



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:51 AM UTC

PDB ID : 1ULH / pdb_00001ulh
Title : A short peptide insertion crucial for angiostatic activity of human tryptophanyl-tRNA synthetase
Authors : Kise, Y.; Sengoku, T.; Ishii, R.; Yokoyama, S.; Park, S.G.; Lee, S.W.; Kim, S.; Nureki, O.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2003-09-12
Resolution : 2.31 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

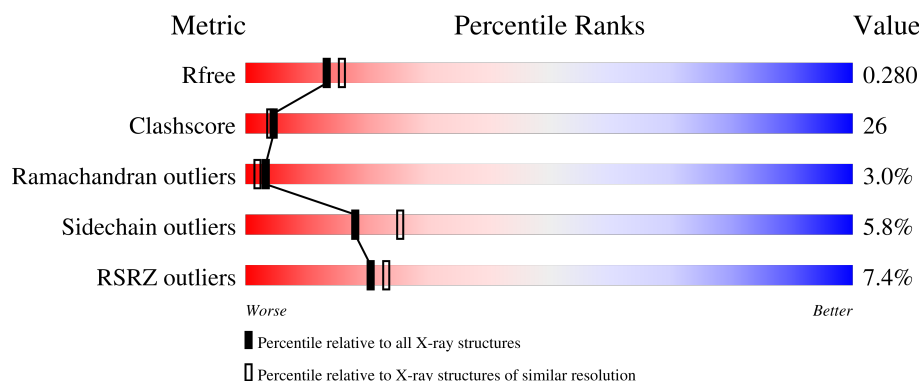
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 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	390	9% 45% 38% 10% 7%
1	B	390	5% 51% 39% 7% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6488 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2958	1903	500	541	14			
1	B	379	Total	C	N	O	S	0	0	0
			3053	1960	513	565	15			

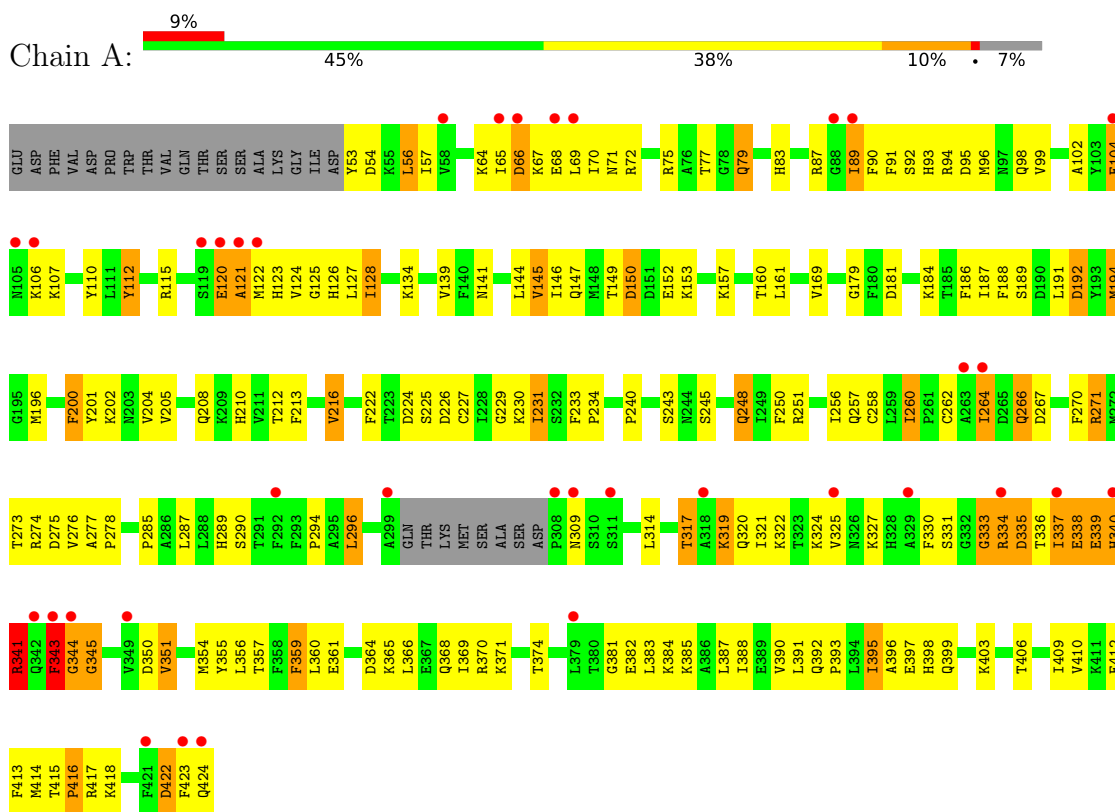
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	219	Total	O	0	0
			219	219		
2	B	258	Total	O	0	0
			258	258		

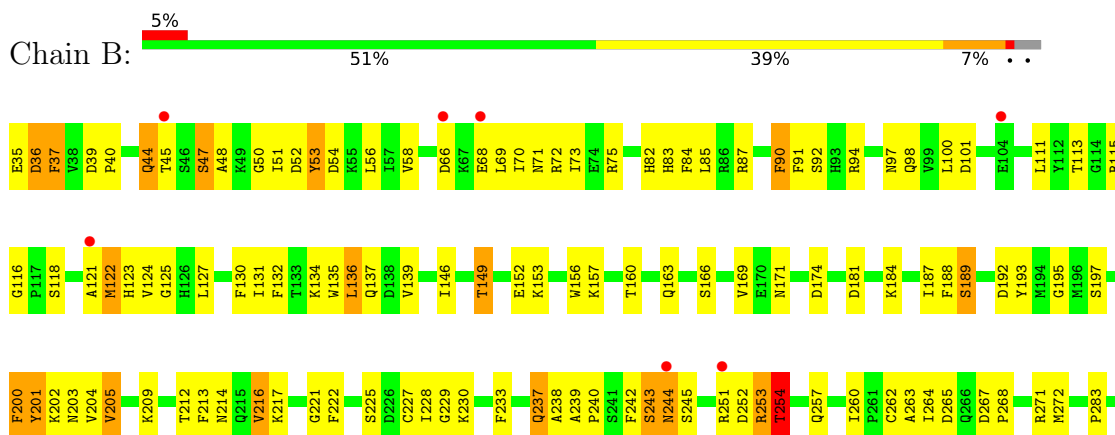
3 Residue-property plots

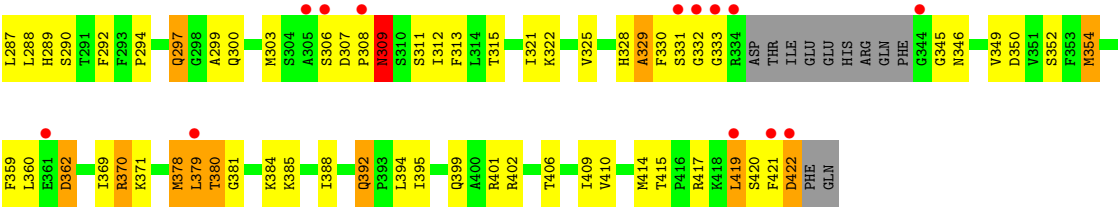
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Tryptophanyl-tRNA synthetase



- Molecule 1: Tryptophanyl-tRNA synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.03Å 96.61Å 98.32Å 90.00° 130.26° 90.00°	Depositor
Resolution (Å)	42.89 – 2.31 42.89 – 2.31	Depositor EDS
% Data completeness (in resolution range)	90.7 (42.89-2.31) 90.7 (42.89-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.292 0.234 , 0.280	Depositor DCC
R_{free} test set	1939 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6488	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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	0.93	1/3031 (0.0%)	1.23	29/4086 (0.7%)
1	B	0.95	2/3127 (0.1%)	1.20	33/4221 (0.8%)
All	All	0.94	3/6158 (0.0%)	1.21	62/8307 (0.7%)

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	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	ILE	CA-CB	7.39	1.57	1.54
1	B	122	MET	SD-CE	-6.05	1.64	1.79
1	B	329	ALA	CA-CB	-5.60	1.45	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	GLU	N-CA-C	-15.58	94.32	111.14
1	B	308	PRO	N-CA-C	-10.97	99.20	113.57
1	A	67	LYS	N-CA-C	-9.43	98.28	113.19
1	B	332	GLY	N-CA-C	-9.19	95.66	111.47
1	A	225	SER	N-CA-C	-8.95	102.36	113.28
1	A	359	PHE	N-CA-C	8.93	124.30	113.23
1	B	37	PHE	N-CA-C	8.78	122.84	108.52
1	B	306	SER	N-CA-C	-8.27	101.95	110.97
1	A	418	LYS	N-CA-C	-8.04	98.58	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	SER	N-CA-C	7.71	123.17	112.45
1	B	121	ALA	N-CA-C	7.69	121.26	108.73
1	A	381	GLY	N-CA-C	-7.65	104.30	114.25
1	A	160	THR	N-CA-C	-7.63	99.17	110.46
1	B	380	THR	N-CA-C	7.45	126.68	110.80
1	A	260	ILE	N-CA-C	7.44	115.56	107.60
1	A	56	LEU	N-CA-C	-7.32	104.50	113.50
1	A	423	PHE	N-CA-C	-7.25	103.41	111.82
1	A	264	ILE	N-CA-C	-7.11	105.10	113.42
1	B	253	ARG	N-CA-C	7.07	121.16	112.54
1	A	66	ASP	CA-C-O	7.04	122.02	117.94
1	B	359	PHE	N-CA-C	6.94	122.73	112.94
1	B	328	HIS	N-CA-C	6.93	121.98	112.90
1	A	200	PHE	N-CA-C	6.92	118.61	111.14
1	B	200	PHE	N-CA-C	6.81	118.39	110.97
1	B	272	MET	N-CA-C	-6.78	103.82	111.14
1	B	263	ALA	N-CA-C	-6.62	101.17	110.50
1	B	90	PHE	N-CA-C	-6.37	95.08	107.62
1	A	194	MET	N-CA-C	-6.37	104.42	111.36
1	B	378	MET	N-CA-C	6.35	118.00	111.14
1	B	47	SER	N-CA-C	6.34	119.47	109.96
1	B	53	TYR	N-CA-C	6.33	119.17	111.82
1	A	89	ILE	N-CA-C	-6.28	104.39	110.42
1	A	382	GLU	N-CA-C	-6.20	104.07	111.69
1	B	254	THR	N-CA-C	6.20	124.00	110.80
1	B	362	ASP	N-CA-C	-6.14	97.73	110.80
1	B	149	THR	N-CA-C	6.05	120.07	110.70
1	A	95	ASP	N-CA-C	5.94	120.48	113.23
1	A	121	ALA	N-CA-C	-5.91	98.22	110.80
1	B	197	SER	N-CA-C	5.86	118.07	108.52
1	B	239	ALA	N-CA-C	5.74	121.32	113.16
1	A	250	PHE	N-CA-C	5.69	119.40	112.23
1	A	341	ARG	N-CA-C	5.67	122.87	110.80
1	B	311	SER	N-CA-C	5.53	118.08	109.52
1	A	243	SER	N-CA-C	5.46	120.37	111.37
1	A	333	GLY	N-CA-C	-5.45	105.57	112.54
1	A	66	ASP	CB-CA-C	-5.40	109.30	117.07
1	B	354	MET	N-CA-C	-5.36	105.35	111.14
1	A	157	LYS	N-CA-C	5.35	118.44	110.14
1	B	188	PHE	N-CA-C	5.30	118.09	109.24
1	B	379	LEU	N-CA-C	5.27	122.02	110.80
1	A	334	ARG	N-CA-C	-5.20	106.77	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	PHE	N-CA-C	5.15	116.58	111.07
1	B	237	GLN	N-CA-C	-5.13	106.86	113.23
1	A	91	PHE	N-CA-C	5.12	119.53	113.12
1	B	205	VAL	CB-CA-C	-5.10	105.35	111.88
1	A	361	GLU	N-CA-C	5.10	119.12	113.01
1	B	244	ASN	N-CA-C	5.06	118.23	111.75
1	B	189	SER	N-CA-C	-5.05	102.23	110.20
1	B	156	TRP	N-CA-C	5.04	117.51	111.71
1	A	351	VAL	N-CA-C	5.04	115.65	110.36
1	B	134	LYS	N-CA-C	-5.04	105.92	111.71
1	A	343	PHE	N-CA-C	-5.01	100.13	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	TYR	Sidechain
1	B	201	TYR	Sidechain

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	2958	0	2917	166	0
1	B	3053	0	3010	148	0
2	A	219	0	0	64	0
2	B	258	0	0	67	0
All	All	6488	0	5927	310	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (310) 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:356:LEU:HD22	1:A:360:LEU:HD22	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ARG:HG2	1:B:100:LEU:HD13	1.53	0.91
1:B:184:LYS:HB3	2:B:573:HOH:O	1.76	0.85
1:A:345:GLY:HA3	1:A:374:THR:HA	1.57	0.85
1:B:329:ALA:HB1	2:B:645:HOH:O	1.77	0.85
1:B:82:HIS:HD2	1:B:84:PHE:H	1.34	0.75
1:B:92:SER:HB3	1:B:289:HIS:HB2	1.68	0.74
1:A:94:ARG:HD2	1:A:287:LEU:HD12	1.70	0.74
1:A:145:VAL:HG13	1:A:188:PHE:HE2	1.52	0.73
1:B:123:HIS:HD2	1:B:125:GLY:H	1.36	0.71
1:A:226:ASP:HB2	2:A:593:HOH:O	1.89	0.71
1:A:99:VAL:HG22	1:A:257:GLN:HG2	1.71	0.71
1:B:395:ILE:HG22	1:B:399:GLN:HE21	1.58	0.69
2:A:492:HOH:O	1:B:228:ILE:HG22	1.94	0.67
1:A:66:ASP:HB2	1:A:68:GLU:H	1.59	0.67
1:A:189:SER:HB3	1:A:192:ASP:HB2	1.77	0.67
1:A:415:THR:O	1:A:417:ARG:HG3	1.96	0.66
1:A:231:ILE:HG23	2:A:492:HOH:O	1.96	0.66
1:A:144:LEU:HD21	2:A:588:HOH:O	1.98	0.64
1:A:325:VAL:HG21	1:A:388:ILE:HG12	1.77	0.64
1:A:187:ILE:O	1:A:414:MET:HA	1.99	0.63
2:A:520:HOH:O	1:B:225:SER:HA	1.98	0.63
1:B:137:GLN:HE22	1:B:181:ASP:H	1.46	0.63
1:A:355:TYR:HB3	2:A:451:HOH:O	1.98	0.63
1:A:92:SER:HB3	1:A:289:HIS:HB2	1.81	0.62
1:B:349:VAL:HB	2:B:649:HOH:O	2.00	0.62
1:B:83:HIS:HB3	2:B:511:HOH:O	2.00	0.61
1:A:141:ASN:O	1:A:422:ASP:HB2	2.01	0.61
1:A:245:SER:HB2	2:A:497:HOH:O	2.01	0.61
1:A:233:PHE:HA	2:A:608:HOH:O	2.00	0.61
1:B:238:ALA:HA	2:B:660:HOH:O	2.00	0.59
1:A:224:ASP:HA	2:A:593:HOH:O	2.02	0.59
1:A:335:ASP:C	1:A:337:ILE:H	2.10	0.59
1:B:379:LEU:HB2	2:B:619:HOH:O	2.03	0.59
1:A:93:HIS:HD2	1:A:96:MET:H	1.49	0.59
1:B:360:LEU:HB3	2:B:446:HOH:O	2.02	0.59
1:A:77:THR:HG23	1:A:139:VAL:HB	1.85	0.59
1:A:68:GLU:HA	1:A:71:ASN:ND2	2.19	0.58
1:B:35:GLU:N	1:B:45:THR:HG23	2.19	0.58
1:B:87:ARG:HB2	2:B:502:HOH:O	2.02	0.58
1:B:73:ILE:HD13	1:B:100:LEU:HD11	1.86	0.58
1:A:204:VAL:O	1:A:208:GLN:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:HB	1:A:287:LEU:HD23	1.86	0.57
1:A:57:ILE:HD13	1:A:64:LYS:HB2	1.86	0.57
1:A:371:LYS:HE3	2:A:542:HOH:O	2.05	0.57
1:B:312:ILE:HG13	2:B:466:HOH:O	2.04	0.56
1:B:115:ARG:HD2	2:B:577:HOH:O	2.03	0.56
1:B:35:GLU:HB3	1:B:52:ASP:H	1.71	0.56
1:A:115:ARG:NH2	1:A:122:MET:HG2	2.21	0.56
1:B:394:LEU:HD23	2:B:570:HOH:O	2.04	0.56
1:B:300:GLN:HA	2:B:523:HOH:O	2.05	0.55
1:A:152:GLU:HB2	1:A:233:PHE:CZ	2.41	0.55
1:B:242:PHE:HA	2:B:433:HOH:O	2.06	0.55
1:B:370:ARG:HH12	1:B:371:LYS:HG3	1.72	0.55
1:A:187:ILE:HG13	2:A:436:HOH:O	2.06	0.55
1:B:209:LYS:HG3	2:B:560:HOH:O	2.05	0.55
1:B:267:ASP:HB3	2:B:545:HOH:O	2.05	0.55
1:A:324:LYS:HG3	2:A:641:HOH:O	2.07	0.55
1:A:320:GLN:HB2	2:A:438:HOH:O	2.07	0.55
1:A:396:ALA:N	2:A:496:HOH:O	2.39	0.55
1:A:213:PHE:HA	2:A:492:HOH:O	2.07	0.55
1:B:139:VAL:HB	2:B:486:HOH:O	2.06	0.54
1:A:392:GLN:HB2	1:A:393:PRO:HD3	1.88	0.54
1:B:136:LEU:HD11	2:B:534:HOH:O	2.07	0.54
1:B:136:LEU:HA	2:B:486:HOH:O	2.08	0.54
1:A:393:PRO:C	2:A:496:HOH:O	2.50	0.54
1:B:288:LEU:HD13	2:B:534:HOH:O	2.08	0.54
1:B:388:ILE:O	1:B:392:GLN:HB2	2.08	0.54
1:B:388:ILE:HG22	1:B:392:GLN:NE2	2.23	0.54
1:A:264:ILE:HA	1:A:289:HIS:CD2	2.42	0.53
1:A:364:ASP:O	1:A:368:GLN:HG3	2.08	0.53
1:B:394:LEU:HD12	2:B:552:HOH:O	2.09	0.53
1:A:248:GLN:HG2	2:A:589:HOH:O	2.06	0.53
1:B:124:VAL:HB	2:B:500:HOH:O	2.07	0.53
1:B:73:ILE:HG22	2:B:605:HOH:O	2.09	0.53
1:B:401:ARG:HD2	2:B:621:HOH:O	2.08	0.53
1:A:384:LYS:O	1:A:388:ILE:HG13	2.09	0.53
1:B:68:GLU:HA	2:B:483:HOH:O	2.08	0.53
1:A:231:ILE:HG13	2:A:628:HOH:O	2.08	0.53
1:B:85:LEU:HB3	2:B:659:HOH:O	2.08	0.53
1:A:271:ARG:HG3	2:A:469:HOH:O	2.09	0.53
1:A:383:LEU:HB3	2:A:452:HOH:O	2.09	0.53
1:B:253:ARG:HH11	1:B:253:ARG:HG2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ASN:HB2	2:B:565:HOH:O	2.08	0.53
1:B:90:PHE:CZ	1:B:290:SER:HB3	2.43	0.52
1:B:346:ASN:HD21	1:B:349:VAL:HG23	1.74	0.52
1:B:48:ALA:HA	1:B:300:GLN:NE2	2.25	0.52
1:A:275:ASP:O	1:A:278:PRO:HD2	2.09	0.52
1:A:77:THR:HG22	1:A:79:GLN:HB2	1.91	0.52
1:B:174:ASP:CG	1:B:402:ARG:HE	2.18	0.52
1:B:216:VAL:HG13	1:B:222:PHE:HD2	1.73	0.52
1:A:384:LYS:HG3	2:A:452:HOH:O	2.10	0.52
1:B:69:LEU:O	1:B:73:ILE:HG12	2.10	0.51
1:B:82:HIS:HB3	2:B:562:HOH:O	2.10	0.51
1:A:212:THR:HA	1:B:227:CYS:HA	1.91	0.51
1:B:181:ASP:HB3	1:B:184:LYS:HB2	1.91	0.51
1:A:365:LYS:O	1:A:369:ILE:HG13	2.11	0.51
1:A:334:ARG:O	1:A:336:THR:N	2.43	0.51
1:A:360:LEU:HD13	1:A:390:VAL:CG2	2.41	0.51
1:B:202:LYS:HG3	2:B:474:HOH:O	2.11	0.51
1:A:229:GLY:HA2	2:B:488:HOH:O	2.11	0.51
1:A:424:GLN:HG2	2:A:507:HOH:O	2.10	0.51
1:A:277:ALA:HB2	2:A:445:HOH:O	2.11	0.51
1:A:53:TYR:HA	1:A:56:LEU:HD12	1.93	0.51
1:B:203:ASN:HD21	1:B:244:ASN:HB2	1.75	0.50
1:A:285:PRO:HD3	2:A:445:HOH:O	2.10	0.50
1:A:327:LYS:HE3	2:A:609:HOH:O	2.11	0.50
1:A:338:GLU:O	1:A:339:GLU:HG3	2.10	0.50
1:B:137:GLN:NE2	1:B:181:ASP:H	2.09	0.50
1:B:243:SER:HB2	2:B:591:HOH:O	2.11	0.50
1:B:94:ARG:HD3	2:B:614:HOH:O	2.10	0.50
1:B:251:ARG:HG3	2:B:652:HOH:O	2.10	0.50
1:B:346:ASN:HB3	2:B:428:HOH:O	2.11	0.50
1:A:123:HIS:HB2	2:A:605:HOH:O	2.12	0.50
1:A:387:LEU:HD11	2:A:451:HOH:O	2.12	0.50
1:A:417:ARG:HD2	2:A:603:HOH:O	2.11	0.50
1:B:350:ASP:HB2	2:B:463:HOH:O	2.12	0.50
1:A:72:ARG:HB2	2:A:458:HOH:O	2.12	0.50
1:A:124:VAL:HG12	2:A:605:HOH:O	2.12	0.50
1:A:360:LEU:HD13	1:A:390:VAL:HG21	1.93	0.50
1:A:266:GLN:HG2	2:A:455:HOH:O	2.12	0.50
1:B:122:MET:HE2	1:B:171:ASN:CG	2.37	0.49
1:A:335:ASP:C	1:A:337:ILE:N	2.70	0.49
1:A:370:ARG:HA	2:A:484:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:THR:HG22	1:B:47:SER:H	1.77	0.49
1:B:283:PRO:HG2	2:B:599:HOH:O	2.12	0.49
1:B:303:MET:HA	2:B:643:HOH:O	2.12	0.49
1:B:66:ASP:HB3	2:B:633:HOH:O	2.12	0.49
1:B:321:ILE:O	1:B:325:VAL:HG23	2.12	0.49
1:A:224:ASP:HB3	2:B:503:HOH:O	2.13	0.49
1:B:100:LEU:HD21	2:B:631:HOH:O	2.12	0.49
1:B:415:THR:O	1:B:417:ARG:HG3	2.12	0.49
1:B:69:LEU:HD23	1:B:73:ILE:HD11	1.93	0.49
1:A:106:LYS:HD2	1:A:424:GLN:HG3	1.93	0.49
1:A:333:GLY:C	1:A:335:ASP:H	2.19	0.49
1:B:35:GLU:HG3	1:B:36:ASP:H	1.77	0.49
1:B:313:PHE:C	1:B:315:THR:H	2.20	0.49
1:A:208:GLN:HB3	1:B:229:GLY:CA	2.43	0.49
1:A:333:GLY:C	1:A:335:ASP:N	2.70	0.49
1:B:240:PRO:HA	2:B:508:HOH:O	2.12	0.49
1:A:72:ARG:HD2	2:A:572:HOH:O	2.13	0.48
1:A:77:THR:CG2	1:A:79:GLN:HB2	2.43	0.48
1:A:161:LEU:HD13	2:A:464:HOH:O	2.11	0.48
1:B:406:THR:HG21	2:B:525:HOH:O	2.12	0.48
1:A:125:GLY:O	1:A:128:ILE:HG12	2.14	0.48
1:A:276:VAL:HG23	2:A:471:HOH:O	2.12	0.48
1:A:337:ILE:HD13	2:A:554:HOH:O	2.13	0.48
1:B:152:GLU:HB2	1:B:233:PHE:CZ	2.48	0.48
1:A:65:ILE:HG23	1:A:69:LEU:HD23	1.95	0.48
1:A:202:LYS:HG3	2:B:611:HOH:O	2.12	0.48
1:A:248:GLN:HG3	1:A:416:PRO:HB3	1.96	0.48
1:B:71:ASN:HB3	2:B:543:HOH:O	2.12	0.48
1:A:395:ILE:O	1:A:398:HIS:HB3	2.14	0.48
1:A:94:ARG:HE	1:A:267:ASP:CG	2.21	0.48
1:B:85:LEU:N	2:B:562:HOH:O	2.47	0.48
1:B:217:LYS:HA	1:B:222:PHE:H	1.78	0.48
1:A:354:MET:O	1:A:357:THR:HB	2.14	0.48
1:A:70:ILE:HG13	2:A:466:HOH:O	2.13	0.48
1:B:313:PHE:HB3	1:B:315:THR:HG22	1.96	0.48
1:A:104:GLU:C	1:A:106:LYS:H	2.21	0.47
1:B:253:ARG:O	1:B:254:THR:HG22	2.13	0.47
1:A:90:PHE:HA	1:A:290:SER:HA	1.96	0.47
1:A:240:PRO:HG2	2:A:544:HOH:O	2.15	0.47
1:B:200:PHE:O	1:B:204:VAL:HG23	2.14	0.47
1:B:169:VAL:HG13	1:B:410:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ILE:HB	1:B:287:LEU:HD23	1.96	0.47
1:A:75:ARG:HB2	2:A:572:HOH:O	2.15	0.47
1:A:391:LEU:HD21	2:A:451:HOH:O	2.14	0.47
1:A:317:THR:C	2:A:438:HOH:O	2.57	0.47
1:A:355:TYR:HB3	1:A:387:LEU:HD11	1.97	0.47
1:B:71:ASN:N	2:B:483:HOH:O	2.35	0.47
1:A:321:ILE:HG13	2:A:438:HOH:O	2.14	0.47
1:B:70:ILE:HG12	2:B:659:HOH:O	2.15	0.47
1:B:187:ILE:O	1:B:414:MET:HA	2.15	0.47
1:A:331:SER:HA	1:A:350:ASP:OD2	2.15	0.46
1:A:413:PHE:HA	1:A:417:ARG:HH21	1.79	0.46
1:B:75:ARG:HG3	2:B:543:HOH:O	2.14	0.46
1:B:90:PHE:CE1	1:B:290:SER:HB3	2.51	0.46
1:A:87:ARG:HB3	1:A:89:ILE:CD1	2.45	0.46
1:A:134:LYS:HA	2:A:560:HOH:O	2.14	0.46
1:A:309:ASN:HA	1:A:324:LYS:HE2	1.98	0.46
1:A:317:THR:HG22	1:A:320:GLN:OE1	2.16	0.46
1:A:398:HIS:HA	2:A:634:HOH:O	2.16	0.46
1:B:45:THR:HB	2:B:523:HOH:O	2.16	0.46
1:A:120:GLU:HB2	2:A:531:HOH:O	2.16	0.46
1:A:406:THR:HG23	2:A:526:HOH:O	2.16	0.46
1:A:356:LEU:HD21	1:A:387:LEU:HA	1.98	0.46
1:B:53:TYR:HB3	1:B:91:PHE:CE2	2.51	0.46
1:A:112:TYR:HD1	1:A:260:ILE:HG12	1.81	0.46
1:A:192:ASP:O	1:A:196:MET:HE3	2.16	0.46
1:A:200:PHE:N	2:A:561:HOH:O	2.48	0.46
1:A:314:LEU:HD13	1:A:398:HIS:NE2	2.30	0.46
1:A:98:GLN:HE21	1:A:257:GLN:HE22	1.64	0.46
1:A:181:ASP:OD2	1:A:184:LYS:HE3	2.15	0.45
1:A:296:LEU:O	1:A:351:VAL:HG21	2.16	0.45
1:A:200:PHE:HD1	1:A:245:SER:HB3	1.81	0.45
1:B:40:PRO:HD3	1:B:268:PRO:HG2	1.98	0.45
1:B:122:MET:HE1	1:B:174:ASP:HB2	1.97	0.45
1:B:300:GLN:HG3	2:B:523:HOH:O	2.16	0.45
1:B:395:ILE:HG13	2:B:570:HOH:O	2.15	0.45
1:B:160:THR:HG23	1:B:163:GLN:NE2	2.32	0.45
1:A:201:TYR:O	1:A:205:VAL:HG23	2.16	0.45
1:A:341:ARG:HG2	2:A:472:HOH:O	2.17	0.45
1:B:50:GLY:HA2	1:B:299:ALA:O	2.16	0.45
1:B:193:TYR:HB3	2:B:439:HOH:O	2.16	0.45
1:A:231:ILE:HD12	2:B:541:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:MET:O	1:B:195:GLY:HA2	2.16	0.45
1:A:359:PHE:HD1	2:A:451:HOH:O	1.99	0.45
1:B:410:VAL:HG13	2:B:554:HOH:O	2.16	0.45
1:A:194:MET:SD	1:A:200:PHE:HD2	2.40	0.45
1:A:260:ILE:HG21	1:A:270:PHE:CE2	2.52	0.45
1:B:369:ILE:HG23	1:B:378:MET:SD	2.57	0.45
1:A:115:ARG:CZ	1:A:122:MET:HG2	2.46	0.45
1:A:146:ILE:HD12	1:A:187:ILE:HG12	1.99	0.45
1:B:420:SER:C	1:B:422:ASP:H	2.24	0.45
1:A:144:LEU:HD22	2:A:560:HOH:O	2.16	0.44
1:A:360:LEU:HG	2:A:636:HOH:O	2.17	0.44
1:B:222:PHE:HA	2:B:451:HOH:O	2.17	0.44
1:B:111:LEU:HD11	1:B:136:LEU:HB3	1.99	0.44
1:A:334:ARG:HG2	1:A:344:GLY:HA2	1.98	0.44
1:B:420:SER:C	1:B:422:ASP:N	2.75	0.44
1:A:110:TYR:HD2	1:A:256:ILE:HG22	1.82	0.44
1:A:317:THR:HG23	1:A:320:GLN:H	1.82	0.44
1:B:97:ASN:HB2	2:B:566:HOH:O	2.18	0.44
1:B:113:THR:O	1:B:146:ILE:HA	2.17	0.44
1:B:330:PHE:CE2	1:B:349:VAL:HG12	2.52	0.44
1:A:257:GLN:HG3	1:A:258:CYS:N	2.32	0.44
1:A:274:ARG:HG2	1:A:285:PRO:HD2	1.98	0.44
1:A:112:TYR:HD2	1:A:145:VAL:HG12	1.82	0.44
1:A:399:GLN:O	1:A:403:LYS:HG3	2.17	0.44
1:A:406:THR:O	1:A:410:VAL:HG23	2.18	0.44
1:A:409:ILE:HG13	2:A:526:HOH:O	2.17	0.44
1:B:98:GLN:HA	1:B:101:ASP:HB2	2.00	0.44
1:B:217:LYS:O	1:B:221:GLY:HA2	2.18	0.44
1:A:343:PHE:HB3	1:A:344:GLY:H	1.52	0.44
1:B:48:ALA:O	1:B:299:ALA:HB3	2.18	0.44
1:A:202:LYS:HE3	2:B:588:HOH:O	2.18	0.44
1:A:216:VAL:HG12	2:A:620:HOH:O	2.17	0.44
1:B:116:GLY:HA3	1:B:153:LYS:HE2	1.99	0.44
1:A:294:PRO:HG2	1:A:354:MET:HB3	2.00	0.43
1:B:333:GLY:HA2	2:B:661:HOH:O	2.17	0.43
1:B:406:THR:HG22	1:B:409:ILE:HD12	2.00	0.43
1:B:294:PRO:HG2	1:B:354:MET:SD	2.58	0.43
1:B:395:ILE:HG22	1:B:399:GLN:NE2	2.29	0.43
1:A:360:LEU:HG	2:A:450:HOH:O	2.18	0.43
1:B:51:ILE:HD12	1:B:51:ILE:H	1.81	0.43
1:A:127:LEU:HD11	1:A:314:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:SER:HB3	1:B:157:LYS:HE3	1.99	0.43
1:B:227:CYS:SG	1:B:230:LYS:HG3	2.59	0.43
1:B:257:GLN:HA	2:B:599:HOH:O	2.18	0.43
1:B:352:SER:N	2:B:645:HOH:O	2.52	0.43
1:A:124:VAL:HG22	1:A:359:PHE:CZ	2.53	0.43
1:A:134:LYS:HE2	1:A:179:GLY:C	2.44	0.43
1:A:216:VAL:HG23	1:A:222:PHE:HD2	1.83	0.43
1:A:150:ASP:OD2	1:A:150:ASP:N	2.51	0.43
1:A:351:VAL:HA	1:A:354:MET:HE3	2.01	0.43
1:A:104:GLU:HG3	2:A:480:HOH:O	2.19	0.43
1:B:297:GLN:CD	1:B:297:GLN:H	2.26	0.43
1:A:147:GLN:NE2	2:A:544:HOH:O	2.52	0.42
1:B:66:ASP:O	1:B:70:ILE:HG13	2.19	0.42
1:A:273:THR:HG22	2:A:445:HOH:O	2.18	0.42
1:A:69:LEU:O	1:A:72:ARG:HB3	2.19	0.42
1:A:210:HIS:ND1	1:A:210:HIS:N	2.67	0.42
1:A:186:PHE:CZ	1:A:188:PHE:HB3	2.55	0.42
1:A:385:LYS:HA	1:A:388:ILE:HD12	2.01	0.42
1:B:381:GLY:O	1:B:385:LYS:HB2	2.19	0.42
1:A:340:HIS:CD2	1:A:344:GLY:HA3	2.55	0.42
1:B:82:HIS:HB2	1:B:135:TRP:CD2	2.55	0.42
1:A:83:HIS:O	1:A:87:ARG:HB2	2.20	0.42
1:A:319:LYS:HD3	1:A:322:LYS:HD2	2.01	0.42
1:A:169:VAL:HG13	1:A:410:VAL:HG11	2.02	0.42
1:A:322:LYS:HG3	2:A:518:HOH:O	2.19	0.42
1:B:54:ASP:O	1:B:58:VAL:HG23	2.19	0.42
1:B:201:TYR:O	1:B:205:VAL:HG23	2.20	0.42
1:A:330:PHE:HB3	1:A:351:VAL:HG23	2.02	0.41
1:B:166:SER:HB3	2:B:638:HOH:O	2.19	0.41
1:B:378:MET:HG2	2:B:447:HOH:O	2.19	0.41
1:B:419:LEU:HD22	2:B:526:HOH:O	2.19	0.41
1:A:264:ILE:HA	1:A:289:HIS:HD2	1.85	0.41
1:B:322:LYS:HG3	1:B:388:ILE:HD13	2.01	0.41
1:A:122:MET:HA	1:A:126:HIS:ND1	2.36	0.41
1:B:44:GLN:HE21	1:B:44:GLN:HB2	1.72	0.41
1:B:213:PHE:CE2	1:B:217:LYS:HD3	2.56	0.41
1:B:271:ARG:HB3	2:B:465:HOH:O	2.20	0.41
1:A:149:THR:HG21	2:A:494:HOH:O	2.20	0.41
1:A:337:ILE:HG21	2:A:554:HOH:O	2.21	0.41
1:B:132:PHE:O	1:B:136:LEU:HD22	2.21	0.41
1:A:102:ALA:HB1	1:A:107:LYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:CYS:HA	1:B:212:THR:HA	2.03	0.41
1:B:84:PHE:CZ	1:B:131:ILE:HD11	2.56	0.41
1:B:262:CYS:O	1:B:289:HIS:HA	2.21	0.41
1:B:409:ILE:HG23	2:B:572:HOH:O	2.21	0.41
1:A:96:MET:N	2:A:598:HOH:O	2.53	0.41
1:B:35:GLU:O	1:B:37:PHE:N	2.55	0.41
1:B:384:LYS:O	1:B:388:ILE:HG13	2.21	0.41
1:B:253:ARG:HH11	1:B:253:ARG:CG	2.34	0.40
1:B:333:GLY:N	2:B:428:HOH:O	2.54	0.40
1:A:413:PHE:HD2	2:A:436:HOH:O	2.05	0.40
1:B:116:GLY:HA2	1:B:149:THR:OG1	2.21	0.40
1:B:127:LEU:HB3	2:B:485:HOH:O	2.19	0.40
1:A:191:LEU:HD22	2:A:464:HOH:O	2.21	0.40
1:A:230:LYS:HB2	2:A:628:HOH:O	2.20	0.40
1:A:262:CYS:O	1:A:289:HIS:HA	2.21	0.40
1:B:330:PHE:HE2	1:B:349:VAL:HG12	1.86	0.40
1:B:123:HIS:CD2	1:B:125:GLY:H	2.25	0.40
1:B:214:ASN:HA	1:B:217:LYS:HE2	2.04	0.40
1:B:265:ASP:HB3	1:B:292:PHE:CE2	2.56	0.40
1:A:145:VAL:HG13	1:A:188:PHE:CE2	2.43	0.40
1:B:87:ARG:NE	2:B:550:HOH:O	2.55	0.40
1:B:313:PHE:C	1:B:315:THR:N	2.79	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	360/390 (92%)	318 (88%)	29 (8%)	13 (4%)	2	1
1	B	375/390 (96%)	343 (92%)	23 (6%)	9 (2%)	4	3
All	All	735/780 (94%)	661 (90%)	52 (7%)	22 (3%)	3	2

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA
1	A	251	ARG
1	A	317	THR
1	A	335	ASP
1	A	337	ILE
1	A	343	PHE
1	B	36	ASP
1	B	309	ASN
1	B	345	GLY
1	B	380	THR
1	A	340	HIS
1	A	344	GLY
1	A	345	GLY
1	B	362	ASP
1	B	419	LEU
1	A	296	LEU
1	B	254	THR
1	A	339	GLU
1	A	341	ARG
1	B	307	ASP
1	B	264	ILE
1	A	395	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	323/346 (93%)	302 (94%)	21 (6%)	15	21
1	B	335/346 (97%)	318 (95%)	17 (5%)	21	31
All	All	658/692 (95%)	620 (94%)	38 (6%)	18	25

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASP

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Mol	Chain	Res	Type
1	A	79	GLN
1	A	104	GLU
1	A	120	GLU
1	A	145	VAL
1	A	150	ASP
1	A	153	LYS
1	A	192	ASP
1	A	216	VAL
1	A	231	ILE
1	A	234	PRO
1	A	248	GLN
1	A	266	GLN
1	A	271	ARG
1	A	319	LYS
1	A	343	PHE
1	A	366	LEU
1	A	397	GLU
1	A	412	GLU
1	A	416	PRO
1	A	422	ASP
1	B	39	ASP
1	B	44	GLN
1	B	56	LEU
1	B	136	LEU
1	B	189	SER
1	B	192	ASP
1	B	216	VAL
1	B	237	GLN
1	B	243	SER
1	B	245	SER
1	B	252	ASP
1	B	297	GLN
1	B	309	ASN
1	B	370	ARG
1	B	392	GLN
1	B	421	PHE
1	B	422	ASP

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	71	ASN

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Mol	Chain	Res	Type
1	A	93	HIS
1	A	98	GLN
1	A	105	ASN
1	A	137	GLN
1	A	141	ASN
1	A	171	ASN
1	A	208	GLN
1	A	266	GLN
1	A	297	GLN
1	A	309	ASN
1	B	44	GLN
1	B	71	ASN
1	B	82	HIS
1	B	83	HIS
1	B	98	GLN
1	B	105	ASN
1	B	123	HIS
1	B	137	GLN
1	B	203	ASN
1	B	208	GLN
1	B	210	HIS
1	B	237	GLN
1	B	244	ASN
1	B	309	ASN
1	B	328	HIS
1	B	346	ASN
1	B	392	GLN
1	B	398	HIS
1	B	399	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	364/390 (93%)	0.75	35 (9%) 13 15	21, 54, 84, 106	0
1	B	379/390 (97%)	0.43	20 (5%) 32 34	27, 48, 68, 90	0
All	All	743/780 (95%)	0.59	55 (7%) 20 23	21, 51, 79, 106	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	422	ASP	5.5
1	A	349	VAL	5.2
1	A	308	PRO	5.1
1	B	66	ASP	4.5
1	A	299	ALA	4.4
1	A	343	PHE	4.0
1	A	263	ALA	3.9
1	B	104	GLU	3.9
1	A	423	PHE	3.8
1	A	340	HIS	3.8
1	A	344	GLY	3.7
1	B	344	GLY	3.6
1	A	121	ALA	3.6
1	A	421	PHE	3.5
1	A	66	ASP	3.3
1	A	337	ILE	3.3
1	A	88	GLY	3.3
1	B	419	LEU	3.3
1	A	65	ILE	3.1
1	B	333	GLY	3.1
1	A	69	LEU	2.9
1	A	119	SER	2.9
1	A	309	ASN	2.9
1	B	306	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	332	GLY	2.8
1	A	318	ALA	2.8
1	A	264	ILE	2.8
1	B	361	GLU	2.8
1	A	325	VAL	2.8
1	B	334	ARG	2.6
1	B	45	THR	2.6
1	A	58	VAL	2.6
1	A	379	LEU	2.5
1	A	104	GLU	2.5
1	B	421	PHE	2.4
1	A	424	GLN	2.4
1	B	308	PRO	2.4
1	A	122	MET	2.4
1	A	120	GLU	2.4
1	B	305	ALA	2.3
1	A	329	ALA	2.3
1	B	121	ALA	2.3
1	B	68	GLU	2.3
1	A	311	SER	2.3
1	A	292	PHE	2.2
1	A	342	GLN	2.2
1	B	331	SER	2.2
1	A	334	ARG	2.2
1	A	105	ASN	2.2
1	A	68	GLU	2.2
1	B	251	ARG	2.1
1	B	379	LEU	2.1
1	B	244	ASN	2.1
1	A	89	ILE	2.0
1	A	106	LYS	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.