



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:35 PM GMT

PDB ID : 3HO5
Title : Crystal structure of Hedgehog-interacting protein (HHIP) and Sonic hedgehog (SHH) complex
Authors : Hymowitz, S.G.; Bosanac, I.
Deposited on : 2009-06-01
Resolution : 3.01 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

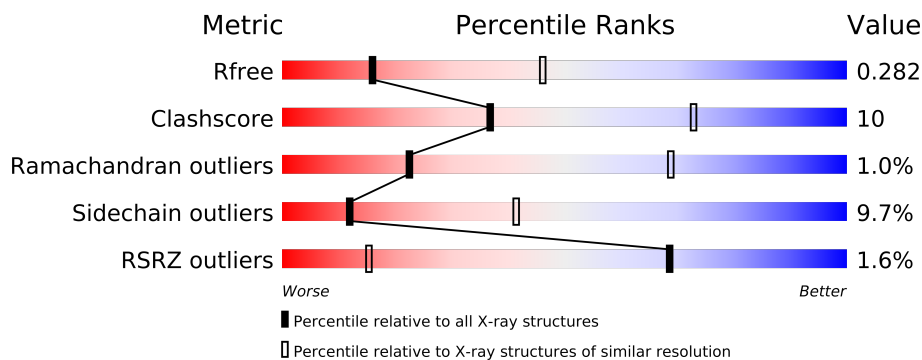
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.01 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}	66092	1332 (3.04-3.00)
Clashscore	79885	1732 (3.04-3.00)
Ramachandran outliers	78287	1669 (3.04-3.00)
Sidechain outliers	78261	1672 (3.04-3.00)
RSRZ outliers	66119	1333 (3.04-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	481	
1	B	481	
2	H	169	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8255 atoms, of which 0 are hydrogen and 0 are deuterium.

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	446	Total	C	N	O	S	19	0	0
			3487	2189	623	647	28			
1	B	451	Total	C	N	O	S	19	0	0
			3529	2213	631	657	28			

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

- Molecule 2 is a protein called Sonic hedgehog protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	154	Total	C	N	O	S	0	0	0
			1235	771	220	239	5			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

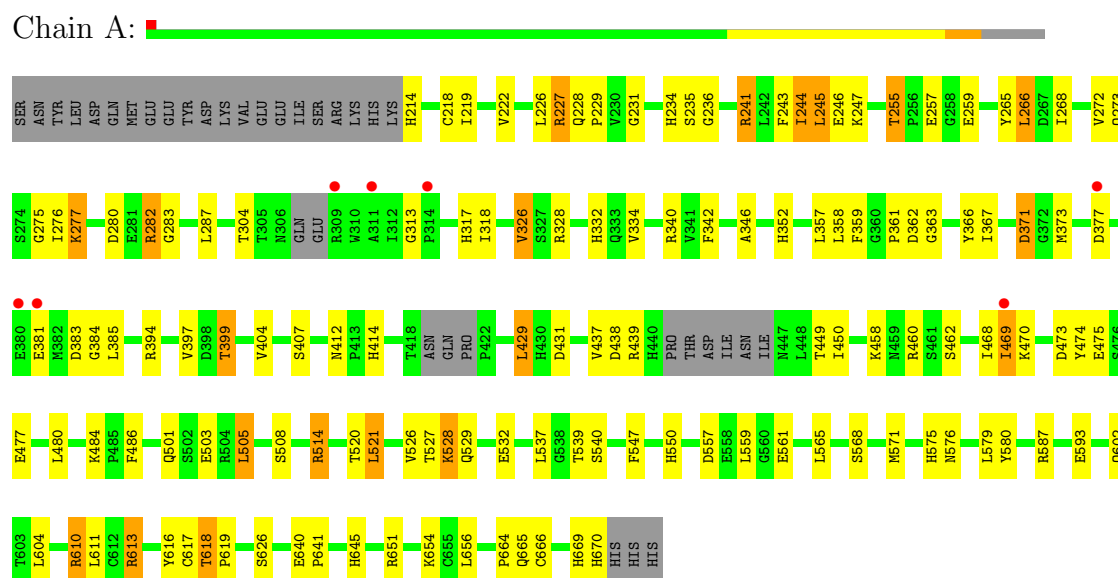
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	2	Total	Ca	0	0
			2	2		

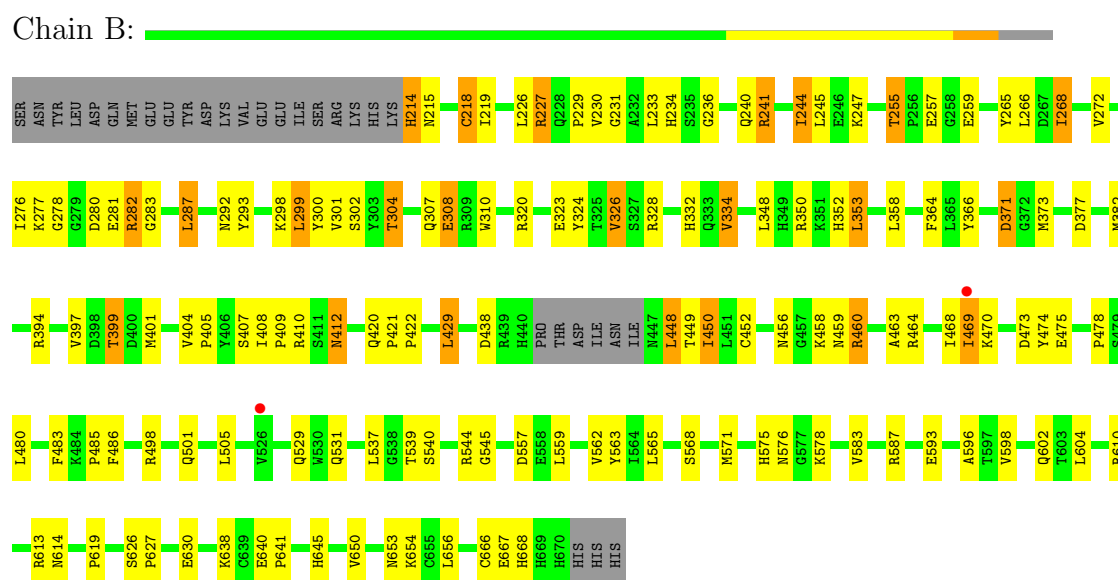
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

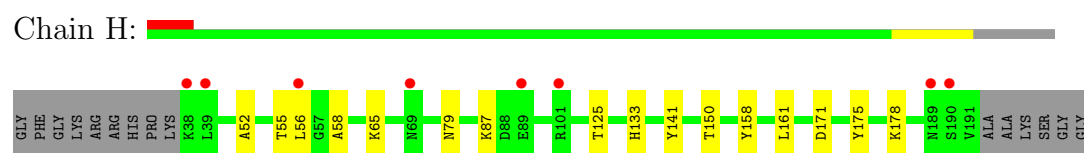


• Molecule 1: Hedgehog-interacting protein



• Molecule 2: Sonic hedgehog protein

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.62Å 101.62Å 302.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.01 29.33 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-3.01) 99.8 (29.33-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.231 , 0.287 0.233 , 0.282	Depositor DCC
R_{free} test set	1874 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 114.4	EDS
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 37023 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8255	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.45	3/3569 (0.1%)	0.63	3/4816 (0.1%)
1	B	0.47	4/3614 (0.1%)	0.64	3/4882 (0.1%)
2	H	0.34	0/1261	0.48	0/1701
All	All	0.44	7/8444 (0.1%)	0.62	6/11399 (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	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	460	ARG	CA-CB	-10.50	1.30	1.53
1	A	460	ARG	CA-CB	-9.56	1.32	1.53
1	B	458	LYS	CA-CB	-6.67	1.39	1.53
1	B	410	ARG	CA-CB	-6.46	1.39	1.53
1	B	218	CYS	CB-SG	-6.38	1.71	1.82
1	A	528	LYS	CE-NZ	5.97	1.64	1.49
1	A	218	CYS	CB-SG	-5.73	1.72	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	460	ARG	N-CA-CB	-10.71	91.33	110.60
1	B	299	LEU	CA-CB-CG	7.91	133.50	115.30
1	A	458	LYS	CB-CA-C	-7.21	95.98	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ARG	N-CA-CB	6.78	122.80	110.60
1	B	458	LYS	CB-CA-C	5.89	122.18	110.40
1	A	245	LEU	CA-CB-CG	5.34	127.58	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3487	0	3388	78	0
1	B	3529	0	3424	85	0
2	H	1235	0	1197	11	0
3	A	1	0	0	0	0
3	H	1	0	0	0	0
4	H	2	0	0	0	0
All	All	8255	0	8009	165	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (165) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:277:LYS:HB2	1:A:280:ASP:HB2	1.51	0.91
1:B:240:GLN:HE22	1:B:596:ALA:HB1	1.38	0.89
1:A:429:LEU:HD13	1:A:480:LEU:HD21	1.55	0.86
1:B:469:ILE:HG22	1:B:470:LYS:H	1.41	0.85
1:A:501:GLN:O	1:A:587:ARG:HD3	1.78	0.83
1:A:645:HIS:HD2	1:A:666:CYS:O	1.63	0.81
1:A:318:ILE:HG22	1:A:346:ALA:HA	1.64	0.80
1:B:429:LEU:HD13	1:B:480:LEU:HD21	1.61	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:527:THR:O	1:A:529:GLN:N	2.15	0.78
1:B:382:MET:HG2	2:H:133:HIS:HB3	1.66	0.78
1:A:469:ILE:HG22	1:A:470:LYS:H	1.49	0.78
1:B:421:PRO:HD3	2:H:178:LYS:HE2	1.66	0.76
1:B:501:GLN:O	1:B:587:ARG:HD3	1.86	0.76
1:A:257:GLU:OE2	1:B:539:THR:HG21	1.85	0.76
1:B:568:SER:H	1:B:571:MET:HB2	1.54	0.72
1:B:397:VAL:HG12	1:B:619:PRO:HG2	1.72	0.71
1:A:399:THR:HG23	1:A:407:SER:HB2	1.72	0.71
1:B:463:ALA:HB2	1:B:486:PHE:HE2	1.55	0.69
1:A:414:HIS:HE1	1:A:477:GLU:HG3	1.57	0.69
1:B:282:ARG:O	1:B:304:THR:HB	1.93	0.69
1:B:667:GLU:HG3	1:B:668:HIS:CD2	2.30	0.67
1:A:394:ARG:HE	1:A:412:ASN:HD21	1.45	0.65
1:B:255:THR:HG22	1:B:259:GLU:H	1.60	0.65
1:B:421:PRO:HG3	2:H:178:LYS:HZ1	1.60	0.65
1:A:257:GLU:CD	1:B:539:THR:HG21	2.18	0.64
1:B:226:LEU:HD13	1:B:244:ILE:CD1	2.28	0.64
1:B:300:TYR:OH	1:B:397:VAL:HG11	1.97	0.64
1:A:255:THR:HG22	1:A:259:GLU:H	1.60	0.64
1:B:300:TYR:CE2	1:B:323:GLU:HG3	2.34	0.63
1:A:640:GLU:HB2	1:A:641:PRO:HD3	1.79	0.63
1:A:313:GLY:HA3	1:A:384:GLY:HA3	1.81	0.62
1:A:359:PHE:O	1:A:439:ARG:NH1	2.29	0.62
1:A:241:ARG:HH11	1:A:332:HIS:HD2	1.46	0.61
2:H:65:LYS:HG3	2:H:141:TYR:HB3	1.84	0.60
1:B:421:PRO:HG3	2:H:178:LYS:NZ	2.17	0.59
1:A:257:GLU:OE2	1:B:539:THR:CG2	2.51	0.59
1:B:645:HIS:HD2	1:B:666:CYS:O	1.86	0.58
1:B:640:GLU:HB2	1:B:641:PRO:HD3	1.87	0.57
1:A:234:HIS:HD2	1:A:236:GLY:H	1.52	0.56
1:B:408:ILE:HD13	1:B:422:PRO:HB2	1.86	0.56
1:A:234:HIS:HD2	1:A:236:GLY:N	2.04	0.56
1:B:226:LEU:HD13	1:B:244:ILE:HD13	1.87	0.55
1:B:244:ILE:HD12	1:B:565:LEU:CD2	2.37	0.54
1:A:468:ILE:O	1:A:474:TYR:OH	2.24	0.54
1:A:340:ARG:HD3	1:A:616:TYR:CG	2.42	0.54
1:B:293:TYR:OH	1:B:326:VAL:HG11	2.08	0.53
1:B:469:ILE:HG22	1:B:470:LYS:N	2.20	0.53
1:B:557:ASP:HB3	1:B:559:LEU:H	1.73	0.53
1:B:240:GLN:NE2	1:B:596:ALA:HB1	2.16	0.52
1:A:414:HIS:CE1	1:A:477:GLU:HG3	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:651:ARG:HD2	1:A:654:LYS:HD3	1.91	0.52
1:A:326:VAL:HA	1:A:334:VAL:HA	1.91	0.52
1:A:571:MET:HB2	1:A:576:ASN:HB3	1.91	0.52
1:B:463:ALA:HB2	1:B:486:PHE:CE2	2.40	0.51
1:B:348:LEU:HD11	1:B:382:MET:HE1	1.92	0.51
1:B:613:ARG:O	1:B:614:ASN:HB2	2.11	0.51
1:B:630:GLU:HB3	1:B:638:LYS:HE3	1.93	0.51
1:A:244:ILE:HD12	1:A:565:LEU:CD2	2.41	0.51
1:B:247:LYS:HG2	1:B:283:GLY:HA3	1.92	0.51
1:B:421:PRO:HD3	2:H:178:LYS:CE	2.40	0.51
1:B:282:ARG:CG	1:B:304:THR:HG21	2.41	0.51
1:B:571:MET:HG2	1:B:576:ASN:O	2.11	0.51
1:A:539:THR:HB	1:B:257:GLU:OE2	2.11	0.50
1:A:227:ARG:HG2	1:A:575:HIS:HD2	1.77	0.50
1:B:429:LEU:CD1	1:B:480:LEU:HD21	2.39	0.50
1:A:394:ARG:HE	1:A:412:ASN:ND2	2.07	0.50
1:A:429:LEU:CD1	1:A:480:LEU:HD21	2.35	0.50
1:B:282:ARG:HG2	1:B:304:THR:HG21	1.92	0.50
1:A:547:PHE:HB2	1:A:580:TYR:CE1	2.46	0.49
1:B:241:ARG:HH11	1:B:332:HIS:HD2	1.60	0.49
1:A:371:ASP:HB3	1:A:373:MET:H	1.76	0.49
1:B:366:TYR:CZ	1:B:394:ARG:HD2	2.48	0.49
2:H:158:TYR:HA	2:H:161:LEU:HB3	1.94	0.49
1:A:664:PRO:HB2	1:A:665:GLN:NE2	2.27	0.49
1:A:383:ASP:C	1:A:385:LEU:H	2.16	0.49
1:B:234:HIS:HD2	1:B:236:GLY:H	1.60	0.49
1:B:645:HIS:CD2	1:B:666:CYS:O	2.65	0.48
1:A:231:GLY:HA2	1:A:565:LEU:HD13	1.94	0.48
1:B:302:SER:HA	1:B:320:ARG:O	2.13	0.48
1:B:268:ILE:HD11	1:B:324:TYR:OH	2.14	0.48
1:B:227:ARG:HB3	1:B:575:HIS:CD2	2.48	0.48
1:A:342:PHE:HE1	1:A:397:VAL:HG12	1.78	0.48
1:B:474:TYR:CE2	1:B:478:PRO:HG3	2.48	0.48
1:A:282:ARG:HG2	1:A:304:THR:HG21	1.95	0.48
1:B:241:ARG:HH11	1:B:332:HIS:CD2	2.31	0.48
1:A:514:ARG:HG2	1:A:550:HIS:HB3	1.94	0.48
1:B:371:ASP:HB3	1:B:373:MET:H	1.78	0.47
1:A:247:LYS:HG2	1:A:283:GLY:HA3	1.96	0.47
1:A:486:PHE:CE1	1:A:521:LEU:HD21	2.49	0.47
1:A:618:THR:HB	1:A:619:PRO:HD2	1.96	0.47
1:A:282:ARG:CG	1:A:304:THR:HG21	2.44	0.47
1:B:529:GLN:HG2	1:B:531:GLN:HG2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:438:ASP:HB3	1:A:449:THR:HB	1.96	0.47
1:A:568:SER:OG	1:A:571:MET:HG2	2.15	0.47
1:A:469:ILE:HG22	1:A:470:LYS:N	2.24	0.47
1:B:241:ARG:NH1	1:B:332:HIS:CD2	2.83	0.46
1:A:282:ARG:O	1:A:304:THR:HB	2.14	0.46
1:A:645:HIS:CD2	1:A:666:CYS:O	2.54	0.46
1:B:307:GLN:O	1:B:310:TRP:N	2.48	0.46
1:A:352:HIS:CD2	1:A:431:ASP:HB2	2.51	0.46
1:A:241:ARG:NH1	1:A:332:HIS:HD2	2.13	0.46
1:B:348:LEU:HD11	1:B:382:MET:CE	2.46	0.46
1:B:420:GLN:HB3	1:B:421:PRO:HD2	1.98	0.46
1:B:448:LEU:HB3	1:B:468:ILE:HG12	1.98	0.46
1:B:399:THR:HG22	1:B:401:MET:H	1.80	0.46
1:B:282:ARG:HD2	1:B:350:ARG:HG2	1.97	0.45
1:B:231:GLY:HA2	1:B:565:LEU:HD13	1.97	0.45
1:B:450:ILE:HD11	1:B:452:CYS:SG	2.56	0.45
2:H:52:ALA:HB3	2:H:55:THR:HG23	1.97	0.45
1:B:276:ILE:HG13	1:B:277:LYS:H	1.82	0.45
1:A:610:ARG:HG3	1:A:611:LEU:HD13	1.99	0.45
1:B:255:THR:HG23	1:B:257:GLU:H	1.81	0.45
1:B:218:CYS:HB3	1:B:583:VAL:HB	1.99	0.45
1:B:214:HIS:HB2	1:B:215:ASN:H	1.55	0.45
1:B:640:GLU:HB2	1:B:653:ASN:HD21	1.82	0.45
1:B:280:ASP:OD2	1:B:282:ARG:NH1	2.50	0.45
1:A:227:ARG:HG3	1:A:246:GLU:OE1	2.17	0.44
1:B:300:TYR:CZ	1:B:397:VAL:HG11	2.51	0.44
1:A:255:THR:HG23	1:A:257:GLU:H	1.82	0.44
1:B:244:ILE:HD12	1:B:565:LEU:HD23	1.99	0.44
1:A:394:ARG:HH21	1:A:412:ASN:HD22	1.65	0.44
2:H:87:LYS:HD2	2:H:125:THR:HG22	1.98	0.44
1:B:281:GLU:HB2	1:B:353:LEU:HD22	1.99	0.44
1:B:229:PRO:HB2	1:B:565:LEU:HB3	1.99	0.44
1:B:438:ASP:HB3	1:B:449:THR:HB	1.98	0.44
1:B:456:ASN:HB2	1:B:459:ASN:HB3	2.00	0.44
1:B:298:LYS:HD2	1:B:619:PRO:HG3	1.99	0.43
1:A:226:LEU:HD13	1:A:244:ILE:CD1	2.48	0.43
1:A:304:THR:HG23	1:A:317:HIS:ND1	2.34	0.43
1:A:669:HIS:O	1:A:670:HIS:HB3	2.18	0.43
1:A:273:GLN:O	1:A:282:ARG:O	2.36	0.43
1:B:562:VAL:HG12	1:B:563:TYR:N	2.32	0.43
1:B:568:SER:N	1:B:571:MET:HB2	2.29	0.43
1:A:358:LEU:HG	1:A:366:TYR:HB2	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:326:VAL:HA	1:B:334:VAL:HA	2.00	0.43
1:A:227:ARG:O	1:A:228:GLN:C	2.56	0.43
1:A:265:TYR:O	1:A:334:VAL:HG13	2.18	0.43
1:A:503:GLU:H	1:A:587:ARG:HD2	1.84	0.43
1:A:520:THR:O	1:A:532:GLU:HA	2.19	0.42
2:H:58:ALA:O	2:H:171:ASP:HB3	2.19	0.42
1:B:233:LEU:HD21	1:B:287:LEU:HB3	2.00	0.42
1:B:404:VAL:CG1	1:B:405:PRO:HD2	2.49	0.42
1:B:483:PHE:CE2	1:B:485:PRO:HG3	2.55	0.42
1:A:277:LYS:HB2	1:A:280:ASP:CB	2.36	0.42
1:B:227:ARG:HB3	1:B:575:HIS:HD2	1.85	0.42
2:H:150:THR:HG23	2:H:161:LEU:HD22	2.02	0.41
1:B:429:LEU:HD12	1:B:464:ARG:HD2	2.03	0.41
1:A:235:SER:HB2	1:A:243:PHE:HE1	1.85	0.41
1:A:377:ASP:O	1:A:381:GLU:HB2	2.20	0.41
1:A:229:PRO:HB2	1:A:565:LEU:HB3	2.02	0.41
1:A:358:LEU:HD22	1:A:437:VAL:HG21	2.03	0.41
1:B:409:PRO:HG2	1:B:412:ASN:CG	2.41	0.41
1:A:361:PRO:C	1:A:363:GLY:H	2.24	0.41
1:A:222:VAL:HB	1:A:579:LEU:HD23	2.03	0.41
1:B:539:THR:HB	1:B:545:GLY:H	1.86	0.41
1:A:366:TYR:CE2	1:A:394:ARG:HD3	2.56	0.41
1:A:462:SER:HB3	1:A:484:LYS:HG2	2.03	0.41
1:A:640:GLU:HB2	1:A:641:PRO:CD	2.50	0.41
1:B:265:TYR:O	1:B:334:VAL:HG13	2.21	0.41
1:B:364:PHE:CZ	1:B:409:PRO:HB3	2.55	0.40
1:A:357:LEU:HD22	1:A:367:ILE:HG13	2.03	0.40
1:A:505:LEU:HD22	1:A:508:SER:HB2	2.02	0.40
1:A:266:LEU:HD13	1:A:268:ILE:HB	2.03	0.40
1:A:557:ASP:HB2	1:A:561:GLU:H	1.87	0.40
1:A:557:ASP:HB3	1:A:559:LEU:H	1.85	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	438/481 (91%)	412 (94%)	21 (5%)	5 (1%)	21	66
1	B	447/481 (93%)	412 (92%)	30 (7%)	5 (1%)	21	66
2	H	152/169 (90%)	147 (97%)	5 (3%)	0	100	100
All	All	1037/1131 (92%)	971 (94%)	56 (5%)	10 (1%)	22	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	ILE
1	A	277	LYS
1	A	469	ILE
1	A	528	LYS
1	A	613	ARG
1	B	460	ARG
1	B	469	ILE
1	B	308	GLU
1	B	627	PRO
1	B	278	GLY

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	387/422 (92%)	351 (91%)	36 (9%)	13	44
1	B	392/422 (93%)	343 (88%)	49 (12%)	7	27
2	H	132/141 (94%)	129 (98%)	3 (2%)	63	92
All	All	911/985 (92%)	823 (90%)	88 (10%)	12	41

All (88) 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
1	A	244	ILE

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Mol	Chain	Res	Type
1	A	245	LEU
1	A	255	THR
1	A	266	LEU
1	A	272	VAL
1	A	282	ARG
1	A	287	LEU
1	A	326	VAL
1	A	328	ARG
1	A	362	ASP
1	A	371	ASP
1	A	399	THR
1	A	404	VAL
1	A	429	LEU
1	A	450	ILE
1	A	473	ASP
1	A	475	GLU
1	A	505	LEU
1	A	514	ARG
1	A	521	LEU
1	A	526	VAL
1	A	537	LEU
1	A	540	SER
1	A	593	GLU
1	A	602	GLN
1	A	604	LEU
1	A	610	ARG
1	A	613	ARG
1	A	617	CYS
1	A	618	THR
1	A	626	SER
1	A	656	LEU
1	B	214	HIS
1	B	219	ILE
1	B	227	ARG
1	B	230	VAL
1	B	241	ARG
1	B	244	ILE
1	B	245	LEU
1	B	255	THR
1	B	266	LEU
1	B	268	ILE
1	B	272	VAL

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Mol	Chain	Res	Type
1	B	282	ARG
1	B	287	LEU
1	B	292	ASN
1	B	299	LEU
1	B	301	VAL
1	B	304	THR
1	B	308	GLU
1	B	326	VAL
1	B	328	ARG
1	B	334	VAL
1	B	352	HIS
1	B	353	LEU
1	B	358	LEU
1	B	371	ASP
1	B	377	ASP
1	B	399	THR
1	B	407	SER
1	B	412	ASN
1	B	429	LEU
1	B	448	LEU
1	B	450	ILE
1	B	473	ASP
1	B	475	GLU
1	B	498	ARG
1	B	505	LEU
1	B	537	LEU
1	B	540	SER
1	B	544	ARG
1	B	578	LYS
1	B	593	GLU
1	B	598	VAL
1	B	602	GLN
1	B	604	LEU
1	B	610	ARG
1	B	626	SER
1	B	650	VAL
1	B	654	LYS
1	B	656	LEU
2	H	56	LEU
2	H	79	ASN
2	H	175	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	HIS
1	A	332	HIS
1	A	412	ASN
1	A	414	HIS
1	A	440	HIS
1	A	447	ASN
1	A	459	ASN
1	A	515	ASN
1	A	550	HIS
1	A	575	HIS
1	A	645	HIS
1	A	665	GLN
1	B	214	HIS
1	B	234	HIS
1	B	240	GLN
1	B	315	HIS
1	B	332	HIS
1	B	412	ASN
1	B	414	HIS
1	B	575	HIS
1	B	614	ASN
1	B	645	HIS
1	B	665	GLN
1	B	668	HIS
2	H	69	ASN
2	H	79	ASN
2	H	91	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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.

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	446/481 (92%)	0.03	7 (1%)	68 15	67, 98, 136, 168	4 (0%)
1	B	451/481 (93%)	-0.09	2 (0%)	90 40	69, 94, 128, 154	4 (0%)
2	H	154/169 (91%)	0.56	8 (5%)	26 5	62, 78, 92, 103	0
All	All	1051/1131 (92%)	0.06	17 (1%)	68 15	62, 94, 131, 168	8 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	ALA	5.0
1	A	314	PRO	3.4
2	H	38	LYS	3.2
1	A	380	GLU	3.2
2	H	56	LEU	3.1
2	H	101	ARG	3.1
1	B	526	VAL	3.0
1	A	381	GLU	2.7
2	H	69	ASN	2.6
2	H	39	LEU	2.6
1	A	377	ASP	2.4
1	A	469	ILE	2.4
2	H	89	GLU	2.3
2	H	190	SER	2.3
1	A	309	ARG	2.3
2	H	189	ASN	2.2
1	B	469	ILE	2.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CA	H	401	1/1	0.38	0.05	90,90,90,90	0
4	CA	H	402	1/1	0.23	-0.93	91,91,91,91	0
3	ZN	H	400	1/1	0.07	-3.48	75,75,75,75	0
3	ZN	A	902	1/1	0.08	-	151,151,151,151	0

6.5 Other polymers ⓘ

There are no such residues in this entry.