



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:18 pm BST

PDB ID : 6OAM
Title : Crystal Structure of ChlaDUB2 DUB domain
Authors : Hausman, J.M.; Das, C.
Deposited on : 2019-03-17
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

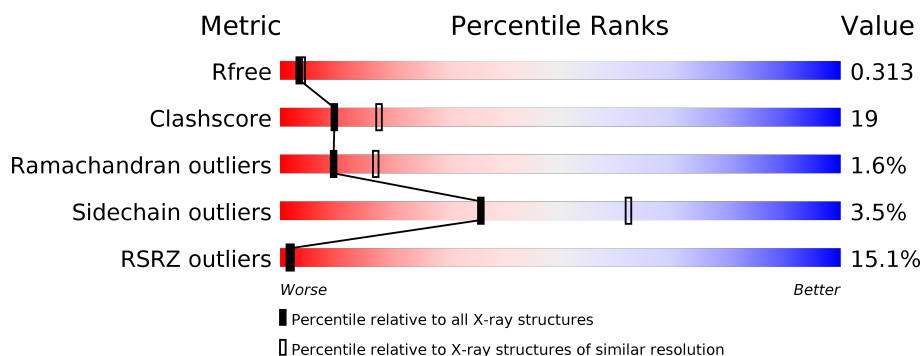
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 $\leq 5\%$. 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	251	
1	B	251	
2	C	76	
2	D	76	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5019 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 Deubiquitinase and deneddylase Dub2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	49	0	0
			1908	1206	318	361	23			
1	B	239	Total	C	N	O	S	23	0	0
			1909	1209	317	361	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	GLY	LEU	conflict	UNP B0B999
A	90	ARG	PRO	conflict	UNP B0B999
A	91	LEU	ILE	conflict	UNP B0B999
A	92	GLU	TRP	conflict	UNP B0B999
B	89	GLY	LEU	conflict	UNP B0B999
B	90	ARG	PRO	conflict	UNP B0B999
B	91	LEU	ILE	conflict	UNP B0B999
B	92	GLU	TRP	conflict	UNP B0B999

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	76	Total	C	N	O	S	18	0	0
			601	379	105	116	1			
2	C	76	Total	C	N	O	S	7	0	0
			601	379	105	116	1			

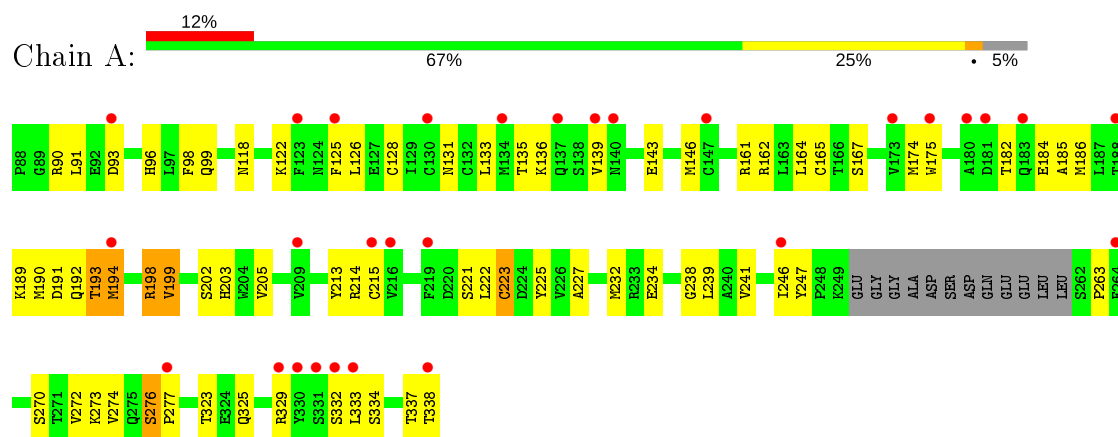
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	76	AYE	-	amidation	UNP J3QS39
C	76	AYE	-	amidation	UNP J3QS39

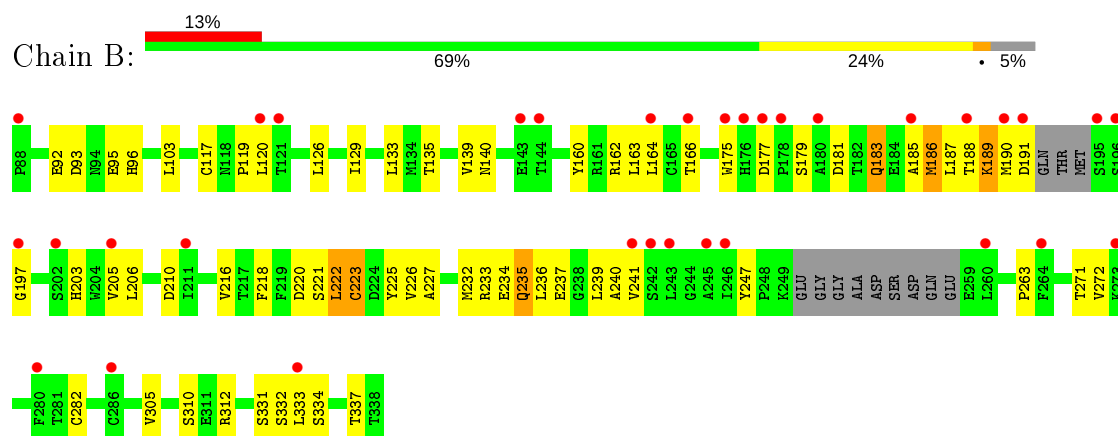
3 Residue-property plots [i](#)

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.

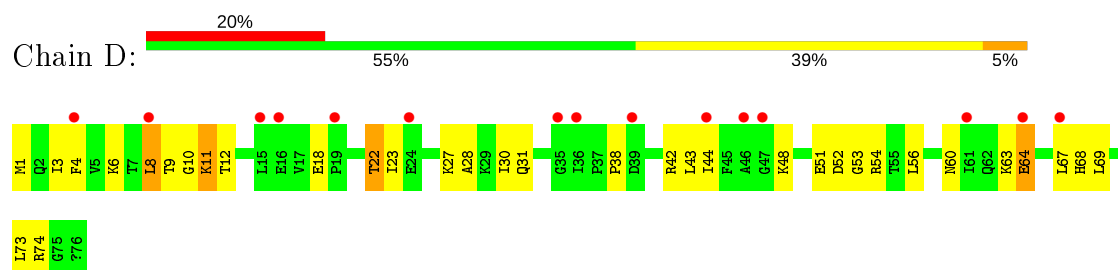
• Molecule 1: Deubiquitinase and deneddylase Dub2



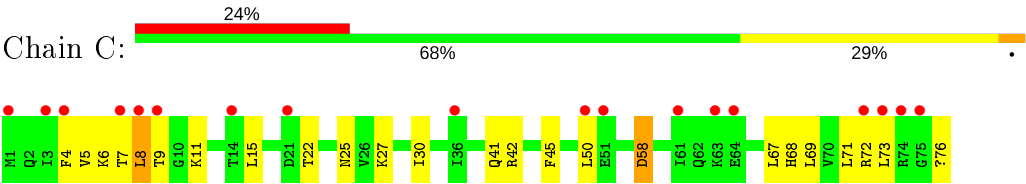
• Molecule 1: Deubiquitinase and deneddylase Dub2



• Molecule 2: Ubiquitin



● Molecule 2: Ubiquitin



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	108.69 Å 108.69 Å 62.28 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 2.50 48.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.61-2.50) 99.9 (48.61-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.51 (at 2.51 Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.283 , 0.306 0.295 , 0.313	Depositor DCC
R_{free} test set	1282 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.179 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5019	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.66	0/1956	0.87	0/2658
1	B	0.67	0/1956	0.89	5/2657 (0.2%)
2	C	0.65	0/603	1.10	0/811
2	D	0.72	0/603	1.13	3/811 (0.4%)
All	All	0.67	0/5118	0.94	8/6937 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	54	ARG	N-CA-C	5.51	125.89	111.00
1	B	210	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	120	LEU	CA-CB-CG	5.18	127.22	115.30
2	D	54	ARG	N-CA-CB	-5.13	101.36	110.60
2	D	53	GLY	N-CA-C	5.10	125.86	113.10
1	B	133	LEU	CA-CB-CG	5.04	126.89	115.30
1	B	197	GLY	N-CA-C	5.04	125.69	113.10
1	B	222	LEU	CB-CA-C	-5.01	100.67	110.20

There are no chirality outliers.

There are no planarity outliers.

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	1908	0	1839	70	0
1	B	1909	0	1842	74	0
2	C	601	0	631	44	0
2	D	601	0	630	23	0
All	All	5019	0	4942	188	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 19.

All (188) 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:B:186:MET:HG3	1:B:190:MET:HE2	1.27	1.12
1:A:135:THR:O	1:A:139:VAL:HG23	1.50	1.09
2:C:6:LYS:O	2:C:68:HIS:HA	1.55	1.04
2:D:6:LYS:O	2:D:68:HIS:HA	1.72	0.89
1:A:213:TYR:HB2	1:A:215:CYS:SG	2.13	0.88
1:B:188:THR:CG2	1:B:189:LYS:H	1.88	0.86
1:B:188:THR:HG23	1:B:189:LYS:H	1.40	0.85
2:C:8:LEU:HD12	2:C:69:LEU:O	1.77	0.85
2:C:8:LEU:HD22	2:C:9:THR:N	1.92	0.85
1:A:276:SER:HB3	1:A:277:PRO:HD2	1.59	0.85
1:A:174:MET:O	1:A:205:VAL:HG22	1.77	0.84
1:B:205:VAL:HG11	1:B:218:PHE:HE1	1.41	0.83
1:B:188:THR:HG23	1:B:189:LYS:N	1.95	0.82
1:A:98:PHE:CE2	1:A:333:LEU:O	2.34	0.81
2:C:8:LEU:HD13	2:C:9:THR:H	1.47	0.80
1:A:184:GLU:OE1	2:C:4:PHE:CE1	2.35	0.80
1:B:185:ALA:O	1:B:188:THR:HG22	1.82	0.79
1:B:205:VAL:HG11	1:B:218:PHE:CE1	2.17	0.79
1:A:93:ASP:OD1	2:D:74:ARG:HG2	1.82	0.79
1:B:175:TRP:CE3	1:B:190:MET:SD	2.77	0.78
1:B:163:LEU:HA	1:B:166:THR:HG22	1.63	0.78
1:A:185:ALA:HB2	2:C:4:PHE:CZ	2.19	0.78
1:B:183:GLN:NE2	1:B:186:MET:HB3	1.98	0.77
1:A:182:THR:HG21	2:C:4:PHE:CE2	2.21	0.76
1:B:333:LEU:HD11	2:C:42:ARG:HD3	1.67	0.76
1:A:175:TRP:HE1	1:A:202:SER:HB3	1.51	0.75
1:B:163:LEU:HA	1:B:166:THR:CG2	2.17	0.74
1:B:175:TRP:CH2	1:B:190:MET:HG2	2.22	0.74
1:A:175:TRP:NE1	1:A:202:SER:HB3	2.03	0.73
1:B:222:LEU:O	1:B:223:CYS:HB2	1.86	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:ILE:HG23	2:D:68:HIS:HB2	1.70	0.73
1:B:186:MET:HG3	1:B:190:MET:CE	2.15	0.72
1:A:189:LYS:O	1:A:193:THR:HB	1.89	0.72
2:D:10:GLY:O	2:D:12:THR:N	2.21	0.72
2:D:1:MET:HB2	2:D:63:LYS:HG2	1.71	0.71
1:B:175:TRP:CZ3	1:B:190:MET:HG2	2.27	0.70
1:A:182:THR:HG21	2:C:4:PHE:CD2	2.27	0.69
1:A:174:MET:HB3	1:A:205:VAL:HG23	1.74	0.69
1:A:184:GLU:OE1	2:C:4:PHE:HE1	1.73	0.68
2:D:23:ILE:HG23	2:D:43:LEU:HD12	1.74	0.68
1:A:276:SER:HB3	1:A:277:PRO:CD	2.22	0.68
1:A:174:MET:HB3	1:A:205:VAL:CG2	2.24	0.67
2:D:8:LEU:HD23	2:D:8:LEU:C	2.15	0.67
1:A:193:THR:HG23	1:A:193:THR:O	1.94	0.66
1:A:213:TYR:CB	1:A:215:CYS:SG	2.85	0.65
1:B:222:LEU:CD1	1:B:225:TYR:CD1	2.79	0.65
1:A:175:TRP:HZ3	1:A:186:MET:SD	2.21	0.64
1:A:139:VAL:HG21	1:A:164:LEU:HD13	1.79	0.64
1:B:93:ASP:OD2	1:B:96:HIS:ND1	2.29	0.64
1:B:117:CYS:HA	2:C:8:LEU:HB2	1.78	0.64
1:B:205:VAL:CG1	1:B:218:PHE:CE1	2.81	0.64
1:B:163:LEU:CA	1:B:166:THR:HG22	2.27	0.63
1:B:126:LEU:HD21	1:B:235:GLN:OE1	1.97	0.63
1:A:223:CYS:SG	1:A:270:SER:HB3	2.39	0.63
1:B:205:VAL:HG21	1:B:226:VAL:HG21	1.79	0.63
1:A:185:ALA:HB2	2:C:4:PHE:CE2	2.34	0.62
1:A:186:MET:O	1:A:190:MET:HG2	2.00	0.62
1:A:199:VAL:HG22	2:D:74:ARG:HB3	1.81	0.62
1:A:162:ARG:HA	1:A:165:CYS:SG	2.39	0.61
1:B:175:TRP:CZ3	2:C:73:LEU:HD13	2.34	0.61
1:B:188:THR:CG2	1:B:189:LYS:N	2.52	0.61
1:A:136:LYS:O	1:A:139:VAL:HB	2.01	0.61
1:A:96:HIS:HA	1:A:99:GLN:HG3	1.82	0.61
1:B:203:HIS:CE1	1:B:221:SER:HB2	2.35	0.61
1:B:183:GLN:HA	1:B:183:GLN:NE2	2.16	0.60
1:B:183:GLN:NE2	1:B:187:LEU:HG	2.17	0.60
2:C:8:LEU:N	2:C:8:LEU:CD1	2.64	0.59
2:C:8:LEU:N	2:C:8:LEU:HD13	2.15	0.59
1:B:205:VAL:CG1	1:B:206:LEU:N	2.66	0.59
1:B:220:ASP:OD2	1:B:223:CYS:O	2.20	0.58
1:A:203:HIS:CE1	1:A:222:LEU:HD12	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:THR:O	1:B:190:MET:N	2.36	0.58
1:A:139:VAL:HG21	1:A:164:LEU:CD1	2.33	0.58
1:B:175:TRP:CZ3	1:B:190:MET:CG	2.86	0.58
1:A:98:PHE:HE2	1:A:333:LEU:O	1.85	0.58
2:C:5:VAL:CG2	2:C:15:LEU:HD12	2.34	0.58
1:B:183:GLN:HE21	1:B:183:GLN:C	2.06	0.58
2:C:8:LEU:CD1	2:C:8:LEU:H	2.17	0.57
1:A:192:GLN:C	1:A:194:MET:H	2.08	0.56
1:B:227:ALA:HB3	1:B:232:MET:HB2	1.86	0.56
1:B:175:TRP:CZ3	1:B:190:MET:SD	2.98	0.56
2:D:22:THR:OG1	2:D:23:ILE:N	2.38	0.56
2:D:18:GLU:O	2:D:56:LEU:HD22	2.06	0.55
1:A:118:ASN:ND2	1:A:128:CYS:SG	2.79	0.55
1:B:162:ARG:O	1:B:166:THR:HG22	2.07	0.55
1:A:136:LYS:HB2	1:A:164:LEU:HD22	1.88	0.55
1:B:222:LEU:HD13	1:B:225:TYR:CD1	2.40	0.55
1:B:203:HIS:HE1	1:B:221:SER:HB2	1.71	0.55
1:B:183:GLN:HE22	1:B:186:MET:HB3	1.71	0.54
2:D:8:LEU:HD23	2:D:8:LEU:O	2.08	0.54
2:D:27:LYS:HD2	2:D:38:PRO:HA	1.89	0.54
1:A:272:VAL:O	1:A:274:VAL:HG13	2.09	0.53
1:A:234:GLU:O	1:A:238:GLY:N	2.38	0.53
1:A:185:ALA:HB2	2:C:4:PHE:HZ	1.68	0.53
1:A:90:ARG:O	1:A:90:ARG:HG2	2.09	0.52
2:C:6:LYS:N	2:C:67:LEU:O	2.42	0.52
2:D:4:PHE:O	2:D:67:LEU:HB2	2.09	0.52
1:A:198:ARG:O	1:A:199:VAL:HB	2.08	0.52
1:B:188:THR:O	1:B:191:ASP:N	2.24	0.52
1:A:337:THR:OG1	1:A:338:THR:N	2.42	0.51
1:B:271:THR:OG1	1:B:272:VAL:N	2.43	0.51
1:A:325:GLN:O	1:A:329:ARG:NH1	2.44	0.51
2:D:51:GLU:O	2:D:52:ASP:C	2.47	0.51
1:B:135:THR:O	1:B:139:VAL:HG23	2.11	0.50
1:A:203:HIS:HB2	1:A:225:TYR:HE2	1.76	0.50
1:B:331:SER:OG	1:B:331:SER:O	2.28	0.50
1:B:162:ARG:NH1	1:B:337:THR:O	2.44	0.50
2:C:45:PHE:HB3	2:C:50:LEU:HD21	1.94	0.50
1:B:234:GLU:HA	1:B:237:GLU:HB2	1.93	0.50
1:B:222:LEU:HD12	1:B:225:TYR:CD1	2.46	0.50
1:B:183:GLN:HE21	1:B:183:GLN:CA	2.25	0.50
1:B:305:VAL:HB	1:B:312:ARG:HD2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:ILE:HD12	2:D:48:LYS:O	2.12	0.49
1:B:233:ARG:O	1:B:236:LEU:N	2.46	0.49
1:B:332:SER:HB2	1:B:334:SER:H	1.77	0.49
1:B:175:TRP:CE3	2:C:73:LEU:HD13	2.47	0.49
1:B:183:GLN:NE2	1:B:183:GLN:CA	2.76	0.49
2:C:8:LEU:HD22	2:C:8:LEU:C	2.33	0.49
2:C:8:LEU:HD13	2:C:9:THR:N	2.23	0.49
1:A:214:ARG:NH1	1:A:247:TYR:O	2.40	0.48
2:C:5:VAL:HG21	2:C:15:LEU:HD12	1.94	0.48
1:B:205:VAL:HG12	1:B:206:LEU:N	2.29	0.48
1:B:177:ASP:OD2	1:B:179:SER:OG	2.30	0.47
1:A:192:GLN:C	1:A:194:MET:N	2.66	0.47
1:A:198:ARG:O	1:A:199:VAL:CB	2.61	0.47
2:D:3:ILE:HA	2:D:64:GLU:HA	1.96	0.47
2:C:7:THR:HG22	2:C:69:LEU:HB3	1.96	0.47
1:B:282:CYS:HB3	2:C:76:AYE:H3A	1.60	0.46
1:A:191:ASP:OD2	2:D:11:LYS:HD2	2.16	0.46
1:A:175:TRP:CZ3	1:A:186:MET:SD	3.06	0.46
1:A:190:MET:HA	1:A:193:THR:HB	1.98	0.46
2:C:8:LEU:HD11	2:C:71:LEU:HD12	1.97	0.46
1:A:133:LEU:HB3	1:A:247:TYR:HE2	1.81	0.46
1:A:182:THR:CG2	2:C:4:PHE:CE2	2.97	0.46
1:A:182:THR:HG23	1:A:185:ALA:HB3	1.97	0.45
2:C:5:VAL:HG23	2:C:15:LEU:HD12	1.98	0.45
1:B:188:THR:HG22	1:B:189:LYS:H	1.77	0.45
1:A:246:ILE:HG22	1:A:246:ILE:O	2.17	0.45
1:B:129:ILE:HG21	1:B:239:LEU:HD21	1.98	0.45
2:C:27:LYS:HG2	2:C:41:GLN:HE21	1.81	0.45
2:C:22:THR:HG23	2:C:25:ASN:H	1.81	0.45
1:A:241:VAL:HG23	1:A:263:PRO:HG3	1.99	0.45
1:A:126:LEU:HD22	1:A:239:LEU:HD22	1.99	0.44
1:B:163:LEU:C	1:B:166:THR:HG22	2.38	0.44
1:B:183:GLN:O	1:B:187:LEU:N	2.39	0.44
1:B:187:LEU:O	1:B:191:ASP:HB2	2.18	0.44
1:B:117:CYS:HA	2:C:8:LEU:CB	2.46	0.44
1:B:92:GLU:OE2	2:C:76:AYE:N1	2.51	0.44
1:B:331:SER:O	1:B:332:SER:HB3	2.17	0.44
1:A:193:THR:CG2	2:D:73:LEU:HD21	2.48	0.44
1:B:160:TYR:O	1:B:164:LEU:HB2	2.18	0.43
1:B:216:VAL:HG11	1:B:236:LEU:HD12	2.00	0.43
1:A:143:GLU:OE2	1:A:146:MET:N	2.46	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:VAL:CG2	1:A:164:LEU:HD13	2.47	0.43
2:D:28:ALA:O	2:D:31:GLN:HG2	2.18	0.43
1:A:128:CYS:HA	1:A:131:ASN:HB2	1.99	0.43
1:A:193:THR:CG2	2:D:73:LEU:CD2	2.96	0.43
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.92	0.43
2:D:23:ILE:HB	2:D:52:ASP:O	2.19	0.43
2:C:7:THR:OG1	2:C:11:LYS:O	2.30	0.43
1:A:143:GLU:O	1:A:161:ARG:NH1	2.52	0.42
1:A:136:LYS:NZ	1:A:167:SER:O	2.48	0.42
2:C:8:LEU:H	2:C:8:LEU:HD12	1.82	0.42
2:D:67:LEU:HA	2:D:67:LEU:HD23	1.88	0.42
1:A:273:LYS:HE2	1:A:273:LYS:HB3	1.73	0.42
1:A:98:PHE:CZ	1:A:333:LEU:O	2.72	0.42
2:C:69:LEU:HD21	2:C:71:LEU:CD2	2.49	0.42
1:B:188:THR:O	1:B:189:LYS:C	2.58	0.42
1:B:241:VAL:HG23	1:B:263:PRO:HG3	2.00	0.42
1:B:95:GLU:HG3	2:C:72:ARG:HH11	1.84	0.42
1:B:222:LEU:HD13	1:B:225:TYR:HD1	1.84	0.42
2:C:58:ASP:OD1	2:C:58:ASP:N	2.53	0.41
1:A:125:PHE:CD1	1:A:125:PHE:C	2.93	0.41
1:B:119:PRO:HB3	1:B:187:LEU:HD21	2.03	0.41
2:C:69:LEU:CD2	2:C:71:LEU:CD2	2.99	0.41
1:B:187:LEU:HD22	2:C:9:THR:OG1	2.21	0.41
1:B:236:LEU:O	1:B:240:ALA:HB2	2.20	0.41
2:D:27:LYS:HA	2:D:30:ILE:HG13	2.03	0.41
1:B:175:TRP:CZ3	2:C:73:LEU:HD22	2.56	0.41
2:C:30:ILE:HD13	2:C:69:LEU:HD12	2.02	0.41
2:C:8:LEU:HD22	2:C:9:THR:CA	2.50	0.41
1:A:91:LEU:HD11	1:A:323:THR:HG21	2.02	0.41
1:A:246:ILE:O	1:A:246:ILE:CG2	2.69	0.41
1:A:227:ALA:HB3	1:A:232:MET:HB2	2.03	0.40
1:B:162:ARG:O	1:B:166:THR:CG2	2.69	0.40
1:A:174:MET:CB	1:A:205:VAL:CG2	2.97	0.40
1:A:162:ARG:O	1:A:165:CYS:SG	2.70	0.40
2:C:5:VAL:HG21	2:C:15:LEU:CD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	235/251 (94%)	210 (89%)	19 (8%)	6 (3%)	5	8
1	B	233/251 (93%)	209 (90%)	21 (9%)	3 (1%)	12	21
2	C	73/76 (96%)	64 (88%)	9 (12%)	0	100	100
2	D	73/76 (96%)	59 (81%)	13 (18%)	1 (1%)	11	20
All	All	614/654 (94%)	542 (88%)	62 (10%)	10 (2%)	9	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	VAL
2	D	11	LYS
1	B	140	ASN
1	B	189	LYS
1	B	223	CYS
1	A	122	LYS
1	A	223	CYS
1	A	276	SER
1	A	332	SER
1	A	334	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	221/230 (96%)	217 (98%)	4 (2%)	59 81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	221/230 (96%)	214 (97%)	7 (3%)	39	65
2	C	68/68 (100%)	66 (97%)	2 (3%)	42	69
2	D	68/68 (100%)	61 (90%)	7 (10%)	7	14
All	All	578/596 (97%)	558 (96%)	20 (4%)	36	62

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	THR
1	A	194	MET
1	A	198	ARG
1	A	221	SER
2	D	8	LEU
2	D	9	THR
2	D	22	THR
2	D	42	ARG
2	D	60	ASN
2	D	64	GLU
2	D	69	LEU
1	B	103	LEU
1	B	181	ASP
1	B	183	GLN
1	B	186	MET
1	B	235	GLN
1	B	247	TYR
1	B	310	SER
2	C	8	LEU
2	C	58	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	124	ASN
1	A	203	HIS
1	A	325	GLN
2	D	68	HIS
1	B	124	ASN
2	C	41	GLN

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

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	239/251 (95%)	0.89	29 (12%) 4 4	30, 73, 105, 113	17 (7%)
1	B	239/251 (95%)	0.86	33 (13%) 2 2	30, 72, 103, 113	12 (5%)
2	C	75/76 (98%)	1.22	18 (24%) 0 0	48, 75, 95, 98	5 (6%)
2	D	75/76 (98%)	1.31	15 (20%) 1 0	69, 91, 107, 120	11 (14%)
All	All	628/654 (96%)	0.97	95 (15%) 2 1	30, 76, 105, 120	45 (7%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	SER	9.1
1	A	338	THR	8.7
2	D	19	PRO	6.7
1	B	175	TRP	6.1
2	D	61	ILE	6.0
1	B	197	GLY	5.8
1	A	175	TRP	5.5
1	A	140	ASN	5.3
2	C	73	LEU	5.2
1	B	144	THR	5.0
1	B	191	ASP	5.0
2	C	8	LEU	4.9
1	A	139	VAL	4.9
1	B	121	THR	4.9
2	D	46	ALA	4.7
1	B	120	LEU	4.6
2	C	64	GLU	4.4
1	A	173	VAL	4.3
1	B	333	LEU	4.2
1	A	216	VAL	4.2
2	C	4	PHE	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	219	PHE	3.9
2	C	1	MET	3.8
2	D	8	LEU	3.8
2	C	3	ILE	3.7
1	B	242	SER	3.7
2	C	9	THR	3.7
2	D	4	PHE	3.6
1	A	134	MET	3.6
1	A	332	SER	3.5
1	A	194	MET	3.5
1	B	176	HIS	3.4
1	B	245	ALA	3.4
2	D	15	LEU	3.4
2	D	64	GLU	3.3
1	B	178	PRO	3.3
1	B	243	LEU	3.2
2	C	61	ILE	3.2
1	A	137	GLN	3.1
1	A	93	ASP	3.1
1	A	147	CYS	3.1
1	A	331	SER	3.1
1	A	209	VAL	3.0
1	B	88	PRO	3.0
1	B	164	LEU	3.0
1	A	246	ILE	3.0
1	B	196	SER	3.0
1	A	123	PHE	2.9
2	C	21	ASP	2.9
2	D	44	ILE	2.9
1	A	329	ARG	2.9
1	B	180	ALA	2.8
1	A	180	ALA	2.8
1	B	280	PHE	2.8
1	A	183	GLN	2.8
1	A	188	THR	2.7
1	A	181	ASP	2.7
1	B	188	THR	2.7
1	B	166	THR	2.7
1	B	246	ILE	2.7
2	C	36	ILE	2.7
2	C	74	ARG	2.6
1	B	143	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	333	LEU	2.6
2	C	63	LYS	2.5
1	B	273	LYS	2.5
1	B	286	CYS	2.4
1	B	205	VAL	2.4
1	B	211	ILE	2.4
1	B	264	PHE	2.4
2	D	67	LEU	2.4
2	C	50	LEU	2.3
2	C	51	GLU	2.3
1	B	260	LEU	2.3
1	A	277	PRO	2.3
1	B	190	MET	2.3
1	A	264	PHE	2.3
1	B	185	ALA	2.2
2	D	36	ILE	2.2
1	A	130	CYS	2.2
2	C	72	ARG	2.2
1	A	125	PHE	2.2
1	B	241	VAL	2.2
1	A	215	CYS	2.1
2	D	16	GLU	2.1
2	C	14	THR	2.1
2	D	39	ASP	2.1
2	D	24	GLU	2.1
2	D	47	GLY	2.1
1	A	330	TYR	2.1
2	C	7	THR	2.1
1	B	177	ASP	2.1
1	B	202	SER	2.0
2	D	35	GLY	2.0
2	C	75	GLY	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.