



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 11:24 AM EDT

PDB ID : 2R62  
Title : Crystal structure of Helicobacter pylori ATP dependent protease, FtsH  
Authors : Kim, S.H.; Kang, G.B.; Song, H.-E.; Park, S.J.; Bae, M.-H.; Eom, S.H.  
Deposited on : 2007-09-05  
Resolution : 3.30 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 : 2.23.2  
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) : 2.23.2

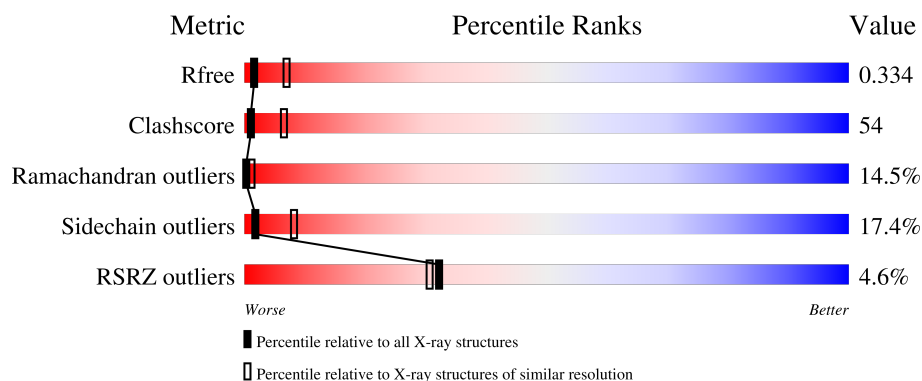
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	268	<div> <div>5%</div> <div>25%</div> <div>47%</div> <div>18%</div> <div>• 7%</div> </div>
1	B	268	<div> <div>3%</div> <div>21%</div> <div>52%</div> <div>17%</div> <div>• 7%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3802 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 Cell division protease ftsH homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1901	1203	336	357	5			
1	B	249	Total	C	N	O	S	0	0	0
			1901	1203	336	357	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	LYS	ASN	engineered mutation	UNP P71408
A	420	LEU	-	expression tag	UNP P71408
A	421	GLU	-	expression tag	UNP P71408
A	422	HIS	-	expression tag	UNP P71408
A	423	HIS	-	expression tag	UNP P71408
A	424	HIS	-	expression tag	UNP P71408
A	425	HIS	-	expression tag	UNP P71408
A	426	HIS	-	expression tag	UNP P71408
A	427	HIS	-	expression tag	UNP P71408
B	170	LYS	ASN	engineered mutation	UNP P71408
B	420	LEU	-	expression tag	UNP P71408
B	421	GLU	-	expression tag	UNP P71408
B	422	HIS	-	expression tag	UNP P71408
B	423	HIS	-	expression tag	UNP P71408
B	424	HIS	-	expression tag	UNP P71408
B	425	HIS	-	expression tag	UNP P71408
B	426	HIS	-	expression tag	UNP P71408
B	427	HIS	-	expression tag	UNP P71408



K418
LYS
LEU
GLU
HIS
HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.22Å 141.22Å 54.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.30 49.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-3.30) 98.4 (49.90-3.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.39 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.280 , 0.336 0.279 , 0.334	Depositor DCC
$R_{free}$ test set	500 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	118.0	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 261.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3802	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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

### 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	1.00	11/1927 (0.6%)	0.89	3/2597 (0.1%)
1	B	0.99	13/1927 (0.7%)	0.91	5/2597 (0.2%)
All	All	0.99	24/3854 (0.6%)	0.90	8/5194 (0.2%)

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	B	0	2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	GLU	CD-OE2	14.05	1.41	1.25
1	B	306	SER	C-N	13.15	1.64	1.34
1	A	367	GLN	CD-OE1	12.04	1.50	1.24
1	A	335	ARG	CZ-NH1	11.99	1.48	1.33
1	A	289	GLU	CG-CD	9.92	1.66	1.51
1	B	181	GLU	CD-OE1	9.12	1.35	1.25
1	B	368	GLU	CD-OE1	7.39	1.33	1.25
1	A	161	ASN	CG-OD1	7.37	1.40	1.24
1	B	287	ASN	CG-OD1	7.28	1.40	1.24
1	B	305	GLY	C-O	6.82	1.34	1.23
1	B	307	GLU	CD-OE1	6.56	1.32	1.25
1	B	250	ARG	CZ-NH1	6.17	1.41	1.33
1	A	161	ASN	CG-ND2	6.14	1.48	1.32
1	B	181	GLU	CD-OE2	6.05	1.32	1.25
1	B	417	GLU	CD-OE2	5.75	1.31	1.25
1	B	304	PHE	C-N	5.73	1.43	1.33
1	B	304	PHE	C-O	5.73	1.34	1.23
1	A	371	LYS	CE-NZ	5.54	1.62	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	SER	CB-OG	5.54	1.49	1.42
1	A	335	ARG	CZ-NH2	5.46	1.40	1.33
1	A	256	GLU	CD-OE1	5.18	1.31	1.25
1	B	306	SER	CA-CB	5.14	1.60	1.52
1	A	252	ARG	CZ-NH1	5.05	1.39	1.33
1	A	184	GLU	CD-OE1	5.04	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ARG	NE-CZ-NH2	-12.25	114.18	120.30
1	A	335	ARG	NE-CZ-NH2	-11.08	114.76	120.30
1	B	306	SER	O-C-N	-6.25	112.69	122.70
1	B	194	ARG	N-CA-C	-5.96	94.91	111.00
1	B	376	LEU	CA-CB-CG	5.89	128.86	115.30
1	A	335	ARG	NH1-CZ-NH2	5.37	125.30	119.40
1	B	306	SER	C-N-CA	-5.35	108.33	121.70
1	B	306	SER	CA-C-O	5.31	131.25	120.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239	PHE	Mainchain
1	B	306	SER	Mainchain

## 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	1901	0	1948	206	0
1	B	1901	0	1948	213	1
All	All	3802	0	3896	413	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 54.



All (413) 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:189:LEU:HD23	1:B:263:PRO:HB2	1.24	1.16
1:B:347:ARG:HH12	1:B:374:ALA:HA	1.07	1.14
1:A:211:PRO:HB2	1:A:212:PRO:CD	1.82	1.09
1:A:211:PRO:HB2	1:A:212:PRO:HD3	1.15	1.08
1:B:355:ILE:HG23	1:B:358:VAL:HG22	1.33	1.07
1:B:185:ILE:HD13	1:B:312:ILE:HG21	1.38	1.05
1:B:175:ASN:HD21	1:B:178:ALA:HB3	1.17	1.04
1:A:202:ILE:HG12	1:A:202:ILE:O	1.60	0.99
1:B:351:LEU:HD11	1:B:366:LEU:HG	1.45	0.99
1:B:347:ARG:NH1	1:B:374:ALA:HA	1.78	0.99
1:A:216:LYS:HD2	1:A:217:THR:H	1.26	0.98
1:B:327:LEU:O	1:B:333:PHE:HB2	1.66	0.95
1:B:355:ILE:HG23	1:B:358:VAL:CG2	1.96	0.94
1:B:175:ASN:HD21	1:B:178:ALA:CB	1.80	0.93
1:A:236:GLY:H	1:A:269:ASP:H	1.16	0.92
1:B:325:PRO:HA	1:B:328:MET:HG3	1.51	0.92
1:B:359:LYS:HG2	1:B:399:GLU:HA	1.52	0.92
1:B:205:GLY:HA3	1:B:333:PHE:H	1.34	0.91
1:A:347:ARG:HB2	1:A:381:LEU:HD11	1.51	0.91
1:B:175:ASN:ND2	1:B:178:ALA:HB3	1.85	0.90
1:B:403:GLN:OE1	1:B:403:GLN:HA	1.73	0.89
1:B:271:ILE:HG13	1:B:315:ALA:HB1	1.53	0.88
1:B:189:LEU:CD2	1:B:263:PRO:HB2	2.04	0.87
1:A:256:GLU:O	1:A:260:LYS:HG2	1.76	0.85
1:A:263:PRO:HB3	1:A:310:PRO:HB2	1.58	0.85
1:B:189:LEU:HD23	1:B:263:PRO:CB	2.07	0.85
1:B:263:PRO:HA	1:B:310:PRO:O	1.77	0.85
1:B:347:ARG:HH12	1:B:374:ALA:CA	1.89	0.82
1:B:359:LYS:CB	1:B:400:VAL:H	1.92	0.82
1:A:369:VAL:HG21	1:A:405:LEU:HB3	1.63	0.81
1:B:188:PHE:CD2	1:B:203:PRO:HG3	2.16	0.81
1:A:361:ALA:HA	1:A:399:GLU:HB3	1.63	0.81
1:B:168:ARG:C	1:B:170:LYS:H	1.85	0.80
1:B:376:LEU:HB3	1:B:380:ASP:HB3	1.65	0.79
1:B:209:VAL:HG12	1:B:337:VAL:O	1.83	0.79
1:B:359:LYS:HB2	1:B:400:VAL:HG23	1.66	0.78
1:A:300:GLU:OE2	1:A:304:PHE:HB3	1.82	0.77
1:B:355:ILE:HG22	1:B:355:ILE:O	1.85	0.77
1:B:401:ARG:H	1:B:404:HIS:CE1	2.03	0.76
1:A:410:GLU:HG2	1:A:411:ARG:HG2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:MET:SD	1:B:254:LEU:HD22	2.25	0.76
1:A:236:GLY:H	1:A:269:ASP:N	1.83	0.76
1:B:408:ALA:HA	1:B:411:ARG:HB2	1.69	0.75
1:A:236:GLY:N	1:A:269:ASP:H	1.84	0.75
1:A:233:SER:HB3	1:A:267:PHE:H	1.51	0.74
1:A:201:LYS:HG3	1:A:203:PRO:HD3	1.67	0.74
1:B:319:ARG:HD3	1:B:322:ILE:HD11	1.68	0.74
1:B:376:LEU:HB3	1:B:380:ASP:CB	2.16	0.74
1:B:173:ALA:HB2	1:B:344:PHE:HD2	1.53	0.74
1:B:306:SER:O	1:B:308:ASN:N	2.20	0.74
1:B:359:LYS:HB2	1:B:400:VAL:H	1.51	0.73
1:B:167:VAL:O	1:B:168:ARG:HG2	1.88	0.73
1:B:205:GLY:HA3	1:B:333:PHE:N	2.04	0.73
1:A:343:ASP:HB2	1:A:345:ASN:OD1	1.89	0.72
1:A:214:THR:H	1:A:216:LYS:HE3	1.53	0.72
1:A:180:GLU:O	1:A:183:VAL:HB	1.90	0.72
1:A:181:GLU:O	1:A:184:GLU:HG2	1.89	0.72
1:B:362:ASN:HB2	1:B:401:ARG:HA	1.71	0.72
1:B:342:PRO:HB2	1:B:347:ARG:HG2	1.69	0.72
1:A:168:ARG:NH1	1:B:166:ASN:OD1	2.23	0.71
1:A:407:GLU:O	1:A:409:VAL:N	2.21	0.71
1:B:194:ARG:O	1:B:194:ARG:HG2	1.90	0.70
1:A:176:GLU:HG3	1:A:179:LYS:HD2	1.73	0.70
1:B:365:ASN:HD22	1:B:368:GLU:HG2	1.55	0.70
1:B:179:LYS:O	1:B:183:VAL:HG12	1.91	0.70
1:B:350:ILE:O	1:B:353:VAL:HG23	1.92	0.69
1:B:351:LEU:HD13	1:B:385:ILE:HD11	1.75	0.69
1:A:207:LEU:HD12	1:A:333:PHE:HB3	1.75	0.69
1:B:351:LEU:C	1:B:351:LEU:HD12	2.13	0.69
1:B:165:PRO:HB3	1:B:221:LYS:HB3	1.74	0.68
1:B:411:ARG:HB3	1:B:411:ARG:NH1	2.08	0.68
1:B:176:GLU:O	1:B:180:GLU:HB2	1.92	0.68
1:B:358:VAL:HG23	1:B:360:LEU:H	1.58	0.68
1:A:179:LYS:O	1:A:183:VAL:N	2.25	0.68
1:A:189:LEU:HD23	1:A:263:PRO:HB2	1.75	0.68
1:A:293:THR:HA	1:A:296:GLN:HE21	1.60	0.67
1:A:182:VAL:CG1	1:A:223:VAL:HG22	2.24	0.67
1:B:366:LEU:H	1:B:366:LEU:HD22	1.59	0.67
1:B:364:VAL:HA	1:B:402:GLN:HG3	1.77	0.67
1:B:359:LYS:HB3	1:B:400:VAL:H	1.60	0.66
1:A:189:LEU:CD2	1:A:263:PRO:HB2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:PRO:O	1:B:194:ARG:N	2.29	0.66
1:A:188:PHE:HA	1:A:195:TYR:CE1	2.30	0.66
1:A:371:LYS:C	1:A:373:THR:H	1.99	0.66
1:B:175:ASN:O	1:B:179:LYS:HD3	1.96	0.66
1:B:380:ASP:O	1:B:384:ILE:HG12	1.95	0.66
1:B:365:ASN:ND2	1:B:368:GLU:HG2	2.09	0.66
1:A:233:SER:HB2	1:A:267:PHE:O	1.95	0.65
1:B:272:ASP:OD1	1:B:319:ARG:HG3	1.96	0.65
1:B:185:ILE:CD1	1:B:312:ILE:HG21	2.22	0.65
1:B:188:PHE:CE2	1:B:203:PRO:HG3	2.31	0.65
1:A:169:PHE:HE1	1:A:183:VAL:HG22	1.62	0.65
1:A:201:LYS:NZ	1:A:202:ILE:H	1.94	0.65
1:B:230:PRO:HD2	1:B:264:SER:HB3	1.79	0.65
1:B:336:GLN:O	1:B:336:GLN:HG3	1.97	0.64
1:B:168:ARG:O	1:B:170:LYS:N	2.30	0.64
1:A:186:VAL:HG22	1:A:223:VAL:HG13	1.80	0.64
1:B:185:ILE:HD11	1:B:206:VAL:HG21	1.78	0.64
1:A:354:HIS:HB2	1:A:385:ILE:HD13	1.79	0.64
1:A:216:LYS:HD2	1:A:217:THR:N	2.07	0.63
1:A:214:THR:N	1:A:216:LYS:HE3	2.11	0.63
1:B:385:ILE:O	1:B:388:ALA:HB3	1.98	0.63
1:A:402:GLN:HE21	1:A:402:GLN:HA	1.63	0.63
1:B:232:PHE:O	1:B:233:SER:HB2	1.97	0.63
1:A:386:ASN:O	1:A:389:ALA:HB3	1.98	0.63
1:A:188:PHE:HA	1:A:195:TYR:HE1	1.64	0.62
1:A:235:GLY:HA2	1:A:269:ASP:H	1.65	0.62
1:A:266:ILE:O	1:A:313:VAL:HA	1.99	0.62
1:B:347:ARG:C	1:B:349:GLU:H	2.01	0.62
1:B:411:ARG:HB3	1:B:411:ARG:CZ	2.29	0.62
1:A:201:LYS:CE	1:A:202:ILE:H	2.12	0.62
1:A:380:ASP:OD2	1:A:380:ASP:N	2.32	0.62
1:B:214:THR:HG21	1:B:339:VAL:HB	1.81	0.62
1:A:222:ALA:O	1:A:226:GLU:HB2	2.00	0.61
1:A:227:ALA:HB3	1:A:229:VAL:HG22	1.82	0.61
1:B:359:LYS:CG	1:B:399:GLU:HA	2.30	0.61
1:B:239:PHE:O	1:B:239:PHE:CD2	2.53	0.61
1:A:313:VAL:O	1:A:314:LEU:HD12	2.00	0.61
1:A:168:ARG:O	1:A:171:ASP:HB3	2.01	0.61
1:A:377:ALA:HB3	1:A:380:ASP:OD2	1.99	0.61
1:A:401:ARG:O	1:A:404:HIS:HB2	2.01	0.61
1:B:192:PRO:O	1:B:193:GLU:C	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:C	1:A:408:ALA:H	2.04	0.61
1:B:209:VAL:HG21	1:B:320:PRO:HG3	1.81	0.61
1:B:293:THR:O	1:B:296:GLN:HB3	2.00	0.61
1:B:230:PRO:HB2	1:B:232:PHE:CE1	2.36	0.61
1:B:383:ASN:O	1:B:384:ILE:C	2.39	0.61
1:A:366:LEU:HA	1:A:369:VAL:HG12	1.83	0.60
1:B:168:ARG:C	1:B:170:LYS:N	2.49	0.60
1:B:192:PRO:C	1:B:194:ARG:N	2.54	0.60
1:B:267:PHE:HE2	1:B:269:ASP:OD1	1.84	0.60
1:A:182:VAL:CG1	1:A:223:VAL:CG2	2.78	0.60
1:A:347:ARG:HD2	1:A:370:ALA:O	2.02	0.60
1:A:330:PRO:HA	1:A:334:ASP:OD1	2.02	0.60
1:B:209:VAL:CG2	1:B:320:PRO:HG3	2.32	0.60
1:A:183:VAL:O	1:A:186:VAL:HG23	2.02	0.60
1:A:210:GLY:O	1:A:318:ASN:HA	2.01	0.59
1:A:185:ILE:HD11	1:A:206:VAL:HG21	1.84	0.59
1:A:409:VAL:HG12	1:A:409:VAL:O	2.03	0.59
1:B:306:SER:O	1:B:307:GLU:C	2.41	0.59
1:B:169:PHE:O	1:B:179:LYS:HE2	2.02	0.59
1:A:211:PRO:CB	1:A:212:PRO:CD	2.68	0.59
1:A:165:PRO:HB2	1:A:167:VAL:HG23	1.83	0.59
1:A:360:LEU:HB3	1:A:364:VAL:HG21	1.83	0.59
1:B:165:PRO:HG3	1:B:231:PHE:HB2	1.84	0.59
1:A:324:ASP:OD1	1:A:326:ALA:N	2.36	0.59
1:B:404:HIS:O	1:B:407:GLU:HB2	2.03	0.59
1:A:343:ASP:C	1:A:345:ASN:H	2.06	0.58
1:B:276:LYS:HD2	1:B:290:ARG:HH22	1.68	0.58
1:B:179:LYS:CB	1:B:179:LYS:NZ	2.67	0.58
1:B:208:LEU:O	1:B:316:ALA:HA	2.03	0.58
1:A:238:SER:HA	1:A:241:GLU:HB3	1.85	0.58
1:B:408:ALA:CA	1:B:411:ARG:HB2	2.33	0.58
1:A:239:PHE:CE1	1:A:251:VAL:HG21	2.39	0.58
1:A:275:GLY:HA2	1:A:294:LEU:HB2	1.85	0.57
1:A:302:ASP:OD1	1:A:302:ASP:N	2.36	0.57
1:B:401:ARG:HG3	1:B:404:HIS:CE1	2.39	0.57
1:A:351:LEU:HB3	1:A:366:LEU:HD12	1.86	0.57
1:B:189:LEU:O	1:B:263:PRO:HG3	2.05	0.57
1:A:239:PHE:HE1	1:A:251:VAL:HG21	1.68	0.57
1:A:347:ARG:HB2	1:A:381:LEU:CD1	2.28	0.57
1:A:300:GLU:OE2	1:A:304:PHE:CB	2.52	0.57
1:B:289:GLU:O	1:B:290:ARG:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:PRO:CD	1:B:231:PHE:HB2	2.35	0.57
1:A:250:ARG:O	1:A:254:LEU:HB2	2.05	0.56
1:A:344:PHE:HA	1:A:347:ARG:HE	1.69	0.56
1:A:168:ARG:HB2	1:A:171:ASP:HB3	1.87	0.56
1:A:266:ILE:HD12	1:A:266:ILE:H	1.70	0.56
1:B:165:PRO:CG	1:B:231:PHE:HB2	2.35	0.56
1:B:409:VAL:O	1:B:413:ILE:HG12	2.06	0.56
1:A:409:VAL:O	1:A:411:ARG:N	2.38	0.56
1:B:262:ALA:HB1	1:B:310:PRO:O	2.05	0.56
1:B:213:GLY:O	1:B:215:GLY:N	2.32	0.56
1:B:347:ARG:O	1:B:350:ILE:N	2.38	0.56
1:A:235:GLY:HA2	1:A:269:ASP:N	2.20	0.56
1:A:168:ARG:O	1:A:169:PHE:C	2.42	0.56
1:A:169:PHE:HB3	1:A:179:LYS:HD3	1.88	0.56
1:B:383:ASN:O	1:B:386:ASN:N	2.39	0.56
1:A:413:ILE:HG12	1:A:413:ILE:O	2.06	0.55
1:A:201:LYS:HZ3	1:A:202:ILE:H	1.55	0.55
1:A:403:GLN:HA	1:A:406:LYS:HB2	1.89	0.55
1:B:347:ARG:NH1	1:B:373:THR:O	2.39	0.55
1:A:344:PHE:HA	1:A:347:ARG:NE	2.20	0.55
1:B:191:TYR:O	1:B:194:ARG:HB3	2.07	0.55
1:B:401:ARG:H	1:B:404:HIS:HE1	1.52	0.55
1:A:267:PHE:HD1	1:A:314:LEU:O	1.89	0.55
1:A:215:GLY:H	1:A:216:LYS:HE3	1.70	0.55
1:B:376:LEU:HD12	1:B:381:LEU:HD23	1.88	0.55
1:B:271:ILE:HG13	1:B:315:ALA:CB	2.33	0.55
1:A:270:GLU:O	1:A:271:ILE:C	2.45	0.54
1:A:387:GLU:O	1:A:390:LEU:N	2.40	0.54
1:B:179:LYS:HZ2	1:B:179:LYS:HB2	1.73	0.54
1:A:297:LEU:HD12	1:A:301:MET:SD	2.47	0.54
1:B:267:PHE:CE2	1:B:269:ASP:OD1	2.61	0.54
1:A:179:LYS:O	1:A:183:VAL:HG23	2.07	0.54
1:B:216:LYS:HG2	1:B:339:VAL:HG21	1.89	0.54
1:A:256:GLU:HG2	1:A:260:LYS:HE2	1.90	0.54
1:A:369:VAL:HA	1:A:373:THR:HG21	1.90	0.54
1:B:336:GLN:O	1:B:336:GLN:CG	2.55	0.54
1:A:204:LYS:HD2	1:A:331:GLY:C	2.29	0.53
1:A:405:LEU:O	1:A:408:ALA:HB2	2.08	0.53
1:B:351:LEU:HB2	1:B:385:ILE:HD11	1.90	0.53
1:B:354:HIS:CD2	1:B:382:ALA:HA	2.43	0.53
1:A:216:LYS:CD	1:A:217:THR:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ILE:O	1:A:353:VAL:HB	2.08	0.53
1:B:210:GLY:O	1:B:318:ASN:HA	2.09	0.53
1:B:375:GLY:O	1:B:376:LEU:HD23	2.09	0.53
1:A:169:PHE:CE1	1:A:183:VAL:HG22	2.43	0.53
1:B:166:ASN:O	1:B:166:ASN:CG	2.46	0.53
1:B:207:LEU:HD21	1:B:317:THR:OG1	2.08	0.53
1:A:207:LEU:HD23	1:A:315:ALA:O	2.08	0.53
1:B:202:ILE:N	1:B:203:PRO:CD	2.71	0.53
1:B:169:PHE:HE2	1:B:170:LYS:HZ2	1.55	0.53
1:A:195:TYR:C	1:A:197:ASN:H	2.13	0.52
1:B:257:THR:HG22	1:B:261:GLN:HE21	1.74	0.52
1:A:369:VAL:CG2	1:A:405:LEU:HB3	2.36	0.52
1:A:230:PRO:HB2	1:A:232:PHE:CE1	2.45	0.52
1:B:227:ALA:O	1:B:228:HIS:HB2	2.09	0.52
1:A:178:ALA:HA	1:A:181:GLU:HG2	1.91	0.52
1:A:271:ILE:O	1:A:274:ILE:HG12	2.10	0.52
1:A:276:LYS:HE2	1:A:290:ARG:HA	1.91	0.52
1:A:407:GLU:C	1:A:409:VAL:H	2.11	0.52
1:B:347:ARG:CZ	1:B:374:ALA:HA	2.39	0.52
1:A:403:GLN:O	1:A:406:LYS:HB3	2.09	0.52
1:B:192:PRO:C	1:B:194:ARG:H	2.13	0.52
1:B:262:ALA:HB3	1:B:309:ALA:HB1	1.91	0.51
1:A:235:GLY:CA	1:A:269:ASP:H	2.22	0.51
1:B:410:GLU:O	1:B:413:ILE:HB	2.09	0.51
1:A:293:THR:HA	1:A:296:GLN:HG3	1.91	0.51
1:B:173:ALA:HB2	1:B:344:PHE:CD2	2.41	0.51
1:A:190:LYS:HG3	1:A:191:TYR:CE1	2.46	0.51
1:B:355:ILE:O	1:B:355:ILE:CG2	2.56	0.51
1:B:296:GLN:O	1:B:298:LEU:N	2.44	0.51
1:B:204:LYS:HD2	1:B:331:GLY:O	2.12	0.50
1:B:216:LYS:O	1:B:219:LEU:HB3	2.12	0.50
1:B:298:LEU:O	1:B:301:MET:HB2	2.12	0.50
1:A:193:GLU:O	1:A:194:ARG:C	2.49	0.50
1:A:199:GLY:O	1:A:200:ALA:HB2	2.11	0.50
1:A:357:GLY:O	1:A:358:VAL:C	2.50	0.50
1:A:366:LEU:O	1:A:370:ALA:N	2.45	0.50
1:A:259:LYS:NZ	1:A:305:GLY:HA3	2.27	0.50
1:A:369:VAL:HG22	1:A:369:VAL:O	2.11	0.50
1:B:167:VAL:HG12	1:B:168:ARG:H	1.77	0.50
1:B:405:LEU:O	1:B:406:LYS:C	2.49	0.50
1:A:185:ILE:HA	1:A:188:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:MET:HA	1:B:333:PHE:O	2.12	0.49
1:A:176:GLU:O	1:A:177:GLU:HB3	2.12	0.49
1:A:240:ILE:HD11	1:A:273:ALA:HA	1.94	0.49
1:A:271:ILE:O	1:A:272:ASP:C	2.51	0.49
1:A:385:ILE:HG22	1:A:386:ASN:N	2.27	0.49
1:B:257:THR:HG22	1:B:261:GLN:NE2	2.28	0.49
1:A:176:GLU:OE1	1:A:179:LYS:NZ	2.45	0.49
1:B:376:LEU:HD13	1:B:380:ASP:HB3	1.95	0.49
1:B:186:VAL:O	1:B:189:LEU:N	2.46	0.49
1:B:229:VAL:HB	1:B:264:SER:HA	1.95	0.48
1:B:276:LYS:HD2	1:B:290:ARG:NH2	2.28	0.48
1:A:291:GLU:H	1:A:291:GLU:CD	2.16	0.48
1:B:376:LEU:HD12	1:B:381:LEU:CD2	2.44	0.48
1:B:379:ALA:O	1:B:382:ALA:N	2.46	0.48
1:B:369:VAL:O	1:B:372:LEU:N	2.47	0.48
1:A:405:LEU:HD22	1:A:405:LEU:H	1.78	0.48
1:A:182:VAL:HG13	1:A:223:VAL:HG21	1.96	0.48
1:B:169:PHE:CD2	1:B:170:LYS:HG3	2.49	0.48
1:A:169:PHE:C	1:A:179:LYS:HZ3	2.17	0.48
1:B:298:LEU:O	1:B:302:ASP:OD2	2.32	0.48
1:A:211:PRO:CB	1:A:212:PRO:HD3	2.11	0.47
1:B:391:LEU:C	1:B:393:GLY:H	2.16	0.47
1:A:300:GLU:C	1:A:302:ASP:H	2.16	0.47
1:A:313:VAL:CG1	1:A:314:LEU:N	2.76	0.47
1:A:388:ALA:CB	1:A:405:LEU:HD13	2.45	0.47
1:B:242:MET:SD	1:B:242:MET:N	2.87	0.47
1:B:366:LEU:HA	1:B:369:VAL:HG23	1.97	0.47
1:A:207:LEU:O	1:A:208:LEU:C	2.53	0.47
1:A:221:LYS:HA	1:A:231:PHE:CE1	2.50	0.47
1:A:202:ILE:O	1:A:202:ILE:CG1	2.40	0.47
1:A:366:LEU:HA	1:A:369:VAL:CG1	2.45	0.47
1:B:161:ASN:O	1:B:232:PHE:HA	2.15	0.47
1:B:167:VAL:C	1:B:168:ARG:HG2	2.34	0.47
1:B:218:LEU:O	1:B:221:LYS:N	2.47	0.47
1:B:389:ALA:O	1:B:392:ALA:N	2.48	0.47
1:A:185:ILE:HG22	1:A:185:ILE:O	2.14	0.47
1:A:232:PHE:O	1:A:233:SER:CB	2.63	0.47
1:B:197:ASN:N	1:B:197:ASN:HD22	2.13	0.47
1:A:356:LYS:HE2	1:B:190:LYS:HZ3	1.80	0.46
1:B:230:PRO:HG2	1:B:264:SER:HB3	1.98	0.46
1:A:267:PHE:CD1	1:A:314:LEU:O	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLY:O	1:A:200:ALA:CB	2.64	0.46
1:B:262:ALA:HA	1:B:263:PRO:C	2.36	0.46
1:B:405:LEU:O	1:B:407:GLU:N	2.48	0.46
1:A:403:GLN:H	1:A:403:GLN:CD	2.19	0.46
1:B:266:ILE:HB	1:B:313:VAL:HB	1.98	0.46
1:A:235:GLY:HA3	1:A:269:ASP:HB2	1.98	0.46
1:B:348:VAL:HG12	1:B:348:VAL:O	2.15	0.46
1:A:164:LYS:HD3	1:B:166:ASN:ND2	2.31	0.46
1:A:297:LEU:HD23	1:A:297:LEU:H	1.81	0.46
1:B:173:ALA:HB3	1:B:343:ASP:HA	1.98	0.46
1:B:213:GLY:C	1:B:215:GLY:H	2.16	0.46
1:A:257:THR:HG22	1:A:261:GLN:OE1	2.16	0.45
1:B:362:ASN:CG	1:B:402:GLN:H	2.20	0.45
1:B:232:PHE:HB3	1:B:254:LEU:HD11	1.98	0.45
1:B:221:LYS:HG2	1:B:231:PHE:CZ	2.51	0.45
1:A:321:GLU:O	1:A:323:LEU:N	2.39	0.45
1:B:347:ARG:O	1:B:349:GLU:N	2.45	0.45
1:B:353:VAL:O	1:B:355:ILE:N	2.50	0.45
1:A:403:GLN:HA	1:A:406:LYS:CB	2.47	0.45
1:B:197:ASN:HD22	1:B:197:ASN:H	1.65	0.45
1:A:181:GLU:O	1:A:182:VAL:C	2.56	0.45
1:A:261:GLN:O	1:A:264:SER:OG	2.35	0.45
1:A:383:ASN:O	1:A:384:ILE:C	2.54	0.45
1:B:175:ASN:ND2	1:B:178:ALA:CB	2.60	0.45
1:B:209:VAL:CG1	1:B:338:LEU:HA	2.47	0.45
1:B:265:ILE:CG2	1:B:266:ILE:N	2.80	0.45
1:A:351:LEU:HD23	1:A:385:ILE:CD1	2.47	0.44
1:B:343:ASP:O	1:B:345:ASN:N	2.49	0.44
1:B:369:VAL:CG1	1:B:409:VAL:HG21	2.47	0.44
1:A:296:GLN:O	1:A:298:LEU:N	2.50	0.44
1:A:351:LEU:HD23	1:A:385:ILE:HD11	1.99	0.44
1:A:243:PHE:CD1	1:A:244:VAL:HG22	2.52	0.44
1:A:348:VAL:H	1:A:348:VAL:HG23	1.43	0.44
1:A:356:LYS:HE2	1:B:191:TYR:OH	2.17	0.44
1:B:351:LEU:C	1:B:351:LEU:CD1	2.85	0.44
1:A:294:LEU:O	1:A:298:LEU:CD1	2.65	0.44
1:A:347:ARG:NH2	1:A:374:ALA:HB1	2.32	0.44
1:B:383:ASN:N	1:B:383:ASN:HD22	2.15	0.44
1:A:267:PHE:HA	1:A:314:LEU:O	2.17	0.44
1:A:205:GLY:HA2	1:A:313:VAL:O	2.17	0.44
1:A:201:LYS:HG3	1:A:202:ILE:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LYS:HG3	1:A:202:ILE:N	2.33	0.44
1:B:302:ASP:OD2	1:B:302:ASP:N	2.50	0.44
1:A:371:LYS:C	1:A:373:THR:N	2.68	0.44
1:B:224:ALA:HB2	1:B:265:ILE:HD13	2.00	0.44
1:B:311:VAL:O	1:B:312:ILE:C	2.55	0.44
1:B:321:GLU:HG3	1:B:322:ILE:H	1.83	0.44
1:B:402:GLN:C	1:B:404:HIS:H	2.21	0.44
1:B:312:ILE:H	1:B:312:ILE:HG12	1.56	0.43
1:B:176:GLU:HA	1:B:179:LYS:HZ2	1.82	0.43
1:B:183:VAL:O	1:B:186:VAL:N	2.51	0.43
1:B:179:LYS:NZ	1:B:179:LYS:HB3	2.32	0.43
1:B:216:LYS:O	1:B:219:LEU:N	2.50	0.43
1:A:200:ALA:O	1:A:201:LYS:HB2	2.18	0.43
1:A:219:LEU:HA	1:A:222:ALA:HB3	2.00	0.43
1:A:258:ALA:O	1:A:262:ALA:HB2	2.18	0.43
1:A:269:ASP:O	1:A:270:GLU:C	2.56	0.43
1:A:289:GLU:HB3	1:A:290:ARG:NH2	2.34	0.43
1:A:402:GLN:HA	1:A:405:LEU:HD23	2.01	0.43
1:B:326:ALA:HA	1:B:329:ARG:HB2	1.99	0.43
1:B:165:PRO:CD	1:B:231:PHE:CB	2.97	0.43
1:A:208:LEU:O	1:A:316:ALA:HA	2.18	0.43
1:A:275:GLY:CA	1:A:294:LEU:HB2	2.49	0.43
1:B:205:GLY:HA3	1:B:333:PHE:CA	2.48	0.43
1:A:218:LEU:O	1:A:221:LYS:N	2.51	0.43
1:A:381:LEU:O	1:A:382:ALA:C	2.57	0.43
1:B:198:LEU:O	1:B:199:GLY:C	2.57	0.43
1:B:300:GLU:HA	1:B:304:PHE:HD1	1.83	0.43
1:A:213:GLY:HA2	1:A:216:LYS:CE	2.49	0.43
1:A:260:LYS:HB2	1:A:261:GLN:H	1.64	0.43
1:A:160:ILE:O	1:A:161:ASN:HB3	2.19	0.43
1:A:201:LYS:HE2	1:A:202:ILE:H	1.83	0.42
1:A:243:PHE:CG	1:A:244:VAL:N	2.86	0.42
1:B:309:ALA:HA	1:B:310:PRO:HD3	1.58	0.42
1:A:321:GLU:C	1:A:323:LEU:H	2.20	0.42
1:B:211:PRO:O	1:B:212:PRO:C	2.56	0.42
1:A:268:ILE:HG22	1:A:269:ASP:O	2.19	0.42
1:A:298:LEU:HD12	1:A:298:LEU:H	1.84	0.42
1:A:368:GLU:HA	1:A:371:LYS:HG3	2.00	0.42
1:B:358:VAL:HB	1:B:400:VAL:HG21	2.01	0.42
1:A:213:GLY:HA2	1:A:216:LYS:HE2	2.02	0.42
1:A:299:ALA:O	1:A:303:GLY:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:VAL:HG12	1:A:314:LEU:N	2.34	0.42
1:A:406:LYS:C	1:A:408:ALA:N	2.71	0.42
1:B:232:PHE:HD1	1:B:265:ILE:O	2.02	0.42
1:B:239:PHE:N	1:B:242:MET:SD	2.92	0.42
1:B:342:PRO:CB	1:B:347:ARG:HG2	2.45	0.42
1:B:351:LEU:HB2	1:B:385:ILE:CD1	2.49	0.42
1:A:232:PHE:HZ	1:A:261:GLN:HB2	1.83	0.42
1:A:269:ASP:OD2	1:A:270:GLU:HG3	2.19	0.42
1:A:186:VAL:O	1:A:187:ASP:C	2.57	0.42
1:A:266:ILE:HB	1:A:313:VAL:HG22	2.01	0.42
1:A:271:ILE:HG12	1:A:315:ALA:HB1	2.02	0.42
1:A:364:VAL:HG11	1:A:400:VAL:O	2.20	0.42
1:B:346:GLY:O	1:B:350:ILE:HG12	2.19	0.42
1:B:347:ARG:C	1:B:349:GLU:N	2.71	0.42
1:B:379:ALA:C	1:B:381:LEU:N	2.72	0.42
1:B:319:ARG:CD	1:B:322:ILE:HD11	2.46	0.42
1:B:405:LEU:HD13	1:B:405:LEU:HA	1.57	0.42
1:B:343:ASP:C	1:B:345:ASN:H	2.23	0.41
1:B:355:ILE:HG23	1:B:358:VAL:HG21	1.91	0.41
1:A:356:LYS:NZ	1:B:190:LYS:HZ1	2.18	0.41
1:A:385:ILE:O	1:A:386:ASN:C	2.59	0.41
1:B:244:VAL:O	1:B:246:LEU:N	2.52	0.41
1:A:168:ARG:NH2	1:B:171:ASP:OD1	2.53	0.41
1:B:205:GLY:HA3	1:B:333:PHE:HA	2.03	0.41
1:B:270:GLU:C	1:B:272:ASP:N	2.73	0.41
1:A:182:VAL:HG11	1:A:223:VAL:HG22	2.01	0.41
1:B:383:ASN:HB3	1:B:387:GLU:HG2	2.02	0.41
1:A:321:GLU:HG2	1:A:322:ILE:H	1.86	0.41
1:A:347:ARG:O	1:A:350:ILE:HB	2.21	0.41
1:B:296:GLN:O	1:B:297:LEU:C	2.59	0.41
1:A:216:LYS:HD2	1:A:216:LYS:N	2.35	0.41
1:A:274:ILE:HG22	1:A:294:LEU:HA	2.03	0.41
1:A:294:LEU:O	1:A:298:LEU:HD11	2.21	0.41
1:B:230:PRO:CD	1:B:264:SER:HB3	2.50	0.41
1:B:314:LEU:HA	1:B:314:LEU:HD23	1.87	0.41
1:A:169:PHE:HE1	1:A:183:VAL:CG2	2.32	0.41
1:B:394:ARG:HG2	1:B:394:ARG:O	2.21	0.41
1:B:323:LEU:HG	1:B:324:ASP:N	2.36	0.40
1:A:189:LEU:HD13	1:A:229:VAL:HG21	2.02	0.40
1:A:216:LYS:CD	1:A:216:LYS:N	2.83	0.40
1:A:181:GLU:O	1:A:184:GLU:N	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLN:C	1:A:298:LEU:H	2.24	0.40
1:A:350:ILE:O	1:A:351:LEU:C	2.58	0.40
1:B:383:ASN:N	1:B:383:ASN:ND2	2.69	0.40
1:B:410:GLU:HA	1:B:413:ILE:HG12	2.03	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:B:361:ALA:O	1:B:361:ALA:O[4_455]	2.03	0.17

## 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	245/268 (91%)	146 (60%)	62 (25%)	37 (15%)	0	1
1	B	245/268 (91%)	152 (62%)	59 (24%)	34 (14%)	0	1
All	All	490/536 (91%)	298 (61%)	121 (25%)	71 (14%)	0	1

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ASP
1	A	177	GLU
1	A	200	ALA
1	A	211	PRO
1	A	243	PHE
1	A	289	GLU
1	A	322	ILE
1	A	358	VAL
1	A	371	LYS

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Mol	Chain	Res	Type
1	A	408	ALA
1	A	410	GLU
1	B	175	ASN
1	B	193	GLU
1	B	214	THR
1	B	307	GLU
1	B	358	VAL
1	B	405	LEU
1	A	233	SER
1	A	245	GLY
1	A	272	ASP
1	A	307	GLU
1	A	344	PHE
1	A	361	ALA
1	A	385	ILE
1	A	415	GLY
1	B	169	PHE
1	B	245	GLY
1	B	297	LEU
1	B	344	PHE
1	B	348	VAL
1	B	396	ASN
1	B	406	LYS
1	B	407	GLU
1	A	169	PHE
1	A	212	PRO
1	A	260	LYS
1	A	270	GLU
1	A	271	ILE
1	B	217	THR
1	B	296	GLN
1	B	384	ILE
1	A	196	ALA
1	A	219	LEU
1	A	238	SER
1	A	288	ASP
1	A	297	LEU
1	A	372	LEU
1	B	199	GLY
1	B	219	LEU
1	B	228	HIS
1	B	288	ASP

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Mol	Chain	Res	Type
1	B	306	SER
1	B	321	GLU
1	B	354	HIS
1	A	292	GLN
1	A	353	VAL
1	A	407	GLU
1	B	298	LEU
1	B	357	GLY
1	B	363	ASP
1	B	392	ALA
1	B	393	GLY
1	A	237	SER
1	A	236	GLY
1	A	384	ILE
1	B	202	ILE
1	A	182	VAL
1	B	165	PRO
1	B	182	VAL
1	B	342	PRO
1	B	364	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	198/212 (93%)	164 (83%)	34 (17%)	2	9
1	B	198/212 (93%)	163 (82%)	35 (18%)	2	8
All	All	396/424 (93%)	327 (83%)	69 (17%)	2	8

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	LYS
1	A	168	ARG
1	A	193	GLU

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Mol	Chain	Res	Type
1	A	201	LYS
1	A	202	ILE
1	A	216	LYS
1	A	218	LEU
1	A	239	PHE
1	A	257	THR
1	A	266	ILE
1	A	270	GLU
1	A	272	ASP
1	A	290	ARG
1	A	297	LEU
1	A	302	ASP
1	A	317	THR
1	A	324	ASP
1	A	338	LEU
1	A	343	ASP
1	A	344	PHE
1	A	347	ARG
1	A	358	VAL
1	A	364	VAL
1	A	367	GLN
1	A	372	LEU
1	A	373	THR
1	A	376	LEU
1	A	380	ASP
1	A	383	ASN
1	A	386	ASN
1	A	394	ARG
1	A	395	ASN
1	A	402	GLN
1	A	403	GLN
1	B	164	LYS
1	B	169	PHE
1	B	172	MET
1	B	177	GLU
1	B	182	VAL
1	B	183	VAL
1	B	194	ARG
1	B	197	ASN
1	B	201	LYS
1	B	217	THR
1	B	226	GLU

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Mol	Chain	Res	Type
1	B	229	VAL
1	B	240	ILE
1	B	242	MET
1	B	253	ASP
1	B	264	SER
1	B	276	LYS
1	B	291	GLU
1	B	296	GLN
1	B	302	ASP
1	B	304	PHE
1	B	313	VAL
1	B	328	MET
1	B	332	ARG
1	B	334	ASP
1	B	336	GLN
1	B	351	LEU
1	B	352	LYS
1	B	353	VAL
1	B	363	ASP
1	B	366	LEU
1	B	369	VAL
1	B	391	LEU
1	B	402	GLN
1	B	403	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	ASN
1	A	296	GLN
1	A	397	GLN
1	A	402	GLN
1	B	161	ASN
1	B	175	ASN
1	B	197	ASN
1	B	261	GLN
1	B	367	GLN
1	B	383	ASN
1	B	386	ASN
1	B	404	HIS

### 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	306:SER	C	307:GLU	N	1.64



## 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	249/268 (92%)	0.24	14 (5%) 24 23	105, 142, 186, 224	0
1	B	249/268 (92%)	0.13	9 (3%) 42 40	94, 133, 186, 222	0
All	All	498/536 (92%)	0.18	23 (4%) 32 30	94, 138, 187, 224	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	GLY	4.6
1	A	399	GLU	4.2
1	A	255	PHE	3.9
1	B	201	LYS	3.9
1	A	276	LYS	3.7
1	A	275	GLY	3.5
1	B	251	VAL	3.4
1	B	202	ILE	3.3
1	B	287	ASN	3.2
1	B	373	THR	3.1
1	A	288	ASP	2.8
1	A	289	GLU	2.6
1	B	239	PHE	2.6
1	A	287	ASN	2.5
1	B	274	ILE	2.4
1	B	273	ALA	2.4
1	A	264	SER	2.3
1	A	378	GLY	2.2
1	A	204	LYS	2.2
1	A	198	LEU	2.2
1	A	405	LEU	2.2
1	A	290	ARG	2.2
1	B	418	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.