



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 09:02 PM EDT

PDB ID : 6BRQ  
Title : Crystal structure of rice ASK1-D3 ubiquitin ligase complex crystal form 3  
Authors : Shabek, N.; Zheng, N.; Mao, H.; Hinds, T.R.; Ticchiarelli, F.; Leyser, O.  
Deposited on : 2017-11-30  
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 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)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

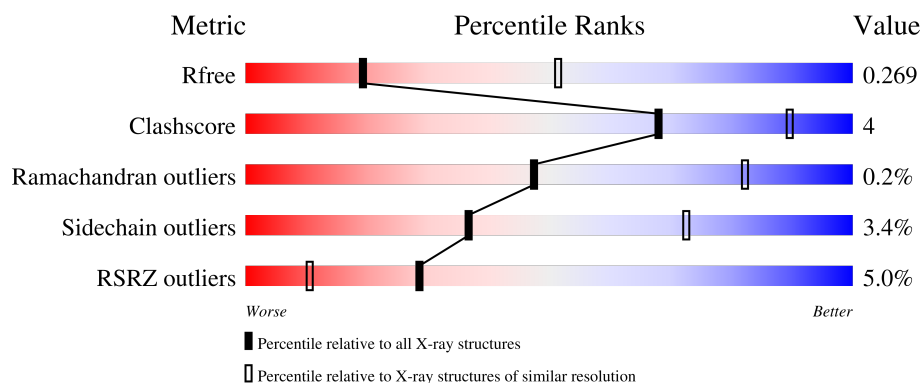
# 1 Overall quality at a glance

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 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	B	688	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>11%</div> <div>16%</div> </div> </div>
1	D	688	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>14%</div> </div> </div>
2	A	160	<div> <div>4%</div> <div> <div></div> <div>54%</div> <div>12%</div> <div>•</div> <div>34%</div> </div> </div>
2	C	160	<div> <div>13%</div> <div> <div></div> <div>49%</div> <div>11%</div> <div>•</div> <div>38%</div> </div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 10771 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 F-box/LRR-repeat MAX2 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	581	Total	C	N	O	S	0	0	0
			4500	2876	784	811	29			
1	D	592	Total	C	N	O	S	0	0	0
			4602	2944	801	828	29			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	509	GLU	-	linker	UNP Q5VMP0
B	510	ASN	-	linker	UNP Q5VMP0
B	511	LEU	-	linker	UNP Q5VMP0
B	512	TYR	-	linker	UNP Q5VMP0
B	513	PHE	-	linker	UNP Q5VMP0
B	514	GLN	-	linker	UNP Q5VMP0
B	515	SER	-	linker	UNP Q5VMP0
D	509	GLU	-	linker	UNP Q5VMP0
D	510	ASN	-	linker	UNP Q5VMP0
D	511	LEU	-	linker	UNP Q5VMP0
D	512	TYR	-	linker	UNP Q5VMP0
D	513	PHE	-	linker	UNP Q5VMP0
D	514	GLN	-	linker	UNP Q5VMP0
D	515	SER	-	linker	UNP Q5VMP0

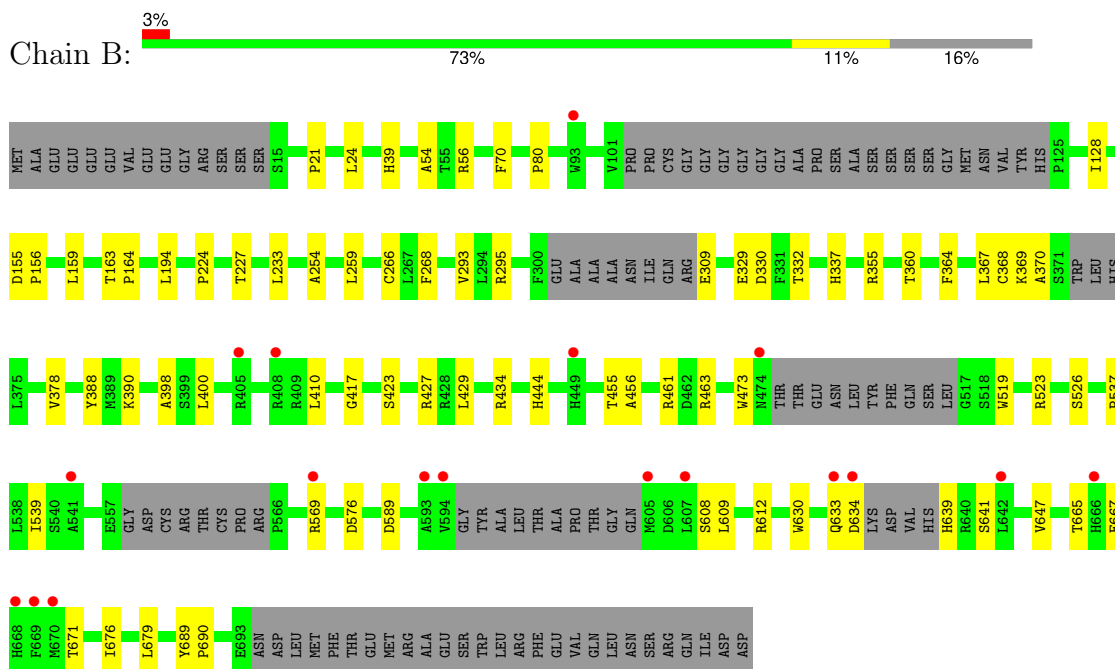
- Molecule 2 is a protein called SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	106	Total	C	N	O	S	0	0	0
			858	545	140	168	5			
2	C	99	Total	C	N	O	S	0	0	0
			811	516	133	158	4			

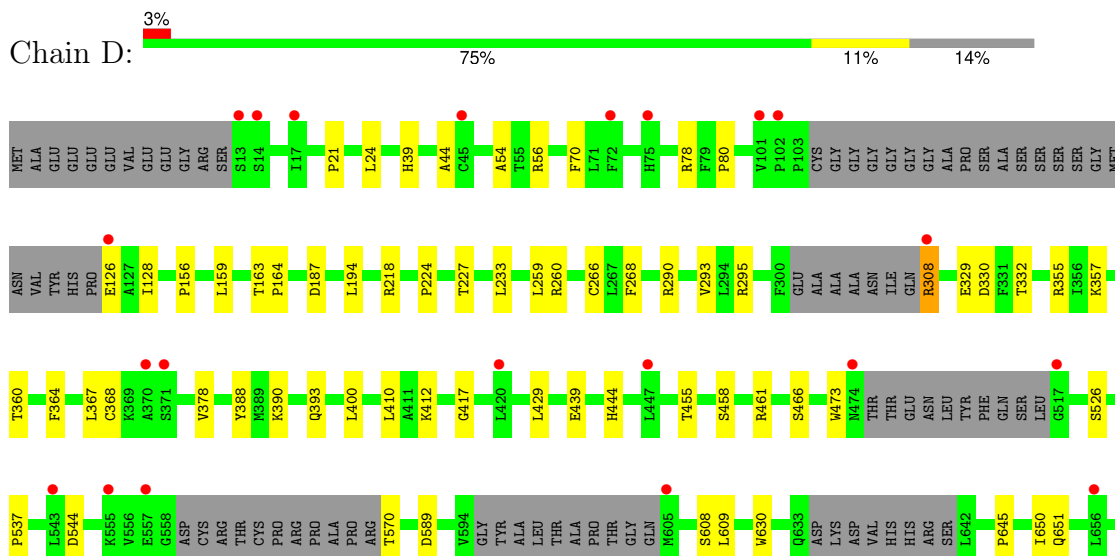
### 3 Residue-property plots

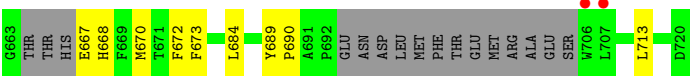
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

- Molecule 1: F-box/LRR-repeat MAX2 homolog

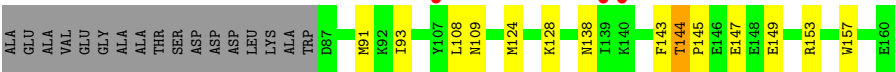


- Molecule 1: F-box/LRR-repeat MAX2 homolog





• Molecule 2: SKP1-like protein 1A



• Molecule 2: SKP1-like protein 1A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.91Å 113.31Å 92.86Å 90.00° 99.00° 90.00°	Depositor
Resolution (Å)	91.71 – 2.99 49.39 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (91.71-2.99) 95.7 (49.39-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.220 , 0.256 0.228 , 0.269	Depositor DCC
$R_{free}$ test set	1582 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.1	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 26.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10771	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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](#)

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	B	0.41	0/4601	0.68	0/6253
1	D	0.42	0/4705	0.67	0/6392
2	A	0.42	0/867	0.64	0/1168
2	C	0.43	0/822	0.65	0/1108
All	All	0.42	0/10995	0.67	0/14921

There are no bond length outliers.

There are no bond angle outliers.

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	B	4500	0	4537	32	0
1	D	4602	0	4628	35	0
2	A	858	0	859	10	0
2	C	811	0	804	9	0
All	All	10771	0	10828	82	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 4.

All (82) 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:D:224:PRO:HA	1:D:227:THR:HG22	1.61	0.82
1:B:224:PRO:HA	1:B:227:THR:HG22	1.63	0.81
1:D:187:ASP:HB2	1:D:218:ARG:HE	1.48	0.78
1:B:423:SER:O	1:B:427:ARG:HG3	1.87	0.74
1:B:309:GLU:HG3	1:B:337:HIS:HD2	1.57	0.70
1:B:254:ALA:O	1:D:78:ARG:HD3	1.93	0.67
1:D:670:MET:HE2	1:D:684:LEU:HB2	1.78	0.65
2:A:27:GLN:HB2	2:A:109:ASN:HB3	1.83	0.61
2:C:27:GLN:HB2	2:C:109:ASN:HB3	1.83	0.61
2:C:144:THR:HG23	2:C:147:GLU:HB2	1.82	0.60
2:A:124:MET:O	2:A:128:LYS:HE2	2.02	0.60
1:D:260:ARG:NH2	1:D:290:ARG:HE	2.00	0.60
2:C:124:MET:O	2:C:128:LYS:HE2	2.02	0.60
1:D:368:CYS:HB2	1:D:378:VAL:HG12	1.85	0.58
1:B:427:ARG:HG2	1:B:456:ALA:HA	1.85	0.58
2:C:50:LYS:HE3	2:C:50:LYS:H	1.69	0.57
1:B:368:CYS:HB2	1:B:378:VAL:HG12	1.86	0.57
2:A:143:PHE:HD1	2:A:147:GLU:HG3	1.69	0.57
2:A:54:LYS:HA	2:A:57:GLU:HG2	1.86	0.56
1:D:266:CYS:HB2	1:D:268:PHE:CE2	2.41	0.55
1:B:266:CYS:HB2	1:B:268:PHE:CE2	2.42	0.54
1:B:54:ALA:HA	1:B:80:PRO:HD2	1.92	0.52
1:D:54:ALA:HA	1:D:80:PRO:HD2	1.92	0.52
1:B:370:ALA:HB3	1:B:398:ALA:HB1	1.92	0.51
1:D:360:THR:HG23	1:D:388:TYR:HB3	1.92	0.51
1:B:360:THR:HG23	1:B:388:TYR:HB3	1.92	0.51
1:B:434:ARG:HD2	1:B:463:ARG:HH21	1.76	0.51
1:B:633:GLN:HG2	1:B:634:ASP:N	2.26	0.51
1:D:650:ILE:HB	1:D:673:PHE:HE1	1.76	0.51
1:B:329:GLU:HG2	1:B:355:ARG:HB3	1.92	0.50
1:B:159:LEU:HD13	1:B:194:LEU:HG	1.94	0.49
1:D:159:LEU:HD13	1:D:194:LEU:HG	1.95	0.49
1:D:329:GLU:HG2	1:D:355:ARG:HB3	1.93	0.48
2:A:144:THR:HG22	2:A:145:PRO:HD2	1.95	0.48
1:B:364:PHE:HB3	1:B:367:LEU:HD21	1.95	0.47
1:D:355:ARG:NH1	1:D:357:LYS:NZ	2.62	0.47
1:B:589:ASP:HA	1:B:630:TRP:HB2	1.97	0.47
1:D:233:LEU:HB2	1:D:259:LEU:HD21	1.96	0.47
1:D:400:LEU:HD13	1:D:429:LEU:HD22	1.97	0.47
1:B:39:HIS:CD2	1:B:56:ARG:HH22	2.33	0.46
1:D:21:PRO:HD2	1:D:24:LEU:HD12	1.97	0.46
1:D:39:HIS:CD2	1:D:56:ARG:HH22	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:PRO:HD2	1:B:24:LEU:HD12	1.98	0.46
1:B:400:LEU:HD13	1:B:429:LEU:HD22	1.98	0.46
1:D:589:ASP:HA	1:D:630:TRP:HB2	1.98	0.46
1:B:233:LEU:HB2	1:B:259:LEU:HD21	1.97	0.46
1:B:293:VAL:HA	1:B:330:ASP:HB3	1.98	0.45
1:D:308:ARG:HD2	1:D:308:ARG:HA	1.76	0.45
1:D:364:PHE:HB3	1:D:367:LEU:HD21	1.97	0.45
1:D:293:VAL:HA	1:D:330:ASP:HB3	1.99	0.45
1:D:70:PHE:HB2	2:C:157:TRP:CH2	2.53	0.44
1:D:689:TYR:HA	1:D:690:PRO:HA	1.72	0.44
2:A:143:PHE:CD1	2:A:147:GLU:HG3	2.51	0.44
1:D:295:ARG:HA	1:D:332:THR:HB	1.99	0.43
1:B:461:ARG:HG3	1:B:519:TRP:CD2	2.53	0.43
1:B:295:ARG:HA	1:B:332:THR:HB	1.99	0.43
2:A:149:GLU:O	2:A:153:ARG:HB2	2.18	0.43
1:D:163:THR:N	1:D:164:PRO:HD2	2.33	0.43
1:B:473:TRP:CE2	1:B:537:PRO:HG2	2.54	0.42
2:A:91:MET:C	2:A:93:ILE:H	2.23	0.42
1:B:163:THR:N	1:B:164:PRO:HD2	2.34	0.42
2:A:55:VAL:HG11	2:A:108:LEU:HD13	2.00	0.42
1:B:689:TYR:HA	1:B:690:PRO:HA	1.71	0.42
1:D:308:ARG:NH1	1:D:393:GLN:HG3	2.35	0.42
1:B:539:ILE:HD13	1:B:576:ASP:HB3	2.01	0.42
1:D:473:TRP:CE2	1:D:537:PRO:HG2	2.55	0.42
1:B:647:VAL:HG21	1:B:667:GLU:HG3	2.01	0.42
2:C:149:GLU:O	2:C:153:ARG:HB2	2.19	0.42
1:D:608:SER:HB2	1:D:645:PRO:HG3	2.01	0.41
1:B:70:PHE:HB2	2:A:157:TRP:CH2	2.56	0.41
2:C:91:MET:C	2:C:93:ILE:H	2.23	0.41
1:B:676:ILE:HD12	1:B:679:LEU:HD22	2.03	0.41
1:B:388:TYR:HE1	1:B:390:LYS:HG2	1.86	0.41
1:D:412:LYS:HG2	1:D:439:GLU:HB2	2.03	0.41
1:D:651:GLN:NE2	1:D:672:PHE:HB3	2.37	0.40
1:B:417:GLY:HA2	1:B:444:HIS:O	2.22	0.40
1:D:44:ALA:O	2:C:134:ARG:HD2	2.21	0.40
1:D:260:ARG:NH2	1:D:290:ARG:NE	2.69	0.40
1:D:388:TYR:HE1	1:D:390:LYS:HG2	1.87	0.40
1:D:417:GLY:HA2	1:D:444:HIS:O	2.22	0.40
2:C:86:TRP:HB3	2:C:87:ASP:H	1.72	0.40
1:D:439:GLU:HG2	1:D:466:SER:HB3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	565/688 (82%)	546 (97%)	18 (3%)	1 (0%)	47	82
1	D	574/688 (83%)	554 (96%)	19 (3%)	1 (0%)	47	82
2	A	98/160 (61%)	95 (97%)	3 (3%)	0	100	100
2	C	93/160 (58%)	89 (96%)	4 (4%)	0	100	100
All	All	1330/1696 (78%)	1284 (96%)	44 (3%)	2 (0%)	47	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	PRO
1	D	156	PRO

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	488/575 (85%)	473 (97%)	15 (3%)	40	75
1	D	498/575 (87%)	484 (97%)	14 (3%)	43	77
2	A	96/137 (70%)	92 (96%)	4 (4%)	30	66
2	C	89/137 (65%)	82 (92%)	7 (8%)	12	41
All	All	1171/1424 (82%)	1131 (97%)	40 (3%)	37	72

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	128	ILE
1	B	155	ASP
1	B	369	LYS
1	B	410	LEU
1	B	455	THR
1	B	523	ARG
1	B	526	SER
1	B	569	ARG
1	B	608	SER
1	B	609	LEU
1	B	612	ARG
1	B	639	HIS
1	B	641	SER
1	B	665	THR
1	B	671	THR
2	A	29	ILE
2	A	50	LYS
2	A	138	ASN
2	A	144	THR
1	D	126	GLU
1	D	128	ILE
1	D	308	ARG
1	D	410	LEU
1	D	455	THR
1	D	458	SER
1	D	461	ARG
1	D	526	SER
1	D	544	ASP
1	D	570	THR
1	D	609	LEU
1	D	667	GLU
1	D	668	HIS
1	D	713	LEU
2	C	24	LEU
2	C	29	ILE
2	C	50	LYS
2	C	61	ARG
2	C	89	ASP
2	C	138	ASN
2	C	144	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	337	HIS
1	D	180	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 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 [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	B	581/688 (84%)	0.21	18 (3%)	49 21	42, 60, 89, 120	0
1	D	592/688 (86%)	0.24	23 (3%)	39 15	41, 60, 87, 132	0
2	A	106/160 (66%)	0.61	7 (6%)	18 5	48, 71, 94, 105	0
2	C	99/160 (61%)	0.88	21 (21%)	0 0	51, 83, 116, 125	0
All	All	1378/1696 (81%)	0.30	69 (5%)	28 10	41, 62, 97, 132	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	474	ASN	6.8
2	C	58	TYR	5.9
1	D	706	TRP	5.2
2	A	24	LEU	5.0
1	B	569	ARG	4.8
2	A	30	ALA	4.8
1	D	102	PRO	4.6
1	B	670	MET	4.6
2	C	56	ILE	4.4
1	B	593	ALA	3.6
2	C	57	GLU	3.5
1	D	605	MET	3.5
1	B	594	VAL	3.5
1	B	669	PHE	3.4
1	D	370	ALA	3.3
2	C	90	PHE	3.3
2	C	112	ASN	3.2
2	C	25	GLU	3.1
2	C	24	LEU	3.1
2	C	30	ALA	2.9
2	A	107	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	96	ALA	2.8
1	B	605	MET	2.7
1	B	666	HIS	2.7
2	C	113	LEU	2.7
1	D	14	SER	2.6
1	D	474	ASN	2.6
1	B	668	HIS	2.6
1	D	517	GLY	2.6
1	B	541	ALA	2.6
1	D	707	LEU	2.5
1	D	72	PHE	2.5
1	D	308	ARG	2.5
2	C	23	ALA	2.5
2	C	147	GLU	2.4
1	D	126	GLU	2.4
1	B	607	LEU	2.4
2	A	140	LYS	2.4
2	C	31	HIS	2.4
1	B	408	ARG	2.4
2	A	31	HIS	2.3
2	C	91	MET	2.3
1	D	13	SER	2.3
1	D	557	GLU	2.3
1	D	447	LEU	2.3
2	C	150	GLU	2.2
1	D	17	ILE	2.2
2	C	59	CYS	2.2
1	D	75	HIS	2.2
2	C	111	LYS	2.1
2	A	22	VAL	2.1
1	B	633	GLN	2.1
1	D	101	VAL	2.1
1	B	405	ARG	2.1
1	B	449	HIS	2.1
1	D	543	LEU	2.1
1	D	656	LEU	2.1
2	C	116	LEU	2.1
1	D	555	LYS	2.1
1	B	93	TRP	2.1
1	B	634	ASP	2.1
1	D	45	CYS	2.1
2	A	139	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	371	SER	2.0
1	B	642	LEU	2.0
1	D	420	LEU	2.0
2	C	94	ASP	2.0
2	C	52	LEU	2.0
2	C	55	VAL	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.