



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:30 AM UTC

PDB ID : 3HHM / pdb_00003hhm
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

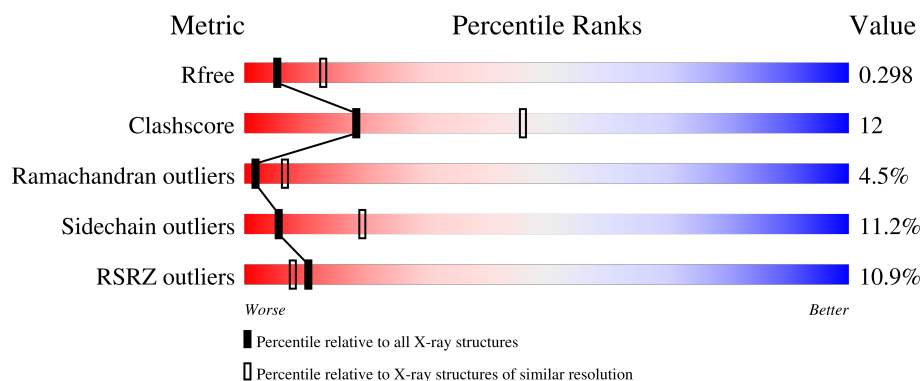
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	1091	9% 64% 22% 7% 5%
2	B	373	10% 52% 13% 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
1	A	1032	Total	C	N	O	S	0	0	0
			8448	5405	1447	1528	68			

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

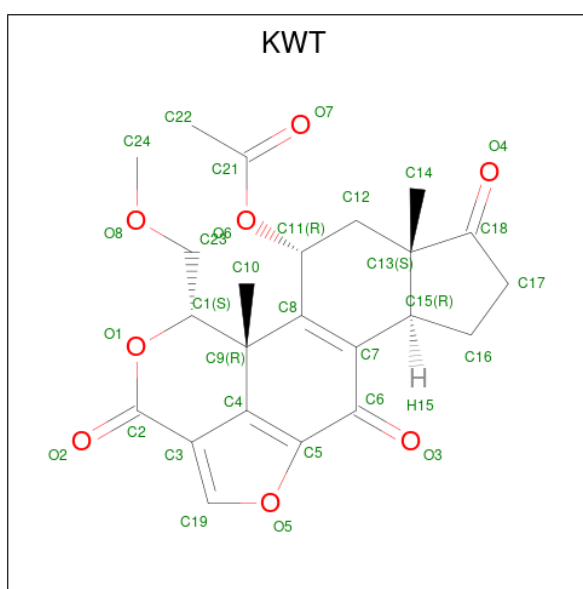
- Molecule 2 is a protein called niSH2 p85alpha.

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

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 (CCD ID: KWT) (formula: C₂₃H₂₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			31	23	8		

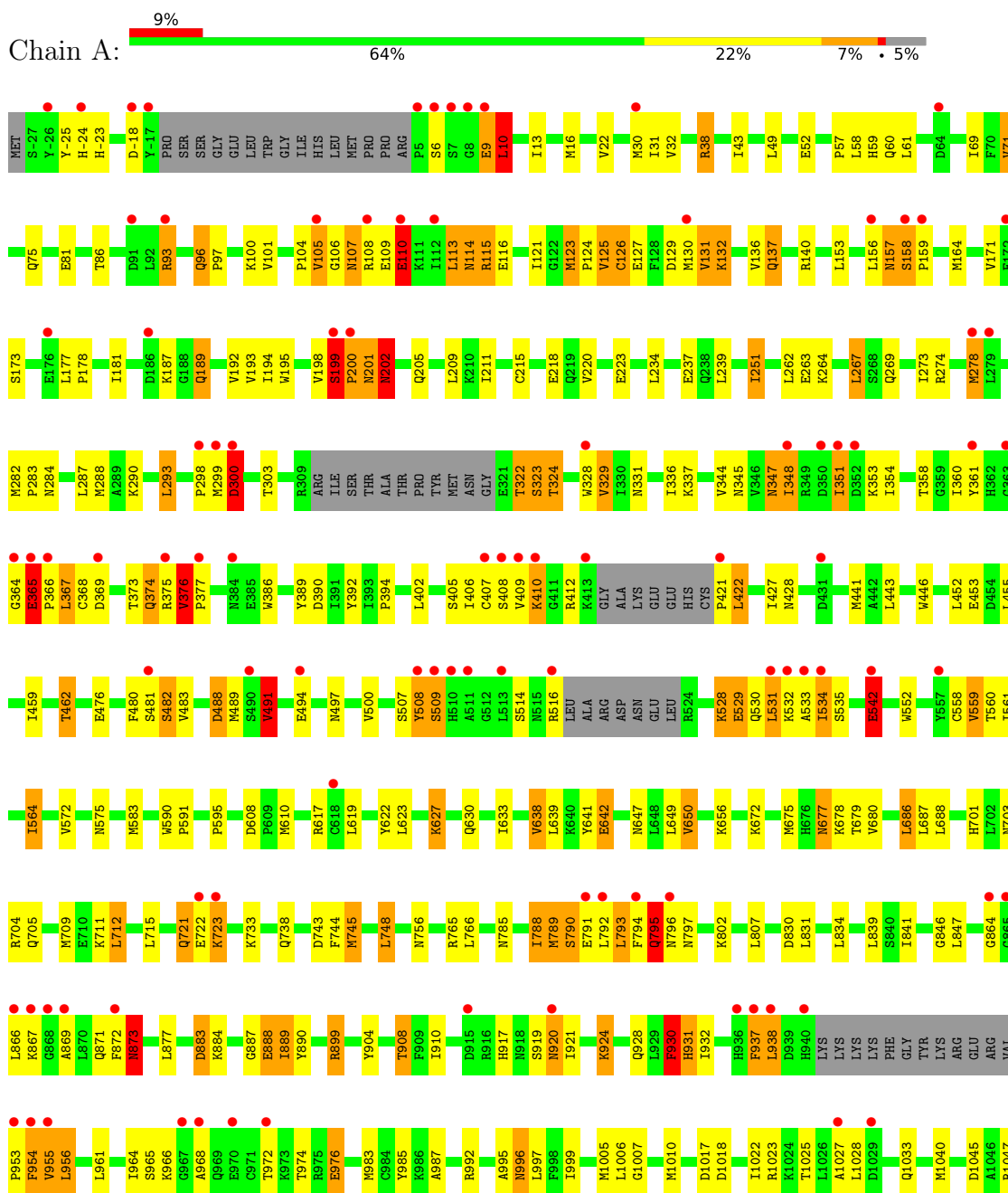
- Molecule 4 is water.

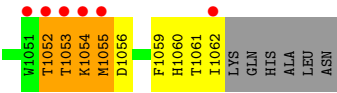
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total	O	0	0
			106	106		
4	B	9	Total	O	0	0
			9	9		

3 Residue-property plots

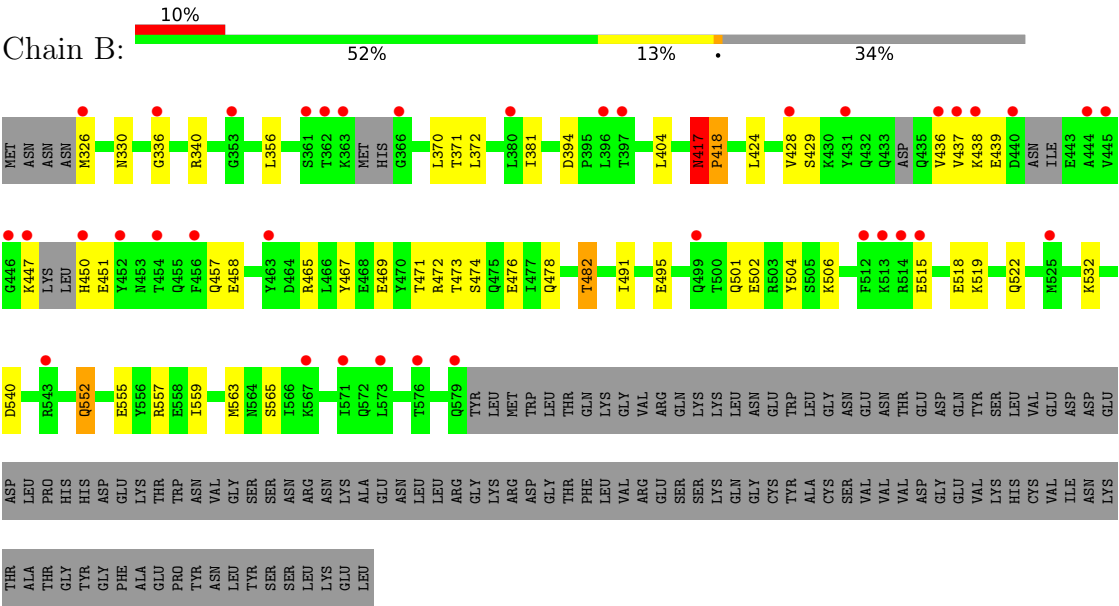
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



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 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 99.7 (50.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.223 , 0.307 0.239 , 0.298	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 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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

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	0.54	0/8644	0.92	20/11681 (0.2%)
2	B	0.48	0/2122	0.86	3/2835 (0.1%)
All	All	0.53	0/10766	0.91	23/14516 (0.2%)

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 (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	199	SER	CA-C-N	8.69	130.71	119.84
1	A	199	SER	C-N-CA	8.69	130.71	119.84
1	A	329	VAL	N-CA-C	-7.71	105.97	113.53
1	A	930	PHE	CA-C-N	7.51	135.23	121.70
1	A	930	PHE	C-N-CA	7.51	135.23	121.70
2	B	417	ASN	CA-C-N	7.08	128.69	119.84
2	B	417	ASN	C-N-CA	7.08	128.69	119.84
1	A	365	GLU	CA-C-N	6.80	128.34	119.84
1	A	365	GLU	C-N-CA	6.80	128.34	119.84
1	A	608	ASP	CA-C-N	6.79	126.75	119.28
1	A	608	ASP	C-N-CA	6.79	126.75	119.28
1	A	534	ILE	N-CA-C	-6.38	106.56	112.43
1	A	930	PHE	N-CA-C	-6.06	97.90	110.80
1	A	797	ASN	N-CA-C	5.55	117.82	107.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	795	GLN	N-CA-C	5.29	116.48	108.07
1	A	376	VAL	CA-C-N	-5.24	114.33	119.99
1	A	376	VAL	C-N-CA	-5.24	114.33	119.99
1	A	189	GLN	N-CA-C	5.23	117.02	109.07
1	A	177	LEU	CA-C-N	5.15	126.28	119.84
1	A	177	LEU	C-N-CA	5.15	126.28	119.84
1	A	482	SER	N-CA-C	5.14	114.92	108.45
2	B	394	ASP	N-CA-C	5.07	121.01	109.81
1	A	883	ASP	N-CA-C	-5.06	103.81	110.43

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	234	0
2	B	2092	0	2059	22	0
3	A	31	0	24	6	0
4	A	106	0	0	8	0
4	B	9	0	0	1	0
All	All	10686	0	10510	252	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 12.

All (252) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:278:MET:HE2	1:A:278:MET:HA	1.52	0.91
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:709:MET:HE1	1:A:847:LEU:HD21	1.63	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:642:GLU:HG2	1:A:647:ASN:CG	2.15	0.72
1:A:30:MET:HE1	1:A:57:PRO:HD2	1.72	0.71
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: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:123:MET:CE	1:A:675:MET:HE1	2.24	0.68
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:351:ILE:C	1:A:353:LYS:H	2.01	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:677:ASN:C	1:A:677:ASN:HD22	2.03	0.67
1:A:364:GLY:C	1:A:365:GLU:HG3	2.21	0.66
1:A:113:LEU:C	1:A:115:ARG:H	2.04	0.65
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:633:ILE:HG22	1:A:1005:MET:HE1	1.79	0.63
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:114:ASN:C	4:A:1085:HOH:O	2.42	0.62
1:A:137:GLN:HE22	1:A:140:ARG:HH11	1.45	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: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
2:B:467:TYR:HD2	2:B:563:MET:HE1	1.67	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:373:THR:C	1:A:375:ARG:H	2.10	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:802:LYS:HZ1	3:A:1833:KWT:C19	2.16	0.58
1:A:405:SER:OG	1:A:455:LEU:O	2.13	0.57
1:A:558:CYS:C	1:A:560:THR:H	2.12	0.57
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: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:351:ILE:C	1:A:353:LYS:N	2.62	0.56
1:A:353:LYS:HB3	1:A:376:VAL:CG1	2.34	0.56
1:A:633:ILE:CG2	1:A:1005:MET:HE1	2.35	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:756:ASN:C	1:A:756:ASN:HD22	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:366:PRO:HB3	1:A:575:ASN:HB3	1.93	0.51
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:796:ASN:ND2	4:A:1092:HOH:O	2.44	0.50
1:A:123:MET:HE2	1:A:675:MET:CE	2.42	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:528:LYS:O	1:A:528:LYS:HG2	2.11	0.49
1:A:126:CYS:HA	1:A:129:ASP:CG	2.37	0.49
1:A:552:TRP:HZ3	1:A:583:MET:HE3	1.78	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:10:LEU:HD13	1:A:16:MET:HE2	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:376:VAL:HG23	1:A:377:PRO:C	2.38	0.49
1:A:745:MET:HE2	1:A:745:MET:HA	1.93	0.49
1:A:872:PHE:O	1:A:873:ASN:CB	2.56	0.48
1:A:552:TRP:HZ3	1:A:583:MET:HE2	1.78	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:164:MET:HE1	1:A:263:GLU:HG3	1.95	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:373:THR:C	1:A:375:ARG:N	2.71	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:802:LYS:HZ3	3:A:1833:KWT:C19	2.26	0.48
1:A:113:LEU:C	1:A:115:ARG:N	2.70	0.47
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:374:GLN:C	1:A:376:VAL:HG12	2.39	0.47
1:A:61:LEU:HD13	2:B:504:TYR:CD2	2.50	0.47
1:A:532:LYS:C	1:A:534:ILE:H	2.22	0.46
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:785:ASN:C	1:A:785:ASN:HD22	2.22	0.46
1:A:421:PRO:HD2	1:A:455:LEU:HD23	1.98	0.46
1:A:507:SER:O	1:A:509:SER:N	2.40	0.46
1:A:558:CYS:C	1:A:560:THR:N	2.71	0.46
1:A:709:MET:HE2	1:A:841:ILE:HD13	1.97	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:617:ARG:NH2	4:A:1174:HOH:O	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:ASP:OD2	1:A:1061:THR:CB	2.64	0.45
1:A:552:TRP:CZ3	1:A:583:MET:CE	2.97	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:1055:MET:HE2	1:A:1055:MET:HA	1.97	0.45
1:A:558:CYS:SG	1:A:564:ILE:HD12	2.56	0.45
1:A:1053:THR:O	1:A:1054:LYS:C	2.60	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:HD22	1:A:678:LYS:N	2.14	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: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: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:106:GLY:C	1:A:108:ARG:H	2.10	0.43
1:A:324:THR:HA	1:A:483:VAL:O	2.17	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:677:ASN:C	1:A:677:ASN:ND2	2.69	0.43
1:A:105:VAL:C	1:A:107:ASN:N	2.75	0.43
1:A:953:PRO:O	1:A:954:PHE:HB2	2.18	0.43
1:A:130:MET:HE2	1:A:132:LYS:HE3	2.01	0.43
1:A:974:THR:HB	1:A:976:GLU:HG2	2.01	0.43
1:A:789:MET:HE2	1:A:793:LEU:HD12	2.00	0.42
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:407:CYS:HB2	1:A:408:SER:H	1.63	0.42
1:A:121:ILE:HG12	1:A:688:LEU:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:489:MET:C	1:A:491:VAL:H	2.28	0.42
1:A:802:LYS:HZ1	3:A:1833:KWT:C3	2.32	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:790:SER:O	1:A:791:GLU:C	2.61	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
2:B:356:LEU:HD23	2:B:428:VAL:HG21	2.02	0.42
1:A:200:PRO:C	1:A:202:ASN:H	2.28	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:480:PHE:O	1:A:481:SER:C	2.63	0.41
1:A:756:ASN:C	1:A:756:ASN:ND2	2.77	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:552:TRP:CZ3	1:A:583:MET:HE2	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
1:A:572:VAL:HG22	1:A:583:MET:HE3	2.03	0.41
1:A:785:ASN:C	1:A:785:ASN:ND2	2.79	0.41
2:B:417:ASN:HA	2:B:418:PRO:HD2	1.85	0.41
1:A:428:ASN:ND2	1:A:462:THR:HG21	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:123:MET:HE1	1:A:675:MET:HE1	2.02	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

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%)	1	6
2	B	237/373 (64%)	215 (91%)	15 (6%)	7 (3%)	3	12
All	All	1257/1464 (86%)	1095 (87%)	105 (8%)	57 (4%)	2	7

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
1	A	793	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
2	B	417	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	828 (88%)	117 (12%)	4 16
2	B	229/342 (67%)	214 (93%)	15 (7%)	15 43
All	All	1174/1337 (88%)	1042 (89%)	132 (11%)	6 19

All (132) 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	22	VAL
1	A	31	ILE
1	A	32	VAL
1	A	38	ARG
1	A	43	ILE
1	A	52	GLU
1	A	60	GLN
1	A	69	ILE
1	A	71	VAL
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	125	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	131	VAL
1	A	137	GLN
1	A	153	LEU
1	A	171	VAL
1	A	173	SER
1	A	187	LYS
1	A	198	VAL
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	278	MET
1	A	287	LEU
1	A	293	LEU
1	A	300	ASP
1	A	303	THR
1	A	322	THR
1	A	323	SER
1	A	329	VAL
1	A	347	ASN
1	A	367	LEU
1	A	368	CYS
1	A	376	VAL
1	A	390	ASP
1	A	441	MET
1	A	452	LEU
1	A	453	GLU
1	A	459	ILE
1	A	462	THR
1	A	488	ASP
1	A	491	VAL
1	A	494	GLU
1	A	516	ARG
1	A	528	LYS
1	A	529	GLU
1	A	530	GLN
1	A	531	LEU
1	A	535	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	542	GLU
1	A	559	VAL
1	A	564	ILE
1	A	610	MET
1	A	619	LEU
1	A	627	LYS
1	A	630	GLN
1	A	638	VAL
1	A	642	GLU
1	A	650	VAL
1	A	656	LYS
1	A	672	LYS
1	A	677	ASN
1	A	680	VAL
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	745	MET
1	A	748	LEU
1	A	766	LEU
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	867	LYS
1	A	871	GLN
1	A	873	ASN
1	A	877	LEU
1	A	888	GLU
1	A	889	ILE
1	A	899	ARG
1	A	908	THR
1	A	920	ASN
1	A	924	LYS
1	A	932	ILE
1	A	937	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	938	LEU
1	A	955	VAL
1	A	972	THR
1	A	976	GLU
1	A	983	MET
1	A	997	LEU
1	A	1006	LEU
1	A	1010	MET
1	A	1017	ASP
1	A	1018	ASP
1	A	1052	THR
1	A	1055	MET
2	B	371	THR
2	B	404	LEU
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	552	GLN
2	B	565	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-23	HIS
1	A	14	HIS
1	A	60	GLN
1	A	75	GLN
1	A	137	GLN
1	A	145	ASN
1	A	157	ASN
1	A	213	HIS
1	A	247	GLN
1	A	284	ASN
1	A	331	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	345	ASN
1	A	347	ASN
1	A	374	GLN
1	A	380	ASN
1	A	388	ASN
1	A	428	ASN
1	A	444	ASN
1	A	467	ASN
1	A	515	ASN
1	A	605	ASN
1	A	630	GLN
1	A	643	GLN
1	A	647	ASN
1	A	677	ASN
1	A	682	GLN
1	A	701	HIS
1	A	703	ASN
1	A	756	ASN
1	A	763	ASN
1	A	785	ASN
1	A	871	GLN
1	A	917	HIS
1	A	920	ASN
1	A	1014	GLN
1	A	1042	GLN
1	A	1048	HIS
2	B	478	GLN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	32,35,35	12.00	7 (21%)	35,57,57	6.89	16 (45%)

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	O5-C19	66.07	2.57	1.37
3	A	1833	KWT	C8-C7	9.45	1.54	1.35
3	A	1833	KWT	O6-C21	6.69	1.50	1.35
3	A	1833	KWT	C11-C8	5.85	1.57	1.51
3	A	1833	KWT	O1-C2	5.66	1.45	1.35
3	A	1833	KWT	O5-C5	-3.10	1.33	1.38
3	A	1833	KWT	C19-C3	-2.53	1.32	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1833	KWT	O5-C19-C3	-27.43	83.20	111.19
3	A	1833	KWT	C19-O5-C5	-18.85	87.33	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1833	KWT	O5-C5-C4	17.81	121.02	110.22
3	A	1833	KWT	O6-C21-C22	7.58	124.61	111.09
3	A	1833	KWT	C15-C7-C8	-5.71	108.34	121.58
3	A	1833	KWT	C11-O6-C21	5.56	125.25	117.00
3	A	1833	KWT	C17-C18-C13	4.73	113.26	108.56
3	A	1833	KWT	C11-C8-C7	-3.55	114.35	121.14
3	A	1833	KWT	C16-C17-C18	-3.15	102.66	105.70
3	A	1833	KWT	O6-C21-O7	-2.89	117.41	122.99
3	A	1833	KWT	C9-C4-C3	-2.83	118.31	124.61
3	A	1833	KWT	C4-C5-C6	-2.76	120.39	124.57
3	A	1833	KWT	O1-C1-C23	2.71	113.17	107.26
3	A	1833	KWT	O4-C18-C13	-2.51	122.69	125.98
3	A	1833	KWT	C14-C13-C18	2.19	109.22	105.18
3	A	1833	KWT	C10-C9-C4	-2.00	106.49	109.13

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

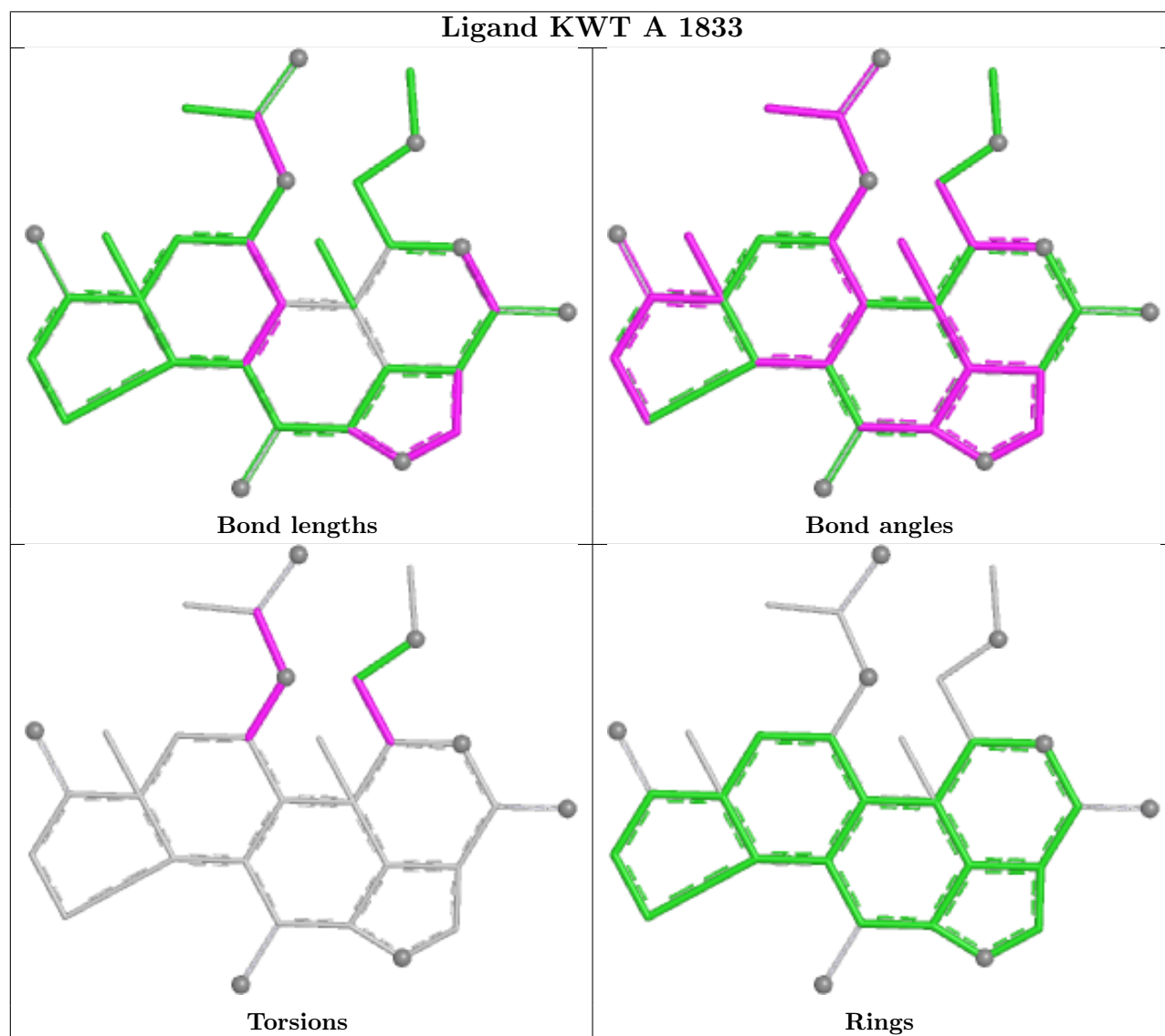
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1833	KWT	6	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 than 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.



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	1032/1091 (94%)	0.63	102 (9%) 13 9	35, 60, 84, 101	0
2	B	247/373 (66%)	1.21	37 (14%) 5 4	62, 89, 117, 131	0
All	All	1279/1464 (87%)	0.74	139 (10%) 10 8	35, 64, 98, 131	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	792	LEU	7.9
2	B	445	VAL	6.0
1	A	791	GLU	5.6
1	A	408	SER	5.4
2	B	362	THR	5.2
1	A	865	GLY	5.2
2	B	436	VAL	5.1
1	A	953	PRO	5.1
1	A	794	PHE	5.1
1	A	5	PRO	5.0
1	A	866	LEU	5.0
1	A	158	SER	4.5
1	A	377	PRO	4.5
2	B	361	SER	4.4
1	A	365	GLU	4.4
2	B	512	PHE	4.3
2	B	437	VAL	4.3
2	B	326	MET	4.2
1	A	513	LEU	4.2
1	A	351	ILE	4.2
2	B	438	LYS	4.0
1	A	723	LYS	4.0
1	A	366	PRO	3.9
2	B	444	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	446	GLY	3.9
1	A	1055	MET	3.8
1	A	350	ASP	3.6
1	A	363	GLY	3.6
1	A	299	MET	3.6
1	A	494	GLU	3.6
1	A	375	ARG	3.5
1	A	130	MET	3.5
1	A	1052	THR	3.5
1	A	968	ALA	3.5
1	A	108	ARG	3.3
1	A	508	TYR	3.3
1	A	1054	LYS	3.3
1	A	409	VAL	3.3
2	B	440	ASP	3.2
1	A	481	SER	3.2
2	B	514	ARG	3.1
2	B	450	HIS	3.1
2	B	515	GLU	3.1
1	A	937	PHE	3.0
1	A	915	ASP	3.0
1	A	110	GLU	3.0
1	A	509	SER	3.0
2	B	447	LYS	3.0
1	A	972	THR	2.9
1	A	872	PHE	2.9
1	A	533	ALA	2.9
1	A	364	GLY	2.8
2	B	431	TYR	2.8
1	A	490	SER	2.8
2	B	428	VAL	2.8
1	A	352	ASP	2.8
1	A	328	TRP	2.8
2	B	396	LEU	2.8
1	A	532	LYS	2.8
1	A	955	VAL	2.7
2	B	452	TYR	2.7
1	A	6	SER	2.7
1	A	348	ILE	2.7
1	A	361	TYR	2.7
2	B	463	TYR	2.7
1	A	8	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	353	GLY	2.7
2	B	454	THR	2.7
1	A	7	SER	2.7
1	A	172	GLU	2.7
1	A	431	ASP	2.7
2	B	513	LYS	2.6
1	A	557	TYR	2.6
1	A	618	CYS	2.6
1	A	516	ARG	2.6
1	A	-26	TYR	2.6
1	A	-17	TYR	2.6
1	A	722	GLU	2.6
1	A	954	PHE	2.5
1	A	1053	THR	2.5
1	A	531	LEU	2.5
1	A	534	ILE	2.5
2	B	336	GLY	2.5
2	B	573	LEU	2.5
1	A	970	GLU	2.5
1	A	796	ASN	2.5
1	A	920	ASN	2.4
1	A	186	ASP	2.4
2	B	576	THR	2.4
1	A	64	ASP	2.4
1	A	864	GLY	2.4
1	A	105	VAL	2.4
2	B	543	ARG	2.4
2	B	579	GLN	2.4
1	A	1062	ILE	2.4
1	A	200	PRO	2.4
1	A	-18	ASP	2.3
1	A	91	ASP	2.3
1	A	300	ASP	2.3
1	A	407	CYS	2.3
2	B	366	GLY	2.3
1	A	1029	ASP	2.3
2	B	363	LYS	2.3
1	A	510	HIS	2.3
1	A	936	HIS	2.3
1	A	278	MET	2.3
1	A	869	ALA	2.3
1	A	542	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	413	LYS	2.2
1	A	967	GLY	2.2
1	A	9	GLU	2.2
1	A	384	ASN	2.2
2	B	571	ILE	2.2
1	A	1051	TRP	2.2
1	A	93	ARG	2.2
2	B	499	GLN	2.2
1	A	421	PRO	2.2
2	B	397	THR	2.2
1	A	199	SER	2.2
1	A	938	LEU	2.2
1	A	511	ALA	2.2
1	A	112	ILE	2.1
2	B	567	LYS	2.1
1	A	298	PRO	2.1
1	A	156	LEU	2.1
1	A	279	LEU	2.1
2	B	456	PHE	2.1
1	A	1027	ALA	2.1
2	B	525	MET	2.1
1	A	369	ASP	2.1
1	A	868	GLY	2.1
1	A	176	GLU	2.1
1	A	410	LYS	2.0
2	B	380	LEU	2.0
1	A	867	LYS	2.0
1	A	30	MET	2.0
1	A	-24	HIS	2.0
1	A	940	HIS	2.0
1	A	159	PRO	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](#)

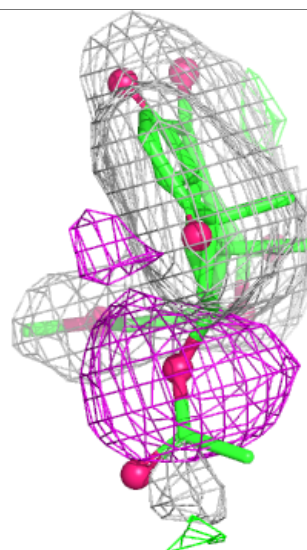
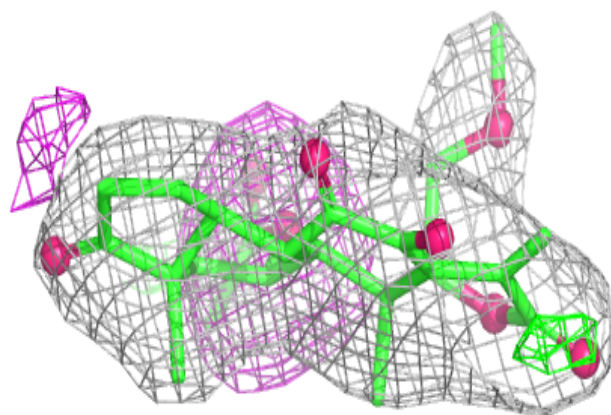
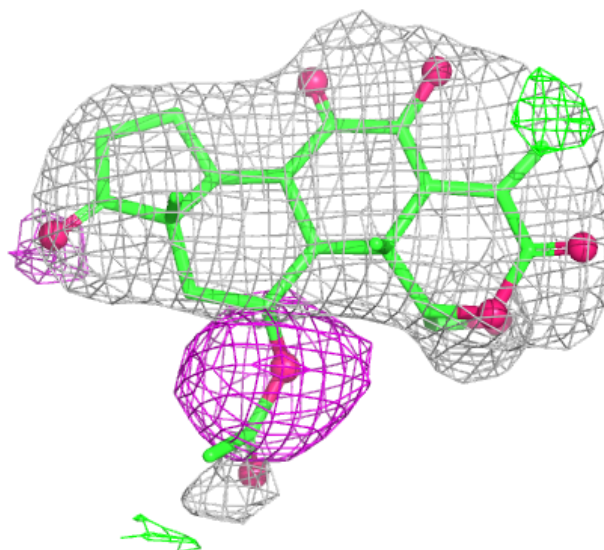
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	KWT	A	1833	31/31	0.86	0.18	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 [i](#)

There are no such residues in this entry.