



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:08 AM UTC

PDB ID : 8BFU / pdb_00008bfu
Title : Crystal structure of the apo p110alpha catalytic subunit from homo sapiens
Authors : Gong, G.Q.; Bellini, D.; Vanhaesebroeck, B.; Williams, R.L.
Deposited on : 2022-10-26
Resolution : 2.41 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

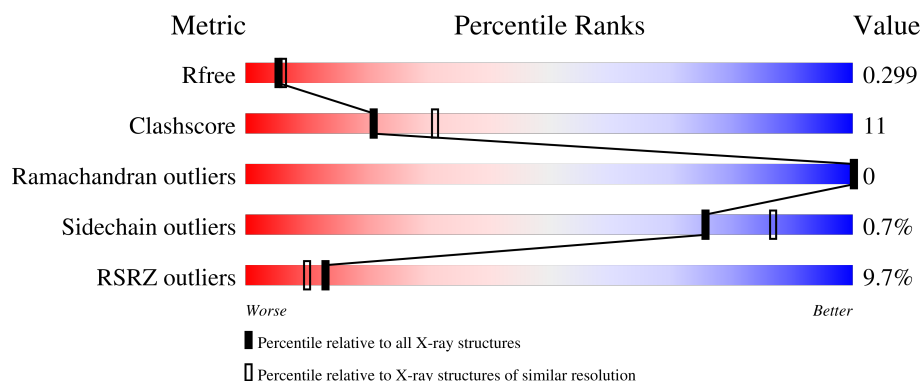
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	946	9% 72% 20% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7237 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	880	Total	C	N	O	S	0	0	0
			7186	4586	1232	1307	61			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLY	-	expression tag	UNP P42336
A	104	SER	-	expression tag	UNP P42336

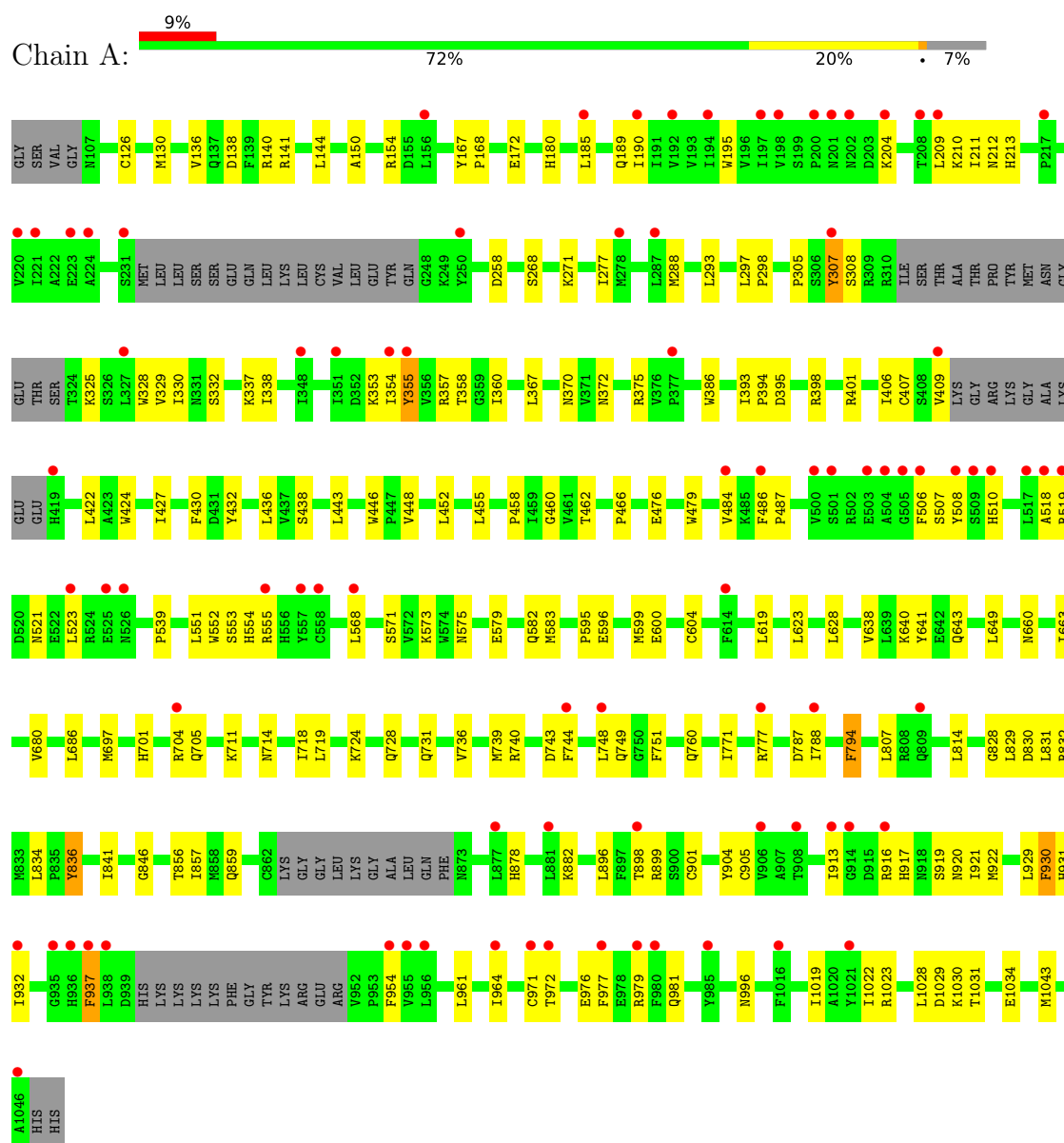
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	51	Total	O	0	0
			51	51		

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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.29Å 135.26Å 142.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 2.41 49.08 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.08-2.41) 99.9 (49.08-2.41)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.42Å)	Xtriage
Refinement program	REFMAC 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.243 , 0.279 0.259 , 0.299	Depositor DCC
R_{free} test set	2216 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	74.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7237	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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	0.18	0/7344	0.44	1/9927 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	582	GLN	CA-CB-CG	5.74	125.59	114.10

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	7186	0	7168	158	0
2	A	51	0	0	3	0
All	All	7237	0	7168	158	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 11.

All (158) 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:922:MET:HB2	1:A:930:PHE:CE1	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:TYR:CE1	1:A:407:CYS:HB2	2.14	0.82
1:A:552:TRP:HA	1:A:555:ARG:HE	1.47	0.79
1:A:209:LEU:HD23	1:A:211:ILE:HD11	1.66	0.77
1:A:555:ARG:NH1	1:A:583:MET:SD	2.59	0.75
1:A:555:ARG:HG2	1:A:568:LEU:HD11	1.70	0.74
1:A:930:PHE:O	1:A:930:PHE:HD1	1.72	0.72
1:A:298:PRO:HB2	1:A:697:MET:HG3	1.72	0.71
1:A:728:GLN:NE2	1:A:771:ILE:O	2.24	0.71
1:A:916:ARG:HH11	1:A:920:ASN:HB3	1.56	0.70
1:A:138:ASP:OD1	1:A:141:ARG:NH2	2.26	0.69
1:A:427:ILE:HD11	1:A:443:LEU:HD22	1.76	0.68
1:A:628:LEU:HD23	1:A:663:ILE:HD13	1.75	0.67
1:A:619:LEU:HD22	1:A:623:LEU:HD22	1.78	0.65
1:A:937:PHE:HD1	1:A:937:PHE:O	1.80	0.65
1:A:258:ASP:OD2	1:A:760:GLN:NE2	2.27	0.64
1:A:913:ILE:HG22	1:A:916:ARG:HE	1.62	0.64
1:A:519:ARG:HG2	1:A:553:SER:O	1.98	0.64
1:A:878:HIS:CE1	1:A:882:LYS:HE3	2.33	0.64
1:A:836:TYR:O	1:A:836:TYR:HD1	1.81	0.63
1:A:724:LYS:HA	1:A:777:ARG:NH2	2.14	0.63
1:A:898:THR:HG22	1:A:964:ILE:HG12	1.80	0.62
1:A:922:MET:HB2	1:A:930:PHE:HE1	1.60	0.62
1:A:555:ARG:NH2	1:A:568:LEU:O	2.32	0.62
1:A:555:ARG:NH1	1:A:568:LEU:HG	2.15	0.61
1:A:213:HIS:N	2:A:1103:HOH:O	2.32	0.61
1:A:794:PHE:O	1:A:794:PHE:HD1	1.84	0.61
1:A:719:LEU:HD13	1:A:777:ARG:HD3	1.84	0.59
1:A:724:LYS:HA	1:A:777:ARG:HH22	1.66	0.59
1:A:141:ARG:HG2	1:A:308:SER:HA	1.85	0.59
1:A:573:LYS:NZ	1:A:579:GLU:OE2	2.36	0.58
1:A:213:HIS:HB2	1:A:268:SER:HB3	1.85	0.58
1:A:552:TRP:HA	1:A:555:ARG:NE	2.19	0.58
1:A:328:TRP:HA	1:A:394:PRO:HB3	1.86	0.58
1:A:338:ILE:HD11	1:A:358:THR:HG21	1.86	0.57
1:A:180:HIS:CD2	1:A:828:GLY:HA2	2.40	0.57
1:A:448:VAL:HG13	1:A:452:LEU:HD23	1.86	0.56
1:A:704:ARG:NH2	1:A:749:GLN:O	2.40	0.55
1:A:180:HIS:HD2	1:A:828:GLY:HA2	1.73	0.54
1:A:1031:THR:HG23	1:A:1034:GLU:H	1.71	0.54
1:A:185:LEU:HD22	1:A:190:ILE:HG22	1.90	0.54
1:A:355:TYR:C	1:A:355:TYR:HD1	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:ARG:NH1	1:A:932:ILE:O	2.32	0.54
1:A:305:PRO:HG2	1:A:307:TYR:CE1	2.43	0.54
1:A:961:LEU:HB3	1:A:971:CYS:SG	2.49	0.53
1:A:604:CYS:HB3	1:A:641:TYR:CE1	2.44	0.53
1:A:917:HIS:CE1	1:A:919:SER:HB2	2.43	0.53
1:A:1023:ARG:NH2	1:A:1029:ASP:OD1	2.42	0.52
1:A:930:PHE:HD1	1:A:930:PHE:C	2.18	0.52
1:A:518:ALA:HB3	1:A:553:SER:HB2	1.92	0.52
1:A:355:TYR:C	1:A:355:TYR:CD1	2.88	0.52
1:A:921:ILE:HG12	1:A:931:HIS:CD2	2.45	0.52
1:A:401:ARG:NH2	2:A:1106:HOH:O	2.36	0.52
1:A:856:THR:HG23	1:A:859:GLN:H	1.74	0.52
1:A:167:TYR:HE2	1:A:297:LEU:HD21	1.74	0.52
1:A:771:ILE:HG23	1:A:777:ARG:HG3	1.91	0.52
1:A:711:LYS:HB2	1:A:748:LEU:HD11	1.90	0.51
1:A:375:ARG:HE	1:A:409:VAL:HG21	1.76	0.51
1:A:596:GLU:HA	1:A:599:MET:HE2	1.93	0.51
1:A:930:PHE:C	1:A:930:PHE:CD1	2.89	0.51
1:A:189:GLN:OE1	1:A:210:LYS:HE2	2.11	0.51
1:A:288:MET:HE3	1:A:293:LEU:HB2	1.92	0.51
1:A:743:ASP:OD1	1:A:744:PHE:N	2.44	0.51
1:A:357:ARG:HH21	1:A:370:ASN:HD22	1.60	0.50
1:A:787:ASP:OD1	1:A:788:ILE:N	2.44	0.50
1:A:126:CYS:O	1:A:130:MET:HG2	2.11	0.50
1:A:539:PRO:HD3	1:A:996:ASN:OD1	2.12	0.50
1:A:972:THR:HA	1:A:977:PHE:CD2	2.46	0.50
1:A:354:ILE:HG22	1:A:355:TYR:H	1.76	0.50
1:A:832:ARG:HD2	1:A:896:LEU:HD11	1.94	0.50
1:A:638:VAL:HA	1:A:641:TYR:CD2	2.47	0.50
1:A:1019:ILE:O	1:A:1022:ILE:HG12	2.11	0.50
1:A:401:ARG:NH2	1:A:458:PRO:O	2.38	0.49
1:A:330:ILE:O	1:A:394:PRO:HD3	2.12	0.49
1:A:916:ARG:NH1	1:A:920:ASN:HB3	2.26	0.49
1:A:436:LEU:HB3	1:A:484:VAL:HB	1.94	0.49
1:A:355:TYR:HD1	1:A:355:TYR:O	1.96	0.49
1:A:901:CYS:HA	1:A:929:LEU:HD22	1.94	0.49
1:A:794:PHE:O	1:A:794:PHE:CD1	2.64	0.48
1:A:552:TRP:CE3	1:A:555:ARG:NE	2.81	0.48
1:A:814:LEU:HD11	1:A:836:TYR:CE1	2.48	0.48
1:A:136:VAL:HG13	1:A:686:LEU:HD11	1.95	0.48
1:A:401:ARG:HD2	1:A:462:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:THR:OG1	1:A:919:SER:HA	2.13	0.48
1:A:930:PHE:O	1:A:930:PHE:CD1	2.61	0.48
1:A:357:ARG:HG3	1:A:372:ASN:OD1	2.14	0.47
1:A:836:TYR:HE2	1:A:932:ILE:HG12	1.79	0.47
1:A:360:ILE:HG22	1:A:367:LEU:HD12	1.96	0.47
1:A:195:TRP:HZ3	1:A:204:LYS:HB2	1.80	0.47
1:A:406:ILE:HG22	1:A:422:LEU:HD12	1.96	0.47
1:A:856:THR:HA	1:A:922:MET:HG2	1.96	0.47
1:A:704:ARG:HG3	1:A:751:PHE:HB3	1.96	0.46
1:A:506:PHE:HB3	1:A:510:HIS:HB3	1.98	0.46
1:A:739:MET:HA	1:A:744:PHE:CD2	2.50	0.46
1:A:771:ILE:CG2	1:A:777:ARG:HG3	2.46	0.46
1:A:905:CYS:HB3	1:A:954:PHE:CZ	2.51	0.46
1:A:916:ARG:HA	1:A:916:ARG:HD3	1.67	0.46
1:A:976:GLU:HG3	1:A:979:ARG:HH21	1.80	0.45
1:A:551:LEU:HB3	1:A:568:LEU:HD12	1.99	0.45
1:A:555:ARG:CZ	1:A:568:LEU:HG	2.45	0.45
1:A:337:LYS:HB3	1:A:476:GLU:HB3	1.97	0.45
1:A:337:LYS:HD2	1:A:386:TRP:CZ2	2.52	0.45
1:A:904:TYR:CE2	1:A:930:PHE:HA	2.52	0.45
1:A:841:ILE:HG12	1:A:846:GLY:HA2	1.97	0.45
1:A:328:TRP:CE2	1:A:487:PRO:HG3	2.52	0.44
1:A:332:SER:HB2	1:A:393:ILE:HD12	1.98	0.44
1:A:486:PHE:CG	1:A:487:PRO:HD2	2.52	0.44
1:A:981:GLN:HG2	1:A:1043:MET:SD	2.57	0.44
1:A:518:ALA:HA	1:A:521:ASN:OD1	2.17	0.44
1:A:168:PRO:HG3	1:A:660:ASN:OD1	2.17	0.44
1:A:1030:LYS:HE2	1:A:1034:GLU:HB3	1.99	0.44
1:A:430:PHE:HE1	1:A:436:LEU:HD13	1.81	0.44
1:A:913:ILE:CG2	1:A:916:ARG:HE	2.29	0.44
1:A:185:LEU:HD11	1:A:277:ILE:HD13	2.00	0.44
1:A:398:ARG:HD2	1:A:430:PHE:HD2	1.83	0.44
1:A:354:ILE:HG22	1:A:355:TYR:N	2.33	0.43
1:A:507:SER:OG	1:A:508:TYR:N	2.51	0.43
1:A:211:ILE:HG22	1:A:212:ASN:N	2.33	0.43
1:A:595:PRO:O	1:A:599:MET:HG3	2.18	0.43
1:A:438:SER:HB2	1:A:479:TRP:HA	2.01	0.43
1:A:424:TRP:CH2	1:A:460:GLY:HA3	2.54	0.43
1:A:937:PHE:C	1:A:937:PHE:CD1	2.97	0.43
1:A:325:LYS:HE3	1:A:329:VAL:HG21	1.99	0.43
1:A:539:PRO:HB3	1:A:600:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ALA:O	1:A:154:ARG:HG3	2.19	0.43
1:A:172:GLU:OE2	1:A:271:LYS:HG2	2.19	0.43
1:A:638:VAL:HG23	1:A:649:LEU:HD21	2.01	0.42
1:A:140:ARG:NH2	1:A:307:TYR:CE2	2.87	0.42
1:A:555:ARG:NH2	1:A:571:SER:HB2	2.33	0.42
1:A:701:HIS:O	1:A:705:GLN:HG3	2.19	0.42
1:A:739:MET:HG2	1:A:744:PHE:CE2	2.54	0.42
1:A:138:ASP:OD2	1:A:432:TYR:OH	2.15	0.42
1:A:523:LEU:HD22	1:A:554:HIS:CE1	2.54	0.42
1:A:857:ILE:HD12	1:A:921:ILE:HB	2.01	0.42
1:A:407:CYS:SG	1:A:455:LEU:HD12	2.59	0.42
1:A:640:LYS:HG2	1:A:680:VAL:HG11	2.01	0.42
1:A:830:ASP:O	1:A:899:ARG:HD3	2.20	0.42
1:A:834:LEU:HD23	1:A:930:PHE:CD2	2.54	0.42
1:A:731:GLN:NE2	1:A:777:ARG:HH21	2.17	0.42
1:A:731:GLN:HE22	1:A:777:ARG:HH21	1.68	0.41
1:A:937:PHE:O	1:A:937:PHE:CD1	2.66	0.41
1:A:954:PHE:CE2	1:A:1043:MET:HG3	2.55	0.41
1:A:807:LEU:HD12	1:A:846:GLY:HA3	2.01	0.41
1:A:307:TYR:C	1:A:307:TYR:CD1	2.98	0.41
1:A:144:LEU:HD11	1:A:307:TYR:HE1	1.85	0.41
1:A:395:ASP:HB3	1:A:575:ASN:O	2.20	0.41
1:A:714:ASN:O	1:A:718:ILE:HG12	2.20	0.41
1:A:829:LEU:HG	1:A:831:LEU:HG	2.02	0.41
1:A:427:ILE:CD1	1:A:443:LEU:HD22	2.48	0.41
1:A:643:GLN:NE2	2:A:1108:HOH:O	2.45	0.41
1:A:711:LYS:HB3	1:A:744:PHE:CD1	2.56	0.41
1:A:836:TYR:C	1:A:836:TYR:CD1	2.99	0.41
1:A:1023:ARG:HG2	1:A:1028:LEU:HD12	2.02	0.41
1:A:736:VAL:O	1:A:740:ARG:HG3	2.21	0.41
1:A:555:ARG:HG2	1:A:568:LEU:HD21	2.02	0.40
1:A:353:LYS:HE2	1:A:375:ARG:HD3	2.03	0.40
1:A:446:TRP:CH2	1:A:466:PRO:HD2	2.57	0.40
1:A:711:LYS:HB3	1:A:744:PHE:CE1	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	868/946 (92%)	836 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	806/860 (94%)	800 (99%)	6 (1%)	76	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	TYR
1	A	355	TYR
1	A	794	PHE
1	A	836	TYR
1	A	930	PHE
1	A	937	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	HIS
1	A	362	HIS

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Mol	Chain	Res	Type
1	A	370	ASN
1	A	510	HIS
1	A	630	GLN
1	A	731	GLN
1	A	878	HIS
1	A	885	ASN
1	A	931	HIS
1	A	936	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, 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	880/946 (93%)	0.79	85 (9%) 13 10	51, 89, 126, 149	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	555	ARG	6.5
1	A	202	ASN	5.5
1	A	506	PHE	4.3
1	A	938	LEU	4.2
1	A	955	VAL	4.2
1	A	954	PHE	4.1
1	A	956	LEU	4.1
1	A	505	GLY	4.1
1	A	517	LEU	4.1
1	A	156	LEU	4.0
1	A	409	VAL	4.0
1	A	937	PHE	4.0
1	A	500	VAL	4.0
1	A	508	TYR	3.7
1	A	204	LYS	3.7
1	A	1046	ALA	3.7
1	A	504	ALA	3.7
1	A	525	GLU	3.6
1	A	935	GLY	3.6
1	A	932	ILE	3.6
1	A	509	SER	3.5
1	A	523	LEU	3.4
1	A	980	PHE	3.3
1	A	348	ILE	3.3
1	A	916	ARG	3.3
1	A	354	ILE	3.3
1	A	198	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	744	PHE	3.2
1	A	221	ILE	3.2
1	A	231	SER	3.1
1	A	501	SER	3.0
1	A	971	CYS	3.0
1	A	223	GLU	2.9
1	A	898	THR	2.9
1	A	972	THR	2.9
1	A	217	PRO	2.9
1	A	250	TYR	2.9
1	A	1021	TYR	2.9
1	A	419	HIS	2.9
1	A	964	ILE	2.8
1	A	307	TYR	2.8
1	A	558	CYS	2.8
1	A	777	ARG	2.8
1	A	224	ALA	2.8
1	A	518	ALA	2.7
1	A	510	HIS	2.7
1	A	519	ARG	2.6
1	A	568	LEU	2.6
1	A	503	GLU	2.6
1	A	192	VAL	2.6
1	A	209	LEU	2.5
1	A	704	ARG	2.5
1	A	788	ILE	2.5
1	A	185	LEU	2.5
1	A	201	ASN	2.5
1	A	985	TYR	2.5
1	A	809	GLN	2.5
1	A	977	PHE	2.5
1	A	377	PRO	2.4
1	A	278	MET	2.4
1	A	979	ARG	2.4
1	A	486	PHE	2.4
1	A	908	THR	2.4
1	A	351	ILE	2.4
1	A	526	ASN	2.4
1	A	194	ILE	2.3
1	A	327	LEU	2.3
1	A	355	TYR	2.3
1	A	914	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	881	LEU	2.3
1	A	208	THR	2.3
1	A	936	HIS	2.3
1	A	484	VAL	2.3
1	A	877	LEU	2.2
1	A	614	PHE	2.2
1	A	190	ILE	2.2
1	A	287	LEU	2.2
1	A	913	ILE	2.2
1	A	200	PRO	2.1
1	A	197	ILE	2.1
1	A	557	TYR	2.1
1	A	1016	PHE	2.0
1	A	748	LEU	2.0
1	A	220	VAL	2.0
1	A	906	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 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.