



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:17 am GMT

PDB ID : 3OQC  
Title : Ubiquitin-fold modifier 1 Specific Protease, UfSP2  
Authors : Ha, B.H.; Chung, C.H.; Kim, E.E.  
Deposited on : 2010-09-02  
Resolution : 2.60 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  
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

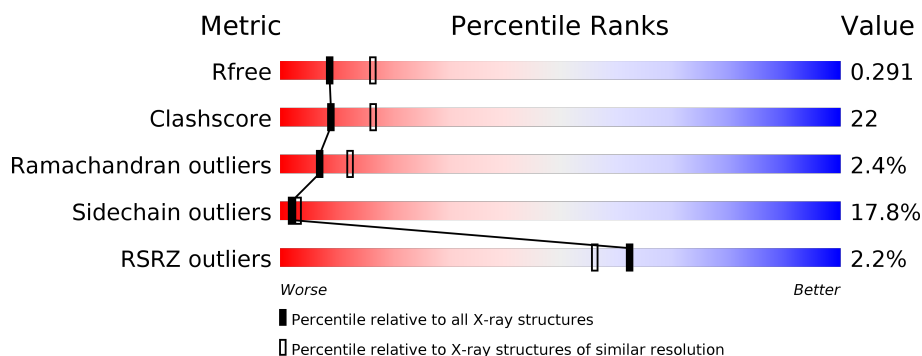
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	481	
1	B	481	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6716 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 Ufm1-specific protease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3328	2131	573	606	18			
1	B	411	Total	C	N	O	S	0	0	0
			3281	2101	561	601	18			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q99K23
A	-18	GLY	-	EXPRESSION TAG	UNP Q99K23
A	-17	SER	-	EXPRESSION TAG	UNP Q99K23
A	-16	SER	-	EXPRESSION TAG	UNP Q99K23
A	-15	HIS	-	EXPRESSION TAG	UNP Q99K23
A	-14	HIS	-	EXPRESSION TAG	UNP Q99K23
A	-13	HIS	-	EXPRESSION TAG	UNP Q99K23
A	-12	HIS	-	EXPRESSION TAG	UNP Q99K23
A	-11	HIS	-	EXPRESSION TAG	UNP Q99K23
A	-10	HIS	-	EXPRESSION TAG	UNP Q99K23
A	-9	SER	-	EXPRESSION TAG	UNP Q99K23
A	-8	SER	-	EXPRESSION TAG	UNP Q99K23
A	-7	GLY	-	EXPRESSION TAG	UNP Q99K23
A	-6	LEU	-	EXPRESSION TAG	UNP Q99K23
A	-5	VAL	-	EXPRESSION TAG	UNP Q99K23
A	-4	PRO	-	EXPRESSION TAG	UNP Q99K23
A	-3	ARG	-	EXPRESSION TAG	UNP Q99K23
A	-2	GLY	-	EXPRESSION TAG	UNP Q99K23
A	-1	SER	-	EXPRESSION TAG	UNP Q99K23
A	0	HIS	-	EXPRESSION TAG	UNP Q99K23
A	94	ARG	LYS	ENGINEERED MUTATION	UNP Q99K23
A	128	ALA	ARG	ENGINEERED MUTATION	UNP Q99K23
A	294	SER	CYS	ENGINEERED MUTATION	UNP Q99K23
B	-19	MET	-	EXPRESSION TAG	UNP Q99K23
B	-18	GLY	-	EXPRESSION TAG	UNP Q99K23

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	EXPRESSION TAG	UNP Q99K23
B	-16	SER	-	EXPRESSION TAG	UNP Q99K23
B	-15	HIS	-	EXPRESSION TAG	UNP Q99K23
B	-14	HIS	-	EXPRESSION TAG	UNP Q99K23
B	-13	HIS	-	EXPRESSION TAG	UNP Q99K23
B	-12	HIS	-	EXPRESSION TAG	UNP Q99K23
B	-11	HIS	-	EXPRESSION TAG	UNP Q99K23
B	-10	HIS	-	EXPRESSION TAG	UNP Q99K23
B	-9	SER	-	EXPRESSION TAG	UNP Q99K23
B	-8	SER	-	EXPRESSION TAG	UNP Q99K23
B	-7	GLY	-	EXPRESSION TAG	UNP Q99K23
B	-6	LEU	-	EXPRESSION TAG	UNP Q99K23
B	-5	VAL	-	EXPRESSION TAG	UNP Q99K23
B	-4	PRO	-	EXPRESSION TAG	UNP Q99K23
B	-3	ARG	-	EXPRESSION TAG	UNP Q99K23
B	-2	GLY	-	EXPRESSION TAG	UNP Q99K23
B	-1	SER	-	EXPRESSION TAG	UNP Q99K23
B	0	HIS	-	EXPRESSION TAG	UNP Q99K23
B	94	ARG	LYS	ENGINEERED MUTATION	UNP Q99K23
B	128	ALA	ARG	ENGINEERED MUTATION	UNP Q99K23
B	294	SER	CYS	ENGINEERED MUTATION	UNP Q99K23

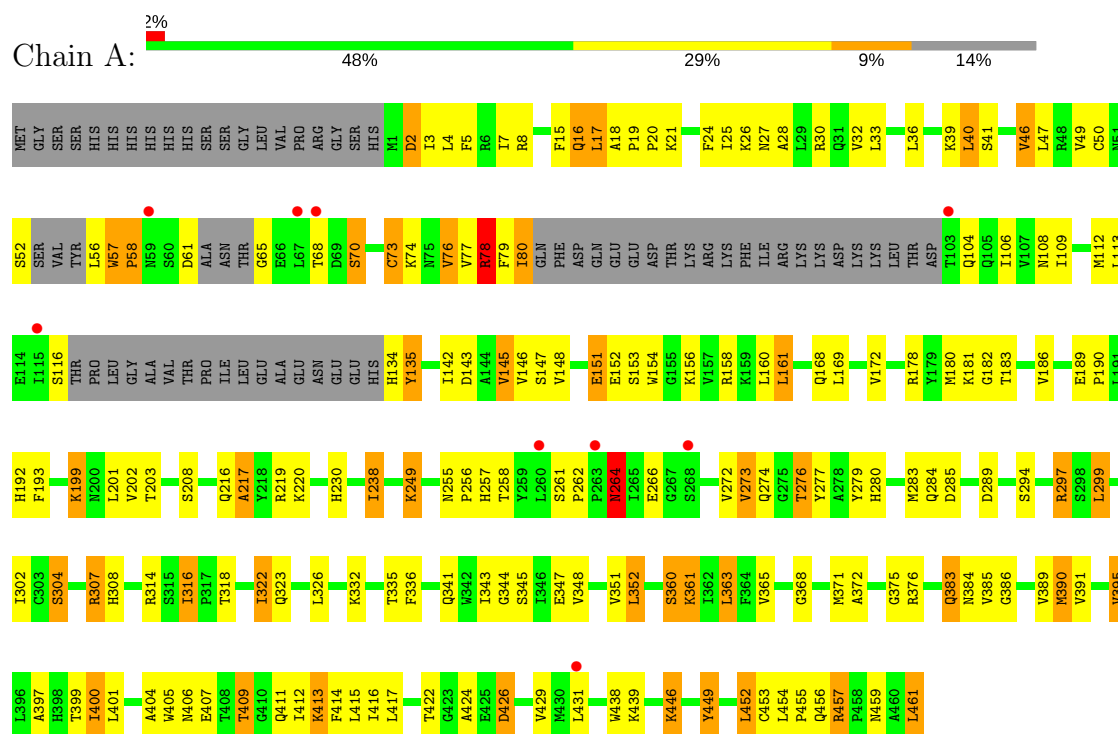
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	53	Total O 53 53	0	0
2	B	54	Total O 54 54	0	0

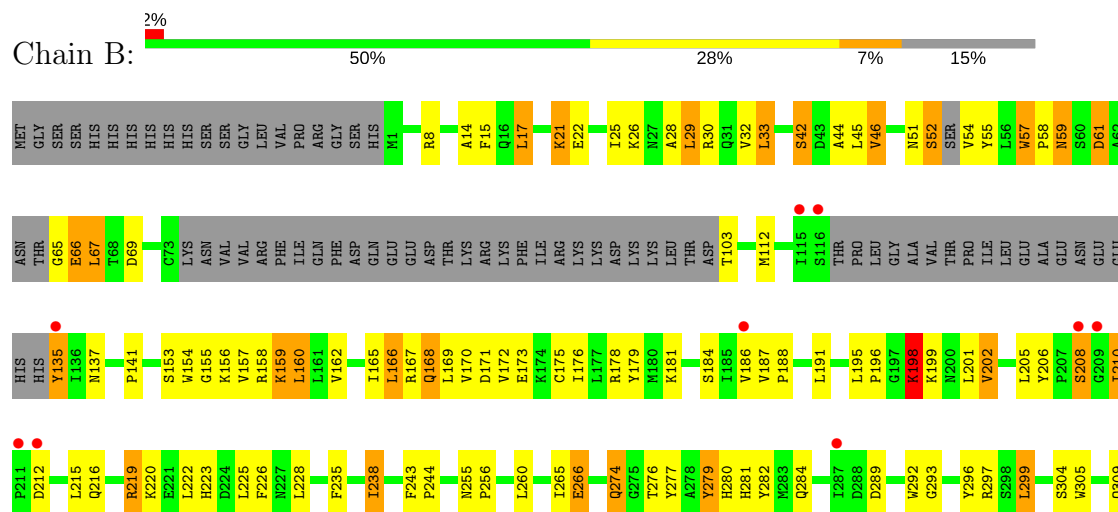
### 3 Residue-property plots

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

#### • Molecule 1: Ufm1-specific protease 2



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G310	Y311	T312	E313	R314	T318	H319	A325	L326	A329	K332	P333	A334	T335	F336	S339	R340	Q341	L355	T356	G357	V358	T359	S360	K361	T362	L363	F364	V365	N366	Q367	G368	S369	E370	S373	Q374	V385	G386	T387	K390	V391	L396	I400	L401	M406	E407	T408	T409
G410	Q411	I416	L417	H420	Y421	T422	G423	A424	E425	D426	L431	G437	W438	K439	S440	P441	D442	F443	W444	N445	K446	D447	A448	Y449	L452	C453	L454	R457	P458	M459	M460	L461															

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.53Å 56.04Å 143.27Å 90.00° 128.01° 90.00°	Depositor
Resolution (Å)	46.10 – 2.60 46.10 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.10-2.60) 98.4 (46.10-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.238 , 0.298 0.233 , 0.291	Depositor DCC
$R_{free}$ test set	1776 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6716	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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	0.76	1/3409 (0.0%)	0.85	1/4627 (0.0%)
1	B	0.71	0/3361	0.84	4/4564 (0.1%)
All	All	0.74	1/6770 (0.0%)	0.84	5/9191 (0.1%)

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
1	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	GLY	N-CA	6.91	1.56	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	B	396	LEU	CA-CB-CG	5.44	127.80	115.30
1	B	8	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	B	201	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	457	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	262	PRO	Peptide
1	A	57	TRP	Peptide
1	B	57	TRP	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	3328	0	3297	167	1
1	B	3281	0	3243	126	0
2	A	53	0	0	15	0
2	B	54	0	0	10	1
All	All	6716	0	6540	293	1

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 22.

All (293) 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:B:65:GLY:HA2	1:B:158:ARG:HH12	0.99	1.09
1:B:409:THR:HG21	2:B:494:HOH:O	1.50	1.08
1:B:260:LEU:HD11	1:B:437:GLY:HA2	1.37	1.07
1:A:216:GLN:HB2	2:A:476:HOH:O	1.58	1.03
1:B:362:ILE:HD11	1:B:364:PHE:CZ	1.94	1.02
1:A:49:VAL:HB	1:A:58:PRO:CG	1.90	1.00
1:A:383:GLN:HA	1:A:383:GLN:HE21	1.22	1.00
1:B:219:ARG:HB2	1:B:219:ARG:HH11	1.26	0.98
1:B:65:GLY:HA2	1:B:158:ARG:NH1	1.78	0.97
1:B:362:ILE:HD11	1:B:364:PHE:CE1	2.04	0.92
1:A:426:ASP:HB3	2:A:487:HOH:O	1.70	0.92
1:A:17:LEU:HD13	1:A:25:ILE:HG23	1.49	0.91
1:A:322:ILE:HD12	1:A:351:VAL:HG21	1.55	0.89
1:A:49:VAL:HB	1:A:58:PRO:HG2	1.55	0.88
1:B:219:ARG:HA	1:B:222:LEU:HD12	1.55	0.88
1:A:406:ASN:HB3	1:A:409:THR:HG22	1.54	0.88
1:B:219:ARG:HH11	1:B:219:ARG:CB	1.88	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:CD2	1:A:352:LEU:HD13	2.07	0.85
1:A:52:SER:HA	1:A:79:PHE:CD2	2.11	0.85
1:B:219:ARG:HB2	1:B:219:ARG:NH1	1.93	0.83
1:A:446:LYS:HD3	1:A:446:LYS:H	1.44	0.83
1:B:198:LYS:HE3	1:B:198:LYS:O	1.80	0.82
1:A:449:TYR:HB2	2:A:462:HOH:O	1.79	0.81
1:B:289:ASP:HA	1:B:292:TRP:CE2	2.17	0.80
1:A:383:GLN:HA	1:A:383:GLN:NE2	1.98	0.79
1:B:363:LEU:HD12	2:B:516:HOH:O	1.82	0.79
1:B:452:LEU:HD22	2:B:516:HOH:O	1.82	0.79
1:A:158:ARG:HD3	2:A:488:HOH:O	1.83	0.78
1:A:19:PRO:HB2	1:A:20:PRO:HD3	1.65	0.77
1:A:283:MET:HG3	1:A:422:THR:HG23	1.66	0.77
1:A:15:PHE:HB3	1:A:32:VAL:HG21	1.65	0.77
1:B:370:GLU:O	1:B:373:SER:HB2	1.84	0.77
1:B:289:ASP:OD1	1:B:297:ARG:HD3	1.85	0.76
1:A:219:ARG:NH1	1:A:461:LEU:OXT	2.18	0.75
1:A:52:SER:HA	1:A:79:PHE:HD2	1.51	0.74
1:A:299:LEU:HD21	1:A:352:LEU:HD13	1.69	0.74
1:A:406:ASN:HB3	1:A:409:THR:CG2	2.18	0.72
1:A:16:GLN:HG3	1:A:135:TYR:HD1	1.54	0.72
1:B:289:ASP:HA	1:B:292:TRP:NE1	2.04	0.72
1:A:78:ARG:HB3	1:A:78:ARG:HH11	1.54	0.72
1:A:429:VAL:HG23	2:A:487:HOH:O	1.90	0.70
1:A:391:VAL:HG12	1:A:452:LEU:HD22	1.74	0.70
1:A:49:VAL:CB	1:A:58:PRO:HG2	2.21	0.70
1:B:198:LYS:HA	2:B:480:HOH:O	1.92	0.70
1:B:416:ILE:HD11	1:B:439:LYS:HD3	1.73	0.70
1:A:255:ASN:O	1:A:258:THR:HG22	1.93	0.69
1:A:409:THR:HG23	1:A:411:GLN:H	1.59	0.68
1:A:189:GLU:OE2	1:A:208:SER:HB2	1.94	0.68
1:B:362:ILE:CD1	1:B:364:PHE:CE1	2.77	0.68
1:A:274:GLN:HG3	1:A:457:ARG:HH21	1.60	0.67
1:B:238:ILE:HG13	1:B:238:ILE:O	1.92	0.67
1:A:322:ILE:HG13	1:A:323:GLN:N	2.09	0.67
1:B:42:SER:HB2	1:B:44:ALA:H	1.61	0.66
1:A:16:GLN:CG	1:A:135:TYR:HD1	2.07	0.66
1:A:255:ASN:OD1	1:A:276:THR:HB	1.96	0.66
1:A:299:LEU:HG	1:A:348:VAL:HG13	1.76	0.66
1:A:70:SER:HB3	1:A:153:SER:HB2	1.77	0.65
1:A:16:GLN:HG3	1:A:135:TYR:CD1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:HB	1:A:58:PRO:HG3	1.78	0.64
1:A:216:GLN:CB	2:A:476:HOH:O	2.27	0.64
1:B:65:GLY:CA	1:B:158:ARG:HH12	1.93	0.64
1:B:407:GLU:HB3	2:B:463:HOH:O	1.99	0.63
1:A:49:VAL:CG2	1:A:58:PRO:HG2	2.28	0.63
1:B:374:GLN:NE2	1:B:374:GLN:HA	2.13	0.62
1:B:168:GLN:O	1:B:172:VAL:HG23	1.99	0.62
1:B:202:VAL:HG21	1:B:226:PHE:CZ	2.35	0.62
1:B:216:GLN:HA	1:B:219:ARG:HH12	1.65	0.62
1:A:219:ARG:NH2	2:A:476:HOH:O	2.32	0.62
1:B:282:TYR:HB2	1:B:421:TYR:O	2.00	0.61
1:A:372:ALA:HA	1:A:412:ILE:HG21	1.82	0.61
1:A:199:LYS:HE3	1:A:199:LYS:O	2.00	0.61
1:B:390:MET:HG3	1:B:453:CYS:HB3	1.83	0.60
1:B:282:TYR:CD1	1:B:420:HIS:HA	2.36	0.60
1:B:391:VAL:O	1:B:391:VAL:HG23	2.00	0.60
1:A:8:ARG:HH21	1:A:108:ASN:ND2	1.99	0.60
1:A:274:GLN:HG2	1:A:386:GLY:HA3	1.83	0.60
1:A:376:ARG:NH2	1:A:407:GLU:OE1	2.34	0.60
1:A:255:ASN:O	1:A:258:THR:CG2	2.51	0.59
1:B:265:ILE:HG22	1:B:266:GLU:O	2.03	0.59
1:B:274:GLN:HG2	1:B:386:GLY:HA3	1.85	0.59
1:A:449:TYR:C	1:A:449:TYR:CD1	2.76	0.59
1:A:257:HIS:HB2	1:A:415:LEU:HD21	1.86	0.58
1:A:143:ASP:HB3	1:A:190:PRO:HG2	1.86	0.58
1:A:220:LYS:HG2	1:A:461:LEU:HD11	1.85	0.58
1:A:17:LEU:HD13	1:A:25:ILE:CG2	2.28	0.57
1:B:391:VAL:HG12	1:B:452:LEU:HG	1.86	0.57
1:B:59:ASN:HB2	2:B:503:HOH:O	2.04	0.57
1:B:362:ILE:HA	1:B:452:LEU:O	2.04	0.57
1:A:49:VAL:O	1:A:52:SER:OG	2.18	0.56
1:B:305:TRP:O	1:B:309:GLN:HG2	2.04	0.56
1:A:25:ILE:HA	1:A:28:ALA:HB3	1.86	0.56
1:B:219:ARG:HD3	1:B:235:PHE:C	2.25	0.56
1:B:45:LEU:O	1:B:58:PRO:HD3	2.04	0.56
1:B:61:ASP:OD2	1:B:61:ASP:N	2.38	0.56
1:B:452:LEU:N	1:B:452:LEU:HD12	2.20	0.56
1:B:175:CYS:SG	1:B:188:PRO:HG3	2.46	0.56
1:A:274:GLN:HG3	1:A:457:ARG:NH2	2.20	0.56
1:B:336:PHE:O	1:B:339:SER:CB	2.53	0.56
1:B:284:GLN:HB2	1:B:297:ARG:NH2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PHE:CB	1:A:32:VAL:HG21	2.33	0.56
1:A:400:ILE:HD12	1:A:415:LEU:O	2.06	0.56
1:A:304:SER:HA	1:A:307:ARG:HG2	1.88	0.56
1:B:162:VAL:O	1:B:166:LEU:HD22	2.06	0.56
1:B:176:ILE:HA	2:B:496:HOH:O	2.05	0.56
1:A:375:GLY:HA3	1:A:412:ILE:HD12	1.89	0.55
1:A:4:LEU:HD23	1:A:106:ILE:HD13	1.89	0.55
1:B:364:PHE:HD2	1:B:449:TYR:HH	1.54	0.55
1:A:383:GLN:CA	1:A:383:GLN:HE21	2.05	0.55
1:A:25:ILE:HD12	1:A:26:LYS:H	1.72	0.55
1:A:46:VAL:HG22	1:A:112:MET:HE3	1.89	0.54
1:A:216:GLN:CA	2:A:476:HOH:O	2.51	0.54
1:B:51:ASN:O	1:B:52:SER:HB2	2.08	0.54
1:A:168:GLN:O	1:A:172:VAL:HG23	2.07	0.54
1:B:409:THR:HG23	1:B:411:GLN:H	1.72	0.54
1:B:336:PHE:HE1	1:B:341:GLN:HB2	1.73	0.54
1:A:401:LEU:HD11	1:A:417:LEU:HB2	1.90	0.54
1:B:256:PRO:HD2	1:B:277:TYR:OH	2.07	0.54
1:B:368:GLY:HA3	1:B:445:ASN:O	2.08	0.54
1:A:376:ARG:HH21	1:A:405:TRP:HZ3	1.55	0.53
1:B:216:GLN:HA	1:B:219:ARG:NH1	2.23	0.53
1:B:385:VAL:HG12	1:B:387:THR:HG23	1.89	0.53
1:B:14:ALA:CB	1:B:137:ASN:OD1	2.56	0.53
1:B:17:LEU:HD12	1:B:21:LYS:HB2	1.90	0.53
1:A:79:PHE:CB	2:A:477:HOH:O	2.56	0.53
1:B:66:GLU:HB3	1:B:154:TRP:HD1	1.72	0.53
1:A:401:LEU:O	1:A:415:LEU:HD23	2.09	0.53
1:A:52:SER:CA	1:A:79:PHE:HD2	2.21	0.53
1:B:181:LYS:HB3	1:B:184:SER:OG	2.08	0.53
1:B:336:PHE:O	1:B:339:SER:HB3	2.09	0.53
1:A:52:SER:CA	1:A:79:PHE:CD2	2.86	0.52
1:B:279:TYR:CE2	1:B:281:HIS:HB3	2.44	0.52
1:A:49:VAL:HB	1:A:58:PRO:CD	2.40	0.52
1:B:195:LEU:HD22	1:B:228:LEU:HD11	1.92	0.52
1:B:401:LEU:HD11	1:B:417:LEU:HB2	1.92	0.52
1:A:280:HIS:NE2	1:A:316:ILE:HD12	2.24	0.52
1:A:360:SER:HB3	1:A:455:PRO:HA	1.92	0.52
1:B:67:LEU:HD22	1:B:67:LEU:H	1.75	0.52
1:A:348:VAL:HG11	1:A:390:MET:HG2	1.92	0.52
1:B:280:HIS:HA	1:B:284:GLN:HE22	1.75	0.52
1:B:153:SER:O	1:B:157:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASP:HB3	1:B:205:LEU:HD12	1.92	0.51
1:B:445:ASN:HD22	1:B:445:ASN:C	2.12	0.51
1:A:79:PHE:HB2	2:A:477:HOH:O	2.11	0.51
1:B:445:ASN:OD1	1:B:448:ALA:HB2	2.11	0.51
1:B:191:LEU:HD12	1:B:206:TYR:HB2	1.93	0.51
1:A:68:THR:OG1	1:A:158:ARG:NH2	2.44	0.51
1:B:445:ASN:ND2	1:B:446:LYS:O	2.44	0.51
1:A:272:VAL:HG23	1:A:401:LEU:O	2.10	0.51
1:B:299:LEU:HD23	1:B:299:LEU:O	2.11	0.51
1:A:216:GLN:N	2:A:476:HOH:O	2.44	0.50
1:B:14:ALA:HB2	1:B:137:ASN:OD1	2.11	0.50
1:A:256:PRO:HD2	1:A:277:TYR:CZ	2.47	0.50
1:B:166:LEU:O	1:B:167:ARG:C	2.50	0.50
1:B:441:PRO:C	1:B:443:PHE:H	2.14	0.50
1:A:68:THR:HG23	1:A:158:ARG:HE	1.77	0.50
1:B:356:ILE:HG13	1:B:358:VAL:HG23	1.94	0.50
1:A:414:PHE:O	1:A:438:TRP:HA	2.11	0.49
1:A:409:THR:CG2	1:A:411:GLN:HB2	2.42	0.49
1:A:409:THR:CG2	1:A:411:GLN:H	2.23	0.49
1:B:416:ILE:HD11	1:B:439:LYS:HB2	1.94	0.49
1:B:173:GLU:OE2	2:B:473:HOH:O	2.20	0.49
1:A:17:LEU:HD12	1:A:21:LYS:HD2	1.93	0.49
1:A:336:PHE:CE1	1:A:341:GLN:HB2	2.47	0.49
1:A:289:ASP:CG	1:A:297:ARG:NH1	2.66	0.49
1:B:289:ASP:HA	1:B:292:TRP:CZ2	2.48	0.49
1:A:8:ARG:HA	1:A:142:ILE:O	2.12	0.49
1:A:18:ALA:HB3	1:A:24:PHE:CE1	2.47	0.48
1:A:322:ILE:CD1	1:A:351:VAL:HG21	2.36	0.48
1:B:374:GLN:NE2	1:B:374:GLN:CA	2.75	0.48
1:A:25:ILE:HD12	1:A:26:LYS:N	2.28	0.48
1:B:279:TYR:CD1	1:B:417:LEU:HD11	2.47	0.48
1:B:325:ALA:HB2	1:B:355:LEU:HD21	1.96	0.48
1:B:336:PHE:CE1	1:B:341:GLN:HB2	2.48	0.48
1:B:26:LYS:O	1:B:30:ARG:HG3	2.12	0.48
1:A:151:GLU:O	1:A:152:GLU:C	2.52	0.48
1:A:406:ASN:ND2	1:A:409:THR:HB	2.29	0.48
1:B:219:ARG:HD3	1:B:235:PHE:O	2.13	0.48
1:A:146:VAL:HG11	1:A:161:LEU:HD12	1.95	0.48
1:A:272:VAL:HG22	1:A:273:VAL:H	1.79	0.47
1:A:73:CYS:HB2	1:A:152:GLU:O	2.13	0.47
1:B:277:TYR:CD2	1:B:277:TYR:C	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ILE:HG21	1:A:352:LEU:HD21	1.95	0.47
1:B:141:PRO:HD3	1:B:187:VAL:HG11	1.96	0.47
1:B:65:GLY:CA	1:B:158:ARG:NH1	2.64	0.47
1:A:363:LEU:HB3	1:A:452:LEU:HB2	1.96	0.47
1:B:178:ARG:HD3	1:B:179:TYR:CZ	2.49	0.47
1:B:141:PRO:HD3	1:B:187:VAL:CG1	2.44	0.47
1:A:453:CYS:C	1:A:454:LEU:HD12	2.35	0.47
1:B:255:ASN:N	1:B:256:PRO:HD3	2.29	0.47
1:A:376:ARG:HB2	1:A:405:TRP:CH2	2.49	0.47
1:A:318:THR:O	1:A:322:ILE:HG23	2.15	0.47
1:A:73:CYS:O	1:A:76:VAL:HG23	2.15	0.47
1:B:206:TYR:CE1	1:B:215:LEU:HD13	2.50	0.47
1:A:52:SER:C	1:A:79:PHE:CE2	2.89	0.46
1:A:219:ARG:NH1	1:A:461:LEU:C	2.68	0.46
1:A:76:VAL:O	1:A:78:ARG:N	2.48	0.46
1:B:336:PHE:O	1:B:339:SER:HB2	2.15	0.46
1:A:284:GLN:HB2	1:A:297:ARG:NH2	2.31	0.46
1:B:406:ASN:CG	1:B:409:THR:HG22	2.36	0.46
1:A:15:PHE:CG	1:A:32:VAL:HG21	2.50	0.46
1:A:389:VAL:HB	1:A:400:ILE:HG23	1.98	0.46
1:A:189:GLU:HB2	2:A:471:HOH:O	2.15	0.46
1:A:216:GLN:O	1:A:217:ALA:C	2.54	0.46
1:A:391:VAL:HG12	1:A:452:LEU:CD2	2.45	0.46
1:B:29:LEU:O	1:B:33:LEU:HB2	2.16	0.46
1:A:18:ALA:HB3	1:A:24:PHE:CD1	2.52	0.45
1:A:289:ASP:OD2	1:A:297:ARG:NH1	2.49	0.45
1:A:56:LEU:HG	2:A:489:HOH:O	2.16	0.45
1:A:449:TYR:HD1	1:A:449:TYR:C	2.19	0.45
1:A:3:ILE:HG22	1:A:148:VAL:O	2.17	0.45
1:B:67:LEU:H	1:B:67:LEU:CD2	2.29	0.45
1:B:220:LYS:O	1:B:223:HIS:HB2	2.17	0.45
1:A:169:LEU:HA	1:A:169:LEU:HD23	1.82	0.45
1:B:28:ALA:O	1:B:32:VAL:HG23	2.17	0.45
1:B:424:ALA:O	1:B:426:ASP:N	2.41	0.45
1:A:3:ILE:HG21	1:A:73:CYS:SG	2.56	0.45
1:A:449:TYR:O	1:A:449:TYR:CD1	2.69	0.45
1:B:14:ALA:HB2	1:B:137:ASN:HA	1.99	0.45
1:B:25:ILE:O	1:B:29:LEU:HB2	2.17	0.45
1:A:4:LEU:HD23	1:A:106:ILE:CD1	2.46	0.44
1:A:238:ILE:HG23	1:A:308:HIS:O	2.18	0.44
1:A:280:HIS:CE1	1:A:316:ILE:HD12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:SER:C	1:A:79:PHE:CD2	2.90	0.44
1:B:159:LYS:O	1:B:162:VAL:HG12	2.17	0.44
1:B:219:ARG:O	1:B:222:LEU:HB2	2.18	0.44
1:A:390:MET:HG3	1:A:453:CYS:HB3	1.98	0.44
1:B:238:ILE:CG1	1:B:238:ILE:O	2.62	0.44
1:B:445:ASN:ND2	1:B:445:ASN:C	2.71	0.44
1:B:135:TYR:N	1:B:135:TYR:CD1	2.84	0.44
1:B:326:LEU:O	1:B:329:ALA:N	2.50	0.44
1:A:389:VAL:HG13	1:A:453:CYS:O	2.18	0.43
1:A:160:LEU:HA	1:A:160:LEU:HD23	1.82	0.43
1:B:157:VAL:O	1:B:160:LEU:N	2.52	0.43
1:B:33:LEU:HA	1:B:33:LEU:HD13	1.78	0.43
1:A:156:LYS:O	1:A:160:LEU:HG	2.19	0.43
1:B:311:TYR:OH	1:B:457:ARG:HD3	2.19	0.43
1:A:5:PHE:HD1	1:A:109:ILE:HD11	1.84	0.43
1:A:390:MET:CE	1:A:397:ALA:HB1	2.48	0.43
1:A:40:LEU:HA	1:A:40:LEU:HD12	1.82	0.43
1:A:46:VAL:HG22	1:A:112:MET:CE	2.49	0.43
1:A:401:LEU:HB2	1:A:415:LEU:HD23	2.01	0.42
1:A:361:LYS:HE3	1:A:361:LYS:HB3	1.79	0.42
1:A:249:LYS:CD	1:A:249:LYS:H	2.31	0.42
1:A:289:ASP:CG	1:A:297:ARG:HH11	2.23	0.42
1:B:210:ILE:O	1:B:215:LEU:HD11	2.19	0.42
1:B:274:GLN:HB3	1:B:274:GLN:HE21	1.73	0.42
1:A:456:GLN:NE2	2:A:490:HOH:O	2.06	0.42
1:A:49:VAL:H	1:A:58:PRO:HD2	1.83	0.42
1:B:284:GLN:CB	1:B:297:ARG:NH2	2.83	0.42
1:A:375:GLY:CA	1:A:412:ILE:HD12	2.49	0.42
1:B:155:GLY:O	1:B:158:ARG:HG2	2.19	0.42
1:A:255:ASN:HD21	1:A:276:THR:HA	1.84	0.42
1:A:375:GLY:CA	1:A:412:ILE:CD1	2.98	0.42
1:A:49:VAL:HG12	1:A:49:VAL:O	2.20	0.42
1:B:54:VAL:CG1	1:B:55:TYR:N	2.82	0.42
1:B:293:GLY:HA2	1:B:296:TYR:CD2	2.55	0.42
1:A:79:PHE:CD1	1:A:80:ILE:N	2.88	0.42
1:B:445:ASN:HD22	1:B:446:LYS:N	2.17	0.42
1:B:454:LEU:HD12	1:B:454:LEU:N	2.34	0.42
1:A:368:GLY:HA3	1:A:446:LYS:HA	2.01	0.41
1:A:277:TYR:CD2	1:A:277:TYR:C	2.93	0.41
1:A:5:PHE:HB2	1:A:146:VAL:HG13	2.00	0.41
1:B:186:VAL:O	1:B:188:PRO:HD3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PHE:HB3	1:A:32:VAL:CG2	2.44	0.41
1:A:21:LYS:O	1:A:25:ILE:HG13	2.21	0.41
1:A:199:LYS:HD2	1:A:199:LYS:HA	1.75	0.41
1:B:318:THR:O	1:B:319:HIS:C	2.58	0.41
1:A:5:PHE:O	1:A:145:VAL:HA	2.21	0.41
1:A:395:VAL:O	1:A:395:VAL:CG1	2.67	0.41
1:A:399:THR:HB	1:A:417:LEU:HB3	2.03	0.41
1:B:445:ASN:HA	2:B:491:HOH:O	2.19	0.41
1:A:192:HIS:ND1	1:A:203:THR:OG1	2.48	0.41
1:A:299:LEU:CD2	1:A:352:LEU:CD1	2.91	0.41
1:A:49:VAL:O	1:A:50:CYS:C	2.59	0.41
1:B:332:LYS:HB3	1:B:333:PRO:HD2	2.02	0.41
1:A:344:GLY:H	1:A:347:GLU:CD	2.24	0.41
1:A:365:VAL:HG11	1:A:371:MET:SD	2.61	0.41
1:A:264:ASN:N	1:A:264:ASN:OD1	2.47	0.41
1:A:332:LYS:HG3	1:A:336:PHE:CD2	2.56	0.40
1:A:193:PHE:O	1:A:202:VAL:HG12	2.21	0.40
1:A:27:ASN:O	1:A:28:ALA:C	2.60	0.40
1:A:299:LEU:HD23	1:A:352:LEU:HD13	1.93	0.40
1:B:46:VAL:HG22	1:B:57:TRP:CZ3	2.56	0.40
1:A:404:ALA:HB3	1:A:413:LYS:HB3	2.03	0.40
1:B:360:SER:HB2	2:B:464:HOH:O	2.20	0.40
1:B:416:ILE:HD11	1:B:439:LYS:CD	2.47	0.40
1:A:16:GLN:HG2	1:A:135:TYR:HD1	1.84	0.40
1:A:395:VAL:O	1:A:395:VAL:HG13	2.21	0.40
1:A:416:ILE:HD12	1:A:416:ILE:C	2.41	0.40
1:B:243:PHE:HA	1:B:244:PRO:HD2	1.93	0.40
1:A:104:GLN:HG3	2:A:484:HOH:O	2.22	0.40
1:A:109:ILE:HD13	1:A:161:LEU:HD21	2.04	0.40
1:A:424:ALA:O	1:A:426:ASP:N	2.52	0.40

All (1) 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:181:LYS:O	2:B:463:HOH:O[2_556]	2.18	0.02



## 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	406/481 (84%)	352 (87%)	45 (11%)	9 (2%)	8	14
1	B	401/481 (83%)	346 (86%)	45 (11%)	10 (2%)	6	11
All	All	807/962 (84%)	698 (86%)	90 (11%)	19 (2%)	7	12

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	PRO
1	A	73	CYS
1	A	182	GLY
1	B	208	SER
1	B	212	ASP
1	B	425	GLU
1	A	2	ASP
1	A	78	ARG
1	A	264	ASN
1	B	196	PRO
1	B	198	LYS
1	B	314	ARG
1	A	217	ALA
1	B	442	ASP
1	A	154	TRP
1	B	22	GLU
1	B	334	ALA
1	B	335	THR
1	A	77	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/424 (86%)	291 (80%)	75 (20%)	1	2
1	B	360/424 (85%)	306 (85%)	54 (15%)	3	6
All	All	726/848 (86%)	597 (82%)	129 (18%)	2	3

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	7	ILE
1	A	16	GLN
1	A	17	LEU
1	A	30	ARG
1	A	33	LEU
1	A	36	LEU
1	A	39	LYS
1	A	40	LEU
1	A	41	SER
1	A	46	VAL
1	A	47	LEU
1	A	57	TRP
1	A	61	ASP
1	A	70	SER
1	A	74	LYS
1	A	76	VAL
1	A	78	ARG
1	A	80	ILE
1	A	113	LEU
1	A	116	SER
1	A	134	HIS
1	A	135	TYR
1	A	145	VAL
1	A	147	SER
1	A	151	GLU
1	A	161	LEU
1	A	178	ARG
1	A	180	MET
1	A	183	THR
1	A	186	VAL
1	A	199	LYS
1	A	201	LEU

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Mol	Chain	Res	Type
1	A	230	HIS
1	A	238	ILE
1	A	249	LYS
1	A	261	SER
1	A	264	ASN
1	A	266	GLU
1	A	273	VAL
1	A	276	THR
1	A	279	TYR
1	A	285	ASP
1	A	294	SER
1	A	297	ARG
1	A	299	LEU
1	A	304	SER
1	A	307	ARG
1	A	314	ARG
1	A	316	ILE
1	A	322	ILE
1	A	326	LEU
1	A	335	THR
1	A	343	ILE
1	A	345	SER
1	A	352	LEU
1	A	360	SER
1	A	361	LYS
1	A	363	LEU
1	A	383	GLN
1	A	384	ASN
1	A	385	VAL
1	A	390	MET
1	A	395	VAL
1	A	400	ILE
1	A	409	THR
1	A	413	LYS
1	A	426	ASP
1	A	431	LEU
1	A	439	LYS
1	A	446	LYS
1	A	449	TYR
1	A	452	LEU
1	A	459	ASN
1	A	461	LEU

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Mol	Chain	Res	Type
1	B	15	PHE
1	B	17	LEU
1	B	21	LYS
1	B	29	LEU
1	B	33	LEU
1	B	42	SER
1	B	46	VAL
1	B	52	SER
1	B	59	ASN
1	B	61	ASP
1	B	66	GLU
1	B	67	LEU
1	B	69	ASP
1	B	103	THR
1	B	112	MET
1	B	135	TYR
1	B	156	LYS
1	B	159	LYS
1	B	160	LEU
1	B	165	ILE
1	B	166	LEU
1	B	168	GLN
1	B	169	LEU
1	B	170	VAL
1	B	198	LYS
1	B	199	LYS
1	B	202	VAL
1	B	208	SER
1	B	210	ILE
1	B	219	ARG
1	B	225	LEU
1	B	238	ILE
1	B	266	GLU
1	B	274	GLN
1	B	276	THR
1	B	279	TYR
1	B	299	LEU
1	B	304	SER
1	B	312	THR
1	B	326	LEU
1	B	332	LYS
1	B	362	ILE

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Mol	Chain	Res	Type
1	B	365	VAL
1	B	367	GLN
1	B	390	MET
1	B	396	LEU
1	B	400	ILE
1	B	411	GLN
1	B	416	ILE
1	B	422	THR
1	B	431	LEU
1	B	439	LYS
1	B	445	ASN
1	B	459	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	59	ASN
1	A	105	GLN
1	A	108	ASN
1	A	200	ASN
1	A	214	GLN
1	A	284	GLN
1	A	383	GLN
1	A	445	ASN
1	B	31	GLN
1	B	104	GLN
1	B	194	GLN
1	B	200	ASN
1	B	274	GLN
1	B	280	HIS
1	B	284	GLN
1	B	354	GLN
1	B	367	GLN
1	B	374	GLN
1	B	383	GLN
1	B	445	ASN
1	B	459	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	416/481 (86%)	-0.29	9 (2%) 62 56	5, 36, 81, 119	0
1	B	411/481 (85%)	-0.24	9 (2%) 62 56	5, 40, 83, 118	0
All	All	827/962 (85%)	-0.26	18 (2%) 62 56	5, 38, 82, 119	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	THR	5.8
1	A	263	PRO	5.5
1	B	135	TYR	4.7
1	A	59	ASN	4.1
1	B	115	ILE	4.0
1	A	67	LEU	3.3
1	A	103	THR	2.9
1	B	186	VAL	2.5
1	B	209	GLY	2.4
1	A	431	LEU	2.3
1	B	212	ASP	2.3
1	A	260	LEU	2.3
1	B	211	PRO	2.3
1	B	208	SER	2.2
1	B	116	SER	2.2
1	B	287	ILE	2.1
1	A	268	SER	2.0
1	A	115	ILE	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.