Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2024 – 06:24 PM EST

PDB ID	:	1HEI
Title	:	STRUCTURE OF THE HEPATITIS C VIRUS RNA HELICASE DOMAIN
Authors	:	Yao, N.; Weber, P.
Deposited on	:	1997-03-31
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

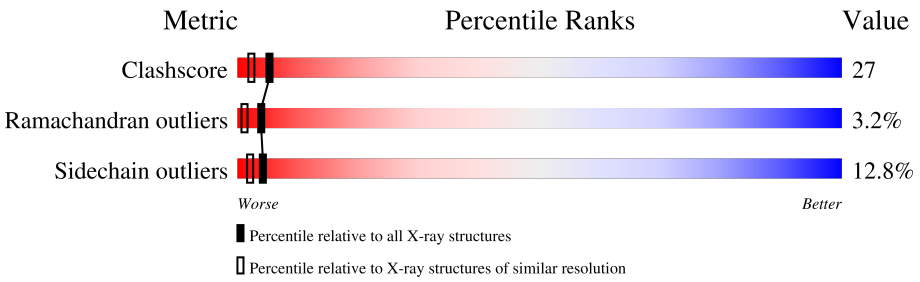
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	451	56% 33% 8% •
1	B	451	51% 33% 6% • 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6759 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 HCV HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	443	3328	2109	562	635	22	0	0	0
1	B	412	3103	1969	520	593	21	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	GLN	LYS	conflict	UNP P27958
A	277	GLY	ALA	conflict	UNP P27958
A	301	LEU	SER	conflict	UNP P27958
A	403	ASN	SER	conflict	UNP P27958
A	505	MET	THR	conflict	UNP P27958
A	530	GLU	GLY	conflict	UNP P27958
A	582	TRP	ARG	conflict	UNP P27958
B	221	GLN	LYS	conflict	UNP P27958
B	277	GLY	ALA	conflict	UNP P27958
B	301	LEU	SER	conflict	UNP P27958
B	403	ASN	SER	conflict	UNP P27958
B	505	MET	THR	conflict	UNP P27958
B	530	GLU	GLY	conflict	UNP P27958
B	582	TRP	ARG	conflict	UNP P27958

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	187	187	187	0	0
			Total	O		
3	B	139	139	139	0	0

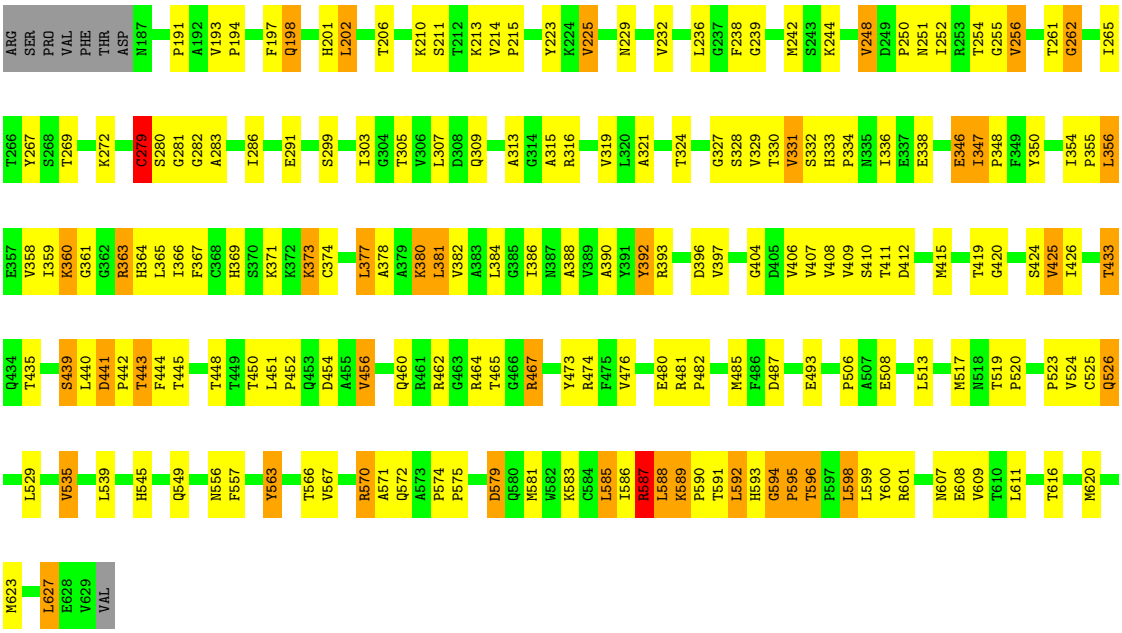
3 Residue-property plots (i)

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. 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. 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.

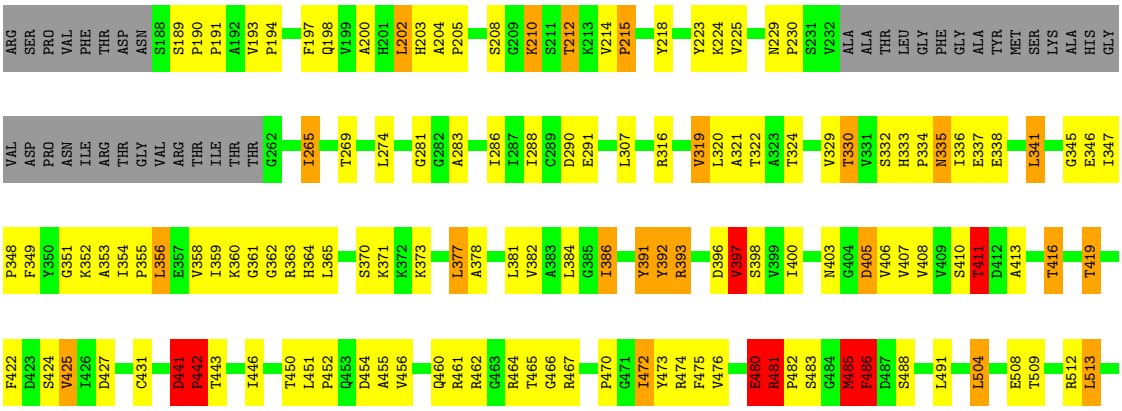
• Molecule 1: HCV HELICASE

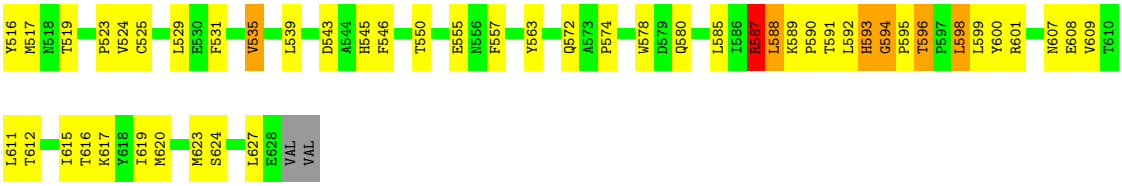
Chain A: 56% 33% 8% •



• Molecule 1: HCV HELICASE

Chain B: 51% 33% 6% • 9%




Y516
M517
N518
T519
P523
V524
C525
L529
E530
F531
V535
L539
D543
A544
H545
F546
T550
E555
N556
F557
Y563
Q572
A573
P574
W578
D579
Q580
L585
I586
R587
L588
K589
P590
T591
L592
H593
G594
P595
T596
P597
L598
L599
Y600
R601
N607
E608
V609
T610
L611
T612
I615
T616
K617
Y618
I619
M620
M623
S624
L627
E628
VAL
VAL

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.54Å 102.73Å 119.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	88.0 (8.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.220 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6759	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.77	4/3409 (0.1%)	0.97	7/4658 (0.2%)
1	B	0.56	0/3179	0.85	8/4343 (0.2%)
All	All	0.68	4/6588 (0.1%)	0.92	15/9001 (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	A	0	3
1	B	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	THR	C-N	20.82	1.81	1.34
1	A	595	PRO	C-N	15.64	1.70	1.34
1	A	279	CYS	C-N	-11.45	1.07	1.34
1	A	589	LYS	C-N	11.08	1.55	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	443	THR	O-C-N	-22.18	87.22	122.70
1	A	279	CYS	O-C-N	-21.53	88.25	122.70
1	A	595	PRO	CA-C-N	-10.04	95.12	117.20
1	B	486	PHE	O-C-N	-9.04	108.23	122.70
1	A	283	ALA	O-C-N	-7.90	110.05	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	481	ARG	NE-CZ-NH2	7.55	124.08	120.30
1	B	441	ASP	N-CA-C	-7.51	90.72	111.00
1	B	441	ASP	C-N-CD	7.15	143.42	128.40
1	A	595	PRO	C-N-CA	-6.27	106.02	121.70
1	B	485	MET	CG-SD-CE	6.13	110.00	100.20
1	A	283	ALA	CA-C-N	5.49	129.28	117.20
1	A	279	CYS	CA-C-N	5.48	129.25	117.20
1	B	411	THR	N-CA-C	-5.07	97.33	111.00
1	B	587	ARG	N-CA-C	-5.03	97.42	111.00
1	B	442	PRO	N-CA-C	-5.00	99.09	112.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	CYS	Mainchain,Peptide
1	A	563	TYR	Sidechain
1	B	486	PHE	Mainchain
1	B	563	TYR	Sidechain

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	3328	0	3289	173	0
1	B	3103	0	3062	172	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	187	0	0	4	0
3	B	139	0	0	7	0
All	All	6759	0	6351	339	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 (339) 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:595:PRO:C	1:A:596:THR:N	1.70	1.45
1:A:443:THR:C	1:A:444:PHE:N	1.81	1.31
1:A:347:ILE:HG12	1:A:354:ILE:HB	1.42	0.98
1:B:225:VAL:HG12	1:B:286:ILE:HB	1.49	0.94
1:B:194:PRO:HG3	1:B:198:GLN:HG2	1.50	0.94
1:B:441:ASP:HB2	1:B:442:PRO:HD3	1.50	0.93
1:A:324:THR:HG21	1:A:456:VAL:HG12	1.50	0.93
1:B:442:PRO:HG3	1:B:611:LEU:HD22	1.50	0.90
1:A:595:PRO:CA	1:A:596:THR:N	2.35	0.89
1:A:366:ILE:HG12	1:A:426:ILE:HD13	1.54	0.89
1:B:441:ASP:HB2	1:B:442:PRO:CD	2.05	0.87
1:A:441:ASP:HB2	1:A:442:PRO:HD2	1.56	0.86
1:B:442:PRO:HD3	1:B:601:ARG:NH1	1.92	0.85
1:A:193:VAL:HG21	1:A:223:TYR:CZ	2.13	0.83
1:A:194:PRO:HG3	1:A:198:GLN:HG2	1.60	0.82
1:B:347:ILE:HD11	1:B:384:LEU:HD12	1.63	0.80
1:A:346:GLU:HG3	1:A:356:LEU:HD23	1.62	0.80
1:A:248:VAL:HG11	1:A:265:ILE:HD12	1.63	0.79
1:A:588:LEU:HD12	1:A:588:LEU:H	1.48	0.79
1:B:578:TRP:CZ2	1:B:588:LEU:HB3	2.18	0.79
1:B:587:ARG:O	1:B:590:PRO:HD2	1.83	0.79
1:A:443:THR:O	1:A:444:PHE:N	2.15	0.78
1:A:442:PRO:HD2	3:A:1005:HOH:O	1.82	0.78
1:A:440:LEU:O	1:A:441:ASP:O	2.02	0.78
1:A:347:ILE:HD11	1:A:354:ILE:HD12	1.66	0.78
1:A:595:PRO:C	1:A:596:THR:CA	2.52	0.77
1:B:355:PRO:O	1:B:358:VAL:HG22	1.83	0.77
1:A:592:LEU:HG	1:A:593:HIS:H	1.51	0.76
1:A:350:TYR:OH	1:A:373:LYS:HG2	1.85	0.76
1:B:197:PHE:HA	1:B:316:ARG:O	1.86	0.76
1:B:517:MET:HE3	1:B:529:LEU:CD1	2.16	0.76
1:B:336:ILE:HD12	1:B:465:THR:HG23	1.67	0.75
1:A:587:ARG:HD2	1:A:587:ARG:O	1.88	0.74
1:A:566:THR:O	1:A:570:ARG:HG2	1.89	0.73
1:A:327:GLY:HA2	1:B:482:PRO:HG2	1.68	0.73
1:B:324:THR:HG21	1:B:456:VAL:HG22	1.69	0.73
1:A:364:HIS:HD2	1:A:424:SER:OG	1.71	0.73
1:B:517:MET:HE3	1:B:529:LEU:HD13	1.71	0.73
1:A:595:PRO:HA	1:A:596:THR:N	2.02	0.73
1:B:370:SER:HB3	1:B:373:LYS:HB2	1.71	0.72
1:B:365:LEU:HD13	1:B:408:VAL:HG13	1.71	0.72
1:A:441:ASP:HB2	1:A:442:PRO:CD	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:LEU:HG	1:A:593:HIS:N	2.04	0.72
1:B:460:GLN:NE2	1:B:461:ARG:HG3	2.05	0.72
1:B:509:THR:HG22	1:B:513:LEU:HD22	1.72	0.71
1:A:443:THR:HG1	1:A:444:PHE:N	1.89	0.71
1:B:411:THR:HG22	1:B:413:ALA:H	1.55	0.71
1:A:360:LYS:HD2	1:A:386:ILE:HG12	1.72	0.71
1:B:442:PRO:HD3	1:B:601:ARG:HH12	1.55	0.71
1:A:332:SER:HA	1:A:462:ARG:HH22	1.57	0.70
1:B:442:PRO:HG3	1:B:611:LEU:CD2	2.22	0.70
1:B:588:LEU:HD23	1:B:588:LEU:H	1.58	0.69
1:B:588:LEU:HA	1:B:591:THR:OG1	1.92	0.69
1:A:464:ARG:HA	1:A:467:ARG:NH2	2.07	0.69
1:A:255:GLY:O	1:A:256:VAL:HB	1.93	0.69
1:A:358:VAL:HG23	1:A:359:ILE:HG23	1.74	0.69
1:B:191:PRO:HG3	1:B:200:ALA:HB1	1.74	0.69
1:B:202:LEU:HD13	1:B:204:ALA:HB3	1.75	0.69
1:A:360:LYS:HE3	1:A:361:GLY:H	1.58	0.68
1:A:587:ARG:O	1:A:590:PRO:HD2	1.93	0.68
1:B:215:PRO:HB2	1:B:265:ILE:HD11	1.74	0.68
1:A:238:PHE:O	1:A:242:MET:HG2	1.94	0.68
1:A:232:VAL:HG23	1:A:254:THR:HG21	1.76	0.68
1:B:288:ILE:HG12	1:B:319:VAL:HG13	1.75	0.67
1:A:388:ALA:HA	1:A:407:VAL:O	1.94	0.67
1:B:589:LYS:HB2	1:B:590:PRO:HD3	1.74	0.67
1:A:347:ILE:HG23	1:A:354:ILE:O	1.95	0.67
1:A:332:SER:HA	1:A:462:ARG:NH2	2.10	0.66
1:A:411:THR:HG22	1:A:412:ASP:H	1.60	0.66
1:B:229:ASN:O	1:B:269:THR:HA	1.96	0.65
1:B:464:ARG:HA	1:B:467:ARG:CZ	2.25	0.65
1:B:574:PRO:O	1:B:596:THR:HB	1.96	0.65
1:B:356:LEU:HA	1:B:359:ILE:HG12	1.78	0.65
1:B:612:THR:O	1:B:617:LYS:HE2	1.97	0.65
1:B:424:SER:HB2	1:B:472:ILE:HG23	1.77	0.65
1:B:587:ARG:O	1:B:587:ARG:HG2	1.97	0.65
1:B:460:GLN:HE22	1:B:461:ARG:HG3	1.62	0.64
1:B:364:HIS:HD2	1:B:424:SER:HB3	1.62	0.64
1:A:445:THR:HG23	1:A:601:ARG:HB2	1.81	0.63
1:A:229:ASN:HB3	3:A:1303:HOH:O	1.98	0.63
1:A:282:GLY:HA2	1:A:313:ALA:O	1.97	0.63
1:B:596:THR:HG22	1:B:607:ASN:OD1	1.98	0.63
1:A:367:PHE:HZ	1:A:464:ARG:HH11	1.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLU:CG	1:A:356:LEU:HD23	2.29	0.62
1:B:480:GLU:C	1:B:481:ARG:HG3	2.19	0.62
1:A:596:THR:HG22	1:A:607:ASN:OD1	2.00	0.62
1:A:526:GLN:HG2	1:B:452:PRO:HD3	1.82	0.62
1:B:203:HIS:CD2	1:B:322:THR:HG22	2.35	0.62
1:B:441:ASP:HB2	1:B:601:ARG:NH1	2.15	0.62
1:A:355:PRO:O	1:A:358:VAL:HG22	1.99	0.61
1:A:439:SER:OG	1:A:441:ASP:OD1	2.13	0.61
1:B:454:ASP:HB2	1:B:481:ARG:O	2.00	0.61
1:A:279:CYS:O	1:A:281:GLY:N	2.31	0.60
1:A:419:THR:HG23	1:A:467:ARG:HH22	1.65	0.60
1:B:202:LEU:HB2	1:B:319:VAL:CG2	2.31	0.60
1:A:441:ASP:CB	1:A:442:PRO:CD	2.80	0.59
1:A:254:THR:HG22	1:A:256:VAL:HG12	1.82	0.59
1:A:360:LYS:HE3	1:A:361:GLY:N	2.17	0.59
1:B:482:PRO:HD2	3:B:1079:HOH:O	2.01	0.59
1:A:239:GLY:HA3	1:A:252:ILE:HD11	1.84	0.59
1:A:354:ILE:HD11	1:A:426:ILE:HG21	1.84	0.58
1:B:365:LEU:CD1	1:B:408:VAL:HG13	2.34	0.58
1:A:590:PRO:O	1:A:592:LEU:HD23	2.04	0.58
1:B:377:LEU:HD22	1:B:381:LEU:HD13	1.85	0.58
1:A:252:ILE:HD13	1:A:267:TYR:HB2	1.86	0.57
1:A:333:HIS:HE1	1:A:336:ILE:HD12	1.69	0.57
1:B:517:MET:HE3	1:B:529:LEU:HD11	1.87	0.57
1:A:439:SER:O	1:A:440:LEU:HB2	2.05	0.57
1:B:393:ARG:HA	1:B:393:ARG:NE	2.20	0.57
1:B:364:HIS:CD2	1:B:424:SER:HB3	2.40	0.57
1:B:364:HIS:HB2	1:B:407:VAL:HG22	1.87	0.57
1:B:365:LEU:O	1:B:425:VAL:HA	2.05	0.56
1:A:598:LEU:HG	1:A:609:VAL:HG11	1.87	0.56
1:B:224:LYS:HD2	1:B:283:ALA:O	2.05	0.56
1:B:336:ILE:HD13	1:B:470:PRO:O	2.06	0.56
1:A:589:LYS:HB3	1:A:590:PRO:HD3	1.88	0.56
1:B:324:THR:HG23	1:B:324:THR:O	2.06	0.56
1:A:194:PRO:O	1:A:316:ARG:HD3	2.06	0.56
1:B:324:THR:HG21	1:B:456:VAL:CG2	2.36	0.56
1:A:545:HIS:O	1:A:549:GLN:HG3	2.06	0.56
1:B:531:PHE:O	1:B:535:VAL:HG13	2.06	0.56
1:B:360:LYS:HD3	1:B:386:ILE:HG13	1.88	0.55
1:A:197:PHE:HA	1:A:316:ARG:O	2.06	0.55
1:A:574:PRO:O	1:A:596:THR:HB	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ASN:ND2	1:B:290:ASP:HB3	2.21	0.55
1:B:419:THR:HG23	1:B:467:ARG:HD2	1.89	0.55
1:B:451:LEU:HB2	3:B:1150:HOH:O	2.06	0.55
1:B:225:VAL:HG12	1:B:286:ILE:CB	2.32	0.55
1:B:585:LEU:O	1:B:587:ARG:HD2	2.07	0.55
1:A:239:GLY:CA	1:A:252:ILE:HD11	2.36	0.55
1:B:508:GLU:O	1:B:512:ARG:HD3	2.06	0.55
1:B:589:LYS:HB2	1:B:590:PRO:CD	2.37	0.55
1:A:474:ARG:HH11	1:A:474:ARG:HG2	1.72	0.55
1:A:347:ILE:CG1	1:A:354:ILE:HB	2.27	0.54
1:A:232:VAL:CG2	1:A:254:THR:HG21	2.37	0.54
1:A:439:SER:CB	1:A:441:ASP:OD1	2.54	0.54
1:B:473:TYR:CE2	1:B:475:PHE:HB3	2.42	0.54
1:B:425:VAL:HG22	1:B:465:THR:HB	1.89	0.53
1:A:411:THR:HG22	1:A:412:ASP:N	2.23	0.53
1:A:356:LEU:CD1	1:A:386:ILE:HD11	2.39	0.53
1:A:425:VAL:HG22	1:A:473:TYR:HD1	1.73	0.53
1:A:350:TYR:HB2	1:A:476:VAL:HG21	1.91	0.53
1:B:362:GLY:O	1:B:405:ASP:HA	2.08	0.53
1:B:202:LEU:HB2	1:B:319:VAL:HG21	1.90	0.53
1:B:446:ILE:HG21	1:B:557:PHE:CE2	2.43	0.53
1:A:360:LYS:CD	1:A:386:ILE:HG12	2.38	0.53
1:A:616:THR:HG22	1:A:620:MET:CE	2.39	0.53
1:B:396:ASP:CG	1:B:397:VAL:H	2.12	0.53
1:B:616:THR:O	1:B:620:MET:HG3	2.09	0.53
1:A:366:ILE:CG1	1:A:426:ILE:HD13	2.34	0.52
1:A:374:CYS:SG	1:A:410:SER:HA	2.50	0.52
1:A:451:LEU:HB3	1:A:452:PRO:HD2	1.92	0.52
1:B:346:GLU:C	1:B:348:PRO:HD3	2.29	0.52
1:A:373:LYS:O	1:A:377:LEU:HB2	2.09	0.52
1:A:616:THR:HG22	1:A:620:MET:HE2	1.91	0.52
1:B:356:LEU:H	1:B:356:LEU:CD2	2.23	0.52
1:B:341:LEU:HD12	1:B:474:ARG:CG	2.39	0.52
1:A:583:LYS:O	1:A:586:ILE:HG13	2.10	0.51
1:B:347:ILE:HD11	1:B:384:LEU:CD1	2.37	0.51
1:B:363:ARG:NH2	1:B:400:ILE:O	2.43	0.51
1:A:363:ARG:HA	1:A:406:VAL:O	2.10	0.51
1:B:356:LEU:H	1:B:356:LEU:HD23	1.74	0.51
1:B:572:GLN:NE2	1:B:590:PRO:HB2	2.25	0.51
1:B:578:TRP:HZ2	1:B:588:LEU:HB3	1.72	0.51
1:B:615:ILE:O	1:B:619:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:PRO:HG3	1:B:200:ALA:CB	2.39	0.51
1:B:202:LEU:O	1:B:321:ALA:HA	2.11	0.51
1:B:204:ALA:O	1:B:210:LYS:HD2	2.11	0.51
1:B:443:THR:HG21	1:B:619:ILE:HB	1.93	0.51
1:A:329:VAL:HG12	1:A:482:PRO:HG3	1.92	0.50
1:B:230:PRO:HD2	1:B:291:GLU:OE1	2.12	0.50
1:A:439:SER:HB2	1:A:441:ASP:OD1	2.11	0.50
1:B:460:GLN:NE2	3:B:1011:HOH:O	2.44	0.50
1:A:327:GLY:CA	1:B:482:PRO:HG2	2.37	0.50
1:B:365:LEU:HD13	1:B:408:VAL:CG1	2.40	0.50
1:A:201:HIS:CE1	1:A:520:PRO:O	2.65	0.50
1:B:473:TYR:CE2	1:B:475:PHE:CD2	3.00	0.50
1:A:229:ASN:O	1:A:269:THR:HA	2.12	0.49
1:B:193:VAL:HG21	1:B:223:TYR:CE2	2.47	0.49
1:B:335:ASN:ND2	1:B:470:PRO:HA	2.26	0.49
1:B:336:ILE:CD1	1:B:465:THR:HG23	2.39	0.49
1:B:265:ILE:HG23	1:B:265:ILE:O	2.12	0.49
1:B:338:GLU:HG2	1:B:473:TYR:HB3	1.95	0.49
1:B:364:HIS:O	1:B:408:VAL:HG12	2.11	0.49
1:B:446:ILE:HG21	1:B:557:PHE:HE2	1.77	0.49
1:B:336:ILE:HD12	1:B:465:THR:CG2	2.39	0.49
1:A:347:ILE:HA	1:A:380:LYS:HE3	1.94	0.49
1:A:441:ASP:HB3	1:A:601:ARG:HH11	1.77	0.49
1:B:391:TYR:CD1	1:B:391:TYR:C	2.86	0.49
1:A:193:VAL:HG11	1:A:286:ILE:HD11	1.95	0.49
1:A:213:LYS:HG3	3:A:1261:HOH:O	2.11	0.49
1:A:366:ILE:HG12	1:A:426:ILE:CD1	2.37	0.49
1:A:575:PRO:HD3	1:A:585:LEU:HD23	1.95	0.49
1:A:299:SER:O	1:A:303:ILE:HG13	2.12	0.49
1:A:330:THR:HG23	1:A:480:GLU:OE1	2.13	0.49
1:A:443:THR:CB	1:A:444:PHE:N	2.76	0.49
1:B:512:ARG:NH1	3:B:1152:HOH:O	2.46	0.49
1:A:380:LYS:O	1:A:384:LEU:HD23	2.13	0.49
1:A:442:PRO:HB3	1:A:611:LEU:HD22	1.95	0.49
1:B:214:VAL:N	1:B:215:PRO:CD	2.75	0.49
1:B:345:GLY:HA3	1:B:354:ILE:O	2.12	0.49
1:B:378:ALA:O	1:B:382:VAL:HG23	2.13	0.49
1:A:338:GLU:HG2	1:A:473:TYR:HB3	1.94	0.49
1:A:363:ARG:HG3	3:A:1197:HOH:O	2.13	0.48
1:A:356:LEU:HD13	1:A:386:ILE:HD11	1.95	0.48
1:B:462:ARG:O	1:B:465:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ASN:ND2	1:A:608:GLU:H	2.11	0.48
1:A:303:ILE:O	1:A:307:LEU:HG	2.12	0.48
1:B:442:PRO:CG	1:B:611:LEU:HD22	2.33	0.48
1:A:193:VAL:CG1	1:A:286:ILE:HD11	2.44	0.48
1:B:442:PRO:HD2	3:B:1003:HOH:O	2.14	0.48
1:B:462:ARG:O	1:B:462:ARG:HG2	2.14	0.48
1:A:366:ILE:O	1:A:409:VAL:HA	2.13	0.48
1:A:590:PRO:C	1:A:592:LEU:H	2.16	0.48
1:A:214:VAL:HB	1:A:215:PRO:HD3	1.95	0.47
1:B:441:ASP:CB	1:B:601:ARG:NH1	2.77	0.47
1:A:202:LEU:O	1:A:321:ALA:HA	2.14	0.47
1:B:416:THR:HG22	1:B:467:ARG:HH22	1.79	0.47
1:B:391:TYR:C	1:B:391:TYR:HD1	2.17	0.47
1:B:473:TYR:CZ	1:B:475:PHE:HB3	2.50	0.47
1:B:442:PRO:HD3	1:B:601:ARG:HH11	1.78	0.47
1:A:571:ALA:O	1:A:572:GLN:HB2	2.15	0.47
1:A:526:GLN:HE21	1:A:526:GLN:HA	1.78	0.47
1:A:193:VAL:HG21	1:A:223:TYR:OH	2.14	0.47
1:A:355:PRO:HG2	1:A:358:VAL:HG13	1.96	0.47
1:B:431:CYS:O	1:B:450:THR:HA	2.14	0.47
1:A:201:HIS:HE1	1:A:520:PRO:O	1.98	0.47
1:A:350:TYR:OH	1:A:369:HIS:HD2	1.98	0.47
1:B:335:ASN:CG	1:B:470:PRO:HA	2.34	0.47
1:A:433:THR:OG1	1:A:451:LEU:HD12	2.15	0.46
1:B:598:LEU:HG	1:B:609:VAL:HG11	1.97	0.46
1:A:623:MET:O	1:A:627:LEU:HB2	2.15	0.46
1:B:480:GLU:O	1:B:481:ARG:HG3	2.15	0.46
1:B:517:MET:CE	1:B:529:LEU:HD13	2.44	0.46
1:A:377:LEU:HD13	1:A:381:LEU:HD22	1.97	0.46
1:A:382:VAL:HA	1:A:386:ILE:O	2.15	0.46
1:B:349:PHE:HB2	1:B:354:ILE:HG13	1.98	0.46
1:B:391:TYR:HD1	1:B:392:TYR:N	2.14	0.46
1:B:620:MET:O	1:B:623:MET:HB2	2.16	0.46
1:B:193:VAL:HG22	1:B:286:ILE:HD11	1.97	0.46
1:B:355:PRO:HB2	1:B:358:VAL:HG13	1.97	0.46
1:A:239:GLY:HA2	1:A:250:PRO:HG3	1.97	0.45
1:B:358:VAL:HG23	1:B:359:ILE:HG23	1.96	0.45
1:B:516:TYR:OH	1:B:523:PRO:HG2	2.15	0.45
1:A:474:ARG:HG2	1:A:474:ARG:NH1	2.31	0.45
1:B:595:PRO:HA	1:B:608:GLU:O	2.16	0.45
1:A:420:GLY:HA2	1:A:467:ARG:CZ	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:GLN:O	1:B:464:ARG:HG3	2.16	0.45
1:A:390:ALA:HA	1:A:409:VAL:O	2.16	0.45
1:B:307:LEU:HD13	1:B:519:THR:OG1	2.17	0.45
1:B:424:SER:CB	1:B:472:ILE:HG23	2.44	0.45
1:A:454:ASP:HA	1:A:481:ARG:O	2.17	0.44
1:B:210:LYS:HA	1:B:214:VAL:HB	1.99	0.44
1:B:337:GLU:O	1:B:472:ILE:HG13	2.16	0.44
1:A:464:ARG:HA	1:A:467:ARG:HH21	1.80	0.44
1:A:574:PRO:HG2	1:A:607:ASN:OD1	2.17	0.44
1:B:218:TYR:HB2	1:B:225:VAL:HG11	1.97	0.44
1:B:332:SER:O	1:B:334:PRO:HD3	2.17	0.44
1:B:361:GLY:O	1:B:364:HIS:HE1	1.99	0.44
1:A:236:LEU:HD23	1:A:252:ILE:HG21	2.00	0.44
1:B:356:LEU:HA	1:B:359:ILE:CG1	2.46	0.44
1:A:378:ALA:O	1:A:382:VAL:HG23	2.18	0.44
1:A:563:TYR:O	1:A:567:VAL:HG13	2.18	0.44
1:B:356:LEU:HD23	1:B:356:LEU:N	2.31	0.44
1:B:473:TYR:CE2	1:B:475:PHE:HD2	2.36	0.44
1:A:255:GLY:N	1:A:272:LYS:HG3	2.33	0.44
1:A:592:LEU:O	1:A:593:HIS:C	2.55	0.44
1:B:352:LYS:CD	1:B:476:VAL:HG13	2.48	0.44
1:A:327:GLY:HA2	1:B:482:PRO:CG	2.44	0.44
1:B:348:PRO:HA	1:B:353:ALA:HA	1.99	0.44
1:A:239:GLY:HA2	1:A:250:PRO:CG	2.48	0.44
1:A:420:GLY:HA2	1:A:467:ARG:NH2	2.32	0.44
1:B:330:THR:HG22	3:B:1149:HOH:O	2.17	0.44
1:B:347:ILE:HD12	1:B:381:LEU:HD12	2.00	0.44
1:B:589:LYS:O	1:B:592:LEU:HD22	2.18	0.44
1:B:189:SER:HB3	1:B:190:PRO:HD2	2.00	0.43
1:B:543:ASP:OD1	1:B:545:HIS:HB2	2.18	0.43
1:A:347:ILE:HA	1:A:348:PRO:HD3	1.87	0.43
1:B:488:SER:O	1:B:491:LEU:HB2	2.18	0.43
1:A:595:PRO:C	1:A:596:THR:HA	2.36	0.43
1:B:329:VAL:HA	1:B:455:ALA:CB	2.48	0.43
1:B:592:LEU:O	1:B:594:GLY:N	2.51	0.43
1:A:517:MET:SD	1:A:529:LEU:HD11	2.59	0.43
1:B:202:LEU:HB2	1:B:319:VAL:HG23	2.00	0.43
1:A:365:LEU:O	1:A:425:VAL:HA	2.19	0.43
1:A:481:ARG:HD3	1:B:485:MET:CE	2.48	0.43
1:A:598:LEU:HG	1:A:609:VAL:CG1	2.48	0.43
1:A:206:THR:HA	1:A:210:LYS:HZ1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:PHE:HB3	1:A:267:TYR:CE1	2.54	0.43
1:A:307:LEU:HD13	1:A:519:THR:OG1	2.18	0.43
1:B:225:VAL:CG2	1:B:265:ILE:HG13	2.49	0.43
1:A:225:VAL:HA	1:A:286:ILE:O	2.18	0.43
1:A:202:LEU:HD13	1:A:210:LYS:HG2	2.01	0.43
1:B:391:TYR:CD1	1:B:392:TYR:N	2.87	0.43
1:A:191:PRO:HD3	1:A:202:LEU:HG	2.00	0.42
1:A:374:CYS:O	1:A:409:VAL:HG21	2.18	0.42
1:A:255:GLY:O	1:A:256:VAL:CB	2.65	0.42
1:A:305:THR:O	1:A:309:GLN:HG3	2.20	0.42
1:A:493:GLU:HG3	1:A:557:PHE:CE1	2.54	0.42
1:B:422:PHE:O	1:B:466:GLY:N	2.51	0.42
1:B:392:TYR:HB3	1:B:411:THR:HB	2.02	0.42
1:A:579:ASP:OD2	1:A:581:MET:HB3	2.20	0.42
1:B:193:VAL:CG2	1:B:286:ILE:HD11	2.50	0.42
1:A:371:LYS:HE3	1:A:392:TYR:CE1	2.55	0.42
1:A:623:MET:HG2	1:A:627:LEU:CD2	2.50	0.42
1:B:416:THR:O	1:B:467:ARG:NH1	2.53	0.42
1:B:546:PHE:O	1:B:550:THR:HG23	2.20	0.42
1:B:210:LYS:HE2	1:B:210:LYS:HB2	1.90	0.42
1:B:485:MET:HB2	1:B:524:VAL:O	2.19	0.42
1:A:197:PHE:HD1	1:A:315:ALA:O	2.03	0.41
1:A:535:VAL:O	1:A:539:LEU:HD13	2.20	0.41
1:B:486:PHE:CZ	1:B:525:CYS:SG	3.13	0.41
1:B:504:LEU:HD21	1:B:512:ARG:CZ	2.50	0.41
1:B:360:LYS:HD2	1:B:360:LYS:HA	1.80	0.41
1:A:373:LYS:HB2	1:A:373:LYS:HE2	1.79	0.41
1:A:485:MET:HA	1:A:524:VAL:O	2.21	0.41
1:A:539:LEU:HG	1:A:563:TYR:CD2	2.55	0.41
1:A:251:ASN:ND2	1:A:251:ASN:H	2.18	0.41
1:A:433:THR:O	1:A:448:THR:HA	2.20	0.41
1:A:435:THR:HA	1:A:487:ASP:OD2	2.21	0.41
1:A:440:LEU:C	1:A:441:ASP:O	2.57	0.41
1:A:462:ARG:O	1:A:465:THR:HG22	2.20	0.41
1:B:480:GLU:HB3	3:B:1028:HOH:O	2.20	0.41
1:A:363:ARG:HG2	1:A:404:GLY:O	2.20	0.41
1:A:254:THR:CG2	1:A:256:VAL:HG12	2.51	0.41
1:B:363:ARG:HA	1:B:406:VAL:O	2.20	0.41
1:A:261:THR:O	1:A:262:GLY:C	2.59	0.41
1:A:425:VAL:HG22	1:A:473:TYR:CD1	2.55	0.41
1:B:481:ARG:O	1:B:483:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ILE:HG21	1:B:403:ASN:CG	2.42	0.40
1:B:427:ASP:HB2	1:B:473:TYR:CE1	2.56	0.40
1:B:341:LEU:HD12	1:B:474:ARG:HD2	2.02	0.40
1:A:327:GLY:CA	1:B:482:PRO:CG	3.00	0.40
1:A:566:THR:O	1:A:570:ARG:CG	2.66	0.40
1:A:574:PRO:HD2	1:A:594:GLY:O	2.21	0.40
1:B:486:PHE:CE1	1:B:525:CYS:HB3	2.56	0.40
1:A:525:CYS:SG	1:A:526:GLN:N	2.94	0.40
1:A:529:LEU:N	1:A:529:LEU:HD12	2.37	0.40
1:B:572:GLN:O	1:B:593:HIS:ND1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/451 (98%)	394 (89%)	37 (8%)	10 (2%)	6	2
1	B	408/451 (90%)	351 (86%)	40 (10%)	17 (4%)	3	0
All	All	849/902 (94%)	745 (88%)	77 (9%)	27 (3%)	4	1

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	VAL
1	A	262	GLY
1	A	441	ASP
1	A	587	ARG
1	B	393	ARG
1	B	441	ASP
1	B	593	HIS
1	A	331	VAL

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Mol	Chain	Res	Type
1	A	397	VAL
1	A	594	GLY
1	B	212	THR
1	B	265	ILE
1	B	281	GLY
1	B	335	ASN
1	B	594	GLY
1	A	591	THR
1	B	480	GLU
1	A	279	CYS
1	B	397	VAL
1	B	405	ASP
1	B	419	THR
1	B	442	PRO
1	B	580	GLN
1	A	334	PRO
1	B	215	PRO
1	B	205	PRO
1	B	351	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	363/371 (98%)	313 (86%)	50 (14%)	3 2
1	B	340/371 (92%)	300 (88%)	40 (12%)	5 2
All	All	703/742 (95%)	613 (87%)	90 (13%)	4 2

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	202	LEU
1	A	211	SER
1	A	225	VAL

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Mol	Chain	Res	Type
1	A	244	LYS
1	A	248	VAL
1	A	280	SER
1	A	291	GLU
1	A	319	VAL
1	A	328	SER
1	A	331	VAL
1	A	346	GLU
1	A	347	ILE
1	A	356	LEU
1	A	360	LYS
1	A	363	ARG
1	A	373	LYS
1	A	377	LEU
1	A	380	LYS
1	A	381	LEU
1	A	392	TYR
1	A	393	ARG
1	A	396	ASP
1	A	408	VAL
1	A	415	MET
1	A	425	VAL
1	A	433	THR
1	A	439	SER
1	A	450	THR
1	A	456	VAL
1	A	460	GLN
1	A	467	ARG
1	A	506	PRO
1	A	508	GLU
1	A	513	LEU
1	A	523	PRO
1	A	526	GLN
1	A	535	VAL
1	A	556	ASN
1	A	570	ARG
1	A	579	ASP
1	A	585	LEU
1	A	587	ARG
1	A	588	LEU
1	A	592	LEU
1	A	596	THR

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Mol	Chain	Res	Type
1	A	598	LEU
1	A	599	LEU
1	A	600	TYR
1	A	627	LEU
1	B	202	LEU
1	B	208	SER
1	B	210	LYS
1	B	212	THR
1	B	274	LEU
1	B	319	VAL
1	B	320	LEU
1	B	330	THR
1	B	333	HIS
1	B	341	LEU
1	B	356	LEU
1	B	371	LYS
1	B	377	LEU
1	B	386	ILE
1	B	391	TYR
1	B	392	TYR
1	B	397	VAL
1	B	398	SER
1	B	410	SER
1	B	411	THR
1	B	416	THR
1	B	425	VAL
1	B	441	ASP
1	B	472	ILE
1	B	480	GLU
1	B	481	ARG
1	B	485	MET
1	B	504	LEU
1	B	513	LEU
1	B	535	VAL
1	B	539	LEU
1	B	555	GLU
1	B	587	ARG
1	B	588	LEU
1	B	596	THR
1	B	598	LEU
1	B	599	LEU
1	B	600	TYR

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Mol	Chain	Res	Type
1	B	624	SER
1	B	627	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	HIS
1	A	221	GLN
1	A	229	ASN
1	A	246	HIS
1	A	293	HIS
1	A	333	HIS
1	A	364	HIS
1	A	369	HIS
1	A	526	GLN
1	A	549	GLN
1	A	556	ASN
1	B	198	GLN
1	B	201	HIS
1	B	203	HIS
1	B	364	HIS
1	B	369	HIS
1	B	460	GLN
1	B	518	ASN
1	B	541	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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	443:THR	C	444:PHE	N	1.81
1	A	595:PRO	C	596:THR	N	1.70
1	A	279:CYS	C	280:SER	N	1.07

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.