Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 06:42 am BST

PDB ID	:	1KOA
Title	:	TWITCHIN KINASE FRAGMENT (C.ELEGANS), AUTOREGULATED PROTEIN KINASE AND IMMUNOGLOBULIN DOMAINS
Authors	:	Kobe, B.; Heierhorst, J.; Feil, S.C.; Parker, M.W.; Benian, G.M.; Weiss, K.R.; Kemp, B.E.
Deposited on	:	1996-06-28
Resolution	:	3.30 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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
Clashscore		42
Ramachandran outliers		4.5%
Sidechain outliers		12.3%
RSRZ outliers		0.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
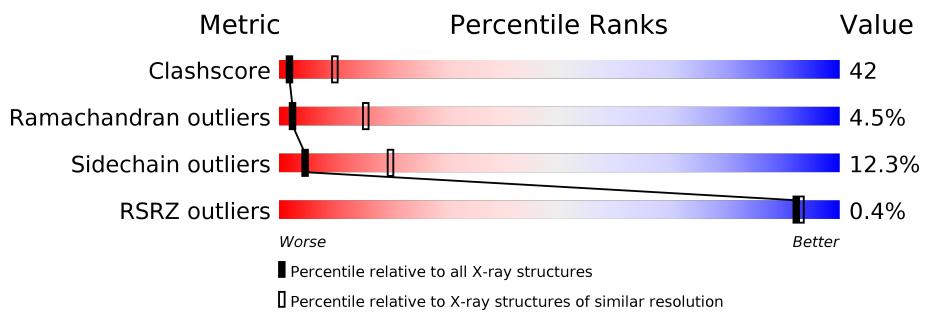
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 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	491	31% 51% 8% · 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3616 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 TWITCHIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3616	2279	625	695	17	0	0	0

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 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: TWITCHIN
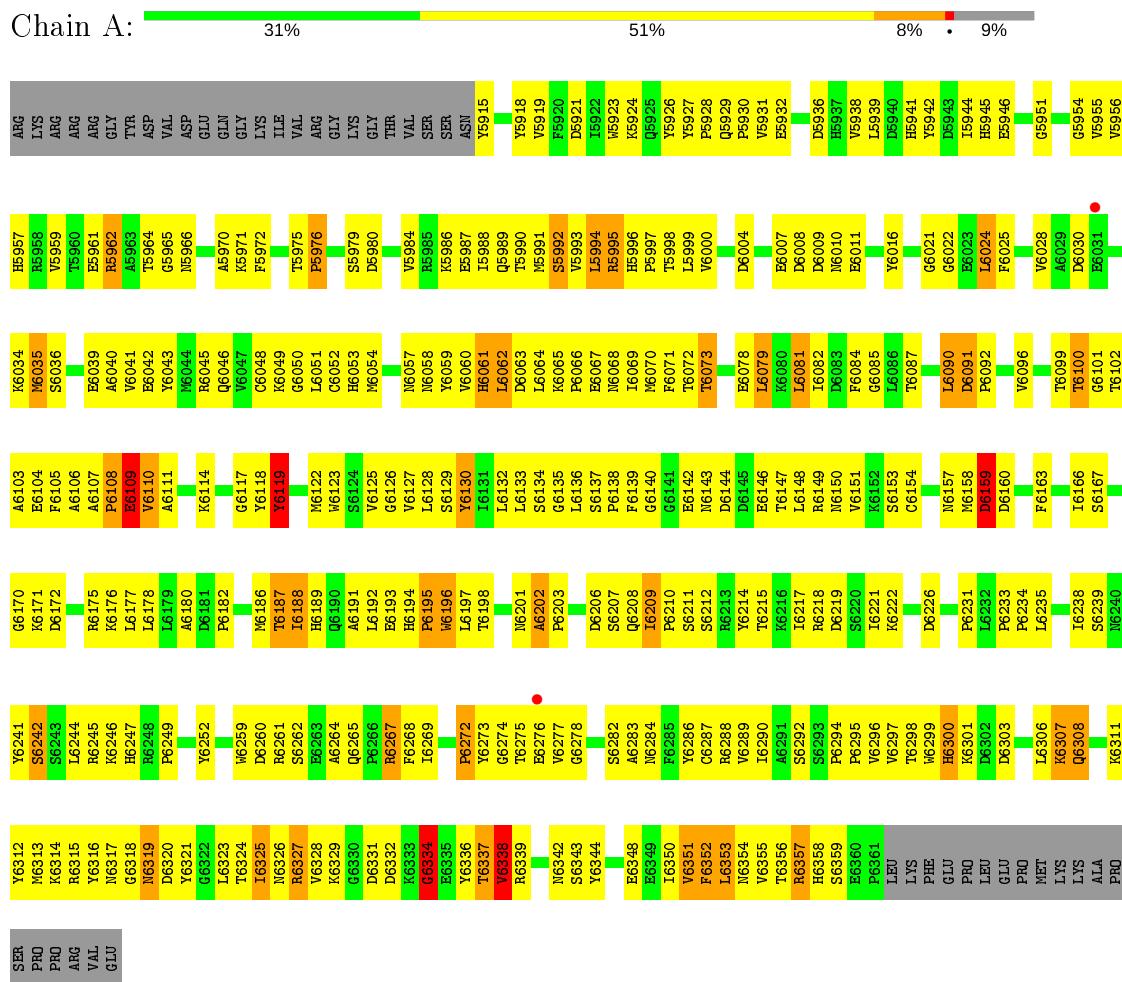
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α, β, γ	195.50Å 195.50Å 195.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 38.34 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.30) 82.4 (38.34-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	0.99 (at 3.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.251 , 0.351 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	99.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 129.9	EDS
L-test for twinning [2]	$<|L|> = 0.43$, $<L^2> = 0.25$	Xtriage
Estimated twinning fraction	0.049 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3616	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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)

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	0.74	1/3710 (0.0%)	1.00	9/5026 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6287	CYS	CB-SG	-5.31	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6079	LEU	CA-CB-CG	7.25	131.97	115.30
1	A	6081	LEU	CA-CB-CG	-6.80	99.66	115.30
1	A	6334	GLY	N-CA-C	6.19	128.57	113.10
1	A	6062	LEU	CA-CB-CG	-5.87	101.79	115.30
1	A	5994	LEU	CA-CB-CG	-5.63	102.34	115.30
1	A	6338	VAL	CB-CA-C	-5.45	101.05	111.40
1	A	6159	ASP	N-CA-C	5.42	125.62	111.00
1	A	6187	THR	N-CA-C	-5.28	96.75	111.00
1	A	6316	TYR	N-CA-C	5.27	125.22	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	6059	TYR	Sidechain
1	A	6119	TYR	Sidechain
1	A	6130	TYR	Sidechain

5.2 Too-close contacts (i)

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	3616	0	3469	301	0
All	All	3616	0	3469	301	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 42.

All (301) 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:6061:HIS:HA	1:A:6087:THR:HG22	1.30	1.13
1:A:6269:ILE:HD11	1:A:6290:ILE:HG12	1.21	1.11
1:A:6134:SER:HB2	1:A:6136:LEU:HD12	1.37	1.04
1:A:6046:GLN:HB2	1:A:6079:LEU:HD12	1.40	1.00
1:A:6301:LYS:HE3	1:A:6334:GLY:HA3	1.48	0.94
1:A:6070:MET:HE1	1:A:6235:LEU:HA	1.51	0.92
1:A:6000:VAL:HG23	1:A:6081:LEU:O	1.70	0.92
1:A:6163:PHE:HA	1:A:6166:ILE:HD12	1.53	0.90
1:A:5931:VAL:HG22	1:A:5992:SER:HB2	1.54	0.89
1:A:6238:ILE:HA	1:A:6241:TYR:CD2	2.08	0.89
1:A:5923:TRP:CZ3	1:A:5928:PRO:HG2	2.10	0.86
1:A:6119:TYR:CE2	1:A:6182:PRO:HB3	2.11	0.86
1:A:6065:LYS:HB2	1:A:6068:ASN:ND2	1.92	0.84
1:A:6233:PRO:HB2	1:A:6234:PRO:HD2	1.62	0.81
1:A:6126:GLY:HA3	1:A:6178:LEU:HD21	1.66	0.77
1:A:6268:PHE:HA	1:A:6289:VAL:HG22	1.67	0.77
1:A:6337:THR:HG22	1:A:6350:ILE:HG12	1.67	0.76
1:A:5956:VAL:HG23	1:A:6239:SER:HB3	1.67	0.76
1:A:6202:ALA:N	1:A:6203:PRO:HD3	2.00	0.76
1:A:6109:GLU:HG2	1:A:6110:VAL:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6065:LYS:H	1:A:6068:ASN:HD22	1.32	0.75
1:A:6090:LEU:HD12	1:A:6259:TRP:CZ3	2.23	0.74
1:A:6048:CYS:CB	1:A:6192:LEU:HD21	2.17	0.73
1:A:5931:VAL:CG2	1:A:5992:SER:HB2	2.20	0.72
1:A:6048:CYS:HB3	1:A:6192:LEU:HD21	1.73	0.71
1:A:6061:HIS:CA	1:A:6087:THR:HG22	2.17	0.71
1:A:6336:TYR:HE2	1:A:6353:LEU:HD23	1.57	0.70
1:A:6146:GLU:HA	1:A:6149:ARG:HD2	1.74	0.69
1:A:6142:GLU:HB3	1:A:6146:GLU:HG3	1.73	0.69
1:A:6119:TYR:CD2	1:A:6182:PRO:HB3	2.27	0.69
1:A:6186:MET:SD	1:A:6191:ALA:HA	2.33	0.68
1:A:6130:TYR:CD1	1:A:6138:PRO:HG3	2.29	0.68
1:A:6288:ARG:HG3	1:A:6319:ASN:HB2	1.76	0.68
1:A:6065:LYS:N	1:A:6068:ASN:HD22	1.92	0.67
1:A:5992:SER:O	1:A:5995:ARG:HG3	1.95	0.67
1:A:6336:TYR:CE2	1:A:6353:LEU:HD23	2.30	0.67
1:A:6278:GLY:HA2	1:A:6356:THR:O	1.95	0.67
1:A:6102:THR:OG1	1:A:6105:PHE:HB2	1.94	0.67
1:A:6046:GLN:HB2	1:A:6079:LEU:CD1	2.22	0.66
1:A:5915:TYR:CE2	1:A:6233:PRO:HD3	2.31	0.66
1:A:6051:LEU:HB2	1:A:6188:ILE:HD12	1.77	0.65
1:A:5930:PRO:HG3	1:A:5995:ARG:HH22	1.61	0.65
1:A:6099:THR:HG22	1:A:6101:GLY:H	1.62	0.65
1:A:6051:LEU:CB	1:A:6188:ILE:HD12	2.26	0.65
1:A:6103:ALA:HB1	1:A:6148:LEU:HG	1.79	0.64
1:A:6000:VAL:HG11	1:A:6016:TYR:HD2	1.62	0.64
1:A:6317:ASN:OD1	1:A:6320:ASP:HB2	1.97	0.64
1:A:6061:HIS:HA	1:A:6087:THR:CG2	2.19	0.64
1:A:6171:LYS:O	1:A:6175:ARG:HG3	1.99	0.63
1:A:5944:ILE:HA	1:A:5959:VAL:HG12	1.79	0.63
1:A:6148:LEU:O	1:A:6151:VAL:HB	1.99	0.62
1:A:5956:VAL:CG2	1:A:6239:SER:HB3	2.30	0.62
1:A:6242:SER:O	1:A:6245:ARG:HG3	1.99	0.62
1:A:6000:VAL:CG2	1:A:6082:ILE:HA	2.30	0.62
1:A:6301:LYS:HD2	1:A:6336:TYR:CE1	2.35	0.62
1:A:6307:LYS:HD3	1:A:6308:GLN:H	1.63	0.62
1:A:6247:HIS:O	1:A:6249:PRO:HD3	2.00	0.62
1:A:6269:ILE:HD11	1:A:6290:ILE:CG1	2.14	0.61
1:A:5996:HIS:CD2	1:A:5997:PRO:HD2	2.35	0.61
1:A:6313:MET:O	1:A:6323:LEU:HD12	2.01	0.61
1:A:6201:ASN:HB2	1:A:6203:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5989:GLN:O	1:A:5992:SER:HB3	2.01	0.61
1:A:6158:MET:HB2	1:A:6175:ARG:HH21	1.66	0.61
1:A:6090:LEU:HA	1:A:6259:TRP:CZ2	2.35	0.60
1:A:6147:THR:O	1:A:6151:VAL:HG23	2.02	0.60
1:A:6036:SER:H	1:A:6039:GLU:HG2	1.66	0.60
1:A:6172:ASP:OD1	1:A:6176:LYS:HE2	2.02	0.59
1:A:6035:MET:HE2	1:A:6043:TYR:HE2	1.68	0.58
1:A:6109:GLU:HA	1:A:6114:LYS:HB2	1.86	0.58
1:A:6048:CYS:HB3	1:A:6188:ILE:HD11	1.85	0.58
1:A:6357:ARG:HG3	1:A:6358:HIS:H	1.69	0.58
1:A:6233:PRO:CB	1:A:6234:PRO:HD2	2.28	0.58
1:A:6066:PRO:HA	1:A:6069:ILE:HD12	1.86	0.57
1:A:6051:LEU:HB2	1:A:6188:ILE:CD1	2.33	0.57
1:A:6042:GLU:O	1:A:6046:GLN:HG3	2.03	0.57
1:A:5956:VAL:HA	1:A:5970:ALA:O	2.04	0.57
1:A:6048:CYS:HB2	1:A:6192:LEU:HD21	1.86	0.57
1:A:6070:MET:CE	1:A:6235:LEU:HA	2.30	0.57
1:A:6065:LYS:HB2	1:A:6068:ASN:HD21	1.66	0.56
1:A:5915:TYR:CD2	1:A:6233:PRO:HD3	2.40	0.56
1:A:5932:GLU:OE1	1:A:5932:GLU:HA	2.06	0.56
1:A:6036:SER:O	1:A:6039:GLU:HB2	2.05	0.56
1:A:6297:VAL:HA	1:A:6339:ARG:O	2.05	0.56
1:A:6058:ASN:ND2	1:A:6267:ARG:HH21	2.03	0.56
1:A:6045:ARG:HG2	1:A:6049:LYS:HE3	1.88	0.56
1:A:6191:ALA:O	1:A:6197:LEU:HD12	2.05	0.56
1:A:6247:HIS:C	1:A:6249:PRO:HD3	2.27	0.55
1:A:6269:ILE:CD1	1:A:6290:ILE:HG12	2.15	0.55
1:A:6129:SER:O	1:A:6133:LEU:N	2.40	0.55
1:A:6300:HIS:N	1:A:6300:HIS:ND1	2.54	0.55
1:A:6172:ASP:O	1:A:6176:LYS:HG2	2.07	0.55
1:A:6297:VAL:HG21	1:A:6321:TYR:CD2	2.42	0.55
1:A:6071:PHE:CZ	1:A:6079:LEU:HD23	2.42	0.54
1:A:6135:GLY:HA3	1:A:6214:TYR:HD1	1.72	0.54
1:A:6342:ASN:O	1:A:6344:TYR:N	2.40	0.54
1:A:6163:PHE:HA	1:A:6166:ILE:CD1	2.30	0.54
1:A:6180:ALA:O	1:A:6182:PRO:HD3	2.08	0.54
1:A:6217:ILE:HG13	1:A:6218:ARG:N	2.22	0.54
1:A:6117:GLY:HA3	1:A:6119:TYR:CE1	2.43	0.54
1:A:6289:VAL:HG12	1:A:6290:ILE:N	2.24	0.53
1:A:5931:VAL:HG21	1:A:5988:ILE:HG22	1.91	0.53
1:A:6070:MET:SD	1:A:6235:LEU:CD1	2.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6202:ALA:H	1:A:6203:PRO:HD3	1.70	0.53
1:A:6051:LEU:O	1:A:6054:MET:N	2.42	0.53
1:A:5951:GLY:HA3	1:A:6239:SER:O	2.09	0.53
1:A:6288:ARG:HA	1:A:6319:ASN:O	2.08	0.53
1:A:6109:GLU:CG	1:A:6110:VAL:H	2.21	0.53
1:A:6045:ARG:NH2	1:A:6197:LEU:O	2.43	0.52
1:A:6119:TYR:HE2	1:A:6182:PRO:HB3	1.73	0.52
1:A:6283:ALA:O	1:A:6324:THR:HA	2.09	0.52
1:A:6000:VAL:HG23	1:A:6082:ILE:HA	1.91	0.52
1:A:6119:TYR:H	1:A:6119:TYR:HD1	1.56	0.52
1:A:6135:GLY:C	1:A:6136:LEU:HG	2.29	0.52
1:A:6327:ARG:HD3	1:A:6327:ARG:C	2.31	0.52
1:A:6007:GLU:HG2	1:A:6008:ASP:N	2.25	0.52
1:A:6050:GLY:O	1:A:6053:HIS:HB3	2.10	0.52
1:A:6323:LEU:HD12	1:A:6324:THR:H	1.75	0.51
1:A:6109:GLU:HG2	1:A:6110:VAL:HG23	1.92	0.51
1:A:6135:GLY:CA	1:A:6214:TYR:HD1	2.23	0.51
1:A:6142:GLU:HB3	1:A:6146:GLU:CG	2.40	0.51
1:A:6090:LEU:HA	1:A:6259:TRP:CE2	2.46	0.51
1:A:6307:LYS:HD3	1:A:6308:GLN:N	2.25	0.51
1:A:6070:MET:SD	1:A:6235:LEU:HD12	2.51	0.51
1:A:6275:THR:HG22	1:A:6277:VAL:HG23	1.92	0.51
1:A:6231:PRO:HB2	1:A:6234:PRO:HA	1.92	0.51
1:A:6312:TYR:CE1	1:A:6325:ILE:HG23	2.46	0.50
1:A:6060:VAL:O	1:A:6087:THR:HA	2.11	0.50
1:A:5955:VAL:HG12	1:A:5956:VAL:N	2.26	0.50
1:A:6235:LEU:O	1:A:6238:ILE:HG13	2.11	0.50
1:A:5938:VAL:HG23	1:A:5939:LEU:N	2.26	0.50
1:A:5988:ILE:O	1:A:5989:GLN:C	2.49	0.50
1:A:6357:ARG:HG3	1:A:6358:HIS:N	2.27	0.50
1:A:6275:THR:O	1:A:6353:LEU:HD12	2.12	0.50
1:A:6289:VAL:CG1	1:A:6290:ILE:N	2.75	0.50
1:A:6142:GLU:HB3	1:A:6146:GLU:CB	2.42	0.50
1:A:6262:SER:O	1:A:6265:GLN:HB2	2.11	0.50
1:A:6035:MET:HE2	1:A:6039:GLU:CB	2.42	0.49
1:A:6264:ALA:HB3	1:A:6344:TYR:CD2	2.47	0.49
1:A:5945:HIS:O	1:A:5957:HIS:HD2	1.95	0.49
1:A:6350:ILE:C	1:A:6351:VAL:HG12	2.32	0.49
1:A:6189:HIS:O	1:A:6193:GLU:HG3	2.13	0.49
1:A:6352:PHE:HD1	1:A:6352:PHE:O	1.96	0.49
1:A:6035:MET:HE2	1:A:6039:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6051:LEU:O	1:A:6052:CYS:C	2.50	0.49
1:A:6099:THR:HG22	1:A:6100:THR:N	2.26	0.49
1:A:6025:PHE:CE1	1:A:6132:LEU:HA	2.47	0.49
1:A:6048:CYS:HA	1:A:6051:LEU:HD12	1.94	0.49
1:A:6090:LEU:HD12	1:A:6259:TRP:CE3	2.47	0.49
1:A:6314:LYS:C	1:A:6315:ARG:HG2	2.33	0.49
1:A:5923:TRP:CE3	1:A:5928:PRO:HG2	2.46	0.49
1:A:6067:GLU:O	1:A:6082:ILE:HD11	2.12	0.49
1:A:6139:PHE:HD1	1:A:6150:ASN:HB2	1.78	0.49
1:A:6024:LEU:O	1:A:6028:VAL:HG13	2.13	0.48
1:A:5930:PRO:HG3	1:A:5995:ARG:NH2	2.26	0.48
1:A:6188:ILE:O	1:A:6192:LEU:HG	2.13	0.48
1:A:6071:PHE:HA	1:A:6078:GLU:O	2.14	0.48
1:A:6299:TRP:C	1:A:6300:HIS:ND1	2.66	0.48
1:A:5955:VAL:HG12	1:A:5956:VAL:H	1.78	0.48
1:A:6065:LYS:HE3	1:A:6067:GLU:OE1	2.13	0.48
1:A:6084:PHE:O	1:A:6085:GLY:C	2.52	0.48
1:A:6277:VAL:O	1:A:6355:VAL:HA	2.14	0.48
1:A:5975:THR:O	1:A:6010:ASN:HA	2.13	0.48
1:A:6108:PRO:HD3	1:A:6123:TRP:CE2	2.48	0.48
1:A:6099:THR:HG22	1:A:6101:GLY:N	2.26	0.48
1:A:6109:GLU:CA	1:A:6114:LYS:HB2	2.44	0.48
1:A:6157:ASN:HB2	1:A:6159:ASP:OD1	2.14	0.48
1:A:6126:GLY:HA2	1:A:6177:LEU:HD12	1.95	0.47
1:A:6194:HIS:CG	1:A:6195:PRO:HD2	2.49	0.47
1:A:5955:VAL:HG11	1:A:5957:HIS:CE1	2.50	0.47
1:A:6201:ASN:HB2	1:A:6203:PRO:CD	2.45	0.47
1:A:6025:PHE:O	1:A:6028:VAL:HG22	2.15	0.47
1:A:6208:GLN:HG2	1:A:6209:ILE:N	2.29	0.47
1:A:6191:ALA:O	1:A:6194:HIS:HB3	2.15	0.47
1:A:6284:ASN:OD1	1:A:6324:THR:HG23	2.14	0.47
1:A:5941:HIS:O	1:A:5962:ARG:HB2	2.15	0.47
1:A:6108:PRO:O	1:A:6111:ALA:N	2.47	0.47
1:A:6070:MET:SD	1:A:6235:LEU:HD13	2.54	0.47
1:A:6081:LEU:HD23	1:A:6081:LEU:HA	1.56	0.47
1:A:6021:GLY:HA3	1:A:6071:PHE:O	2.15	0.46
1:A:6264:ALA:CB	1:A:6344:TYR:CD2	2.98	0.46
1:A:6201:ASN:HB2	1:A:6203:PRO:CG	2.45	0.46
1:A:6063:ASP:OD1	1:A:6065:LYS:HD3	2.15	0.46
1:A:6109:GLU:HG2	1:A:6110:VAL:N	2.26	0.46
1:A:6282:SER:HB3	1:A:6326:ASN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6202:ALA:N	1:A:6203:PRO:CD	2.72	0.46
1:A:6294:PRO:HA	1:A:6295:PRO:HD3	1.69	0.46
1:A:6314:LYS:O	1:A:6315:ARG:HG2	2.15	0.46
1:A:6187:THR:O	1:A:6188:ILE:C	2.54	0.46
1:A:6278:GLY:HA2	1:A:6356:THR:OG1	2.16	0.45
1:A:6036:SER:H	1:A:6039:GLU:CG	2.28	0.45
1:A:6153:SER:O	1:A:6154:CYS:HB3	2.16	0.45
1:A:6041:VAL:O	1:A:6045:ARG:HB2	2.16	0.45
1:A:6000:VAL:HG21	1:A:6082:ILE:HA	1.98	0.45
1:A:6244:LEU:HD23	1:A:6244:LEU:HA	1.63	0.45
1:A:6048:CYS:O	1:A:6049:LYS:C	2.55	0.45
1:A:6091:ASP:HA	1:A:6092:PRO:HD3	1.90	0.45
1:A:6350:ILE:HG22	1:A:6351:VAL:N	2.31	0.45
1:A:6323:LEU:HG	1:A:6324:THR:N	2.31	0.45
1:A:6099:THR:CG2	1:A:6100:THR:N	2.80	0.44
1:A:6130:TYR:HE1	1:A:6136:LEU:O	2.00	0.44
1:A:5998:THR:C	1:A:5999:LEU:HD23	2.38	0.44
1:A:6118:TYR:CZ	1:A:6267:ARG:NH2	2.85	0.44
1:A:6110:VAL:HB	1:A:6111:ALA:H	1.62	0.44
1:A:5989:GLN:O	1:A:5993:VAL:HG23	2.18	0.44
1:A:6022:GLY:HA2	1:A:6234:PRO:HG3	1.99	0.44
1:A:6036:SER:OG	1:A:6039:GLU:HG2	2.17	0.44
1:A:6119:TYR:O	1:A:6122:MET:N	2.50	0.44
1:A:6107:ALA:O	1:A:6110:VAL:HB	2.18	0.44
1:A:6118:TYR:CE2	1:A:6267:ARG:NH2	2.86	0.44
1:A:6210:PRO:C	1:A:6212:SER:H	2.21	0.44
1:A:6218:ARG:HG2	1:A:6222:LYS:HE3	2.00	0.44
1:A:6283:ALA:O	1:A:6325:ILE:N	2.50	0.44
1:A:6119:TYR:HA	1:A:6122:MET:HG2	2.00	0.44
1:A:6067:GLU:H	1:A:6067:GLU:HG3	1.55	0.44
1:A:6194:HIS:CD2	1:A:6195:PRO:HD2	2.53	0.44
1:A:6221:ILE:HG22	1:A:6222:LYS:N	2.31	0.44
1:A:6288:ARG:CG	1:A:6319:ASN:HB2	2.45	0.44
1:A:6324:THR:HG22	1:A:6325:ILE:N	2.33	0.44
1:A:6327:ARG:NH1	1:A:6329:LYS:HG2	2.33	0.44
1:A:6272:PRO:HA	1:A:6286:TYR:O	2.18	0.44
1:A:6328:VAL:HG11	1:A:6355:VAL:HG21	1.99	0.44
1:A:6103:ALA:CB	1:A:6148:LEU:HG	2.46	0.43
1:A:6000:VAL:HG11	1:A:6016:TYR:CD2	2.46	0.43
1:A:6099:THR:CG2	1:A:6101:GLY:H	2.27	0.43
1:A:6041:VAL:HG22	1:A:6196:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6108:PRO:O	1:A:6109:GLU:C	2.56	0.43
1:A:6048:CYS:CB	1:A:6188:ILE:HD11	2.48	0.43
1:A:6296:VAL:O	1:A:6296:VAL:CG2	2.66	0.43
1:A:6102:THR:O	1:A:6106:ALA:N	2.51	0.43
1:A:6103:ALA:HB3	1:A:6147:THR:HG21	2.00	0.43
1:A:6107:ALA:HA	1:A:6123:TRP:CD1	2.54	0.43
1:A:6127:VAL:O	1:A:6128:LEU:C	2.57	0.43
1:A:6142:GLU:HB3	1:A:6146:GLU:HB2	2.00	0.43
1:A:6036:SER:C	1:A:6209:ILE:HD11	2.39	0.43
1:A:6137:SER:HA	1:A:6138:PRO:HD3	1.80	0.43
1:A:6160:ASP:O	1:A:6163:PHE:HB2	2.18	0.43
1:A:5976:PRO:HD2	1:A:5980:ASP:OD2	2.18	0.43
1:A:5984:VAL:O	1:A:5988:ILE:HG13	2.19	0.43
1:A:5986:LYS:O	1:A:5987:GLU:C	2.57	0.43
1:A:6109:GLU:CG	1:A:6110:VAL:N	2.82	0.43
1:A:6119:TYR:O	1:A:6122:MET:HB2	2.19	0.43
1:A:5972:PHE:CD1	1:A:5972:PHE:N	2.85	0.43
1:A:5915:TYR:O	1:A:5918:TYR:HB2	2.19	0.42
1:A:5961:GLU:O	1:A:5965:GLY:N	2.46	0.42
1:A:6282:SER:HB2	1:A:6326:ASN:HA	2.00	0.42
1:A:5939:LEU:C	1:A:5941:HIS:H	2.23	0.42
1:A:5990:THR:O	1:A:5991:MET:C	2.57	0.42
1:A:5954:GLY:HA3	1:A:5972:PHE:O	2.19	0.42
1:A:6103:ALA:CB	1:A:6147:THR:HB	2.50	0.42
1:A:6276:GLU:OE1	1:A:6354:ASN:HB3	2.20	0.42
1:A:5994:LEU:HA	1:A:5994:LEU:HD23	1.38	0.42
1:A:5961:GLU:O	1:A:5962:ARG:O	2.37	0.42
1:A:6129:SER:O	1:A:6130:TYR:C	2.57	0.42
1:A:6195:PRO:HA	1:A:6198:THR:OG1	2.19	0.42
1:A:6107:ALA:HA	1:A:6123:TRP:NE1	2.34	0.42
1:A:6133:LEU:HD23	1:A:6133:LEU:HA	1.77	0.42
1:A:6051:LEU:HB3	1:A:6188:ILE:HD12	2.00	0.42
1:A:5923:TRP:HH2	1:A:5995:ARG:HB3	1.84	0.42
1:A:6064:LEU:HA	1:A:6064:LEU:HD12	1.69	0.42
1:A:6122:MET:O	1:A:6125:VAL:N	2.52	0.42
1:A:6275:THR:HG22	1:A:6276:GLU:N	2.34	0.42
1:A:6043:TYR:O	1:A:6046:GLN:N	2.53	0.42
1:A:6122:MET:HG3	1:A:6186:MET:O	2.20	0.42
1:A:6166:ILE:HG22	1:A:6167:SER:N	2.35	0.42
1:A:6035:MET:HE2	1:A:6043:TYR:CE2	2.53	0.41
1:A:6060:VAL:O	1:A:6062:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5919:VAL:HG21	1:A:6073:THR:HG22	2.01	0.41
1:A:6103:ALA:HB3	1:A:6147:THR:CG2	2.50	0.41
1:A:5938:VAL:CG2	1:A:5939:LEU:N	2.83	0.41
1:A:6034:LYS:HD2	1:A:6208:GLN:OE1	2.20	0.41
1:A:6274:GLY:HA2	1:A:6351:VAL:HG21	2.02	0.41
1:A:6048:CYS:CA	1:A:6188:ILE:HD11	2.50	0.41
1:A:6260:ASP:O	1:A:6261:ARG:C	2.58	0.41
1:A:5921:ASP:HB3	1:A:5924:LYS:HB3	2.01	0.41
1:A:5996:HIS:HA	1:A:5997:PRO:HD3	1.85	0.41
1:A:6035:MET:CE	1:A:6039:GLU:HB2	2.50	0.41
1:A:6245:ARG:HG2	1:A:6252:TYR:CE2	2.55	0.41
1:A:6324:THR:C	1:A:6325:ILE:CG1	2.88	0.41
1:A:6039:GLU:O	1:A:6040:ALA:C	2.59	0.41
1:A:6122:MET:CE	1:A:6188:ILE:HA	2.50	0.41
1:A:6284:ASN:HA	1:A:6323:LEU:O	2.21	0.41
1:A:6245:ARG:HG2	1:A:6252:TYR:CD2	2.56	0.41
1:A:6311:LYS:O	1:A:6312:TYR:CD1	2.74	0.41
1:A:6338:VAL:O	1:A:6348:GLU:HA	2.21	0.41
1:A:5915:TYR:HA	1:A:5918:TYR:HD2	1.86	0.41
1:A:5927:TYR:CD2	1:A:5929:GLN:HG2	2.56	0.41
1:A:6048:CYS:C	1:A:6050:GLY:N	2.74	0.41
1:A:6057:ASN:O	1:A:6058:ASN:HB2	2.20	0.41
1:A:6061:HIS:CE1	1:A:6063:ASP:H	2.39	0.41
1:A:6194:HIS:HA	1:A:6195:PRO:HD3	1.94	0.41
1:A:6195:PRO:O	1:A:6198:THR:O	2.38	0.41
1:A:6065:LYS:N	1:A:6068:ASN:ND2	2.66	0.41
1:A:6135:GLY:HA3	1:A:6214:TYR:CD1	2.54	0.41
1:A:6126:GLY:CA	1:A:6178:LEU:HD21	2.45	0.41
1:A:5964:THR:HG21	1:A:5966:ASN:ND2	2.35	0.40
1:A:6170:GLY:O	1:A:6171:LYS:C	2.59	0.40
1:A:6128:LEU:HD12	1:A:6128:LEU:HA	1.84	0.40
1:A:5941:HIS:HB3	1:A:5942:TYR:CD1	2.56	0.40
1:A:5956:VAL:HG22	1:A:5971:LYS:HA	2.04	0.40
1:A:6301:LYS:HB2	1:A:6336:TYR:CD1	2.57	0.40
1:A:6135:GLY:CA	1:A:6214:TYR:CD1	3.04	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	445/491 (91%)	346 (78%)	79 (18%)	20 (4%)	2	15

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6108	PRO
1	A	6334	GLY
1	A	5976	PRO
1	A	5992	SER
1	A	6024	LEU
1	A	6109	GLU
1	A	6140	GLY
1	A	6332	ASP
1	A	6343	SER
1	A	5962	ARG
1	A	6215	THR
1	A	6226	ASP
1	A	6207	SER
1	A	6246	LYS
1	A	6318	GLY
1	A	6143	ASN
1	A	6202	ALA
1	A	6206	ASP
1	A	6110	VAL
1	A	6325	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	397/436 (91%)	348 (88%)	49 (12%)	4 20

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5926	TYR
1	A	5936	ASP
1	A	5946	GLU
1	A	5979	SER
1	A	5995	ARG
1	A	6004	ASP
1	A	6009	ASP
1	A	6011	GLU
1	A	6030	ASP
1	A	6035	MET
1	A	6061	HIS
1	A	6072	THR
1	A	6073	THR
1	A	6090	LEU
1	A	6091	ASP
1	A	6096	VAL
1	A	6100	THR
1	A	6104	GLU
1	A	6109	GLU
1	A	6119	TYR
1	A	6144	ASP
1	A	6159	ASP
1	A	6188	ILE
1	A	6195	PRO
1	A	6196	TRP
1	A	6209	ILE
1	A	6211	SER
1	A	6219	ASP
1	A	6242	SER
1	A	6267	ARG
1	A	6272	PRO
1	A	6273	TYR
1	A	6292	SER
1	A	6298	THR
1	A	6300	HIS
1	A	6303	ASP

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Mol	Chain	Res	Type
1	A	6306	LEU
1	A	6307	LYS
1	A	6308	GLN
1	A	6319	ASN
1	A	6327	ARG
1	A	6331	ASP
1	A	6337	THR
1	A	6338	VAL
1	A	6351	VAL
1	A	6352	PHE
1	A	6353	LEU
1	A	6357	ARG
1	A	6359	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5941	HIS
1	A	5945	HIS
1	A	5957	HIS
1	A	5996	HIS
1	A	6001	ASN
1	A	6058	ASN
1	A	6068	ASN
1	A	6150	ASN
1	A	6247	HIS
1	A	6326	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (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(Å²)	Q<0.9
1	A	447/491 (91%)	-0.47	2 (0%)	92	93	25, 83, 143, 203	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6031	GLU	3.1
1	A	6276	GLU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.