



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 01:56 pm GMT

PDB ID : 3KL4  
Title : Recognition of a signal peptide by the signal recognition particle  
Authors : Janda, C.Y.; Nagai, K.; Li, J.; Oubridge, C.  
Deposited on : 2009-11-06  
Resolution : 3.50 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.

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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 : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

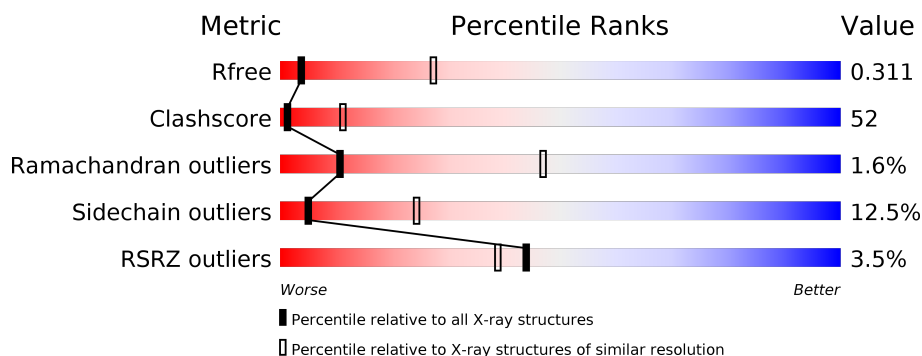
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

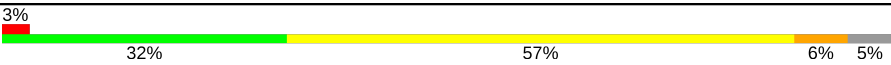

The reported resolution of this entry is 3.50 Å.

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))
$R_{free}$	111664	1391 (3.60-3.40)
Clashscore	122126	1485 (3.60-3.40)
Ramachandran outliers	120053	1446 (3.60-3.40)
Sidechain outliers	120020	1447 (3.60-3.40)
RSRZ outliers	108989	1303 (3.60-3.40)

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	433	
2	B	42	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3385 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 Signal recognition 54 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	1
			3229	2067	548	602	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q97ZE7
A	1	GLY	-	EXPRESSION TAG	UNP Q97ZE7

- Molecule 2 is a protein called Signal peptide of yeast dipeptidyl aminopeptidase B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	21	Total	C	N	O	0	0	1
			156	109	25	22			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	433	ALA	-	LINKER	UNP P18962
B	434	ARG	-	LINKER	UNP P18962
B	435	SER	-	LINKER	UNP P18962
B	436	GLY	-	LINKER	UNP P18962
B	437	SER	-	LINKER	UNP P18962
B	438	GLY	-	LINKER	UNP P18962
B	439	SER	-	LINKER	UNP P18962
B	440	GLY	-	LINKER	UNP P18962
B	441	SER	-	LINKER	UNP P18962
B	442	GLY	-	LINKER	UNP P18962
B	443	SER	-	LINKER	UNP P18962
B	470	HIS	-	EXPRESSION TAG	UNP P18962
B	471	HIS	-	EXPRESSION TAG	UNP P18962
B	472	HIS	-	EXPRESSION TAG	UNP P18962

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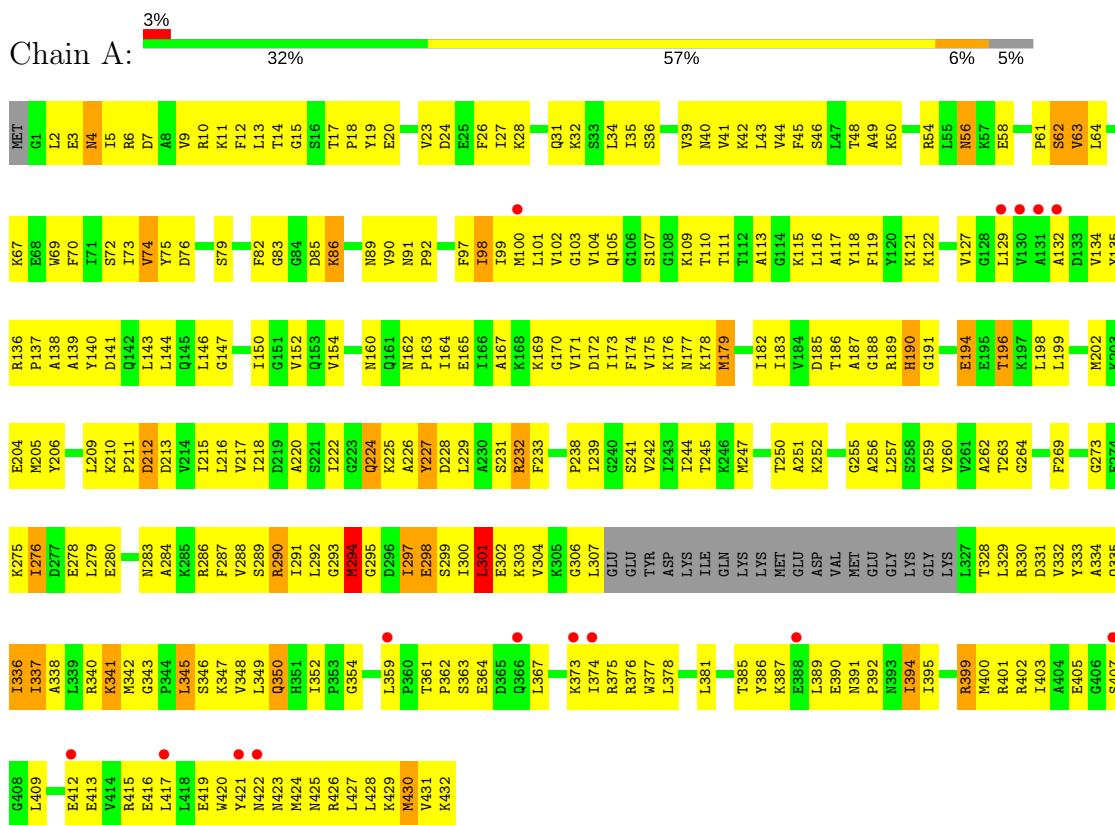
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Chain	Residue	Modelled	Actual	Comment	Reference
B	473	HIS	-	EXPRESSION TAG	UNP P18962
B	474	HIS	-	EXPRESSION TAG	UNP P18962

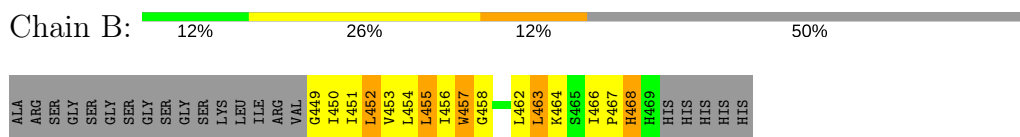
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Signal recognition 54 kDa protein



#### • Molecule 2: Signal peptide of yeast dipeptidyl aminopeptidase B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.88Å 91.88Å 133.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.42 – 3.50 58.40 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (58.42-3.50) 99.7 (58.40-3.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.301 , 0.322 0.299 , 0.311	Depositor DCC
$R_{free}$ test set	353 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	138.4	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 121.0	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	0.90	EDS
Total number of atoms	3385	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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	A	0.66	0/3278	0.78	1/4413 (0.0%)
2	B	0.70	0/159	0.85	0/218
All	All	0.66	0/3437	0.79	1/4631 (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	301	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	3229	0	3365	342	0
2	B	156	0	182	23	0
All	All	3385	0	3547	360	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 52.

All (360) 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:177:ASN:HB2	1:A:179:MET:SD	1.81	1.21
1:A:297:ILE:O	1:A:297:ILE:HD13	1.61	0.99
2:B:451:ILE:O	2:B:455:LEU:HG	1.67	0.94
1:A:392:PRO:HA	1:A:395:ILE:HD13	1.49	0.94
1:A:306:GLY:HA2	1:A:341:LYS:HE3	1.47	0.93
1:A:392:PRO:CA	1:A:395:ILE:HD13	2.00	0.91
1:A:177:ASN:HD22	1:A:179:MET:CE	1.83	0.90
1:A:199:LEU:HD11	1:A:232:ARG:HB3	1.54	0.89
1:A:67:LYS:O	1:A:70:PHE:HB3	1.73	0.88
1:A:134:VAL:H	1:A:187:ALA:HB2	1.39	0.87
1:A:167:ALA:HB1	1:A:209:LEU:HD12	1.57	0.87
1:A:255:GLY:O	1:A:259:ALA:HB2	1.74	0.87
1:A:129:LEU:HD23	1:A:183:ILE:HB	1.54	0.87
1:A:392:PRO:HA	1:A:395:ILE:CD1	2.05	0.85
1:A:40:ASN:ND2	1:A:42:LYS:HE3	1.91	0.85
1:A:117:ALA:HB1	1:A:127:VAL:HG11	1.57	0.85
1:A:391:ASN:O	1:A:394:ILE:HG23	1.76	0.85
1:A:209:LEU:HD23	1:A:209:LEU:O	1.77	0.84
1:A:46:SER:O	1:A:49:ALA:HB3	1.77	0.84
1:A:329:LEU:HD23	1:A:329:LEU:O	1.78	0.83
1:A:334:ALA:O	1:A:337:ILE:HG22	1.78	0.83
1:A:276:ILE:H	1:A:276:ILE:HD12	1.43	0.82
1:A:301:LEU:HD12	1:A:302:GLU:N	1.93	0.82
1:A:329:LEU:HD21	1:A:381:LEU:CD2	2.09	0.81
1:A:385:THR:HG22	1:A:387:LYS:H	1.45	0.81
2:B:466:ILE:HG23	2:B:467:PRO:HD2	1.64	0.80
1:A:336:ILE:HD13	1:A:336:ILE:O	1.82	0.80
1:A:103:GLY:HA3	1:A:109:LYS:HB2	1.65	0.78
1:A:98:ILE:H	1:A:98:ILE:HD12	1.47	0.78
1:A:98:ILE:N	1:A:98:ILE:HD12	1.97	0.78
1:A:61:PRO:HB2	1:A:64:LEU:HD12	1.64	0.78
1:A:17:THR:HB	1:A:18:PRO:CD	2.14	0.77
1:A:400:MET:HA	1:A:403:ILE:HD11	1.66	0.77
2:B:462:LEU:C	2:B:464:LYS:H	1.87	0.77
1:A:177:ASN:CB	1:A:179:MET:SD	2.70	0.77
1:A:283:ASN:ND2	1:A:286:ARG:HG3	2.00	0.77
2:B:452:LEU:C	2:B:452:LEU:HD12	2.05	0.77
1:A:102:VAL:HG21	1:A:202:MET:HE2	1.65	0.77
1:A:40:ASN:OD1	1:A:42:LYS:HG2	1.84	0.76
1:A:17:THR:HB	1:A:18:PRO:HD2	1.68	0.75
1:A:359:LEU:O	1:A:362:PRO:HD2	1.86	0.74
1:A:227:TYR:CD1	1:A:227:TYR:O	2.40	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:HD12	1:A:44:VAL:HG13	1.69	0.74
1:A:390:GLU:O	1:A:392:PRO:HD3	1.87	0.74
1:A:24:ASP:O	1:A:28:LYS:HG2	1.86	0.74
1:A:76:ASP:O	1:A:79:SER:HB3	1.88	0.74
2:B:453:VAL:O	2:B:457:TRP:HB2	1.88	0.74
1:A:297:ILE:C	1:A:297:ILE:HD13	2.08	0.74
2:B:452:LEU:HD12	2:B:453:VAL:N	2.03	0.73
1:A:256:ALA:O	1:A:260:VAL:HG23	1.89	0.73
1:A:298:GLU:O	1:A:301:LEU:HG	1.89	0.72
1:A:134:VAL:HG21	1:A:163:PRO:HD3	1.71	0.72
1:A:102:VAL:HG21	1:A:202:MET:CE	2.18	0.72
1:A:79:SER:HA	1:A:288:VAL:HG21	1.70	0.71
1:A:329:LEU:HB3	1:A:389:LEU:O	1.91	0.71
1:A:381:LEU:HD21	1:A:421:TYR:OH	1.91	0.70
1:A:424:MET:CE	2:B:455:LEU:HD22	2.21	0.70
1:A:75:TYR:O	1:A:79:SER:HB2	1.90	0.70
1:A:336:ILE:CD1	1:A:378:LEU:HD11	2.21	0.70
1:A:42:LYS:HG3	1:A:43:LEU:HD23	1.73	0.70
1:A:26:PHE:HE2	1:A:74:VAL:HG21	1.56	0.70
1:A:395:ILE:CG2	1:A:400:MET:HG3	2.23	0.69
1:A:250:THR:HG22	1:A:252:LYS:H	1.57	0.69
1:A:190:HIS:HB3	1:A:194:GLU:HA	1.74	0.69
1:A:61:PRO:O	1:A:64:LEU:HB2	1.93	0.69
1:A:189:ARG:HG2	1:A:190:HIS:H	1.58	0.68
1:A:116:LEU:O	1:A:119:PHE:HB3	1.92	0.68
1:A:412:GLU:O	1:A:416:GLU:HG2	1.94	0.68
1:A:392:PRO:O	1:A:395:ILE:HD13	1.94	0.68
1:A:137:PRO:HA	1:A:140:TYR:HD2	1.59	0.68
1:A:287:PHE:O	1:A:291:ILE:HG23	1.95	0.67
1:A:227:TYR:HD1	1:A:227:TYR:O	1.78	0.67
1:A:62:SER:O	1:A:63:VAL:HG12	1.94	0.67
1:A:177:ASN:ND2	1:A:179:MET:SD	2.66	0.67
1:A:139:ALA:O	1:A:143:LEU:HB2	1.94	0.67
1:A:196:THR:HG23	1:A:232:ARG:HD3	1.75	0.67
1:A:347:LYS:HD2	1:A:350:GLN:OE1	1.95	0.67
1:A:269:PHE:CD1	1:A:279:LEU:HD21	2.29	0.66
1:A:32:LYS:O	1:A:36:SER:HB3	1.95	0.66
1:A:44:VAL:O	1:A:48:THR:HG23	1.96	0.66
1:A:210:LYS:O	1:A:210:LYS:HG3	1.96	0.66
1:A:54:ARG:HD3	1:A:73:ILE:HG23	1.76	0.66
1:A:177:ASN:ND2	1:A:179:MET:CE	2.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ARG:HH11	1:A:399:ARG:HG2	1.60	0.66
1:A:329:LEU:HA	1:A:332:VAL:CG2	2.26	0.65
1:A:422:ASN:HA	1:A:425:ASN:HB2	1.77	0.65
1:A:336:ILE:HD12	1:A:378:LEU:HD21	1.78	0.65
1:A:227:TYR:CD1	1:A:227:TYR:C	2.70	0.65
1:A:40:ASN:HA	1:A:224:GLN:OE1	1.97	0.65
1:A:291:ILE:HG13	1:A:292:LEU:N	2.11	0.64
1:A:136:ARG:HG3	1:A:139:ALA:H	1.62	0.64
1:A:121:LYS:HE2	1:A:150:ILE:O	1.97	0.64
1:A:31:GLN:HE21	1:A:48:THR:HG21	1.63	0.64
1:A:330:ARG:HH11	1:A:330:ARG:HG2	1.63	0.64
1:A:199:LEU:CD1	1:A:232:ARG:HB3	2.26	0.63
1:A:295:GLY:O	1:A:298:GLU:CB	2.46	0.63
1:A:213:ASP:OD2	1:A:215:ILE:HD11	1.98	0.63
1:A:225:LYS:O	1:A:227:TYR:N	2.31	0.63
1:A:345:LEU:HD12	1:A:347:LYS:HB2	1.81	0.63
1:A:129:LEU:O	1:A:154:VAL:HA	1.98	0.62
1:A:399:ARG:O	1:A:403:ILE:HG12	1.99	0.62
1:A:42:LYS:NZ	1:A:43:LEU:HD21	2.14	0.62
1:A:336:ILE:HD11	1:A:378:LEU:HD11	1.80	0.62
1:A:399:ARG:HG2	1:A:399:ARG:NH1	2.15	0.62
1:A:376:ARG:HB3	1:A:409:LEU:HD21	1.80	0.62
1:A:415:ARG:O	1:A:419:GLU:HG2	1.99	0.62
1:A:14:THR:O	1:A:14:THR:HG22	1.98	0.62
1:A:295:GLY:O	1:A:298:GLU:N	2.32	0.62
1:A:335:GLN:NE2	2:B:456:ILE:HD13	2.14	0.62
1:A:137:PRO:O	1:A:140:TYR:HB2	2.00	0.62
1:A:423:ASN:O	1:A:427:LEU:HG	2.00	0.62
1:A:12:PHE:CE2	1:A:67:LYS:HB2	2.35	0.61
1:A:424:MET:HE1	2:B:455:LEU:HD22	1.82	0.61
2:B:462:LEU:O	2:B:464:LYS:N	2.33	0.61
1:A:375:ARG:HB3	1:A:378:LEU:HD13	1.81	0.61
1:A:340:ARG:CZ	1:A:374:ILE:HB	2.31	0.61
1:A:390:GLU:C	1:A:392:PRO:HD3	2.21	0.61
1:A:61:PRO:HD2	1:A:64:LEU:HD12	1.82	0.61
1:A:431:VAL:HG12	1:A:432:LYS:N	2.15	0.61
1:A:378:LEU:HD12	1:A:378:LEU:N	2.16	0.61
1:A:105:GLN:HB3	1:A:191:GLY:HA2	1.84	0.60
1:A:336:ILE:HD12	1:A:378:LEU:CG	2.30	0.60
1:A:92:PRO:HB3	1:A:97:PHE:CG	2.36	0.60
1:A:329:LEU:O	1:A:332:VAL:HB	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:MET:HE2	2:B:455:LEU:HD22	1.83	0.60
1:A:136:ARG:HD2	1:A:138:ALA:HB3	1.82	0.60
1:A:31:GLN:NE2	1:A:45:PHE:CD1	2.69	0.60
1:A:27:ILE:O	1:A:31:GLN:HG3	2.02	0.60
1:A:377:TRP:HZ3	1:A:420:TRP:HD1	1.49	0.60
1:A:42:LYS:HZ1	1:A:43:LEU:HD21	1.66	0.59
1:A:392:PRO:C	1:A:395:ILE:HD13	2.22	0.59
1:A:61:PRO:CB	1:A:64:LEU:HD12	2.32	0.59
2:B:452:LEU:O	2:B:456:ILE:HG22	2.02	0.59
1:A:273:GLY:HA3	1:A:278:GLU:OE2	2.02	0.59
1:A:110:THR:HG23	1:A:143:LEU:HD13	1.84	0.59
2:B:462:LEU:C	2:B:464:LYS:N	2.56	0.58
1:A:144:LEU:HD22	1:A:154:VAL:HB	1.84	0.58
1:A:349:LEU:HD23	1:A:352:ILE:HD12	1.86	0.58
1:A:6:ARG:HD2	1:A:294:MET:HG2	1.86	0.58
1:A:376:ARG:HD2	1:A:409:LEU:HG	1.86	0.58
1:A:247:MET:CE	1:A:257:LEU:HD21	2.32	0.58
1:A:297:ILE:CD1	1:A:297:ILE:O	2.45	0.57
1:A:146:LEU:O	1:A:150:ILE:HG23	2.03	0.57
1:A:276:ILE:N	1:A:276:ILE:HD12	2.16	0.57
1:A:378:LEU:HD12	1:A:378:LEU:H	1.69	0.57
1:A:134:VAL:CG2	1:A:163:PRO:HB3	2.36	0.56
1:A:215:ILE:HA	1:A:241:SER:O	2.06	0.56
1:A:50:LYS:O	1:A:54:ARG:HG3	2.06	0.56
1:A:329:LEU:CD2	1:A:389:LEU:HD22	2.35	0.56
1:A:417:LEU:HD11	1:A:421:TYR:OH	2.05	0.56
1:A:255:GLY:O	1:A:259:ALA:CB	2.50	0.56
1:A:329:LEU:HA	1:A:332:VAL:HG21	1.85	0.56
1:A:40:ASN:HB3	1:A:43:LEU:HG	1.87	0.56
2:B:453:VAL:C	2:B:457:TRP:HB2	2.24	0.56
1:A:250:THR:HG22	1:A:251:ALA:H	1.71	0.56
1:A:300:ILE:O	1:A:304:VAL:HG23	2.06	0.56
1:A:377:TRP:CZ3	1:A:420:TRP:HD1	2.24	0.56
1:A:101:LEU:HB2	1:A:185:ASP:HA	1.88	0.56
1:A:337:ILE:CG2	1:A:338:ALA:N	2.68	0.56
1:A:329:LEU:HD21	1:A:381:LEU:HD23	1.88	0.55
2:B:453:VAL:O	2:B:457:TRP:CB	2.55	0.55
1:A:340:ARG:NH2	1:A:374:ILE:HD12	2.21	0.55
1:A:377:TRP:CZ3	1:A:420:TRP:CD1	2.94	0.55
1:A:336:ILE:HD12	1:A:378:LEU:HD11	1.89	0.55
1:A:244:ILE:HD11	1:A:260:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LYS:HB3	1:A:278:GLU:HG2	1.89	0.55
1:A:363:SER:O	1:A:367:LEU:HG	2.07	0.55
1:A:400:MET:HA	1:A:403:ILE:CD1	2.34	0.55
1:A:227:TYR:HD1	1:A:227:TYR:C	2.07	0.55
1:A:222:ILE:O	1:A:222:ILE:HG22	2.07	0.55
1:A:137:PRO:HA	1:A:140:TYR:CD2	2.42	0.55
1:A:110:THR:CG2	1:A:143:LEU:HD13	2.37	0.54
2:B:468:HIS:ND1	2:B:468:HIS:N	2.55	0.54
1:A:3:GLU:H	1:A:3:GLU:CD	2.11	0.54
1:A:129:LEU:CD2	1:A:183:ILE:HB	2.33	0.54
1:A:31:GLN:NE2	1:A:45:PHE:HD1	2.05	0.54
1:A:6:ARG:HA	1:A:292:LEU:O	2.08	0.54
1:A:69:TRP:O	1:A:72:SER:HB3	2.08	0.54
1:A:336:ILE:HD12	1:A:378:LEU:CD2	2.38	0.53
1:A:176:LYS:C	1:A:178:LYS:H	2.11	0.53
1:A:340:ARG:HD3	1:A:378:LEU:HD22	1.91	0.53
1:A:102:VAL:HG23	1:A:102:VAL:O	2.08	0.53
1:A:165:GLU:O	1:A:169:LYS:HG3	2.08	0.53
1:A:134:VAL:N	1:A:187:ALA:HB2	2.17	0.53
1:A:247:MET:HE1	1:A:257:LEU:HD21	1.90	0.53
1:A:100:MET:SD	1:A:211:PRO:HG3	2.49	0.52
1:A:118:TYR:O	1:A:119:PHE:C	2.48	0.52
1:A:238:PRO:HG2	1:A:239:ILE:HD12	1.91	0.52
1:A:117:ALA:CB	1:A:127:VAL:HG11	2.34	0.52
1:A:209:LEU:C	1:A:209:LEU:HD23	2.29	0.52
1:A:63:VAL:HG21	1:A:345:LEU:HD11	1.91	0.52
1:A:171:VAL:HG23	1:A:182:ILE:HG21	1.90	0.52
1:A:206:TYR:CD2	1:A:211:PRO:HD2	2.45	0.52
1:A:6:ARG:NH1	1:A:294:MET:HE3	2.25	0.52
1:A:134:VAL:HG23	1:A:163:PRO:HB3	1.92	0.51
1:A:295:GLY:O	1:A:298:GLU:HB3	2.10	0.51
1:A:174:PHE:O	1:A:179:MET:HB2	2.10	0.51
1:A:289:SER:O	1:A:290:ARG:C	2.47	0.51
1:A:98:ILE:HD12	1:A:212:ASP:HB2	1.92	0.51
1:A:146:LEU:HD12	1:A:147:GLY:N	2.25	0.51
1:A:330:ARG:HG2	1:A:330:ARG:NH1	2.25	0.51
1:A:332:VAL:HG21	1:A:421:TYR:CE1	2.45	0.51
1:A:375:ARG:NH2	2:B:466:ILE:HD11	2.25	0.51
1:A:31:GLN:HE22	1:A:45:PHE:HD1	1.57	0.51
1:A:61:PRO:CD	1:A:64:LEU:HD12	2.40	0.51
1:A:348:VAL:HG23	1:A:349:LEU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ILE:H	1:A:276:ILE:CD1	2.19	0.50
1:A:376:ARG:HD2	1:A:409:LEU:CD1	2.41	0.50
1:A:222:ILE:HG22	1:A:225:LYS:HB2	1.94	0.50
1:A:250:THR:HG22	1:A:251:ALA:N	2.26	0.50
2:B:452:LEU:C	2:B:452:LEU:CD1	2.77	0.50
1:A:222:ILE:O	1:A:225:LYS:HB2	2.11	0.49
1:A:61:PRO:HB2	1:A:64:LEU:CD1	2.38	0.49
1:A:150:ILE:O	1:A:150:ILE:HG13	2.13	0.49
1:A:23:VAL:O	1:A:27:ILE:HG12	2.11	0.49
1:A:206:TYR:HD2	1:A:211:PRO:HD2	1.78	0.49
1:A:399:ARG:HH11	1:A:399:ARG:CG	2.26	0.49
1:A:170:GLY:O	1:A:173:ILE:HG22	2.12	0.49
1:A:190:HIS:O	1:A:191:GLY:C	2.50	0.49
1:A:83:GLY:HA3	1:A:284:ALA:HB1	1.95	0.49
1:A:218:ILE:HG23	1:A:222:ILE:HD12	1.93	0.49
1:A:375:ARG:HB3	1:A:378:LEU:CD1	2.42	0.48
1:A:89:ASN:C	1:A:91:ASN:H	2.16	0.48
1:A:39:VAL:HA	1:A:255:GLY:HA2	1.94	0.48
1:A:216:LEU:HB3	1:A:233:PHE:CE2	2.48	0.48
1:A:298:GLU:OE1	1:A:301:LEU:HD23	2.13	0.48
1:A:377:TRP:CE3	1:A:417:LEU:HD12	2.48	0.48
1:A:171:VAL:CG1	1:A:172:ASP:N	2.75	0.48
1:A:225:LYS:C	1:A:227:TYR:N	2.64	0.48
1:A:83:GLY:HA3	1:A:284:ALA:CB	2.42	0.48
1:A:289:SER:O	1:A:291:ILE:N	2.46	0.48
1:A:336:ILE:CD1	1:A:378:LEU:HD21	2.43	0.48
1:A:409:LEU:HD23	1:A:413:GLU:HB3	1.96	0.48
1:A:177:ASN:HD22	1:A:179:MET:HE1	1.71	0.48
1:A:76:ASP:O	1:A:79:SER:CB	2.59	0.48
1:A:26:PHE:CD2	1:A:70:PHE:HE2	2.31	0.48
1:A:54:ARG:CZ	1:A:73:ILE:HD12	2.44	0.48
1:A:259:ALA:O	1:A:262:ALA:HB3	2.13	0.48
1:A:218:ILE:HD12	1:A:242:VAL:HG11	1.94	0.47
1:A:225:LYS:C	1:A:227:TYR:H	2.17	0.47
1:A:333:TYR:O	1:A:337:ILE:HB	2.15	0.47
1:A:40:ASN:OD1	1:A:42:LYS:N	2.46	0.47
1:A:135:TYR:CD2	1:A:187:ALA:HB1	2.50	0.47
1:A:46:SER:O	1:A:49:ALA:CB	2.55	0.47
1:A:4:ASN:OD1	1:A:4:ASN:N	2.47	0.47
1:A:376:ARG:HB3	1:A:409:LEU:CD2	2.44	0.47
1:A:54:ARG:HA	1:A:58:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:TYR:CE2	1:A:122:LYS:HD2	2.50	0.47
1:A:422:ASN:O	1:A:425:ASN:N	2.47	0.47
1:A:297:ILE:CD1	1:A:297:ILE:C	2.77	0.47
1:A:377:TRP:CH2	1:A:420:TRP:CD1	3.03	0.47
1:A:135:TYR:CE2	1:A:189:ARG:HB2	2.50	0.47
1:A:329:LEU:HD21	1:A:389:LEU:HD22	1.96	0.47
1:A:359:LEU:O	1:A:362:PRO:CD	2.60	0.47
1:A:43:LEU:O	1:A:46:SER:HB3	2.15	0.47
1:A:98:ILE:CD1	1:A:98:ILE:N	2.67	0.47
1:A:89:ASN:C	1:A:91:ASN:N	2.68	0.46
1:A:98:ILE:HG23	1:A:182:ILE:HB	1.96	0.46
1:A:146:LEU:C	1:A:146:LEU:HD12	2.36	0.46
1:A:269:PHE:CD1	1:A:279:LEU:CD2	2.99	0.46
1:A:31:GLN:O	1:A:35:ILE:HG13	2.15	0.46
1:A:171:VAL:O	1:A:175:VAL:HG23	2.15	0.46
1:A:100:MET:CE	1:A:186:THR:HG21	2.45	0.46
1:A:206:TYR:O	1:A:210:LYS:HA	2.16	0.46
1:A:307:LEU:C	1:A:307:LEU:HD23	2.36	0.46
1:A:424:MET:HA	1:A:424:MET:HE3	1.97	0.46
1:A:407:SER:HB2	1:A:409:LEU:HD13	1.97	0.45
1:A:5:ILE:O	1:A:6:ARG:C	2.53	0.45
2:B:466:ILE:HG23	2:B:467:PRO:CD	2.41	0.45
1:A:227:TYR:O	1:A:231:SER:HB2	2.17	0.45
1:A:336:ILE:HD12	1:A:378:LEU:CD1	2.46	0.45
1:A:329:LEU:HD22	1:A:389:LEU:HD22	1.98	0.45
1:A:188:GLY:HA2	1:A:198:LEU:HD21	1.99	0.45
1:A:104:VAL:O	1:A:107:SER:CB	2.65	0.45
1:A:332:VAL:HG11	1:A:421:TYR:CE1	2.52	0.45
1:A:377:TRP:O	1:A:381:LEU:HD12	2.16	0.45
1:A:426:ARG:HG3	1:A:430:MET:HE1	1.98	0.45
1:A:134:VAL:HG21	1:A:163:PRO:CD	2.43	0.45
1:A:132:ALA:O	1:A:134:VAL:HG23	2.17	0.44
1:A:247:MET:HE3	1:A:257:LEU:HD21	1.97	0.44
1:A:40:ASN:C	1:A:40:ASN:OD1	2.55	0.44
1:A:54:ARG:C	1:A:56:ASN:N	2.69	0.44
1:A:337:ILE:HG23	1:A:338:ALA:N	2.32	0.44
1:A:75:TYR:O	1:A:76:ASP:C	2.54	0.44
1:A:86:LYS:HD2	1:A:86:LYS:HA	1.69	0.44
1:A:343:GLY:C	1:A:345:LEU:HD23	2.38	0.44
1:A:54:ARG:HD3	1:A:73:ILE:CG2	2.47	0.44
1:A:289:SER:C	1:A:291:ILE:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:451:ILE:O	2:B:455:LEU:CG	2.53	0.44
1:A:99:ILE:HA	1:A:213:ASP:O	2.18	0.43
1:A:359:LEU:C	1:A:361:THR:N	2.70	0.43
1:A:136:ARG:HG3	1:A:139:ALA:N	2.31	0.43
1:A:342:MET:HB3	1:A:343:GLY:H	1.50	0.43
1:A:329:LEU:HG	1:A:421:TYR:CZ	2.53	0.43
1:A:19:TYR:CD2	1:A:20:GLU:HG2	2.53	0.43
1:A:263:THR:OG1	1:A:264:GLY:N	2.51	0.43
1:A:5:ILE:O	1:A:9:VAL:HG23	2.18	0.43
2:B:463:LEU:HG	2:B:466:ILE:HD12	2.01	0.43
1:A:376:ARG:HB3	1:A:409:LEU:CG	2.48	0.43
1:A:111:THR:HG22	1:A:115:LYS:HD3	1.99	0.43
1:A:54:ARG:NH1	1:A:73:ILE:HD12	2.33	0.43
2:B:449:GLY:O	2:B:453:VAL:HG23	2.18	0.43
1:A:385:THR:O	1:A:389:LEU:HG	2.18	0.43
1:A:100:MET:HE3	1:A:186:THR:HG21	2.00	0.43
1:A:375:ARG:HG3	1:A:377:TRP:H	1.84	0.43
1:A:385:THR:HG22	1:A:386:TYR:N	2.33	0.43
1:A:58:GLU:HB2	1:A:69:TRP:HZ2	1.82	0.43
1:A:229:LEU:O	1:A:229:LEU:HD12	2.19	0.43
1:A:220:ALA:HB2	1:A:244:ILE:HG22	2.01	0.43
1:A:381:LEU:HD21	1:A:421:TYR:HH	1.81	0.43
1:A:40:ASN:OD1	1:A:41:VAL:N	2.52	0.43
1:A:164:ILE:HG13	1:A:165:GLU:N	2.34	0.42
1:A:301:LEU:HD12	1:A:302:GLU:CA	2.48	0.42
1:A:82:PHE:N	1:A:82:PHE:CD1	2.84	0.42
1:A:104:VAL:O	1:A:107:SER:HB3	2.20	0.42
1:A:14:THR:O	1:A:15:GLY:C	2.57	0.42
1:A:329:LEU:HD21	1:A:381:LEU:HD21	1.95	0.42
1:A:340:ARG:HH21	1:A:374:ILE:HD12	1.82	0.42
1:A:392:PRO:C	1:A:394:ILE:H	2.22	0.42
1:A:61:PRO:HD2	1:A:64:LEU:CD1	2.50	0.42
1:A:284:ALA:O	1:A:287:PHE:HB3	2.20	0.42
1:A:101:LEU:CD1	1:A:113:ALA:HB2	2.50	0.42
1:A:150:ILE:HG13	1:A:152:VAL:HG23	2.02	0.42
1:A:63:VAL:HG22	1:A:303:LYS:HD3	2.00	0.42
1:A:328:THR:O	1:A:330:ARG:N	2.52	0.42
1:A:376:ARG:HD2	1:A:409:LEU:CG	2.49	0.42
1:A:425:ASN:O	1:A:429:LYS:HG3	2.19	0.42
1:A:63:VAL:HG22	1:A:63:VAL:O	2.20	0.42
1:A:170:GLY:O	1:A:173:ILE:CG2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:MET:C	1:A:204:GLU:N	2.73	0.42
1:A:39:VAL:HG12	1:A:40:ASN:N	2.34	0.42
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.81	0.41
1:A:162:ASN:ND2	1:A:165:GLU:HB2	2.35	0.41
1:A:269:PHE:CD2	1:A:269:PHE:N	2.88	0.41
1:A:359:LEU:C	1:A:361:THR:H	2.23	0.41
1:A:401:ARG:O	1:A:405:GLU:HG2	2.21	0.41
1:A:336:ILE:HD12	1:A:378:LEU:HG	2.02	0.41
1:A:72:SER:O	1:A:76:ASP:HB2	2.20	0.41
1:A:283:ASN:ND2	1:A:286:ARG:CG	2.76	0.41
1:A:336:ILE:C	1:A:336:ILE:HD13	2.41	0.41
1:A:352:ILE:O	1:A:354:GLY:N	2.53	0.41
1:A:407:SER:CB	1:A:409:LEU:HD13	2.50	0.41
1:A:7:ASP:C	1:A:9:VAL:N	2.74	0.41
1:A:170:GLY:HA2	1:A:173:ILE:HG22	2.00	0.41
1:A:6:ARG:HH12	1:A:10:ARG:NH1	2.19	0.41
1:A:54:ARG:HB3	1:A:58:GLU:HG3	2.01	0.41
1:A:431:VAL:CG1	1:A:432:LYS:N	2.82	0.41
1:A:160:ASN:C	1:A:162:ASN:H	2.24	0.41
1:A:256:ALA:O	1:A:259:ALA:HB3	2.21	0.41
1:A:11:LYS:C	1:A:13:LEU:N	2.73	0.41
1:A:426:ARG:HG3	1:A:430:MET:CE	2.51	0.41
1:A:134:VAL:HG21	1:A:163:PRO:HB3	2.03	0.41
1:A:90:VAL:HG12	1:A:90:VAL:O	2.20	0.40
1:A:101:LEU:HD12	1:A:113:ALA:HB2	2.03	0.40
1:A:135:TYR:H	1:A:187:ALA:HB1	1.86	0.40
1:A:293:GLY:O	1:A:294:MET:C	2.59	0.40
1:A:178:LYS:O	1:A:179:MET:C	2.60	0.40
1:A:361:THR:OG1	1:A:362:PRO:CD	2.69	0.40
1:A:170:GLY:C	1:A:173:ILE:HG22	2.42	0.40
2:B:452:LEU:C	2:B:454:LEU:H	2.25	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	A	409/433 (94%)	329 (80%)	75 (18%)	5 (1%)	14	53
2	B	19/42 (45%)	14 (74%)	3 (16%)	2 (10%)	0	6
All	All	428/475 (90%)	343 (80%)	78 (18%)	7 (2%)	11	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	ALA
2	B	463	LEU
1	A	294	MET
2	B	458	GLY
1	A	290	ARG
1	A	63	VAL
1	A	74	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	351/370 (95%)	310 (88%)	41 (12%)	6	27
2	B	18/35 (51%)	13 (72%)	5 (28%)	0	3
All	All	369/405 (91%)	323 (88%)	46 (12%)	5	24

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	4	ASN
1	A	56	ASN
1	A	62	SER
1	A	85	ASP
1	A	86	LYS

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Mol	Chain	Res	Type
1	A	98	ILE
1	A	141	ASP
1	A	179	MET
1	A	190	HIS
1	A	194	GLU
1	A	196	THR
1	A	205	MET
1	A	212	ASP
1	A	217	VAL
1	A	224	GLN
1	A	227	TYR
1	A	228	ASP
1	A	232	ARG
1	A	245	THR
1	A	276	ILE
1	A	280	GLU
1	A	294	MET
1	A	297	ILE
1	A	298	GLU
1	A	299	SER
1	A	301	LEU
1	A	331	ASP
1	A	336	ILE
1	A	337	ILE
1	A	341	LYS
1	A	345	LEU
1	A	346	SER
1	A	350	GLN
1	A	364	GLU
1	A	373	LYS
1	A	394	ILE
1	A	399	ARG
1	A	402	ARG
1	A	428	LEU
1	A	430	MET
2	B	450	ILE
2	B	452	LEU
2	B	455	LEU
2	B	457	TRP
2	B	468	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	145	GLN
1	A	177	ASN
1	A	283	ASN
1	A	335	GLN
1	A	366	GLN
1	A	423	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	413/433 (95%)	0.04	15 (3%) 42 38	79, 154, 195, 200	0
2	B	21/42 (50%)	0.31	0 100 100	145, 169, 200, 200	0
All	All	434/475 (91%)	0.06	15 (3%) 44 39	79, 155, 196, 200	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	VAL	5.2
1	A	373	LYS	4.6
1	A	374	ILE	3.7
1	A	131	ALA	3.5
1	A	129	LEU	3.2
1	A	100	MET	2.8
1	A	407	SER	2.6
1	A	359	LEU	2.6
1	A	366	GLN	2.5
1	A	388	GLU	2.4
1	A	421	TYR	2.3
1	A	422	ASN	2.3
1	A	132	ALA	2.3
1	A	417	LEU	2.2
1	A	412	GLU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.