Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2023 – 06:10 pm GMT

PDB ID	:	8BFU
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:

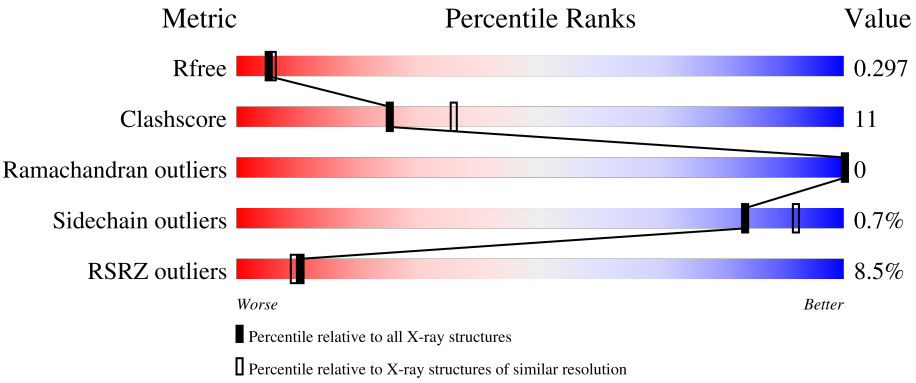
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (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 <=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	8% 73% 20% 7%

2 Entry composition (i)

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 subunit alpha isoform.

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

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.

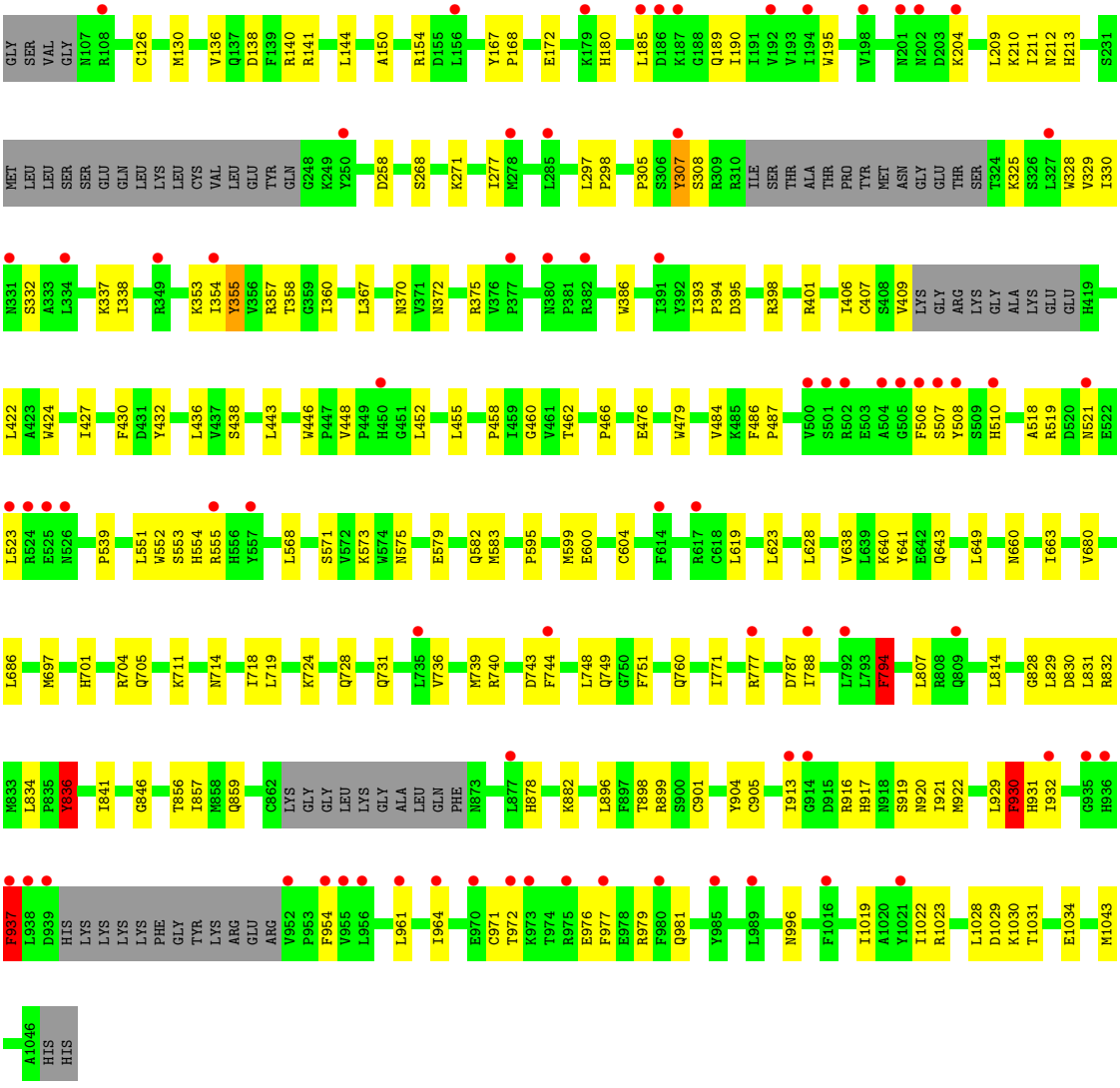
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	51	51	51	0	0

3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

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 67.63 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.08-2.41) 100.0 (67.63-2.41)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 0.297	Depositor DCC
R_{free} test set	2215 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)	0.32 , 59.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.28	0/7344	0.51	7/9927 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	937	PHE	CB-CG-CD2	-7.57	115.50	120.80
1	A	930	PHE	CB-CG-CD2	-7.08	115.85	120.80
1	A	794	PHE	CB-CG-CD2	-6.74	116.08	120.80
1	A	937	PHE	CB-CG-CD1	6.02	125.01	120.80
1	A	930	PHE	CB-CG-CD1	5.96	124.97	120.80
1	A	582	GLN	CA-CB-CG	5.54	125.59	113.40
1	A	836	TYR	CB-CG-CD2	-5.21	117.88	121.00

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	153	0
2	A	51	0	0	3	0
All	All	7237	0	7168	153	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 (153) 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
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:213:HIS:HB2	1:A:268:SER:HB3	1.85	0.58
1:A:573:LYS:NZ	1:A:579:GLU:OE2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:HD22	1:A:190:ILE:HG22	1.90	0.54
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:518:ALA:HB3	1:A:553:SER:HB2	1.92	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:189:GLN:OE1	1:A:210:LYS:HE2	2.11	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:355:TYR:HD1	1:A:355:TYR:C	2.15	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
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:930:PHE:HD1	1:A:930:PHE:C	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:TYR:C	1:A:355:TYR:CD1	2.88	0.47
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:930:PHE:CD1	1:A:930:PHE:C	2.89	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: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
1:A:150:ALA:O	1:A:154:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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 (i)

5.3.1 Protein backbone (i)

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 (i)

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%)	84 92

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 (2) such sidechains are listed below:

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

5.3.3 RNA (i)

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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%)	0.57	75 (8%)	10	9	51, 89, 126, 149	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	PHE	11.1
1	A	505	GLY	9.5
1	A	555	ARG	8.1
1	A	525	GLU	7.6
1	A	937	PHE	7.5
1	A	204	LYS	7.0
1	A	938	LEU	6.6
1	A	202	ASN	5.8
1	A	508	TYR	5.7
1	A	502	ARG	5.6
1	A	526	ASN	5.6
1	A	201	ASN	5.2
1	A	501	SER	4.6
1	A	377	PRO	4.3
1	A	1021	TYR	3.9
1	A	936	HIS	3.7
1	A	956	LEU	3.5
1	A	354	ILE	3.4
1	A	507	SER	3.4
1	A	914	GLY	3.3
1	A	250	TYR	3.3
1	A	964	ILE	3.2
1	A	349	ARG	3.1
1	A	500	VAL	3.1
1	A	307	TYR	3.1
1	A	980	PHE	3.0
1	A	450	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	977	PHE	2.9
1	A	380	ASN	2.9
1	A	510	HIS	2.9
1	A	331	ASN	2.8
1	A	809	GLN	2.8
1	A	985	TYR	2.8
1	A	955	VAL	2.8
1	A	777	ARG	2.8
1	A	617	ARG	2.8
1	A	877	LEU	2.7
1	A	954	PHE	2.7
1	A	334	LEU	2.6
1	A	187	LYS	2.6
1	A	198	VAL	2.5
1	A	194	ILE	2.5
1	A	327	LEU	2.5
1	A	557	TYR	2.5
1	A	970	GLU	2.5
1	A	744	PHE	2.4
1	A	179	LYS	2.4
1	A	156	LEU	2.4
1	A	285	LEU	2.4
1	A	932	ILE	2.3
1	A	1016	PHE	2.3
1	A	961	LEU	2.3
1	A	614	PHE	2.3
1	A	192	VAL	2.3
1	A	913	ILE	2.2
1	A	935	GLY	2.2
1	A	524	ARG	2.2
1	A	108	ARG	2.2
1	A	952	VAL	2.2
1	A	972	THR	2.2
1	A	792	LEU	2.2
1	A	973	LYS	2.1
1	A	382	ARG	2.1
1	A	521	ASN	2.1
1	A	975	ARG	2.1
1	A	788	ILE	2.1
1	A	504	ALA	2.1
1	A	989	LEU	2.1
1	A	186	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	939	ASP	2.1
1	A	278	MET	2.1
1	A	735	LEU	2.1
1	A	523	LEU	2.1
1	A	185	LEU	2.0
1	A	391	ILE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.