



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2017 – 05:42 PM EDT

PDB ID : 2YU2
Title : Crystal structure of hJHDM1A without a-ketoglutarate
Authors : Han, Z.
Deposited on : unknown
Resolution : 2.70 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

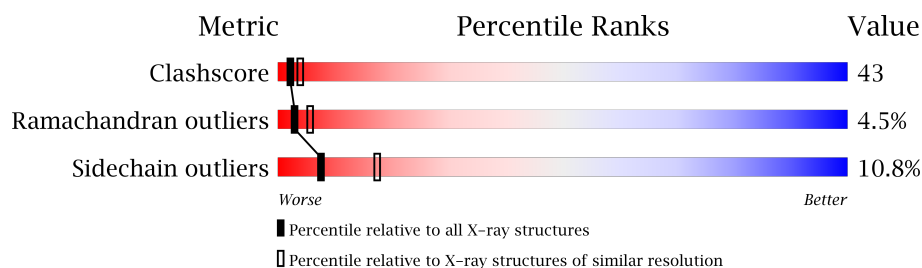
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	451	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3296 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 JmjC domain-containing histone demethylation protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3178	2045	529	582	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	SER	LYS	ENGINEERED	UNP Q9Y2K7

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 3 is water.

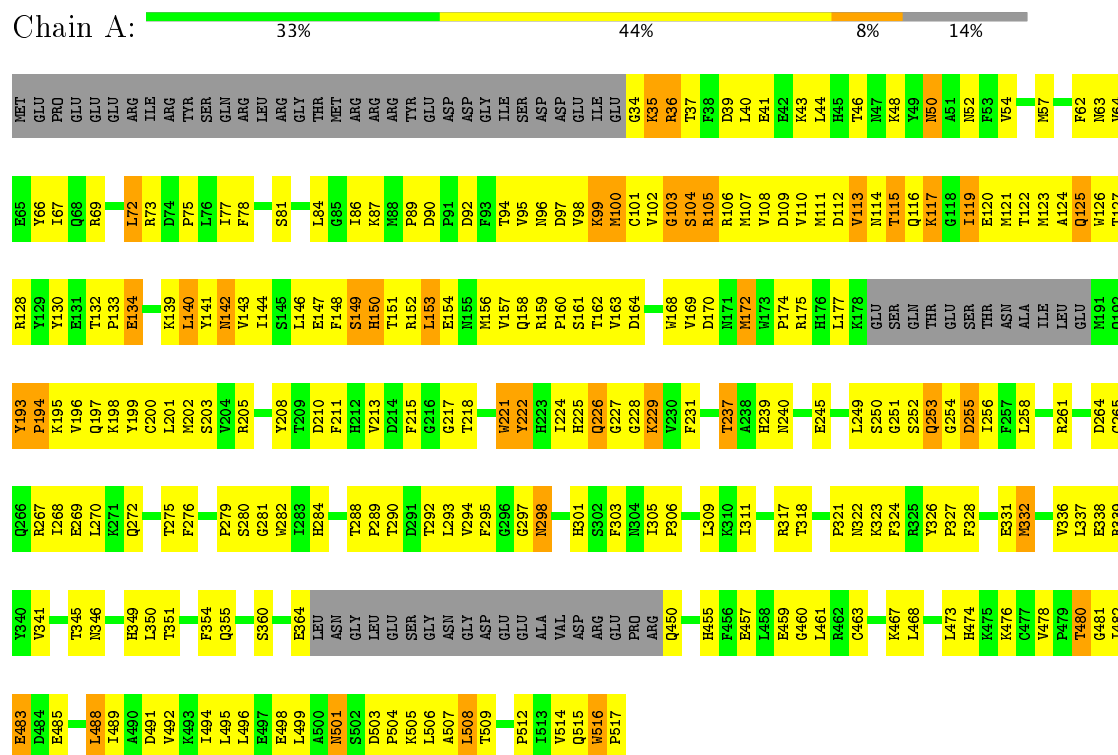
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total	O	0	0
			117	117		

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.

Note EDS was not executed.

- Molecule 1: JmjC domain-containing histone demethylation protein 1A



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	81.15Å 81.15Å 124.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.7 (20.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3296	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

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	0.46	0/3264	0.71	0/4427

There are no bond length outliers.

There are no bond angle outliers.

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	3178	0	3077	269	0
2	A	1	0	0	0	0
3	A	117	0	0	18	0
All	All	3296	0	3077	269	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 43.

All (269) 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:281:GLY:HA2	1:A:311:ILE:HD11	1.36	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:SER:HB2	1:A:86:ILE:HD11	1.32	1.05
1:A:115:THR:HG23	1:A:116:GLN:H	1.24	1.01
1:A:102:VAL:HG12	1:A:151:THR:HG21	1.40	1.00
1:A:198:LYS:HD3	3:A:643:HOH:O	1.69	0.92
1:A:227:GLY:HA3	1:A:292:THR:HG22	1.52	0.91
1:A:100:MET:HG3	1:A:101:CYS:N	1.87	0.88
1:A:94:THR:HG22	1:A:95:VAL:H	1.37	0.88
1:A:100:MET:HG3	1:A:101:CYS:H	1.39	0.86
1:A:205:ARG:HG3	1:A:289:PRO:O	1.78	0.83
1:A:201:LEU:HB2	1:A:294:VAL:HB	1.59	0.82
1:A:81:SER:CB	1:A:86:ILE:HD11	2.09	0.82
1:A:228:GLY:H	1:A:292:THR:CG2	1.93	0.81
1:A:99:LYS:HE2	1:A:104:SER:HB3	1.60	0.81
1:A:172:MET:HG2	1:A:336:VAL:HG22	1.62	0.80
1:A:106:ARG:HH11	1:A:106:ARG:HG2	1.48	0.79
1:A:290:THR:O	1:A:292:THR:HG23	1.82	0.79
1:A:147:GLU:HG2	1:A:198:LYS:O	1.82	0.79
1:A:473:LEU:HD22	1:A:473:LEU:H	1.48	0.79
1:A:99:LYS:HB2	1:A:123:MET:HB3	1.64	0.78
1:A:104:SER:HB2	1:A:124:ALA:HB2	1.65	0.78
1:A:170:ASP:O	1:A:517:PRO:HB3	1.85	0.77
1:A:146:LEU:HD22	1:A:200:CYS:HB3	1.68	0.76
1:A:256:ILE:HD13	1:A:261:ARG:NH1	2.01	0.76
1:A:153:LEU:O	1:A:156:MET:HB3	1.86	0.75
1:A:228:GLY:H	1:A:292:THR:HG21	1.52	0.74
1:A:338:GLU:HG2	1:A:349:HIS:HB2	1.70	0.74
1:A:110:VAL:HG22	1:A:143:VAL:HG22	1.70	0.74
1:A:108:VAL:HG21	1:A:123:MET:HE2	1.70	0.73
1:A:237:THR:HG22	1:A:240:ASN:H	1.55	0.72
1:A:279:PRO:HG2	1:A:282:TRP:CD1	2.26	0.71
1:A:174:PRO:HG2	1:A:177:LEU:HD12	1.74	0.69
1:A:318:THR:HG22	1:A:318:THR:O	1.93	0.69
1:A:81:SER:HB2	1:A:86:ILE:CD1	2.18	0.68
1:A:64:VAL:HG11	1:A:512:PRO:HD3	1.76	0.67
1:A:351:THR:O	1:A:355:GLN:HG3	1.93	0.67
1:A:111:MET:HG3	1:A:117:LYS:N	2.10	0.66
1:A:512:PRO:HG2	1:A:515:GLN:OE1	1.95	0.66
1:A:44:LEU:HB3	3:A:667:HOH:O	1.95	0.66
1:A:115:THR:HG23	1:A:116:GLN:N	2.05	0.66
1:A:501:ASN:H	1:A:501:ASN:ND2	1.93	0.66
1:A:198:LYS:HE3	3:A:697:HOH:O	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:TYR:O	1:A:195:LYS:N	2.27	0.65
1:A:114:ASN:HD21	1:A:140:LEU:HB2	1.59	0.65
1:A:154:GLU:HG3	1:A:198:LYS:HE2	1.78	0.65
1:A:39:ASP:OD1	1:A:41:GLU:HB2	1.96	0.65
1:A:298:ASN:N	1:A:298:ASN:HD22	1.93	0.65
1:A:98:VAL:O	1:A:102:VAL:HG22	1.97	0.64
1:A:105:ARG:H	1:A:124:ALA:HB2	1.62	0.64
1:A:148:PHE:O	1:A:150:HIS:N	2.31	0.64
1:A:455:HIS:O	1:A:459:GLU:HG2	1.98	0.64
1:A:123:MET:CE	1:A:123:MET:HA	2.27	0.64
1:A:95:VAL:O	1:A:98:VAL:HB	1.98	0.63
1:A:175:ARG:HD2	1:A:517:PRO:C	2.18	0.63
1:A:213:VAL:HG11	1:A:311:ILE:HD13	1.78	0.63
1:A:144:ILE:HG22	1:A:201:LEU:HD12	1.81	0.63
1:A:109:ASP:C	1:A:119:ILE:HG22	2.19	0.62
1:A:110:VAL:HG22	1:A:143:VAL:CG2	2.29	0.62
1:A:194:PRO:HD3	1:A:328:PHE:HD1	1.63	0.62
1:A:281:GLY:CA	1:A:311:ILE:HD11	2.23	0.62
1:A:122:THR:OG1	1:A:125:GLN:HG3	1.99	0.62
1:A:351:THR:HG22	1:A:483:GLU:OE2	2.00	0.61
1:A:159:ARG:HB2	1:A:160:PRO:HD2	1.83	0.61
1:A:354:PHE:CZ	1:A:480:THR:HG22	2.36	0.60
1:A:160:PRO:HG2	1:A:163:VAL:CG2	2.30	0.60
1:A:142:ASN:ND2	1:A:203:SER:OG	2.33	0.59
1:A:503:ASP:OD1	1:A:505:LYS:HB2	2.01	0.59
1:A:73:ARG:NH1	1:A:303:PHE:O	2.35	0.59
1:A:301:HIS:CD2	1:A:303:PHE:H	2.20	0.59
1:A:515:GLN:O	1:A:516:TRP:HB2	2.03	0.59
1:A:106:ARG:HG2	1:A:106:ARG:NH1	2.16	0.59
1:A:351:THR:HA	1:A:483:GLU:HG2	1.83	0.59
1:A:450:GLN:HB2	3:A:672:HOH:O	2.03	0.59
1:A:503:ASP:HB3	1:A:506:LEU:HG	1.85	0.58
1:A:321:PRO:C	1:A:323:LYS:H	2.07	0.58
1:A:495:LEU:HD23	1:A:499:LEU:HD12	1.86	0.57
1:A:224:ILE:N	1:A:224:ILE:HD12	2.19	0.57
1:A:112:ASP:C	1:A:114:ASN:H	2.07	0.57
1:A:168:TRP:HB3	1:A:332:MET:HE3	1.87	0.57
1:A:221:TRP:HZ3	3:A:657:HOH:O	1.87	0.57
1:A:222:TYR:HB3	1:A:276:PHE:HB3	1.87	0.57
1:A:228:GLY:H	1:A:292:THR:HG22	1.67	0.57
1:A:354:PHE:HZ	1:A:480:THR:HG22	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LYS:NZ	1:A:288:THR:OG1	2.38	0.56
1:A:213:VAL:CG1	1:A:311:ILE:HD13	2.35	0.56
1:A:107:MET:HA	1:A:122:THR:HG22	1.87	0.56
1:A:199:TYR:HB2	3:A:620:HOH:O	2.05	0.56
1:A:252:SER:O	1:A:254:GLY:N	2.39	0.56
1:A:473:LEU:HD13	1:A:476:LYS:HE2	1.88	0.56
1:A:37:THR:HB	1:A:255:ASP:HA	1.88	0.56
1:A:94:THR:HG22	1:A:95:VAL:N	2.15	0.56
1:A:144:ILE:HA	1:A:201:LEU:HD13	1.88	0.55
1:A:57:MET:HG3	1:A:78:PHE:CE2	2.41	0.55
1:A:306:PRO:HD3	1:A:460:GLY:HA2	1.89	0.55
1:A:160:PRO:HG2	1:A:163:VAL:HG23	1.87	0.54
1:A:113:VAL:HG22	1:A:140:LEU:HB3	1.89	0.54
1:A:200:CYS:SG	1:A:295:PHE:HE2	2.30	0.54
1:A:148:PHE:HE1	3:A:643:HOH:O	1.90	0.54
1:A:249:LEU:O	1:A:251:GLY:N	2.40	0.54
1:A:256:ILE:HD13	1:A:261:ARG:HH12	1.72	0.54
1:A:321:PRO:HG2	1:A:324:PHE:HD1	1.71	0.54
1:A:87:LYS:HG2	1:A:158:GLN:HB2	1.90	0.54
1:A:473:LEU:H	1:A:473:LEU:CD2	2.17	0.54
1:A:112:ASP:O	1:A:114:ASN:N	2.37	0.53
1:A:224:ILE:HD12	1:A:224:ILE:H	1.74	0.53
1:A:321:PRO:HG2	1:A:324:PHE:CD1	2.44	0.53
1:A:172:MET:SD	1:A:514:VAL:HG11	2.49	0.53
1:A:208:TYR:CZ	1:A:210:ASP:HA	2.44	0.53
1:A:102:VAL:HG23	1:A:123:MET:HG3	1.90	0.52
1:A:226:GLN:HG3	1:A:226:GLN:O	2.07	0.52
1:A:501:ASN:ND2	1:A:501:ASN:N	2.57	0.52
1:A:104:SER:CB	1:A:124:ALA:HB2	2.38	0.52
1:A:194:PRO:HB3	1:A:327:PRO:HG2	1.91	0.52
1:A:132:THR:O	1:A:133:PRO:C	2.47	0.52
1:A:483:GLU:HB2	3:A:680:HOH:O	2.08	0.52
1:A:102:VAL:HG12	1:A:151:THR:CG2	2.26	0.52
1:A:89:PRO:HG2	1:A:225:HIS:CE1	2.44	0.52
1:A:217:GLY:HA2	1:A:311:ILE:HD12	1.91	0.52
1:A:96:ASN:HB2	1:A:127:THR:HG21	1.90	0.52
1:A:159:ARG:HD3	3:A:657:HOH:O	2.10	0.52
1:A:193:TYR:CG	1:A:193:TYR:O	2.62	0.52
1:A:201:LEU:HD21	3:A:620:HOH:O	2.09	0.52
1:A:109:ASP:CA	1:A:119:ILE:HG22	2.40	0.51
1:A:288:THR:HG22	1:A:290:THR:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG21	1:A:123:MET:CE	2.38	0.51
1:A:495:LEU:CD2	1:A:499:LEU:HD12	2.40	0.51
1:A:115:THR:O	1:A:116:GLN:HB3	2.11	0.51
1:A:200:CYS:SG	1:A:295:PHE:CE2	3.01	0.51
1:A:115:THR:CG2	1:A:116:GLN:H	2.06	0.51
1:A:148:PHE:O	1:A:149:SER:C	2.50	0.51
1:A:97:ASP:HA	1:A:100:MET:HG2	1.93	0.51
1:A:337:LEU:O	1:A:341:VAL:HG23	2.10	0.50
1:A:121:MET:CE	1:A:126:TRP:HA	2.41	0.50
1:A:126:TRP:HZ3	1:A:141:TYR:CB	2.23	0.50
1:A:144:ILE:HA	1:A:201:LEU:CD1	2.42	0.50
1:A:63:ASN:O	1:A:66:TYR:HB3	2.11	0.50
1:A:501:ASN:H	1:A:501:ASN:HD22	1.56	0.50
1:A:504:PRO:O	1:A:508:LEU:HG	2.11	0.50
1:A:225:HIS:O	1:A:272:GLN:HG3	2.12	0.50
1:A:148:PHE:C	1:A:150:HIS:N	2.65	0.50
1:A:99:LYS:O	1:A:99:LYS:HD2	2.12	0.50
1:A:505:LYS:NZ	3:A:665:HOH:O	2.45	0.49
1:A:109:ASP:HA	1:A:119:ILE:HB	1.95	0.49
1:A:100:MET:HE2	1:A:101:CYS:HA	1.94	0.49
1:A:507:ALA:O	1:A:509:THR:N	2.42	0.49
1:A:515:GLN:HG3	1:A:516:TRP:CZ3	2.47	0.49
1:A:211:PHE:HA	1:A:284:HIS:O	2.12	0.49
1:A:67:ILE:HD12	1:A:67:ILE:N	2.28	0.49
1:A:231:PHE:O	1:A:267:ARG:HA	2.13	0.49
1:A:147:GLU:HA	1:A:198:LYS:O	2.13	0.48
1:A:237:THR:CG2	1:A:239:HIS:HB3	2.43	0.48
1:A:104:SER:C	1:A:106:ARG:H	2.15	0.48
1:A:121:MET:HA	1:A:125:GLN:NE2	2.28	0.48
1:A:249:LEU:C	1:A:251:GLY:H	2.16	0.48
1:A:105:ARG:O	1:A:105:ARG:HG2	2.12	0.48
1:A:350:LEU:HA	1:A:481:GLY:O	2.13	0.48
1:A:132:THR:HG21	3:A:647:HOH:O	2.11	0.48
1:A:321:PRO:O	1:A:323:LYS:N	2.45	0.48
1:A:35:LYS:HG2	1:A:35:LYS:O	2.11	0.48
1:A:301:HIS:HD2	1:A:303:PHE:H	1.58	0.48
1:A:237:THR:HG22	1:A:239:HIS:N	2.29	0.48
1:A:298:ASN:N	1:A:298:ASN:ND2	2.62	0.48
1:A:109:ASP:HA	1:A:119:ILE:CG2	2.44	0.47
1:A:360:SER:O	1:A:364:GLU:HG3	2.13	0.47
1:A:168:TRP:O	1:A:332:MET:HE1	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLY:O	1:A:35:LYS:CB	2.61	0.47
1:A:332:MET:O	1:A:336:VAL:HG23	2.15	0.47
1:A:102:VAL:CG2	1:A:123:MET:HG3	2.44	0.47
1:A:237:THR:CG2	1:A:239:HIS:H	2.27	0.47
1:A:270:LEU:HD11	1:A:276:PHE:CD1	2.50	0.47
1:A:134:GLU:N	1:A:134:GLU:CD	2.68	0.47
1:A:168:TRP:O	1:A:172:MET:HB2	2.15	0.47
1:A:309:LEU:HD12	1:A:463:CYS:HB3	1.97	0.47
1:A:494:ILE:O	1:A:498:GLU:HG3	2.15	0.47
1:A:202:MET:HG2	1:A:293:LEU:HD23	1.97	0.47
1:A:99:LYS:HB2	1:A:123:MET:CB	2.41	0.47
1:A:96:ASN:OD1	1:A:99:LYS:HG2	2.15	0.47
1:A:516:TRP:O	1:A:517:PRO:C	2.52	0.47
1:A:75:PRO:HA	1:A:279:PRO:HD3	1.96	0.47
1:A:34:GLY:O	1:A:35:LYS:HB3	2.15	0.46
1:A:112:ASP:CG	1:A:112:ASP:O	2.54	0.46
1:A:197:GLN:O	1:A:297:GLY:HA3	2.15	0.46
1:A:331:GLU:N	1:A:331:GLU:OE1	2.49	0.46
1:A:488:LEU:O	1:A:492:VAL:HG23	2.16	0.46
1:A:126:TRP:HZ3	1:A:141:TYR:HB2	1.81	0.46
1:A:152:ARG:O	1:A:154:GLU:N	2.49	0.46
1:A:159:ARG:HB3	1:A:221:TRP:CH2	2.50	0.46
1:A:96:ASN:O	1:A:100:MET:N	2.47	0.46
1:A:201:LEU:CD2	3:A:620:HOH:O	2.64	0.46
1:A:354:PHE:CE1	1:A:481:GLY:HA2	2.51	0.46
1:A:245:GLU:OE2	1:A:317:ARG:HD2	2.15	0.46
1:A:168:TRP:C	1:A:332:MET:HE1	2.37	0.46
1:A:100:MET:CG	1:A:101:CYS:N	2.70	0.45
1:A:146:LEU:CD2	1:A:200:CYS:HB3	2.42	0.45
1:A:202:MET:HG2	1:A:293:LEU:CD2	2.46	0.45
1:A:106:ARG:O	1:A:122:THR:HA	2.15	0.45
1:A:318:THR:CG2	1:A:318:THR:O	2.62	0.45
1:A:107:MET:N	1:A:122:THR:HG22	2.31	0.45
1:A:201:LEU:N	1:A:201:LEU:HD22	2.32	0.45
1:A:323:LYS:HD2	1:A:324:PHE:CE1	2.52	0.45
1:A:107:MET:CA	1:A:122:THR:HG22	2.46	0.45
1:A:478:VAL:HG21	1:A:485:GLU:HG2	1.97	0.45
1:A:112:ASP:HB3	1:A:141:TYR:HE2	1.82	0.45
1:A:228:GLY:O	1:A:292:THR:HG21	2.16	0.44
1:A:50:ASN:H	1:A:50:ASN:ND2	2.15	0.44
1:A:154:GLU:C	1:A:156:MET:H	2.20	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LEU:O	1:A:160:PRO:HA	2.18	0.44
1:A:87:LYS:HE2	1:A:158:GLN:HB2	2.00	0.44
1:A:170:ASP:O	1:A:517:PRO:CB	2.61	0.44
1:A:112:ASP:OD2	1:A:115:THR:HG22	2.17	0.44
1:A:37:THR:CB	1:A:255:ASP:HA	2.47	0.43
1:A:46:THR:HG22	1:A:48:LYS:HB3	2.00	0.43
1:A:111:MET:CG	1:A:117:LYS:N	2.79	0.43
1:A:249:LEU:C	1:A:251:GLY:N	2.71	0.43
1:A:341:VAL:O	1:A:345:THR:HB	2.18	0.43
1:A:473:LEU:N	1:A:473:LEU:HD22	2.26	0.43
1:A:128:ARG:HD3	1:A:128:ARG:HA	1.77	0.42
1:A:148:PHE:O	1:A:151:THR:N	2.52	0.42
1:A:104:SER:O	1:A:106:ARG:N	2.52	0.42
1:A:305:ILE:N	1:A:306:PRO:HD2	2.34	0.42
1:A:489:ILE:HA	1:A:489:ILE:HD13	1.90	0.42
1:A:139:LYS:HG3	1:A:141:TYR:OH	2.19	0.42
1:A:172:MET:HG3	1:A:336:VAL:HA	2.00	0.42
1:A:99:LYS:O	1:A:103:GLY:CA	2.67	0.42
1:A:253:GLN:HB3	1:A:255:ASP:HB3	2.01	0.42
1:A:222:TYR:O	1:A:276:PHE:N	2.48	0.42
1:A:346:ASN:OD1	1:A:346:ASN:O	2.37	0.42
1:A:39:ASP:O	1:A:43:LYS:HG2	2.19	0.42
1:A:457:GLU:O	1:A:461:LEU:HG	2.20	0.42
1:A:339:ARG:HD2	3:A:605:HOH:O	2.20	0.42
1:A:112:ASP:HA	1:A:140:LEU:O	2.20	0.42
1:A:222:TYR:O	1:A:275:THR:HA	2.18	0.42
1:A:294:VAL:HG12	1:A:295:PHE:N	2.33	0.42
1:A:321:PRO:C	1:A:323:LYS:N	2.73	0.42
1:A:54:VAL:HG11	1:A:77:ILE:HD12	2.01	0.42
1:A:121:MET:CE	1:A:126:TRP:HB2	2.50	0.42
1:A:268:ILE:HG13	1:A:269:GLU:N	2.35	0.42
1:A:36:ARG:HG2	3:A:694:HOH:O	2.20	0.42
1:A:114:ASN:HB3	3:A:618:HOH:O	2.19	0.41
1:A:168:TRP:HB3	1:A:332:MET:CE	2.48	0.41
1:A:515:GLN:HG3	1:A:516:TRP:CE3	2.55	0.41
1:A:62:PHE:O	1:A:162:THR:OG1	2.22	0.41
1:A:516:TRP:HE3	1:A:516:TRP:N	2.18	0.41
1:A:111:MET:CG	1:A:117:LYS:H	2.34	0.41
1:A:116:GLN:O	1:A:117:LYS:O	2.38	0.41
1:A:160:PRO:HG2	1:A:163:VAL:HG21	2.02	0.41
1:A:321:PRO:HB2	1:A:323:LYS:HG3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLY:CA	1:A:311:ILE:HD12	2.51	0.41
1:A:217:GLY:HA2	1:A:311:ILE:CD1	2.50	0.41
1:A:326:TYR:HA	1:A:327:PRO:HD2	1.91	0.41
1:A:112:ASP:C	1:A:114:ASN:N	2.74	0.41
1:A:104:SER:C	1:A:106:ARG:N	2.74	0.41
1:A:194:PRO:O	1:A:196:VAL:HG22	2.21	0.41
1:A:280:SER:HB2	3:A:616:HOH:O	2.21	0.41
1:A:297:GLY:C	1:A:298:ASN:HD22	2.24	0.41
1:A:157:VAL:HB	3:A:643:HOH:O	2.20	0.40
1:A:146:LEU:O	1:A:146:LEU:HD23	2.20	0.40
1:A:467:LYS:HD2	1:A:467:LYS:HA	1.74	0.40
1:A:482:ILE:HD13	1:A:488:LEU:HD12	2.02	0.40
1:A:95:VAL:HG21	1:A:130:TYR:CG	2.56	0.40
1:A:96:ASN:OD1	1:A:99:LYS:CG	2.70	0.40
1:A:169:VAL:HB	1:A:197:GLN:NE2	2.36	0.40
1:A:66:TYR:HD2	1:A:67:ILE:HD12	1.87	0.40
1:A:72:LEU:HA	1:A:72:LEU:HD23	1.91	0.40
1:A:106:ARG:CG	1:A:106:ARG:NH1	2.82	0.40
1:A:338:GLU:HB2	1:A:482:ILE:HD11	2.04	0.40
1:A:120:GLU:CD	1:A:120:GLU:N	2.73	0.40
1:A:496:LEU:HA	1:A:496:LEU:HD23	1.90	0.40
1:A:95:VAL:HG21	1:A:130:TYR:CD2	2.56	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	381/451 (84%)	328 (86%)	36 (9%)	17 (4%)	3 6

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	VAL
1	A	115	THR
1	A	117	LYS
1	A	194	PRO
1	A	253	GLN
1	A	322	ASN
1	A	483	GLU
1	A	36	ARG
1	A	103	GLY
1	A	105	ARG
1	A	119	ILE
1	A	149	SER
1	A	153	LEU
1	A	250	SER
1	A	508	LEU
1	A	35	LYS
1	A	104	SER

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	352/413 (85%)	314 (89%)	38 (11%)	7 17

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	50	ASN
1	A	52	ASN
1	A	69	ARG
1	A	72	LEU
1	A	90	ASP
1	A	92	ASP
1	A	99	LYS
1	A	100	MET
1	A	125	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	134	GLU
1	A	140	LEU
1	A	142	ASN
1	A	150	HIS
1	A	161	SER
1	A	164	ASP
1	A	172	MET
1	A	193	TYR
1	A	215	PHE
1	A	218	THR
1	A	221	TRP
1	A	222	TYR
1	A	226	GLN
1	A	229	LYS
1	A	237	THR
1	A	255	ASP
1	A	258	LEU
1	A	264	ASP
1	A	265	CYS
1	A	298	ASN
1	A	332	MET
1	A	468	LEU
1	A	474	HIS
1	A	480	THR
1	A	488	LEU
1	A	491	ASP
1	A	501	ASN
1	A	516	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	50	ASN
1	A	52	ASN
1	A	114	ASN
1	A	142	ASN
1	A	197	GLN
1	A	225	HIS
1	A	226	GLN
1	A	272	GLN
1	A	298	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	301	HIS
1	A	346	ASN
1	A	349	HIS
1	A	455	HIS
1	A	501	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](#)

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 [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 ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.