



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 04:06 AM EDT

PDB ID : 3MH4  
Title : HtrA proteases are activated by a conserved mechanism that can be triggered by distinct molecular cues  
Authors : Krojer, T.; Sawa, J.; Huber, R.; Clausen, T.  
Deposited on : 2010-04-07  
Resolution : 3.10 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

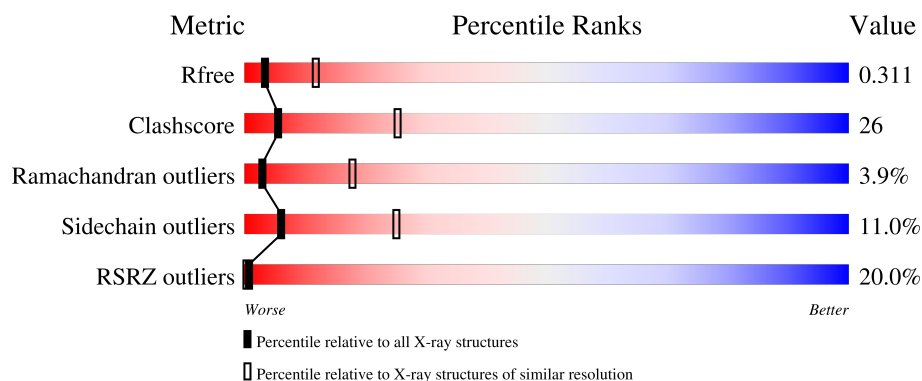
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	456	<div> <div>15%</div> <div>36%</div> <div>25%</div> <div>5%</div> <div>34%</div> </div>
1	B	456	<div> <div>15%</div> <div>47%</div> <div>31%</div> <div>5%</div> <div>16%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5007 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.

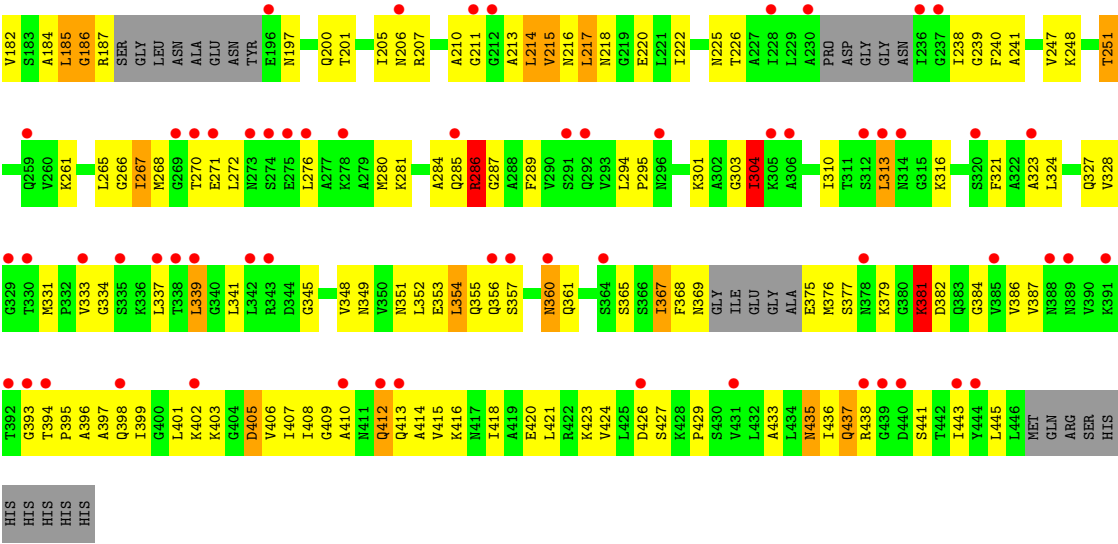
- Molecule 1 is a protein called Protease do.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2194	1367	390	425	12			
1	B	383	Total	C	N	O	S	0	0	0
			2813	1752	499	549	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	ALA	SER	engineered mutation	UNP P0C0V0
A	449	ARG	-	expression tag	UNP P0C0V0
A	450	SER	-	expression tag	UNP P0C0V0
A	451	HIS	-	expression tag	UNP P0C0V0
A	452	HIS	-	expression tag	UNP P0C0V0
A	453	HIS	-	expression tag	UNP P0C0V0
A	454	HIS	-	expression tag	UNP P0C0V0
A	455	HIS	-	expression tag	UNP P0C0V0
A	456	HIS	-	expression tag	UNP P0C0V0
B	210	ALA	SER	engineered mutation	UNP P0C0V0
B	449	ARG	-	expression tag	UNP P0C0V0
B	450	SER	-	expression tag	UNP P0C0V0
B	451	HIS	-	expression tag	UNP P0C0V0
B	452	HIS	-	expression tag	UNP P0C0V0
B	453	HIS	-	expression tag	UNP P0C0V0
B	454	HIS	-	expression tag	UNP P0C0V0
B	455	HIS	-	expression tag	UNP P0C0V0
B	456	HIS	-	expression tag	UNP P0C0V0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.71Å 120.71Å 232.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.07 – 3.10 24.07 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (24.07-3.10) 97.6 (24.07-3.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 3.10Å)	Xtriage
Refinement program	CNS, PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.257 , 0.309 0.260 , 0.311	Depositor DCC
$R_{free}$ test set	958 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	104.4	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 95.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5007	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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	0.32	0/2215	0.52	0/2991
1	B	0.30	0/2835	0.49	0/3824
All	All	0.31	0/5050	0.50	0/6815

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2194	0	2270	127	0
1	B	2813	0	2919	137	0
All	All	5007	0	5189	263	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 26.

All (263) 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:409:GLY:HA3	1:B:435:ASN:HB2	1.55	0.88
1:A:318:ILE:HG21	1:A:324:LEU:HG	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:HG23	1:A:342:LEU:HB3	1.59	0.83
1:A:293:VAL:HG23	1:A:299:ALA:HB1	1.60	0.81
1:A:19:LEU:HD21	1:A:177:VAL:HG21	1.62	0.81
1:A:313:LEU:HD11	1:A:337:LEU:HD12	1.63	0.80
1:B:313:LEU:HD21	1:B:337:LEU:HD12	1.63	0.79
1:B:382:ASP:HB3	1:B:416:LYS:HB2	1.64	0.79
1:B:121:ARG:NH2	1:B:145:LYS:O	2.14	0.79
1:A:298:SER:HA	1:A:301:LYS:HB3	1.65	0.79
1:B:247:VAL:O	1:B:251:THR:HB	1.84	0.78
1:A:29:ILE:HG23	1:A:113:ILE:HD13	1.67	0.76
1:B:276:LEU:HB3	1:B:280:MET:HE2	1.67	0.76
1:A:197:ASN:HD22	1:A:197:ASN:N	1.84	0.74
1:A:262:ARG:HH12	1:A:332:PRO:HG3	1.52	0.73
1:A:273:ASN:HA	1:A:278:LYS:HG2	1.69	0.73
1:A:343:ARG:HH11	1:A:346:LYS:HD2	1.53	0.73
1:B:399:ILE:HG23	1:B:401:LEU:HD13	1.70	0.72
1:A:187:ARG:HB2	1:A:197:ASN:HB3	1.71	0.72
1:A:267:ILE:HG21	1:A:293:VAL:HA	1.72	0.72
1:A:289:PHE:HA	1:A:309:VAL:HG12	1.73	0.71
1:B:410:ALA:HB1	1:B:424:VAL:HG21	1.72	0.71
1:B:367:ILE:HG23	1:B:368:PHE:H	1.54	0.71
1:B:384:GLY:HA3	1:B:408:ILE:HD13	1.74	0.70
1:B:304:ILE:HG12	1:B:341:LEU:HD11	1.75	0.68
1:B:225:ASN:ND2	1:B:241:ALA:HB2	2.08	0.68
1:B:394:THR:HB	1:B:397:ALA:HB3	1.76	0.67
1:A:293:VAL:HG21	1:A:304:ILE:O	1.95	0.66
1:B:361:GLN:HG3	1:B:375:GLU:HG2	1.77	0.66
1:A:304:ILE:HA	1:A:346:LYS:NZ	2.10	0.65
1:A:341:LEU:HD22	1:A:346:LYS:HD3	1.77	0.65
1:B:402:LYS:HG2	1:B:403:LYS:H	1.61	0.65
1:B:267:ILE:HD11	1:B:321:PHE:HE1	1.61	0.64
1:B:82:GLN:OE1	1:B:82:GLN:HA	1.96	0.64
1:A:126:LYS:HG2	1:A:142:GLN:NE2	2.13	0.64
1:A:272:LEU:O	1:A:273:ASN:HB2	1.98	0.63
1:A:343:ARG:NH1	1:A:346:LYS:HZ2	1.97	0.63
1:A:236:ILE:HG21	1:A:240:PHE:HE1	1.64	0.62
1:A:290:VAL:HG21	1:A:310:ILE:HD13	1.81	0.62
1:A:305:LYS:HG3	1:A:306:ALA:H	1.64	0.62
1:A:304:ILE:HA	1:A:346:LYS:HZ3	1.63	0.61
1:B:367:ILE:HG23	1:B:368:PHE:N	2.15	0.61
1:B:310:ILE:HD12	1:B:310:ILE:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:HD12	1:A:297:SER:HB2	1.83	0.61
1:B:354:LEU:HD13	1:B:355:GLN:N	2.17	0.60
1:B:369:ASN:HD22	1:B:396:ALA:HB2	1.66	0.60
1:A:42:MET:HB3	1:A:43:PRO:HA	1.84	0.59
1:A:114:LYS:HE2	1:A:124:ASP:OD1	2.02	0.59
1:A:311:THR:HA	1:A:318:ILE:HB	1.85	0.59
1:B:113:ILE:HG13	1:B:125:ALA:HB3	1.84	0.59
1:A:23:MET:N	1:A:24:PRO:HD2	2.19	0.58
1:B:348:VAL:HG12	1:B:349:ASN:H	1.68	0.58
1:A:264:GLU:HA	1:A:329:GLY:HA2	1.84	0.58
1:A:267:ILE:O	1:A:268:MET:HB2	2.02	0.58
1:A:293:VAL:HG11	1:A:305:LYS:HD3	1.85	0.58
1:B:313:LEU:HD13	1:B:327:GLN:HE21	1.67	0.58
1:B:410:ALA:C	1:B:412:GLN:H	2.05	0.58
1:A:200:GLN:HA	1:A:239:GLY:O	2.03	0.58
1:B:405:ASP:HA	1:B:438:ARG:HB3	1.85	0.58
1:A:18:MET:HA	1:A:21:LYS:HE3	1.85	0.58
1:B:394:THR:N	1:B:395:PRO:HD3	2.19	0.57
1:B:396:ALA:O	1:B:399:ILE:HG22	2.05	0.57
1:A:261:LYS:O	1:A:333:VAL:HG23	2.05	0.57
1:B:376:MET:HG3	1:B:387:VAL:HG23	1.86	0.57
1:A:343:ARG:HH12	1:A:346:LYS:HZ2	1.53	0.56
1:B:303:GLY:O	1:B:304:ILE:HG13	2.05	0.56
1:B:408:ILE:H	1:B:437:GLN:NE2	2.04	0.56
1:B:141:ILE:O	1:B:144:PRO:HD3	2.05	0.56
1:B:384:GLY:HA2	1:B:415:VAL:O	2.04	0.56
1:A:263:GLY:O	1:A:265:LEU:HD22	2.06	0.56
1:B:113:ILE:CG1	1:B:125:ALA:HB3	2.36	0.55
1:B:379:LYS:HB2	1:B:386:VAL:HB	1.89	0.55
1:A:113:ILE:HD12	1:A:114:LYS:N	2.22	0.55
1:A:29:ILE:HG23	1:A:113:ILE:CD1	2.37	0.55
1:A:269:GLY:HA2	1:A:291:SER:OG	2.06	0.55
1:A:335:SER:HB2	1:A:352:LEU:HD22	1.89	0.55
1:B:381:LYS:HD3	1:B:381:LYS:H	1.72	0.54
1:A:283:ASP:O	1:A:284:ALA:HB3	2.08	0.54
1:A:230:ALA:HA	1:A:232:ASP:H	1.73	0.54
1:B:348:VAL:HG12	1:B:349:ASN:N	2.22	0.54
1:A:94:ASP:HB3	1:A:99:TYR:HB2	1.88	0.54
1:B:386:VAL:HG22	1:B:406:VAL:HG22	1.90	0.54
1:B:333:VAL:HG13	1:B:353:GLU:HA	1.90	0.54
1:A:23:MET:N	1:A:24:PRO:CD	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LEU:HD23	1:A:342:LEU:N	2.23	0.54
1:A:87:LEU:C	1:A:87:LEU:HD23	2.28	0.53
1:B:160:VAL:HG13	1:B:182:VAL:O	2.08	0.53
1:B:365:SER:HB3	1:B:367:ILE:HG22	1.90	0.53
1:A:91:VAL:CG2	1:A:213:ALA:HB2	2.39	0.53
1:A:243:PRO:O	1:A:247:VAL:HG23	2.09	0.53
1:B:19:LEU:O	1:B:23:MET:HG2	2.08	0.53
1:A:244:SER:O	1:A:247:VAL:HB	2.09	0.53
1:A:293:VAL:HG11	1:A:305:LYS:HA	1.90	0.52
1:B:225:ASN:HD22	1:B:241:ALA:HB2	1.74	0.52
1:A:214:LEU:HG	1:A:225:ASN:HD21	1.74	0.52
1:B:141:ILE:HD12	1:B:147:LEU:HD21	1.89	0.52
1:A:160:VAL:HG13	1:A:182:VAL:O	2.09	0.52
1:A:337:LEU:HD21	1:A:352:LEU:HD11	1.90	0.52
1:B:272:LEU:HD11	1:B:287:GLY:H	1.75	0.52
1:A:163:TYR:HB2	1:A:217:LEU:CD2	2.40	0.52
1:A:266:GLY:C	1:A:267:ILE:HG13	2.30	0.52
1:B:81:GLN:O	1:B:82:GLN:OE1	2.28	0.52
1:B:286:ARG:HD2	1:B:286:ARG:O	2.10	0.51
1:A:31:VAL:HG21	1:A:106:VAL:O	2.11	0.51
1:A:141:ILE:O	1:A:144:PRO:HD3	2.11	0.51
1:A:304:ILE:HG23	1:A:308:ASP:OD2	2.11	0.50
1:B:310:ILE:HD12	1:B:310:ILE:N	2.27	0.50
1:A:312:SER:HB2	1:A:340:GLY:HA3	1.93	0.50
1:A:313:LEU:HD11	1:A:337:LEU:CD1	2.39	0.50
1:A:163:TYR:HB2	1:A:217:LEU:HD21	1.94	0.50
1:B:267:ILE:HD11	1:B:321:PHE:CE1	2.46	0.50
1:B:367:ILE:HG13	1:B:368:PHE:N	2.26	0.50
1:B:94:ASP:HB3	1:B:99:TYR:HB2	1.93	0.49
1:A:170:PRO:HG3	1:A:205:ILE:HG12	1.93	0.49
1:A:312:SER:HB2	1:A:340:GLY:H	1.78	0.49
1:B:206:ASN:OD1	1:B:207:ARG:HG3	2.13	0.49
1:A:256:GLU:HG2	1:A:257:TYR:CZ	2.48	0.49
1:A:128:VAL:HG13	1:A:138:LEU:O	2.13	0.49
1:B:185:LEU:O	1:B:186:GLY:C	2.51	0.49
1:B:226:THR:HG22	1:B:240:PHE:O	2.13	0.49
1:B:437:GLN:HA	1:B:441:SER:O	2.13	0.49
1:A:205:ILE:O	1:A:235:ASN:ND2	2.45	0.48
1:B:100:VAL:O	1:B:138:LEU:HD23	2.12	0.48
1:B:159:ARG:O	1:B:162:ASP:HB2	2.14	0.48
1:B:443:ILE:HD12	1:B:445:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ALA:HB3	1:B:17:PRO:HD3	1.96	0.48
1:B:301:LYS:HD3	1:B:301:LYS:C	2.32	0.48
1:A:113:ILE:HG13	1:A:125:ALA:HB3	1.95	0.48
1:A:197:ASN:N	1:A:197:ASN:ND2	2.57	0.48
1:A:324:LEU:O	1:A:328:VAL:HG22	2.14	0.48
1:B:185:LEU:O	1:B:187:ARG:N	2.47	0.48
1:B:313:LEU:HA	1:B:339:LEU:HB3	1.95	0.48
1:B:360:ASN:O	1:B:375:GLU:HA	2.14	0.48
1:A:117:LEU:HG	1:A:123:PHE:HE1	1.79	0.47
1:B:200:GLN:HA	1:B:239:GLY:O	2.14	0.47
1:A:312:SER:HB2	1:A:340:GLY:CA	2.44	0.47
1:A:93:ILE:HG13	1:A:152:MET:CE	2.44	0.47
1:B:272:LEU:HD23	1:B:289:PHE:HB2	1.96	0.47
1:A:225:ASN:ND2	1:A:241:ALA:HB2	2.30	0.47
1:A:266:GLY:O	1:A:267:ILE:HG13	2.15	0.47
1:B:153:ALA:HB2	1:B:220:GLU:HB3	1.96	0.47
1:B:185:LEU:O	1:B:187:ARG:HB2	2.15	0.47
1:B:266:GLY:O	1:B:294:LEU:HB2	2.15	0.47
1:B:126:LYS:HG3	1:B:142:GLN:CD	2.34	0.47
1:A:133:ARG:HD3	1:A:330:THR:O	2.15	0.47
1:B:396:ALA:O	1:B:401:LEU:HB2	2.15	0.47
1:A:229:LEU:O	1:A:232:ASP:HB3	2.15	0.47
1:B:18:MET:CE	1:B:165:VAL:HG11	2.45	0.47
1:A:282:VAL:HG12	1:A:282:VAL:O	2.16	0.46
1:A:352:LEU:O	1:A:353:GLU:HB2	2.15	0.46
1:B:337:LEU:HD23	1:B:337:LEU:H	1.81	0.46
1:B:113:ILE:HG13	1:B:113:ILE:O	2.16	0.46
1:B:399:ILE:O	1:B:445:LEU:HG	2.16	0.46
1:A:16:ALA:O	1:A:20:GLU:HG3	2.16	0.46
1:B:355:GLN:HG2	1:B:356:GLN:H	1.81	0.46
1:A:185:LEU:C	1:A:187:ARG:H	2.20	0.45
1:A:16:ALA:HB3	1:A:17:PRO:HD3	1.98	0.45
1:A:127:MET:HG3	1:A:128:VAL:N	2.31	0.45
1:B:410:ALA:HB2	1:B:415:VAL:HG23	1.98	0.45
1:B:413:GLN:HB3	1:B:414:ALA:H	1.46	0.45
1:A:313:LEU:HD23	1:A:327:GLN:HE21	1.82	0.45
1:A:272:LEU:O	1:A:273:ASN:CB	2.64	0.45
1:B:393:GLY:C	1:B:395:PRO:HD3	2.36	0.45
1:B:415:VAL:O	1:B:415:VAL:HG12	2.14	0.45
1:B:420:GLU:O	1:B:423:LYS:HB3	2.17	0.45
1:A:16:ALA:N	1:A:17:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:VAL:HG22	1:A:293:VAL:O	2.16	0.45
1:A:236:ILE:HG21	1:A:240:PHE:CE1	2.46	0.45
1:A:342:LEU:HD23	1:A:343:ARG:N	2.32	0.45
1:B:87:LEU:HD23	1:B:87:LEU:O	2.16	0.45
1:B:216:ASN:OD1	1:B:218:ASN:N	2.50	0.45
1:A:133:ARG:HH11	1:A:330:THR:HG23	1.82	0.45
1:B:272:LEU:CD1	1:B:287:GLY:H	2.30	0.45
1:A:225:ASN:HD22	1:A:241:ALA:HB2	1.82	0.45
1:B:153:ALA:HB2	1:B:220:GLU:CB	2.47	0.45
1:B:165:VAL:HG12	1:B:215:VAL:O	2.17	0.45
1:A:180:GLY:HA3	1:A:203:ALA:HB2	1.99	0.45
1:B:128:VAL:HG13	1:B:138:LEU:HB3	1.99	0.45
1:A:31:VAL:HB	1:A:86:ALA:HB3	1.99	0.44
1:B:93:ILE:HD12	1:B:93:ILE:HA	1.84	0.44
1:A:337:LEU:HG	1:A:350:VAL:HG22	2.00	0.44
1:B:265:LEU:HD21	1:B:339:LEU:HD21	1.98	0.44
1:A:345:GLY:O	1:A:346:LYS:HB2	2.16	0.44
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.89	0.44
1:A:246:MET:HA	1:A:246:MET:HE1	1.99	0.44
1:A:318:ILE:CG2	1:A:324:LEU:HG	2.40	0.44
1:B:410:ALA:C	1:B:412:GLN:N	2.70	0.43
1:A:271:GLU:HG2	1:A:272:LEU:N	2.31	0.43
1:B:270:THR:HB	1:B:271:GLU:H	1.64	0.43
1:B:433:ALA:HA	1:B:445:LEU:O	2.18	0.43
1:A:337:LEU:HD23	1:A:337:LEU:H	1.84	0.43
1:B:184:ALA:HB3	1:B:200:GLN:HB3	2.01	0.43
1:B:410:ALA:CA	1:B:415:VAL:HG23	2.49	0.43
1:A:331:MET:HA	1:A:332:PRO:HD3	1.85	0.43
1:B:381:LYS:HB2	1:B:382:ASP:H	1.60	0.43
1:B:386:VAL:CG2	1:B:406:VAL:HG22	2.49	0.43
1:A:19:LEU:O	1:A:23:MET:HG2	2.19	0.43
1:B:91:VAL:HG21	1:B:213:ALA:HB2	2.00	0.43
1:B:126:LYS:HG3	1:B:142:GLN:OE1	2.18	0.43
1:A:18:MET:SD	1:A:18:MET:C	2.97	0.43
1:B:268:MET:HE3	1:B:294:LEU:HD21	2.01	0.43
1:B:360:ASN:N	1:B:360:ASN:ND2	2.67	0.43
1:A:93:ILE:HG13	1:A:152:MET:HE1	2.00	0.42
1:A:246:MET:HA	1:A:246:MET:CE	2.49	0.42
1:B:294:LEU:HA	1:B:295:PRO:HD3	1.87	0.42
1:A:294:LEU:N	1:A:295:PRO:CD	2.83	0.42
1:B:424:VAL:C	1:B:426:ASP:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ILE:HG13	1:A:341:LEU:HG	2.01	0.42
1:B:91:VAL:CG2	1:B:213:ALA:HB2	2.49	0.42
1:A:262:ARG:HA	1:A:262:ARG:HD3	1.74	0.42
1:B:409:GLY:HA2	1:B:413:GLN:O	2.19	0.42
1:B:427:SER:C	1:B:429:PRO:HD3	2.39	0.42
1:B:165:VAL:CG1	1:B:215:VAL:HG12	2.49	0.42
1:A:147:LEU:HD12	1:A:147:LEU:HA	1.85	0.42
1:B:408:ILE:H	1:B:437:GLN:HE21	1.67	0.42
1:A:269:GLY:HA2	1:A:291:SER:H	1.85	0.42
1:B:248:LYS:O	1:B:251:THR:HG22	2.20	0.42
1:B:408:ILE:HG12	1:B:437:GLN:HE21	1.84	0.42
1:A:308:ASP:HB3	1:A:341:LEU:HD21	2.01	0.42
1:B:80:GLN:CD	1:B:82:GLN:HE22	2.23	0.42
1:B:272:LEU:HD13	1:B:285:GLN:HA	2.01	0.42
1:A:262:ARG:HH12	1:A:332:PRO:CG	2.28	0.42
1:B:381:LYS:H	1:B:381:LYS:CD	2.30	0.42
1:B:402:LYS:HG2	1:B:403:LYS:N	2.32	0.42
1:A:341:LEU:HD13	1:A:346:LYS:HE2	2.02	0.41
1:B:108:ASP:O	1:B:109:ASN:HB2	2.19	0.41
1:B:169:ASN:C	1:B:169:ASN:HD22	2.22	0.41
1:A:170:PRO:CG	1:A:205:ILE:HG12	2.50	0.41
1:A:321:PHE:H	1:A:321:PHE:HD2	1.60	0.41
1:B:333:VAL:HG21	1:B:354:LEU:HD23	2.02	0.41
1:B:387:VAL:CG1	1:B:405:ASP:H	2.33	0.41
1:B:238:ILE:HG12	1:B:239:GLY:H	1.84	0.41
1:B:331:MET:SD	1:B:337:LEU:HD13	2.60	0.41
1:B:333:VAL:HG12	1:B:334:GLY:N	2.35	0.41
1:A:205:ILE:H	1:A:205:ILE:HD12	1.86	0.41
1:A:321:PHE:CD2	1:A:321:PHE:N	2.80	0.41
1:A:142:GLN:HB3	1:B:119:ASP:O	2.20	0.41
1:A:290:VAL:HG21	1:A:310:ILE:CD1	2.50	0.41
1:A:312:SER:HB2	1:A:340:GLY:N	2.34	0.41
1:B:324:LEU:O	1:B:328:VAL:HG22	2.20	0.41
1:B:415:VAL:CG1	1:B:421:LEU:HB2	2.50	0.41
1:A:107:VAL:HG22	1:A:127:MET:HE1	2.03	0.41
1:A:160:VAL:O	1:A:182:VAL:HB	2.20	0.41
1:A:230:ALA:HA	1:A:232:ASP:N	2.35	0.41
1:B:104:ASN:O	1:B:108:ASP:HB2	2.21	0.41
1:B:323:ALA:O	1:B:327:GLN:HG3	2.21	0.41
1:A:125:ALA:HA	1:A:140:GLN:O	2.21	0.41
1:B:407:ILE:HG12	1:B:436:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASN:C	1:A:216:ASN:OD1	2.59	0.41
1:B:216:ASN:OD1	1:B:216:ASN:C	2.59	0.41
1:B:394:THR:O	1:B:398:GLN:HG3	2.21	0.41
1:B:12:MET:HA	1:B:13:PRO:HD3	1.94	0.41
1:B:214:LEU:O	1:B:222:ILE:HG12	2.21	0.41
1:B:355:GLN:HG2	1:B:357:SER:H	1.86	0.40
1:A:343:ARG:HH11	1:A:346:LYS:CD	2.30	0.40
1:B:435:ASN:OD1	1:B:435:ASN:N	2.54	0.40
1:B:18:MET:HE3	1:B:165:VAL:HG11	2.04	0.40
1:B:23:MET:N	1:B:24:PRO:CD	2.84	0.40
1:B:201:THR:O	1:B:238:ILE:HG12	2.21	0.40
1:B:377:SER:HA	1:B:418:ILE:HD11	2.03	0.40
1:A:264:GLU:H	1:A:264:GLU:HG2	1.68	0.40
1:A:22:VAL:C	1:A:24:PRO:HD2	2.41	0.40
1:B:39:THR:HA	1:B:40:PRO:HD3	1.90	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	295/456 (65%)	249 (84%)	32 (11%)	14 (5%)	2	14
1	B	373/456 (82%)	319 (86%)	42 (11%)	12 (3%)	4	22
All	All	668/912 (73%)	568 (85%)	74 (11%)	26 (4%)	3	18

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	MET
1	A	281	LYS
1	A	343	ARG

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Mol	Chain	Res	Type
1	B	367	ILE
1	B	381	LYS
1	A	267	ILE
1	A	282	VAL
1	A	285	GLN
1	A	293	VAL
1	B	186	GLY
1	B	412	GLN
1	A	210	ALA
1	B	197	ASN
1	B	281	LYS
1	A	264	GLU
1	A	271	GLU
1	A	319	SER
1	B	304	ILE
1	B	345	GLY
1	A	186	GLY
1	A	346	LYS
1	B	210	ALA
1	B	284	ALA
1	B	286	ARG
1	A	211	GLY
1	B	211	GLY

### 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	238/364 (65%)	210 (88%)	28 (12%)	5	21
1	B	309/364 (85%)	277 (90%)	32 (10%)	7	27
All	All	547/728 (75%)	487 (89%)	60 (11%)	6	25

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	18	MET
1	A	25	SER
1	A	41	ARG
1	A	93	ILE
1	A	113	ILE
1	A	114	LYS
1	A	128	VAL
1	A	133	ARG
1	A	138	LEU
1	A	147	LEU
1	A	165	VAL
1	A	177	VAL
1	A	197	ASN
1	A	198	PHE
1	A	205	ILE
1	A	214	LEU
1	A	217	LEU
1	A	251	THR
1	A	265	LEU
1	A	267	ILE
1	A	268	MET
1	A	272	LEU
1	A	275	GLU
1	A	305	LYS
1	A	309	VAL
1	A	337	LEU
1	A	343	ARG
1	B	12	MET
1	B	18	MET
1	B	42	MET
1	B	87	LEU
1	B	104	ASN
1	B	113	ILE
1	B	128	VAL
1	B	138	LEU
1	B	164	THR
1	B	169	ASN
1	B	177	VAL
1	B	185	LEU
1	B	205	ILE
1	B	214	LEU
1	B	215	VAL

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Mol	Chain	Res	Type
1	B	217	LEU
1	B	251	THR
1	B	261	LYS
1	B	267	ILE
1	B	286	ARG
1	B	304	ILE
1	B	313	LEU
1	B	316	LYS
1	B	339	LEU
1	B	351	ASN
1	B	352	LEU
1	B	354	LEU
1	B	360	ASN
1	B	381	LYS
1	B	405	ASP
1	B	435	ASN
1	B	437	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	140	GLN
1	A	142	GLN
1	A	169	ASN
1	A	225	ASN
1	A	235	ASN
1	A	245	ASN
1	A	327	GLN
1	A	347	GLN
1	B	80	GLN
1	B	82	GLN
1	B	104	ASN
1	B	140	GLN
1	B	169	ASN
1	B	225	ASN
1	B	245	ASN
1	B	292	GLN
1	B	296	ASN
1	B	327	GLN
1	B	347	GLN
1	B	355	GLN

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Mol	Chain	Res	Type
1	B	360	ASN
1	B	383	GLN
1	B	388	ASN
1	B	413	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	301/456 (66%)	0.98	69 (22%) <b>0</b> <b>0</b>	66, 107, 226, 235	0
1	B	383/456 (83%)	0.84	68 (17%) <b>1</b> <b>0</b>	67, 143, 211, 220	0
All	All	684/912 (75%)	0.90	137 (20%) <b>1</b> <b>0</b>	66, 125, 218, 235	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	SER	11.0
1	B	439	GLY	10.8
1	A	287	GLY	8.9
1	B	337	LEU	8.9
1	A	232	ASP	8.6
1	A	188	SER	8.0
1	A	293	VAL	7.8
1	B	38	ASN	7.7
1	A	349	ASN	7.6
1	A	292	GLN	7.1
1	A	206	ASN	6.5
1	B	43	PRO	6.5
1	B	42	MET	6.4
1	A	266	GLY	6.2
1	A	345	GLY	6.1
1	A	276	LEU	5.9
1	B	274	SER	5.9
1	B	431	VAL	5.7
1	A	233	GLY	5.6
1	A	307	GLY	5.6
1	B	392	THR	5.5
1	A	342	LEU	5.4
1	A	323	ALA	5.3
1	A	329	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	283	ASP	5.2
1	B	444	TYR	5.2
1	B	236	ILE	5.0
1	B	230	ALA	4.9
1	B	443	ILE	4.9
1	A	285	GLN	4.9
1	B	271	GLU	4.8
1	A	265	LEU	4.8
1	A	234	GLY	4.8
1	B	333	VAL	4.8
1	A	294	LEU	4.7
1	A	264	GLU	4.7
1	B	440	ASP	4.6
1	B	385	VAL	4.5
1	B	438	ARG	4.5
1	A	277	ALA	4.4
1	A	231	PRO	4.4
1	B	338	THR	4.3
1	B	275	GLU	4.3
1	B	269	GLY	4.0
1	B	410	ALA	4.0
1	A	315	GLY	4.0
1	A	317	PRO	3.9
1	B	196	GLU	3.9
1	A	273	ASN	3.9
1	B	323	ALA	3.9
1	B	278	LYS	3.9
1	B	360	ASN	3.8
1	A	275	GLU	3.7
1	B	391	LYS	3.7
1	B	314	ASN	3.7
1	B	39	THR	3.6
1	B	330	THR	3.6
1	B	79	GLY	3.5
1	B	388	ASN	3.4
1	B	342	LEU	3.4
1	B	402	LYS	3.3
1	A	272	LEU	3.3
1	B	313	LEU	3.3
1	B	339	LEU	3.2
1	A	343	ARG	3.2
1	A	236	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	394	THR	3.2
1	A	90	GLY	3.2
1	B	276	LEU	3.2
1	A	286	ARG	3.2
1	A	325	ARG	3.1
1	A	314	ASN	3.0
1	B	291	SER	3.0
1	A	211	GLY	3.0
1	B	212	GLY	3.0
1	B	273	ASN	3.0
1	B	171	PHE	3.0
1	B	335	SER	2.9
1	A	350	VAL	2.9
1	B	320	SER	2.9
1	B	211	GLY	2.9
1	B	306	ALA	2.9
1	B	356	GLN	2.9
1	B	228	ILE	2.8
1	B	270	THR	2.8
1	A	263	GLY	2.8
1	A	80	GLN	2.8
1	A	351	ASN	2.7
1	A	259	GLN	2.7
1	A	281	LYS	2.7
1	B	413	GLN	2.7
1	B	393	GLY	2.7
1	A	38	ASN	2.7
1	A	229	LEU	2.7
1	A	306	ALA	2.7
1	A	320	SER	2.6
1	A	344	ASP	2.6
1	A	42	MET	2.6
1	A	336	LYS	2.5
1	A	169	ASN	2.5
1	A	348	VAL	2.5
1	B	292	GLN	2.5
1	A	43	PRO	2.5
1	A	237	GLY	2.5
1	A	291	SER	2.5
1	A	212	GLY	2.4
1	A	89	SER	2.4
1	B	343	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	426	ASP	2.4
1	A	319	SER	2.4
1	B	285	GLN	2.4
1	B	41	ARG	2.4
1	A	39	THR	2.3
1	B	412	GLN	2.3
1	A	322	ALA	2.3
1	B	389	ASN	2.3
1	A	228	ILE	2.3
1	B	237	GLY	2.3
1	B	206	ASN	2.3
1	A	207	ARG	2.2
1	A	284	ALA	2.2
1	B	305	LYS	2.2
1	B	329	GLY	2.2
1	A	224	ILE	2.2
1	B	357	SER	2.2
1	A	230	ALA	2.2
1	B	364	SER	2.2
1	A	271	GLU	2.2
1	A	102	THR	2.1
1	B	312	SER	2.1
1	B	398	GLN	2.1
1	B	296	ASN	2.1
1	A	36	THR	2.0
1	B	378	ASN	2.0
1	B	259	GLN	2.0
1	A	324	LEU	2.0
1	A	133	ARG	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.