



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:10 AM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

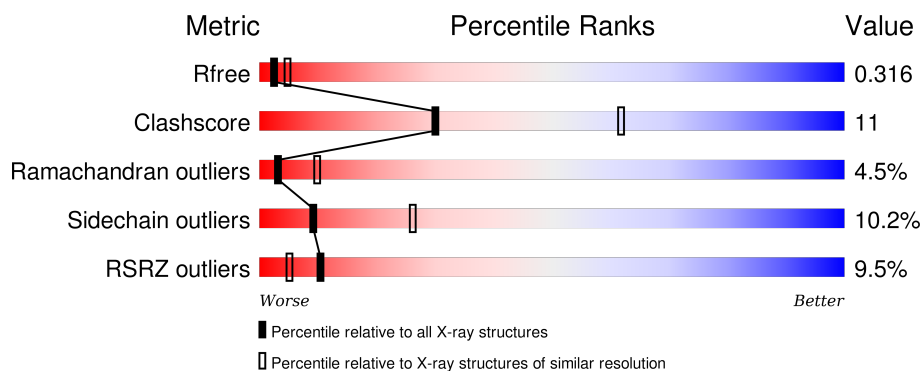
1 Overall quality at a glance

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
2	B	373	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	KWT	A	1833	-	-	-	X

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	UNP P42336

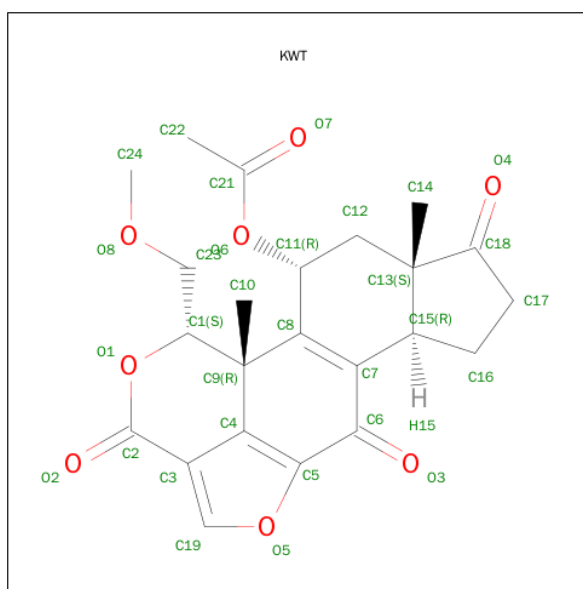
- Molecule 2 is a protein called niSH2 p85alpha.

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	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: C₂₃H₂₄O₈).



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

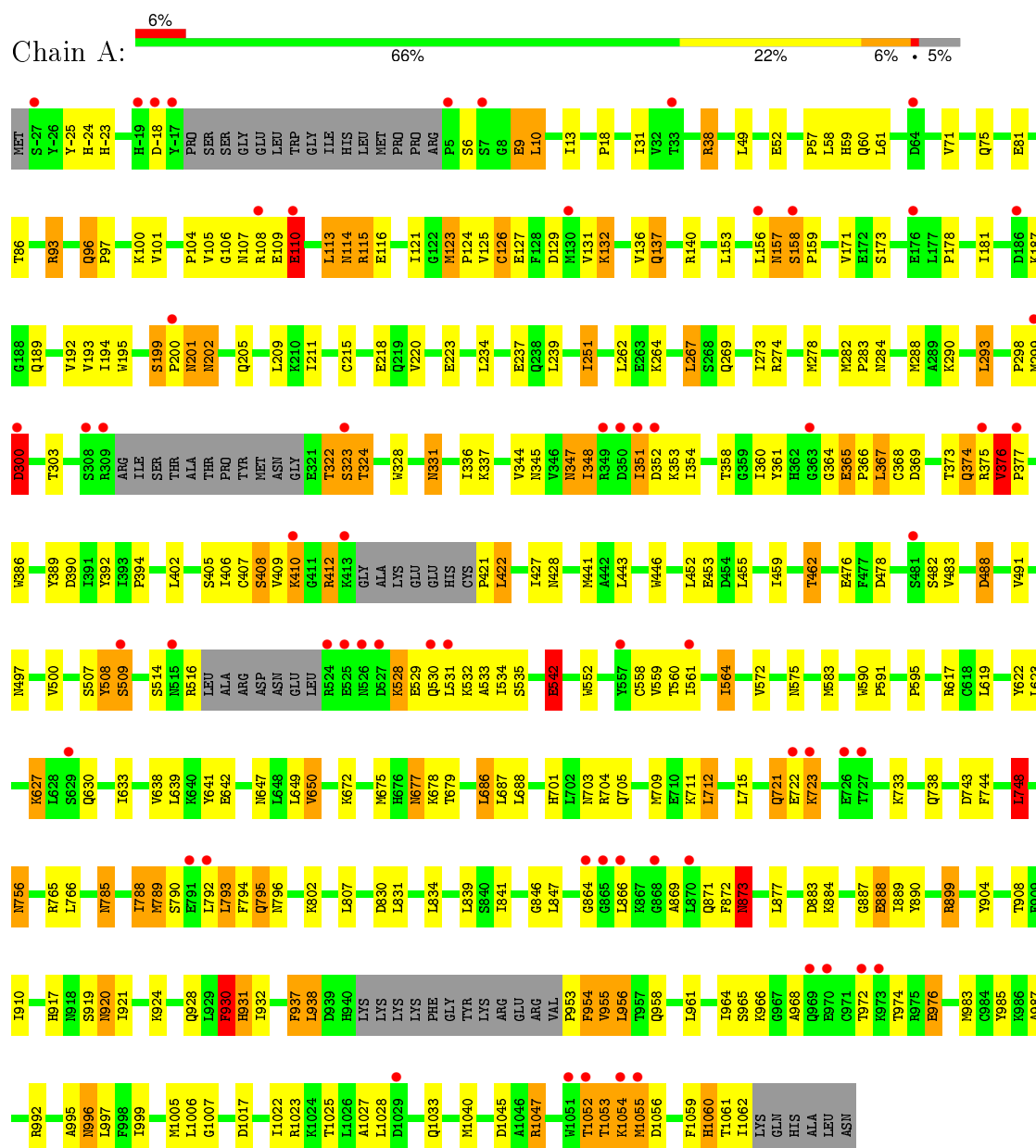
- Molecule 4 is water.

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

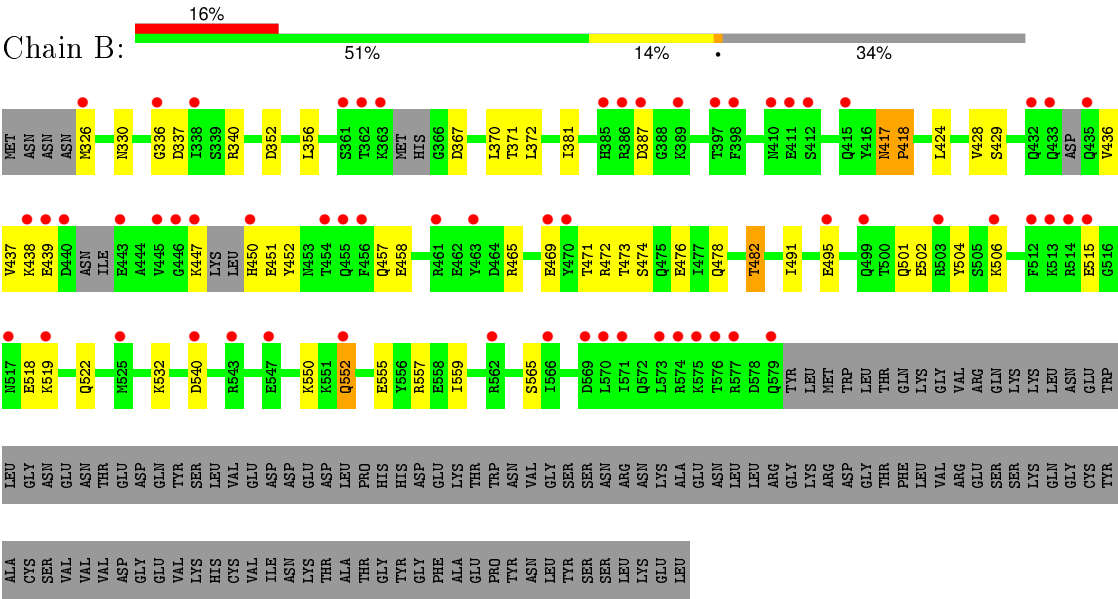
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 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
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.307 0.250 , 0.316	Depositor DCC
R_{free} test set	2678 reflections (5.30%)	DCC
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 , 44.1	EDS
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 53236 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.44	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($^{\circ}$)	Ideal($^{\circ}$)
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:364:GLY:C	1:A:365:GLU:HG3	2.21	0.61
1:A:351:ILE:C	1:A:353:LYS:H	2.01	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:995:ALA:O	1:A:996:ASN:CB	2.50	0.59
1:A:337:LYS:HB3	1:A:476:GLU:HB3	1.85	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: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:HG2	1:A:529:GLU:O	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:558:CYS:C	1:A:560:THR:H	2.12	0.53
1:A:209:LEU:HD13	1:A:223:GLU:HB3	1.90	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:796:ASN:ND2	4:A:1092:HOH:O	2.44	0.50
1:A:278:MET:HA	1:A:278:MET:HE3	1.94	0.50
1:A:178:PRO:HG2	1:A:181:ILE:HD12	1.93	0.50
1:A:9:GLU:OE2	1:A:38:ARG:NH1	2.45	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:701:HIS:CD2	1:A:704:ARG:HH21	2.31	0.49
1:A:533:ALA:N	4:A:1117:HOH:O	2.45	0.49
1:A:872:PHE:O	1:A:873:ASN:CB	2.56	0.48
1:A:802:LYS:HZ1	3:A:1833:KWT:C19	2.26	0.48
1:A:123:MET:HE2	1:A:675:MET:CE	2.42	0.48
3:A:1833:KWT:O5	3:A:1833:KWT:C19	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:1056:ASP:OD2	1:A:1061:THR:CB	2.64	0.45
1:A:617:ARG:NH2	4:A:1174:HOH:O	2.49	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:709:MET:CE	1:A:841:ILE:HD13	2.47	0.45
1:A:126:CYS:HA	1:A:129:ASP:CG	2.37	0.45
1:A:251:ILE:HG22	1:A:288:MET:HB3	1.99	0.44
1:A:677:ASN:C	1:A:677:ASN:ND2	2.69	0.44
1:A:595:PRO:HG3	1:A:622:TYR:HB2	1.99	0.44
1:A:116:GLU:HB3	1:A:703:ASN:HD21	1.81	0.44
1:A:641:TYR:OH	1:A:1007:GLY:N	2.50	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:HB2	1:A:93:ARG:HH11	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:709:MET:HE3	1:A:841:ILE:HD13	2.00	0.43
1:A:376:VAL:HG23	1:A:377:PRO:C	2.38	0.43
1:A:324:THR:HA	1:A:483:VAL:O	2.17	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: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:788:ILE:H	1:A:788:ILE:HG13	1.55	0.43
1:A:937:PHE:HB3	1:A:938:LEU:HG	2.00	0.43
1:A:376:VAL:HG22	1:A:376:VAL:O	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:407:CYS:HB2	1:A:408:SER:H	1.63	0.42
1:A:278:MET:HA	1:A:278:MET:HE2	1.98	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:361:TYR:CD2	1:A:365:GLU:HB3	2.54	0.42
1:A:344:VAL:HG21	1:A:422:LEU:HD13	2.00	0.42
1:A:124:PRO:HG2	1:A:127:GLU:HG3	2.01	0.42
1:A:924:LYS:HE3	1:A:928:GLN:HB3	2.01	0.42
1:A:121:ILE:HG12	1:A:688:LEU: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:211:ILE:HG13	1:A:215:CYS:SG	2.60	0.41
1:A:192:VAL:HG13	1:A:283:PRO:HB2	2.02	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:328:TRP:CB	1:A:394:PRO:HB3	2.50	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:361:TYR:CG	1:A:365:GLU:HB3	2.55	0.41
1:A:158:SER:HB3	1:A:159:PRO:CD	2.51	0.41
1:A:956:LEU:HD23	1:A:956:LEU:HA	1.90	0.41
1:A:1054:LYS:CG	1:A:1055:MET:N	2.83	0.41
1:A:269:GLN:HA	1:A:274:ARG:NH2	2.35	0.41
1:A:328:TRP:HB2	1:A:394:PRO:HB3	2.03	0.41
1:A:49:LEU:HD21	1:A:101:VAL:HG21	2.02	0.41
2:B:518:GLU:O	2:B:519:LYS:HB2	2.21	0.41
1:A:792:LEU:O	1:A:793:LEU:CB	2.68	0.41
1:A:712:LEU:HD13	1:A:748:LEU:HD11	2.03	0.41
2:B:473:THR:HG23	2:B:552:GLN:NE2	2.36	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:H	1:A:412:ARG:HD2	1.86	0.40
1:A:1053:THR:O	1:A:1054:LYS:C	2.60	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%)	3	8
2	B	237/373 (64%)	215 (91%)	15 (6%)	7 (3%)	5	18
All	All	1257/1464 (86%)	1095 (87%)	105 (8%)	57 (4%)	3	10

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%)	8	24
2	B	229/342 (67%)	209 (91%)	20 (9%)	13	35
All	All	1174/1337 (88%)	1054 (90%)	120 (10%)	9	26

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

Some 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 carbohydrates 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	-	28,35,35	2.93	5 (17%)	26,57,57	4.05	11 (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	-	-	0/7/75/75	0/4/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1833	KWT	C19-C3	-3.90	1.32	1.37
3	A	1833	KWT	O6-C21	6.36	1.50	1.35
3	A	1833	KWT	O1-C2	6.97	1.45	1.35
3	A	1833	KWT	C3-C4	7.03	1.46	1.38
3	A	1833	KWT	C8-C7	8.22	1.54	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1833	KWT	C9-C8-C7	-7.20	109.87	122.90
3	A	1833	KWT	C16-C17-C18	-2.88	102.66	105.65
3	A	1833	KWT	O6-C21-O7	-2.76	117.41	122.92
3	A	1833	KWT	C5-C6-C7	-2.45	116.67	118.14
3	A	1833	KWT	O4-C18-C13	-2.19	122.69	125.93
3	A	1833	KWT	O1-C2-O2	2.00	120.28	117.66
3	A	1833	KWT	C17-C18-C13	4.67	113.26	108.64
3	A	1833	KWT	C11-O6-C21	5.02	125.25	117.14
3	A	1833	KWT	O6-C21-C22	7.16	124.61	111.10
3	A	1833	KWT	C19-C3-C4	9.80	123.07	111.31
3	A	1833	KWT	C3-C4-C5	11.28	118.84	108.01

There are no chirality outliers.

There are no torsion outliers.

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

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(Å ²)	Q<0.9
1	A	1032/1091 (94%)	0.46	62 (6%) 25 15	35, 60, 84, 101	0
2	B	247/373 (66%)	1.37	60 (24%) 1 0	62, 89, 117, 131	0
All	All	1279/1464 (87%)	0.64	122 (9%) 10 5	35, 64, 98, 131	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	445	VAL	8.7
2	B	579	GLN	7.6
1	A	866	LEU	7.4
2	B	362	THR	6.3
2	B	326	MET	6.0
1	A	792	LEU	5.8
2	B	361	SER	5.6
1	A	723	LYS	5.2
2	B	512	PHE	5.0
2	B	576	THR	5.0
2	B	410	ASN	4.7
1	A	350	ASP	4.7
2	B	397	THR	4.6
2	B	415	GLN	4.6
1	A	865	GLY	4.5
2	B	575	LYS	4.4
1	A	186	ASP	4.4
1	A	375	ARG	4.3
2	B	447	LYS	4.2
1	A	158	SER	4.2
2	B	454	THR	4.2
1	A	300	ASP	4.1
2	B	440	ASP	4.0
2	B	456	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	514	ARG	3.9
1	A	-27	SER	3.9
1	A	-18	ASP	3.9
1	A	299	MET	3.8
2	B	433	GLN	3.8
1	A	524	ARG	3.8
2	B	435	GLN	3.8
1	A	791	GLU	3.7
2	B	469	GLU	3.7
2	B	515	GLU	3.7
1	A	1052	THR	3.6
1	A	413	LYS	3.5
2	B	387	ASP	3.5
2	B	363	LYS	3.5
1	A	557	TYR	3.4
1	A	972	THR	3.4
1	A	309	ARG	3.4
1	A	525	GLU	3.4
1	A	5	PRO	3.3
1	A	1054	LYS	3.3
2	B	463	TYR	3.3
1	A	722	GLU	3.3
2	B	438	LYS	3.2
2	B	443	GLU	3.2
1	A	969	GLN	3.1
2	B	389	LYS	3.1
2	B	411	GLU	3.1
1	A	1055	MET	3.0
1	A	531	LEU	3.0
2	B	569	ASP	3.0
2	B	525	MET	3.0
1	A	352	ASP	2.9
1	A	868	GLY	2.9
2	B	446	GLY	2.9
1	A	377	PRO	2.9
2	B	450	HIS	2.9
1	A	200	PRO	2.8
2	B	385	HIS	2.8
2	B	543	ARG	2.8
1	A	864	GLY	2.8
2	B	432	GLN	2.8
1	A	323	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	351	ILE	2.7
2	B	574	ARG	2.6
2	B	519	LYS	2.6
1	A	410	LYS	2.6
2	B	470	TYR	2.6
2	B	517	ASN	2.6
2	B	506	LYS	2.6
2	B	439	GLU	2.6
2	B	562	ARG	2.5
2	B	573	LEU	2.5
2	B	461	ARG	2.5
2	B	547	GLU	2.5
1	A	156	LEU	2.5
1	A	363	GLY	2.5
2	B	386	ARG	2.5
1	A	349	ARG	2.4
1	A	110	GLU	2.4
1	A	970	GLU	2.4
1	A	481	SER	2.4
1	A	527	ASP	2.4
2	B	570	LEU	2.4
2	B	455	GLN	2.4
1	A	526	ASN	2.4
1	A	1051	TRP	2.4
1	A	64	ASP	2.4
2	B	412	SER	2.3
1	A	308	SER	2.3
2	B	495	GLU	2.3
1	A	130	MET	2.3
2	B	577	ARG	2.3
1	A	726	GLU	2.3
2	B	499	GLN	2.3
1	A	530	GLN	2.2
1	A	-19	HIS	2.2
1	A	515	ASN	2.2
2	B	338	ILE	2.2
1	A	727	THR	2.2
2	B	336	GLY	2.2
2	B	503	ARG	2.1
1	A	176	GLU	2.1
2	B	566	ILE	2.1
1	A	-17	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	513	LYS	2.1
2	B	571	ILE	2.1
1	A	870	LEU	2.1
2	B	398	PHE	2.1
1	A	33	THR	2.1
1	A	973	LYS	2.1
2	B	540	ASP	2.1
1	A	629	SER	2.1
2	B	552	GLN	2.1
1	A	108	ARG	2.0
1	A	7	SER	2.0
1	A	509	SER	2.0
1	A	1029	ASP	2.0
1	A	561	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	KWT	A	1833	31/31	0.86	0.32	2.24	57,61,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.