



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:18 AM EDT

PDB ID : 4D1E / pdb_00004d1e
Title : THE CRYSTAL STRUCTURE OF HUMAN MUSCLE ALPHA-ACTININ-2
Authors : Pinotsis, N.; Salmazo, A.; Sjoebloom, 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

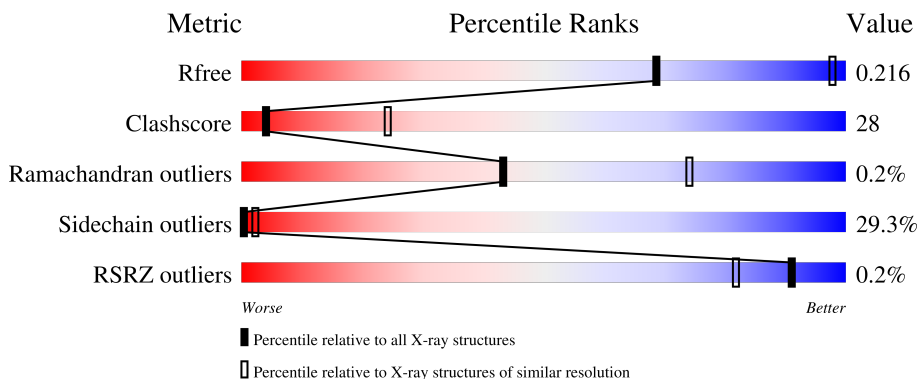
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

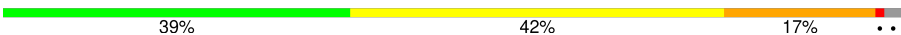
The reported resolution of this entry is 3.50 Å.

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))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 of 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	876	 39% 42% 17% ..

2 Entry composition

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
1	A	859	Total	C	N	O	S	0	0	0
			6865	4305	1226	1301	33			

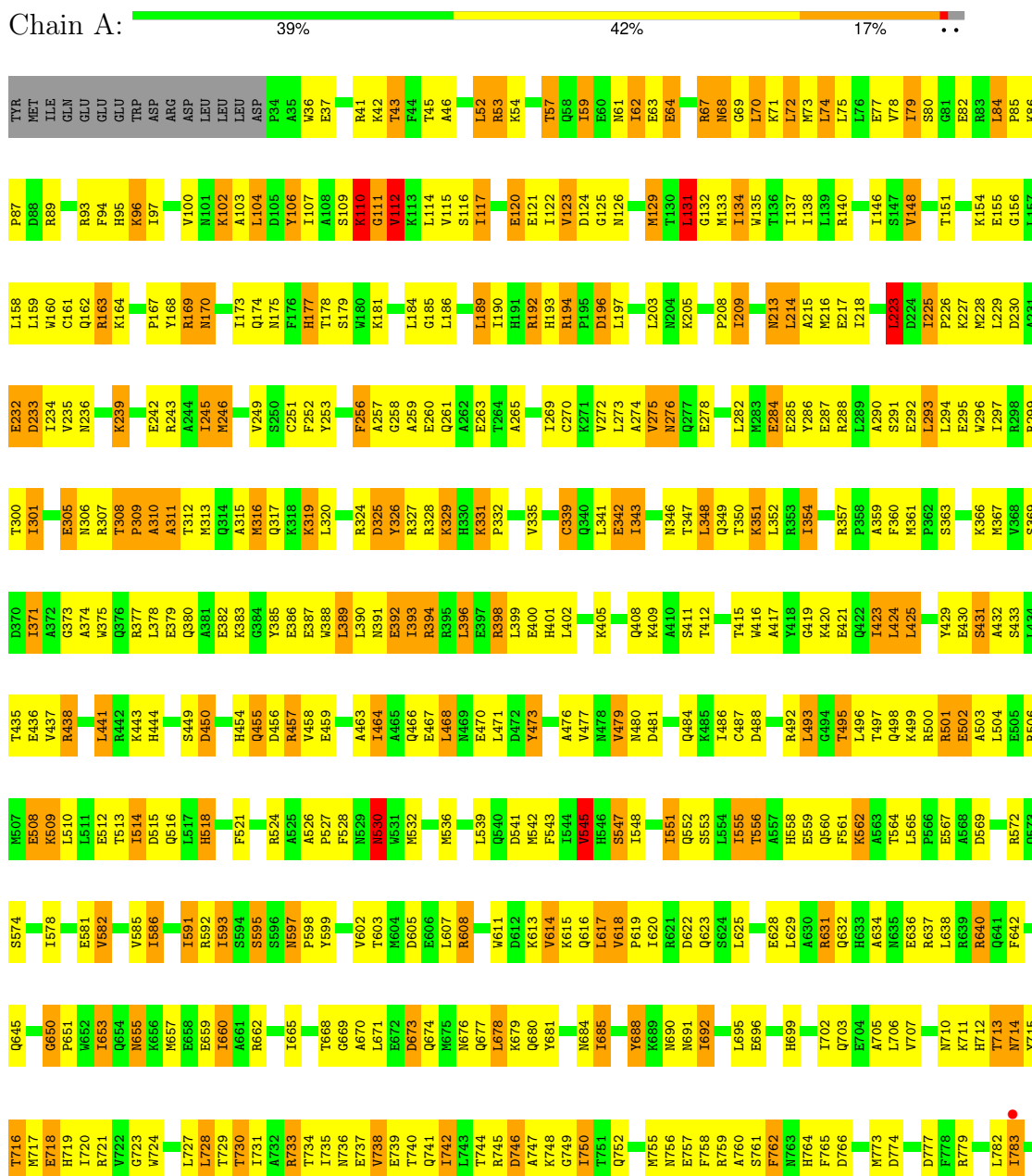
There are 2 discrepancies between the modelled and reference sequences:

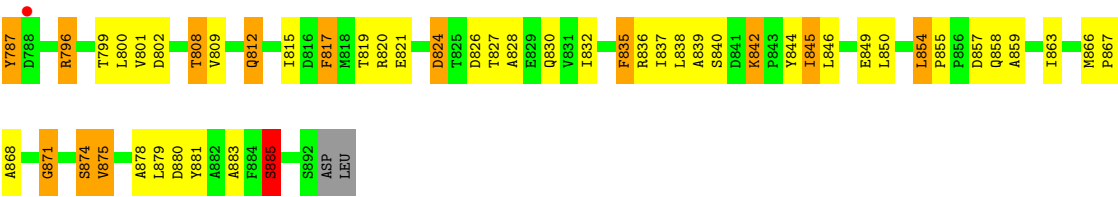
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	ALA	GLU	engineered mutation	UNP P35609
A	311	ALA	LYS	engineered mutation	UNP P35609

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: ALPHA-ACTININ-2





4 Data and refinement statistics

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) 99.7 (51.31-3.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.205 , 0.258 0.213 , 0.216	Depositor DCC
R_{free} test set	918 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	97.7	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 104.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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

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	0.69	0/6846	1.15	49/9243 (0.5%)

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 (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	597	ASN	CA-C-N	9.42	129.12	118.85
1	A	597	ASN	C-N-CA	9.42	129.12	118.85
1	A	112	VAL	N-CA-C	9.23	121.42	108.12
1	A	706	LEU	N-CA-C	9.08	123.95	113.15
1	A	68	ASN	N-CA-C	8.96	121.86	111.11
1	A	885	SER	N-CA-C	8.71	120.77	111.28
1	A	802	ASP	CA-C-N	7.67	127.83	120.31
1	A	802	ASP	C-N-CA	7.67	127.83	120.31
1	A	430	GLU	N-CA-C	7.51	119.46	111.28
1	A	296	TRP	N-CA-C	7.42	120.07	111.02
1	A	111	GLY	CA-C-N	-6.79	113.55	122.99
1	A	111	GLY	C-N-CA	-6.79	113.55	122.99
1	A	233	ASP	N-CA-C	6.75	118.64	111.28
1	A	707	VAL	CB-CA-C	-6.63	100.42	111.29
1	A	292	GLU	N-CA-C	6.41	118.14	111.03
1	A	226	PRO	CA-C-O	-6.40	113.89	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	711	LYS	N-CA-C	-6.35	105.29	113.16
1	A	874	SER	N-CA-C	6.25	117.94	110.19
1	A	787	TYR	N-CA-C	6.25	121.04	113.17
1	A	871	GLY	CA-C-N	6.12	125.74	119.56
1	A	871	GLY	C-N-CA	6.12	125.74	119.56
1	A	53	ARG	N-CA-C	-6.11	104.70	111.36
1	A	530	ASN	N-CA-C	-6.01	104.65	112.23
1	A	335	VAL	N-CA-C	-6.00	104.67	110.72
1	A	839	ALA	CA-C-N	-5.91	114.63	122.85
1	A	839	ALA	C-N-CA	-5.91	114.63	122.85
1	A	855	PRO	CA-C-N	5.86	126.27	119.47
1	A	855	PRO	C-N-CA	5.86	126.27	119.47
1	A	310	ALA	N-CA-C	5.85	119.25	111.30
1	A	653	ILE	N-CA-C	-5.75	104.72	110.30
1	A	223	LEU	CA-C-N	-5.67	114.08	122.41
1	A	223	LEU	C-N-CA	-5.67	114.08	122.41
1	A	236	ASN	N-CA-C	5.60	118.58	111.69
1	A	766	ASP	N-CA-C	-5.60	102.51	111.02
1	A	842	LYS	CA-C-N	5.58	125.28	119.82
1	A	842	LYS	C-N-CA	5.58	125.28	119.82
1	A	749	GLY	N-CA-C	5.57	118.37	110.74
1	A	839	ALA	N-CA-C	-5.57	103.19	110.53
1	A	716	THR	N-CA-C	5.56	119.06	111.39
1	A	875	VAL	CA-C-N	5.52	126.75	119.84
1	A	875	VAL	C-N-CA	5.52	126.75	119.84
1	A	650	GLY	N-CA-C	5.33	121.59	115.09
1	A	812	GLN	N-CA-C	5.32	116.77	110.97
1	A	391	ASN	N-CA-C	5.31	119.86	113.17
1	A	311	ALA	N-CA-C	-5.30	102.45	110.24
1	A	746	ASP	N-CA-C	5.29	118.19	111.69
1	A	185	GLY	N-CA-C	-5.26	106.41	112.83
1	A	545	VAL	N-CA-C	5.25	116.07	107.24
1	A	325	ASP	N-CA-C	-5.13	105.60	111.14

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

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Mol	Chain	Res	Type	Group
1	A	312	THR	Peptide
1	A	705	ALA	Peptide
1	A	787	TYR	Peptide

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	6865	0	6706	376	0
All	All	6865	0	6706	376	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 28.

All (376) 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:H	1:A:394:ARG:CD	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:HH11	1:A:457:ARG:HB3	1.48	0.77
1:A:867:PRO:HG2	1:A:880:ASP:HB3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:LEU:HD12	1:A:468:LEU:HD13	1.66	0.77
1:A:394:ARG:H	1:A:394:ARG:HD2	1.49	0.76
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: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:290:ALA:HA	1:A:366:LYS:HZ3	1.52	0.72
1:A:748:LYS:O	1:A:820:ARG:NH2	2.22	0.72
1:A:532:MET:HE2	1:A:611:TRP:HE3	1.55	0.72
1:A:638:LEU:HB3	1:A:702:ILE:HG22	1.71	0.71
1:A:528:PHE:CE2	1:A:532:MET:HE3	2.26	0.70
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:HG22	1:A:229:LEU:HA	1.74	0.68
1:A:43:THR:HA	1:A:228:MET:HB2	1.76	0.68
1:A:170:ASN:OD1	1:A:170:ASN:N	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:454:HIS:O	1:A:458:VAL:HG23	1.96	0.66
1:A:521:PHE:HB2	1:A:578:ILE:HG21	1.77	0.66
1:A:528:PHE:CZ	1:A:572:ARG:HB2	2.30	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:310:ALA:HA	1:A:316:MET:HE3	1.78	0.64
1:A:547:SER:O	1:A:632:GLN:HG2	1.99	0.63
1:A:846:LEU:N	1:A:849:GLU:OE2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ILE:O	1:A:138:ILE:HG13	1.98	0.63
1:A:618:VAL:HG22	1:A:619:PRO:HD3	1.79	0.63
1:A:276:ASN:HB2	1:A:357:ARG:HH12	1.63	0.63
1:A:466:GLN:HG3	1:A:467:GLU:N	2.13	0.62
1:A:761:SER:O	1:A:764:HIS:ND1	2.32	0.62
1:A:258:GLY:HA2	1:A:261:GLN:HB2	1.82	0.62
1:A:393:ILE:HG22	1:A:394:ARG:NE	2.14	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:835:PHE:HA	1:A:838:LEU:HD12	1.82	0.62
1:A:840:SER:H	1:A:842:LYS:HE3	1.63	0.62
1:A:536:MET:HG3	1:A:614:VAL:HG23	1.82	0.62
1:A:216:MET:HE3	1:A:227:LYS:HA	1.82	0.61
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:536:MET:HE3	1:A:613:LYS:HD3	1.82	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:282:LEU:HB3	1:A:348:LEU:HD11	1.83	0.60
1:A:457:ARG:HH11	1:A:457:ARG:CB	2.13	0.60
1:A:74:LEU:O	1:A:78:VAL:HG23	2.01	0.60
1:A:569:ASP:OD1	1:A:572:ARG:NH1	2.33	0.60
1:A:290:ALA:HA	1:A:366:LYS:NZ	2.17	0.60
1:A:608:ARG:HG3	1:A:608:ARG:HH11	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:162:GLN:HB3	1:A:173:ILE:HD11	1.86	0.58
1:A:390:LEU:C	1:A:394:ARG:HD3	2.27	0.58
1:A:741:GLN:HG3	1:A:812:GLN:HG3	1.86	0.58
1:A:435:THR:OG1	1:A:436:GLU:N	2.34	0.58
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:528:PHE:CE2	1:A:572:ARG:HB2	2.39	0.57
1:A:106:TYR:CD1	1:A:106:TYR:C	2.82	0.57
1:A:516:GLN:OE1	1:A:516:GLN:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:106:TYR:C	1:A:106:TYR:HD1	2.14	0.56
1:A:41:ARG:HG2	1:A:62:ILE:HG21	1.88	0.56
1:A:388:TRP:CE3	1:A:389:LEU:HD22	2.40	0.56
1:A:484:GLN:O	1:A:488:ASP:N	2.33	0.56
1:A:670:ALA:HB1	1:A:673:ASP:CG	2.31	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:OE1	1:A:421:GLU:N	2.35	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:741:GLN:HE21	1:A:812:GLN:HE21	1.55	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:842:LYS:O	1:A:881:TYR:OH	2.23	0.54
1:A:94:PHE:HA	1:A:97:ILE:HD12	1.88	0.54
1:A:169:ARG:HH11	1:A:169:ARG:CG	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: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:135:TRP:CG	1:A:243:ARG:HD3	2.44	0.53
1:A:408:GLN:O	1:A:412:THR:HG23	2.09	0.53
1:A:779:ARG:O	1:A:783:ILE:HG13	2.09	0.52
1:A:514:ILE:HD11	1:A:586:ILE:HG22	1.91	0.52
1:A:678:LEU:HD11	1:A:735:ILE:HD12	1.92	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:74:LEU:C	1:A:74:LEU:HD12	2.34	0.52
1:A:473:TYR:OH	1:A:479:VAL:HG11	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:36:TRP:CD1	1:A:37:GLU:H	2.28	0.51
1:A:93:ARG:HG2	1:A:97:ILE:HD11	1.92	0.51
1:A:845:ILE:HG21	1:A:866:MET:HE1	1.92	0.51
1:A:70:LEU:HA	1:A:73:MET:HG3	1.91	0.51
1:A:476:ALA:O	1:A:480:ASN:ND2	2.43	0.51
1:A:824:ASP:OD1	1:A:824:ASP:N	2.42	0.51
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:230:ASP:OD2	1:A:233:ASP:HB2	2.11	0.51
1:A:291:SER:O	1:A:295:GLU:HB3	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:196:ASP:OD1	1:A:196:ASP:N	2.34	0.50
1:A:274:ALA:O	1:A:278:GLU:HG2	2.11	0.50
1:A:373:GLY:O	1:A:377:ARG:HG3	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:87:PRO:HG2	1:A:89:ARG:HH22	1.76	0.50
1:A:832:ILE:HA	1:A:835:PHE:HB2	1.93	0.50
1:A:257:ALA:C	1:A:259:ALA:H	2.20	0.50
1:A:695:LEU:HD23	1:A:696:GLU:N	2.27	0.50
1:A:275:VAL:HB	1:A:357:ARG:NH2	2.26	0.50
1:A:431:SER:HA	1:A:592:ARG:HD3	1.94	0.50
1:A:290:ALA:O	1:A:294:LEU:HB2	2.12	0.49
1:A:628:GLU:OE1	1:A:628:GLU:HA	2.12	0.49
1:A:64:GLU:HA	1:A:67:ARG:HG3	1.93	0.49
1:A:214:LEU:O	1:A:214:LEU:HG	2.06	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:424:LEU:CD1	1:A:496:LEU:HB3	2.43	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:316:MET:HE2	1:A:319:MLZ:HD3	1.93	0.49
1:A:61:ASN:OD1	1:A:63:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLN:H	1:A:179:SER:HG	1.60	0.49
1:A:844:TYR:HB3	1:A:878:ALA:HB1	1.95	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:561:PHE:CD1	1:A:561:PHE:C	2.91	0.48
1:A:684:ASN:C	1:A:684:ASN:HD22	2.21	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:252:PHE:O	1:A:256:PHE:HB2	2.14	0.48
1:A:551:ILE:HG21	1:A:629:LEU:HA	1.96	0.48
1:A:502:GLU:HG2	1:A:503:ALA:N	2.28	0.47
1:A:710:ASN:OD1	1:A:712:HIS:HB2	2.14	0.47
1:A:750:ILE:CG2	1:A:758:PHE:HZ	2.27	0.47
1:A:859:ALA:O	1:A:863:ILE:HG12	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:95:HIS:O	1:A:96:MLZ:C	2.60	0.47
1:A:714:ASN:OD1	1:A:714:ASN:N	2.47	0.47
1:A:74:LEU:O	1:A:77:GLU:HG2	2.15	0.47
1:A:441:LEU:HD13	1:A:504:LEU:HD13	1.97	0.47
1:A:158:LEU:O	1:A:162:GLN:HG2	2.14	0.47
1:A:293:LEU:HD21	1:A:371:ILE:CD1	2.41	0.47
1:A:551:ILE:HG22	1:A:629:LEU:HD13	1.97	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:107:ILE:HG22	1:A:112:VAL:CG1	2.45	0.46
1:A:532:MET:HE2	1:A:611:TRP:CE3	2.44	0.46
1:A:642:PHE:CE2	1:A:699:HIS:HB2	2.50	0.46
1:A:374:ALA:HA	1:A:377:ARG:NE	2.30	0.46
1:A:737:GLU:O	1:A:741:GLN:HG2	2.14	0.46
1:A:467:GLU:O	1:A:471:LEU:HD13	2.16	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:109:SER:OG	1:A:110:LYS:N	2.48	0.46
1:A:316:MET:HB3	1:A:393:ILE:HD12	1.96	0.46
1:A:746:ASP:OD1	1:A:747:ALA:N	2.48	0.46
1:A:466:GLN:HG3	1:A:467:GLU:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:52:LEU:HD13	1:A:75:LEU:HD13	1.98	0.46
1:A:67:ARG:HD2	1:A:125:GLY:CA	2.46	0.46
1:A:121:GLU:HG2	1:A:129:MET:SD	2.55	0.46
1:A:215:ALA:O	1:A:218:ILE:HG22	2.16	0.46
1:A:504:LEU:HA	1:A:504:LEU:HD23	1.62	0.46
1:A:692:ILE:HD12	1:A:692:ILE:HA	1.73	0.46
1:A:773:MET:HB2	1:A:808:THR:CG2	2.46	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:858:GLN:OE1	1:A:858:GLN:N	2.46	0.45
1:A:868:ALA:HA	1:A:879:LEU:HA	1.98	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:636:GLU:OE1	1:A:636:GLU:HA	2.17	0.45
1:A:845:ILE:HD13	1:A:850:LEU:HD21	1.99	0.45
1:A:197:LEU:HD12	1:A:197:LEU:H	1.80	0.45
1:A:764:HIS:CG	1:A:765:PHE:N	2.84	0.45
1:A:311:ALA:O	1:A:315:ALA:HB3	2.17	0.45
1:A:367:MET:HE3	1:A:369:SER:H	1.82	0.45
1:A:495:THR:O	1:A:499:LYS:NZ	2.47	0.45
1:A:696:GLU:HG2	1:A:717:MET:CE	2.46	0.45
1:A:796:ARG:HD3	1:A:796:ARG:HA	1.65	0.45
1:A:84:LEU:HD12	1:A:84:LEU:H	1.81	0.45
1:A:551:ILE:HG13	1:A:628:GLU:HG3	1.97	0.45
1:A:194:ARG:CZ	1:A:197:LEU:HD11	2.47	0.45
1:A:840:SER:N	1:A:842:LYS:HE3	2.30	0.45
1:A:253:TYR:O	1:A:256:PHE:N	2.46	0.45
1:A:331:MLZ:HCM1	1:A:379:GLU:OE1	2.17	0.45
1:A:419:GLY:O	1:A:423:ILE:HG23	2.17	0.45
1:A:526:ALA:N	1:A:527:PRO:HD2	2.31	0.45
1:A:828:ALA:HB1	1:A:885:SER:OG	2.17	0.45
1:A:245:ILE:O	1:A:249:VAL:HG23	2.17	0.45
1:A:253:TYR:CD1	1:A:253:TYR:C	2.94	0.45
1:A:288:ARG:HD3	1:A:341:LEU:CD1	2.47	0.45
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:293:LEU:HD12	1:A:293:LEU:HA	1.85	0.44
1:A:400:GLU:N	1:A:400:GLU:OE1	2.50	0.44
1:A:676:ASN:O	1:A:680:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLU:N	1:A:394:ARG:NH1	2.43	0.44
1:A:524:ARG:NH2	1:A:574:SER:OG	2.39	0.44
1:A:713:THR:HG1	1:A:715:TYR:H	1.66	0.44
1:A:850:LEU:O	1:A:854:LEU:HB2	2.18	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:650:GLY:N	1:A:651:PRO:HD2	2.32	0.44
1:A:671:LEU:HD13	1:A:671:LEU:C	2.41	0.44
1:A:716:THR:O	1:A:718:GLU:N	2.50	0.44
1:A:875:VAL:HB	1:A:878:ALA:HB2	1.98	0.44
1:A:351:LYS:O	1:A:354:ILE:HG13	2.17	0.44
1:A:416:TRP:CE3	1:A:417:ALA:HB2	2.53	0.44
1:A:70:LEU:H	1:A:70:LEU:HG	1.46	0.44
1:A:84:LEU:HB2	1:A:85:PRO:CD	2.43	0.44
1:A:308:THR:HA	1:A:309:PRO:HD3	1.82	0.44
1:A:657:MET:O	1:A:660:ILE:HG22	2.17	0.44
1:A:669:GLY:HA2	1:A:670:ALA:CB	2.35	0.44
1:A:223:LEU:O	1:A:225:ILE:HG23	2.18	0.44
1:A:762:PHE:HD2	1:A:815:ILE:HG21	1.83	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:87:PRO:HG2	1:A:89:ARG:NH2	2.33	0.43
1:A:163:ARG:HD3	1:A:163:ARG:HA	1.39	0.43
1:A:671:LEU:HG	1:A:742:ILE:HD11	1.98	0.43
1:A:117:ILE:HG13	1:A:117:ILE:O	2.18	0.43
1:A:500:ARG:O	1:A:504:LEU:HB2	2.18	0.43
1:A:558:HIS:CD2	1:A:558:HIS:C	2.96	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:301:ILE:O	1:A:305:GLU:HB2	2.18	0.43
1:A:468:LEU:HD12	1:A:468:LEU:HA	1.82	0.43
1:A:695:LEU:HD21	1:A:717:MET:SD	2.58	0.43
1:A:327:ARG:O	1:A:332:PRO:HD3	2.19	0.43
1:A:421:GLU:O	1:A:425:LEU:HD22	2.19	0.43
1:A:651:PRO:O	1:A:655:ASN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLU:N	1:A:82:GLU:OE1	2.52	0.42
1:A:115:VAL:HG12	1:A:116:SER:HB2	2.01	0.42
1:A:306:ASN:OD1	1:A:307:ARG:N	2.52	0.42
1:A:351:LYS:HE2	1:A:354:ILE:HD11	2.00	0.42
1:A:155:GLU:CD	1:A:155:GLU:H	2.28	0.42
1:A:432:ALA:HB3	1:A:437:VAL:HG23	2.01	0.42
1:A:521:PHE:CD1	1:A:521:PHE:C	2.96	0.42
1:A:324:ARG:HA	1:A:324:ARG:HD3	1.61	0.42
1:A:366:LYS:HA	1:A:366:LYS:HD3	1.62	0.42
1:A:405:LYS:O	1:A:409:LYS:HG3	2.19	0.42
1:A:640:ARG:HD2	1:A:712:HIS:CD2	2.55	0.42
1:A:371:ILE:HA	1:A:371:ILE:HD12	1.47	0.42
1:A:424:LEU:CD2	1:A:497:THR:HG22	2.41	0.42
1:A:473:TYR:HD1	1:A:473:TYR:H	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
1:A:77:GLU:HA	1:A:80:SER:HB2	2.02	0.42
1:A:593:ILE:HG23	1:A:595:SER:H	1.84	0.42
1:A:242:GLU:HG2	1:A:246:MET:HE2	2.02	0.42
1:A:431:SER:O	1:A:431:SER:OG	2.28	0.42
1:A:528:PHE:HE2	1:A:532:MET:HE3	1.78	0.42
1:A:69:GLY:O	1:A:72:LEU:HB3	2.19	0.42
1:A:102:MLZ:HCM3	1:A:102:MLZ:HD3	1.75	0.42
1:A:131:LEU:HD13	1:A:131:LEU:HA	1.82	0.42
1:A:339:CYS:HA	1:A:342:GLU:OE2	2.20	0.42
1:A:671:LEU:HD13	1:A:671:LEU:O	2.20	0.42
1:A:733:ARG:HG2	1:A:734:THR:N	2.35	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:389:LEU:C	1:A:394:ARG:NH1	2.78	0.41
1:A:673:ASP:OD1	1:A:673:ASP:C	2.63	0.41
1:A:273:LEU:O	1:A:273:LEU:HD23	2.21	0.41
1:A:696:GLU:HG2	1:A:717:MET:HE1	2.03	0.41
1:A:745:ARG:HD3	1:A:746:ASP:HB3	2.02	0.41
1:A:253:TYR:C	1:A:253:TYR:HD1	2.29	0.41
1:A:742:ILE:HA	1:A:742:ILE:HD13	1.49	0.41
1:A:68:ASN:N	1:A:69:GLY:HA2	2.34	0.41
1:A:177:HIS:CD2	1:A:239:MLZ:HD3	2.56	0.41
1:A:715:TYR:HB3	1:A:720:ILE:HD13	2.02	0.41
1:A:741:GLN:HE21	1:A:812:GLN:HG3	1.85	0.41
1:A:285:GLU:HA	1:A:288:ARG:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LEU:HD13	1:A:389:LEU:HA	1.65	0.41
1:A:551:ILE:HG23	1:A:551:ILE:HD12	1.78	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:532:MET:HE1	1:A:611:TRP:HB2	2.02	0.41
1:A:605:ASP:HA	1:A:608:ARG:HB2	2.03	0.41
1:A:45:THR:OG1	1:A:62:ILE:HB	2.20	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:133:MET:CG	1:A:134:ILE:N	2.83	0.41
1:A:167:PRO:HB2	1:A:168:TYR:HD1	1.86	0.41
1:A:327:ARG:NH2	1:A:386:GLU:OE2	2.44	0.41
1:A:509:LYS:HG2	1:A:510:LEU:N	2.33	0.40
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:64:GLU:O	1:A:67:ARG:HG3	2.21	0.40
1:A:272:VAL:O	1:A:357:ARG:NH2	2.54	0.40
1:A:343:ILE:O	1:A:347:THR:HG23	2.20	0.40
1:A:530:ASN:OD1	1:A:530:ASN:C	2.65	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:750:ILE:HG23	1:A:758:PHE:HZ	1.85	0.40
1:A:134:ILE:O	1:A:137:ILE:HB	2.21	0.40
1:A:243:ARG:HA	1:A:246:MET:HE3	2.04	0.40
1:A:285:GLU:HA	1:A:288:ARG:CD	2.52	0.40
1:A:305:GLU:O	1:A:307:ARG:HG2	2.22	0.40
1:A:186:LEU:C	1:A:186:LEU:HD23	2.46	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 ⓘ

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	844/876 (96%)	790 (94%)	52 (6%)	2 (0%)	43 74

All (2) Ramachandran outliers are listed below:

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

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	702/752 (93%)	496 (71%)	206 (29%)	0 2

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	62	ILE
1	A	64	GLU
1	A	67	ARG
1	A	70	LEU
1	A	72	LEU
1	A	74	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

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Mol	Chain	Res	Type
1	A	117	ILE
1	A	120	GLU
1	A	122	ILE
1	A	123	VAL
1	A	129	MET
1	A	131	LEU
1	A	134	ILE
1	A	140	ARG
1	A	146	ILE
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	177	HIS
1	A	178	THR
1	A	189	LEU
1	A	192	ARG
1	A	194	ARG
1	A	196	ASP
1	A	203	LEU
1	A	205	LYS
1	A	209	ILE
1	A	213	ASN
1	A	214	LEU
1	A	223	LEU
1	A	225	ILE
1	A	232	GLU
1	A	234	ILE
1	A	245	ILE
1	A	246	MET
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	284	GLU
1	A	286	TYR
1	A	293	LEU

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Mol	Chain	Res	Type
1	A	297	ILE
1	A	300	THR
1	A	301	ILE
1	A	305	GLU
1	A	308	THR
1	A	313	MET
1	A	316	MET
1	A	317	GLN
1	A	320	LEU
1	A	326	TYR
1	A	328	ARG
1	A	339	CYS
1	A	342	GLU
1	A	343	ILE
1	A	346	ASN
1	A	348	LEU
1	A	349	GLN
1	A	350	THR
1	A	351	LYS
1	A	352	LEU
1	A	354	ILE
1	A	361	MET
1	A	363	SER
1	A	371	ILE
1	A	375	TRP
1	A	378	LEU
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	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

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Mol	Chain	Res	Type
1	A	438	ARG
1	A	441	LEU
1	A	450	ASP
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	477	VAL
1	A	479	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	501	ARG
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	514	ILE
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	555	ILE
1	A	556	THR
1	A	560	GLN
1	A	565	LEU
1	A	581	GLU
1	A	582	VAL
1	A	585	VAL
1	A	586	ILE
1	A	591	ILE

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Mol	Chain	Res	Type
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	614	VAL
1	A	615	LYS
1	A	616	GLN
1	A	617	LEU
1	A	618	VAL
1	A	620	ILE
1	A	631	ARG
1	A	640	ARG
1	A	653	ILE
1	A	655	ASN
1	A	659	GLU
1	A	660	ILE
1	A	662	ARG
1	A	665	ILE
1	A	668	THR
1	A	673	ASP
1	A	678	LEU
1	A	685	ILE
1	A	688	TYR
1	A	690	ASN
1	A	692	ILE
1	A	703	GLN
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	738	VAL
1	A	740	THR
1	A	742	ILE
1	A	750	ILE
1	A	752	GLN

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Mol	Chain	Res	Type
1	A	756	ASN
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	819	THR
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	885	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	222	HIS
1	A	444	HIS
1	A	454	HIS
1	A	489	GLN
1	A	529	ASN
1	A	552	GLN
1	A	558	HIS
1	A	616	GLN
1	A	641	GLN
1	A	655	ASN
1	A	674	GLN
1	A	677	GLN
1	A	683	HIS
1	A	684	ASN
1	A	699	HIS
1	A	812	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	329	1	8,9,10	0.73	0	4,9,11	1.65	1 (25%)
1	MLZ	A	562	1	8,9,10	0.71	0	4,9,11	1.54	1 (25%)
1	MLZ	A	164	1	8,9,10	0.77	0	4,9,11	1.41	1 (25%)
1	MLZ	A	331	1	8,9,10	0.64	0	4,9,11	1.33	1 (25%)
1	MLZ	A	102	1	8,9,10	0.58	0	4,9,11	1.39	1 (25%)
1	MLZ	A	443	1	8,9,10	0.84	0	4,9,11	1.64	1 (25%)
1	MLZ	A	689	1	8,9,10	0.85	0	4,9,11	0.71	0
1	MLZ	A	71	1	8,9,10	0.58	0	4,9,11	1.84	1 (25%)
1	MLZ	A	181	1	8,9,10	0.69	0	4,9,11	1.51	1 (25%)
1	MLZ	A	42	1	8,9,10	0.66	0	4,9,11	1.31	1 (25%)
1	MLZ	A	96	1	8,9,10	0.57	0	4,9,11	1.33	1 (25%)
1	MLZ	A	239	1	8,9,10	0.68	0	4,9,11	1.51	1 (25%)
1	MLZ	A	319	1	8,9,10	0.83	0	4,9,11	1.49	1 (25%)

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	329	1	-	3/7/8/10	-
1	MLZ	A	562	1	-	2/7/8/10	-
1	MLZ	A	164	1	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLZ	A	331	1	-	5/7/8/10	-
1	MLZ	A	102	1	-	3/7/8/10	-
1	MLZ	A	443	1	-	5/7/8/10	-
1	MLZ	A	689	1	-	4/7/8/10	-
1	MLZ	A	71	1	-	4/7/8/10	-
1	MLZ	A	181	1	-	3/7/8/10	-
1	MLZ	A	42	1	-	1/7/8/10	-
1	MLZ	A	96	1	-	3/7/8/10	-
1	MLZ	A	239	1	-	2/7/8/10	-
1	MLZ	A	319	1	-	2/7/8/10	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	MLZ	CM-NZ-CE	3.36	121.36	112.01
1	A	329	MLZ	CM-NZ-CE	3.13	120.74	112.01
1	A	562	MLZ	CM-NZ-CE	3.00	120.36	112.01
1	A	164	MLZ	CM-NZ-CE	2.69	119.50	112.01
1	A	319	MLZ	CM-NZ-CE	2.68	119.47	112.01
1	A	181	MLZ	CM-NZ-CE	2.67	119.46	112.01
1	A	239	MLZ	CM-NZ-CE	2.64	119.36	112.01
1	A	102	MLZ	CM-NZ-CE	2.48	118.91	112.01
1	A	443	MLZ	CM-NZ-CE	2.47	118.89	112.01
1	A	96	MLZ	CM-NZ-CE	2.32	118.47	112.01
1	A	331	MLZ	CM-NZ-CE	2.32	118.47	112.01
1	A	42	MLZ	CM-NZ-CE	2.16	118.04	112.01

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	42	MLZ	CD-CE-NZ-CM
1	A	71	MLZ	N-CA-CB-CG
1	A	71	MLZ	C-CA-CB-CG
1	A	71	MLZ	CD-CE-NZ-CM
1	A	96	MLZ	CD-CE-NZ-CM
1	A	102	MLZ	CD-CE-NZ-CM
1	A	164	MLZ	CD-CE-NZ-CM

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Mol	Chain	Res	Type	Atoms
1	A	181	MLZ	CD-CE-NZ-CM
1	A	319	MLZ	CD-CE-NZ-CM
1	A	329	MLZ	CD-CE-NZ-CM
1	A	331	MLZ	C-CA-CB-CG
1	A	331	MLZ	CD-CE-NZ-CM
1	A	443	MLZ	N-CA-CB-CG
1	A	443	MLZ	C-CA-CB-CG
1	A	443	MLZ	CD-CE-NZ-CM
1	A	562	MLZ	C-CA-CB-CG
1	A	689	MLZ	C-CA-CB-CG
1	A	689	MLZ	CD-CE-NZ-CM
1	A	319	MLZ	CG-CD-CE-NZ
1	A	329	MLZ	CG-CD-CE-NZ
1	A	443	MLZ	CG-CD-CE-NZ
1	A	689	MLZ	CG-CD-CE-NZ
1	A	102	MLZ	CG-CD-CE-NZ
1	A	331	MLZ	CA-CB-CG-CD
1	A	331	MLZ	CE-CD-CG-CB
1	A	443	MLZ	CE-CD-CG-CB
1	A	164	MLZ	CE-CD-CG-CB
1	A	239	MLZ	CE-CD-CG-CB
1	A	164	MLZ	CA-CB-CG-CD
1	A	102	MLZ	CA-CB-CG-CD
1	A	96	MLZ	CE-CD-CG-CB
1	A	181	MLZ	CE-CD-CG-CB
1	A	331	MLZ	N-CA-CB-CG
1	A	181	MLZ	CG-CD-CE-NZ
1	A	689	MLZ	CE-CD-CG-CB
1	A	562	MLZ	CE-CD-CG-CB
1	A	239	MLZ	CA-CB-CG-CD
1	A	71	MLZ	CA-CB-CG-CD
1	A	96	MLZ	N-CA-CB-CG
1	A	329	MLZ	N-CA-CB-CG

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	329	MLZ	1	0
1	A	562	MLZ	1	0
1	A	331	MLZ	1	0
1	A	102	MLZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	96	MLZ	1	0
1	A	239	MLZ	1	0
1	A	319	MLZ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	846/876 (96%)	-0.37	2 (0%) 91 82	49, 130, 244, 277	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	788	ASP	3.2
1	A	783	ILE	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
1	MLZ	A	329	10/11	0.88	0.07	110,130,139,142	0
1	MLZ	A	239	10/11	0.91	0.08	129,135,148,148	0
1	MLZ	A	319	10/11	0.92	0.11	104,118,125,130	0
1	MLZ	A	181	10/11	0.93	0.10	125,138,152,153	0
1	MLZ	A	102	10/11	0.93	0.09	72,79,81,83	0
1	MLZ	A	443	10/11	0.94	0.07	57,64,74,80	0
1	MLZ	A	331	10/11	0.95	0.12	122,125,132,133	0
1	MLZ	A	42	10/11	0.95	0.08	81,87,102,103	0
1	MLZ	A	689	10/11	0.95	0.08	126,135,139,139	0
1	MLZ	A	71	10/11	0.97	0.06	64,70,84,93	0
1	MLZ	A	164	10/11	0.97	0.09	76,94,100,101	0
1	MLZ	A	562	10/11	0.97	0.07	51,57,86,86	0
1	MLZ	A	96	10/11	0.97	0.07	64,74,77,79	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.