Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:40 PM GMT

PDB ID	:	4D1E
Title	:	THE CRYSTAL STRUCTURE OF HUMAN MUSCLE ALPHA-ACTININ-2
Authors	:	Pinotsis, N.; Salmazo, A.; Sjoeblom, B.; Gkougkoulia, E.; Djinovic-Carugo, K.
Deposited on	:	2014-05-01
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

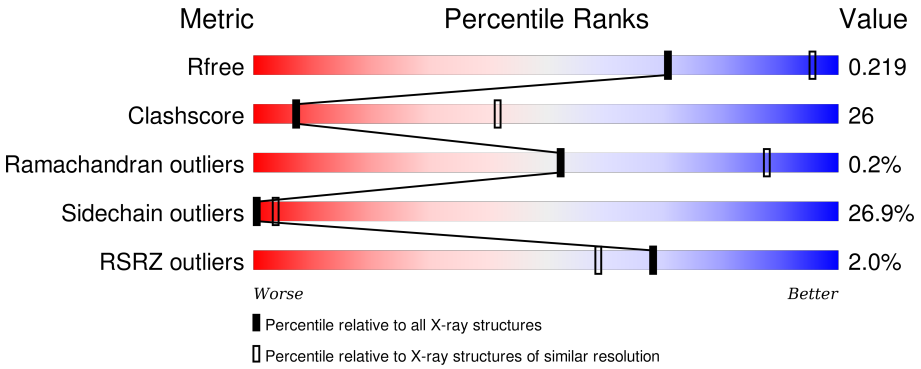
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (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 <=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	876	2% 43% 42% 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6865 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 ALPHA-ACTININ-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	859	6865	4305	1226	1301	33	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

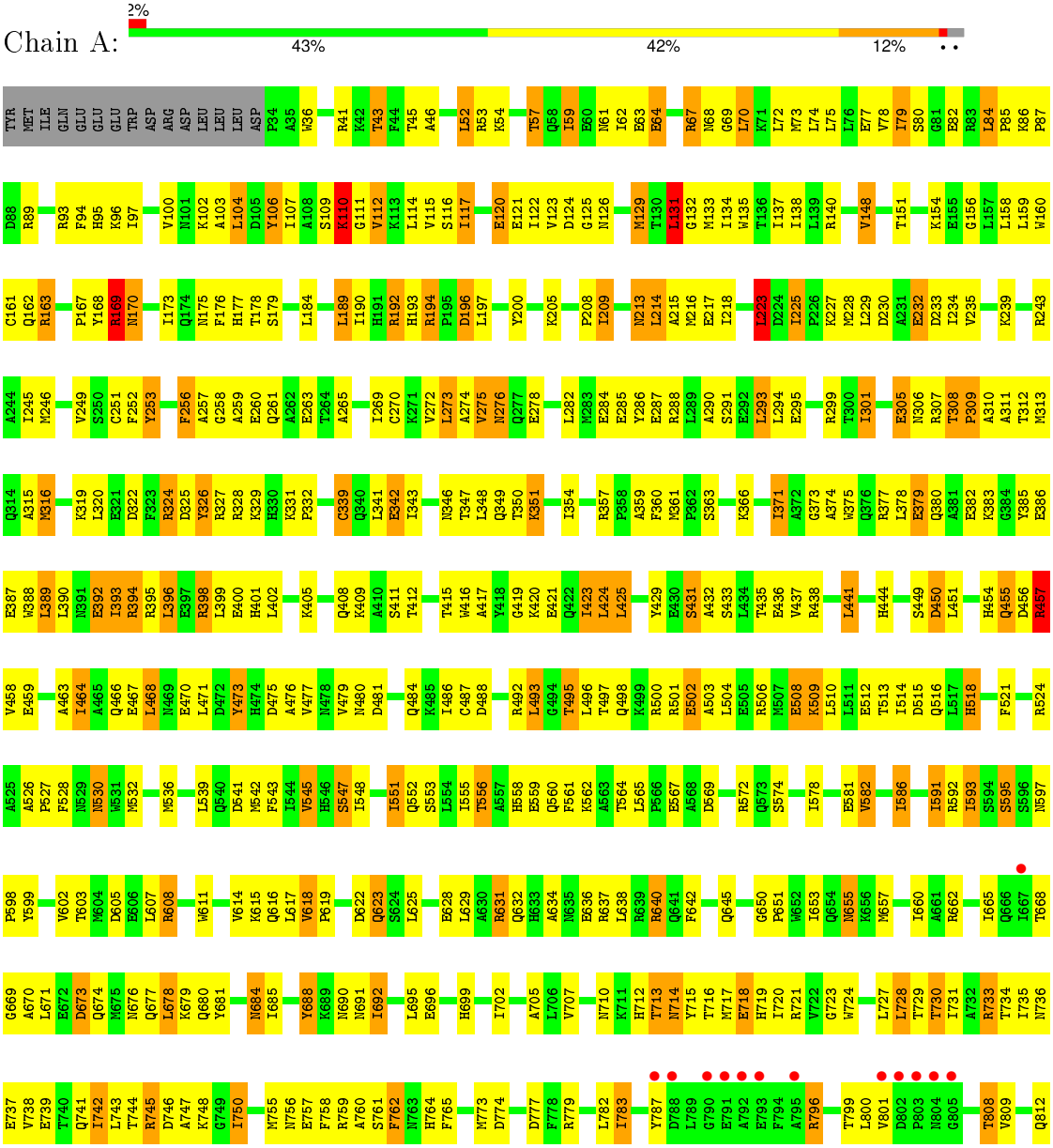
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	ALA	GLU	ENGINEERED MUTATION	UNP P35609
A	311	ALA	LYS	ENGINEERED MUTATION	UNP P35609

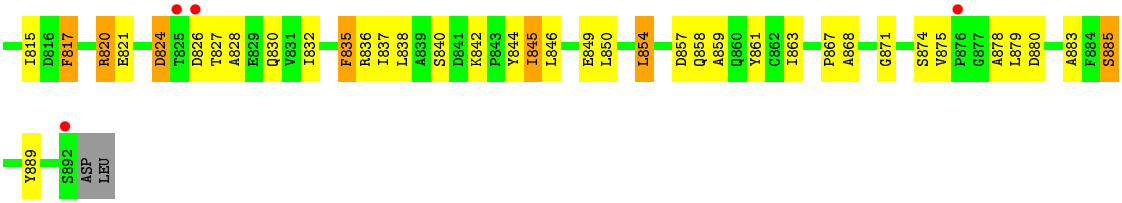
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ALPHA-ACTININ-2

Chain A:




I815
D816
F817
A820
E821
D824
T825
D826
T827
A828
E829
Q830
V831
I832
F835
R836
I837
L838
A839
S840
D841
K842
P843
Y844
I845
L846
E849
L850
L854
D857
Q858
A859
Q860
Y861
C862
I863
P867
A868
G871
S874
V875
P876
G877
A878
L879
D880
A883
F884
S885
Y889
S892
ASP
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.33Å 102.61Å 182.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.31 – 3.50 51.31 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (51.31-3.50) 99.8 (51.31-3.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.205 , 0.258 0.216 , 0.219	Depositor DCC
R_{free} test set	918 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	97.7	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 89.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Outliers	2 of 18008 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6865	wwPDB-VP
Average B, all atoms (Å^2)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.51	0/6846	0.76	4/9243 (0.0%)

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	7

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	169	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	707	VAL	CB-CA-C	-5.78	100.42	111.40
1	A	457	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	273	LEU	CB-CG-CD2	5.15	119.76	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	GLY	Peptide
1	A	131	LEU	Peptide
1	A	223	LEU	Peptide
1	A	309	PRO	Peptide
1	A	312	THR	Peptide
1	A	705	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	787	TYR	Peptide

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	6865	0	6706	352	0
All	All	6865	0	6706	352	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 26.

All (352) 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:392:GLU:H	1:A:394:ARG:NH1	1.58	1.01
1:A:545:VAL:HG11	1:A:551:ILE:HG12	1.48	0.93
1:A:392:GLU:N	1:A:394:ARG:HH11	1.68	0.91
1:A:169:ARG:HG2	1:A:169:ARG:HH11	1.36	0.89
1:A:591:ILE:HG22	1:A:593:ILE:H	1.40	0.86
1:A:431:SER:HB2	1:A:592:ARG:HH11	1.41	0.85
1:A:285:GLU:OE1	1:A:288:ARG:NH1	2.10	0.85
1:A:295:GLU:HG3	1:A:299:ARG:HH11	1.42	0.84
1:A:539:LEU:HD23	1:A:617:LEU:HB3	1.59	0.84
1:A:495:THR:HA	1:A:498:GLN:HE22	1.42	0.82
1:A:424:LEU:HD21	1:A:497:THR:HG22	1.62	0.81
1:A:678:LEU:HD21	1:A:735:ILE:HG13	1.63	0.81
1:A:394:ARG:CD	1:A:394:ARG:H	1.93	0.80
1:A:669:GLY:HA2	1:A:670:ALA:HB3	1.64	0.79
1:A:392:GLU:H	1:A:394:ARG:HH11	0.84	0.79
1:A:293:LEU:HD21	1:A:371:ILE:HD11	1.64	0.78
1:A:84:LEU:HB2	1:A:85:PRO:HD2	1.66	0.77
1:A:457:ARG:HB3	1:A:457:ARG:HH11	1.48	0.77
1:A:867:PRO:HG2	1:A:880:ASP:HB3	1.65	0.77
1:A:402:LEU:HD12	1:A:468:LEU:HD13	1.66	0.77
1:A:394:ARG:HD2	1:A:394:ARG:H	1.49	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:HIS:HD2	1:A:500:ARG:HD3	1.50	0.76
1:A:628:GLU:OE2	1:A:631:ARG:NH2	2.19	0.75
1:A:46:ALA:HB3	1:A:228:MET:HB3	1.68	0.74
1:A:389:LEU:O	1:A:394:ARG:NH2	2.21	0.74
1:A:151:THR:HG23	1:A:156:GLY:HA2	1.70	0.74
1:A:290:ALA:HA	1:A:366:LYS:HZ3	1.52	0.73
1:A:559:GLU:N	1:A:559:GLU:OE1	2.21	0.73
1:A:498:GLN:OE1	1:A:498:GLN:N	2.20	0.73
1:A:773:MET:HB3	1:A:774:ASP:HA	1.71	0.72
1:A:867:PRO:HG3	1:A:883:ALA:HB3	1.71	0.72
1:A:748:LYS:O	1:A:820:ARG:NH2	2.22	0.72
1:A:638:LEU:HB3	1:A:702:ILE:HG22	1.71	0.71
1:A:393:ILE:HG22	1:A:394:ARG:HE	1.57	0.70
1:A:114:LEU:HD21	1:A:117:ILE:HG13	1.72	0.70
1:A:539:LEU:HD21	1:A:618:VAL:HG12	1.74	0.69
1:A:175:ASN:OD1	1:A:177:HIS:NE2	2.25	0.69
1:A:43:THR:HA	1:A:228:MET:HB2	1.76	0.68
1:A:43:THR:HG22	1:A:229:LEU:HA	1.74	0.68
1:A:170:ASN:N	1:A:170:ASN:OD1	2.27	0.67
1:A:551:ILE:HG23	1:A:555:ILE:HD13	1.74	0.67
1:A:444:HIS:CD2	1:A:500:ARG:HD3	2.30	0.67
1:A:467:GLU:HA	1:A:470:GLU:HB3	1.74	0.66
1:A:622:ASP:OD1	1:A:623:GLN:N	2.27	0.66
1:A:295:GLU:HG3	1:A:299:ARG:NH1	2.10	0.66
1:A:528:PHE:CZ	1:A:572:ARG:HB2	2.30	0.66
1:A:521:PHE:HB2	1:A:578:ILE:HG21	1.77	0.66
1:A:454:HIS:O	1:A:458:VAL:HG23	1.96	0.66
1:A:390:LEU:O	1:A:394:ARG:HD3	1.96	0.66
1:A:209:ILE:HG22	1:A:235:VAL:HG21	1.76	0.65
1:A:431:SER:HB2	1:A:592:ARG:NH1	2.12	0.65
1:A:827:THR:HG22	1:A:828:ALA:H	1.60	0.65
1:A:730:THR:HA	1:A:733:ARG:HD2	1.79	0.65
1:A:170:ASN:HD22	1:A:184:LEU:HD22	1.62	0.64
1:A:518:HIS:O	1:A:597:ASN:ND2	2.30	0.64
1:A:547:SER:O	1:A:632:GLN:HG2	1.99	0.63
1:A:466:GLN:HG3	1:A:467:GLU:N	2.13	0.63
1:A:846:LEU:N	1:A:849:GLU:OE2	2.26	0.63
1:A:618:VAL:HG22	1:A:619:PRO:HD3	1.79	0.63
1:A:134:ILE:O	1:A:138:ILE:HG13	1.98	0.63
1:A:276:ASN:HB2	1:A:357:ARG:HH12	1.63	0.63
1:A:761:SER:O	1:A:764:HIS:ND1	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ILE:HG22	1:A:394:ARG:NE	2.14	0.62
1:A:258:GLY:HA2	1:A:261:GLN:HB2	1.82	0.62
1:A:741:GLN:HA	1:A:744:THR:HG22	1.80	0.62
1:A:755:MET:HA	1:A:758:PHE:CE2	2.34	0.62
1:A:840:SER:H	1:A:842:LYS:HE3	1.63	0.62
1:A:835:PHE:HA	1:A:838:LEU:HD12	1.82	0.62
1:A:536:MET:HG3	1:A:614:VAL:HG23	1.82	0.62
1:A:399:LEU:HD11	1:A:471:LEU:HD23	1.82	0.61
1:A:216:MET:SD	1:A:229:LEU:HB2	2.40	0.61
1:A:160:TRP:HZ2	1:A:193:HIS:HE1	1.49	0.61
1:A:209:ILE:O	1:A:213:ASN:HB2	2.01	0.61
1:A:464:ILE:O	1:A:468:LEU:HB2	2.01	0.60
1:A:564:THR:O	1:A:567:GLU:N	2.32	0.60
1:A:736:ASN:HA	1:A:739:GLU:HB3	1.84	0.60
1:A:457:ARG:CB	1:A:457:ARG:HH11	2.13	0.60
1:A:216:MET:HE3	1:A:227:LYS:HA	1.84	0.60
1:A:282:LEU:HB3	1:A:348:LEU:HD11	1.83	0.60
1:A:569:ASP:OD1	1:A:572:ARG:NH1	2.33	0.60
1:A:74:LEU:O	1:A:78:VAL:HG23	2.01	0.60
1:A:290:ALA:HA	1:A:366:LYS:NZ	2.17	0.60
1:A:608:ARG:HH11	1:A:608:ARG:HG3	1.67	0.60
1:A:129:MET:O	1:A:132:GLY:HA3	2.02	0.59
1:A:817:PHE:O	1:A:821:GLU:N	2.35	0.59
1:A:120:GLU:OE1	1:A:121:GLU:N	2.34	0.59
1:A:273:LEU:O	1:A:276:ASN:N	2.36	0.58
1:A:741:GLN:HG3	1:A:812:GLN:HG3	1.86	0.58
1:A:162:GLN:HB3	1:A:173:ILE:HD11	1.86	0.58
1:A:435:THR:OG1	1:A:436:GLU:N	2.34	0.58
1:A:528:PHE:CE2	1:A:572:ARG:HB2	2.39	0.57
1:A:52:LEU:HB3	1:A:57:THR:O	2.04	0.57
1:A:59:ILE:HG12	1:A:59:ILE:O	2.04	0.57
1:A:93:ARG:NH1	1:A:124:ASP:OD1	2.36	0.57
1:A:516:GLN:HA	1:A:516:GLN:OE1	2.05	0.57
1:A:217:GLU:OE1	1:A:217:GLU:N	2.38	0.57
1:A:761:SER:HA	1:A:764:HIS:HB3	1.86	0.57
1:A:796:ARG:O	1:A:800:LEU:N	2.38	0.56
1:A:359:ALA:HB3	1:A:360:PHE:HA	1.86	0.56
1:A:67:ARG:NE	1:A:123:VAL:O	2.22	0.56
1:A:388:TRP:CE3	1:A:389:LEU:HD22	2.40	0.56
1:A:214:LEU:HG	1:A:214:LEU:O	2.06	0.56
1:A:41:ARG:HG2	1:A:62:ILE:HG21	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLN:O	1:A:488:ASP:N	2.33	0.56
1:A:548:ILE:O	1:A:552:GLN:HG2	2.06	0.55
1:A:121:GLU:HG3	1:A:126:ASN:HB3	1.88	0.55
1:A:421:GLU:N	1:A:421:GLU:OE1	2.35	0.55
1:A:741:GLN:HE21	1:A:812:GLN:HE21	1.55	0.55
1:A:173:ILE:HA	1:A:179:SER:HB3	1.89	0.55
1:A:411:SER:O	1:A:415:THR:HG23	2.06	0.55
1:A:799:THR:HB	1:A:809:VAL:HG22	1.88	0.55
1:A:73:MET:HG2	1:A:103:ALA:HB2	1.89	0.55
1:A:169:ARG:HG2	1:A:169:ARG:NH1	2.13	0.54
1:A:844:TYR:CZ	1:A:874:SER:HA	2.43	0.54
1:A:94:PHE:HA	1:A:97:ILE:HD12	1.88	0.54
1:A:169:ARG:CG	1:A:169:ARG:HH11	2.16	0.54
1:A:845:ILE:HG22	1:A:879:LEU:HB2	1.89	0.54
1:A:316:MET:HA	1:A:319:MLZ:HB2	1.89	0.54
1:A:399:LEU:CD1	1:A:471:LEU:HD23	2.37	0.54
1:A:160:TRP:CZ2	1:A:193:HIS:HE1	2.25	0.54
1:A:326:TYR:OH	1:A:382:GLU:OE2	2.25	0.53
1:A:390:LEU:C	1:A:394:ARG:HD3	2.27	0.53
1:A:555:ILE:HD12	1:A:625:LEU:HG	1.90	0.53
1:A:100:VAL:O	1:A:104:LEU:N	2.37	0.53
1:A:265:ALA:O	1:A:269:ILE:HG12	2.09	0.53
1:A:374:ALA:HA	1:A:377:ARG:HE	1.73	0.53
1:A:408:GLN:O	1:A:412:THR:HG23	2.09	0.53
1:A:135:TRP:CG	1:A:243:ARG:HD3	2.44	0.53
1:A:106:TYR:CD1	1:A:106:TYR:C	2.82	0.52
1:A:779:ARG:O	1:A:783:ILE:HG13	2.09	0.52
1:A:678:LEU:HD11	1:A:735:ILE:HD12	1.92	0.52
1:A:514:ILE:HD11	1:A:586:ILE:HG22	1.91	0.52
1:A:284:GLU:O	1:A:287:GLU:N	2.41	0.52
1:A:232:GLU:O	1:A:235:VAL:HG12	2.09	0.52
1:A:473:TYR:OH	1:A:479:VAL:HG11	2.09	0.52
1:A:631:ARG:NH2	1:A:632:GLN:OE1	2.43	0.52
1:A:438:ARG:HD3	1:A:508:GLU:OE2	2.09	0.51
1:A:449:SER:OG	1:A:450:ASP:N	2.43	0.51
1:A:93:ARG:HG2	1:A:97:ILE:HD11	1.92	0.51
1:A:670:ALA:HB1	1:A:673:ASP:CG	2.31	0.51
1:A:70:LEU:HA	1:A:73:MET:HG3	1.91	0.51
1:A:106:TYR:C	1:A:106:TYR:HD1	2.14	0.51
1:A:476:ALA:O	1:A:480:ASN:ND2	2.43	0.51
1:A:824:ASP:N	1:A:824:ASP:OD1	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LEU:HG	1:A:473:TYR:CZ	2.45	0.51
1:A:750:ILE:HG13	1:A:758:PHE:CE2	2.45	0.51
1:A:463:ALA:O	1:A:466:GLN:HG2	2.11	0.51
1:A:678:LEU:HD23	1:A:679:LYS:HG2	1.93	0.51
1:A:291:SER:O	1:A:295:GLU:HB3	2.11	0.51
1:A:230:ASP:OD2	1:A:233:ASP:HB2	2.11	0.51
1:A:75:LEU:O	1:A:79:ILE:HG23	2.12	0.50
1:A:455:GLN:HG3	1:A:456:ASP:N	2.25	0.50
1:A:73:MET:SD	1:A:87:PRO:HB3	2.51	0.50
1:A:373:GLY:O	1:A:377:ARG:HG3	2.11	0.50
1:A:196:ASP:N	1:A:196:ASP:OD1	2.34	0.50
1:A:274:ALA:O	1:A:278:GLU:HG2	2.11	0.50
1:A:388:TRP:HE3	1:A:389:LEU:HD22	1.75	0.50
1:A:498:GLN:HA	1:A:501:ARG:HB3	1.92	0.50
1:A:731:ILE:HG13	1:A:735:ILE:CD1	2.41	0.50
1:A:832:ILE:HA	1:A:835:PHE:HB2	1.93	0.50
1:A:87:PRO:HG2	1:A:89:ARG:HH22	1.76	0.50
1:A:431:SER:OG	1:A:431:SER:O	2.28	0.50
1:A:695:LEU:HD23	1:A:696:GLU:N	2.27	0.50
1:A:431:SER:HA	1:A:592:ARG:HD3	1.94	0.50
1:A:275:VAL:HB	1:A:357:ARG:NH2	2.26	0.50
1:A:628:GLU:HA	1:A:628:GLU:OE1	2.12	0.49
1:A:290:ALA:O	1:A:294:LEU:HB2	2.12	0.49
1:A:64:GLU:HA	1:A:67:ARG:HG3	1.93	0.49
1:A:424:LEU:CD1	1:A:496:LEU:HB3	2.43	0.49
1:A:189:LEU:HA	1:A:192:ARG:HB3	1.93	0.49
1:A:325:ASP:HA	1:A:329:MLZ:HCM2	1.95	0.49
1:A:674:GLN:HG2	1:A:738:VAL:HG21	1.94	0.49
1:A:634:ALA:HA	1:A:637:ARG:HH11	1.76	0.49
1:A:844:TYR:HB3	1:A:878:ALA:HB1	1.95	0.49
1:A:61:ASN:OD1	1:A:63:GLU:N	2.46	0.49
1:A:527:PRO:O	1:A:530:ASN:N	2.44	0.48
1:A:309:PRO:HA	1:A:388:TRP:HZ2	1.79	0.48
1:A:493:LEU:O	1:A:497:THR:HG23	2.13	0.48
1:A:673:ASP:OD1	1:A:674:GLN:N	2.45	0.48
1:A:532:MET:HE2	1:A:611:TRP:HE3	1.78	0.48
1:A:688:TYR:O	1:A:691:ASN:N	2.46	0.48
1:A:553:SER:O	1:A:556:THR:HG22	2.13	0.48
1:A:551:ILE:HG21	1:A:629:LEU:HA	1.96	0.48
1:A:252:PHE:O	1:A:256:PHE:HB2	2.14	0.48
1:A:750:ILE:CG2	1:A:758:PHE:HZ	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLU:HG2	1:A:503:ALA:N	2.28	0.47
1:A:859:ALA:O	1:A:863:ILE:HG12	2.14	0.47
1:A:710:ASN:OD1	1:A:712:HIS:HB2	2.14	0.47
1:A:385:TYR:O	1:A:389:LEU:HB2	2.14	0.47
1:A:750:ILE:HG13	1:A:758:PHE:CZ	2.49	0.47
1:A:518:HIS:CD2	1:A:598:PRO:HD3	2.49	0.47
1:A:714:ASN:OD1	1:A:714:ASN:N	2.47	0.47
1:A:95:HIS:O	1:A:96:MLZ:C	2.60	0.47
1:A:441:LEU:HD13	1:A:504:LEU:HD13	1.97	0.47
1:A:74:LEU:O	1:A:77:GLU:HG2	2.15	0.47
1:A:551:ILE:HG22	1:A:629:LEU:HD13	1.97	0.47
1:A:293:LEU:HD21	1:A:371:ILE:CD1	2.41	0.47
1:A:74:LEU:C	1:A:74:LEU:HD12	2.34	0.47
1:A:158:LEU:O	1:A:162:GLN:HG2	2.14	0.47
1:A:208:PRO:HG2	1:A:235:VAL:HG23	1.97	0.47
1:A:310:ALA:HB1	1:A:396:LEU:HD11	1.96	0.47
1:A:731:ILE:HG13	1:A:735:ILE:HD13	1.97	0.47
1:A:642:PHE:CE2	1:A:699:HIS:HB2	2.50	0.46
1:A:107:ILE:HG22	1:A:112:VAL:CG1	2.45	0.46
1:A:737:GLU:O	1:A:741:GLN:HG2	2.14	0.46
1:A:374:ALA:HA	1:A:377:ARG:NE	2.30	0.46
1:A:467:GLU:O	1:A:471:LEU:HD13	2.16	0.46
1:A:696:GLU:HG2	1:A:717:MET:HE1	1.98	0.46
1:A:673:ASP:O	1:A:677:GLN:HB2	2.16	0.46
1:A:759:ARG:HA	1:A:762:PHE:HB3	1.98	0.46
1:A:316:MET:HB3	1:A:393:ILE:HD12	1.96	0.46
1:A:109:SER:OG	1:A:110:LYS:N	2.48	0.46
1:A:746:ASP:OD1	1:A:747:ALA:N	2.48	0.46
1:A:674:GLN:O	1:A:678:LEU:HB3	2.16	0.46
1:A:773:MET:HB2	1:A:808:THR:OG1	2.16	0.46
1:A:466:GLN:HG3	1:A:467:GLU:H	1.79	0.46
1:A:504:LEU:HD23	1:A:504:LEU:HA	1.62	0.46
1:A:773:MET:HB2	1:A:808:THR:CG2	2.46	0.46
1:A:52:LEU:HD13	1:A:75:LEU:HD13	1.98	0.46
1:A:121:GLU:HG2	1:A:129:MET:SD	2.55	0.46
1:A:67:ARG:HD2	1:A:125:GLY:CA	2.46	0.46
1:A:692:ILE:HA	1:A:692:ILE:HD12	1.73	0.46
1:A:215:ALA:O	1:A:218:ILE:HG22	2.16	0.46
1:A:79:ILE:HG12	1:A:80:SER:N	2.31	0.45
1:A:844:TYR:OH	1:A:871:GLY:O	2.34	0.45
1:A:868:ALA:HA	1:A:879:LEU:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:GLN:N	1:A:858:GLN:OE1	2.46	0.45
1:A:393:ILE:H	1:A:394:ARG:CZ	2.29	0.45
1:A:773:MET:CB	1:A:774:ASP:HA	2.41	0.45
1:A:257:ALA:C	1:A:259:ALA:H	2.20	0.45
1:A:845:ILE:HD13	1:A:850:LEU:HD21	1.99	0.45
1:A:636:GLU:HA	1:A:636:GLU:OE1	2.17	0.45
1:A:764:HIS:CG	1:A:765:PHE:N	2.84	0.45
1:A:197:LEU:H	1:A:197:LEU:HD12	1.80	0.45
1:A:311:ALA:O	1:A:315:ALA:HB3	2.17	0.45
1:A:713:THR:HG1	1:A:715:TYR:HD2	1.64	0.45
1:A:796:ARG:HA	1:A:796:ARG:HD3	1.65	0.45
1:A:696:GLU:HG2	1:A:717:MET:CE	2.46	0.45
1:A:551:ILE:HG13	1:A:628:GLU:HG3	1.97	0.45
1:A:84:LEU:HD12	1:A:84:LEU:H	1.81	0.45
1:A:840:SER:N	1:A:842:LYS:HE3	2.30	0.45
1:A:194:ARG:CZ	1:A:197:LEU:HD11	2.47	0.45
1:A:828:ALA:HB1	1:A:885:SER:OG	2.17	0.45
1:A:253:TYR:O	1:A:256:PHE:N	2.46	0.45
1:A:526:ALA:N	1:A:527:PRO:HD2	2.31	0.45
1:A:419:GLY:O	1:A:423:ILE:HG23	2.17	0.45
1:A:331:MLZ:HCM1	1:A:379:GLU:OE1	2.17	0.45
1:A:288:ARG:HD3	1:A:341:LEU:CD1	2.47	0.45
1:A:245:ILE:O	1:A:249:VAL:HG23	2.17	0.45
1:A:293:LEU:HA	1:A:293:LEU:HD12	1.85	0.44
1:A:148:VAL:O	1:A:151:THR:HG22	2.16	0.44
1:A:193:HIS:ND1	1:A:256:PHE:CG	2.79	0.44
1:A:676:ASN:O	1:A:680:GLN:HG2	2.17	0.44
1:A:400:GLU:OE1	1:A:400:GLU:N	2.50	0.44
1:A:392:GLU:N	1:A:394:ARG:NH1	2.43	0.44
1:A:850:LEU:O	1:A:854:LEU:HB2	2.18	0.44
1:A:524:ARG:NH2	1:A:574:SER:OG	2.39	0.44
1:A:285:GLU:HA	1:A:288:ARG:HD2	2.00	0.44
1:A:515:ASP:HA	1:A:518:HIS:HB2	1.99	0.44
1:A:875:VAL:HB	1:A:878:ALA:HB2	1.98	0.44
1:A:716:THR:O	1:A:718:GLU:N	2.50	0.44
1:A:650:GLY:N	1:A:651:PRO:HD2	2.32	0.44
1:A:416:TRP:CE3	1:A:417:ALA:HB2	2.53	0.44
1:A:351:LYS:O	1:A:354:ILE:HG13	2.17	0.44
1:A:308:THR:HA	1:A:309:PRO:HD3	1.82	0.44
1:A:669:GLY:HA2	1:A:670:ALA:CB	2.35	0.44
1:A:84:LEU:HB2	1:A:85:PRO:CD	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HG	1:A:70:LEU:H	1.46	0.44
1:A:657:MET:O	1:A:660:ILE:HG22	2.17	0.44
1:A:762:PHE:HD2	1:A:815:ILE:HG21	1.83	0.44
1:A:223:LEU:O	1:A:225:ILE:HG23	2.18	0.44
1:A:225:ILE:HD12	1:A:251:CYS:HB3	2.00	0.44
1:A:316:MET:CB	1:A:393:ILE:HD12	2.48	0.43
1:A:684:ASN:HD22	1:A:684:ASN:C	2.21	0.43
1:A:117:ILE:HG13	1:A:117:ILE:O	2.18	0.43
1:A:87:PRO:HG2	1:A:89:ARG:NH2	2.33	0.43
1:A:671:LEU:HG	1:A:742:ILE:HD11	1.98	0.43
1:A:163:ARG:HA	1:A:163:ARG:HD3	1.39	0.43
1:A:561:PHE:C	1:A:561:PHE:CD1	2.91	0.43
1:A:500:ARG:O	1:A:504:LEU:HB2	2.18	0.43
1:A:741:GLN:NE2	1:A:812:GLN:HE21	2.15	0.43
1:A:671:LEU:CG	1:A:742:ILE:HD11	2.48	0.43
1:A:681:TYR:O	1:A:685:ILE:N	2.48	0.43
1:A:719:HIS:O	1:A:723:GLY:N	2.23	0.43
1:A:208:PRO:HG2	1:A:235:VAL:CG2	2.48	0.43
1:A:398:ARG:HA	1:A:401:HIS:HB2	2.01	0.43
1:A:597:ASN:HA	1:A:598:PRO:HD3	1.67	0.43
1:A:727:LEU:HD23	1:A:728:LEU:N	2.34	0.43
1:A:468:LEU:HA	1:A:468:LEU:HD12	1.82	0.43
1:A:695:LEU:HD21	1:A:717:MET:SD	2.58	0.43
1:A:301:ILE:O	1:A:305:GLU:HB2	2.18	0.43
1:A:421:GLU:O	1:A:425:LEU:HD22	2.19	0.43
1:A:327:ARG:O	1:A:332:PRO:HD3	2.19	0.43
1:A:651:PRO:O	1:A:655:ASN:N	2.50	0.43
1:A:351:LYS:HE2	1:A:354:ILE:HD11	2.00	0.42
1:A:306:ASN:OD1	1:A:307:ARG:N	2.52	0.42
1:A:115:VAL:HG12	1:A:116:SER:HB2	2.01	0.42
1:A:82:GLU:N	1:A:82:GLU:OE1	2.52	0.42
1:A:432:ALA:HB3	1:A:437:VAL:HG23	2.01	0.42
1:A:366:LYS:HD3	1:A:366:LYS:HA	1.62	0.42
1:A:324:ARG:HD3	1:A:324:ARG:HA	1.61	0.42
1:A:640:ARG:HD2	1:A:712:HIS:CD2	2.55	0.42
1:A:405:LYS:O	1:A:409:LYS:HG3	2.19	0.42
1:A:424:LEU:CD2	1:A:497:THR:HG22	2.41	0.42
1:A:371:ILE:HA	1:A:371:ILE:HD12	1.47	0.42
1:A:473:TYR:H	1:A:473:TYR:HD1	1.66	0.42
1:A:598:PRO:HD2	1:A:599:TYR:CD1	2.55	0.42
1:A:699:HIS:CD2	1:A:717:MET:HG2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:ILE:HG23	1:A:595:SER:H	1.84	0.42
1:A:733:ARG:HG2	1:A:734:THR:N	2.35	0.42
1:A:77:GLU:HA	1:A:80:SER:HB2	2.02	0.42
1:A:671:LEU:O	1:A:671:LEU:HD13	2.20	0.42
1:A:69:GLY:O	1:A:72:LEU:HB3	2.19	0.42
1:A:131:LEU:HD13	1:A:131:LEU:HA	1.82	0.42
1:A:102:MLZ:HCM3	1:A:102:MLZ:HD3	1.75	0.42
1:A:339:CYS:HA	1:A:342:GLU:OE2	2.20	0.42
1:A:326:TYR:CD1	1:A:327:ARG:N	2.88	0.41
1:A:645:GLN:HG2	1:A:695:LEU:HB2	2.01	0.41
1:A:273:LEU:HD23	1:A:273:LEU:O	2.21	0.41
1:A:745:ARG:HD3	1:A:746:ASP:HB3	2.02	0.41
1:A:742:ILE:HA	1:A:742:ILE:HD13	1.49	0.41
1:A:177:HIS:CD2	1:A:239:MLZ:HD3	2.56	0.41
1:A:741:GLN:HE21	1:A:812:GLN:HG3	1.85	0.41
1:A:715:TYR:HB3	1:A:720:ILE:HD13	2.02	0.41
1:A:68:ASN:N	1:A:69:GLY:HA2	2.34	0.41
1:A:389:LEU:HA	1:A:389:LEU:HD13	1.65	0.41
1:A:551:ILE:HG23	1:A:551:ILE:HD12	1.78	0.41
1:A:285:GLU:HA	1:A:288:ARG:CG	2.51	0.41
1:A:558:HIS:CD2	1:A:562:MLZ:HD2	2.56	0.41
1:A:473:TYR:CD1	1:A:476:ALA:HB2	2.55	0.41
1:A:605:ASP:HA	1:A:608:ARG:HB2	2.03	0.41
1:A:133:MET:HG3	1:A:134:ILE:N	2.35	0.41
1:A:189:LEU:HD13	1:A:252:PHE:HD2	1.85	0.41
1:A:45:THR:OG1	1:A:62:ILE:HB	2.20	0.41
1:A:133:MET:CG	1:A:134:ILE:N	2.83	0.41
1:A:327:ARG:NH2	1:A:386:GLU:OE2	2.44	0.41
1:A:167:PRO:HB2	1:A:168:TYR:HD1	1.86	0.41
1:A:582:VAL:O	1:A:586:ILE:HG23	2.20	0.40
1:A:757:GLU:O	1:A:760:ALA:HB3	2.21	0.40
1:A:509:LYS:HG2	1:A:510:LEU:N	2.33	0.40
1:A:272:VAL:O	1:A:357:ARG:NH2	2.54	0.40
1:A:750:ILE:HG23	1:A:758:PHE:HZ	1.85	0.40
1:A:64:GLU:O	1:A:67:ARG:HG3	2.21	0.40
1:A:671:LEU:HD11	1:A:742:ILE:CG1	2.52	0.40
1:A:742:ILE:HD12	1:A:745:ARG:HH11	1.85	0.40
1:A:343:ILE:O	1:A:347:THR:HG23	2.20	0.40
1:A:285:GLU:HA	1:A:288:ARG:CD	2.52	0.40
1:A:134:ILE:O	1:A:137:ILE:HB	2.21	0.40
1:A:305:GLU:O	1:A:307:ARG:HG2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:TYR:CD1	1:A:253:TYR:C	2.94	0.40
1:A:190:ILE:HA	1:A:256:PHE:HZ	1.85	0.40
1:A:728:LEU:HA	1:A:728:LEU:HD13	1.64	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	844/876 (96%)	790 (94%)	52 (6%)	2 (0%)	52 88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	801	VAL
1	A	110	LYS

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	702/752 (93%)	513 (73%)	189 (27%)	0 4

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	TRP
1	A	43	THR
1	A	52	LEU
1	A	53	ARG
1	A	54	LYS
1	A	57	THR
1	A	59	ILE
1	A	64	GLU
1	A	67	ARG
1	A	70	LEU
1	A	79	ILE
1	A	84	LEU
1	A	86	LYS
1	A	104	LEU
1	A	106	TYR
1	A	110	LYS
1	A	112	VAL
1	A	117	ILE
1	A	120	GLU
1	A	122	ILE
1	A	129	MET
1	A	131	LEU
1	A	140	ARG
1	A	148	VAL
1	A	154	LYS
1	A	159	LEU
1	A	161	CYS
1	A	163	ARG
1	A	169	ARG
1	A	170	ASN
1	A	176	PHE
1	A	178	THR
1	A	189	LEU
1	A	192	ARG
1	A	194	ARG
1	A	196	ASP
1	A	200	TYR
1	A	205	LYS
1	A	209	ILE
1	A	213	ASN
1	A	214	LEU
1	A	223	LEU
1	A	225	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	232	GLU
1	A	234	ILE
1	A	246	MET
1	A	253	TYR
1	A	256	PHE
1	A	260	GLU
1	A	263	GLU
1	A	270	CYS
1	A	275	VAL
1	A	276	ASN
1	A	286	TYR
1	A	293	LEU
1	A	301	ILE
1	A	305	GLU
1	A	308	THR
1	A	313	MET
1	A	316	MET
1	A	320	LEU
1	A	322	ASP
1	A	324	ARG
1	A	326	TYR
1	A	328	ARG
1	A	339	CYS
1	A	342	GLU
1	A	346	ASN
1	A	349	GLN
1	A	350	THR
1	A	351	LYS
1	A	361	MET
1	A	363	SER
1	A	371	ILE
1	A	375	TRP
1	A	378	LEU
1	A	379	GLU
1	A	380	GLN
1	A	383	LYS
1	A	387	GLU
1	A	389	LEU
1	A	392	GLU
1	A	393	ILE
1	A	394	ARG
1	A	395	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	396	LEU
1	A	398	ARG
1	A	420	LYS
1	A	423	ILE
1	A	424	LEU
1	A	425	LEU
1	A	429	TYR
1	A	431	SER
1	A	433	SER
1	A	441	LEU
1	A	450	ASP
1	A	451	LEU
1	A	455	GLN
1	A	457	ARG
1	A	459	GLU
1	A	464	ILE
1	A	468	LEU
1	A	473	TYR
1	A	475	ASP
1	A	477	VAL
1	A	481	ASP
1	A	486	ILE
1	A	487	CYS
1	A	492	ARG
1	A	493	LEU
1	A	495	THR
1	A	502	GLU
1	A	506	ARG
1	A	508	GLU
1	A	509	LYS
1	A	512	GLU
1	A	513	THR
1	A	518	HIS
1	A	530	ASN
1	A	541	ASP
1	A	542	MET
1	A	543	PHE
1	A	545	VAL
1	A	547	SER
1	A	551	ILE
1	A	556	THR
1	A	560	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	565	LEU
1	A	581	GLU
1	A	582	VAL
1	A	586	ILE
1	A	591	ILE
1	A	593	ILE
1	A	595	SER
1	A	602	VAL
1	A	603	THR
1	A	607	LEU
1	A	608	ARG
1	A	615	LYS
1	A	616	GLN
1	A	618	VAL
1	A	623	GLN
1	A	631	ARG
1	A	640	ARG
1	A	653	ILE
1	A	655	ASN
1	A	662	ARG
1	A	665	ILE
1	A	668	THR
1	A	673	ASP
1	A	678	LEU
1	A	684	ASN
1	A	688	TYR
1	A	690	ASN
1	A	692	ILE
1	A	713	THR
1	A	714	ASN
1	A	718	GLU
1	A	721	ARG
1	A	724	TRP
1	A	728	LEU
1	A	729	THR
1	A	730	THR
1	A	733	ARG
1	A	742	ILE
1	A	743	LEU
1	A	745	ARG
1	A	750	ILE
1	A	756	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	762	PHE
1	A	777	ASP
1	A	782	LEU
1	A	783	ILE
1	A	796	ARG
1	A	808	THR
1	A	817	PHE
1	A	820	ARG
1	A	824	ASP
1	A	826	ASP
1	A	830	GLN
1	A	835	PHE
1	A	836	ARG
1	A	837	ILE
1	A	845	ILE
1	A	854	LEU
1	A	857	ASP
1	A	861	TYR
1	A	885	SER
1	A	889	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	ASN
1	A	444	HIS
1	A	454	HIS
1	A	489	GLN
1	A	529	ASN
1	A	558	HIS
1	A	684	ASN
1	A	812	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)

13 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
1	MLZ	A	102	1	8,9,10	0.57	0	7,9,11	1.27	1 (14%)
1	MLZ	A	164	1	8,9,10	1.08	1 (12%)	7,9,11	1.41	2 (28%)
1	MLZ	A	181	1	8,9,10	0.75	0	7,9,11	1.53	2 (28%)
1	MLZ	A	239	1	8,9,10	0.88	0	7,9,11	1.52	2 (28%)
1	MLZ	A	319	1	8,9,10	1.16	1 (12%)	7,9,11	1.30	1 (14%)
1	MLZ	A	329	1	8,9,10	0.69	0	7,9,11	1.47	2 (28%)
1	MLZ	A	331	1	8,9,10	0.74	0	7,9,11	1.48	2 (28%)
1	MLZ	A	42	1	8,9,10	0.66	0	7,9,11	1.73	2 (28%)
1	MLZ	A	443	1	8,9,10	1.13	1 (12%)	7,9,11	1.40	1 (14%)
1	MLZ	A	562	1	8,9,10	0.83	0	7,9,11	1.38	1 (14%)
1	MLZ	A	689	1	8,9,10	1.00	0	7,9,11	1.14	1 (14%)
1	MLZ	A	71	1	8,9,10	0.66	0	7,9,11	1.67	2 (28%)
1	MLZ	A	96	1	8,9,10	0.59	0	7,9,11	1.42	2 (28%)

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
1	MLZ	A	102	1	-	0/6/8/10	0/0/0/0
1	MLZ	A	164	1	-	0/6/8/10	0/0/0/0
1	MLZ	A	181	1	-	0/6/8/10	0/0/0/0
1	MLZ	A	239	1	-	0/6/8/10	0/0/0/0
1	MLZ	A	319	1	-	0/6/8/10	0/0/0/0
1	MLZ	A	329	1	-	0/6/8/10	0/0/0/0
1	MLZ	A	331	1	-	0/6/8/10	0/0/0/0
1	MLZ	A	42	1	-	0/6/8/10	0/0/0/0
1	MLZ	A	443	1	-	0/6/8/10	0/0/0/0
1	MLZ	A	562	1	-	0/6/8/10	0/0/0/0
1	MLZ	A	689	1	-	0/6/8/10	0/0/0/0
1	MLZ	A	71	1	-	0/6/8/10	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLZ	A	96	1	-	0/6/8/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	MLZ	CB-CA	-2.85	1.51	1.53
1	A	443	MLZ	CB-CA	-2.68	1.51	1.53
1	A	164	MLZ	CB-CA	-2.55	1.51	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	331	MLZ	O-C-CA	-2.93	117.85	125.49
1	A	42	MLZ	O-C-CA	-2.81	118.18	125.49
1	A	96	MLZ	O-C-CA	-2.72	118.40	125.49
1	A	239	MLZ	O-C-CA	-2.55	118.86	125.49
1	A	71	MLZ	O-C-CA	-2.53	118.89	125.49
1	A	164	MLZ	O-C-CA	-2.50	118.98	125.49
1	A	689	MLZ	O-C-CA	-2.46	119.07	125.49
1	A	181	MLZ	O-C-CA	-2.18	119.81	125.49
1	A	329	MLZ	O-C-CA	-2.17	119.85	125.49
1	A	331	MLZ	CM-NZ-CE	2.13	118.47	112.23
1	A	96	MLZ	CM-NZ-CE	2.13	118.47	112.23
1	A	42	MLZ	CB-CA-N	2.17	116.70	110.52
1	A	443	MLZ	CM-NZ-CE	2.27	118.89	112.23
1	A	102	MLZ	CM-NZ-CE	2.28	118.91	112.23
1	A	239	MLZ	CM-NZ-CE	2.44	119.36	112.23
1	A	181	MLZ	CM-NZ-CE	2.47	119.46	112.23
1	A	319	MLZ	CM-NZ-CE	2.47	119.47	112.23
1	A	164	MLZ	CM-NZ-CE	2.49	119.50	112.23
1	A	562	MLZ	CM-NZ-CE	2.78	120.36	112.23
1	A	329	MLZ	CM-NZ-CE	2.91	120.74	112.23
1	A	71	MLZ	CM-NZ-CE	3.12	121.36	112.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	102	MLZ	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	239	MLZ	1	0
1	A	319	MLZ	1	0
1	A	329	MLZ	1	0
1	A	331	MLZ	1	0
1	A	562	MLZ	1	0
1	A	96	MLZ	1	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

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, 95^{th} 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	846/876 (96%)	-0.30	17 (2%) 68 59	49, 130, 244, 277	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	791	GLU	9.2
1	A	792	ALA	7.1
1	A	801	VAL	6.5
1	A	804	ASN	5.1
1	A	790	GLY	4.7
1	A	787	TYR	4.6
1	A	788	ASP	4.6
1	A	826	ASP	3.5
1	A	803	PRO	3.2
1	A	876	PRO	3.1
1	A	793	GLU	2.8
1	A	825	THR	2.6
1	A	892	SER	2.5
1	A	802	ASP	2.5
1	A	795	ALA	2.4
1	A	667	ILE	2.1
1	A	805	GLY	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	MLZ	A	71	10/11	0.98	0.22	-	64,70,84,93	0
1	MLZ	A	689	10/11	0.94	0.32	-	126,135,139,139	0
1	MLZ	A	181	10/11	0.94	0.26	-	125,138,152,153	0
1	MLZ	A	164	10/11	0.97	0.30	-	76,94,100,101	0
1	MLZ	A	443	10/11	0.95	0.16	-	57,64,74,80	0
1	MLZ	A	329	10/11	0.92	0.18	-	110,130,139,142	0
1	MLZ	A	319	10/11	0.93	0.25	-	104,118,125,130	0
1	MLZ	A	96	10/11	0.97	0.26	-	64,74,77,79	0
1	MLZ	A	42	10/11	0.96	0.18	-	81,87,102,103	0
1	MLZ	A	562	10/11	0.97	0.24	-	51,57,86,86	0
1	MLZ	A	102	10/11	0.97	0.15	-	72,79,81,83	0
1	MLZ	A	239	10/11	0.95	0.19	-	129,135,148,148	0
1	MLZ	A	331	10/11	0.94	0.30	-	122,125,132,133	0

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.