WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 07:46 AM EDT

PDB ID	:	3HHM
Title	:	Crystal structure of p110alpha H1047R mutant in complex with niSH2 of p85alpha and the drug wortmannin
Authors	:	Amzel, L.M.; Vogelstein, B.; Gabelli, S.B.; Mandelker, D.
Deposited on	:	2009-05-15
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*
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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
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)	:	2.35

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	Percentile Ranks	Value
Rfree		0.303
Clashscore		11
Ramachandran outliers		4.5%
Sidechain outliers		10.2%
RSRZ outliers		9.1%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
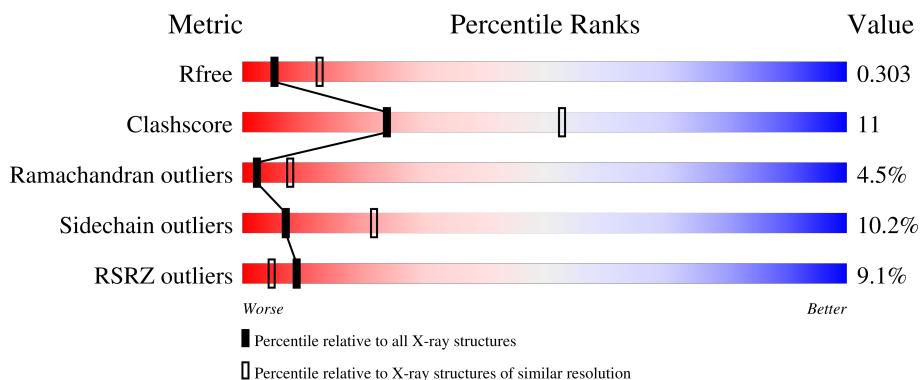
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 >=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	1091	5% · 66% · 22% · 6% · 5%
2	B	373	16% · 51% · 14% · · 34%
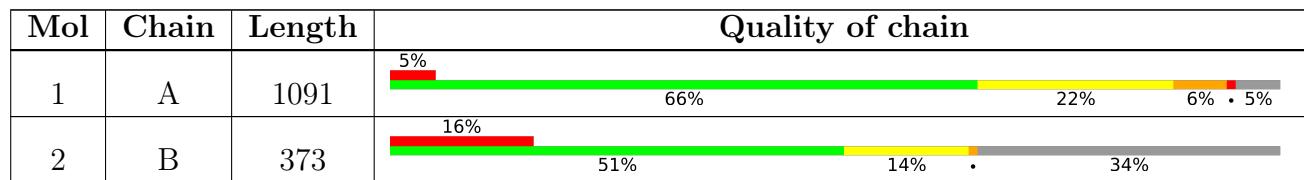
2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 10686 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	1032	8448	5405	1447	1528	68	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	expression tag	UNP P42336
A	-27	SER	-	expression tag	UNP P42336
A	-26	TYR	-	expression tag	UNP P42336
A	-25	TYR	-	expression tag	UNP P42336
A	-24	HIS	-	expression tag	UNP P42336
A	-23	HIS	-	expression tag	UNP P42336
A	-22	HIS	-	expression tag	UNP P42336
A	-21	HIS	-	expression tag	UNP P42336
A	-20	HIS	-	expression tag	UNP P42336
A	-19	HIS	-	expression tag	UNP P42336
A	-18	ASP	-	expression tag	UNP P42336
A	-17	TYR	-	expression tag	UNP P42336
A	-10	PRO	-	expression tag	UNP P42336
A	-9	SER	-	expression tag	UNP P42336
A	-8	SER	-	expression tag	UNP P42336
A	-7	GLY	-	expression tag	UNP P42336
A	-6	GLU	-	expression tag	UNP P42336
A	-5	LEU	-	expression tag	UNP P42336
A	-4	TRP	-	expression tag	UNP P42336
A	-3	GLY	-	expression tag	UNP P42336
A	-2	ILE	-	expression tag	UNP P42336
A	-1	HIS	-	expression tag	UNP P42336
A	0	LEU	-	expression tag	UNP P42336
A	1047	ARG	HIS	engineered mutation	UNP P42336

- Molecule 2 is a protein called niSH2 p85alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	247	Total 2092	C 1306	N 373	O 408	S 5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	330	ASN	ASP	engineered mutation	UNP P27986

- Molecule 3 is (1S,6BR,9AS,11R,11BR)-9A,11B-DIMETHYL-1-[(METHYLOXY)METHYL]
  -3,6,9-TRIOXO-1,6,6B,7,8,9,9A,10,11,11B-DECAHYDRO-3H-FURO[4, 3,2-DE]INDENO[4,
  5-H][2]BENZOPYRAN-11-YL ACETATE (three-letter code: KWT) (formula: $C_{23}H_{24}O_8$).
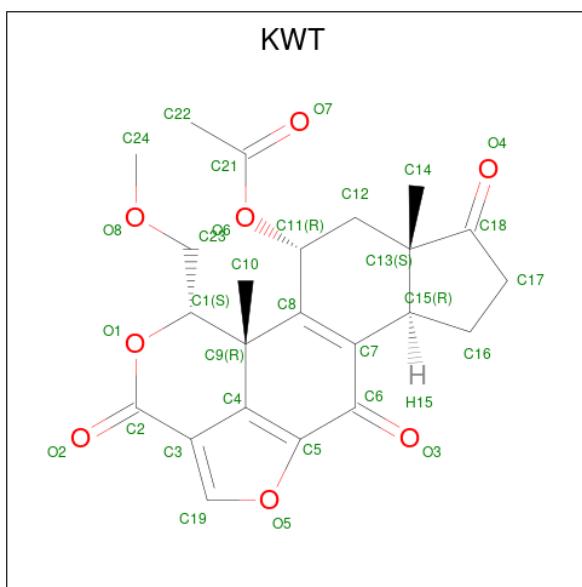
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 31	C 23	O 8	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total 106	O 106	0	0
4	B	9	Total 9	O 9	0	0

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
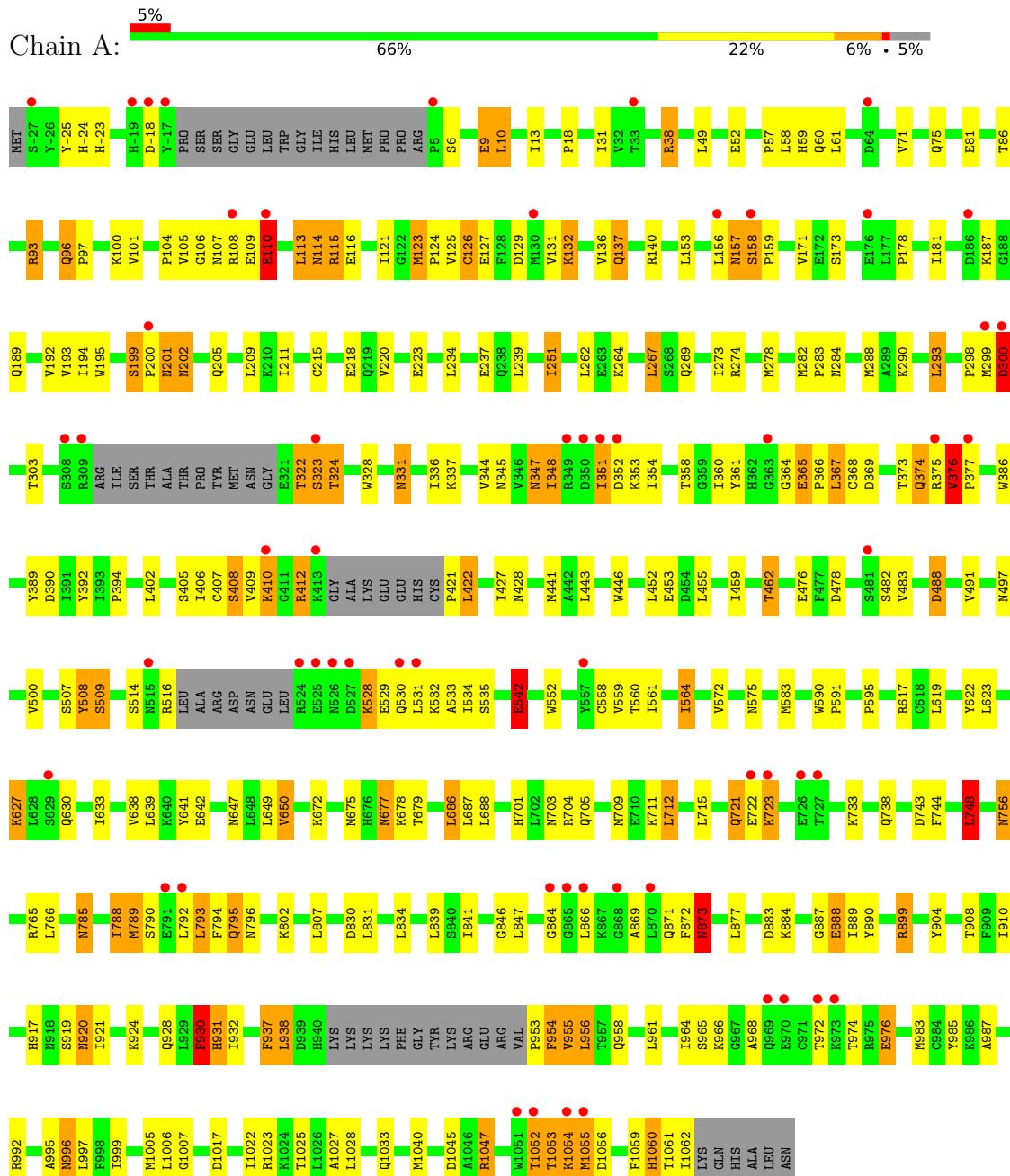
• Molecule 2: niSH2 p85alpha

Chain B:
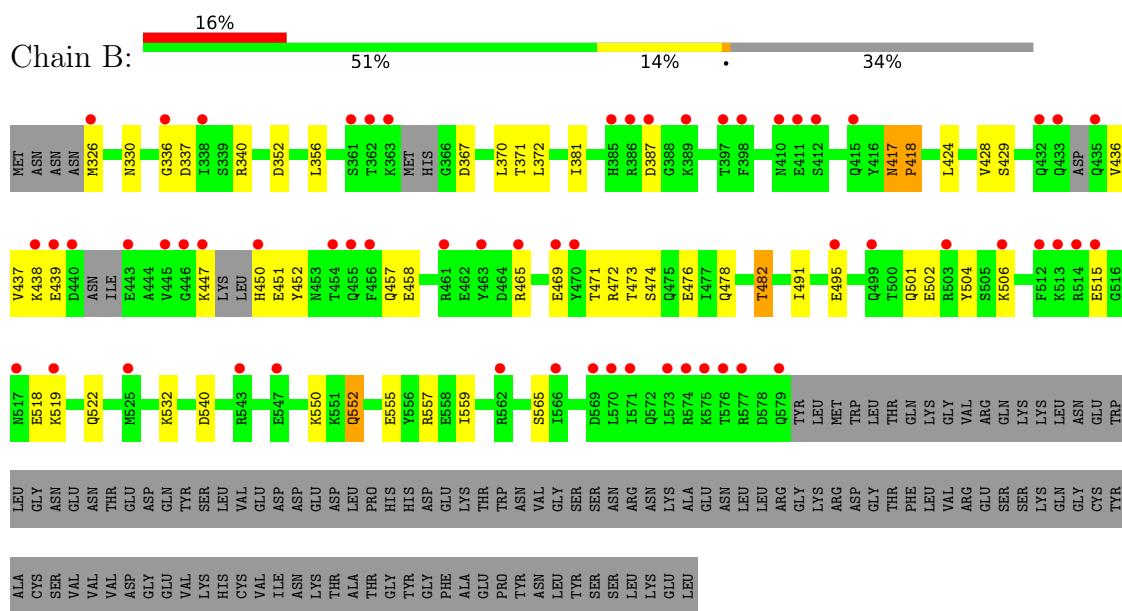
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.31Å 121.45Å 152.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 43.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 99.7 (43.92-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.223 , 0.307 0.242 , 0.303	Depositor DCC
R_{free} test set	2678 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	67.2	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10686	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.44	0/8644	0.64	2/11681 (0.0%)
2	B	0.38	0/2122	0.54	0/2835
All	All	0.43	0/10766	0.62	2/14516 (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	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	930	PHE	C-N-CA	5.41	135.23	121.70
1	A	748	LEU	CA-CB-CG	-5.20	103.34	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	VAL	Peptide
1	A	514	SER	Peptide
1	A	795	GLN	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	8448	0	8427	216	0
2	B	2092	0	2059	21	0
3	A	31	0	24	5	0
4	A	106	0	0	8	0
4	B	9	0	0	1	0
All	All	10686	0	10510	233	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 (233) 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:115:ARG:HA	4:A:1083:HOH:O	1.22	1.29
1:A:364:GLY:O	1:A:365:GLU:HG3	1.58	1.02
1:A:367:LEU:HD11	1:A:389:TYR:HB3	1.44	1.00
1:A:323:SER:HB3	1:A:482:SER:HB2	1.47	0.96
1:A:106:GLY:O	1:A:108:ARG:N	2.03	0.92
1:A:195:TRP:HE1	1:A:284:ASN:HD22	1.17	0.90
1:A:542:GLU:HG2	2:B:340:ARG:NH2	1.91	0.85
1:A:358:THR:O	1:A:369:ASP:HB2	1.80	0.81
1:A:542:GLU:HG2	2:B:340:ARG:HH21	1.44	0.80
1:A:765:ARG:HH12	1:A:796:ASN:HB2	1.47	0.79
1:A:406:ILE:O	1:A:422:LEU:HB2	1.83	0.78
1:A:-18:ASP:HB2	1:A:889:ILE:HD11	1.65	0.77
1:A:323:SER:HB3	1:A:482:SER:CB	2.15	0.77
1:A:830:ASP:O	1:A:899:ARG:HG2	1.84	0.77
1:A:872:PHE:O	1:A:873:ASN:HB3	1.84	0.77
1:A:409:VAL:O	1:A:410:LYS:HB2	1.85	0.76
1:A:347:ASN:O	1:A:348:ILE:HB	1.86	0.76
1:A:251:ILE:HD12	1:A:290:LYS:HG2	1.68	0.75
1:A:965:SER:HA	1:A:976:GLU:HG3	1.70	0.73
1:A:995:ALA:O	1:A:996:ASN:HB2	1.90	0.72
1:A:267:LEU:HD13	1:A:273:ILE:HG12	1.70	0.72
1:A:552:TRP:HZ3	1:A:583:MET:HE2	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:TRP:HE1	1:A:284:ASN:ND2	1.88	0.71
1:A:199:SER:O	1:A:201:ASN:N	2.22	0.71
1:A:1054:LYS:HG3	1:A:1055:MET:H	1.56	0.71
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.73	0.70
1:A:367:LEU:CD1	1:A:389:TYR:HB3	2.20	0.70
1:A:351:ILE:HG12	1:A:353:LYS:HG2	1.74	0.69
1:A:561:ILE:O	1:A:564:ILE:HG12	1.93	0.67
1:A:125:VAL:O	1:A:126:CYS:HB3	1.92	0.67
1:A:360:ILE:HB	1:A:367:LEU:HD22	1.77	0.67
2:B:519:LYS:HA	2:B:522:GLN:HB3	1.76	0.67
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.15	0.66
1:A:278:MET:HA	1:A:278:MET:CE	2.26	0.65
1:A:353:LYS:HD3	1:A:376:VAL:HG13	1.79	0.65
1:A:354:ILE:H	1:A:376:VAL:HG21	1.59	0.65
1:A:802:LYS:NZ	3:A:1833:KWT:C19	2.60	0.65
1:A:873:ASN:HA	1:A:1052:THR:OG1	1.97	0.65
1:A:552:TRP:HZ3	1:A:583:MET:CE	2.11	0.64
1:A:883:ASP:O	1:A:884:LYS:HB2	1.98	0.64
1:A:96:GLN:HG3	1:A:97:PRO:HD2	1.80	0.63
1:A:1052:THR:O	1:A:1054:LYS:N	2.32	0.63
1:A:109:GLU:O	1:A:110:GLU:HB2	1.98	0.63
1:A:137:GLN:HE22	1:A:140:ARG:HH11	1.45	0.62
1:A:677:ASN:C	1:A:677:ASN:HD22	2.03	0.62
1:A:125:VAL:O	1:A:126:CYS:CB	2.47	0.62
1:A:361:TYR:HA	1:A:365:GLU:HA	1.82	0.61
1:A:351:ILE:C	1:A:353:LYS:H	2.01	0.61
1:A:364:GLY:C	1:A:365:GLU:HG3	2.21	0.61
1:A:113:LEU:C	1:A:115:ARG:H	2.04	0.61
1:A:336:ILE:HD13	1:A:402:LEU:HD22	1.84	0.60
1:A:985:TYR:CE2	1:A:1040:MET:HG2	2.36	0.60
1:A:364:GLY:O	1:A:365:GLU:CG	2.42	0.59
1:A:158:SER:HB3	1:A:159:PRO:HD3	1.85	0.59
1:A:299:MET:O	1:A:300:ASP:HB3	2.03	0.59
1:A:337:LYS:HB3	1:A:476:GLU:HB3	1.85	0.59
1:A:995:ALA:O	1:A:996:ASN:CB	2.50	0.59
1:A:1054:LYS:CG	1:A:1055:MET:H	2.15	0.58
1:A:100:LYS:HE2	4:B:29:HOH:O	2.04	0.58
1:A:721:GLN:O	1:A:723:LYS:N	2.36	0.58
1:A:354:ILE:H	1:A:376:VAL:HG11	1.67	0.58
1:A:405:SER:OG	1:A:455:LEU:O	2.13	0.57
1:A:114:ASN:C	4:A:1085:HOH:O	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:TYR:OH	1:A:966:LYS:HG2	2.04	0.57
1:A:529:GLU:O	1:A:529:GLU:HG2	2.05	0.57
1:A:347:ASN:HD22	1:A:348:ILE:H	1.52	0.57
2:B:491:ILE:O	2:B:495:GLU:HG2	2.05	0.57
1:A:131:VAL:O	1:A:132:LYS:HB2	2.03	0.57
1:A:802:LYS:HZ3	3:A:1833:KWT:C19	2.17	0.57
1:A:1056:ASP:OD2	1:A:1061:THR:HB	2.04	0.57
2:B:437:VAL:HG13	2:B:438:LYS:HG2	1.86	0.57
1:A:353:LYS:HB3	1:A:376:VAL:CG1	2.34	0.56
1:A:961:LEU:O	1:A:964:ILE:O	2.24	0.56
1:A:354:ILE:HA	4:A:1079:HOH:O	2.04	0.56
1:A:354:ILE:HG12	1:A:376:VAL:HG21	1.87	0.55
1:A:992:ARG:HH12	1:A:1027:ALA:HB3	1.70	0.55
1:A:488:ASP:N	1:A:488:ASP:OD1	2.38	0.55
1:A:354:ILE:N	1:A:376:VAL:HG11	2.22	0.55
1:A:189:GLN:HB2	1:A:211:ILE:O	2.07	0.54
1:A:123:MET:CE	1:A:675:MET:HE1	2.38	0.54
1:A:552:TRP:CZ3	1:A:583:MET:HE2	2.40	0.54
1:A:910:ILE:HA	1:A:1025:THR:HG21	1.89	0.54
1:A:917:HIS:HD2	1:A:919:SER:H	1.54	0.54
1:A:-25:TYR:O	1:A:-23:HIS:N	2.37	0.54
1:A:373:THR:C	1:A:375:ARG:H	2.10	0.53
1:A:123:MET:CE	1:A:675:MET:CE	2.87	0.53
1:A:1023:ARG:HA	1:A:1028:LEU:HD22	1.90	0.53
1:A:705:GLN:O	1:A:709:MET:HG2	2.08	0.53
1:A:209:LEU:HD13	1:A:223:GLU:HB3	1.90	0.53
1:A:558:CYS:C	1:A:560:THR:H	2.12	0.53
1:A:351:ILE:C	1:A:353:LYS:N	2.62	0.53
1:A:427:ILE:HD11	1:A:443:LEU:HD22	1.91	0.52
1:A:992:ARG:HG3	1:A:992:ARG:HH11	1.74	0.52
1:A:1061:THR:O	1:A:1062:ILE:HB	2.10	0.52
1:A:446:TRP:CZ3	1:A:679:THR:HG22	2.43	0.52
1:A:497:ASN:O	1:A:500:VAL:HG12	2.10	0.52
1:A:109:GLU:HG3	1:A:113:LEU:HD12	1.92	0.51
1:A:353:LYS:HB3	1:A:376:VAL:HG13	1.91	0.51
1:A:508:TYR:CD1	1:A:509:SER:N	2.78	0.51
1:A:1059:PHE:O	1:A:1060:HIS:HB2	2.08	0.51
1:A:409:VAL:HG22	1:A:455:LEU:HD21	1.92	0.51
1:A:572:VAL:HG21	1:A:583:MET:HG2	1.92	0.51
1:A:756:ASN:C	1:A:756:ASN:HD22	2.14	0.51
1:A:366:PRO:HB3	1:A:575:ASN:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLU:O	1:A:110:GLU:CB	2.58	0.51
1:A:193:VAL:HG23	1:A:282:MET:HG2	1.92	0.51
1:A:953:PRO:HA	4:A:1097:HOH:O	2.11	0.51
1:A:61:LEU:HD13	2:B:504:TYR:HD2	1.75	0.51
2:B:555:GLU:O	2:B:559:ILE:HG12	2.11	0.50
1:A:251:ILE:HD13	1:A:293:LEU:HD12	1.94	0.50
1:A:9:GLU:OE2	1:A:38:ARG:NH1	2.45	0.50
1:A:178:PRO:HG2	1:A:181:ILE:HD12	1.93	0.50
1:A:278:MET:HA	1:A:278:MET:HE3	1.94	0.50
1:A:796:ASN:ND2	4:A:1092:HOH:O	2.44	0.50
1:A:194:ILE:HD11	1:A:220:VAL:HG12	1.94	0.50
1:A:647:ASN:HD22	1:A:649:LEU:H	1.59	0.50
1:A:789:MET:HE2	1:A:793:LEU:HD12	1.93	0.50
1:A:528:LYS:O	1:A:528:LYS:HG2	2.11	0.49
1:A:71:VAL:CG2	1:A:81:GLU:HG2	2.42	0.49
1:A:802:LYS:NZ	3:A:1833:KWT:C3	2.75	0.49
1:A:904:TYR:O	1:A:908:THR:HB	2.13	0.49
1:A:136:VAL:HG13	1:A:686:LEU:HD21	1.95	0.49
1:A:533:ALA:N	4:A:1117:HOH:O	2.45	0.49
1:A:701:HIS:CD2	1:A:704:ARG:HH21	2.31	0.49
1:A:802:LYS:HZ1	3:A:1833:KWT:C19	2.26	0.48
1:A:872:PHE:O	1:A:873:ASN:CB	2.56	0.48
1:A:123:MET:HE2	1:A:675:MET:CE	2.42	0.48
3:A:1833:KWT:C19	3:A:1833:KWT:O5	2.57	0.48
1:A:298:PRO:O	1:A:299:MET:HG2	2.13	0.48
1:A:807:LEU:HD23	1:A:846:GLY:HA3	1.96	0.48
1:A:360:ILE:HB	1:A:367:LEU:CD2	2.43	0.48
1:A:406:ILE:O	1:A:421:PRO:O	2.32	0.48
1:A:711:LYS:HE3	1:A:743:ASP:OD2	2.14	0.48
1:A:744:PHE:CZ	1:A:748:LEU:HD13	2.50	0.47
1:A:347:ASN:O	1:A:348:ILE:CB	2.60	0.47
1:A:590:TRP:HD1	1:A:591:PRO:O	1.97	0.47
1:A:354:ILE:O	1:A:376:VAL:HG11	2.14	0.47
1:A:337:LYS:HD2	1:A:386:TRP:CE2	2.50	0.47
2:B:437:VAL:HG22	2:B:438:LYS:H	1.79	0.47
2:B:326:MET:SD	2:B:330:ASN:ND2	2.88	0.47
1:A:61:LEU:HD13	2:B:504:TYR:CD2	2.50	0.47
1:A:639:LEU:HD22	1:A:650:VAL:HG13	1.97	0.46
1:A:873:ASN:HA	1:A:1052:THR:CB	2.45	0.46
1:A:156:LEU:O	1:A:157:ASN:CB	2.63	0.46
1:A:421:PRO:HD2	1:A:455:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:SER:O	1:A:509:SER:N	2.40	0.46
1:A:917:HIS:O	1:A:920:ASN:HB2	2.16	0.46
1:A:331:ASN:ND2	1:A:392:TYR:OH	2.49	0.46
1:A:638:VAL:HG12	1:A:649:LEU:HD21	1.97	0.46
1:A:677:ASN:HD22	1:A:678:LYS:N	2.14	0.46
1:A:617:ARG:NH2	4:A:1174:HOH:O	2.49	0.45
1:A:1056:ASP:OD2	1:A:1061:THR:CB	2.64	0.45
1:A:75:GLN:HG2	1:A:93:ARG:O	2.16	0.45
1:A:831:LEU:HD11	1:A:987:ALA:HB2	1.98	0.45
1:A:921:ILE:HA	1:A:931:HIS:H	1.81	0.45
1:A:558:CYS:SG	1:A:564:ILE:HD12	2.56	0.45
1:A:126:CYS:HA	1:A:129:ASP:CG	2.37	0.45
1:A:709:MET:CE	1:A:841:ILE:HD13	2.47	0.45
1:A:116:GLU:HB3	1:A:703:ASN:HD21	1.81	0.44
1:A:251:ILE:HG22	1:A:288:MET:HB3	1.99	0.44
1:A:595:PRO:HG3	1:A:622:TYR:HB2	1.99	0.44
1:A:641:TYR:OH	1:A:1007:GLY:N	2.50	0.44
1:A:677:ASN:C	1:A:677:ASN:ND2	2.69	0.44
2:B:370:LEU:HD23	2:B:381:ILE:HD12	2.00	0.44
2:B:478:GLN:O	2:B:482:THR:HG23	2.17	0.44
1:A:93:ARG:HH11	1:A:93:ARG:HB2	1.83	0.44
2:B:447:LYS:HD2	2:B:450:HIS:ND1	2.32	0.44
1:A:113:LEU:C	1:A:115:ARG:N	2.70	0.44
1:A:930:PHE:HA	1:A:931:HIS:HB2	2.00	0.44
1:A:354:ILE:HG12	1:A:376:VAL:CG2	2.48	0.44
1:A:558:CYS:C	1:A:560:THR:N	2.71	0.44
1:A:113:LEU:O	1:A:115:ARG:N	2.51	0.44
1:A:883:ASP:O	1:A:884:LYS:CB	2.63	0.44
1:A:407:CYS:HA	1:A:422:LEU:HG	1.99	0.43
1:A:324:THR:HA	1:A:483:VAL:O	2.17	0.43
1:A:376:VAL:HG23	1:A:377:PRO:C	2.38	0.43
1:A:709:MET:HE3	1:A:841:ILE:HD13	2.00	0.43
1:A:373:THR:C	1:A:375:ARG:N	2.71	0.43
1:A:623:LEU:HD22	1:A:627:LYS:HB3	2.00	0.43
1:A:788:ILE:H	1:A:788:ILE:HG13	1.55	0.43
1:A:985:TYR:CZ	1:A:1040:MET:HG2	2.53	0.43
2:B:469:GLU:HG3	2:B:472:ARG:HH12	1.84	0.43
1:A:937:PHE:HB3	1:A:938:LEU:HG	2.00	0.43
1:A:376:VAL:O	1:A:376:VAL:HG22	2.18	0.43
1:A:953:PRO:O	1:A:954:PHE:HB2	2.18	0.43
1:A:552:TRP:CZ3	1:A:583:MET:CE	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:THR:HB	1:A:976:GLU:HG2	2.01	0.43
2:B:502:GLU:O	2:B:506:LYS:HB2	2.18	0.42
1:A:373:THR:O	1:A:375:ARG:N	2.42	0.42
1:A:278:MET:HA	1:A:278:MET:HE2	1.98	0.42
1:A:407:CYS:HB2	1:A:408:SER:H	1.63	0.42
1:A:532:LYS:C	1:A:534:ILE:H	2.22	0.42
1:A:633:ILE:HG22	1:A:1005:MET:CE	2.49	0.42
1:A:121:ILE:HG12	1:A:688:LEU:HB3	2.01	0.42
1:A:124:PRO:HG2	1:A:127:GLU:HG3	2.01	0.42
1:A:344:VAL:HG21	1:A:422:LEU:HD13	2.00	0.42
1:A:361:TYR:CD2	1:A:365:GLU:HB3	2.54	0.42
1:A:924:LYS:HE3	1:A:928:GLN:HB3	2.01	0.42
1:A:1052:THR:OG1	1:A:1052:THR:O	2.32	0.42
1:A:353:LYS:HB3	1:A:376:VAL:HG11	2.00	0.42
1:A:374:GLN:C	1:A:376:VAL:HG12	2.39	0.42
1:A:792:LEU:O	1:A:793:LEU:HB2	2.20	0.42
1:A:57:PRO:O	1:A:58:LEU:HB2	2.20	0.42
1:A:785:ASN:C	1:A:785:ASN:HD22	2.22	0.42
2:B:356:LEU:HD23	2:B:428:VAL:HG21	2.02	0.42
1:A:192:VAL:HG13	1:A:283:PRO:HB2	2.02	0.41
1:A:211:ILE:HG13	1:A:215:CYS:SG	2.60	0.41
1:A:328:TRP:CB	1:A:394:PRO:HB3	2.50	0.41
1:A:528:LYS:HG2	1:A:531:LEU:HD23	2.01	0.41
2:B:372:LEU:HD13	2:B:424:LEU:HD23	2.02	0.41
1:A:251:ILE:HD11	1:A:262:LEU:HD22	2.03	0.41
1:A:409:VAL:O	1:A:410:LYS:CB	2.63	0.41
1:A:910:ILE:HA	1:A:1025:THR:CG2	2.50	0.41
1:A:158:SER:HB3	1:A:159:PRO:CD	2.51	0.41
1:A:361:TYR:CG	1:A:365:GLU:HB3	2.55	0.41
1:A:956:LEU:HD23	1:A:956:LEU:HA	1.90	0.41
1:A:269:GLN:HA	1:A:274:ARG:NH2	2.35	0.41
1:A:1054:LYS:CG	1:A:1055:MET:N	2.83	0.41
1:A:49:LEU:HD21	1:A:101:VAL:HG21	2.02	0.41
1:A:328:TRP:HB2	1:A:394:PRO:HB3	2.03	0.41
1:A:712:LEU:HD13	1:A:748:LEU:HD11	2.03	0.41
1:A:792:LEU:O	1:A:793:LEU:CB	2.68	0.41
2:B:473:THR:HG23	2:B:552:GLN:NE2	2.36	0.41
2:B:518:GLU:O	2:B:519:LYS:HB2	2.21	0.41
1:A:59:HIS:HB2	4:A:1112:HOH:O	2.19	0.41
1:A:345:ASN:HD21	2:B:557:ARG:HG2	1.86	0.41
2:B:417:ASN:HA	2:B:418:PRO:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ASN:ND2	1:A:462:THR:HG21	2.36	0.40
1:A:322:THR:HG22	1:A:323:SER:H	1.86	0.40
1:A:1033:GLN:OE1	1:A:1033:GLN:HA	2.22	0.40
1:A:412:ARG:HD2	1:A:412:ARG:H	1.86	0.40
1:A:999:ILE:HD13	1:A:1022:ILE:HD11	2.02	0.40
1:A:1053:THR:O	1:A:1054:LYS:C	2.60	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	1020/1091 (94%)	880 (86%)	90 (9%)	50 (5%)	2	7
2	B	237/373 (64%)	215 (91%)	15 (6%)	7 (3%)	4	15
All	All	1257/1464 (86%)	1095 (87%)	105 (8%)	57 (4%)	2	8

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	107	ASN
1	A	110	GLU
1	A	114	ASN
1	A	157	ASN
1	A	158	SER
1	A	200	PRO
1	A	300	ASP
1	A	324	THR
1	A	348	ILE
1	A	508	TYR
1	A	722	GLU

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Mol	Chain	Res	Type
1	A	793	LEU
1	A	887	GLY
1	A	996	ASN
1	A	126	CYS
1	A	132	LYS
1	A	410	LYS
1	A	542	GLU
1	A	723	LYS
1	A	790	SER
1	A	864	GLY
1	A	866	LEU
1	A	888	GLU
1	A	931	HIS
1	A	955	VAL
1	A	1047	ARG
1	A	1053	THR
1	A	1054	LYS
2	B	336	GLY
1	A	10	LEU
1	A	374	GLN
1	A	491	VAL
1	A	509	SER
1	A	873	ASN
1	A	954	PHE
1	A	968	ALA
2	B	451	GLU
1	A	-24	HIS
1	A	199	SER
1	A	202	ASN
1	A	351	ILE
1	A	365	GLU
1	A	422	LEU
1	A	559	VAL
1	A	1045	ASP
1	A	104	PRO
1	A	201	ASN
1	A	234	LEU
1	A	930	PHE
1	A	956	LEU
2	B	429	SER
2	B	439	GLU
1	A	869	ALA

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Mol	Chain	Res	Type
2	B	417	ASN
2	B	418	PRO
2	B	436	VAL

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	945/995 (95%)	845 (89%)	100 (11%)	6	20
2	B	229/342 (67%)	209 (91%)	20 (9%)	10	30
All	All	1174/1337 (88%)	1054 (90%)	120 (10%)	7	22

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	10	LEU
1	A	13	ILE
1	A	18	PRO
1	A	31	ILE
1	A	38	ARG
1	A	52	GLU
1	A	60	GLN
1	A	86	THR
1	A	93	ARG
1	A	96	GLN
1	A	105	VAL
1	A	110	GLU
1	A	113	LEU
1	A	115	ARG
1	A	123	MET
1	A	137	GLN
1	A	153	LEU
1	A	171	VAL
1	A	173	SER

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Mol	Chain	Res	Type
1	A	187	LYS
1	A	202	ASN
1	A	205	GLN
1	A	218	GLU
1	A	237	GLU
1	A	239	LEU
1	A	251	ILE
1	A	264	LYS
1	A	267	LEU
1	A	293	LEU
1	A	300	ASP
1	A	303	THR
1	A	322	THR
1	A	323	SER
1	A	331	ASN
1	A	347	ASN
1	A	352	ASP
1	A	367	LEU
1	A	368	CYS
1	A	376	VAL
1	A	390	ASP
1	A	408	SER
1	A	412	ARG
1	A	441	MET
1	A	452	LEU
1	A	453	GLU
1	A	459	ILE
1	A	462	THR
1	A	478	ASP
1	A	488	ASP
1	A	516	ARG
1	A	528	LYS
1	A	530	GLN
1	A	535	SER
1	A	542	GLU
1	A	564	ILE
1	A	619	LEU
1	A	627	LYS
1	A	630	GLN
1	A	650	VAL
1	A	672	LYS
1	A	677	ASN

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Mol	Chain	Res	Type
1	A	686	LEU
1	A	687	LEU
1	A	712	LEU
1	A	715	LEU
1	A	721	GLN
1	A	733	LYS
1	A	738	GLN
1	A	748	LEU
1	A	756	ASN
1	A	766	LEU
1	A	785	ASN
1	A	788	ILE
1	A	789	MET
1	A	794	PHE
1	A	795	GLN
1	A	834	LEU
1	A	839	LEU
1	A	871	GLN
1	A	873	ASN
1	A	877	LEU
1	A	888	GLU
1	A	899	ARG
1	A	920	ASN
1	A	932	ILE
1	A	937	PHE
1	A	938	LEU
1	A	955	VAL
1	A	958	GLN
1	A	972	THR
1	A	976	GLU
1	A	983	MET
1	A	997	LEU
1	A	1006	LEU
1	A	1017	ASP
1	A	1047	ARG
1	A	1052	THR
1	A	1055	MET
1	A	1060	HIS
2	B	337	ASP
2	B	352	ASP
2	B	367	ASP
2	B	371	THR

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Mol	Chain	Res	Type
2	B	387	ASP
2	B	452	TYR
2	B	457	GLN
2	B	458	GLU
2	B	465	ARG
2	B	471	THR
2	B	474	SER
2	B	476	GLU
2	B	482	THR
2	B	501	GLN
2	B	515	GLU
2	B	532	LYS
2	B	540	ASP
2	B	550	LYS
2	B	552	GLN
2	B	565	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	59	HIS
1	A	60	GLN
1	A	137	GLN
1	A	213	HIS
1	A	269	GLN
1	A	284	ASN
1	A	331	ASN
1	A	347	ASN
1	A	374	GLN
1	A	444	ASN
1	A	467	ASN
1	A	556	HIS
1	A	597	GLN
1	A	605	ASN
1	A	647	ASN
1	A	677	ASN
1	A	701	HIS
1	A	714	ASN
1	A	756	ASN
1	A	763	ASN
1	A	785	ASN

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Mol	Chain	Res	Type
1	A	825	GLN
1	A	871	GLN
1	A	917	HIS
1	A	918	ASN
2	B	517	ASN
2	B	564	ASN
2	B	572	GLN

5.3.3 RNA ⓘ

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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	KWT	A	1833	-	30,35,35	3.06	7 (23%)	35,57,57	5.99	15 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KWT	A	1833	-	-	6/7/75/75	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1833	KWT	C8-C7	8.97	1.54	1.35
3	A	1833	KWT	C3-C4	7.01	1.46	1.38
3	A	1833	KWT	O1-C2	6.76	1.45	1.35
3	A	1833	KWT	O6-C21	6.55	1.50	1.35
3	A	1833	KWT	C5-C6	-4.48	1.45	1.49
3	A	1833	KWT	C19-C3	-3.96	1.32	1.37
3	A	1833	KWT	C9-C8	2.70	1.55	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1833	KWT	C5-C4-C3	30.27	118.84	107.42
3	A	1833	KWT	C9-C8-C7	-8.26	109.87	123.18
3	A	1833	KWT	C19-C3-C4	7.46	123.07	110.89
3	A	1833	KWT	O6-C21-C22	7.35	124.61	111.09
3	A	1833	KWT	C15-C7-C8	-5.60	108.34	121.60
3	A	1833	KWT	C11-O6-C21	5.39	125.25	117.06
3	A	1833	KWT	C17-C18-C13	4.73	113.26	108.59
3	A	1833	KWT	C16-C17-C18	-3.02	102.66	105.70
3	A	1833	KWT	O6-C21-O7	-2.79	117.41	122.96
3	A	1833	KWT	O1-C1-C23	2.65	113.17	107.31
3	A	1833	KWT	C5-C6-C7	-2.54	116.67	118.14
3	A	1833	KWT	O4-C18-C13	-2.46	122.69	125.96
3	A	1833	KWT	O1-C2-O2	2.40	120.28	117.60
3	A	1833	KWT	C14-C13-C18	2.20	109.22	105.18
3	A	1833	KWT	C15-C7-C6	-2.14	115.12	118.10

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1833	KWT	C8-C11-O6-C21
3	A	1833	KWT	C12-C11-O6-C21
3	A	1833	KWT	O7-C21-O6-C11
3	A	1833	KWT	C22-C21-O6-C11
3	A	1833	KWT	O1-C1-C23-O8
3	A	1833	KWT	C9-C1-C23-O8

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1833	KWT	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand KWT A 1833

Bond lengths

Bond angles

Torsions

Rings
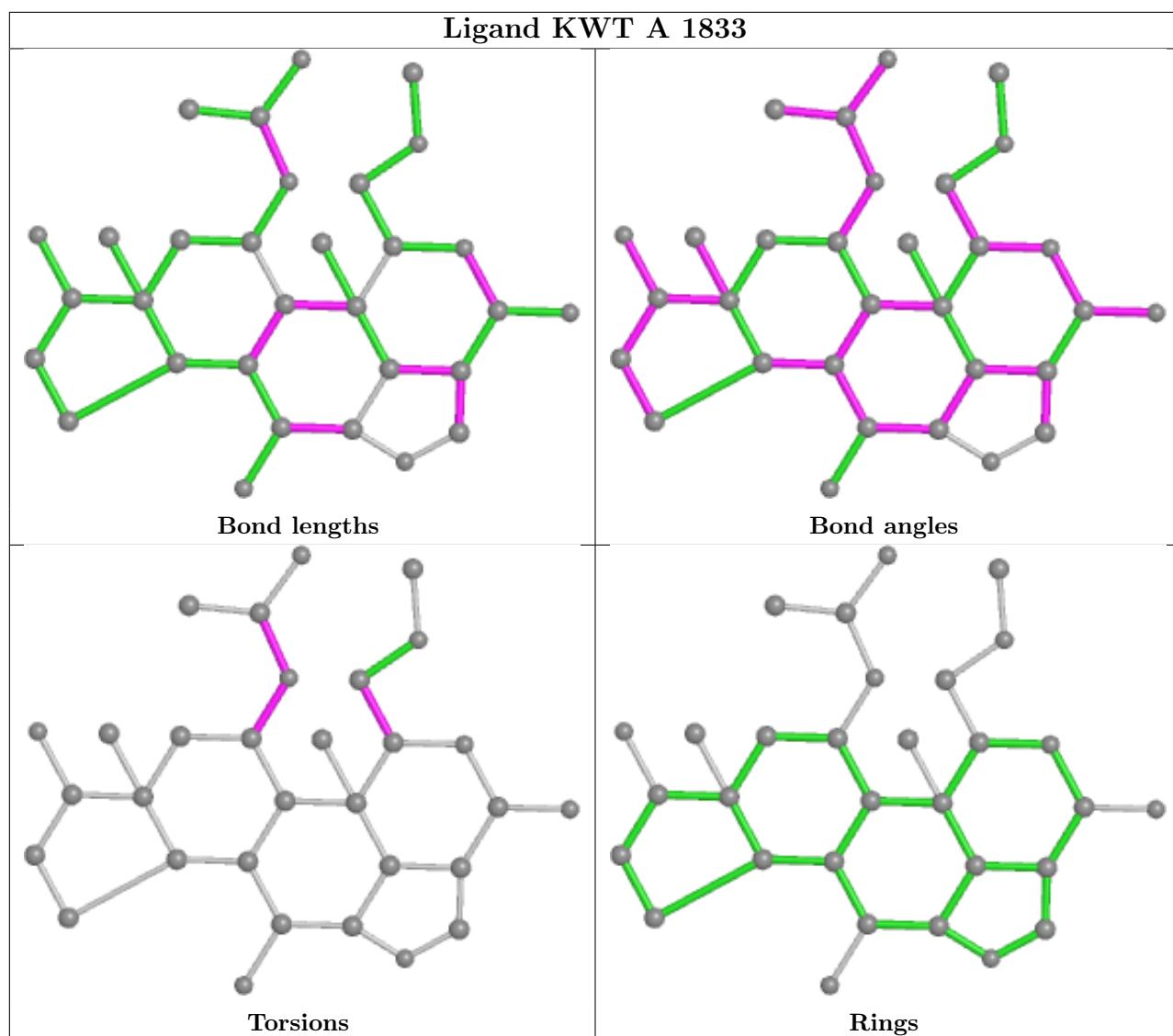
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	1032/1091 (94%)	0.44	58 (5%)	24	16	35, 60, 84, 101	0
2	B	247/373 (66%)	1.34	59 (23%)	0	0	62, 89, 117, 131	0
All	All	1279/1464 (87%)	0.62	117 (9%)	9	5	35, 64, 98, 131	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	445	VAL	8.6
2	B	579	GLN	7.3
1	A	866	LEU	7.3
2	B	362	THR	6.1
2	B	326	MET	5.9
1	A	792	LEU	5.8
2	B	361	SER	5.5
1	A	723	LYS	5.1
2	B	512	PHE	5.0
2	B	576	THR	4.9
2	B	410	ASN	4.6
2	B	397	THR	4.5
1	A	350	ASP	4.5
1	A	375	ARG	4.5
1	A	865	GLY	4.5
2	B	415	GLN	4.4
2	B	575	LYS	4.3
1	A	186	ASP	4.3
2	B	447	LYS	4.2
1	A	158	SER	4.1
2	B	454	THR	4.1
2	B	514	ARG	4.1
1	A	300	ASP	3.9
1	A	524	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	440	ASP	3.9
2	B	456	PHE	3.8
1	A	-27	SER	3.8
1	A	-18	ASP	3.8
2	B	433	GLN	3.7
1	A	299	MET	3.7
1	A	791	GLU	3.7
2	B	469	GLU	3.6
2	B	435	GLN	3.6
2	B	515	GLU	3.5
1	A	1052	THR	3.5
1	A	309	ARG	3.5
1	A	413	LYS	3.5
2	B	363	LYS	3.4
2	B	387	ASP	3.4
1	A	557	TYR	3.4
1	A	972	THR	3.3
1	A	525	GLU	3.3
2	B	463	TYR	3.2
1	A	5	PRO	3.2
1	A	1054	LYS	3.2
1	A	722	GLU	3.2
2	B	438	LYS	3.2
2	B	443	GLU	3.1
2	B	389	LYS	3.1
1	A	969	GLN	3.0
2	B	411	GLU	3.0
1	A	1055	MET	3.0
1	A	531	LEU	2.9
1	A	868	GLY	2.9
2	B	525	MET	2.9
2	B	446	GLY	2.9
2	B	543	ARG	2.9
2	B	569	ASP	2.9
1	A	352	ASP	2.8
2	B	450	HIS	2.8
1	A	377	PRO	2.8
1	A	200	PRO	2.7
2	B	385	HIS	2.7
1	A	864	GLY	2.7
2	B	574	ARG	2.7
2	B	432	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	351	ILE	2.7
2	B	562	ARG	2.6
2	B	461	ARG	2.6
1	A	323	SER	2.6
2	B	386	ARG	2.6
2	B	470	TYR	2.6
1	A	410	LYS	2.6
2	B	519	LYS	2.6
1	A	349	ARG	2.5
2	B	573	LEU	2.5
2	B	506	LYS	2.5
1	A	363	GLY	2.5
1	A	156	LEU	2.5
2	B	517	ASN	2.5
2	B	547	GLU	2.5
2	B	439	GLU	2.4
2	B	577	ARG	2.4
1	A	481	SER	2.4
2	B	570	LEU	2.4
1	A	110	GLU	2.4
1	A	970	GLU	2.4
2	B	455	GLN	2.3
1	A	527	ASP	2.3
2	B	412	SER	2.3
1	A	526	ASN	2.3
1	A	1051	TRP	2.3
1	A	308	SER	2.3
1	A	64	ASP	2.2
1	A	130	MET	2.2
2	B	495	GLU	2.2
2	B	503	ARG	2.2
1	A	726	GLU	2.2
2	B	499	GLN	2.2
2	B	338	ILE	2.2
1	A	-19	HIS	2.2
1	A	530	GLN	2.1
2	B	336	GLY	2.1
1	A	515	ASN	2.1
2	B	566	ILE	2.1
1	A	108	ARG	2.1
1	A	727	THR	2.1
1	A	-17	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	176	GLU	2.1
2	B	513	LYS	2.1
2	B	571	ILE	2.1
2	B	465	ARG	2.1
1	A	870	LEU	2.0
2	B	398	PHE	2.0
1	A	973	LYS	2.0
1	A	33	THR	2.0
1	A	629	SER	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 ⓘ

There are no monosaccharides 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. 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	KWT	A	1833	31/31	0.86	0.32	57,61,70,71	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around KWT A 1833:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.