



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:44 PM UTC

PDB ID : 3HO4 / pdb_00003ho4
Title : Crystal structure of Hedgehog-interacting protein (HHIP)
Authors : Hymowitz, S.G.; Bosanac, I.
Deposited on : 2009-06-01
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

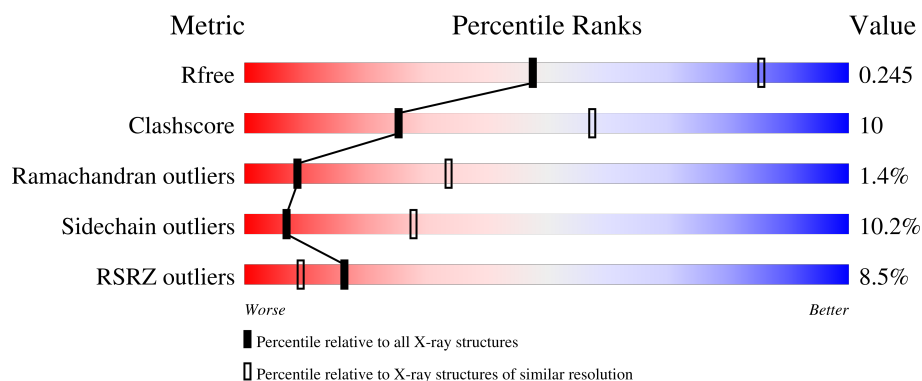
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	481	5% 67% 20% . . 9%
1	B	481	11% 65% 21% 5% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6868 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 Hedgehog-interacting protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	Se	5	0	0
			3414	2143	608	636	22	5			
1	B	442	Total	C	N	O	S	Se	9	0	0
			3454	2166	616	644	22	6			

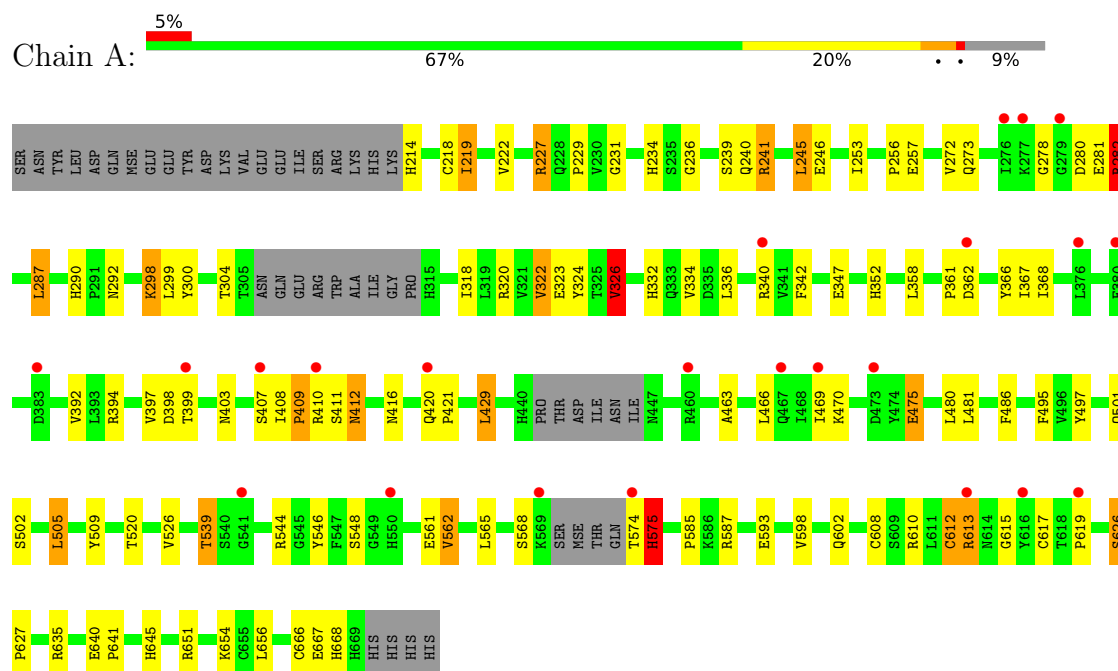
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	668	HIS	-	expression tag	UNP Q96QV1
A	669	HIS	-	expression tag	UNP Q96QV1
A	670	HIS	-	expression tag	UNP Q96QV1
A	671	HIS	-	expression tag	UNP Q96QV1
A	672	HIS	-	expression tag	UNP Q96QV1
A	673	HIS	-	expression tag	UNP Q96QV1
B	668	HIS	-	expression tag	UNP Q96QV1
B	669	HIS	-	expression tag	UNP Q96QV1
B	670	HIS	-	expression tag	UNP Q96QV1
B	671	HIS	-	expression tag	UNP Q96QV1
B	672	HIS	-	expression tag	UNP Q96QV1
B	673	HIS	-	expression tag	UNP Q96QV1

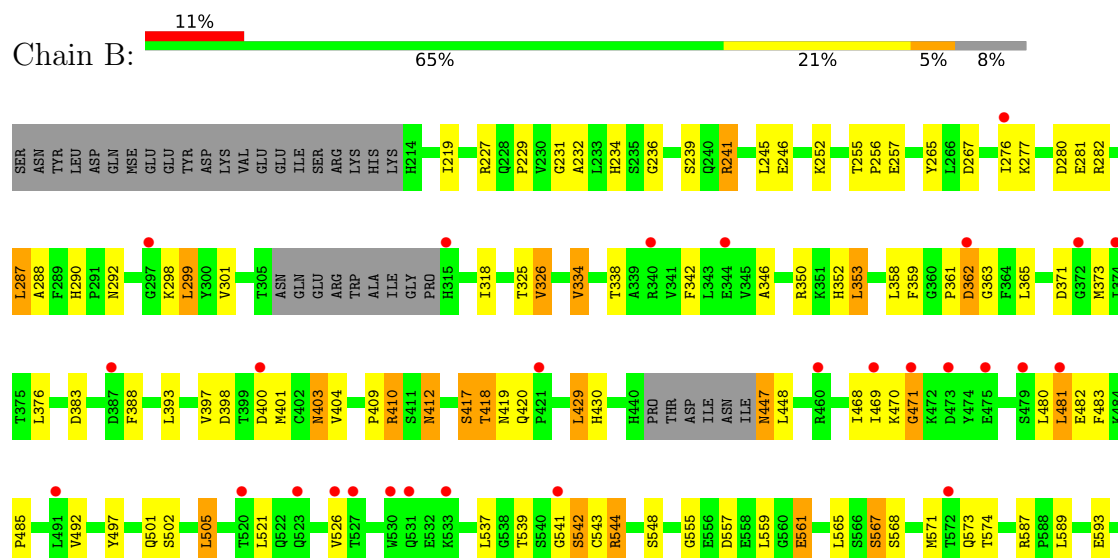
3 Residue-property plots

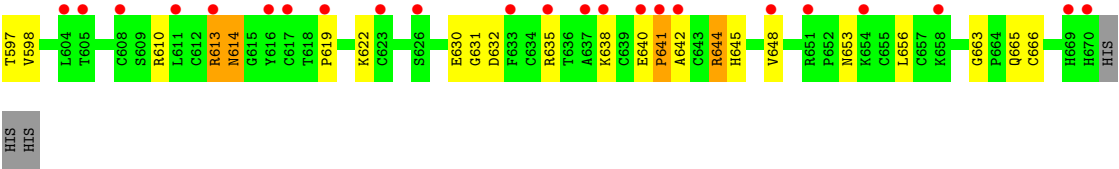
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Hedgehog-interacting protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.04Å 101.04Å 304.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.10 30.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-3.10) 99.8 (30.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.36 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.252 0.210 , 0.245	Depositor DCC
R_{free} test set	1709 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 76.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6868	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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	0.50	0/3488	0.87	6/4699 (0.1%)
1	B	0.49	1/3529 (0.0%)	0.85	7/4754 (0.1%)
All	All	0.50	1/7017 (0.0%)	0.86	13/9453 (0.1%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	277	LYS	CA-CB	6.35	1.61	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	LYS	CB-CA-C	-12.85	98.33	114.40
1	A	615	GLY	N-CA-C	-11.14	101.37	111.95
1	B	383	ASP	CA-CB-CG	-7.70	104.90	112.60
1	B	276	ILE	N-CA-C	-6.85	106.36	112.12
1	B	420	GLN	N-CA-C	5.65	122.29	109.81
1	A	421	PRO	CA-C-N	5.56	125.92	119.47
1	A	421	PRO	C-N-CA	5.56	125.92	119.47
1	A	326	VAL	CB-CA-C	-5.45	104.21	111.13
1	A	282	ARG	N-CA-C	5.42	119.88	113.16
1	B	644	ARG	N-CA-C	5.20	117.23	110.53
1	A	298	LYS	N-CA-C	5.16	116.81	108.41
1	B	663	GLY	CA-C-N	5.09	125.38	119.47
1	B	663	GLY	C-N-CA	5.09	125.38	119.47

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	281	GLU	Peptide
1	A	409	PRO	Peptide

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	3414	0	3317	63	0
1	B	3454	0	3354	68	0
All	All	6868	0	6671	128	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 10.

All (128) 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:574:THR:O	1:A:575:HIS:HB2	1.80	0.82
1:B:544:ARG:HG2	1:B:544:ARG:HH11	1.46	0.80
1:A:241:ARG:HH11	1:A:332:HIS:HD2	1.31	0.77
1:B:281:GLU:HB3	1:B:353:LEU:HD22	1.69	0.75
1:B:544:ARG:HH11	1:B:544:ARG:CG	1.99	0.75
1:B:231:GLY:HA2	1:B:565:LEU:HD13	1.70	0.72
1:B:290:HIS:HD2	1:B:292:ASN:H	1.37	0.72
1:B:567:SER:HA	1:B:571:MSE:HE2	1.70	0.72
1:B:501:GLN:O	1:B:587:ARG:HD3	1.94	0.67
1:A:290:HIS:HD2	1:A:292:ASN:H	1.42	0.67
1:A:241:ARG:HH11	1:A:332:HIS:CD2	2.11	0.67
1:B:410:ARG:H	1:B:410:ARG:CD	2.08	0.67
1:A:290:HIS:CD2	1:A:292:ASN:H	2.13	0.66
1:A:539:THR:HB	1:A:544:ARG:HA	1.76	0.66
1:A:394:ARG:HE	1:A:412:ASN:HD21	1.44	0.65
1:A:469:ILE:HG12	1:A:470:LYS:H	1.62	0.64
1:B:290:HIS:CD2	1:B:292:ASN:H	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:LEU:HD13	1:B:480:LEU:HD21	1.79	0.63
1:A:234:HIS:CD2	1:A:236:GLY:H	2.16	0.62
1:A:234:HIS:HD2	1:A:236:GLY:H	1.47	0.62
1:B:630:GLU:HB3	1:B:638:LYS:HE3	1.81	0.62
1:A:358:LEU:HG	1:A:366:TYR:HB2	1.82	0.61
1:A:429:LEU:HD13	1:A:480:LEU:HD21	1.82	0.61
1:A:368:ILE:HG12	1:A:392:VAL:HG22	1.83	0.60
1:A:282:ARG:O	1:A:304:THR:HB	2.02	0.60
1:B:342:PHE:HE1	1:B:397:VAL:HG12	1.69	0.58
1:A:501:GLN:O	1:A:587:ARG:HD3	2.04	0.57
1:A:394:ARG:HE	1:A:412:ASN:ND2	2.03	0.57
1:B:613:ARG:O	1:B:614:ASN:HB2	2.05	0.56
1:A:231:GLY:HA2	1:A:565:LEU:HD13	1.87	0.56
1:B:401:MSE:HE3	1:B:403:ASN:HD21	1.71	0.56
1:A:495:PHE:CZ	1:A:562:VAL:HG11	2.41	0.55
1:B:568:SER:H	1:B:571:MSE:HB2	1.70	0.55
1:A:475:GLU:HA	1:A:475:GLU:OE1	2.06	0.55
1:A:495:PHE:CE2	1:A:562:VAL:HG11	2.42	0.55
1:B:645:HIS:HD2	1:B:666:CYS:O	1.90	0.54
1:A:466:LEU:HB2	1:A:480:LEU:HD12	1.89	0.54
1:B:544:ARG:CG	1:B:544:ARG:NH1	2.64	0.54
1:A:651:ARG:HH11	1:A:654:LYS:HG2	1.72	0.54
1:B:227:ARG:HG3	1:B:246:GLU:CD	2.32	0.53
1:A:640:GLU:HB2	1:A:641:PRO:CD	2.38	0.53
1:A:651:ARG:NH1	1:A:654:LYS:HG2	2.23	0.53
1:B:326:VAL:HA	1:B:334:VAL:HA	1.90	0.52
1:A:227:ARG:HG3	1:A:246:GLU:CD	2.35	0.52
1:B:267:ASP:OD1	1:B:267:ASP:C	2.52	0.51
1:B:448:LEU:HD23	1:B:468:ILE:HD12	1.92	0.51
1:A:245:LEU:HD11	1:A:287:LEU:HB2	1.92	0.51
1:A:463:ALA:HB2	1:A:486:PHE:CE2	2.46	0.51
1:B:497:TYR:OH	1:B:561:GLU:OE2	2.25	0.51
1:A:241:ARG:NH1	1:A:332:HIS:CD2	2.79	0.50
1:A:300:TYR:OH	1:A:397:VAL:HG11	2.12	0.50
1:B:290:HIS:HD2	1:B:292:ASN:N	2.08	0.50
1:A:361:PRO:O	1:A:362:ASP:HB2	2.10	0.50
1:A:229:PRO:HB2	1:A:565:LEU:HB3	1.93	0.50
1:B:219:ILE:HD13	1:B:537:LEU:HD13	1.94	0.50
1:A:219:ILE:HD11	1:A:546:TYR:C	2.37	0.49
1:B:229:PRO:HB2	1:B:565:LEU:HB3	1.94	0.49
1:A:326:VAL:HA	1:A:334:VAL:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LYS:NZ	1:B:325:THR:OG1	2.46	0.49
1:B:557:ASP:HB3	1:B:559:LEU:H	1.78	0.49
1:B:265:TYR:O	1:B:334:VAL:HG13	2.13	0.48
1:B:287:LEU:HD23	1:B:288:ALA:N	2.29	0.48
1:B:641:PRO:HG2	1:B:665:GLN:HG2	1.95	0.48
1:B:280:ASP:OD1	1:B:282:ARG:NH1	2.46	0.48
1:B:410:ARG:H	1:B:410:ARG:HD3	1.79	0.48
1:B:388:PHE:HB3	1:B:393:LEU:HD11	1.95	0.47
1:A:539:THR:HG21	1:B:257:GLU:CD	2.39	0.47
1:B:447:ASN:HB3	1:B:469:ILE:HA	1.95	0.47
1:B:255:THR:HB	1:B:256:PRO:HD2	1.96	0.47
1:A:509:TYR:O	1:A:520:THR:HA	2.15	0.47
1:A:273:GLN:O	1:A:282:ARG:O	2.32	0.46
1:B:290:HIS:HE1	1:B:398:ASP:OD2	1.99	0.46
1:A:397:VAL:HG12	1:A:619:PRO:HG3	1.97	0.46
1:B:469:ILE:HG12	1:B:470:LYS:H	1.80	0.46
1:A:239:SER:C	1:A:241:ARG:H	2.22	0.46
1:A:320:ARG:HG2	1:A:322:VAL:HG22	1.97	0.46
1:A:340:ARG:HD2	1:A:342:PHE:HE2	1.80	0.46
1:A:342:PHE:HE1	1:A:397:VAL:HG13	1.80	0.46
1:B:282:ARG:HD2	1:B:350:ARG:HG2	1.98	0.46
1:B:246:GLU:OE2	1:B:252:LYS:HE3	2.16	0.46
1:B:318:ILE:HG22	1:B:346:ALA:HA	1.97	0.46
1:B:631:GLY:O	1:B:632:ASP:C	2.60	0.45
1:A:613:ARG:HB3	1:A:613:ARG:HH11	1.81	0.45
1:A:240:GLN:HB2	1:A:256:PRO:HB3	1.97	0.45
1:A:645:HIS:HD2	1:A:666:CYS:O	2.00	0.45
1:A:218:CYS:HB2	1:A:585:PRO:HG3	1.98	0.45
1:A:222:VAL:HG22	1:B:542:SER:HB3	1.98	0.45
1:A:300:TYR:CZ	1:A:397:VAL:HG11	2.52	0.45
1:A:241:ARG:HG2	1:A:253:ILE:HG23	1.98	0.45
1:A:608:CYS:O	1:A:612:CYS:HB3	2.17	0.44
1:B:231:GLY:CA	1:B:565:LEU:HD13	2.43	0.44
1:B:234:HIS:HD2	1:B:236:GLY:H	1.64	0.44
1:B:400:ASP:O	1:B:622:LYS:HD3	2.17	0.44
1:B:418:THR:HG23	1:B:419:ASN:H	1.82	0.44
1:A:257:GLU:OE2	1:B:539:THR:HG21	2.19	0.43
1:B:298:LYS:HD2	1:B:619:PRO:HG3	1.99	0.43
1:B:359:PHE:CE2	1:B:365:LEU:HB2	2.54	0.43
1:B:541:GLY:O	1:B:543:CYS:N	2.52	0.43
1:A:640:GLU:CB	1:A:641:PRO:CD	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:GLU:HG2	1:A:668:HIS:CD2	2.53	0.43
1:B:502:SER:OG	1:B:505:LEU:HB2	2.19	0.43
1:B:361:PRO:O	1:B:362:ASP:HB2	2.19	0.42
1:B:361:PRO:C	1:B:363:GLY:H	2.26	0.42
1:B:371:ASP:OD1	1:B:430:HIS:HA	2.20	0.42
1:A:278:GLY:C	1:A:280:ASP:H	2.26	0.42
1:A:290:HIS:HE1	1:A:398:ASP:OD2	2.03	0.42
1:A:342:PHE:CE1	1:A:397:VAL:HG13	2.54	0.42
1:A:245:LEU:HD23	1:A:245:LEU:N	2.35	0.41
1:B:409:PRO:HG2	1:B:412:ASN:CG	2.45	0.41
1:A:497:TYR:CD1	1:A:505:LEU:HB3	2.54	0.41
1:A:626:SER:O	1:A:627:PRO:C	2.63	0.41
1:A:502:SER:OG	1:A:505:LEU:HB2	2.20	0.41
1:B:232:ALA:O	1:B:555:GLY:HA2	2.21	0.41
1:B:410:ARG:H	1:B:410:ARG:NE	2.18	0.41
1:B:417:SER:O	1:B:419:ASN:N	2.53	0.41
1:B:239:SER:C	1:B:241:ARG:H	2.29	0.41
1:B:470:LYS:O	1:B:471:GLY:C	2.63	0.41
1:A:408:ILE:HA	1:A:409:PRO:HD3	1.82	0.41
1:A:613:ARG:HB3	1:A:613:ARG:NH1	2.36	0.41
1:B:352:HIS:HB3	1:B:371:ASP:HB2	2.02	0.41
1:B:573:GLN:HG3	1:B:574:THR:HG23	2.03	0.41
1:A:324:TYR:HB3	1:A:334:VAL:HG11	2.02	0.40
1:B:640:GLU:HG2	1:B:653:ASN:OD1	2.21	0.40
1:B:371:ASP:HB3	1:B:373:MSE:H	1.86	0.40
1:A:298:LYS:HE3	1:A:617:CYS:O	2.22	0.40
1:B:299:LEU:HD12	1:B:299:LEU:N	2.36	0.40
1:B:481:LEU:HD23	1:B:482:GLU:H	1.86	0.40
1:B:483:PHE:CE2	1:B:485:PRO:HG3	2.57	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	429/481 (89%)	399 (93%)	25 (6%)	5 (1%)	10	37
1	B	436/481 (91%)	395 (91%)	34 (8%)	7 (2%)	7	30
All	All	865/962 (90%)	794 (92%)	59 (7%)	12 (1%)	9	34

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	ARG
1	A	575	HIS
1	B	418	THR
1	B	471	GLY
1	A	612	CYS
1	B	542	SER
1	B	614	ASN
1	B	642	ALA
1	A	613	ARG
1	B	417	SER
1	B	641	PRO
1	A	420	GLN

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	380/415 (92%)	339 (89%)	41 (11%)	6	25
1	B	385/415 (93%)	348 (90%)	37 (10%)	8	30
All	All	765/830 (92%)	687 (90%)	78 (10%)	7	28

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	HIS
1	A	219	ILE
1	A	227	ARG
1	A	241	ARG

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Mol	Chain	Res	Type
1	A	245	LEU
1	A	272	VAL
1	A	282	ARG
1	A	287	LEU
1	A	299	LEU
1	A	318	ILE
1	A	322	VAL
1	A	323	GLU
1	A	326	VAL
1	A	336	LEU
1	A	347	GLU
1	A	352	HIS
1	A	367	ILE
1	A	399	THR
1	A	403	ASN
1	A	407	SER
1	A	411	SER
1	A	412	ASN
1	A	416	ASN
1	A	429	LEU
1	A	475	GLU
1	A	481	LEU
1	A	505	LEU
1	A	526	VAL
1	A	539	THR
1	A	548	SER
1	A	561	GLU
1	A	562	VAL
1	A	568	SER
1	A	575	HIS
1	A	593	GLU
1	A	598	VAL
1	A	602	GLN
1	A	610	ARG
1	A	626	SER
1	A	635	ARG
1	A	656	LEU
1	B	241	ARG
1	B	245	LEU
1	B	287	LEU
1	B	299	LEU
1	B	301	VAL

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Mol	Chain	Res	Type
1	B	326	VAL
1	B	334	VAL
1	B	338	THR
1	B	353	LEU
1	B	358	LEU
1	B	362	ASP
1	B	376	LEU
1	B	403	ASN
1	B	404	VAL
1	B	410	ARG
1	B	412	ASN
1	B	429	LEU
1	B	447	ASN
1	B	481	LEU
1	B	492	VAL
1	B	505	LEU
1	B	521	LEU
1	B	526	VAL
1	B	544	ARG
1	B	548	SER
1	B	561	GLU
1	B	567	SER
1	B	589	LEU
1	B	593	GLU
1	B	597	THR
1	B	598	VAL
1	B	610	ARG
1	B	613	ARG
1	B	635	ARG
1	B	644	ARG
1	B	648	VAL
1	B	656	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	HIS
1	A	215	ASN
1	A	234	HIS
1	A	273	GLN
1	A	290	HIS
1	A	332	HIS

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Mol	Chain	Res	Type
1	A	412	ASN
1	A	416	ASN
1	A	419	ASN
1	A	427	HIS
1	A	488	ASN
1	A	602	GLN
1	A	645	HIS
1	A	668	HIS
1	B	234	HIS
1	B	269	HIS
1	B	290	HIS
1	B	332	HIS
1	B	403	ASN
1	B	412	ASN
1	B	419	ASN
1	B	576	ASN
1	B	645	HIS
1	B	668	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 oligosaccharides 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 ⓘ

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	432/481 (89%)	0.57	23 (5%)	32 17	34, 66, 96, 122	8 (1%)
1	B	436/481 (90%)	0.90	51 (11%)	9 5	33, 69, 112, 136	6 (1%)
All	All	868/962 (90%)	0.74	74 (8%)	16 9	33, 68, 103, 136	14 (1%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	ARG	9.2
1	B	533	LYS	9.1
1	B	460	ARG	8.5
1	B	475	GLU	8.5
1	A	420	GLN	8.4
1	A	380	GLU	8.2
1	A	376	LEU	7.6
1	A	277	LYS	7.3
1	A	383	ASP	7.0
1	B	526	VAL	5.0
1	A	340	ARG	4.9
1	B	469	ILE	4.7
1	B	297	GLY	4.3
1	A	569	LYS	4.1
1	B	276	ILE	3.8
1	B	640	GLU	3.8
1	B	481	LEU	3.6
1	B	530	TRP	3.5
1	B	619	PRO	3.5
1	B	527	THR	3.3
1	B	638	LYS	3.2
1	B	344	GLU	3.1
1	B	641	PRO	3.1
1	A	362	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	340	ARG	3.1
1	B	626	SER	3.0
1	B	642	ALA	3.0
1	A	469	ILE	2.9
1	B	541	GLY	2.9
1	A	276	ILE	2.9
1	B	648	VAL	2.8
1	A	541	GLY	2.7
1	B	637	ALA	2.6
1	B	362	ASP	2.6
1	B	400	ASP	2.5
1	B	604	LEU	2.5
1	B	658	LYS	2.5
1	B	651	ARG	2.4
1	B	654	LYS	2.4
1	B	572	THR	2.4
1	B	315	HIS	2.4
1	B	473	ASP	2.4
1	A	616	TYR	2.3
1	B	372	GLY	2.3
1	B	374	ILE	2.3
1	B	605	THR	2.3
1	B	669	HIS	2.3
1	B	670	HIS	2.3
1	A	279	GLY	2.3
1	B	616	TYR	2.3
1	B	523	GLN	2.3
1	A	550	HIS	2.2
1	A	407	SER	2.2
1	B	635	ARG	2.2
1	A	467	GLN	2.2
1	B	617	CYS	2.2
1	A	399	THR	2.2
1	B	611	LEU	2.2
1	A	410	ARG	2.2
1	B	531	GLN	2.2
1	A	619	PRO	2.2
1	B	520	THR	2.2
1	B	491	LEU	2.1
1	B	421	PRO	2.1
1	B	633	PHE	2.1
1	B	479	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	473	ASP	2.1
1	B	387	ASP	2.1
1	A	574	THR	2.1
1	B	608	CYS	2.1
1	B	623	CYS	2.1
1	B	471	GLY	2.0
1	B	613	ARG	2.0
1	A	613	ARG	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.