG:HG2	2.03	0.41
1:A:221:LYS:HA	1:A:221:LYS:HE2	2.01	0.41
1:A:26:ARG:NH1	1:A:35:ASP:OD1	2.53	0.41
1:A:52:GLU:HG2	1:A:128:PHE:CE2	2.55	0.41
1:A:232:LEU:HD11	1:A:254:LEU:HD23	2.03	0.41
1:A:381:PRO:CD	1:A:384:PRO:HB3	2.51	0.41
1:A:677:ASN:CG	1:A:680:SER:HB2	2.41	0.41
1:A:133:ALA:O	1:A:137:THR:HB	2.21	0.41
1:A:270:LEU:CD2	1:A:275:LEU:HD21	2.51	0.41
1:A:506:ASN:ND2	1:A:507:LEU:HD23	2.36	0.41
1:A:565:SER:O	1:A:574:PRO:HG3	2.20	0.41
1:A:336:VAL:HG21	1:A:360:MET:CE	2.51	0.40
1:A:449:ASN:HD22	1:A:449:ASN:HA	1.67	0.40
1:A:566:LEU:HB3	1:A:608:PHE:CD2	2.56	0.40
1:A:602:ILE:H	1:A:602:ILE:CD1	2.34	0.40
1:A:213:VAL:CG1	1:A:223:VAL:HG21	2.50	0.40
1:A:586:PHE:HE2	1:A:711:ILE:HD11	1.85	0.40
1:A:562:LEU:O	1:A:565:SER:N	2.43	0.40

All (20) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLN:NE2	1:A:379:PHE:CA[5_554]	1.26	0.94
1:A:5:GLN:NE2	1:A:379:PHE:N[5_554]	1.27	0.93
1:A:5:GLN:CD	1:A:379:PHE:CA[5_554]	1.29	0.91
1:A:5:GLN:CD	1:A:379:PHE:C[5_554]	1.32	0.88
1:A:5:GLN:CD	1:A:379:PHE:N[5_554]	1.37	0.83
1:A:5:GLN:CG	1:A:379:PHE:CA[5_554]	1.45	0.75
1:A:5:GLN:OE1	1:A:379:PHE:O[5_554]	1.47	0.73
1:A:5:GLN:NE2	1:A:378:TYR:C[5_554]	1.62	0.58
1:A:5:GLN:CG	1:A:379:PHE:CB[5_554]	1.66	0.54
1:A:5:GLN:CD	1:A:379:PHE:O[5_554]	1.68	0.52
1:A:5:GLN:CG	1:A:379:PHE:C[5_554]	1.75	0.45
1:A:5:GLN:NE2	1:A:378:TYR:O[5_554]	1.83	0.37
2:A:900:HOH:O	2:A:905:HOH:O[2_455]	1.87	0.33
1:A:5:GLN:OE1	1:A:379:PHE:C[5_554]	1.90	0.30
1:A:5:GLN:CG	1:A:379:PHE:O[5_554]	1.94	0.26
2:A:916:HOH:O	2:A:922:HOH:O[5_554]	1.96	0.24
1:A:8:ILE:CG2	1:A:405:ASN:OD1[5_554]	2.01	0.19
1:A:5:GLN:CG	1:A:379:PHE:N[5_554]	2.06	0.14
1:A:5:GLN:NE2	1:A:379:PHE:C[5_554]	2.08	0.12
1:A:5:GLN:CB	1:A:379:PHE:O[5_554]	2.11	0.09

## 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	668/731 (91%)	621 (93%)	44 (7%)	3 (0%)	34 60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	PRO
1	A	89	ARG
1	A	380	ASP

### 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	622/668 (93%)	564 (91%)	58 (9%)	9 21

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	13	ILE
1	A	19	THR
1	A	32	LEU
1	A	34	SER
1	A	38	SER
1	A	60	LYS
1	A	62	LEU
1	A	71	MET
1	A	125	VAL
1	A	127	GLN
1	A	188	SER
1	A	197	MET
1	A	234	SER
1	A	242	LEU
1	A	249	ASN
1	A	253	SER
1	A	264	SER
1	A	272	THR
1	A	290	GLU
1	A	319	VAL
1	A	336	VAL
1	A	363	SER
1	A	376	VAL
1	A	380	ASP
1	A	383	LEU
1	A	388	THR
1	A	390	ASN
1	A	399	VAL
1	A	412	SER

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Mol	Chain	Res	Type
1	A	452	THR
1	A	490	PHE
1	A	504	GLU
1	A	512	LEU
1	A	527	HIS
1	A	528	LYS
1	A	532	GLU
1	A	556	GLN
1	A	560	GLU
1	A	567	THR
1	A	571	ILE
1	A	611	GLN
1	A	612	ILE
1	A	615	GLU
1	A	626	LEU
1	A	640	PHE
1	A	643	LYS
1	A	644	GLU
1	A	655	LYS
1	A	666	LYS
1	A	667	LYS
1	A	673	LYS
1	A	675	ASP
1	A	680	SER
1	A	681	ILE
1	A	688	GLU
1	A	689	THR
1	A	718	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	10	GLN
1	A	64	ASN
1	A	103	GLN
1	A	104	GLN
1	A	124	GLN
1	A	144	HIS
1	A	449	ASN
1	A	453	ASN
1	A	544	ASN

### 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 monosaccharides 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	676/731 (92%)	0.60	72 (10%) <b>6</b> <b>4</b>	44, 73, 149, 197	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	455	VAL	13.0
1	A	390	ASN	10.9
1	A	389	ALA	9.5
1	A	452	THR	9.4
1	A	458	ASN	9.3
1	A	454	ASN	9.0
1	A	457	ASP	8.6
1	A	118	MET	8.5
1	A	388	THR	7.6
1	A	456	GLY	7.5
1	A	453	ASN	7.5
1	A	385	VAL	7.4
1	A	544	ASN	7.1
1	A	688	GLU	6.6
1	A	551	PRO	6.4
1	A	451	SER	6.1
1	A	391	GLY	5.6
1	A	543	GLY	5.5
1	A	387	SER	5.4
1	A	679	ASP	5.4
1	A	115	PRO	5.0
1	A	545	ASP	4.8
1	A	450	ASN	4.6
1	A	197	MET	4.6
1	A	677	ASN	4.4
1	A	392	GLY	4.3
1	A	8	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	613	GLN	4.0
1	A	718	ASP	3.9
1	A	394	ILE	3.9
1	A	636	LYS	3.8
1	A	378	TYR	3.8
1	A	123	GLU	3.7
1	A	383	LEU	3.6
1	A	379	PHE	3.6
1	A	676	MET	3.5
1	A	717	HIS	3.5
1	A	116	LEU	3.5
1	A	678	GLU	3.4
1	A	318	THR	3.3
1	A	381	PRO	3.3
1	A	687	ASP	3.3
1	A	114	SER	3.3
1	A	386	ASN	3.3
1	A	32	LEU	3.0
1	A	672	SER	2.8
1	A	6	GLY	2.8
1	A	119	LYS	2.7
1	A	689	THR	2.7
1	A	393	PRO	2.6
1	A	17	ASP	2.6
1	A	525	GLN	2.5
1	A	5	GLN	2.5
1	A	30	SER	2.5
1	A	9	GLN	2.5
1	A	663	LYS	2.5
1	A	225	PHE	2.5
1	A	589	PHE	2.5
1	A	449	ASN	2.4
1	A	31	THR	2.4
1	A	690	GLY	2.4
1	A	675	ASP	2.4
1	A	16	VAL	2.3
1	A	184	PRO	2.3
1	A	666	LYS	2.2
1	A	614	ASP	2.1
1	A	198	HIS	2.1
1	A	218	HIS	2.1
1	A	686	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	33	ILE	2.1
1	A	637	GLU	2.1
1	A	667	LYS	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 monosaccharides 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.