



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:18 PM UTC

PDB ID : 3MH4 / pdb_00003mh4
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

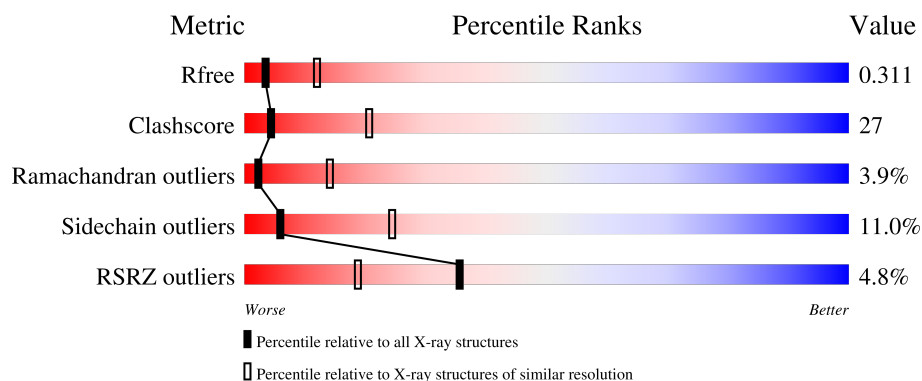
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 ≥ 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	
1	B	456	

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			

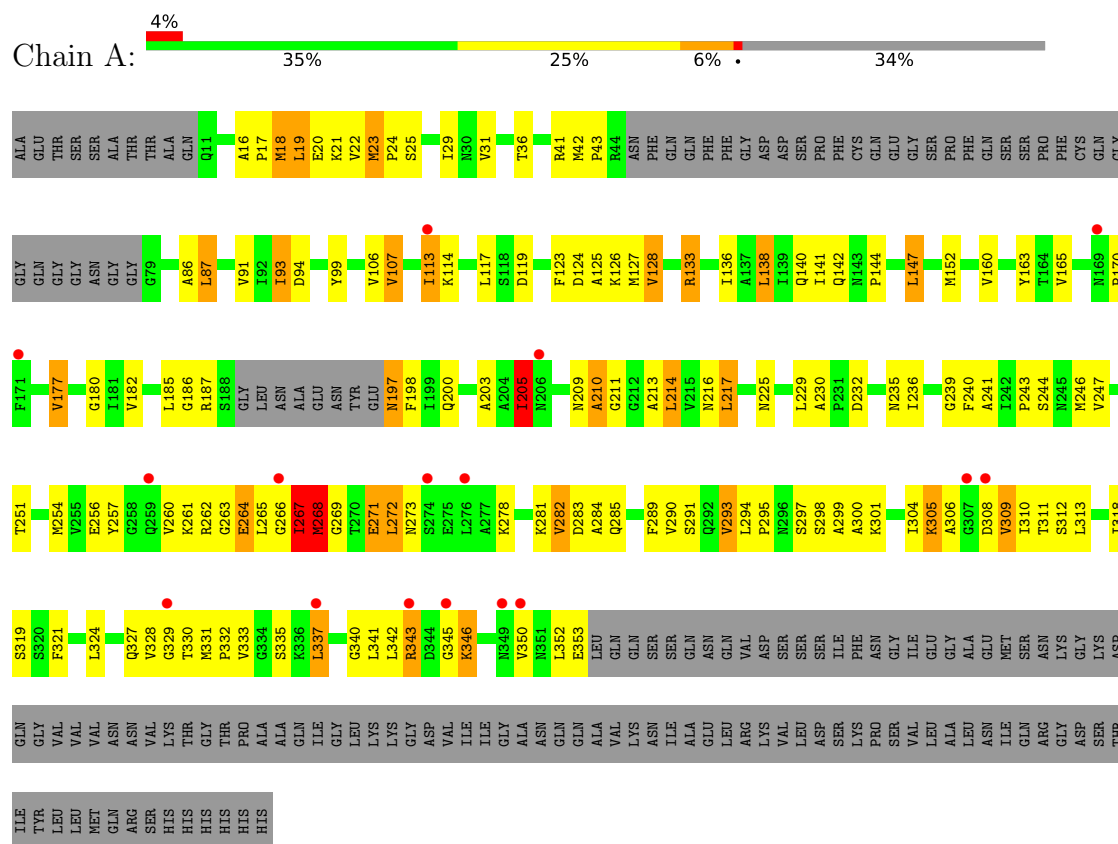
There are 18 discrepancies between the modelled and reference sequences:

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

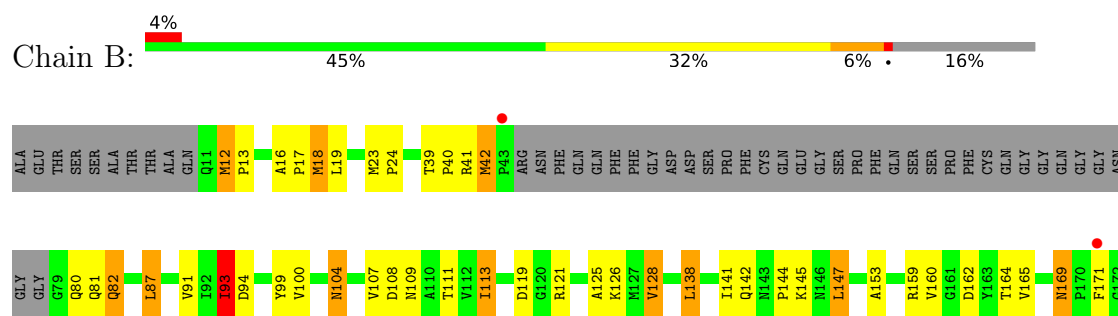
3 Residue-property plots [i](#)

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

• Molecule 1: Protease do



• Molecule 1: Protease do



D405	V406	I407	I408	G409	A410	N411	Q412	Q413	A414	V415	K416	N417	I418	A419	E420	L421	R422	K423	V424	L425	D426	S427	K428	P429	A433	L434	N435	I436	Q437	R438	S441	T442	I443	Y444	L445	L446	MET	GLN	ARG	SER	HIS	HIS	HIS	HIS	HIS										
L338	L339	G340	L341	D344	G345	V348	N349	V350	N351	L352	E353	L354	Q355	Q356	S357	S358	Q359	N360	Q361	S364	S365	S366	L367	F368	N369	GLY	ILE	GLY	GLY	ALA	E375	N376	G377	N378	K379	G380	D381	Q382	Q383	G384	V385	V386	V387	G393	T394	P395	A396	A397	Q398	I399	G400	L401	K402	K403	G404
F240	A241	V247	K248	T251	L265	G266	T267	N268	G269	T270	E271	L272	L276	M280	K281	V282	D283	A284	Q285	R286	G287	F289	L294	P295	K301	A302	G303	I304	T310	L313	K316	F321	A322	A323	L324	R325	A326	Q327	V328	G329	T330	M331	P332	V333	G334	L337									
L173	G174	E175	T176	V177	V182	S183	A184	L185	G186	R187	SER	GLY	LEU	ASN	ALA	GLU	ASN	TYR	E196	N197	F198	I199	Q200	T201	T205	N206	R207	A210	G211	G212	A213	L214	V215	N216	L217	N218	E219	E220	L221	L222	N225	T226	A227	L228	L229	A230	PRO	ASP	GLY	GLY	ASN	T236	G237	T238	G239

4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	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) 97.3 (24.07-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	104.4	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 92.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.43	0/2215	0.85	5/2991 (0.2%)
1	B	0.39	0/2835	0.84	8/3824 (0.2%)
All	All	0.41	0/5050	0.84	13/6815 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	ASN	CA-C-N	6.43	126.65	119.32
1	B	169	ASN	C-N-CA	6.43	126.65	119.32
1	B	344	ASP	N-CA-C	-6.07	107.10	114.75
1	B	93	ILE	N-CA-C	-5.79	107.21	111.90
1	A	300	ALA	N-CA-C	-5.78	106.21	113.20
1	B	111	THR	N-CA-C	-5.77	105.90	113.12
1	A	23	MET	CA-C-N	5.69	125.16	119.24
1	A	23	MET	C-N-CA	5.69	125.16	119.24
1	A	205	ILE	N-CA-C	5.36	115.96	108.89
1	B	12	MET	CA-C-N	5.18	125.09	119.76
1	B	12	MET	C-N-CA	5.18	125.09	119.76
1	B	350	VAL	N-CA-C	5.14	114.81	108.53
1	A	107	VAL	N-CA-C	-5.14	107.97	112.90

There are no chirality outliers.

There are no planarity outliers.

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	2194	0	2270	131	0
1	B	2813	0	2919	142	0
All	All	5007	0	5189	272	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 27.

All (272) 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:304:ILE:HA	1:A:346:LYS:HZ1	1.22	1.04
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
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:18:MET:HE1	1:B:165:VAL:HG11	1.74	0.70
1:B:384:GLY:HA3	1:B:408:ILE:HD13	1.74	0.70
1:A:246:MET:HE2	1:A:246:MET:HA	1.74	0.69
1:B:304:ILE:HG12	1:B:341:LEU:HD11	1.75	0.68
1:A:93:ILE:HG13	1:A:152:MET:HE2	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:GLN:HG3	1:B:375:GLU:HG2	1.77	0.66
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:B:410:ALA:C	1:B:412:GLN:H	2.05	0.63
1:A:272:LEU:O	1:A:273:ASN:HB2	1.98	0.63
1:A:236:ILE:HG21	1:A:240:PHE:HE1	1.64	0.62
1:B:41:ARG:C	1:B:42:MET:HE3	2.24	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: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
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:87:LEU:C	1:A:87:LEU:HD23	2.28	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: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: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:A:266:GLY:C	1:A:267:ILE:HG13	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:341:LEU:HD23	1:A:342:LEU:N	2.23	0.54
1:B:185:LEU:O	1:B:186:GLY:C	2.51	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:B:301:LYS:HD3	1:B:301:LYS:C	2.32	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:107:VAL:O	1:A:127:MET:HE1	2.10	0.52
1:B:81:GLN:O	1:B:82:GLN:OE1	2.28	0.52
1:B:126:LYS:HG3	1:B:142:GLN:CD	2.34	0.52
1:B:286:ARG:HD2	1:B:286:ARG:O	2.10	0.51
1:A:304:ILE:HA	1:A:346:LYS:NZ	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:A:185:LEU:C	1:A:187:ARG:H	2.20	0.50
1:B:310:ILE:HD12	1:B:310:ILE:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:393:GLY:C	1:B:395:PRO:HD3	2.36	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: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
1:B:16:ALA:HB3	1:B:17:PRO:HD3	1.96	0.48
1:A:113:ILE:HG13	1:A:125:ALA:HB3	1.95	0.48
1:A:324:LEU:O	1:A:328:VAL:HG22	2.14	0.48
1:B:410:ALA:C	1:B:412:GLN:N	2.70	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:18:MET:SD	1:A:18:MET:C	2.97	0.47
1:A:312:SER:HB2	1:A:340:GLY:CA	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:A:93:ILE:HG13	1:A:152:MET:CE	2.44	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:B:427:SER:C	1:B:429:PRO:HD3	2.39	0.47
1:A:229:LEU:O	1:A:232:ASP:HB3	2.15	0.47
1:B:424:VAL:C	1:B:426:ASP:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:VAL:HG12	1:A:282:VAL:O	2.16	0.46
1:B:80:GLN:CD	1:B:82:GLN:HE22	2.23	0.46
1:B:337:LEU:HD23	1:B:337:LEU:H	1.81	0.46
1:B:268:MET:HE3	1:B:294:LEU:HD21	1.97	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:B:169:ASN:C	1:B:169:ASN:HD22	2.22	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:22:VAL:C	1:A:24:PRO:HD2	2.41	0.45
1:A:216:ASN:C	1:A:216:ASN:OD1	2.59	0.45
1:B:216:ASN:OD1	1:B:216:ASN:C	2.59	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:A:352:LEU:O	1:A:353:GLU:HB2	2.15	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: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
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:B:268:MET:HE3	1:B:294:LEU:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:CG2	1:A:324:LEU:HG	2.40	0.44
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:136:ILE:O	1:A:254:MET:HE1	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:41:ARG:HD3	1:A:41:ARG:C	2.43	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:342:LEU:HD23	1:A:342:LEU:C	2.42	0.43
1:A:107:VAL:HG22	1:A:127:MET:HE1	1.99	0.43
1:B:360:ASN:N	1:B:360:ASN:ND2	2.67	0.43
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: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: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:197:ASN:N	1:A:197:ASN:ND2	2.57	0.42
1:A:269:GLY:HA2	1:A:291:SER:H	1.85	0.42
1:A:311:THR:C	1:A:318:ILE:H	2.28	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:272:LEU:HD13	1:B:285:GLN:HA	2.01	0.42
1:B:365:SER:C	1:B:367:ILE:N	2.78	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:A:170:PRO:CG	1:A:205:ILE:HG12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:330:THR:C	1:B:331:MET:HG3	2.45	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:209:ASN:O	1:A:210:ALA:C	2.63	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: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:119:ASP:OD1	1:A:119:ASP:C	2.62	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
1:B:171:PHE:C	1:B:173:LEU:H	2.29	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: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:B:18:MET:CE	1:B:165:VAL:HG11	2.45	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	11
1	B	373/456 (82%)	319 (86%)	42 (11%)	12 (3%)	3	18
All	All	668/912 (73%)	568 (85%)	74 (11%)	26 (4%)	2	14

All (26) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	212 (89%)	26 (11%)	6	24
1	B	309/364 (85%)	275 (89%)	34 (11%)	6	24
All	All	547/728 (75%)	487 (89%)	60 (11%)	6	24

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

Mol	Chain	Res	Type
1	A	18	MET
1	A	19	LEU
1	A	25	SER
1	A	36	THR
1	A	87	LEU
1	A	93	ILE
1	A	113	ILE
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	260	VAL
1	A	267	ILE
1	A	268	MET

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Mol	Chain	Res	Type
1	A	272	LEU
1	A	305	LYS
1	A	309	VAL
1	A	337	LEU
1	B	18	MET
1	B	42	MET
1	B	82	GLN
1	B	87	LEU
1	B	93	ILE
1	B	104	ASN
1	B	107	VAL
1	B	113	ILE
1	B	128	VAL
1	B	138	LEU
1	B	147	LEU
1	B	164	THR
1	B	177	VAL
1	B	185	LEU
1	B	205	ILE
1	B	214	LEU
1	B	215	VAL
1	B	217	LEU
1	B	251	THR
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	386	VAL
1	B	413	GLN
1	B	435	ASN
1	B	443	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	116	GLN
1	A	140	GLN
1	A	142	GLN
1	A	169	ASN
1	A	206	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	197	ASN
1	B	225	ASN
1	B	245	ASN
1	B	249	ASN
1	B	292	GLN
1	B	296	ASN
1	B	327	GLN
1	B	347	GLN
1	B	351	ASN
1	B	355	GLN
1	B	360	ASN
1	B	383	GLN
1	B	388	ASN
1	B	413	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	301/456 (66%)	0.35	16 (5%) 32 17	66, 107, 226, 235	0
1	B	383/456 (83%)	0.22	17 (4%) 39 21	67, 143, 211, 220	0
All	All	684/912 (75%)	0.28	33 (4%) 35 19	66, 125, 218, 235	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	GLY	6.0
1	A	329	GLY	5.2
1	B	356	GLN	3.8
1	A	349	ASN	3.8
1	A	266	GLY	3.5
1	B	175	GLU	3.4
1	B	198	PHE	3.1
1	A	343	ARG	3.0
1	B	337	LEU	2.8
1	B	331	MET	2.7
1	A	274	SER	2.6
1	A	276	LEU	2.6
1	B	364	SER	2.5
1	A	113	ILE	2.5
1	B	385	VAL	2.5
1	B	323	ALA	2.5
1	B	358	SER	2.5
1	A	337	LEU	2.4
1	A	169	ASN	2.4
1	A	171	PHE	2.3
1	B	205	ILE	2.3
1	B	228	ILE	2.3
1	A	259	GLN	2.3
1	A	308	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	43	PRO	2.2
1	B	326	ALA	2.2
1	A	206	ASN	2.2
1	B	282	VAL	2.2
1	A	350	VAL	2.1
1	B	171	PHE	2.1
1	B	425	LEU	2.1
1	A	345	GLY	2.0
1	B	330	THR	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 oligosaccharides 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.