



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:35 PM UTC

PDB ID : 2AC5 / pdb_00002ac5
Title : Structure of human Mnk2 Kinase Domain mutant D228G
Authors : Jauch, R.; Wahl, M.C.; Jakel, S.; Schreiter, K.; Aicher, B.; Jackle, H.
Deposited on : 2005-07-18
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

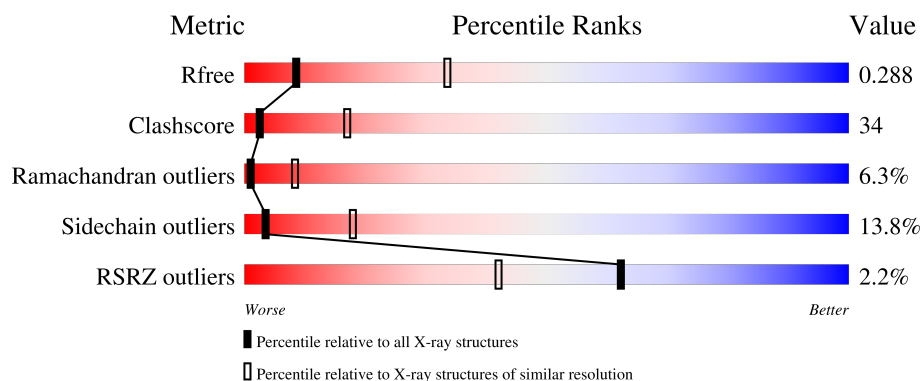
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	316	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2260 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 MAP kinase-interacting serine/threonine kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	5	0
			2241	1421	387	417	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	GLY	-	expression tag	UNP Q9HBH9
A	71	SER	-	expression tag	UNP Q9HBH9
A	228	GLY	ASP	engineered mutation	UNP Q9HBH9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.65Å 104.65Å 73.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-3.20) 98.1 (30.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.22Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.306 0.235 , 0.288	Depositor DCC
R_{free} test set	401 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	93.6	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2260	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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: ZN

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	0.55	0/2291	1.08	16/3090 (0.5%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	ARG	N-CA-C	-7.42	100.70	110.43
1	A	316	ASN	N-CA-C	-7.38	103.31	111.36
1	A	158	VAL	N-CA-C	6.66	118.12	107.73
1	A	300	GLY	N-CA-C	-5.97	106.79	114.85
1	A	253	SER	N-CA-C	-5.92	106.30	112.93
1	A	88	ASP	N-CA-C	5.82	123.19	110.80
1	A	267	GLU	N-CA-C	-5.78	104.89	111.07
1	A	200	GLY	N-CA-C	5.40	122.54	115.47
1	A	358	SER	N-CA-C	-5.38	102.55	110.52
1	A	328	GLU	N-CA-C	5.28	122.04	110.80
1	A	118	GLN	CA-C-N	5.17	126.30	119.84
1	A	118	GLN	C-N-CA	5.17	126.30	119.84
1	A	340	ALA	N-CA-C	-5.15	105.75	111.36
1	A	190	ALA	N-CA-C	-5.10	105.80	111.36
1	A	81	ASP	N-CA-C	-5.08	106.34	112.54
1	A	114	ILE	CB-CA-C	-5.01	106.24	112.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2241	0	2164	152	0
2	A	1	0	0	0	0
3	A	18	0	0	0	0
All	All	2260	0	2164	152	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 34.

All (152) 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:332:LYS:HD3	1:A:332:LYS:H	1.19	1.05
1:A:178:ASN:ND2	1:A:180:LEU:H	1.62	0.97
1:A:178:ASN:HD22	1:A:180:LEU:H	1.08	0.96
1:A:334:TRP:HA	1:A:337:ILE:HD12	1.49	0.93
1:A:365:HIS:HD2	1:A:367:TRP:H	1.22	0.87
1:A:178:ASN:HD22	1:A:178:ASN:C	1.84	0.86
1:A:105:ILE:HG13	1:A:106:THR:HG23	1.61	0.83
1:A:203:HIS:CE1	1:A:226[A]:ASP:HB3	2.17	0.79
1:A:117:LYS:HD2	1:A:152:GLU:O	1.84	0.78
1:A:332:LYS:H	1:A:332:LYS:CD	1.94	0.75
1:A:212:LEU:HD21	1:A:225[B]:CYS:SG	2.26	0.74
1:A:365:HIS:CD2	1:A:367:TRP:H	2.05	0.73
1:A:321:SER:OG	1:A:326:LYS:HE3	1.88	0.72
1:A:178:ASN:HD22	1:A:180:LEU:N	1.84	0.72
1:A:280:SER:O	1:A:284:ILE:HG12	1.88	0.72
1:A:258:ALA:HB3	1:A:261:VAL:HG23	1.72	0.71
1:A:83:TYR:HA	1:A:102:ILE:O	1.94	0.68
1:A:178:ASN:ND2	1:A:178:ASN:C	2.52	0.68
1:A:85:LEU:HD23	1:A:86:GLN:H	1.60	0.66
1:A:170:HIS:HB3	1:A:177:PHE:HZ	1.59	0.66
1:A:258:ALA:O	1:A:262:VAL:HG12	1.96	0.66
1:A:325:GLY:H	1:A:351:ARG:HD3	1.59	0.66
1:A:178:ASN:ND2	1:A:180:LEU:N	2.40	0.65
1:A:284:ILE:O	1:A:288:LEU:HD22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLU:O	1:A:326:LYS:N	2.29	0.65
1:A:226[B]:ASP:O	1:A:227[B]:PHE:HB2	1.97	0.64
1:A:121:HIS:HE1	1:A:123:ARG:HB3	1.61	0.63
1:A:70:GLY:O	1:A:71:SER:HB2	1.98	0.63
1:A:146:ILE:HB	1:A:158:VAL:O	1.99	0.62
1:A:181:GLU:O	1:A:184:VAL:HG12	2.00	0.62
1:A:303:CYS:HB2	1:A:305:TRP:CD1	2.36	0.61
1:A:343:ASP:OD2	1:A:365:HIS:HE1	1.83	0.61
1:A:79:PHE:O	1:A:82:VAL:O	2.20	0.60
1:A:364:GLN:HE21	1:A:364:GLN:HA	1.65	0.60
1:A:150:GLU:HB2	1:A:155:PHE:CE2	2.38	0.59
1:A:334:TRP:HB3	1:A:342:LYS:HE2	1.84	0.58
1:A:114:ILE:HD12	1:A:114:ILE:N	2.19	0.58
1:A:139:HIS:HD2	1:A:141:ASN:HB2	1.68	0.58
1:A:257:MET:HE3	1:A:261:VAL:HG12	1.85	0.58
1:A:311:CYS:HB3	1:A:314:CYS:HB2	1.87	0.57
1:A:330:PRO:HB3	1:A:332:LYS:HE2	1.85	0.57
1:A:267:GLU:C	1:A:269:ALA:H	2.12	0.56
1:A:121:HIS:CE1	1:A:123:ARG:HB3	2.39	0.56
1:A:139:HIS:CD2	1:A:141:ASN:HB2	2.41	0.56
1:A:123:ARG:NH2	1:A:150:GLU:OE2	2.39	0.55
1:A:360:ALA:O	1:A:364:GLN:HG2	2.07	0.55
1:A:183:SER:HA	1:A:367:TRP:CZ3	2.42	0.55
1:A:285:LEU:HA	1:A:288:LEU:HD23	1.88	0.55
1:A:334:TRP:HA	1:A:337:ILE:CD1	2.31	0.55
1:A:278:LEU:HD12	1:A:362:VAL:HG21	1.89	0.54
1:A:126:VAL:O	1:A:130:VAL:HG23	2.07	0.54
1:A:174:ARG:HH22	1:A:181:GLU:CD	2.16	0.54
1:A:365:HIS:CD2	1:A:366:PRO:HD2	2.43	0.54
1:A:100:THR:HG22	1:A:101:CYS:N	2.23	0.54
1:A:103:ASN:ND2	1:A:106:THR:H	2.05	0.53
1:A:218:GLN:HG2	1:A:220:SER:O	2.09	0.53
1:A:272:TYR:CE1	1:A:354:LYS:HG2	2.43	0.53
1:A:83:TYR:HB3	1:A:101:CYS:HB2	1.90	0.52
1:A:347:LYS:HB3	1:A:357:LEU:CD1	2.39	0.52
1:A:203:HIS:NE2	1:A:226[A]:ASP:HB3	2.23	0.52
1:A:347:LYS:O	1:A:357:LEU:HD13	2.09	0.52
1:A:328:GLU:C	1:A:330:PRO:HD3	2.36	0.51
1:A:365:HIS:HD2	1:A:367:TRP:N	2.00	0.51
1:A:279:TRP:C	1:A:279:TRP:CD1	2.88	0.50
1:A:294:PRO:HG2	1:A:295:PHE:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ARG:C	1:A:125:ARG:H	2.19	0.50
1:A:170:HIS:HB3	1:A:177:PHE:CZ	2.44	0.50
1:A:186:VAL:HG21	1:A:285:LEU:HD22	1.93	0.50
1:A:226[B]:ASP:O	1:A:227[B]:PHE:CB	2.60	0.50
1:A:290:SER:HB3	1:A:334:TRP:CE2	2.47	0.50
1:A:326:LYS:HG3	1:A:327:TYR:H	1.75	0.49
1:A:334:TRP:CA	1:A:337:ILE:HD12	2.32	0.49
1:A:122:ILE:O	1:A:125:ARG:HB2	2.12	0.49
1:A:278:LEU:HG	1:A:357:LEU:O	2.13	0.49
1:A:215:HIS:HB2	1:A:218:GLN:HB3	1.94	0.48
1:A:103:ASN:HD21	1:A:105:ILE:HG12	1.77	0.48
1:A:290:SER:HB2	1:A:292:TYR:CE1	2.49	0.48
1:A:284:ILE:C	1:A:288:LEU:HD22	2.38	0.48
1:A:258:ALA:HB1	1:A:260:GLU:OE1	2.13	0.48
1:A:111:ALA:HB2	1:A:161:LYS:HD3	1.96	0.48
1:A:116:GLU:OE1	1:A:154:ARG:NE	2.47	0.48
1:A:267:GLU:O	1:A:269:ALA:N	2.47	0.47
1:A:347:LYS:HB3	1:A:357:LEU:HD13	1.97	0.47
1:A:114:ILE:O	1:A:114:ILE:HG22	2.14	0.47
1:A:78:ARG:O	1:A:79:PHE:C	2.56	0.47
1:A:139:HIS:HB3	1:A:142:VAL:HG23	1.97	0.47
1:A:225[A]:CYS:O	1:A:226[A]:ASP:CB	2.63	0.47
1:A:260:GLU:HG2	1:A:261:VAL:N	2.30	0.47
1:A:122:ILE:O	1:A:122:ILE:HG23	2.15	0.47
1:A:358:SER:H	1:A:361:GLN:HB2	1.80	0.47
1:A:82:VAL:O	1:A:83:TYR:O	2.33	0.46
1:A:285:LEU:HD12	1:A:285:LEU:O	2.15	0.46
1:A:98:VAL:HA	1:A:112:VAL:O	2.16	0.46
1:A:100:THR:HG23	1:A:161:LYS:HE3	1.98	0.46
1:A:129:GLU:O	1:A:133:LEU:HG	2.16	0.46
1:A:285:LEU:HA	1:A:288:LEU:CD2	2.45	0.46
1:A:147:GLU:HG2	1:A:148:PHE:H	1.81	0.46
1:A:259:PRO:HA	1:A:262:VAL:CG1	2.45	0.46
1:A:290:SER:HB3	1:A:334:TRP:CZ2	2.51	0.46
1:A:174:ARG:NH2	1:A:181:GLU:OE1	2.48	0.46
1:A:141:ASN:ND2	1:A:188:ASP:OD1	2.42	0.45
1:A:326:LYS:O	1:A:327:TYR:HB2	2.17	0.45
1:A:258:ALA:HB3	1:A:261:VAL:CG2	2.46	0.45
1:A:70:GLY:O	1:A:71:SER:CB	2.62	0.44
1:A:364:GLN:HA	1:A:364:GLN:NE2	2.31	0.44
1:A:168:LEU:HD13	1:A:208:PRO:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:VAL:HG13	1:A:185:VAL:N	2.32	0.44
1:A:199:LYS:HB2	1:A:199:LYS:HE3	1.71	0.44
1:A:267:GLU:C	1:A:269:ALA:N	2.75	0.44
1:A:318:LEU:O	1:A:322:ILE:HG13	2.17	0.44
1:A:121:HIS:O	1:A:122:ILE:C	2.60	0.44
1:A:102:ILE:HG23	1:A:107:SER:O	2.17	0.44
1:A:224[A]:ILE:O	1:A:225[A]:CYS:HB3	2.17	0.44
1:A:78:ARG:HD2	1:A:78:ARG:HA	1.83	0.43
1:A:72:THR:O	1:A:72:THR:HG23	2.17	0.43
1:A:164:GLY:HA2	1:A:216:PRO:HA	2.01	0.43
1:A:344:LEU:O	1:A:345:ILE:C	2.60	0.43
1:A:174:ARG:NH2	1:A:181:GLU:OE2	2.46	0.43
1:A:225[A]:CYS:O	1:A:226[A]:ASP:HB2	2.18	0.43
1:A:204:ARG:NH2	1:A:204:ARG:HG2	2.33	0.43
1:A:303:CYS:HB2	1:A:305:TRP:HD1	1.83	0.43
1:A:123:ARG:C	1:A:125:ARG:N	2.76	0.42
1:A:256:TYR:CD2	1:A:256:TYR:N	2.87	0.42
1:A:178:ASN:ND2	1:A:181:GLU:H	2.17	0.42
1:A:131:GLU:O	1:A:134:TYR:HB3	2.19	0.42
1:A:132:MET:O	1:A:133:LEU:C	2.63	0.42
1:A:263:GLU:O	1:A:263:GLU:HG2	2.20	0.42
1:A:341:ALA:C	1:A:343:ASP:N	2.77	0.42
1:A:364:GLN:HE21	1:A:364:GLN:CA	2.29	0.42
1:A:86:GLN:OE1	1:A:102:ILE:HG12	2.20	0.42
1:A:343:ASP:OD2	1:A:347:LYS:HD2	2.20	0.42
1:A:334:TRP:O	1:A:335:ALA:C	2.63	0.42
1:A:118:GLN:O	1:A:119:PRO:C	2.63	0.41
1:A:100:THR:HG21	1:A:109:GLU:OE1	2.20	0.41
1:A:259:PRO:HA	1:A:262:VAL:HG12	2.01	0.41
1:A:343:ASP:OD2	1:A:365:HIS:CE1	2.69	0.41
1:A:102:ILE:HD13	1:A:109:GLU:HG2	2.02	0.41
1:A:304:GLY:HA3	1:A:310:ALA:O	2.21	0.41
1:A:296:VAL:HG12	1:A:297:GLY:N	2.34	0.41
1:A:178:ASN:ND2	1:A:178:ASN:O	2.54	0.41
1:A:295:PHE:CD2	1:A:326:LYS:HG2	2.56	0.41
1:A:76:SER:O	1:A:77:GLY:C	2.63	0.41
1:A:314:CYS:O	1:A:317:MET:HB2	2.21	0.41
1:A:326:LYS:CG	1:A:327:TYR:H	2.34	0.41
1:A:184:VAL:HG13	1:A:220:SER:HB2	2.01	0.41
1:A:148:PHE:CD1	1:A:148:PHE:C	2.99	0.40
1:A:343:ASP:O	1:A:346:SER:OG	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LYS:HG3	1:A:327:TYR:N	2.36	0.40
1:A:298:ARG:HH11	1:A:298:ARG:HG2	1.85	0.40
1:A:329:PHE:HD2	1:A:329:PHE:HA	1.78	0.40
1:A:128:ARG:HH11	1:A:128:ARG:HG2	1.86	0.40
1:A:185:VAL:O	1:A:189:VAL:HG23	2.22	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	274/316 (87%)	219 (80%)	37 (14%)	18 (7%)	1 7

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	SER
1	A	79	PHE
1	A	83	TYR
1	A	88	ASP
1	A	119	PRO
1	A	268	GLU
1	A	325	GLY
1	A	326	LYS
1	A	327	TYR
1	A	335	ALA
1	A	95	HIS
1	A	80	GLU
1	A	90	LEU
1	A	179	GLU
1	A	227[A]	PHE
1	A	227[B]	PHE

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Mol	Chain	Res	Type
1	A	122	ILE
1	A	89	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	243/274 (89%)	210 (86%)	33 (14%)	3 18

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	85	LEU
1	A	95	HIS
1	A	99	GLN
1	A	116	GLU
1	A	119	PRO
1	A	123	ARG
1	A	125	ARG
1	A	143	LEU
1	A	144	GLU
1	A	174	ARG
1	A	178	ASN
1	A	199	LYS
1	A	209	GLU
1	A	212	LEU
1	A	251	CYS
1	A	262	VAL
1	A	263	GLU
1	A	267	GLU
1	A	268	GLU
1	A	275	ARG
1	A	287	ILE
1	A	288	LEU
1	A	303	CYS

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Mol	Chain	Res	Type
1	A	314	CYS
1	A	315	GLN
1	A	327	TYR
1	A	328	GLU
1	A	329	PHE
1	A	332	LYS
1	A	355	GLN
1	A	368	VAL
1	A	369	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	103	ASN
1	A	118	GLN
1	A	121	HIS
1	A	135	GLN
1	A	139	HIS
1	A	170	HIS
1	A	172	HIS
1	A	178	ASN
1	A	215	HIS
1	A	315	GLN
1	A	316	ASN
1	A	364	GLN
1	A	365	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	276/316 (87%)	-0.23	6 (2%) 62 42	24, 70, 120, 134	6 (2%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228[A]	GLY	5.6
1	A	227[A]	PHE	4.5
1	A	226[A]	ASP	3.1
1	A	305	TRP	2.8
1	A	88	ASP	2.4
1	A	90	LEU	2.1

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(Å ²)	Q<0.9
2	ZN	A	386	1/1	0.98	0.03	136,136,136,136	0

6.5 Other polymers [i](#)

There are no such residues in this entry.