



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2024 – 02:34 am GMT

PDB ID : 2WFT  
Title : Crystal structure of the human HIP ectodomain  
Authors : Bishop, B.; Aricescu, A.R.; Harlos, K.; O'Callaghan, C.A.; Jones, E.Y.; Siebold, C.  
Deposited on : 2009-04-15  
Resolution : 2.80 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
Xtriage (Phenix)	:	1.13
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

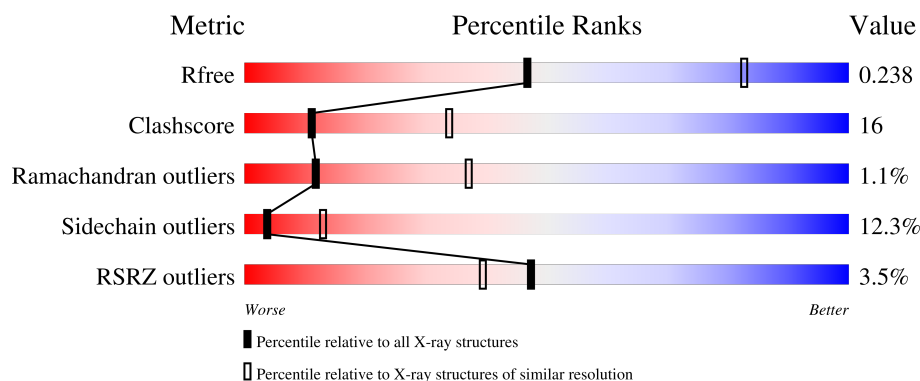
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


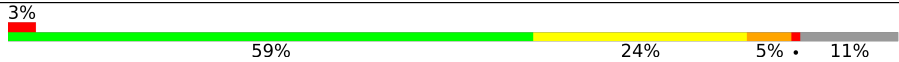
The reported resolution of this entry is 2.80 Å.

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	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	458	
1	B	458	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	A	1673	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6624 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	438	Total	C	N	O	S	0	0	0
			3414	2141	605	640	28			
1	B	409	Total	C	N	O	S	0	0	1
			3166	1986	560	592	28			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

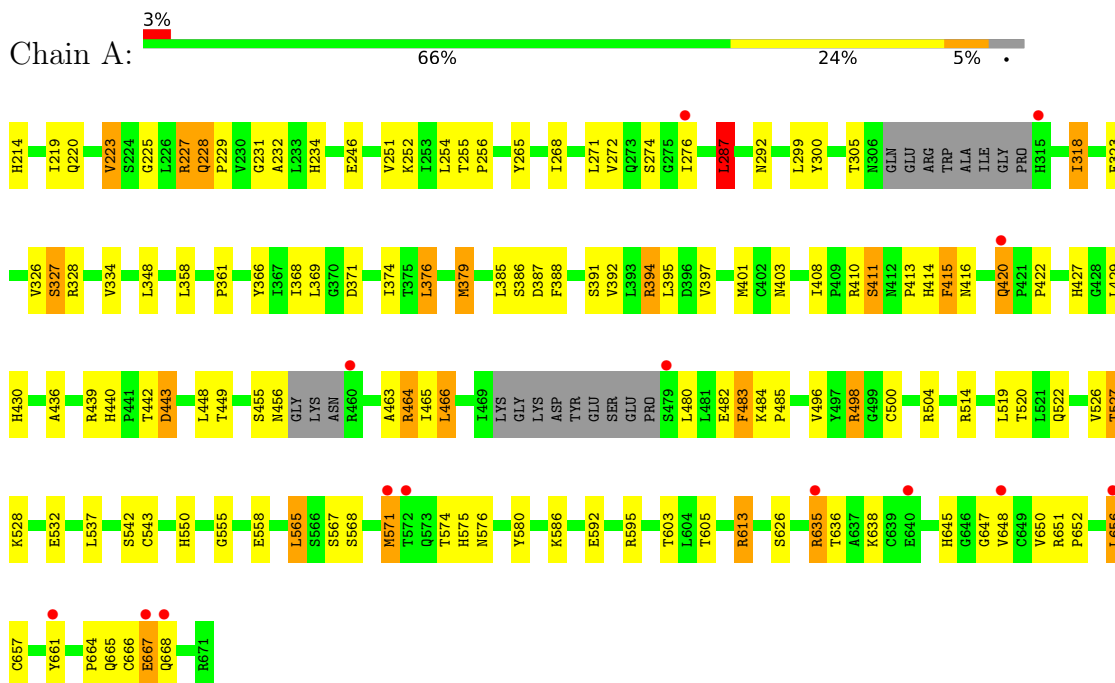
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	19	Total	O	0	0
			19	19		

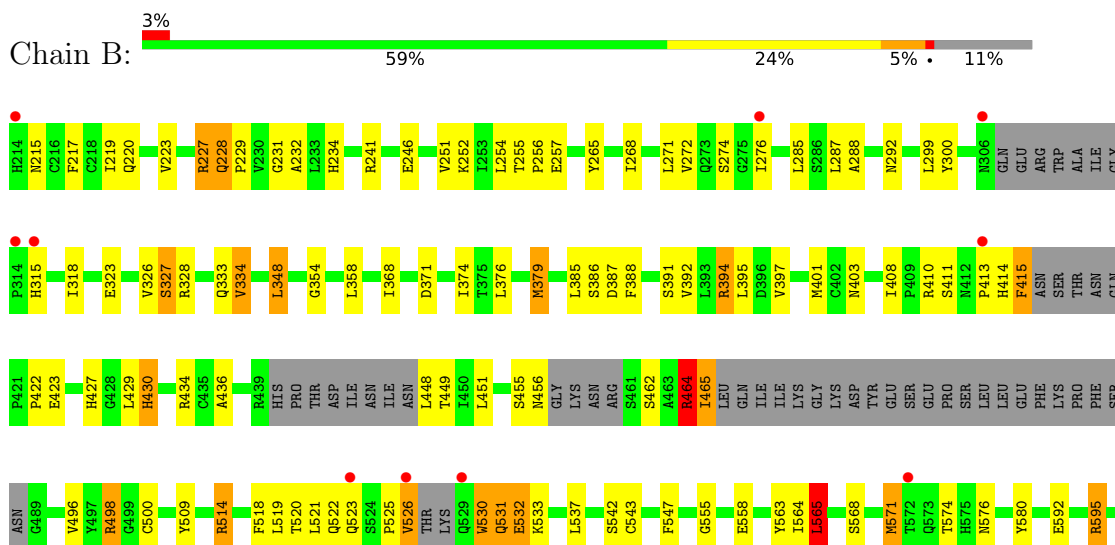
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	100.98Å 100.98Å 305.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 2.80 19.89 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.89-2.80) 99.4 (19.89-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.71Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.199 , 0.238 0.198 , 0.238	Depositor DCC
$R_{free}$ test set	2289 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.0	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 78.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6624	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL

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	0.63	0/3490	1.08	21/4714 (0.4%)
1	B	0.68	0/3234	1.09	26/4362 (0.6%)
All	All	0.66	0/6724	1.08	47/9076 (0.5%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	ARG	NE-CZ-NH2	-14.19	113.20	120.30
1	A	635	ARG	NE-CZ-NH1	13.92	127.26	120.30
1	A	635	ARG	NE-CZ-NH2	-13.45	113.58	120.30
1	B	595	ARG	NE-CZ-NH1	-13.34	113.63	120.30
1	A	498	ARG	NE-CZ-NH2	-13.17	113.71	120.30
1	B	635	ARG	NE-CZ-NH1	-13.14	113.73	120.30
1	A	595	ARG	NE-CZ-NH2	-13.07	113.76	120.30
1	B	394	ARG	NE-CZ-NH2	-13.05	113.78	120.30
1	B	613	ARG	NE-CZ-NH1	-12.66	113.97	120.30
1	A	394	ARG	NE-CZ-NH1	-12.61	114.00	120.30
1	A	613	ARG	NE-CZ-NH1	12.55	126.58	120.30
1	A	328	ARG	NE-CZ-NH2	-12.45	114.07	120.30
1	B	635	ARG	NE-CZ-NH2	12.40	126.50	120.30
1	A	498	ARG	NE-CZ-NH1	12.37	126.48	120.30
1	B	227	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	A	328	ARG	NE-CZ-NH1	12.15	126.38	120.30
1	B	595	ARG	NE-CZ-NH2	12.11	126.36	120.30
1	B	328	ARG	NE-CZ-NH2	12.02	126.31	120.30
1	B	394	ARG	NE-CZ-NH1	11.90	126.25	120.30
1	A	394	ARG	NE-CZ-NH2	11.71	126.16	120.30
1	B	498	ARG	NE-CZ-NH1	-11.63	114.49	120.30
1	A	227	ARG	NE-CZ-NH2	11.59	126.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	595	ARG	NE-CZ-NH1	11.43	126.01	120.30
1	B	613	ARG	NE-CZ-NH2	11.14	125.87	120.30
1	B	328	ARG	NE-CZ-NH1	-10.90	114.85	120.30
1	A	227	ARG	NE-CZ-NH1	-10.86	114.87	120.30
1	B	227	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	B	498	ARG	NE-CZ-NH2	9.45	125.03	120.30
1	B	635	ARG	CD-NE-CZ	7.27	133.78	123.60
1	A	635	ARG	CD-NE-CZ	6.84	133.18	123.60
1	B	328	ARG	CD-NE-CZ	6.66	132.92	123.60
1	A	613	ARG	CD-NE-CZ	6.65	132.91	123.60
1	A	498	ARG	CD-NE-CZ	6.58	132.81	123.60
1	A	328	ARG	CD-NE-CZ	6.52	132.72	123.60
1	B	595	ARG	CD-NE-CZ	6.29	132.41	123.60
1	B	613	ARG	CD-NE-CZ	6.25	132.34	123.60
1	A	394	ARG	CD-NE-CZ	6.22	132.30	123.60
1	A	595	ARG	CD-NE-CZ	6.16	132.22	123.60
1	A	287	LEU	CA-CB-CG	6.15	129.44	115.30
1	B	227	ARG	CD-NE-CZ	5.79	131.70	123.60
1	B	394	ARG	CD-NE-CZ	5.41	131.17	123.60
1	B	514	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	498	ARG	CD-NE-CZ	5.35	131.09	123.60
1	B	241	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	662	LEU	CA-CB-CG	5.20	127.25	115.30
1	B	662	LEU	CB-CG-CD1	5.09	119.66	111.00
1	B	565	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3319	107	1
1	B	3166	0	3071	103	1
2	A	2	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	1	0
3	B	2	0	0	0	0
4	A	19	0	0	2	0
4	B	19	0	0	1	0
All	All	6624	0	6390	209	1

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 16.

All (209) 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:568:SER:H	1:A:571:MET:CB	1.81	0.94
1:B:659:LYS:O	1:B:661:TYR:HE2	1.51	0.93
1:B:660:GLY:C	1:B:661:TYR:CD2	2.42	0.93
1:A:410:ARG:HA	1:A:415:PHE:HD2	1.35	0.91
1:A:483:PHE:H	1:A:483:PHE:HD2	1.19	0.90
1:B:410:ARG:HA	1:B:415:PHE:HD2	1.36	0.89
1:B:532:GLU:O	1:B:533:LYS:HG3	1.72	0.89
1:B:410:ARG:HA	1:B:415:PHE:CD2	2.09	0.87
1:A:410:ARG:HA	1:A:415:PHE:CD2	2.09	0.86
1:A:645:HIS:CG	1:A:661:TYR:CD1	2.64	0.85
1:A:568:SER:H	1:A:571:MET:HB2	1.42	0.85
1:B:659:LYS:O	1:B:661:TYR:CE2	2.33	0.82
1:B:348:LEU:HD22	1:B:374:ILE:HD12	1.64	0.79
1:A:568:SER:OG	1:A:571:MET:HB2	1.85	0.76
1:A:231:GLY:HA2	1:A:565:LEU:HD13	1.67	0.75
1:A:219:ILE:HD13	1:A:537:LEU:HD13	1.68	0.74
1:B:568:SER:H	1:B:571:MET:CB	2.01	0.74
1:B:650:VAL:HG12	1:B:651:ARG:HG3	1.68	0.74
1:A:568:SER:N	1:A:571:MET:HB2	2.02	0.73
1:A:568:SER:H	1:A:571:MET:HB3	1.52	0.73
1:A:645:HIS:ND1	1:A:661:TYR:CD1	2.56	0.73
1:B:613:ARG:HA	1:B:613:ARG:NE	2.04	0.73
1:B:532:GLU:C	1:B:533:LYS:HG3	2.10	0.72
1:B:568:SER:OG	1:B:571:MET:HB2	1.90	0.70
1:B:660:GLY:C	1:B:661:TYR:CG	2.65	0.70
1:A:440:HIS:HA	3:A:1674:CL:CL	2.28	0.69
1:A:571:MET:HG3	1:A:576:ASN:O	1.93	0.69
1:A:645:HIS:CD2	1:A:661:TYR:CE1	2.80	0.69
1:B:386:SER:O	1:B:387:ASP:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ILE:CD1	1:A:537:LEU:HD13	2.24	0.68
1:B:660:GLY:CA	1:B:661:TYR:CD2	2.77	0.68
1:A:645:HIS:CG	1:A:661:TYR:CE1	2.82	0.68
1:B:658:LYS:O	1:B:661:TYR:HD2	1.77	0.68
1:B:408:ILE:HD12	1:B:422:PRO:HB2	1.75	0.67
1:A:465:ILE:O	1:A:466:LEU:HG	1.94	0.67
1:B:451:LEU:HD13	1:B:509:TYR:CE2	2.31	0.66
1:A:379:MET:HA	1:A:385:LEU:HD12	1.78	0.66
1:A:386:SER:O	1:A:387:ASP:HB2	1.95	0.66
1:A:386:SER:OG	1:A:388:PHE:HB2	1.96	0.66
1:B:246:GLU:OE2	1:B:252:LYS:HE3	1.96	0.66
1:B:568:SER:H	1:B:571:MET:HB3	1.61	0.66
1:A:408:ILE:HD12	1:A:422:PRO:HB2	1.78	0.65
1:B:379:MET:HA	1:B:385:LEU:HD12	1.78	0.65
1:A:246:GLU:OE2	1:A:252:LYS:HE3	1.97	0.65
1:B:231:GLY:HA2	1:B:565:LEU:HD13	1.79	0.65
1:B:523:GLN:HA	1:B:530:TRP:CD1	2.31	0.65
1:B:661:TYR:CD2	1:B:661:TYR:N	2.64	0.64
1:A:394:ARG:C	1:A:395:LEU:HD23	2.17	0.64
1:B:386:SER:OG	1:B:388:PHE:HB2	1.98	0.64
1:A:665:GLN:O	1:A:666:CYS:HB2	1.97	0.64
1:A:255:THR:HB	1:A:256:PRO:HD2	1.81	0.63
1:B:451:LEU:HD13	1:B:509:TYR:HE2	1.63	0.63
1:B:658:LYS:O	1:B:661:TYR:CD2	2.52	0.62
1:A:394:ARG:HH12	1:A:411:SER:HB2	1.65	0.61
1:A:408:ILE:CD1	1:A:422:PRO:HB2	2.31	0.61
1:A:667:GLU:HG2	1:A:668:GLN:HE21	1.63	0.61
1:A:464:ARG:HE	1:A:482:GLU:HG3	1.67	0.60
1:B:568:SER:H	1:B:571:MET:HB2	1.66	0.60
1:A:214:HIS:O	1:A:586:LYS:NZ	2.35	0.60
1:A:571:MET:CG	1:A:576:ASN:O	2.49	0.60
1:A:483:PHE:CD2	1:A:483:PHE:N	2.66	0.59
1:B:571:MET:HG3	1:B:576:ASN:O	2.03	0.59
1:B:531:GLN:H	1:B:531:GLN:HE21	1.51	0.59
1:B:665:GLN:O	1:B:666:CYS:HB2	2.02	0.58
1:A:300:TYR:CE2	1:A:323:GLU:HG3	2.38	0.58
1:A:463:ALA:O	1:A:464:ARG:HG2	2.04	0.58
1:B:436:ALA:HB1	1:B:496:VAL:HG23	1.85	0.57
1:A:464:ARG:HH21	1:A:482:GLU:HG3	1.69	0.57
1:A:532:GLU:HG3	1:A:532:GLU:O	2.04	0.57
1:B:660:GLY:O	1:B:661:TYR:CG	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:GLY:HA3	1:B:661:TYR:CE2	2.40	0.56
1:A:214:HIS:NE2	1:B:595:ARG:HD3	2.21	0.56
1:A:550:HIS:HB2	4:A:2013:HOH:O	2.05	0.56
1:A:526:VAL:HG12	1:A:527:THR:HG22	1.88	0.56
1:B:430:HIS:CD2	1:B:456:ASN:HB2	2.41	0.56
1:B:219:ILE:HD13	1:B:537:LEU:HD13	1.88	0.56
1:B:408:ILE:CD1	1:B:422:PRO:HB2	2.35	0.56
1:A:480:LEU:O	1:A:480:LEU:HD12	2.05	0.56
1:B:522:GLN:O	1:B:530:TRP:HD1	1.89	0.56
1:A:568:SER:N	1:A:571:MET:CB	2.59	0.55
1:B:660:GLY:N	1:B:661:TYR:CD2	2.74	0.55
1:B:394:ARG:C	1:B:395:LEU:HD23	2.27	0.55
1:B:646:GLY:O	1:B:647:GLY:O	2.25	0.55
1:A:229:PRO:HB2	1:A:565:LEU:HD22	1.89	0.54
1:B:430:HIS:HD2	1:B:456:ASN:HB2	1.72	0.54
1:A:647:GLY:HA2	1:A:656:LEU:O	2.07	0.54
1:B:300:TYR:CE2	1:B:323:GLU:HG3	2.43	0.54
1:A:413:PRO:O	1:A:414:HIS:CD2	2.61	0.54
1:B:255:THR:HB	1:B:256:PRO:HD2	1.90	0.54
1:A:483:PHE:CD1	1:A:485:PRO:HG3	2.43	0.54
1:A:219:ILE:HG23	1:A:580:TYR:HB3	1.90	0.54
1:A:645:HIS:ND1	1:A:661:TYR:HD1	2.05	0.54
1:B:523:GLN:HA	1:B:530:TRP:HD1	1.73	0.53
1:A:436:ALA:HB1	1:A:496:VAL:HG23	1.89	0.53
1:A:480:LEU:HD12	1:A:480:LEU:C	2.28	0.53
1:B:251:VAL:HG21	1:B:287:LEU:CD1	2.38	0.53
1:B:415:PHE:C	1:B:415:PHE:HD1	2.12	0.53
1:B:415:PHE:C	1:B:415:PHE:CD1	2.81	0.53
1:B:348:LEU:HD22	1:B:374:ILE:CD1	2.38	0.53
1:A:271:LEU:N	1:A:271:LEU:HD23	2.24	0.52
1:B:568:SER:N	1:B:571:MET:HB2	2.23	0.52
1:B:613:ARG:HA	1:B:613:ARG:HE	1.73	0.52
1:A:415:PHE:CD1	1:A:415:PHE:C	2.83	0.52
1:B:667:GLU:HG2	1:B:668:GLN:HE21	1.75	0.52
1:A:415:PHE:C	1:A:415:PHE:HD1	2.13	0.52
1:A:567:SER:HA	1:A:571:MET:HG2	1.90	0.52
1:A:265:TYR:O	1:A:334:VAL:HG13	2.11	0.51
1:B:229:PRO:HB2	1:B:565:LEU:HD22	1.91	0.51
1:A:650:VAL:HG12	1:A:651:ARG:HG3	1.91	0.51
1:B:268:ILE:O	1:B:272:VAL:HG13	2.11	0.51
1:A:504:ARG:HG2	4:A:2015:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:GLY:CA	1:B:661:TYR:CE2	2.93	0.51
1:A:395:LEU:HD23	1:A:395:LEU:N	2.25	0.51
1:B:326:VAL:HA	1:B:334:VAL:HA	1.92	0.51
1:B:464:ARG:C	1:B:465:ILE:HG22	2.31	0.50
1:B:521:LEU:HD23	1:B:532:GLU:HB2	1.92	0.50
1:A:326:VAL:HA	1:A:334:VAL:HA	1.94	0.50
1:A:234:HIS:ND1	1:A:558:GLU:HG3	2.27	0.50
1:B:659:LYS:C	1:B:661:TYR:CD2	2.85	0.49
1:A:455:SER:O	1:A:456:ASN:HB2	2.12	0.49
1:A:231:GLY:CA	1:A:565:LEU:HD13	2.40	0.49
1:B:571:MET:CG	1:B:576:ASN:O	2.61	0.49
1:B:265:TYR:O	1:B:334:VAL:HG13	2.13	0.49
1:A:300:TYR:OH	1:A:397:VAL:HG11	2.13	0.49
1:A:368:ILE:HG23	1:A:429:LEU:HD13	1.94	0.48
1:B:451:LEU:HD22	1:B:509:TYR:CD2	2.49	0.48
1:A:268:ILE:O	1:A:272:VAL:HG13	2.13	0.48
1:A:466:LEU:HD21	1:A:480:LEU:HB3	1.95	0.48
1:B:219:ILE:HG23	1:B:580:TYR:HB3	1.94	0.48
1:A:449:THR:HA	1:A:466:LEU:O	2.13	0.48
1:B:547:PHE:HB2	1:B:580:TYR:CE2	2.49	0.48
1:A:305:THR:HG22	1:A:318:ILE:HG22	1.95	0.48
1:A:251:VAL:HG21	1:A:287:LEU:HD23	1.96	0.47
1:B:223:VAL:HG11	1:B:254:LEU:HD13	1.94	0.47
1:A:656:LEU:HD12	1:A:657:CYS:N	2.30	0.47
1:B:234:HIS:ND1	1:B:558:GLU:HG3	2.30	0.47
1:B:271:LEU:HD23	1:B:271:LEU:N	2.29	0.47
1:B:386:SER:HB2	4:B:2009:HOH:O	2.14	0.47
1:B:659:LYS:C	1:B:661:TYR:CE2	2.88	0.47
1:B:523:GLN:CA	1:B:530:TRP:CD1	2.96	0.47
1:B:392:VAL:HG23	1:B:429:LEU:HD11	1.97	0.46
1:A:455:SER:O	1:A:456:ASN:CB	2.63	0.46
1:B:219:ILE:CD1	1:B:537:LEU:HD13	2.46	0.46
1:A:414:HIS:ND1	1:A:420:GLN:HB2	2.30	0.46
1:A:483:PHE:HD1	1:A:485:PRO:HG3	1.81	0.45
1:B:232:ALA:O	1:B:555:GLY:HA2	2.17	0.45
1:A:232:ALA:O	1:A:555:GLY:HA2	2.16	0.45
1:A:366:TYR:CE1	1:A:394:ARG:HD3	2.52	0.45
1:B:519:LEU:C	1:B:519:LEU:HD12	2.37	0.45
1:A:361:PRO:HD3	1:A:448:LEU:HD13	1.99	0.44
1:B:413:PRO:O	1:B:414:HIS:CD2	2.70	0.44
1:A:255:THR:HB	1:A:256:PRO:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:SER:HA	1:B:427:HIS:HA	1.99	0.44
1:A:368:ILE:HG23	1:A:429:LEU:CD1	2.47	0.44
1:A:326:VAL:HG22	1:A:327:SER:N	2.33	0.44
1:A:371:ASP:O	1:A:374:ILE:HG12	2.18	0.44
1:A:415:PHE:HD1	1:A:416:ASN:HB2	1.82	0.44
1:A:227:ARG:O	1:A:228:GLN:C	2.55	0.43
1:A:519:LEU:HD12	1:A:519:LEU:C	2.38	0.43
1:A:645:HIS:CE1	1:A:661:TYR:CD1	3.06	0.43
1:B:518:PHE:CZ	1:B:564:ILE:HD11	2.53	0.43
1:B:568:SER:N	1:B:571:MET:CB	2.76	0.43
1:B:664:PRO:HB2	1:B:665:GLN:OE1	2.18	0.43
1:A:376:LEU:HD12	1:A:376:LEU:HA	1.77	0.43
1:B:464:ARG:H	1:B:464:ARG:HG2	1.31	0.43
1:A:348:LEU:HD12	1:A:374:ILE:HD12	2.00	0.43
1:B:217:PHE:O	1:B:537:LEU:HA	2.18	0.43
1:A:251:VAL:HG21	1:A:287:LEU:CD2	2.49	0.43
1:B:371:ASP:O	1:B:374:ILE:HG12	2.18	0.43
1:B:518:PHE:HZ	1:B:564:ILE:HD11	1.84	0.43
1:A:413:PRO:C	1:A:414:HIS:CD2	2.92	0.43
1:B:227:ARG:O	1:B:228:GLN:C	2.57	0.43
1:B:368:ILE:HG23	1:B:429:LEU:HD13	2.01	0.43
1:B:663:GLY:HA3	1:B:667:GLU:OE1	2.18	0.43
1:A:305:THR:CG2	1:A:318:ILE:HG22	2.49	0.43
1:A:439:ARG:O	1:A:440:HIS:C	2.57	0.43
1:A:391:SER:HA	1:A:427:HIS:HA	2.01	0.42
1:B:300:TYR:OH	1:B:397:VAL:HG11	2.19	0.42
1:B:410:ARG:HA	1:B:415:PHE:CE2	2.54	0.42
1:A:413:PRO:O	1:A:414:HIS:CG	2.72	0.42
1:A:527:THR:O	1:A:528:LYS:HB2	2.19	0.42
1:B:229:PRO:HB2	1:B:565:LEU:CD2	2.49	0.42
1:A:410:ARG:HA	1:A:415:PHE:CE2	2.52	0.42
1:A:647:GLY:C	1:A:648:VAL:HG23	2.40	0.42
1:A:667:GLU:HG2	1:A:668:GLN:NE2	2.32	0.42
1:B:604:LEU:HD12	1:B:604:LEU:HA	1.86	0.42
1:A:638:LYS:O	1:A:652:PRO:HA	2.20	0.42
1:B:368:ILE:HG23	1:B:429:LEU:CD1	2.50	0.42
1:B:397:VAL:HG12	1:B:397:VAL:O	2.20	0.42
1:A:220:GLN:OE1	1:A:543:CYS:HB2	2.20	0.41
1:B:522:GLN:C	1:B:530:TRP:HD1	2.23	0.41
1:B:220:GLN:OE1	1:B:543:CYS:HB2	2.20	0.41
1:A:664:PRO:HB2	1:A:665:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:LYS:HE2	1:B:533:LYS:HB2	1.68	0.41
1:A:229:PRO:HB2	1:A:565:LEU:CD2	2.49	0.41
1:B:525:PRO:C	1:B:526:VAL:HG12	2.40	0.41
1:B:287:LEU:HD23	1:B:288:ALA:N	2.35	0.41
1:B:327:SER:HB3	1:B:333:GLN:O	2.20	0.41
1:A:225:GLY:HA2	1:A:575:HIS:O	2.21	0.41
1:B:388:PHE:HE1	1:B:423:GLU:HB2	1.85	0.41
1:A:366:TYR:CZ	1:A:394:ARG:HD3	2.56	0.41
1:A:386:SER:O	1:A:387:ASP:CB	2.66	0.41
1:A:571:MET:HG2	1:A:576:ASN:O	2.21	0.41
1:B:563:TYR:N	1:B:563:TYR:CD2	2.88	0.41
1:A:223:VAL:HG11	1:A:254:LEU:HD13	2.03	0.40
1:A:420:GLN:HB2	1:A:420:GLN:HE21	1.68	0.40
1:A:392:VAL:HG23	1:A:429:LEU:HD11	2.03	0.40
1:B:285:LEU:HD13	1:B:354:GLY:O	2.21	0.40
1:B:646:GLY:O	1:B:647:GLY:C	2.60	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:TYR:OH	1:B:257:GLU:OE1[5_665]	2.03	0.17

## 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	430/458 (94%)	397 (92%)	30 (7%)	3 (1%)	19	48
1	B	395/458 (86%)	360 (91%)	29 (7%)	6 (2%)	8	29
All	All	825/916 (90%)	757 (92%)	59 (7%)	9 (1%)	12	37



All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	464	ARG
1	A	274	SER
1	B	647	GLY
1	B	670	ASP
1	B	274	SER
1	A	443	ASP
1	B	215	ASN
1	A	626	SER
1	B	626	SER

### 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	382/399 (96%)	340 (89%)	42 (11%)	5	17
1	B	352/399 (88%)	304 (86%)	48 (14%)	3	10
All	All	734/798 (92%)	644 (88%)	90 (12%)	4	13

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	VAL
1	A	228	GLN
1	A	276	ILE
1	A	287	LEU
1	A	292	ASN
1	A	299	LEU
1	A	318	ILE
1	A	327	SER
1	A	358	LEU
1	A	369	LEU
1	A	376	LEU
1	A	379	MET
1	A	401	MET
1	A	403	ASN

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Mol	Chain	Res	Type
1	A	411	SER
1	A	415	PHE
1	A	420	GLN
1	A	430	HIS
1	A	442	THR
1	A	443	ASP
1	A	464	ARG
1	A	466	LEU
1	A	483	PHE
1	A	484	LYS
1	A	498	ARG
1	A	500	CYS
1	A	514	ARG
1	A	520	THR
1	A	522	GLN
1	A	527	THR
1	A	542	SER
1	A	565	LEU
1	A	571	MET
1	A	574	THR
1	A	592	GLU
1	A	603	THR
1	A	605	THR
1	A	613	ARG
1	A	635	ARG
1	A	636	THR
1	A	656	LEU
1	A	667	GLU
1	B	228	GLN
1	B	276	ILE
1	B	292	ASN
1	B	299	LEU
1	B	315	HIS
1	B	318	ILE
1	B	327	SER
1	B	334	VAL
1	B	348	LEU
1	B	358	LEU
1	B	376	LEU
1	B	379	MET
1	B	401	MET
1	B	403	ASN

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Mol	Chain	Res	Type
1	B	411	SER
1	B	415	PHE
1	B	430	HIS
1	B	434	ARG
1	B	448	LEU
1	B	449	THR
1	B	455	SER
1	B	462	SER
1	B	464	ARG
1	B	465	ILE
1	B	498	ARG
1	B	500	CYS
1	B	514	ARG
1	B	520	THR
1	B	526	VAL
1	B	530	TRP
1	B	531	GLN
1	B	532	GLU
1	B	542	SER
1	B	565	LEU
1	B	571	MET
1	B	574	THR
1	B	592	GLU
1	B	603	THR
1	B	604	LEU
1	B	605	THR
1	B	613	ARG
1	B	622	LYS
1	B	635	ARG
1	B	636	THR
1	B	656	LEU
1	B	661	TYR
1	B	667	GLU
1	B	669	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	ASN
1	A	414	HIS
1	A	420	GLN
1	A	430	HIS

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Mol	Chain	Res	Type
1	A	456	ASN
1	A	529	GLN
1	A	668	GLN
1	B	292	ASN
1	B	414	HIS
1	B	522	GLN
1	B	529	GLN
1	B	531	GLN
1	B	668	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	438/458 (95%)	-0.34	14 (3%)	50 42	39, 74, 137, 196	0
1	B	409/458 (89%)	-0.18	16 (3%)	44 36	36, 74, 134, 174	0
All	All	847/916 (92%)	-0.26	30 (3%)	47 39	36, 74, 137, 196	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	661	TYR	6.3
1	B	648	VAL	5.9
1	B	214	HIS	4.9
1	A	656	LEU	4.8
1	B	314	PRO	4.8
1	A	572	THR	4.6
1	A	661	TYR	4.3
1	B	306	ASN	3.9
1	B	657	CYS	3.7
1	B	656	LEU	3.4
1	B	276	ILE	3.4
1	A	668	GLN	3.1
1	B	315	HIS	2.8
1	A	460	ARG	2.8
1	B	647	GLY	2.7
1	A	571	MET	2.5
1	B	526	VAL	2.5
1	A	635	ARG	2.4
1	B	662	LEU	2.4
1	B	523	GLN	2.3
1	B	413	PRO	2.3
1	B	529	GLN	2.2
1	A	315	HIS	2.2
1	A	479	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	572	THR	2.1
1	A	640	GLU	2.1
1	A	420	GLN	2.1
1	A	276	ILE	2.0
1	A	667	GLU	2.0
1	A	648	VAL	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NA	A	1673	1/1	0.71	0.44	116,116,116,116	0
3	CL	B	1673	1/1	0.86	0.12	105,105,105,105	0
3	CL	A	1674	1/1	0.87	0.17	133,133,133,133	0
3	CL	B	1672	1/1	0.94	0.13	113,113,113,113	0
2	NA	A	1672	1/1	0.95	0.11	83,83,83,83	0
2	NA	B	1671	1/1	0.96	0.11	75,75,75,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.