



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:29 am GMT

PDB ID : 2AYO
Title : Structure of USP14 bound to ubiquitin aldehyde
Authors : Hu, M.; Li, P.; Jeffrey, P.D.; Shi, Y.
Deposited on : 2005-09-07
Resolution : 3.50 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
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) : recalc28949

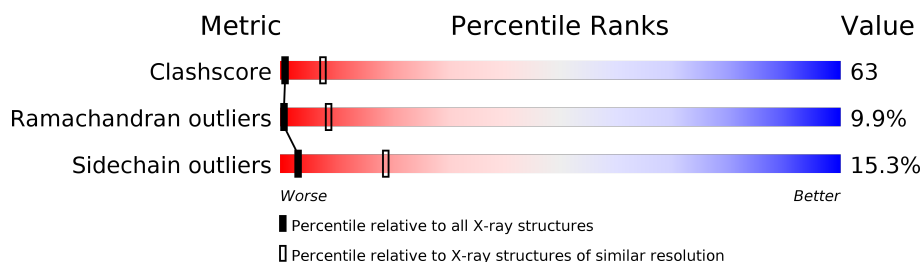
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

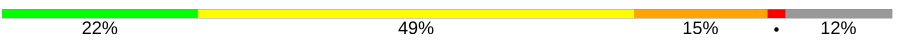

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)

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	404	
2	B	76	

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
2	GLZ	B	76	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3411 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 Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2810	1782	470	538	20			

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	10	0	0
			601	378	105	117	1			

There is a discrepancy between the modelled and reference sequences:

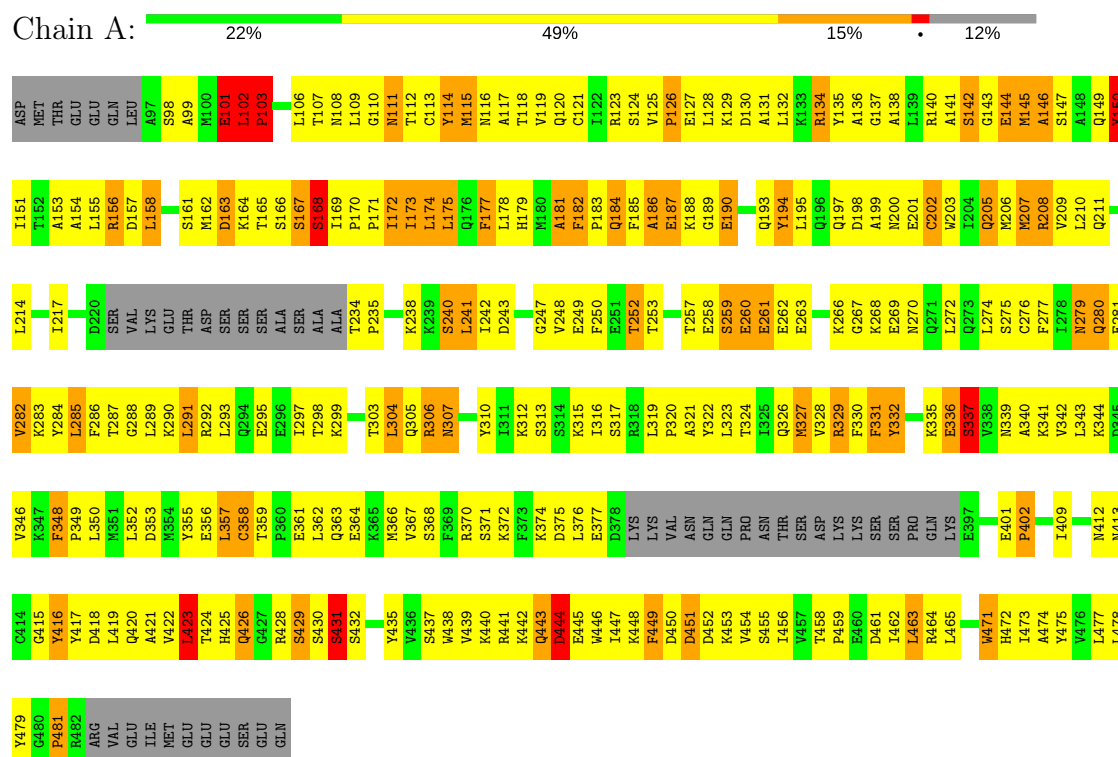
Chain	Residue	Modelled	Actual	Comment	Reference
B	76	GLZ	GLY	MODIFIED RESIDUE	UNP P62988

3 Residue-property plots

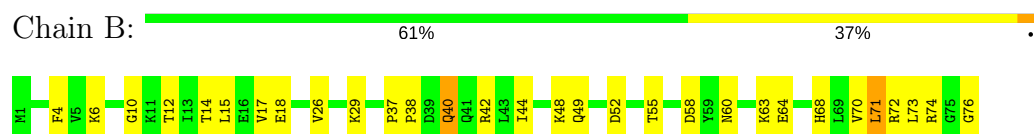
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Ubiquitin carboxyl-terminal hydrolase 14



- Molecule 2: Ubiquitin



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	183.93Å 183.93Å 45.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (99.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.290 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3411	wwPDB-VP
Average B, all atoms (Å ²)	93.0	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: GLZ

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	0.63	0/2860	0.92	6/3852 (0.2%)
2	B	0.47	0/603	0.75	1/811 (0.1%)
All	All	0.60	0/3463	0.89	7/4663 (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	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	102	LEU	N-CA-C	8.92	135.07	111.00
1	A	103	PRO	N-CA-C	6.79	129.74	112.10
1	A	402	PRO	N-CA-CB	6.43	111.01	103.30
1	A	101	GLU	N-CA-C	6.06	127.36	111.00
1	A	423	LEU	N-CA-C	-5.47	96.23	111.00
2	B	52	ASP	N-CA-C	5.11	124.81	111.00
1	A	279	ASN	N-CA-C	-5.04	97.38	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	TYR	Sidechain

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	2810	0	2766	414	0
2	B	601	0	630	60	0
All	All	3411	0	3396	426	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 63.

All (426) 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:319:LEU:O	1:A:412:ASN:HB3	1.37	1.24
1:A:424:THR:HG21	1:A:472:HIS:HB3	1.24	1.17
1:A:292:ARG:NH2	2:B:68:HIS:CE1	2.19	1.11
1:A:282:VAL:HG13	1:A:287:THR:HB	1.25	1.10
1:A:238:LYS:NZ	1:A:412:ASN:HD21	1.50	1.09
1:A:203:TRP:HE1	1:A:207:MET:CE	1.64	1.08
1:A:165:THR:HG22	1:A:166:SER:N	1.66	1.07
1:A:165:THR:CG2	1:A:166:SER:H	1.68	1.06
1:A:165:THR:HG22	1:A:166:SER:H	0.93	1.03
2:B:15:LEU:HD11	2:B:29:LYS:HB3	1.40	1.02
1:A:203:TRP:HE1	1:A:207:MET:HE2	1.27	1.00
1:A:280:GLN:HE22	1:A:344:LYS:HD3	1.28	0.98
1:A:359:THR:O	1:A:363:GLN:HG3	1.65	0.96
1:A:292:ARG:HG3	2:B:6:LYS:NZ	1.81	0.96
1:A:443:GLN:O	1:A:444:ASP:HB2	1.65	0.96
1:A:115:MET:HE2	1:A:174:LEU:HD11	1.47	0.95
1:A:113:CYS:SG	2:B:76:GLZ:C	2.55	0.94
1:A:199:ALA:HB2	1:A:435:TYR:CE1	2.02	0.94
1:A:292:ARG:HH22	2:B:68:HIS:CE1	1.83	0.91
1:A:292:ARG:HG3	2:B:6:LYS:HZ1	1.34	0.91
1:A:307:ASN:H	1:A:307:ASN:HD22	1.14	0.91
1:A:114:TYR:CD2	1:A:115:MET:N	2.40	0.89
1:A:292:ARG:NE	2:B:6:LYS:HZ3	1.70	0.88
1:A:367:VAL:O	1:A:371:SER:HB2	1.73	0.88
1:A:292:ARG:NH2	2:B:68:HIS:ND1	2.21	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:THR:CG2	1:A:472:HIS:HB3	2.03	0.88
1:A:292:ARG:HE	2:B:6:LYS:NZ	1.71	0.88
1:A:426:GLN:HB3	1:A:472:HIS:ND1	1.89	0.87
1:A:165:THR:HG22	1:A:167:SER:H	1.39	0.87
1:A:131:ALA:HB1	1:A:214:LEU:HD22	1.55	0.87
1:A:277:PHE:HE1	1:A:292:ARG:HD2	1.39	0.86
1:A:175:LEU:O	1:A:175:LEU:HD12	1.76	0.86
1:A:292:ARG:HE	2:B:6:LYS:HZ3	0.87	0.86
1:A:277:PHE:CE1	1:A:292:ARG:HD2	2.12	0.85
1:A:292:ARG:HG3	2:B:6:LYS:CE	2.07	0.84
1:A:203:TRP:HE1	1:A:207:MET:HE1	1.42	0.84
1:A:442:LYS:HD3	1:A:445:GLU:OE1	1.76	0.84
1:A:298:THR:O	2:B:14:THR:HG21	1.77	0.83
1:A:352:LEU:HB3	1:A:417:TYR:HB2	1.61	0.82
1:A:316:ILE:HG21	1:A:319:LEU:HD21	1.62	0.81
1:A:275:SER:HB2	1:A:292:ARG:HH11	1.45	0.81
1:A:124:SER:O	1:A:126:PRO:HD3	1.80	0.81
1:A:238:LYS:NZ	1:A:412:ASN:ND2	2.29	0.81
1:A:154:ALA:HB2	1:A:177:PHE:HD1	1.46	0.80
1:A:115:MET:CE	1:A:174:LEU:HD11	2.11	0.80
1:A:238:LYS:HZ2	1:A:412:ASN:HD21	1.28	0.80
2:B:15:LEU:HD11	2:B:29:LYS:CB	2.12	0.80
1:A:430:SER:O	1:A:431:SER:HB2	1.78	0.80
1:A:102:LEU:CD1	1:A:103:PRO:HD3	2.13	0.79
1:A:441:ARG:O	1:A:442:LYS:HG3	1.83	0.79
1:A:123:ARG:HH21	1:A:162:MET:HB3	1.48	0.77
1:A:174:LEU:HD22	1:A:174:LEU:O	1.85	0.77
1:A:283:LYS:HA	1:A:283:LYS:HE2	1.65	0.77
1:A:292:ARG:CG	2:B:6:LYS:HZ1	1.97	0.77
1:A:425:HIS:HB2	1:A:435:TYR:CE2	2.20	0.76
1:A:173:ILE:HG13	1:A:174:LEU:H	1.50	0.76
1:A:293:LEU:HD11	1:A:357:LEU:HD21	1.65	0.76
1:A:250:PHE:O	1:A:268:LYS:HG2	1.86	0.76
1:A:114:TYR:HD2	1:A:115:MET:N	1.82	0.75
1:A:154:ALA:HB2	1:A:177:PHE:CD1	2.21	0.75
1:A:259:SER:O	1:A:261:GLU:N	2.19	0.75
1:A:316:ILE:HG21	1:A:319:LEU:CD2	2.15	0.75
1:A:103:PRO:HB3	1:A:454:VAL:HG11	1.66	0.75
1:A:101:GLU:C	1:A:102:LEU:HG	2.07	0.75
1:A:165:THR:HG22	1:A:167:SER:N	2.02	0.74
1:A:203:TRP:NE1	1:A:207:MET:HE2	2.02	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:HD21	1:A:463:LEU:HD11	1.70	0.73
1:A:292:ARG:HH21	2:B:68:HIS:CE1	2.02	0.73
1:A:292:ARG:HG3	2:B:6:LYS:HE2	1.69	0.73
1:A:319:LEU:O	1:A:412:ASN:CB	2.30	0.73
1:A:199:ALA:HB2	1:A:435:TYR:CD1	2.24	0.72
1:A:197:GLN:NE2	2:B:74:ARG:HH12	1.86	0.72
1:A:307:ASN:ND2	1:A:307:ASN:H	1.86	0.72
1:A:238:LYS:HZ1	1:A:412:ASN:HD21	1.36	0.72
1:A:199:ALA:CB	1:A:435:TYR:CE1	2.72	0.72
1:A:350:LEU:HD11	1:A:463:LEU:HD11	1.72	0.71
1:A:422:VAL:HG12	1:A:423:LEU:N	2.05	0.71
1:A:111:ASN:CA	2:B:76:GLZ:HA1	2.20	0.71
1:A:292:ARG:CG	2:B:6:LYS:NZ	2.52	0.71
1:A:115:MET:O	1:A:119:VAL:HG23	1.92	0.70
1:A:200:ASN:HB2	1:A:475:TYR:HE2	1.55	0.70
1:A:343:LEU:O	1:A:343:LEU:HG	1.91	0.69
1:A:352:LEU:HD23	1:A:417:TYR:HD1	1.58	0.69
1:A:193:GLN:O	1:A:194:TYR:HB2	1.92	0.69
1:A:425:HIS:CD2	1:A:435:TYR:HE2	2.11	0.69
1:A:448:LYS:O	1:A:448:LYS:HG2	1.91	0.69
1:A:426:GLN:HG2	1:A:472:HIS:CE1	2.28	0.68
1:A:275:SER:HB2	1:A:292:ARG:NH1	2.08	0.68
1:A:330:PHE:N	1:A:342:VAL:HG23	2.07	0.68
1:A:127:GLU:HG2	1:A:322:TYR:OH	1.92	0.68
1:A:331:PHE:O	1:A:340:ALA:HB3	1.94	0.68
1:A:158:LEU:HD12	1:A:173:ILE:HD11	1.76	0.68
1:A:363:GLN:O	1:A:367:VAL:HG23	1.93	0.68
1:A:234:THR:HB	1:A:235:PRO:HD3	1.74	0.67
1:A:113:CYS:HA	1:A:116:ASN:HD22	1.61	0.66
1:A:203:TRP:NE1	1:A:207:MET:CE	2.49	0.66
1:A:111:ASN:HA	2:B:76:GLZ:HA1	1.75	0.66
1:A:242:ILE:CG2	1:A:272:LEU:HD21	2.26	0.66
1:A:326:GLN:HG2	1:A:326:GLN:O	1.94	0.65
1:A:446:TRP:CD1	1:A:462:ILE:HD11	2.31	0.65
1:A:295:GLU:OE2	1:A:312:LYS:HD2	1.97	0.65
1:A:286:PHE:CZ	1:A:357:LEU:HD12	2.32	0.65
1:A:317:SER:O	1:A:362:LEU:HD12	1.96	0.65
1:A:249:GLU:O	1:A:250:PHE:HD2	1.79	0.64
1:A:102:LEU:HD13	1:A:103:PRO:HD3	1.78	0.64
1:A:140:ARG:HB2	1:A:149:GLN:NE2	2.13	0.64
1:A:183:PRO:O	1:A:185:PHE:N	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:PHE:HA	1:A:289:LEU:HD12	1.78	0.63
1:A:475:TYR:CE1	2:B:73:LEU:HD12	2.33	0.63
1:A:307:ASN:N	1:A:307:ASN:HD22	1.91	0.63
1:A:143:GLY:O	1:A:144:GLU:HB2	1.99	0.63
1:A:475:TYR:CD1	2:B:73:LEU:HD12	2.32	0.63
1:A:435:TYR:OH	2:B:73:LEU:O	2.13	0.63
1:A:206:MET:O	1:A:209:VAL:HG23	1.99	0.63
1:A:113:CYS:N	2:B:76:GLZ:O	2.30	0.63
1:A:140:ARG:HB2	1:A:149:GLN:HE21	1.64	0.63
1:A:207:MET:HG3	1:A:242:ILE:HD13	1.79	0.63
1:A:114:TYR:HA	1:A:435:TYR:HD1	1.63	0.62
1:A:280:GLN:HE22	1:A:344:LYS:CD	2.07	0.62
1:A:286:PHE:O	1:A:289:LEU:HB2	1.98	0.62
1:A:123:ARG:HH11	1:A:123:ARG:HG2	1.65	0.62
1:A:329:ARG:HG2	1:A:342:VAL:O	1.99	0.62
1:A:330:PHE:CE2	2:B:70:VAL:HG13	2.35	0.62
1:A:366:MET:O	1:A:370:ARG:HB3	2.00	0.62
1:A:238:LYS:HZ2	1:A:412:ASN:ND2	1.95	0.62
1:A:153:ALA:HA	1:A:156:ARG:HE	1.64	0.62
1:A:185:PHE:O	1:A:186:ALA:HB2	1.99	0.61
1:A:290:LYS:C	1:A:292:ARG:H	2.04	0.61
1:A:199:ALA:N	1:A:435:TYR:HE1	1.99	0.61
1:A:339:ASN:OD1	2:B:40:GLN:NE2	2.34	0.61
1:A:258:GLU:O	1:A:260:GLU:N	2.34	0.61
1:A:173:ILE:CG1	1:A:174:LEU:H	2.14	0.61
1:A:165:THR:CG2	1:A:167:SER:H	2.09	0.60
1:A:280:GLN:NE2	1:A:344:LYS:HD3	2.09	0.60
1:A:120:GLN:CD	1:A:449:PHE:HD2	2.04	0.60
1:A:307:ASN:ND2	1:A:307:ASN:N	2.47	0.60
1:A:440:LYS:HD2	1:A:446:TRP:CZ3	2.36	0.60
1:A:339:ASN:O	1:A:429:SER:HB3	2.02	0.59
1:A:173:ILE:O	1:A:177:PHE:HB2	2.03	0.59
1:A:141:ALA:O	1:A:142:SER:HB3	2.02	0.59
1:A:366:MET:HE2	1:A:415:GLY:H	1.67	0.59
1:A:422:VAL:HG12	1:A:423:LEU:H	1.66	0.59
1:A:370:ARG:O	1:A:374:LYS:HB2	2.01	0.59
1:A:175:LEU:CD1	1:A:179:HIS:ND1	2.66	0.59
1:A:168:SER:O	1:A:170:PRO:HD3	2.03	0.59
1:A:199:ALA:H	1:A:435:TYR:HE1	1.48	0.58
1:A:113:CYS:SG	2:B:76:GLZ:CA	2.91	0.58
1:A:291:LEU:HD12	1:A:291:LEU:N	2.17	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:HIS:CD2	1:A:185:PHE:O	2.55	0.58
1:A:275:SER:CB	1:A:292:ARG:NH1	2.66	0.58
1:A:128:LEU:O	1:A:131:ALA:HB3	2.02	0.58
1:A:118:THR:HG21	1:A:202:CYS:SG	2.44	0.58
1:A:138:ALA:C	1:A:140:ARG:H	2.05	0.58
1:A:203:TRP:NE1	1:A:207:MET:HE1	2.15	0.58
1:A:303:THR:O	1:A:304:LEU:HG	2.04	0.58
1:A:198:ASP:CB	2:B:72:ARG:HG2	2.33	0.57
1:A:329:ARG:HG2	1:A:329:ARG:NH1	2.18	0.57
2:B:17:VAL:HG12	2:B:29:LYS:HE3	1.85	0.57
1:A:299:LYS:HD2	1:A:310:TYR:CD2	2.40	0.57
1:A:329:ARG:NH1	1:A:342:VAL:O	2.37	0.57
1:A:208:ARG:HG2	2:B:48:LYS:CD	2.34	0.57
1:A:165:THR:HG21	1:A:167:SER:OG	2.05	0.57
1:A:458:THR:O	1:A:461:ASP:HB2	2.03	0.57
1:A:446:TRP:CD1	1:A:462:ILE:CD1	2.87	0.57
1:A:419:LEU:HD12	1:A:420:GLN:H	1.70	0.57
1:A:353:ASP:CG	1:A:370:ARG:HH21	2.08	0.56
1:A:178:LEU:O	1:A:181:ALA:HB3	2.04	0.56
1:A:199:ALA:HB2	1:A:435:TYR:HE1	1.64	0.56
1:A:282:VAL:HG11	1:A:288:GLY:N	2.20	0.56
1:A:438:TRP:N	1:A:438:TRP:CD1	2.73	0.56
1:A:447:ILE:HG21	1:A:449:PHE:HE1	1.69	0.56
1:A:320:PRO:O	1:A:417:TYR:OH	2.18	0.56
1:A:329:ARG:HH11	1:A:329:ARG:HG2	1.70	0.56
1:A:150:TYR:HD1	1:A:151:ILE:N	2.04	0.56
1:A:422:VAL:CG1	1:A:423:LEU:N	2.69	0.56
1:A:287:THR:O	1:A:291:LEU:HD13	2.06	0.56
1:A:121:CYS:SG	1:A:423:LEU:HD23	2.45	0.56
1:A:368:SER:O	1:A:372:LYS:CB	2.54	0.55
1:A:420:GLN:OE1	1:A:478:LEU:HD23	2.06	0.55
1:A:150:TYR:HB2	1:A:177:PHE:CZ	2.41	0.55
1:A:282:VAL:O	1:A:283:LYS:CE	2.54	0.55
1:A:279:ASN:C	1:A:281:GLU:H	2.08	0.55
1:A:174:LEU:O	1:A:178:LEU:N	2.39	0.55
1:A:442:LYS:HB2	1:A:445:GLU:HB2	1.87	0.55
1:A:329:ARG:HA	1:A:342:VAL:HB	1.88	0.55
1:A:162:MET:HA	1:A:169:ILE:CD1	2.37	0.55
1:A:366:MET:CE	1:A:415:GLY:O	2.55	0.55
1:A:364:GLU:HA	1:A:367:VAL:HG23	1.89	0.55
1:A:153:ALA:O	1:A:156:ARG:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HD12	1:A:175:LEU:C	2.27	0.54
1:A:248:VAL:HG12	1:A:320:PRO:HD3	1.89	0.54
1:A:257:THR:O	1:A:257:THR:HG22	2.08	0.54
1:A:252:THR:O	1:A:267:GLY:N	2.41	0.54
1:A:282:VAL:HG11	1:A:288:GLY:H	1.73	0.54
1:A:425:HIS:CD2	1:A:435:TYR:CE2	2.94	0.54
1:A:252:THR:O	1:A:266:LYS:HA	2.07	0.54
1:A:425:HIS:HD2	1:A:435:TYR:HE2	1.52	0.54
1:A:116:ASN:O	1:A:120:GLN:HG3	2.07	0.54
1:A:282:VAL:O	1:A:283:LYS:HE2	2.08	0.54
1:A:299:LYS:HD2	1:A:310:TYR:CE2	2.42	0.54
1:A:114:TYR:HE1	1:A:197:GLN:H	1.54	0.54
1:A:290:LYS:O	1:A:292:ARG:N	2.41	0.54
1:A:447:ILE:HG21	1:A:449:PHE:CE1	2.43	0.54
1:A:102:LEU:HB2	1:A:103:PRO:HD3	1.89	0.54
1:A:103:PRO:HB3	1:A:454:VAL:CG1	2.36	0.54
1:A:174:LEU:HD22	1:A:174:LEU:C	2.28	0.54
1:A:179:HIS:NE2	1:A:185:PHE:O	2.41	0.54
1:A:343:LEU:HD23	1:A:343:LEU:H	1.73	0.54
1:A:442:LYS:O	1:A:444:ASP:N	2.40	0.54
1:A:115:MET:CE	1:A:174:LEU:CD1	2.85	0.54
1:A:240:SER:OG	1:A:243:ASP:HB2	2.08	0.53
1:A:364:GLU:O	1:A:367:VAL:HB	2.09	0.53
1:A:121:CYS:O	1:A:124:SER:OG	2.17	0.53
1:A:205:GLN:O	1:A:209:VAL:HG22	2.08	0.53
1:A:211:GLN:N	1:A:242:ILE:HD12	2.23	0.53
1:A:366:MET:O	1:A:370:ARG:CB	2.57	0.53
2:B:63:LYS:O	2:B:64:GLU:HB2	2.09	0.53
1:A:119:VAL:O	1:A:119:VAL:HG12	2.09	0.53
1:A:331:PHE:CD2	1:A:342:VAL:HG22	2.43	0.53
1:A:108:ASN:C	1:A:108:ASN:OD1	2.47	0.53
1:A:199:ALA:CB	1:A:435:TYR:HE1	2.19	0.53
1:A:242:ILE:HG22	1:A:272:LEU:HD21	1.90	0.53
1:A:422:VAL:CG1	1:A:423:LEU:H	2.22	0.53
1:A:120:GLN:NE2	1:A:449:PHE:CD2	2.77	0.53
1:A:450:ASP:HB3	1:A:453:LYS:HB2	1.91	0.53
1:A:428:ARG:O	1:A:429:SER:C	2.48	0.52
1:A:102:LEU:CB	1:A:103:PRO:HD3	2.39	0.52
1:A:348:PHE:CD1	1:A:348:PHE:N	2.78	0.52
1:A:297:ILE:HD11	1:A:312:LYS:HE3	1.92	0.52
1:A:123:ARG:HH21	1:A:162:MET:CB	2.22	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:PRO:O	1:A:184:GLN:C	2.48	0.52
1:A:275:SER:OG	1:A:292:ARG:NH1	2.43	0.52
1:A:210:LEU:HD22	1:A:214:LEU:HD11	1.92	0.51
1:A:359:THR:C	1:A:363:GLN:HE21	2.13	0.51
1:A:183:PRO:C	1:A:185:PHE:N	2.63	0.51
1:A:439:VAL:HG12	1:A:440:LYS:N	2.24	0.51
1:A:366:MET:CE	1:A:415:GLY:H	2.23	0.51
1:A:425:HIS:ND1	1:A:425:HIS:C	2.64	0.51
1:A:355:TYR:CE1	1:A:363:GLN:HB3	2.45	0.51
1:A:366:MET:O	1:A:370:ARG:N	2.43	0.51
1:A:137:GLY:N	1:A:156:ARG:HH22	2.09	0.51
1:A:362:LEU:C	1:A:362:LEU:HD23	2.31	0.51
2:B:42:ARG:HB2	2:B:70:VAL:O	2.11	0.51
1:A:352:LEU:HB3	1:A:417:TYR:CB	2.37	0.51
1:A:353:ASP:OD2	1:A:370:ARG:NH2	2.44	0.51
1:A:258:GLU:O	1:A:260:GLU:HB3	2.11	0.51
2:B:42:ARG:HD2	2:B:49:GLN:OE1	2.11	0.51
1:A:102:LEU:HD12	1:A:103:PRO:HD3	1.90	0.50
1:A:249:GLU:HG2	1:A:270:ASN:OD1	2.11	0.50
1:A:259:SER:O	1:A:260:GLU:C	2.50	0.50
1:A:130:ASP:O	1:A:134:ARG:HG2	2.11	0.50
1:A:475:TYR:CE1	2:B:73:LEU:CD1	2.95	0.50
1:A:125:VAL:O	1:A:128:LEU:HB3	2.11	0.50
1:A:320:PRO:HG2	1:A:323:LEU:HD12	1.93	0.50
1:A:450:ASP:O	1:A:451:ASP:C	2.50	0.50
1:A:108:ASN:OD1	1:A:109:LEU:N	2.44	0.50
1:A:279:ASN:O	1:A:281:GLU:N	2.45	0.50
1:A:330:PHE:N	1:A:342:VAL:CG2	2.74	0.50
1:A:153:ALA:CA	1:A:156:ARG:HE	2.24	0.49
1:A:172:ILE:HG13	1:A:173:ILE:H	1.77	0.49
1:A:185:PHE:CD2	1:A:185:PHE:N	2.79	0.49
1:A:260:GLU:O	1:A:261:GLU:CB	2.61	0.49
1:A:290:LYS:HA	1:A:293:LEU:CD1	2.43	0.49
1:A:252:THR:CG2	1:A:267:GLY:O	2.61	0.49
1:A:336:GLU:O	1:A:337:SER:HB2	2.12	0.49
1:A:315:LYS:HD3	1:A:358:CYS:O	2.12	0.49
1:A:137:GLY:CA	1:A:140:ARG:HD2	2.43	0.49
1:A:252:THR:HG22	1:A:267:GLY:O	2.13	0.49
1:A:253:THR:HG22	1:A:266:LYS:HD3	1.94	0.49
1:A:299:LYS:O	1:A:307:ASN:HA	2.13	0.49
1:A:329:ARG:CA	1:A:342:VAL:HB	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:PHE:CE1	1:A:205:GLN:HG2	2.47	0.49
1:A:137:GLY:HA3	1:A:140:ARG:HD2	1.95	0.48
1:A:145:MET:O	1:A:146:ALA:HB2	2.12	0.48
1:A:198:ASP:HB3	2:B:72:ARG:HG2	1.94	0.48
1:A:291:LEU:CD1	1:A:291:LEU:H	2.26	0.48
1:A:419:LEU:HA	1:A:479:TYR:CD2	2.48	0.48
1:A:326:GLN:HE22	2:B:70:VAL:HG21	1.78	0.48
1:A:108:ASN:OD1	1:A:110:GLY:N	2.31	0.48
1:A:277:PHE:CE2	2:B:10:GLY:HA2	2.48	0.48
1:A:141:ALA:O	1:A:142:SER:CB	2.61	0.48
1:A:247:GLY:O	1:A:320:PRO:HG3	2.13	0.48
1:A:199:ALA:O	1:A:202:CYS:HB3	2.14	0.48
1:A:181:ALA:O	1:A:183:PRO:HD3	2.13	0.48
1:A:208:ARG:HG2	2:B:48:LYS:HD3	1.95	0.48
1:A:368:SER:O	1:A:372:LYS:HB3	2.13	0.48
1:A:471:TRP:CG	1:A:472:HIS:N	2.81	0.48
1:A:274:LEU:HD22	1:A:323:LEU:HD21	1.96	0.48
1:A:290:LYS:HA	1:A:293:LEU:HD12	1.95	0.48
1:A:201:GLU:OE2	2:B:72:ARG:HD3	2.13	0.48
1:A:298:THR:CG2	1:A:307:ASN:HB3	2.44	0.48
1:A:425:HIS:HD2	1:A:435:TYR:CE2	2.30	0.47
1:A:426:GLN:HB3	1:A:472:HIS:HA	1.96	0.47
1:A:106:LEU:HD21	1:A:162:MET:SD	2.54	0.47
1:A:353:ASP:OD1	1:A:370:ARG:NH2	2.47	0.47
1:A:364:GLU:HA	1:A:367:VAL:CG2	2.44	0.47
1:A:290:LYS:C	1:A:292:ARG:N	2.68	0.47
1:A:291:LEU:CD1	1:A:291:LEU:N	2.76	0.47
1:A:287:THR:HG22	1:A:291:LEU:HD11	1.95	0.47
1:A:321:ALA:HA	1:A:413:ASN:HB2	1.95	0.47
1:A:103:PRO:CB	1:A:454:VAL:HG11	2.41	0.47
1:A:329:ARG:HB3	1:A:342:VAL:H	1.80	0.47
1:A:447:ILE:HG22	1:A:448:LYS:N	2.29	0.47
1:A:114:TYR:HA	1:A:435:TYR:CD1	2.47	0.47
2:B:15:LEU:CD2	2:B:26:VAL:HG13	2.44	0.47
1:A:114:TYR:CD2	1:A:114:TYR:C	2.87	0.47
1:A:171:PRO:HB3	1:A:174:LEU:HD12	1.96	0.47
1:A:284:TYR:O	1:A:285:LEU:C	2.51	0.47
1:A:170:PRO:O	1:A:172:ILE:HG12	2.15	0.47
1:A:189:GLY:O	1:A:190:GLU:C	2.53	0.47
1:A:112:THR:O	1:A:116:ASN:ND2	2.47	0.47
1:A:361:GLU:O	1:A:364:GLU:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:TYR:CD1	1:A:416:TYR:N	2.82	0.47
1:A:143:GLY:O	1:A:144:GLU:CB	2.61	0.46
1:A:282:VAL:O	1:A:283:LYS:HE3	2.14	0.46
1:A:316:ILE:HG21	1:A:319:LEU:HD23	1.94	0.46
1:A:280:GLN:NE2	1:A:344:LYS:CD	2.75	0.46
1:A:242:ILE:CG2	1:A:272:LEU:CD2	2.94	0.46
1:A:141:ALA:CB	1:A:150:TYR:HD2	2.29	0.46
1:A:197:GLN:NE2	2:B:74:ARG:NH1	2.62	0.46
1:A:368:SER:O	1:A:372:LYS:HB2	2.15	0.46
1:A:474:ALA:HB1	1:A:477:LEU:HD21	1.98	0.46
1:A:174:LEU:O	1:A:178:LEU:CB	2.64	0.46
1:A:240:SER:O	1:A:241:LEU:C	2.53	0.46
1:A:355:TYR:O	1:A:357:LEU:N	2.43	0.46
1:A:113:CYS:O	1:A:117:ALA:N	2.32	0.46
1:A:173:ILE:HG13	1:A:174:LEU:N	2.23	0.46
1:A:444:ASP:O	1:A:459:PRO:HD3	2.15	0.46
1:A:459:PRO:O	1:A:462:ILE:N	2.48	0.46
1:A:425:HIS:HD1	1:A:425:HIS:C	2.19	0.46
1:A:150:TYR:O	1:A:153:ALA:N	2.46	0.45
1:A:440:LYS:HD2	1:A:446:TRP:CH2	2.51	0.45
1:A:107:THR:CB	1:A:170:PRO:HG3	2.46	0.45
1:A:185:PHE:O	1:A:186:ALA:CB	2.64	0.45
1:A:117:ALA:HA	1:A:437:SER:HB2	1.98	0.45
1:A:162:MET:HA	1:A:169:ILE:HD11	1.97	0.45
1:A:422:VAL:HG11	1:A:465:LEU:HD13	1.98	0.45
1:A:129:LYS:O	1:A:132:LEU:N	2.48	0.45
1:A:167:SER:OG	1:A:168:SER:N	2.48	0.45
1:A:198:ASP:C	1:A:198:ASP:OD1	2.54	0.45
1:A:206:MET:O	1:A:209:VAL:CG2	2.64	0.45
1:A:107:THR:HB	1:A:170:PRO:HG3	1.97	0.45
1:A:298:THR:O	2:B:14:THR:CG2	2.59	0.45
1:A:150:TYR:HD1	1:A:151:ILE:H	1.64	0.45
1:A:162:MET:HA	1:A:169:ILE:HD12	1.98	0.45
1:A:279:ASN:C	1:A:281:GLU:N	2.68	0.45
1:A:280:GLN:NE2	1:A:344:LYS:NZ	2.64	0.45
1:A:328:VAL:O	1:A:328:VAL:HG12	2.16	0.45
1:A:173:ILE:O	1:A:177:PHE:N	2.45	0.45
1:A:120:GLN:HA	1:A:123:ARG:HB2	1.99	0.45
1:A:117:ALA:O	1:A:118:THR:C	2.55	0.45
1:A:366:MET:HE1	1:A:415:GLY:O	2.17	0.45
1:A:359:THR:HG22	1:A:361:GLU:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:SER:OG	1:A:169:ILE:HD13	2.17	0.44
1:A:200:ASN:HB2	1:A:475:TYR:CE2	2.45	0.44
1:A:111:ASN:HA	2:B:76:GLZ:CA	2.44	0.44
1:A:138:ALA:C	1:A:140:ARG:N	2.70	0.44
1:A:425:HIS:HB2	1:A:435:TYR:HE2	1.77	0.44
1:A:330:PHE:HE2	2:B:70:VAL:HG13	1.80	0.44
1:A:282:VAL:CG1	1:A:288:GLY:N	2.80	0.44
1:A:352:LEU:HD23	1:A:417:TYR:CD1	2.45	0.44
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.82	0.44
1:A:428:ARG:O	1:A:429:SER:O	2.36	0.43
1:A:292:ARG:NE	2:B:6:LYS:NZ	2.47	0.43
1:A:198:ASP:HB2	2:B:72:ARG:HG2	2.00	0.43
1:A:426:GLN:CB	1:A:472:HIS:HA	2.49	0.43
1:A:285:LEU:O	1:A:286:PHE:C	2.57	0.43
1:A:341:LYS:NZ	1:A:473:ILE:HD12	2.34	0.43
1:A:120:GLN:CD	1:A:449:PHE:CD2	2.89	0.43
1:A:353:ASP:CG	1:A:370:ARG:NH2	2.73	0.43
1:A:439:VAL:CG1	1:A:440:LYS:N	2.82	0.43
1:A:277:PHE:CD2	2:B:10:GLY:HA2	2.54	0.43
1:A:198:ASP:OD1	1:A:200:ASN:N	2.52	0.43
1:A:118:THR:HG22	1:A:206:MET:HE2	2.01	0.43
1:A:241:LEU:HD13	1:A:241:LEU:O	2.19	0.42
2:B:4:PHE:HB3	2:B:12:THR:CG2	2.49	0.42
1:A:349:PRO:HG2	1:A:352:LEU:HD12	2.01	0.42
1:A:366:MET:HE2	1:A:415:GLY:O	2.19	0.42
1:A:425:HIS:HB2	1:A:435:TYR:CD2	2.54	0.42
1:A:110:GLY:O	1:A:111:ASN:ND2	2.51	0.42
1:A:165:THR:CG2	1:A:166:SER:N	2.39	0.42
2:B:37:PRO:HA	2:B:38:PRO:HD3	1.90	0.42
1:A:201:GLU:HG3	2:B:49:GLN:OE1	2.19	0.42
1:A:163:ASP:C	1:A:164:LYS:HG3	2.40	0.42
1:A:332:TYR:C	1:A:332:TYR:CD1	2.93	0.42
1:A:170:PRO:HA	1:A:171:PRO:HD3	1.91	0.42
1:A:107:THR:OG1	1:A:170:PRO:HG3	2.19	0.42
1:A:106:LEU:HD22	1:A:171:PRO:HG3	2.02	0.42
1:A:315:LYS:HB3	1:A:358:CYS:O	2.19	0.42
1:A:113:CYS:CB	2:B:76:GLZ:O	2.67	0.42
1:A:276:CYS:SG	1:A:276:CYS:O	2.77	0.42
1:A:123:ARG:HH11	1:A:123:ARG:CG	2.32	0.42
1:A:370:ARG:O	1:A:374:LYS:CB	2.67	0.42
1:A:424:THR:HG1	1:A:438:TRP:HE1	1.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASN:HA	2:B:76:GLZ:C	2.50	0.42
1:A:177:PHE:HA	1:A:177:PHE:HD2	1.71	0.42
1:A:249:GLU:C	1:A:317:SER:HB3	2.41	0.42
2:B:44:ILE:HD13	2:B:49:GLN:HA	2.02	0.42
1:A:292:ARG:NH2	2:B:68:HIS:HE1	2.05	0.41
1:A:420:GLN:HB3	1:A:421:ALA:H	1.66	0.41
1:A:119:VAL:O	1:A:119:VAL:CG1	2.68	0.41
1:A:421:ALA:HB3	1:A:478:LEU:HB3	2.02	0.41
1:A:181:ALA:HB1	1:A:182:PHE:CE2	2.56	0.41
1:A:187:GLU:HB2	1:A:195:LEU:HD12	2.01	0.41
1:A:442:LYS:CB	1:A:445:GLU:HB2	2.50	0.41
1:A:462:ILE:C	1:A:464:ARG:H	2.23	0.41
1:A:130:ASP:N	1:A:130:ASP:OD2	2.49	0.41
1:A:151:ILE:HD11	1:A:181:ALA:CB	2.51	0.41
1:A:250:PHE:HB2	1:A:269:GLU:O	2.21	0.41
1:A:208:ARG:HG2	2:B:48:LYS:HZ3	1.85	0.41
1:A:135:TYR:CD1	1:A:136:ALA:N	2.87	0.41
1:A:321:ALA:O	1:A:481:PRO:HD3	2.21	0.41
1:A:471:TRP:CE3	1:A:471:TRP:HA	2.56	0.41
1:A:113:CYS:HG	2:B:76:GLZ:C	2.33	0.41
1:A:210:LEU:HD22	1:A:214:LEU:CD1	2.51	0.41
1:A:260:GLU:O	1:A:261:GLU:HB3	2.21	0.41
1:A:330:PHE:HB3	2:B:71:LEU:HD22	2.03	0.41
2:B:71:LEU:HB3	2:B:72:ARG:H	1.55	0.41
1:A:292:ARG:HH21	2:B:68:HIS:HE1	1.61	0.41
1:A:156:ARG:HD2	1:A:157:ASP:N	2.36	0.40
1:A:375:ASP:O	1:A:377:GLU:N	2.53	0.40
2:B:55:THR:O	2:B:58:ASP:HB2	2.21	0.40
1:A:262:GLU:O	1:A:263:GLU:C	2.59	0.40
1:A:305:GLN:O	1:A:306:ARG:HB3	2.22	0.40
1:A:330:PHE:CA	1:A:342:VAL:HG23	2.51	0.40
1:A:182:PHE:CD1	1:A:205:GLN:HG2	2.57	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	349/404 (86%)	240 (69%)	67 (19%)	42 (12%)	0	6
2	B	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
All	All	423/480 (88%)	311 (74%)	70 (16%)	42 (10%)	1	8

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ALA
1	A	167	SER
1	A	168	SER
1	A	181	ALA
1	A	190	GLU
1	A	259	SER
1	A	260	GLU
1	A	261	GLU
1	A	337	SER
1	A	356	GLU
1	A	376	LEU
1	A	402	PRO
1	A	409	ILE
1	A	449	PHE
1	A	451	ASP
1	A	142	SER
1	A	144	GLU
1	A	145	MET
1	A	173	ILE
1	A	184	GLN
1	A	186	ALA
1	A	280	GLN
1	A	291	LEU
1	A	327	MET
1	A	429	SER
1	A	431	SER
1	A	443	GLN
1	A	444	ASP
1	A	463	LEU
1	A	481	PRO
1	A	102	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	103	PRO
1	A	187	GLU
1	A	304	LEU
1	A	335	LYS
1	A	240	SER
1	A	285	LEU
1	A	306	ARG
1	A	471	TRP
1	A	194	TYR
1	A	99	ALA
1	A	401	GLU

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	305/363 (84%)	252 (83%)	53 (17%)	2	13
2	B	68/68 (100%)	64 (94%)	4 (6%)	23	61
All	All	373/431 (86%)	316 (85%)	57 (15%)	3	19

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	SER
1	A	101	GLU
1	A	102	LEU
1	A	103	PRO
1	A	111	ASN
1	A	114	TYR
1	A	115	MET
1	A	126	PRO
1	A	134	ARG
1	A	147	SER
1	A	150	TYR
1	A	155	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	156	ARG
1	A	158	LEU
1	A	163	ASP
1	A	168	SER
1	A	172	ILE
1	A	174	LEU
1	A	175	LEU
1	A	177	PHE
1	A	182	PHE
1	A	188	LYS
1	A	202	CYS
1	A	205	GLN
1	A	207	MET
1	A	208	ARG
1	A	217	ILE
1	A	241	LEU
1	A	252	THR
1	A	282	VAL
1	A	307	ASN
1	A	313	SER
1	A	324	THR
1	A	327	MET
1	A	329	ARG
1	A	331	PHE
1	A	332	TYR
1	A	336	GLU
1	A	337	SER
1	A	346	VAL
1	A	348	PHE
1	A	357	LEU
1	A	358	CYS
1	A	416	TYR
1	A	418	ASP
1	A	423	LEU
1	A	426	GLN
1	A	431	SER
1	A	432	SER
1	A	444	ASP
1	A	452	ASP
1	A	455	SER
1	A	456	ILE
2	B	18	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	40	GLN
2	B	60	ASN
2	B	71	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	116	ASN
1	A	149	GLN
1	A	197	GLN
1	A	205	GLN
1	A	280	GLN
1	A	307	ASN
1	A	326	GLN
1	A	339	ASN
1	A	363	GLN
1	A	412	ASN
1	A	426	GLN
1	A	443	GLN
2	B	25	ASN
2	B	40	GLN
2	B	60	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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
2	GLZ	B	76	2	3,3,3	2.26	1 (33%)	1,2,2	3.28	1 (100%)

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
2	GLZ	B	76	2	-	0/0/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	76	GLZ	O-C	3.86	1.43	1.19

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	76	GLZ	O-C-CA	-3.28	109.90	125.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	76	GLZ	9	0

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

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.