



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2024 – 07:26 PM EDT

PDB ID : 3HO4  
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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

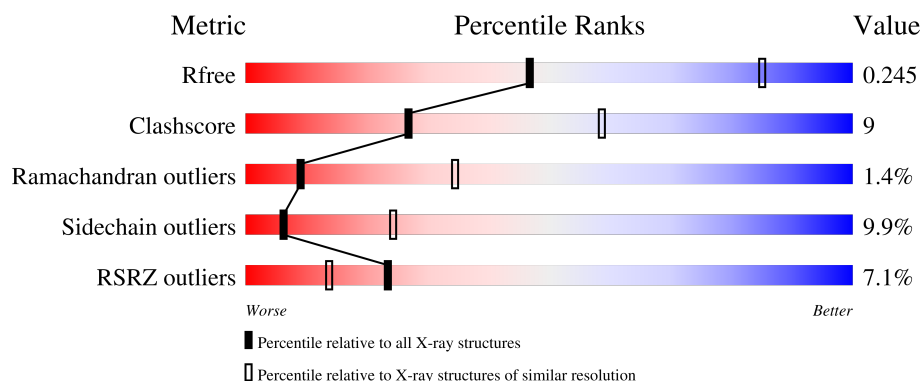
# 1 Overall quality at a glance

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))
$R_{free}$	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (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  $\geq 3$ , 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	<div> <div>4%</div> <div>68%</div> <div>20%</div> <div>•</div> <div>9%</div> </div>
1	B	481	<div> <div>9%</div> <div>67%</div> <div>21%</div> <div>•</div> <div>8%</div> </div>

## 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			

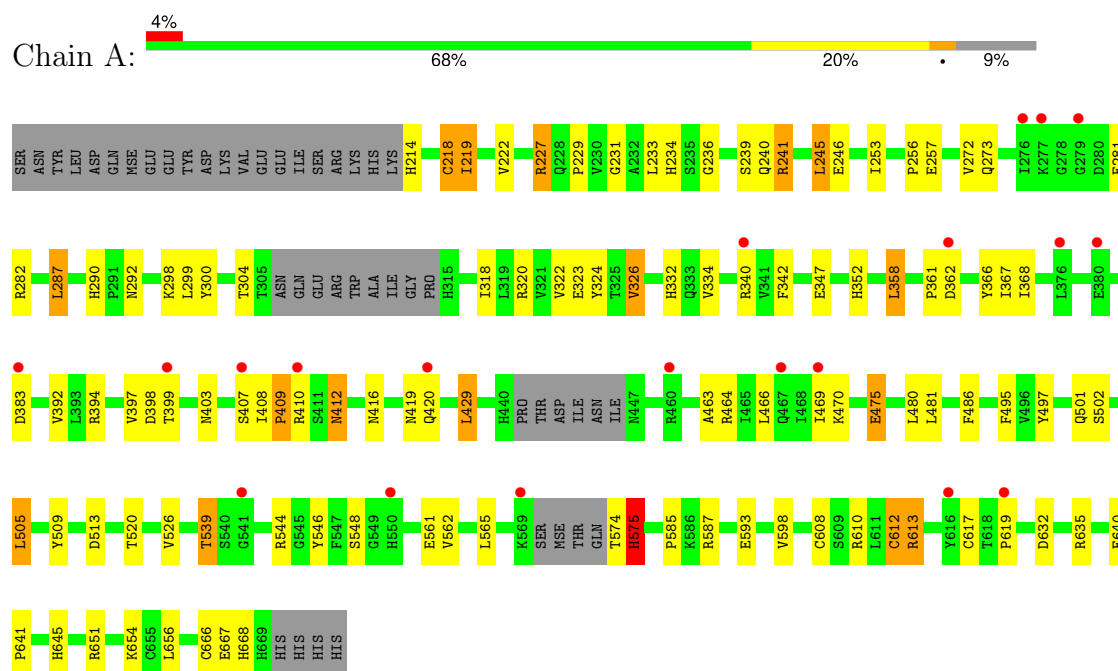
There are 12 discrepancies between the modelled and reference sequences:

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

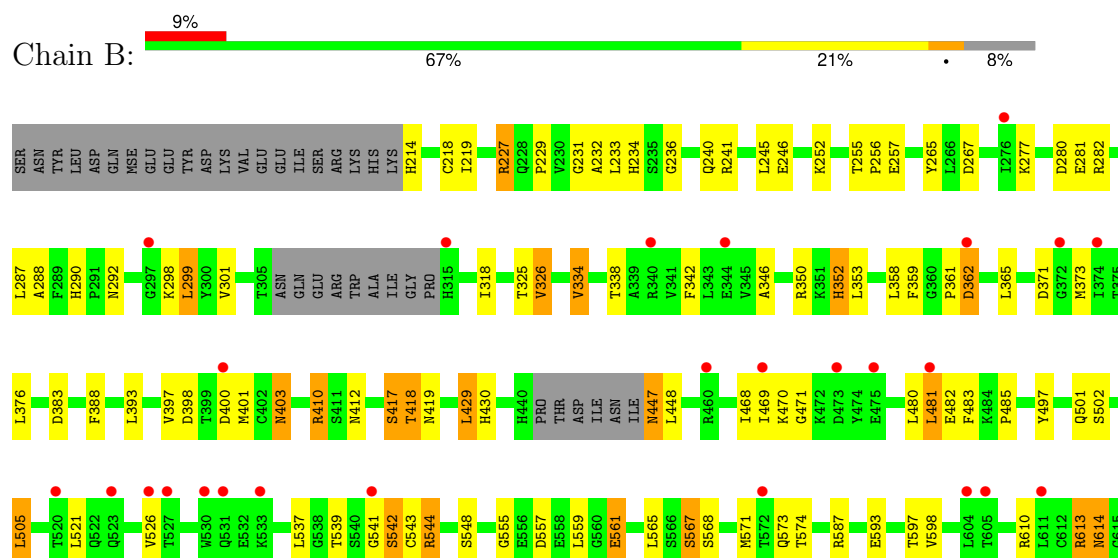
### 3 Residue-property plots

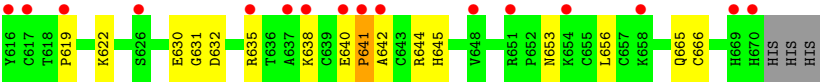
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 76.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.42	1/3488 (0.0%)	0.61	1/4699 (0.0%)
1	B	0.41	1/3529 (0.0%)	0.60	1/4754 (0.0%)
All	All	0.41	2/7017 (0.0%)	0.61	2/9453 (0.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	CYS	CB-SG	-5.94	1.72	1.81
1	A	218	CYS	CB-SG	-5.68	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	LYS	CB-CA-C	-6.03	98.33	110.40
1	A	299	LEU	CA-CB-CG	5.52	128.00	115.30

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	61	0
1	B	3454	0	3354	64	0
All	All	6868	0	6671	122	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 9.

All (122) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
1:B:227:ARG:HG3	1:B:246:GLU:CD	2.32	0.49
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:227:ARG:HG3	1:A:246:GLU:CD	2.35	0.47
1:B:447:ASN:HB3	1:B:469:ILE:HA	1.95	0.47
1:B:267:ASP:OD1	1:B:267:ASP:C	2.52	0.47
1:B:255:THR:HB	1:B:256:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:219:ILE:HD11	1:A:546:TYR:C	2.37	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:497:TYR:OH	1:B:561:GLU:OE2	2.25	0.43
1:A:539:THR:HG21	1:B:257:GLU:CD	2.39	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
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:371:ASP:OD1	1:B:430:HIS:HA	2.20	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:239:SER:C	1:A:241:ARG:H	2.22	0.41
1:A:245:LEU:HD23	1:A:245:LEU:N	2.35	0.41
1:A:497:TYR:CD1	1:A:505:LEU:HB3	2.54	0.41
1:A:502:SER:OG	1:A:505:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:631:GLY:O	1:B:632:ASP:C	2.60	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%)	11	38
1	B	436/481 (91%)	395 (91%)	34 (8%)	7 (2%)	8	31
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

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Mol	Chain	Res	Type
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%)	341 (90%)	39 (10%)	6	22
1	B	385/415 (93%)	348 (90%)	37 (10%)	7	26
All	All	765/830 (92%)	689 (90%)	76 (10%)	6	24

All (76) 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	233	LEU
1	A	241	ARG
1	A	245	LEU
1	A	272	VAL
1	A	287	LEU
1	A	318	ILE
1	A	323	GLU
1	A	326	VAL
1	A	347	GLU
1	A	352	HIS
1	A	358	LEU

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Mol	Chain	Res	Type
1	A	367	ILE
1	A	383	ASP
1	A	399	THR
1	A	403	ASN
1	A	407	SER
1	A	412	ASN
1	A	416	ASN
1	A	419	ASN
1	A	429	LEU
1	A	464	ARG
1	A	475	GLU
1	A	481	LEU
1	A	505	LEU
1	A	513	ASP
1	A	526	VAL
1	A	539	THR
1	A	548	SER
1	A	561	GLU
1	A	575	HIS
1	A	593	GLU
1	A	598	VAL
1	A	610	ARG
1	A	632	ASP
1	A	635	ARG
1	A	656	LEU
1	B	214	HIS
1	B	227	ARG
1	B	233	LEU
1	B	240	GLN
1	B	241	ARG
1	B	245	LEU
1	B	299	LEU
1	B	301	VAL
1	B	326	VAL
1	B	334	VAL
1	B	338	THR
1	B	352	HIS
1	B	358	LEU
1	B	362	ASP
1	B	376	LEU
1	B	383	ASP
1	B	403	ASN

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Mol	Chain	Res	Type
1	B	410	ARG
1	B	412	ASN
1	B	429	LEU
1	B	447	ASN
1	B	481	LEU
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	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	656	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	HIS
1	A	234	HIS
1	A	290	HIS
1	A	332	HIS
1	A	412	ASN
1	A	416	ASN
1	A	419	ASN
1	A	427	HIS
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

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Mol	Chain	Res	Type
1	B	522	GLN
1	B	576	ASN
1	B	602	GLN
1	B	645	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 [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	432/481 (89%)	0.42	20 (4%) 38 22	34, 66, 96, 122	8 (1%)
1	B	436/481 (90%)	0.76	42 (9%) 15 9	33, 69, 112, 136	6 (1%)
All	All	868/962 (90%)	0.59	62 (7%) 23 14	33, 68, 103, 136	14 (1%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	ARG	9.2
1	B	533	LYS	9.0
1	B	460	ARG	8.5
1	B	475	GLU	8.5
1	A	420	GLN	8.3
1	A	380	GLU	8.2
1	A	376	LEU	7.4
1	A	277	LYS	7.2
1	A	383	ASP	6.8
1	A	340	ARG	4.8
1	B	526	VAL	4.8
1	B	469	ILE	4.6
1	B	297	GLY	4.2
1	A	569	LYS	4.0
1	B	276	ILE	3.7
1	B	640	GLU	3.6
1	B	481	LEU	3.5
1	B	619	PRO	3.3
1	B	530	TRP	3.3
1	B	527	THR	3.1
1	B	638	LYS	3.1
1	B	344	GLU	3.0
1	B	340	ARG	3.0
1	B	641	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	362	ASP	2.9
1	B	642	ALA	2.8
1	B	626	SER	2.8
1	A	469	ILE	2.8
1	A	276	ILE	2.7
1	B	541	GLY	2.7
1	B	648	VAL	2.7
1	A	541	GLY	2.5
1	B	637	ALA	2.5
1	B	362	ASP	2.4
1	B	658	LYS	2.4
1	B	604	LEU	2.3
1	B	400	ASP	2.3
1	B	651	ARG	2.3
1	B	654	LYS	2.3
1	B	572	THR	2.2
1	B	315	HIS	2.2
1	B	473	ASP	2.2
1	B	374	ILE	2.2
1	B	605	THR	2.2
1	A	616	TYR	2.2
1	B	372	GLY	2.2
1	B	669	HIS	2.2
1	B	670	HIS	2.2
1	A	279	GLY	2.1
1	B	523	GLN	2.1
1	B	635	ARG	2.1
1	B	616	TYR	2.1
1	A	410	ARG	2.1
1	A	467	GLN	2.1
1	A	550	HIS	2.1
1	A	399	THR	2.1
1	A	407	SER	2.1
1	B	611	LEU	2.1
1	B	617	CYS	2.1
1	B	531	GLN	2.0
1	B	520	THR	2.0
1	A	619	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.