



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:32 AM UTC

PDB ID : 1JF6 / pdb_00001jf6
Title : Crystal structure of thermoactinomyces vulgaris r-47 alpha-amylase mutant F286Y
Authors : Ohtaki, A.; Kondo, S.; Shimura, Y.; Tonozuka, T.; Sakano, Y.; Kamitori, S.
Deposited on : 2001-06-20
Resolution : 3.20 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

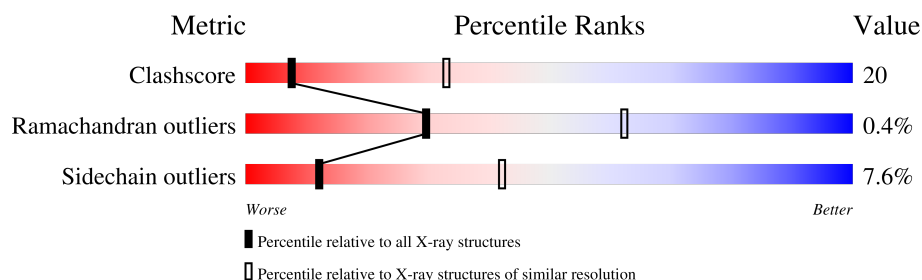
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	585	 56% 39% .
1	B	585	 58% 38% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9556 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 ALPHA AMYLASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4777	3056	831	875	15			
1	B	585	Total	C	N	O	S	0	0	0
			4777	3056	831	875	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	TYR	PHE	engineered mutation	UNP Q08751
B	286	TYR	PHE	engineered mutation	UNP Q08751

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

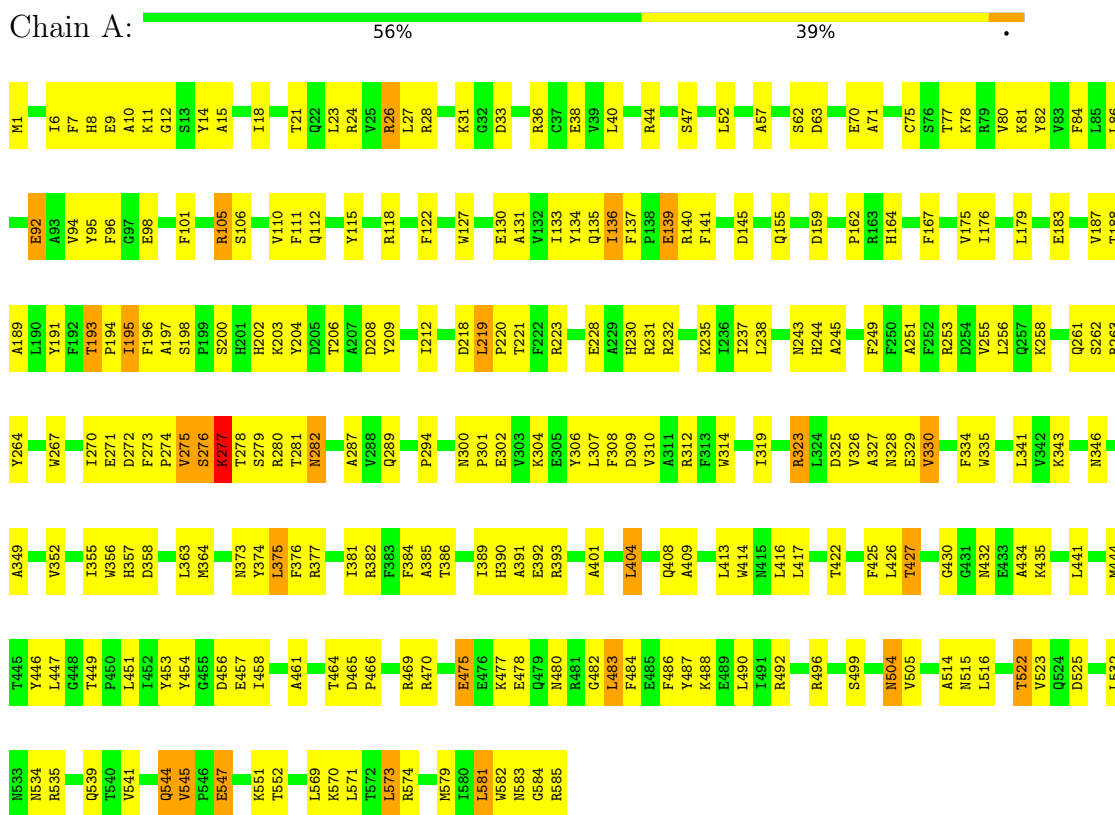
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

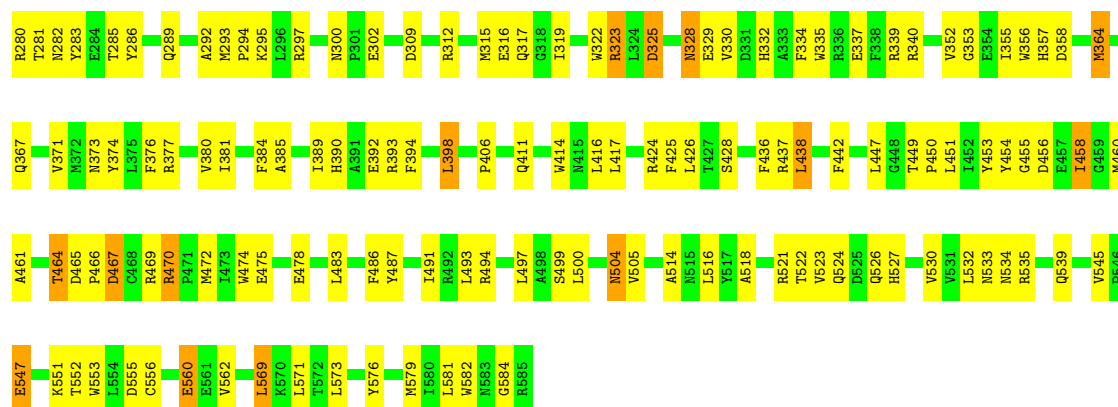
3 Residue-property plots

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: ALPHA AMYLASE II





4 Data and refinement statistics

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	112.25Å 117.94Å 113.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.39 – 3.20	Depositor
% Data completeness (in resolution range)	91.7 (38.39-3.20)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9556	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.60	0/4907	1.00	12/6643 (0.2%)
1	B	0.60	0/4907	0.98	12/6643 (0.2%)
All	All	0.60	0/9814	0.99	24/13286 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	145	ASP	CA-C-N	9.74	129.50	119.56
1	A	145	ASP	C-N-CA	9.74	129.50	119.56
1	A	18	ILE	N-CA-C	-8.57	105.13	113.53
1	B	18	ILE	N-CA-C	-6.85	105.97	113.43
1	B	213	ASP	CA-C-N	6.50	127.01	119.47
1	B	213	ASP	C-N-CA	6.50	127.01	119.47
1	B	417	LEU	N-CA-C	-6.18	105.88	113.41
1	B	88	GLY	CA-C-N	5.88	125.57	119.05
1	B	88	GLY	C-N-CA	5.88	125.57	119.05
1	B	161	ARG	CA-C-N	5.74	125.67	119.76
1	B	161	ARG	C-N-CA	5.74	125.67	119.76
1	A	287	ALA	CB-CA-C	-5.67	110.02	116.54
1	A	136	ILE	N-CA-C	5.58	116.13	107.99
1	A	482	GLY	N-CA-C	-5.57	105.75	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	581	LEU	N-CA-C	5.49	117.68	108.96
1	A	391	ALA	N-CA-C	5.41	117.87	111.33
1	B	80	VAL	N-CA-C	5.35	116.07	108.42
1	B	67	ASP	N-CA-C	-5.32	101.49	109.95
1	A	47	SER	CA-C-N	5.12	124.83	119.82
1	A	47	SER	C-N-CA	5.12	124.83	119.82
1	B	394	PHE	N-CA-C	-5.08	105.63	111.07
1	A	275	VAL	N-CA-C	5.06	114.47	106.32
1	A	522	THR	N-CA-C	5.04	117.63	109.06
1	B	270	ILE	N-CA-C	5.01	115.31	107.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	14	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	4777	0	4607	192	0
1	B	4777	0	4607	191	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	9556	0	9214	379	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 (379) 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:328:ASN:HB3	1:A:355:ILE:HD12	1.40	1.02
1:A:255:VAL:HA	1:A:262:SER:OG	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PRO:HG2	1:A:470:ARG:HA	1.60	0.83
1:B:26:ARG:HG2	1:B:70:GLU:HG2	1.62	0.81
1:A:197:ALA:HB3	1:A:208:ASP:HB3	1.62	0.79
1:A:416:LEU:H	1:A:416:LEU:HD23	1.47	0.79
1:B:328:ASN:HB3	1:B:355:ILE:HG12	1.67	0.76
1:B:499:SER:HB3	1:B:523:VAL:HG12	1.67	0.75
1:B:247:ASP:HB3	1:B:292:ALA:HA	1.69	0.73
1:B:255:VAL:O	1:B:275:VAL:HG21	1.89	0.72
1:B:569:LEU:HD23	1:B:571:LEU:HD21	1.69	0.72
1:A:401:ALA:O	1:A:404:LEU:HB2	1.90	0.72
1:B:26:ARG:HG2	1:B:70:GLU:CG	2.21	0.70
1:B:138:PRO:HG3	1:B:195:ILE:HG22	1.73	0.70
1:A:582:TRP:CZ2	1:A:584:GLY:HA2	2.27	0.70
1:B:467:ASP:CG	1:B:470:ARG:HH12	2.00	0.69
1:A:275:VAL:O	1:A:276:SER:HB2	1.91	0.69
1:A:133:ILE:HG13	1:A:189:ALA:HB3	1.76	0.68
1:A:514:ALA:HB1	1:A:539:GLN:HE22	1.59	0.68
1:A:98:GLU:OE2	1:B:357:HIS:HB2	1.94	0.67
1:B:504:ASN:C	1:B:504:ASN:HD22	2.00	0.67
1:B:202:HIS:CD2	1:B:204:TYR:HB2	2.30	0.66
1:B:198:SER:HB3	1:B:203:LYS:HG3	1.77	0.66
1:A:583:ASN:HD21	1:A:585:ARG:HD2	1.61	0.66
1:B:312:ARG:O	1:B:316:GLU:HG3	1.97	0.65
1:A:195:ILE:O	1:A:196:PHE:HD2	1.79	0.65
1:B:228:GLU:O	1:B:231:ARG:HG2	1.97	0.65
1:B:573:LEU:HD13	1:B:579:MET:HE3	1.79	0.65
1:A:92:GLU:O	1:A:92:GLU:HG2	1.97	0.64
1:A:374:TYR:CE1	1:A:375:LEU:HD13	2.33	0.64
1:A:409:ALA:O	1:A:413:LEU:HD13	1.96	0.64
1:A:326:VAL:HG12	1:A:329:GLU:HB2	1.78	0.64
1:B:555:ASP:OD1	1:B:579:MET:HG2	1.98	0.64
1:B:228:GLU:OE2	1:B:231:ARG:HD3	1.96	0.64
1:A:515:ASN:ND2	1:A:534:ASN:HB3	2.12	0.63
1:A:31:LYS:HE2	1:A:63:ASP:O	2.00	0.62
1:A:195:ILE:O	1:A:195:ILE:HG13	2.00	0.61
1:A:243:ASN:HD22	1:A:244:HIS:HD2	1.47	0.61
1:A:426:LEU:HD23	1:A:461:ALA:HB2	1.81	0.61
1:B:447:LEU:HB2	1:B:505:VAL:CG2	2.31	0.61
1:B:353:GLY:O	1:B:371:VAL:HA	2.01	0.61
1:B:453:TYR:HB3	1:B:456:ASP:OD2	2.01	0.61
1:A:253:ARG:HA	1:A:256:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ILE:O	1:A:385:ALA:HB3	2.02	0.60
1:B:143:ASN:ND2	1:B:169:GLY:HA3	2.16	0.60
1:A:183:GLU:OE2	1:A:232:ARG:HD3	2.02	0.60
1:A:84:PHE:HB2	1:A:96:PHE:HB3	1.84	0.60
1:A:551:LYS:HG3	1:A:552:THR:HG23	1.84	0.59
1:A:84:PHE:O	1:A:95:TYR:HA	2.01	0.59
1:A:140:ARG:HG2	1:A:469:ARG:O	2.02	0.59
1:A:162:PRO:CG	1:A:470:ARG:HA	2.33	0.58
1:A:535:ARG:HH21	1:A:535:ARG:HG3	1.68	0.58
1:B:82:TYR:C	1:B:110:VAL:HG23	2.29	0.58
1:A:441:LEU:HD22	1:A:532:LEU:HD21	1.84	0.58
1:A:258:LYS:HB3	1:A:261:GLN:HB2	1.85	0.58
1:A:582:TRP:CE2	1:A:584:GLY:HA2	2.38	0.58
1:B:455:GLY:O	1:B:458:ILE:HG13	2.04	0.58
1:A:218:ASP:OD1	1:A:220:PRO:HD2	2.03	0.58
1:A:544:GLN:CD	1:A:544:GLN:N	2.61	0.58
1:B:458:ILE:HD11	1:B:460:MET:HG3	1.85	0.58
1:B:82:TYR:O	1:B:110:VAL:HG23	2.03	0.57
1:B:390:HIS:CE1	1:B:392:GLU:HB2	2.38	0.57
1:A:514:ALA:HB1	1:A:539:GLN:NE2	2.19	0.57
1:B:127:TRP:CD2	1:B:235:LYS:HE3	2.39	0.57
1:B:36:ARG:HB3	1:B:87:THR:HB	1.85	0.57
1:A:134:TYR:HB2	1:A:187:VAL:HG11	1.86	0.57
1:B:136:ILE:HD12	1:B:190:LEU:HG	1.86	0.56
1:B:447:LEU:HB2	1:B:505:VAL:HG21	1.85	0.56
1:B:31:LYS:HG2	1:B:67:ASP:OD1	2.05	0.56
1:A:416:LEU:H	1:A:416:LEU:CD2	2.18	0.56
1:A:277:LYS:HB2	1:A:277:LYS:NZ	2.20	0.56
1:A:574:ARG:HH11	1:A:574:ARG:HB3	1.70	0.56
1:B:240:ALA:HB1	1:B:242:PHE:CE1	2.41	0.56
1:B:259:GLY:HA2	1:B:275:VAL:CG2	2.35	0.56
1:B:436:PHE:HE2	1:B:483:LEU:HD21	1.70	0.56
1:B:465:ASP:OD2	1:B:466:PRO:HA	2.05	0.56
1:A:105:ARG:HG3	1:A:106:SER:N	2.21	0.56
1:B:84:PHE:HB2	1:B:96:PHE:HB3	1.87	0.56
1:A:11:LYS:N	1:A:15:ALA:HB3	2.21	0.55
1:B:12:GLY:HA2	1:B:364:MET:HE2	1.88	0.55
1:B:43:ASP:O	1:B:81:LYS:HE2	2.06	0.55
1:B:273:PHE:HA	1:B:274:PRO:C	2.32	0.55
1:A:122:PHE:O	1:A:408:GLN:HG2	2.07	0.55
1:A:544:GLN:CD	1:A:544:GLN:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PHE:HD1	1:A:175:VAL:HG22	1.73	0.54
1:B:300:ASN:OD1	1:B:302:GLU:N	2.41	0.54
1:B:522:THR:HG23	1:B:527:HIS:CD2	2.43	0.54
1:B:183:GLU:OE2	1:B:232:ARG:HG3	2.07	0.54
1:B:139:GLU:OE2	1:B:140:ARG:NH1	2.40	0.54
1:B:518:ALA:HA	1:B:530:VAL:O	2.07	0.54
1:A:82:TYR:N	1:A:110:VAL:HG23	2.23	0.54
1:A:278:THR:O	1:A:279:SER:HB3	2.07	0.54
1:A:544:GLN:N	1:A:544:GLN:OE1	2.40	0.54
1:B:504:ASN:C	1:B:504:ASN:ND2	2.66	0.54
1:A:570:LYS:O	1:A:571:LEU:HD12	2.07	0.54
1:A:346:ASN:HB3	1:A:349:ALA:HB2	1.89	0.53
1:B:323:ARG:HD2	1:B:323:ARG:C	2.33	0.53
1:B:467:ASP:CG	1:B:470:ARG:NH1	2.66	0.53
1:A:162:PRO:CD	1:A:470:ARG:HG2	2.38	0.53
1:A:276:SER:O	1:A:277:LYS:HB2	2.08	0.53
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.89	0.53
1:A:583:ASN:ND2	1:A:585:ARG:HD2	2.23	0.53
1:A:12:GLY:HA2	1:A:364:MET:HE1	1.90	0.52
1:B:193:THR:O	1:B:194:PRO:C	2.52	0.52
1:A:133:ILE:HD12	1:A:133:ILE:N	2.23	0.52
1:B:26:ARG:NE	1:B:70:GLU:OE2	2.41	0.52
1:B:138:PRO:HG3	1:B:195:ILE:CG2	2.39	0.52
1:A:202:HIS:HB2	1:A:204:TYR:HD2	1.74	0.52
1:B:332:HIS:HD2	1:B:367:GLN:HE22	1.56	0.52
1:A:523:VAL:O	1:A:523:VAL:HG13	2.09	0.52
1:A:135:GLN:HG3	1:A:191:TYR:CD2	2.45	0.52
1:B:332:HIS:CD2	1:B:367:GLN:HE22	2.28	0.52
1:B:197:ALA:HB3	1:B:208:ASP:HB3	1.92	0.51
1:A:309:ASP:OD2	1:A:312:ARG:NH1	2.43	0.51
1:A:579:MET:HE2	1:A:581:LEU:HD21	1.91	0.51
1:B:497:LEU:HB2	1:B:500:LEU:HD12	1.91	0.51
1:B:153:THR:HA	1:B:167:PHE:O	2.10	0.51
1:B:240:ALA:HB2	1:B:322:TRP:CE3	2.45	0.51
1:A:82:TYR:C	1:A:110:VAL:HG23	2.36	0.51
1:A:390:HIS:HD2	1:A:392:GLU:H	1.57	0.51
1:B:389:ILE:HB	1:B:393:ARG:HG2	1.93	0.51
1:A:1:MET:HB2	1:A:33:ASP:OD2	2.11	0.51
1:B:250:PHE:CG	1:B:251:ALA:N	2.79	0.51
1:A:202:HIS:HB2	1:A:204:TYR:CD2	2.46	0.51
1:A:139:GLU:OE2	1:A:140:ARG:NH1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:O	1:A:276:SER:CB	2.57	0.50
1:B:244:HIS:CD2	1:B:286:TYR:HB2	2.47	0.50
1:A:206:THR:HG21	1:A:209:TYR:CD2	2.46	0.50
1:A:488:LYS:HB3	1:A:492:ARG:HH12	1.77	0.50
1:B:8:HIS:CG	1:B:9:GLU:N	2.79	0.50
1:B:193:THR:O	1:B:195:ILE:HG23	2.11	0.50
1:B:352:VAL:HG21	1:B:414:TRP:CZ2	2.46	0.50
1:B:137:PHE:HE1	1:B:469:ARG:HH11	1.58	0.50
1:B:545:VAL:HG21	1:B:569:LEU:HD13	1.93	0.50
1:A:133:ILE:HD13	1:A:449:THR:HG21	1.94	0.50
1:A:230:HIS:C	1:A:232:ARG:N	2.69	0.50
1:B:438:LEU:HD11	1:B:532:LEU:HB3	1.93	0.50
1:B:144:GLY:HA3	1:B:173:LYS:HG3	1.94	0.49
1:A:232:ARG:HH21	1:A:232:ARG:HG3	1.77	0.49
1:A:357:HIS:O	1:A:358:ASP:C	2.55	0.49
1:B:2:LEU:N	1:B:33:ASP:OD2	2.44	0.49
1:B:315:MET:HA	1:B:319:ILE:HG12	1.95	0.49
1:A:304:LYS:HG2	1:A:308:PHE:CE1	2.48	0.49
1:A:335:TRP:HA	1:A:335:TRP:CE3	2.48	0.49
1:A:44:ARG:HA	1:A:81:LYS:HD3	1.94	0.49
1:A:92:GLU:O	1:A:92:GLU:CG	2.60	0.49
1:B:271:GLU:N	1:B:271:GLU:OE2	2.46	0.49
1:A:200:SER:OG	1:A:202:HIS:CE1	2.66	0.49
1:B:436:PHE:CE2	1:B:483:LEU:HD21	2.48	0.49
1:A:118:ARG:NH2	1:B:297:ARG:HH12	2.11	0.49
1:B:92:GLU:H	1:B:92:GLU:CD	2.21	0.49
1:B:218:ASP:OD2	1:B:220:PRO:HD2	2.12	0.49
1:B:255:VAL:HA	1:B:262:SER:HB2	1.95	0.49
1:B:464:THR:O	1:B:465:ASP:C	2.55	0.49
1:B:494:ARG:NH1	1:B:494:ARG:HG3	2.28	0.49
1:B:547:GLU:OE1	1:B:551:LYS:HD2	2.12	0.49
1:A:82:TYR:O	1:A:110:VAL:HG23	2.12	0.49
1:A:356:TRP:HA	1:A:356:TRP:CE3	2.48	0.49
1:B:137:PHE:HE1	1:B:469:ARG:NH1	2.11	0.49
1:A:82:TYR:N	1:A:110:VAL:CG2	2.75	0.48
1:A:195:ILE:O	1:A:195:ILE:CG1	2.59	0.48
1:A:162:PRO:HD3	1:A:470:ARG:HG2	1.94	0.48
1:A:228:GLU:OE2	1:A:231:ARG:HD3	2.13	0.48
1:B:514:ALA:O	1:B:535:ARG:HD2	2.14	0.48
1:A:384:PHE:O	1:A:435:LYS:HD3	2.12	0.48
1:A:516:LEU:HD22	1:A:541:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ALA:CB	1:A:208:ASP:HB3	2.38	0.48
1:A:282:ASN:C	1:A:282:ASN:HD22	2.22	0.48
1:A:432:ASN:OD1	1:A:434:ALA:N	2.46	0.48
1:B:193:THR:HB	1:B:194:PRO:HD2	1.96	0.48
1:B:357:HIS:HA	1:B:374:TYR:OH	2.13	0.48
1:A:356:TRP:HA	1:A:356:TRP:HE3	1.77	0.48
1:B:40:LEU:HD22	1:B:54:HIS:CE1	2.49	0.48
1:B:271:GLU:OE2	1:B:283:TYR:HA	2.14	0.48
1:A:7:PHE:CZ	1:A:9:GLU:HG2	2.49	0.48
1:A:57:ALA:HB2	1:A:71:ALA:HB2	1.96	0.48
1:A:504:ASN:HD21	1:A:522:THR:HB	1.79	0.48
1:A:357:HIS:HB2	1:B:98:GLU:OE2	2.13	0.48
1:A:574:ARG:HB3	1:A:574:ARG:NH1	2.29	0.48
1:B:118:ARG:HA	1:B:121:VAL:HG23	1.96	0.48
1:B:121:VAL:O	1:B:122:PHE:C	2.56	0.48
1:A:416:LEU:HB3	1:A:451:LEU:HD23	1.96	0.47
1:B:281:THR:HG21	1:B:289:GLN:HA	1.96	0.47
1:B:416:LEU:HD23	1:B:416:LEU:H	1.79	0.47
1:A:23:LEU:HD22	1:A:80:VAL:HG11	1.96	0.47
1:B:16:TYR:CE2	1:B:406:PRO:HA	2.49	0.47
1:B:140:ARG:HD2	1:B:469:ARG:O	2.13	0.47
1:A:271:GLU:HG3	1:A:272:ASP:OD2	2.13	0.47
1:B:312:ARG:NH2	1:B:312:ARG:HG3	2.29	0.47
1:A:492:ARG:HD2	1:A:496:ARG:NH1	2.29	0.47
1:A:249:PHE:CE2	1:A:251:ALA:HB3	2.50	0.47
1:A:525:ASP:O	1:A:585:ARG:HD2	2.14	0.47
1:B:494:ARG:HG3	1:B:494:ARG:HH11	1.78	0.47
1:A:270:ILE:HD13	1:A:275:VAL:HG21	1.96	0.47
1:B:77:THR:O	1:B:79:ARG:HG3	2.14	0.47
1:B:278:THR:C	1:B:280:ARG:H	2.23	0.47
1:B:312:ARG:HG3	1:B:312:ARG:HH21	1.80	0.47
1:B:385:ALA:HB1	1:B:428:SER:O	2.15	0.47
1:B:22:GLN:HB3	1:B:72:LEU:HD11	1.97	0.47
1:A:300:ASN:OD1	1:A:301:PRO:HD2	2.15	0.47
1:B:243:ASN:HD22	1:B:329:GLU:HB2	1.80	0.47
1:A:7:PHE:CG	1:A:8:HIS:N	2.83	0.46
1:A:457:GLU:HG2	1:A:458:ILE:N	2.29	0.46
1:A:504:ASN:N	1:A:504:ASN:HD22	2.14	0.46
1:A:573:LEU:N	1:A:573:LEU:HD22	2.30	0.46
1:B:259:GLY:HA2	1:B:275:VAL:HG21	1.98	0.46
1:A:488:LYS:HB3	1:A:492:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:PHE:CD2	1:B:28:ARG:CZ	2.99	0.46
1:B:137:PHE:HD2	1:B:138:PRO:HD2	1.81	0.46
1:A:478:GLU:OE2	1:A:478:GLU:HA	2.16	0.46
1:B:146:PRO:HA	1:B:149:ASP:OD2	2.15	0.46
1:A:454:TYR:CD1	1:A:454:TYR:C	2.93	0.46
1:B:381:ILE:HG12	1:B:425:PHE:HE1	1.81	0.46
1:A:271:GLU:HG3	1:A:272:ASP:CG	2.41	0.46
1:B:269:PHE:CE2	1:B:295:LYS:HG2	2.50	0.46
1:B:285:THR:HB	1:B:293:MET:O	2.16	0.46
1:B:358:ASP:OD1	1:B:358:ASP:C	2.58	0.46
1:B:487:TYR:O	1:B:491:ILE:HG13	2.16	0.46
1:B:253:ARG:HH11	1:B:253:ARG:HB3	1.81	0.46
1:A:24:ARG:HD2	1:A:70:GLU:CG	2.45	0.46
1:A:535:ARG:HG3	1:A:535:ARG:NH2	2.30	0.46
1:B:206:THR:HG21	1:B:209:TYR:CD2	2.51	0.46
1:A:373:ASN:O	1:A:376:PHE:HB3	2.16	0.45
1:A:382:ARG:HA	1:A:386:THR:OG1	2.16	0.45
1:A:373:ASN:HB2	1:A:413:LEU:HB3	1.98	0.45
1:A:486:PHE:CZ	1:A:490:LEU:HD11	2.51	0.45
1:B:193:THR:HB	1:B:194:PRO:CD	2.47	0.45
1:A:27:LEU:C	1:A:27:LEU:HD23	2.42	0.45
1:A:499:SER:HB3	1:A:523:VAL:HG12	1.98	0.45
1:B:330:VAL:HB	1:B:335:TRP:NE1	2.31	0.45
1:B:526:GLN:C	1:B:527:HIS:HD2	2.23	0.45
1:A:326:VAL:HG12	1:A:326:VAL:O	2.15	0.45
1:A:377:ARG:HD2	1:A:417:LEU:C	2.41	0.45
1:A:122:PHE:HE1	1:A:363:LEU:O	1.99	0.45
1:A:327:ALA:O	1:A:330:VAL:HG13	2.17	0.45
1:B:241:VAL:HG13	1:B:325:ASP:HB3	1.99	0.45
1:A:10:ALA:O	1:A:11:LYS:HB3	2.16	0.45
1:B:228:GLU:O	1:B:232:ARG:HD3	2.17	0.45
1:B:381:ILE:HG12	1:B:425:PHE:CE1	2.51	0.45
1:B:582:TRP:CE2	1:B:584:GLY:HA2	2.52	0.45
1:A:230:HIS:C	1:A:232:ARG:H	2.23	0.45
1:A:273:PHE:HA	1:A:274:PRO:C	2.42	0.45
1:B:377:ARG:CZ	1:B:381:ILE:HD11	2.46	0.45
1:B:140:ARG:HG3	1:B:469:ARG:HB3	1.99	0.45
1:B:493:LEU:HD21	1:B:556:CYS:HB3	1.99	0.45
1:A:427:THR:O	1:A:430:GLY:N	2.45	0.45
1:B:18:ILE:HD12	1:B:19:SER:HB3	1.98	0.45
1:B:533:ASN:O	1:B:576:TYR:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ALA:O	1:B:294:PRO:HD2	2.18	0.44
1:B:504:ASN:O	1:B:521:ARG:HA	2.17	0.44
1:B:179:LEU:N	1:B:180:PRO:CD	2.80	0.44
1:A:573:LEU:CD1	1:A:579:MET:SD	3.05	0.44
1:A:7:PHE:CD2	1:A:28:ARG:NH1	2.86	0.44
1:B:202:HIS:O	1:B:203:LYS:HB2	2.17	0.44
1:A:176:ILE:HA	1:A:179:LEU:HG	1.99	0.44
1:A:209:TYR:HB3	1:A:310:VAL:HG11	1.98	0.44
1:B:218:ASP:HB2	1:B:220:PRO:HD2	1.99	0.44
1:B:533:ASN:HB2	1:B:573:LEU:CB	2.47	0.44
1:A:306:TYR:O	1:A:310:VAL:HG23	2.17	0.44
1:B:26:ARG:HE	1:B:70:GLU:CD	2.24	0.44
1:A:112:GLN:HB2	1:B:357:HIS:CD2	2.53	0.44
1:B:437:ARG:HB3	1:B:486:PHE:CE1	2.53	0.44
1:B:315:MET:HG2	1:B:319:ILE:HD11	1.99	0.44
1:A:8:HIS:CG	1:A:9:GLU:N	2.86	0.44
1:A:381:ILE:HD13	1:A:425:PHE:CE1	2.53	0.44
1:B:246:GLY:HA2	1:B:292:ALA:O	2.18	0.44
1:B:245:ALA:O	1:B:293:MET:HA	2.18	0.43
1:B:190:LEU:HD13	1:B:234:ILE:CG2	2.48	0.43
1:B:243:ASN:OD1	1:B:243:ASN:C	2.62	0.43
1:B:553:TRP:HB3	1:B:581:LEU:HB3	2.00	0.43
1:A:12:GLY:H	1:A:364:MET:HE1	1.83	0.43
1:A:6:ILE:HD13	1:A:86:LEU:HD13	2.01	0.43
1:A:127:TRP:O	1:A:131:ALA:HB2	2.18	0.43
1:A:198:SER:HB3	1:A:203:LYS:HD2	2.00	0.43
1:B:110:VAL:HG22	1:B:111:PHE:O	2.18	0.43
1:B:455:GLY:HA2	1:B:472:MET:SD	2.59	0.43
1:A:277:LYS:HG2	1:A:280:ARG:HB3	1.99	0.43
1:A:127:TRP:CG	1:A:235:LYS:HE2	2.54	0.43
1:A:133:ILE:HD13	1:A:449:THR:CG2	2.48	0.43
1:A:465:ASP:OD1	1:A:466:PRO:HA	2.19	0.43
1:B:458:ILE:HG12	1:B:472:MET:HE1	2.01	0.43
1:A:191:TYR:CE1	1:A:323:ARG:HG3	2.54	0.43
1:A:453:TYR:HB3	1:A:456:ASP:OD2	2.18	0.43
1:B:285:THR:HG22	1:B:294:PRO:HA	2.00	0.43
1:A:307:LEU:HD12	1:A:334:PHE:CE2	2.53	0.43
1:A:343:LYS:HE2	1:A:349:ALA:O	2.19	0.43
1:A:352:VAL:HG21	1:A:414:TRP:CZ2	2.53	0.43
1:A:504:ASN:ND2	1:A:522:THR:HB	2.33	0.43
1:A:12:GLY:HA2	1:A:364:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:GLU:HA	1:A:487:TYR:CE1	2.53	0.43
1:A:464:THR:OG1	1:A:465:ASP:N	2.49	0.43
1:A:545:VAL:HG21	1:A:569:LEU:HB2	2.00	0.43
1:B:26:ARG:HA	1:B:69:PHE:O	2.19	0.43
1:B:271:GLU:HB2	1:B:282:ASN:O	2.19	0.43
1:A:191:TYR:HA	1:A:237:ILE:HB	2.01	0.42
1:B:16:TYR:CD1	1:B:16:TYR:C	2.97	0.42
1:A:264:TYR:HD2	1:A:267:TRP:CE2	2.37	0.42
1:B:18:ILE:HD11	1:B:22:GLN:CD	2.44	0.42
1:B:426:LEU:HD23	1:B:461:ALA:HB2	2.01	0.42
1:B:465:ASP:HA	1:B:466:PRO:HA	1.89	0.42
1:A:475:GLU:OE1	1:A:477:LYS:HB2	2.18	0.42
1:B:37:CYS:O	1:B:57:ALA:HB3	2.19	0.42
1:A:78:LYS:HE3	1:A:115:TYR:OH	2.20	0.42
1:A:96:PHE:CD2	1:A:101:PHE:CZ	3.08	0.42
1:B:276:SER:HA	1:B:282:ASN:OD1	2.18	0.42
1:A:232:ARG:HG3	1:A:232:ARG:NH2	2.34	0.42
1:A:453:TYR:O	1:A:454:TYR:C	2.62	0.42
1:B:190:LEU:HD13	1:B:234:ILE:HG21	2.01	0.42
1:A:14:TYR:HA	1:A:26:ARG:HB2	2.00	0.42
1:A:75:CYS:SG	1:A:80:VAL:HB	2.58	0.42
1:B:330:VAL:HG11	1:B:334:PHE:CD1	2.55	0.42
1:B:534:ASN:O	1:B:534:ASN:CG	2.62	0.42
1:A:237:ILE:C	1:A:238:LEU:HD23	2.45	0.42
1:A:358:ASP:C	1:A:358:ASP:OD1	2.63	0.42
1:A:574:ARG:NH1	1:A:574:ARG:CB	2.83	0.42
1:B:206:THR:HG21	1:B:209:TYR:CG	2.55	0.42
1:A:255:VAL:HG22	1:A:262:SER:CB	2.49	0.42
1:A:446:TYR:CG	1:A:447:LEU:N	2.88	0.42
1:B:424:ARG:NH1	1:B:454:TYR:O	2.42	0.42
1:B:373:ASN:ND2	1:B:376:PHE:HB2	2.34	0.42
1:B:398:LEU:HD21	1:B:442:PHE:CZ	2.55	0.42
1:B:499:SER:OG	1:B:526:GLN:OE1	2.21	0.42
1:A:193:THR:HB	1:A:194:PRO:CD	2.49	0.41
1:A:245:ALA:O	1:A:294:PRO:HD2	2.20	0.41
1:B:40:LEU:CD2	1:B:54:HIS:ND1	2.83	0.41
1:B:178:ARG:HD2	1:B:474:TRP:CZ3	2.55	0.41
1:A:110:VAL:HG22	1:A:111:PHE:O	2.20	0.41
1:A:134:TYR:CE2	1:A:136:ILE:CD1	3.03	0.41
1:A:218:ASP:O	1:A:219:LEU:C	2.61	0.41
1:A:480:ASN:OD1	1:A:483:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLU:OE2	1:B:11:LYS:HE3	2.19	0.41
1:B:280:ARG:HD2	1:B:281:THR:N	2.36	0.41
1:B:355:ILE:CG2	1:B:357:HIS:CE1	3.03	0.41
1:B:377:ARG:O	1:B:380:VAL:HG22	2.19	0.41
1:A:137:PHE:HD1	1:A:140:ARG:HB2	1.86	0.41
1:A:281:THR:OG1	1:A:289:GLN:NE2	2.53	0.41
1:A:484:PHE:O	1:A:488:LYS:HG3	2.20	0.41
1:B:309:ASP:HA	1:B:312:ARG:HH21	1.83	0.41
1:B:560:GLU:OE2	1:B:562:VAL:HG12	2.20	0.41
1:A:52:LEU:HD12	1:A:105:ARG:HH11	1.86	0.41
1:A:312:ARG:NE	1:A:341:LEU:HD11	2.34	0.41
1:B:384:PHE:CE2	1:B:438:LEU:HD12	2.55	0.41
1:A:36:ARG:HG2	1:A:36:ARG:HH11	1.85	0.41
1:A:141:PHE:CD1	1:A:175:VAL:HG22	2.54	0.41
1:B:158:LYS:HD2	1:B:478:GLU:HB3	2.02	0.41
1:A:202:HIS:O	1:A:203:LYS:HB2	2.21	0.41
1:A:270:ILE:HG21	1:A:275:VAL:HG22	2.03	0.41
1:A:432:ASN:OD1	1:A:432:ASN:C	2.63	0.41
1:B:16:TYR:CD1	1:B:16:TYR:O	2.73	0.41
1:B:523:VAL:O	1:B:524:GLN:C	2.64	0.41
1:B:535:ARG:HD3	1:B:539:GLN:OE1	2.20	0.41
1:B:172:LEU:HG	1:B:216:PHE:HB3	2.03	0.41
1:B:219:LEU:HD11	1:B:317:GLN:OE1	2.21	0.41
1:B:356:TRP:CZ3	1:B:374:TYR:HB3	2.56	0.41
1:B:335:TRP:CE3	1:B:335:TRP:HA	2.56	0.41
1:A:264:TYR:O	1:A:267:TRP:HB2	2.20	0.41
1:A:277:LYS:HB2	1:A:277:LYS:HZ2	1.83	0.41
1:A:314:TRP:O	1:A:319:ILE:HG12	2.20	0.41
1:A:389:ILE:HB	1:A:393:ARG:HG2	2.02	0.41
1:B:449:THR:HA	1:B:450:PRO:HD3	1.92	0.41
1:B:464:THR:OG1	1:B:465:ASP:N	2.54	0.41
1:A:249:PHE:CD2	1:A:251:ALA:HB3	2.55	0.41
1:A:374:TYR:CE1	1:A:375:LEU:CD1	3.03	0.41
1:B:7:PHE:CD2	1:B:28:ARG:NH1	2.89	0.41
1:B:82:TYR:N	1:B:110:VAL:CG2	2.84	0.41
1:B:332:HIS:HD2	1:B:367:GLN:NE2	2.18	0.41
1:B:569:LEU:CD2	1:B:571:LEU:HD21	2.46	0.41
1:B:232:ARG:HH11	1:B:232:ARG:CG	2.34	0.40
1:B:243:ASN:ND2	1:B:329:GLU:HB2	2.35	0.40
1:B:389:ILE:HB	1:B:393:ARG:CG	2.50	0.40
1:B:17:PRO:HA	1:B:23:LEU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ILE:HA	1:B:28:ARG:O	2.21	0.40
1:B:158:LYS:HD3	1:B:478:GLU:OE1	2.21	0.40
1:B:516:LEU:C	1:B:516:LEU:HD23	2.45	0.40
1:A:465:ASP:HA	1:A:466:PRO:HA	1.79	0.40
1:B:242:PHE:N	1:B:242:PHE:CD1	2.88	0.40
1:A:374:TYR:CD1	1:A:375:LEU:HD13	2.56	0.40
1:B:339:ARG:HD2	1:B:367:GLN:O	2.21	0.40
1:B:454:TYR:O	1:B:454:TYR:CG	2.74	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	583/585 (100%)	551 (94%)	28 (5%)	4 (1%)	18	52
1	B	583/585 (100%)	552 (95%)	30 (5%)	1 (0%)	43	73
All	All	1166/1170 (100%)	1103 (95%)	58 (5%)	5 (0%)	30	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	SER
1	A	547	GLU
1	B	547	GLU
1	A	277	LYS
1	A	195	ILE

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	493/493 (100%)	452 (92%)	41 (8%)	10	38
1	B	493/493 (100%)	459 (93%)	34 (7%)	14	45
All	All	986/986 (100%)	911 (92%)	75 (8%)	12	42

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	26	ARG
1	A	38	GLU
1	A	40	LEU
1	A	62	SER
1	A	77	THR
1	A	92	GLU
1	A	94	VAL
1	A	105	ARG
1	A	130	GLU
1	A	139	GLU
1	A	155	GLN
1	A	159	ASP
1	A	164	HIS
1	A	167	PHE
1	A	188	THR
1	A	193	THR
1	A	212	ILE
1	A	219	LEU
1	A	221	THR
1	A	223	ARG
1	A	263	ARG
1	A	277	LYS
1	A	282	ASN
1	A	302	GLU
1	A	323	ARG
1	A	325	ASP

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Mol	Chain	Res	Type
1	A	330	VAL
1	A	375	LEU
1	A	404	LEU
1	A	422	THR
1	A	427	THR
1	A	444	MET
1	A	475	GLU
1	A	483	LEU
1	A	504	ASN
1	A	505	VAL
1	A	544	GLN
1	A	545	VAL
1	A	547	GLU
1	A	573	LEU
1	B	13	SER
1	B	52	LEU
1	B	64	GLU
1	B	92	GLU
1	B	139	GLU
1	B	167	PHE
1	B	232	ARG
1	B	241	VAL
1	B	248	GLN
1	B	250	PHE
1	B	255	VAL
1	B	261	GLN
1	B	265	LYS
1	B	275	VAL
1	B	277	LYS
1	B	323	ARG
1	B	325	ASP
1	B	328	ASN
1	B	337	GLU
1	B	340	ARG
1	B	364	MET
1	B	398	LEU
1	B	411	GLN
1	B	438	LEU
1	B	451	LEU
1	B	458	ILE
1	B	464	THR
1	B	467	ASP

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Mol	Chain	Res	Type
1	B	470	ARG
1	B	475	GLU
1	B	504	ASN
1	B	552	THR
1	B	560	GLU
1	B	569	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	135	GLN
1	A	215	GLN
1	A	243	ASN
1	A	244	HIS
1	A	261	GLN
1	A	282	ASN
1	A	289	GLN
1	A	332	HIS
1	A	346	ASN
1	A	390	HIS
1	A	411	GLN
1	A	504	ASN
1	A	526	GLN
1	A	527	HIS
1	A	539	GLN
1	B	135	GLN
1	B	243	ASN
1	B	257	GLN
1	B	261	GLN
1	B	328	ASN
1	B	332	HIS
1	B	357	HIS
1	B	495	HIS
1	B	504	ASN
1	B	524	GLN
1	B	527	HIS
1	B	534	ASN
1	B	539	GLN
1	B	544	GLN
1	B	566	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 oligosaccharides 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](#)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.