



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:03 PM GMT

PDB ID : 1NB8
Title : Structure of the catalytic domain of USP7 (HAUSP)
Authors : Hu, M.; Li, P.; Li, M.; Li, W.; Yao, T.; Wu, J.-W.; Gu, W.; Cohen, R.E.; Shi, Y.
Deposited on : 2002-12-02
Resolution : 2.30 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

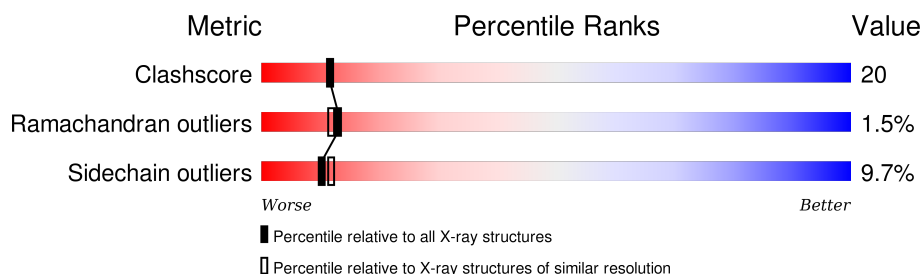
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

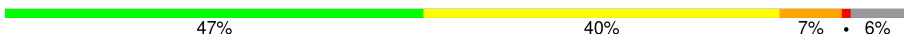

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	353	
1	B	353	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5714 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 Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	Se	0	0	0
			2696	1709	461	510	7	9			
1	B	333	Total	C	N	O	S	Se	0	0	0
			2707	1715	465	511	7	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	MSE	MET	MODIFIED RESIDUE	UNP Q93009
A	244	MSE	MET	MODIFIED RESIDUE	UNP Q93009
A	245	MSE	MET	MODIFIED RESIDUE	UNP Q93009
A	292	MSE	MET	MODIFIED RESIDUE	UNP Q93009
A	311	MSE	MET	MODIFIED RESIDUE	UNP Q93009
A	328	MSE	MET	MODIFIED RESIDUE	UNP Q93009
A	407	MSE	MET	MODIFIED RESIDUE	UNP Q93009
A	410	MSE	MET	MODIFIED RESIDUE	UNP Q93009
A	515	MSE	MET	MODIFIED RESIDUE	UNP Q93009
B	225	MSE	MET	MODIFIED RESIDUE	UNP Q93009
B	244	MSE	MET	MODIFIED RESIDUE	UNP Q93009
B	245	MSE	MET	MODIFIED RESIDUE	UNP Q93009
B	292	MSE	MET	MODIFIED RESIDUE	UNP Q93009
B	311	MSE	MET	MODIFIED RESIDUE	UNP Q93009
B	328	MSE	MET	MODIFIED RESIDUE	UNP Q93009
B	407	MSE	MET	MODIFIED RESIDUE	UNP Q93009
B	410	MSE	MET	MODIFIED RESIDUE	UNP Q93009
B	515	MSE	MET	MODIFIED RESIDUE	UNP Q93009

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	139	Total	O	0	0
			139	139		

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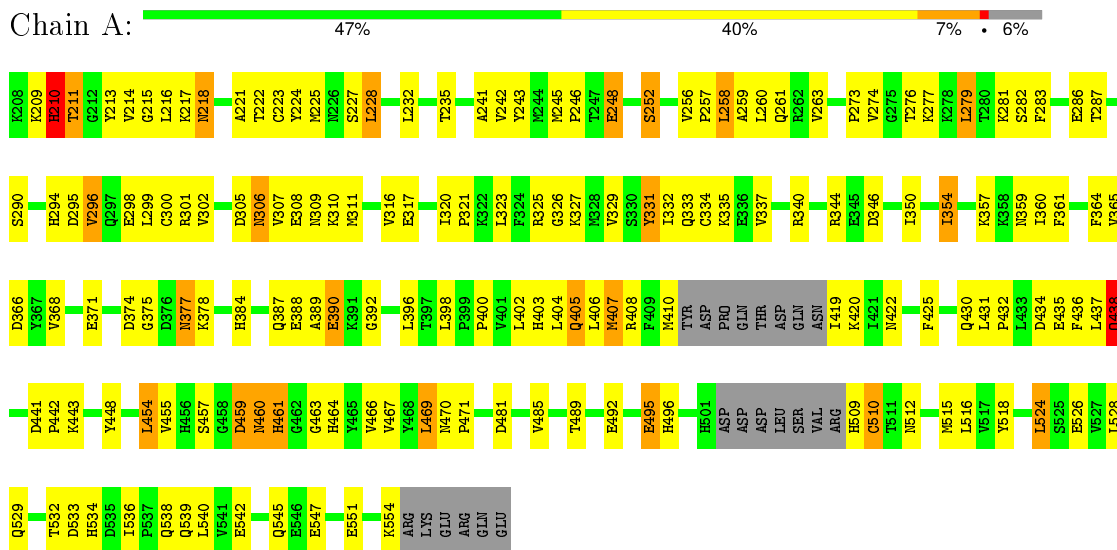
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	172	Total	O	0	0
			172	172		

3 Residue-property plots

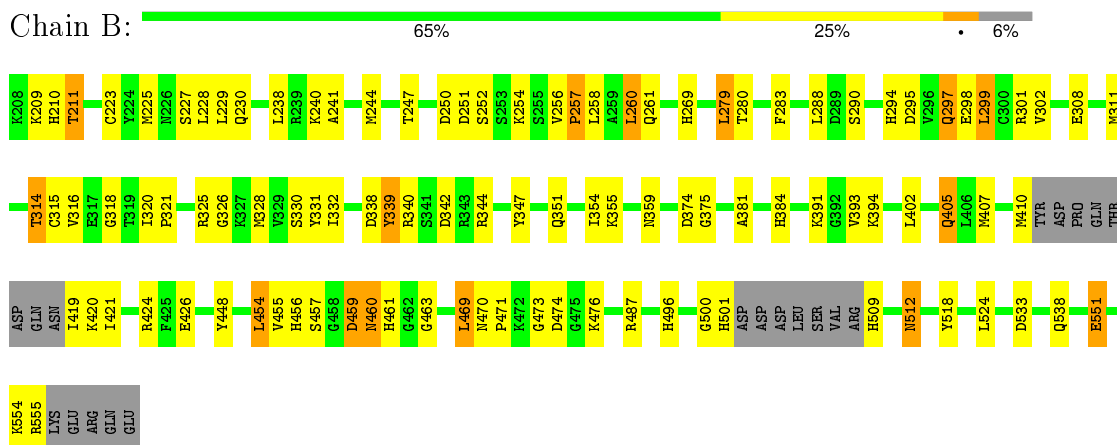
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.65Å 68.51Å 76.26Å 90.00° 95.36° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5714	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

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	0.42	0/2743	0.71	4/3679 (0.1%)
1	B	0.45	1/2754 (0.0%)	0.72	0/3693
All	All	0.43	1/5497 (0.0%)	0.71	4/7372 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	223	CYS	CB-SG	5.04	1.90	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	HIS	N-CA-C	6.28	127.96	111.00
1	A	510	CYS	N-CA-C	6.07	127.39	111.00
1	A	235	THR	N-CA-C	-5.60	95.88	111.00
1	A	463	GLY	N-CA-C	5.15	125.97	113.10

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	2696	0	2649	136	0
1	B	2707	0	2662	81	0
2	A	139	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	172	0	0	13	0
All	All	5714	0	5311	217	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 20.

All (217) 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:244:MSE:HG2	2:B:563:HOH:O	1.62	0.99
1:A:419:ILE:HG22	1:A:420:LYS:H	1.32	0.95
1:B:314:THR:HG22	1:B:316:VAL:H	1.32	0.94
1:B:410:MSE:HE2	1:B:421:ILE:HD11	1.49	0.93
1:A:359:ASN:ND2	1:A:361:PHE:HB3	1.86	0.91
1:A:408:ARG:NH2	1:A:512:ASN:HB2	1.89	0.88
1:B:419:ILE:HA	1:B:460:ASN:HD21	1.41	0.86
1:A:509:HIS:HB3	2:A:671:HOH:O	1.77	0.84
1:A:407:MSE:HG3	2:A:564:HOH:O	1.77	0.83
1:B:314:THR:CG2	1:B:316:VAL:H	1.93	0.82
1:B:240:LYS:HG2	1:B:244:MSE:HE2	1.63	0.80
1:A:408:ARG:HH22	1:A:512:ASN:HB2	1.46	0.79
1:A:545:GLN:HG2	2:A:696:HOH:O	1.87	0.75
1:B:407:MSE:HG3	2:B:562:HOH:O	1.87	0.75
1:A:442:PRO:O	1:A:443:LYS:HB2	1.86	0.74
1:A:354:ILE:HD12	1:A:406:LEU:HB3	1.71	0.71
1:A:526:GLU:O	1:A:529:GLN:HG3	1.90	0.71
1:A:547:GLU:O	1:A:551:GLU:HG3	1.89	0.71
1:A:387:GLN:HB3	2:A:580:HOH:O	1.90	0.70
1:B:410:MSE:HE2	1:B:421:ILE:CD1	2.22	0.69
1:A:331:TYR:HD2	1:A:340:ARG:HH21	1.41	0.69
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.75	0.69
1:A:279:LEU:O	1:A:282:SER:HB3	1.92	0.68
1:A:227:SER:HB3	1:A:454:LEU:HD13	1.73	0.68
1:A:210:HIS:CG	1:A:211:THR:H	2.11	0.68
1:A:298:GLU:O	1:A:302:VAL:HG23	1.94	0.68
1:B:227:SER:HB3	1:B:454:LEU:HD13	1.74	0.67
1:B:459:ASP:O	1:B:460:ASN:HB2	1.92	0.67
1:A:256:VAL:HG22	1:A:282:SER:OG	1.94	0.67
1:A:405:GLN:OE1	1:A:515:MSE:HE3	1.95	0.67
1:A:334:CYS:HA	1:A:389:ALA:HB2	1.77	0.67
1:A:279:LEU:HD22	1:A:283:PHE:HE1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:VAL:O	1:A:311:MSE:HG3	1.95	0.66
1:A:277:LYS:O	1:A:281:LYS:HG3	1.96	0.66
1:A:335:LYS:HD2	1:A:388:GLU:HB3	1.77	0.66
1:B:470:ASN:ND2	1:B:473:GLY:HA2	2.12	0.64
1:A:301:ARG:HG2	2:A:577:HOH:O	1.97	0.64
1:A:419:ILE:HG22	1:A:420:LYS:N	2.10	0.64
1:B:554:LYS:O	1:B:555:ARG:HB2	1.99	0.63
1:A:448:TYR:HB3	1:A:518:TYR:HB3	1.81	0.63
1:A:210:HIS:CD2	1:A:211:THR:H	2.17	0.63
1:A:308:GLU:HB2	1:A:320:ILE:HG13	1.81	0.63
1:B:211:THR:HG23	2:B:661:HOH:O	1.99	0.63
1:B:448:TYR:HB3	1:B:518:TYR:HB3	1.80	0.62
1:A:532:THR:HG21	1:A:534:HIS:CD2	2.34	0.62
1:A:256:VAL:HB	1:A:257:PRO:HD3	1.81	0.62
1:A:295:ASP:OD2	1:A:298:GLU:HG3	1.99	0.62
1:A:454:LEU:HD22	1:A:467:VAL:HG23	1.82	0.62
1:B:391:LYS:HE3	2:B:654:HOH:O	2.00	0.61
1:B:311:MSE:O	1:B:314:THR:HB	2.00	0.60
1:B:279:LEU:HD22	1:B:283:PHE:HE1	1.65	0.60
1:B:209:LYS:HA	2:B:661:HOH:O	2.02	0.60
1:B:314:THR:HG22	1:B:316:VAL:N	2.11	0.60
1:A:359:ASN:HD22	1:A:361:PHE:HB3	1.66	0.60
1:B:410:MSE:CE	1:B:421:ILE:HD11	2.28	0.60
1:B:420:LYS:H	1:B:460:ASN:ND2	1.99	0.60
1:A:538:GLN:O	1:A:542:GLU:HG3	2.02	0.60
1:A:301:ARG:O	1:A:305:ASP:HB2	2.02	0.59
1:A:242:VAL:HG13	1:A:245:MSE:HE2	1.84	0.59
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.83	0.59
1:B:311:MSE:SE	1:B:316:VAL:HG12	2.53	0.59
1:A:350:ILE:HB	1:A:404:LEU:HD23	1.85	0.59
1:A:359:ASN:HD21	1:A:361:PHE:HB3	1.68	0.58
1:A:210:HIS:CG	1:A:211:THR:N	2.71	0.58
1:A:551:GLU:O	1:A:554:LYS:HD3	2.04	0.58
1:A:354:ILE:HG12	1:A:425:PHE:CD2	2.38	0.58
1:B:331:TYR:HE1	1:B:394:LYS:HD2	1.68	0.58
1:B:419:ILE:CA	1:B:460:ASN:HD21	2.15	0.58
1:B:298:GLU:O	1:B:302:VAL:HG23	2.03	0.58
1:A:532:THR:HG22	1:A:533:ASP:N	2.19	0.58
1:A:252:SER:HA	1:A:258:LEU:HD12	1.84	0.57
1:A:225:MSE:HE1	1:A:276:THR:OG1	2.05	0.57
1:B:381:ALA:HB3	1:B:384:HIS:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LEU:O	1:A:400:PRO:HD2	2.05	0.56
1:A:333:GLN:O	1:A:389:ALA:HB1	2.04	0.56
1:B:331:TYR:HB2	2:B:676:HOH:O	2.05	0.56
1:B:325:ARG:C	1:B:325:ARG:HD2	2.26	0.56
1:B:279:LEU:HD22	1:B:283:PHE:CE1	2.41	0.56
1:A:489:THR:OG1	1:A:492:GLU:HG3	2.05	0.56
1:B:295:ASP:OD2	1:B:298:GLU:HG3	2.06	0.56
1:A:359:ASN:HD22	1:A:361:PHE:H	1.53	0.55
1:A:378:LYS:HE2	1:A:388:GLU:HG3	1.88	0.55
1:B:227:SER:HB3	1:B:454:LEU:CD1	2.36	0.55
1:A:374:ASP:O	1:A:377:ASN:N	2.37	0.54
1:A:209:LYS:HD3	2:A:576:HOH:O	2.07	0.54
1:B:500:GLY:O	1:B:509:HIS:N	2.40	0.54
1:A:290:SER:O	1:A:294:HIS:HD2	1.91	0.54
1:A:248:GLU:HB3	1:A:539:GLN:NE2	2.22	0.54
1:B:457:SER:O	1:B:463:GLY:HA3	2.08	0.54
1:B:256:VAL:N	1:B:257:PRO:CD	2.71	0.54
1:A:325:ARG:HD2	2:A:572:HOH:O	2.07	0.53
1:B:318:GLY:O	1:B:321:PRO:HD2	2.08	0.53
1:B:308:GLU:HB2	1:B:320:ILE:HG13	1.91	0.53
1:A:217:LYS:CG	1:A:273:PRO:HB2	2.39	0.53
1:A:256:VAL:HB	1:A:306:ASN:HD22	1.74	0.53
1:A:360:ILE:HD11	1:A:516:LEU:CD1	2.38	0.53
1:B:338:ASP:O	1:B:339:TYR:HB2	2.09	0.53
1:A:216:LEU:HD23	1:A:274:VAL:HB	1.91	0.52
1:A:361:PHE:HE2	1:A:435:GLU:OE1	1.92	0.52
1:B:420:LYS:N	1:B:460:ASN:ND2	2.57	0.52
1:A:466:VAL:HG12	1:A:467:VAL:N	2.24	0.52
1:A:256:VAL:HA	1:A:282:SER:OG	2.09	0.52
1:A:354:ILE:CD1	1:A:406:LEU:HB3	2.39	0.52
1:B:393:VAL:HG12	1:B:394:LYS:N	2.25	0.51
1:A:311:MSE:O	1:A:317:GLU:HB2	2.10	0.51
1:B:554:LYS:O	1:B:555:ARG:CB	2.58	0.51
1:A:357:LYS:HZ1	1:A:366:ASP:CG	2.14	0.51
1:A:256:VAL:HB	1:A:306:ASN:ND2	2.26	0.51
1:B:551:GLU:O	1:B:554:LYS:HB2	2.11	0.51
1:A:422:ASN:HB3	2:A:684:HOH:O	2.11	0.51
1:A:217:LYS:CE	1:A:273:PRO:HB2	2.41	0.50
1:A:403:HIS:HE1	2:A:567:HOH:O	1.93	0.50
1:A:259:ALA:O	1:A:263:VAL:HG23	2.12	0.50
1:A:257:PRO:HD3	1:A:306:ASN:HD22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:VAL:CG1	1:A:467:VAL:N	2.74	0.50
1:B:351:GLN:HB3	1:B:407:MSE:HE2	1.94	0.50
1:B:474:ASP:OD2	1:B:476:LYS:HB2	2.11	0.50
1:A:419:ILE:HA	2:A:675:HOH:O	2.12	0.50
1:A:332:ILE:O	1:A:340:ARG:HA	2.12	0.50
1:A:331:TYR:HE1	1:A:392:GLY:CA	2.25	0.50
1:A:455:VAL:HG13	1:A:512:ASN:O	2.12	0.49
1:A:217:LYS:HE3	1:A:273:PRO:HB2	1.94	0.49
1:B:469:LEU:C	1:B:471:PRO:HD3	2.33	0.49
1:B:420:LYS:HE2	1:B:512:ASN:HD21	1.77	0.49
1:A:217:LYS:HE3	1:A:273:PRO:O	2.12	0.49
1:A:273:PRO:HD3	2:A:589:HOH:O	2.12	0.49
1:B:500:GLY:N	1:B:509:HIS:N	2.61	0.49
1:A:228:LEU:O	1:A:232:LEU:HG	2.13	0.49
1:A:459:ASP:HB2	2:A:653:HOH:O	2.13	0.49
1:A:360:ILE:HD11	1:A:516:LEU:HD12	1.94	0.49
1:A:532:THR:HG22	1:A:533:ASP:H	1.76	0.49
1:A:364:PHE:O	1:A:368:VAL:HG22	2.13	0.49
1:B:241:ALA:HB1	1:B:316:VAL:HG11	1.95	0.49
1:B:331:TYR:CE1	1:B:394:LYS:HD2	2.48	0.48
1:A:419:ILE:CG2	1:A:420:LYS:H	2.13	0.48
1:A:241:ALA:HA	1:A:316:VAL:HG21	1.95	0.48
1:A:551:GLU:O	1:A:554:LYS:HB3	2.13	0.48
1:A:405:GLN:HE21	1:A:405:GLN:HB2	1.43	0.48
1:B:290:SER:O	1:B:294:HIS:HD2	1.95	0.48
1:A:243:TYR:CD1	1:A:536:ILE:HG12	2.49	0.48
1:A:410:MSE:O	1:A:419:ILE:HD12	2.13	0.48
1:A:211:THR:HG22	1:A:213:TYR:H	1.78	0.48
1:B:328:MSE:O	1:B:344:ARG:HG2	2.14	0.48
1:A:461:HIS:HD2	2:B:657:HOH:O	1.97	0.47
1:B:297:GLN:HE21	1:B:297:GLN:H	1.63	0.47
1:B:424:ARG:NH2	1:B:426:GLU:OE2	2.46	0.47
1:B:457:SER:O	1:B:463:GLY:CA	2.62	0.47
1:A:464:HIS:CE1	1:A:481:ASP:OD1	2.68	0.47
1:A:290:SER:O	1:A:294:HIS:CD2	2.67	0.47
1:A:359:ASN:HD22	1:A:361:PHE:N	2.12	0.47
1:B:209:LYS:O	1:B:209:LYS:HG3	2.13	0.47
1:B:251:ASP:OD2	1:B:254:LYS:HB2	2.14	0.47
1:B:381:ALA:CB	1:B:384:HIS:HB2	2.45	0.46
1:A:337:VAL:HG11	1:A:384:HIS:ND1	2.30	0.46
1:A:217:LYS:HG2	1:A:273:PRO:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ARG:HG2	2:B:619:HOH:O	2.16	0.46
1:B:247:THR:HG21	1:B:261:GLN:OE1	2.14	0.46
1:B:501:HIS:C	1:B:501:HIS:CD2	2.89	0.46
1:A:325:ARG:HG2	1:A:326:GLY:N	2.31	0.45
1:B:256:VAL:HB	1:B:257:PRO:HD3	1.98	0.45
1:A:245:MSE:HA	1:A:246:PRO:HD3	1.80	0.45
1:A:263:VAL:HG21	1:A:279:LEU:HD12	1.98	0.45
1:A:287:THR:OG1	1:A:290:SER:HB3	2.16	0.45
1:A:327:LYS:HD3	1:A:346:ASP:OD1	2.17	0.45
1:A:357:LYS:NZ	1:A:366:ASP:CG	2.70	0.45
1:A:221:ALA:C	1:A:223:CYS:N	2.68	0.45
1:A:398:LEU:HD12	1:A:437:LEU:HD11	1.99	0.45
1:B:325:ARG:HH11	1:B:325:ARG:HG3	1.81	0.45
1:A:334:CYS:HA	1:A:389:ALA:CB	2.44	0.44
1:B:225:MSE:HG3	1:B:299:LEU:HD11	1.99	0.44
1:A:469:LEU:C	1:A:471:PRO:HD3	2.36	0.44
1:B:455:VAL:HG12	1:B:456:HIS:N	2.33	0.44
1:B:375:GLY:N	2:B:726:HOH:O	2.40	0.44
1:B:328:MSE:HG2	1:B:393:VAL:CG1	2.48	0.44
1:A:470:ASN:CG	1:A:470:ASN:O	2.55	0.44
1:B:314:THR:HG23	1:B:315:CYS:N	2.33	0.43
1:B:316:VAL:HG12	1:B:316:VAL:O	2.17	0.43
1:B:354:ILE:HG13	1:B:355:LYS:N	2.32	0.43
1:A:218:ASN:C	1:A:218:ASN:HD22	2.22	0.43
1:A:256:VAL:N	1:A:257:PRO:CD	2.81	0.43
1:A:257:PRO:O	1:A:261:GLN:HG3	2.18	0.43
1:B:314:THR:CG2	1:B:315:CYS:N	2.82	0.43
1:A:419:ILE:CA	1:A:460:ASN:HD22	2.31	0.43
1:A:211:THR:HG21	1:A:485:VAL:HG12	2.01	0.43
1:B:326:GLY:HA3	1:B:347:TYR:CZ	2.53	0.43
1:A:361:PHE:O	1:A:365:VAL:HG23	2.19	0.43
1:B:210:HIS:CE1	1:B:487:ARG:H	2.37	0.43
1:A:524:LEU:HD22	1:A:528:LEU:HD12	2.00	0.42
1:B:269:HIS:NE2	1:B:533:ASP:OD2	2.47	0.42
1:A:281:LYS:HG2	1:A:286:GLU:OE2	2.18	0.42
1:A:430:GLN:HB3	2:A:615:HOH:O	2.19	0.42
1:A:214:VAL:HG22	1:A:215:GLY:N	2.33	0.42
1:A:396:LEU:HD23	1:A:438:GLN:HG3	2.01	0.42
1:B:230:GLN:HE21	1:B:230:GLN:HA	1.84	0.42
1:A:364:PHE:HB3	1:A:436:PHE:CE2	2.55	0.42
1:B:332:ILE:O	1:B:340:ARG:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLU:HA	1:A:311:MSE:HE2	2.02	0.42
1:A:374:ASP:O	1:A:378:LYS:N	2.53	0.42
1:A:454:LEU:HD22	1:A:467:VAL:CG2	2.47	0.41
1:A:495:GLU:HG2	1:A:495:GLU:H	1.48	0.41
1:B:405:GLN:HE21	1:B:405:GLN:HB2	1.56	0.41
1:A:246:PRO:O	1:A:310:LYS:HE3	2.20	0.41
1:A:329:VAL:HG22	1:A:344:ARG:HG2	2.02	0.41
1:B:240:LYS:HD2	2:B:615:HOH:O	2.20	0.41
1:B:260:LEU:HD23	1:B:260:LEU:HA	1.88	0.41
1:A:224:TYR:HB2	1:A:296:VAL:CG1	2.50	0.41
1:A:222:THR:O	1:A:223:CYS:HB2	2.20	0.41
1:B:555:ARG:HD2	2:B:711:HOH:O	2.20	0.41
1:A:441:ASP:HB2	2:A:596:HOH:O	2.21	0.41
1:A:441:ASP:O	1:A:441:ASP:OD2	2.39	0.41
1:A:224:TYR:OH	1:A:294:HIS:HB2	2.21	0.40
1:B:355:LYS:HG3	2:B:671:HOH:O	2.20	0.40
1:B:209:LYS:HE3	2:B:717:HOH:O	2.20	0.40
1:A:532:THR:CG2	1:A:534:HIS:CD2	3.04	0.40
1:A:431:LEU:HA	1:A:432:PRO:HD3	1.82	0.40
1:A:371:GLU:O	1:A:390:GLU:HA	2.21	0.40
1:A:242:VAL:HG12	1:A:261:GLN:HG2	2.04	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	326/353 (92%)	293 (90%)	26 (8%)	7 (2%)	9	7
1	B	327/353 (93%)	304 (93%)	20 (6%)	3 (1%)	21	24
All	All	653/706 (92%)	597 (91%)	46 (7%)	10 (2%)	13	12

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	ASN
1	A	510	CYS
1	B	460	ASN
1	A	375	GLY
1	A	407	MSE
1	A	438	GLN
1	B	339	TYR
1	A	252	SER
1	A	211	THR
1	B	288	LEU

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	299/311 (96%)	270 (90%)	29 (10%)	10	12
1	B	300/311 (96%)	271 (90%)	29 (10%)	10	12
All	All	599/622 (96%)	541 (90%)	58 (10%)	10	12

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	HIS
1	A	218	ASN
1	A	228	LEU
1	A	248	GLU
1	A	258	LEU
1	A	260	LEU
1	A	279	LEU
1	A	296	VAL
1	A	299	LEU
1	A	300	CYS
1	A	306	ASN
1	A	309	ASN
1	A	331	TYR

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Mol	Chain	Res	Type
1	A	354	ILE
1	A	377	ASN
1	A	390	GLU
1	A	402	LEU
1	A	405	GLN
1	A	434	ASP
1	A	438	GLN
1	A	454	LEU
1	A	457	SER
1	A	459	ASP
1	A	461	HIS
1	A	469	LEU
1	A	495	GLU
1	A	496	HIS
1	A	524	LEU
1	A	540	LEU
1	B	211	THR
1	B	228	LEU
1	B	229	LEU
1	B	238	LEU
1	B	250	ASP
1	B	252	SER
1	B	257	PRO
1	B	258	LEU
1	B	260	LEU
1	B	279	LEU
1	B	280	THR
1	B	297	GLN
1	B	299	LEU
1	B	314	THR
1	B	330	SER
1	B	342	ASP
1	B	359	ASN
1	B	374	ASP
1	B	402	LEU
1	B	405	GLN
1	B	454	LEU
1	B	459	ASP
1	B	461	HIS
1	B	469	LEU
1	B	496	HIS
1	B	512	ASN

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Mol	Chain	Res	Type
1	B	524	LEU
1	B	538	GLN
1	B	551	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	HIS
1	A	218	ASN
1	A	230	GLN
1	A	237	GLN
1	A	268	GLN
1	A	269	HIS
1	A	294	HIS
1	A	306	ASN
1	A	333	GLN
1	A	359	ASN
1	A	403	HIS
1	A	405	GLN
1	A	451	HIS
1	A	534	HIS
1	A	539	GLN
1	A	545	GLN
1	B	210	HIS
1	B	230	GLN
1	B	237	GLN
1	B	268	GLN
1	B	294	HIS
1	B	297	GLN
1	B	359	ASN
1	B	405	GLN
1	B	447	ASN
1	B	460	ASN
1	B	470	ASN
1	B	501	HIS
1	B	512	ASN

5.3.3 RNA ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.