



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:22 AM EDT

PDB ID : 2NUB / pdb_00002nub
Title : Structure of Aquifex aeolicus Argonuate
Authors : Rashid, U.J.; Paterok, D.; Koglin, A.; Gohlke, H.; Piehler, J.; Chen, J.C.-H.
Deposited on : 2006-11-09
Resolution : 3.20 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
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

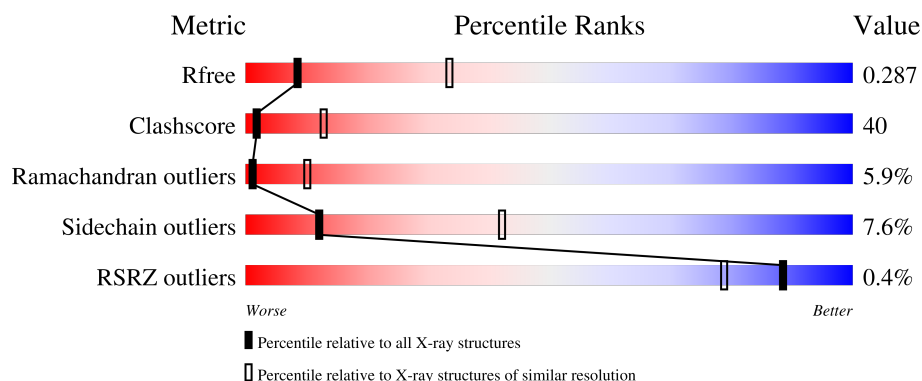
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

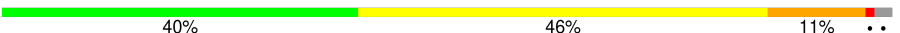
The reported resolution of this entry is 3.20 Å.

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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	706	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5814 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 Argonaute.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	690	Total	C	N	O	S	0	0	0
			5734	3743	971	1008	12			

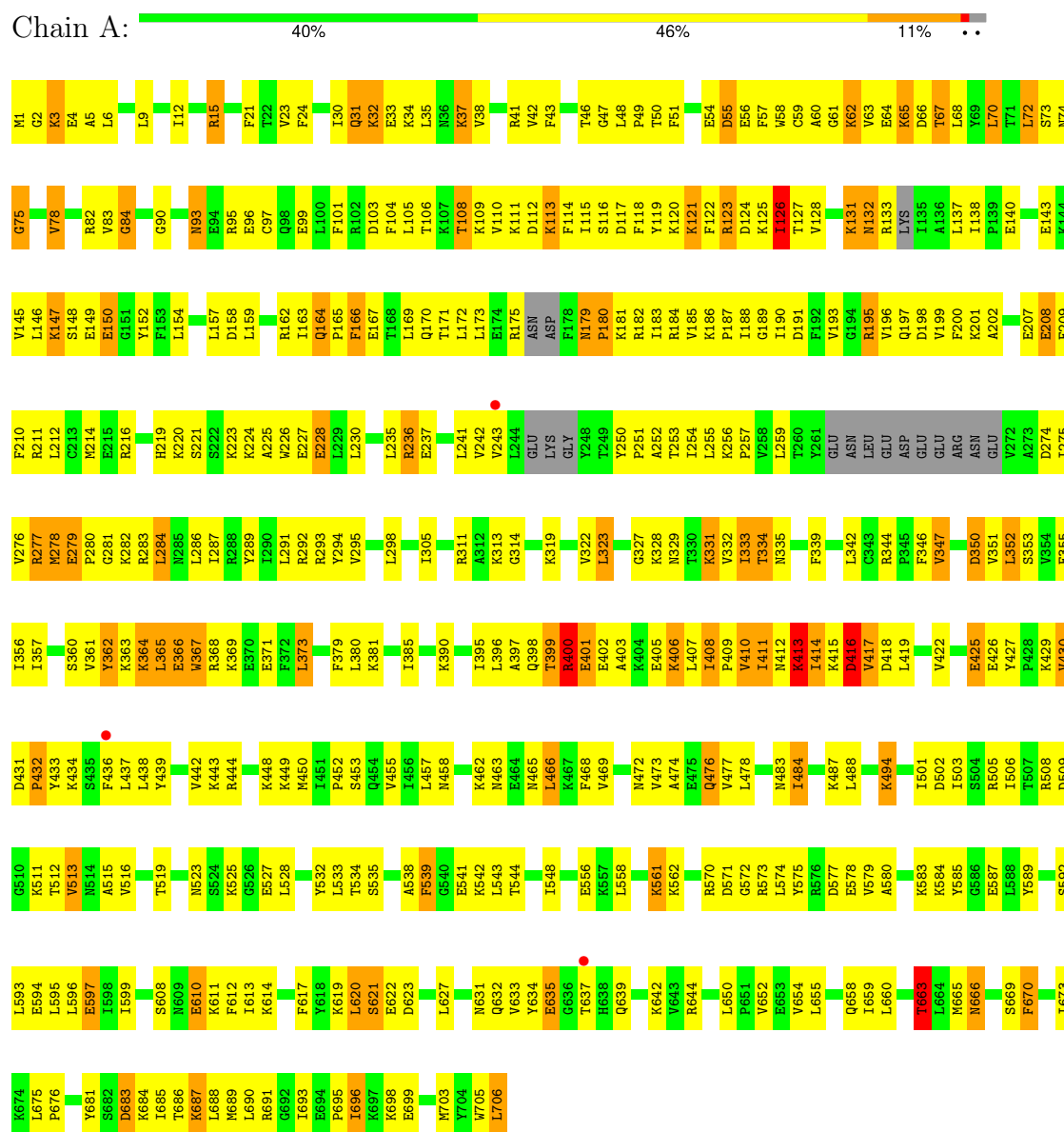
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total	O	0	0
			80	80		

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: Argonaute



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	125.00Å 125.00Å 253.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.50 – 3.20 72.50 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.50-3.20) 100.0 (72.50-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.82Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.311 0.217 , 0.287	Depositor DCC
R_{free} test set	2434 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 90.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5814	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.54	0/5844	1.03	31/7840 (0.4%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	GLU	N-CA-C	-10.53	99.84	112.89
1	A	126	ILE	N-CA-C	-8.64	102.87	112.80
1	A	279	GLU	CA-C-N	8.17	128.11	119.05
1	A	279	GLU	C-N-CA	8.17	128.11	119.05
1	A	538	ALA	N-CA-C	8.15	121.56	109.24
1	A	331	LYS	N-CA-C	-7.92	102.63	111.82
1	A	666	ASN	N-CA-C	-7.88	103.56	113.02
1	A	417	VAL	N-CA-C	-7.73	93.27	109.34
1	A	37	LYS	N-CA-C	-7.72	101.07	111.96
1	A	663	THR	N-CA-C	-7.13	103.55	111.82
1	A	75	GLY	N-CA-C	-7.06	106.03	115.21
1	A	350	ASP	N-CA-C	7.05	120.98	112.38
1	A	334	THR	N-CA-C	6.78	118.67	111.28
1	A	670	PHE	N-CA-C	-6.73	106.27	114.75
1	A	55	ASP	N-CA-C	-6.38	106.14	114.04
1	A	425	GLU	N-CA-C	-6.18	100.12	109.95
1	A	617	PHE	N-CA-C	5.96	118.25	109.24
1	A	346	PHE	N-CA-C	-5.91	102.46	110.68
1	A	367	TRP	N-CA-C	-5.91	104.78	112.23
1	A	400	ARG	N-CA-C	-5.59	105.38	113.21
1	A	675	LEU	N-CA-C	5.59	118.01	110.29
1	A	209	PHE	N-CA-C	-5.55	104.92	110.97
1	A	352	LEU	N-CA-C	5.43	117.81	109.07
1	A	113	LYS	N-CA-C	-5.30	105.50	111.28
1	A	505	ARG	N-CA-C	5.25	117.45	108.90
1	A	597	GLU	N-CA-C	-5.18	101.71	109.95
1	A	381	LYS	N-CA-C	-5.14	105.76	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	610	GLU	N-CA-C	5.11	117.98	111.69
1	A	484	ILE	CA-C-N	5.04	124.64	119.56
1	A	484	ILE	C-N-CA	5.04	124.64	119.56
1	A	627	LEU	N-CA-C	5.00	117.13	109.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5734	0	6017	468	0
2	A	80	0	0	1	0
All	All	5814	0	6017	468	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 40.

All (468) 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:277:ARG:HD3	1:A:277:ARG:H	1.11	1.08
1:A:596:LEU:HD11	1:A:655:LEU:HD13	1.37	1.03
1:A:512:THR:HG22	1:A:513:VAL:H	1.25	0.99
1:A:30:ILE:HB	1:A:35:LEU:HD11	1.45	0.98
1:A:313:LYS:HE3	1:A:619:LYS:HB2	1.45	0.96
1:A:12:ILE:HG13	1:A:305:ILE:HG12	1.51	0.92
1:A:123:ARG:HA	1:A:126:ILE:HD12	1.50	0.91
1:A:179:ASN:HB3	1:A:180:PRO:HA	1.52	0.89
1:A:166:PHE:H	1:A:166:PHE:HD2	1.19	0.88
1:A:32:LYS:HA	1:A:35:LEU:HD12	1.56	0.88
1:A:31:GLN:H	1:A:34:LYS:NZ	1.71	0.87
1:A:159:LEU:HD22	1:A:287:ILE:HG22	1.57	0.87
1:A:93:ASN:ND2	1:A:96:GLU:H	1.72	0.86
1:A:167:GLU:OE1	1:A:171:THR:HB	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:HB3	1:A:34:LYS:HG2	1.57	0.85
1:A:159:LEU:HD11	1:A:286:LEU:HD23	1.58	0.84
1:A:179:ASN:HB3	1:A:180:PRO:CA	2.08	0.84
1:A:291:LEU:HD11	1:A:305:ILE:HG21	1.60	0.83
1:A:108:THR:HG22	1:A:110:VAL:H	1.42	0.83
1:A:38:VAL:HG13	1:A:70:LEU:HD11	1.60	0.83
1:A:187:PRO:HB2	1:A:190:ILE:HB	1.61	0.82
1:A:356:ILE:HD13	1:A:373:LEU:HD21	1.62	0.81
1:A:93:ASN:HD21	1:A:96:GLU:H	1.29	0.81
1:A:476:GLN:HA	1:A:476:GLN:HE21	1.46	0.80
1:A:291:LEU:O	1:A:295:VAL:HG23	1.83	0.79
1:A:411:ILE:HG22	1:A:449:LYS:HZ3	1.46	0.79
1:A:333:ILE:HD11	1:A:339:PHE:HA	1.64	0.78
1:A:138:ILE:HG21	1:A:162:ARG:HH21	1.48	0.78
1:A:6:LEU:HD11	1:A:311:ARG:HH21	1.50	0.77
1:A:214:MET:HE2	1:A:227:GLU:HA	1.65	0.77
1:A:277:ARG:HD3	1:A:277:ARG:N	1.95	0.77
1:A:364:LYS:N	1:A:364:LYS:HE3	2.00	0.77
1:A:95:ARG:O	1:A:99:GLU:HG3	1.85	0.77
1:A:512:THR:HG22	1:A:513:VAL:N	1.99	0.76
1:A:659:ILE:HG23	1:A:676:PRO:HG3	1.64	0.76
1:A:361:VAL:HG13	1:A:425:GLU:HG2	1.65	0.76
1:A:276:VAL:HG22	1:A:278:MET:H	1.50	0.75
1:A:367:TRP:O	1:A:371:GLU:HG2	1.86	0.75
1:A:476:GLN:HA	1:A:476:GLN:NE2	2.02	0.75
1:A:166:PHE:HD2	1:A:166:PHE:N	1.85	0.75
1:A:399:THR:HG23	1:A:400:ARG:H	1.52	0.75
1:A:165:PRO:C	1:A:167:GLU:H	1.95	0.74
1:A:181:LYS:O	1:A:196:VAL:HB	1.87	0.74
1:A:122:PHE:C	1:A:124:ASP:H	1.95	0.74
1:A:411:ILE:HA	1:A:449:LYS:HE2	1.69	0.74
1:A:277:ARG:H	1:A:277:ARG:CD	1.93	0.74
1:A:406:LYS:HZ2	1:A:406:LYS:CB	2.01	0.74
1:A:364:LYS:HE3	1:A:364:LYS:H	1.53	0.73
1:A:259:LEU:HD21	1:A:433:TYR:HA	1.70	0.73
1:A:448:LYS:HA	1:A:689:MET:HE1	1.69	0.73
1:A:31:GLN:HB3	1:A:34:LYS:CG	2.17	0.73
1:A:494:LYS:HD2	1:A:494:LYS:O	1.87	0.73
1:A:38:VAL:O	1:A:42:VAL:HG23	1.90	0.72
1:A:462:LYS:C	1:A:463:ASN:HD22	1.98	0.72
1:A:226:TRP:CZ3	1:A:251:PRO:HG3	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:VAL:CG2	1:A:56:GLU:HB3	2.21	0.71
1:A:93:ASN:C	1:A:93:ASN:HD22	1.96	0.71
1:A:180:PRO:HB2	1:A:183:ILE:HD12	1.71	0.71
1:A:31:GLN:H	1:A:34:LYS:HZ3	1.38	0.71
1:A:431:ASP:OD2	1:A:434:LYS:HE2	1.91	0.71
1:A:659:ILE:HG23	1:A:676:PRO:CG	2.21	0.70
1:A:488:LEU:HG	1:A:665:MET:HE3	1.74	0.69
1:A:138:ILE:HG21	1:A:162:ARG:NH2	2.07	0.69
1:A:610:GLU:O	1:A:611:LYS:HB2	1.93	0.69
1:A:24:PHE:CE2	1:A:82:ARG:HB2	2.27	0.69
1:A:690:LEU:C	1:A:691:ARG:HD2	2.17	0.68
1:A:1:MET:SD	1:A:314:GLY:HA2	2.33	0.68
1:A:280:PRO:HA	1:A:283:ARG:HB2	1.76	0.68
1:A:580:ALA:O	1:A:584:LYS:HB2	1.93	0.68
1:A:291:LEU:HD11	1:A:305:ILE:CG2	2.24	0.67
1:A:170:GLN:HG2	1:A:253:THR:HG22	1.76	0.67
1:A:211:ARG:HH11	1:A:230:LEU:HD21	1.58	0.67
1:A:333:ILE:HD11	1:A:339:PHE:CA	2.25	0.67
1:A:173:LEU:HD13	1:A:199:VAL:HG11	1.76	0.67
1:A:284:LEU:O	1:A:287:ILE:HG12	1.94	0.67
1:A:398:GLN:HA	1:A:427:TYR:HE2	1.59	0.67
1:A:210:PHE:O	1:A:214:MET:HB2	1.94	0.66
1:A:147:LYS:HB3	1:A:621:SER:HB3	1.76	0.66
1:A:42:VAL:O	1:A:46:THR:HB	1.96	0.66
1:A:46:THR:CG2	1:A:48:LEU:HB2	2.25	0.66
1:A:356:ILE:HD11	1:A:373:LEU:HD11	1.77	0.66
1:A:65:LYS:C	1:A:67:THR:H	2.04	0.66
1:A:347:VAL:HB	1:A:385:ILE:HD11	1.77	0.66
1:A:399:THR:HG23	1:A:401:GLU:H	1.61	0.66
1:A:333:ILE:CD1	1:A:339:PHE:HA	2.26	0.65
1:A:573:ARG:HH12	1:A:644:ARG:HD3	1.61	0.65
1:A:1:MET:HG2	1:A:2:GLY:H	1.60	0.65
1:A:62:LYS:CE	1:A:62:LYS:H	2.09	0.65
1:A:512:THR:CG2	1:A:513:VAL:H	2.04	0.65
1:A:406:LYS:C	1:A:408:ILE:H	2.04	0.64
1:A:190:ILE:N	1:A:190:ILE:HD12	2.12	0.64
1:A:279:GLU:HB2	1:A:280:PRO:HD2	1.78	0.64
1:A:408:ILE:HD12	1:A:408:ILE:N	2.13	0.64
1:A:64:GLU:O	1:A:65:LYS:HG3	1.97	0.64
1:A:62:LYS:HE2	1:A:62:LYS:O	1.98	0.63
1:A:108:THR:CG2	1:A:110:VAL:HB	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ASN:CG	1:A:413:LYS:H	2.02	0.63
1:A:584:LYS:HD2	1:A:585:TYR:CD1	2.34	0.62
1:A:313:LYS:CE	1:A:619:LYS:HB2	2.26	0.62
1:A:23:VAL:HG23	1:A:58:TRP:CD1	2.35	0.62
1:A:24:PHE:CE2	1:A:68:LEU:HG	2.34	0.62
1:A:368:ARG:HG3	1:A:368:ARG:HH11	1.64	0.62
1:A:406:LYS:HZ2	1:A:406:LYS:HB3	1.63	0.62
1:A:46:THR:HG22	1:A:48:LEU:HB2	1.81	0.62
1:A:34:LYS:O	1:A:37:LYS:HB2	1.99	0.62
1:A:120:LYS:HE2	1:A:121:LYS:HG2	1.81	0.62
1:A:73:SER:C	1:A:75:GLY:H	2.08	0.62
1:A:202:ALA:HB2	1:A:241:LEU:HG	1.82	0.62
1:A:398:GLN:O	1:A:398:GLN:HG3	1.99	0.62
1:A:211:ARG:NH1	1:A:230:LEU:HD21	2.14	0.61
1:A:397:ALA:HB1	1:A:402:GLU:OE2	1.99	0.61
1:A:574:LEU:HB2	1:A:597:GLU:HG2	1.82	0.61
1:A:542:LYS:O	1:A:542:LYS:HG2	1.99	0.61
1:A:395:ILE:HD11	1:A:409:PRO:HG2	1.82	0.61
1:A:502:ASP:OD1	1:A:686:THR:HG21	2.00	0.61
1:A:408:ILE:HB	1:A:409:PRO:HD3	1.81	0.61
1:A:501:ILE:O	1:A:501:ILE:HD12	2.01	0.61
1:A:523:ASN:ND2	1:A:527:GLU:HB2	2.16	0.61
1:A:367:TRP:H	1:A:367:TRP:CD1	2.17	0.61
1:A:508:ARG:O	1:A:509:ASP:HB2	2.01	0.61
1:A:83:VAL:HG12	1:A:84:GLY:H	1.66	0.61
1:A:140:GLU:OE2	1:A:162:ARG:HB2	2.01	0.60
1:A:574:LEU:N	1:A:597:GLU:OE2	2.32	0.60
1:A:687:LYS:HB2	1:A:687:LYS:NZ	2.15	0.60
1:A:65:LYS:O	1:A:67:THR:N	2.34	0.60
1:A:323:LEU:O	1:A:323:LEU:HD12	2.02	0.60
1:A:333:ILE:HD11	1:A:339:PHE:N	2.16	0.60
1:A:352:LEU:HA	1:A:418:ASP:OD1	2.00	0.60
1:A:595:LEU:O	1:A:596:LEU:HD12	2.02	0.60
1:A:6:LEU:HD11	1:A:311:ARG:NH2	2.15	0.60
1:A:132:ASN:O	1:A:133:ARG:HB2	2.02	0.60
1:A:450:MET:HE1	1:A:698:LYS:HD2	1.83	0.60
1:A:122:PHE:C	1:A:124:ASP:N	2.59	0.60
1:A:250:TYR:HB3	1:A:254:ILE:HD11	1.84	0.60
1:A:31:GLN:HB3	1:A:34:LYS:CD	2.32	0.59
1:A:621:SER:O	1:A:623:ASP:N	2.35	0.59
1:A:705:TRP:O	1:A:706:LEU:C	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:C	1:A:32:LYS:H	2.09	0.59
1:A:199:VAL:HG22	1:A:242:VAL:HG22	1.85	0.59
1:A:93:ASN:HD21	1:A:96:GLU:HG3	1.66	0.59
1:A:418:ASP:O	1:A:452:PRO:HG2	2.03	0.59
1:A:54:GLU:HG3	1:A:55:ASP:OD1	2.03	0.58
1:A:506:ILE:HG13	1:A:690:LEU:HD22	1.84	0.58
1:A:31:GLN:H	1:A:34:LYS:HZ2	1.52	0.58
1:A:198:ASP:O	1:A:243:VAL:HG22	2.02	0.58
1:A:401:GLU:O	1:A:405:GLU:N	2.35	0.58
1:A:614:LYS:NZ	1:A:663:THR:HG21	2.19	0.58
1:A:21:PHE:HD2	1:A:58:TRP:HB3	1.67	0.58
1:A:32:LYS:HA	1:A:35:LEU:CD1	2.31	0.58
1:A:104:PHE:O	1:A:108:THR:HB	2.03	0.57
1:A:406:LYS:C	1:A:408:ILE:N	2.60	0.57
1:A:30:ILE:O	1:A:30:ILE:HG13	2.04	0.57
1:A:398:GLN:HA	1:A:427:TYR:CE2	2.39	0.57
1:A:438:LEU:O	1:A:442:VAL:HG23	2.05	0.57
1:A:523:ASN:OD1	1:A:525:LYS:N	2.36	0.57
1:A:365:LEU:HD13	1:A:365:LEU:O	2.05	0.57
1:A:406:LYS:HA	1:A:409:PRO:HD2	1.85	0.57
1:A:503:ILE:HD12	1:A:578:GLU:OE2	2.04	0.57
1:A:200:PHE:CE1	1:A:241:LEU:HB2	2.40	0.57
1:A:117:ASP:HA	1:A:120:LYS:CG	2.34	0.57
1:A:410:VAL:C	1:A:412:ASN:H	2.12	0.57
1:A:439:TYR:CD1	1:A:455:VAL:HG11	2.40	0.57
1:A:118:PHE:O	1:A:122:PHE:HB2	2.05	0.56
1:A:23:VAL:HG21	1:A:56:GLU:HB3	1.87	0.56
1:A:333:ILE:O	1:A:333:ILE:CG1	2.52	0.56
1:A:476:GLN:HE21	1:A:476:GLN:CA	2.09	0.56
1:A:501:ILE:HD12	1:A:501:ILE:C	2.30	0.56
1:A:654:VAL:O	1:A:658:GLN:HG3	2.05	0.56
1:A:83:VAL:HG12	1:A:84:GLY:N	2.21	0.56
1:A:279:GLU:CB	1:A:280:PRO:HD2	2.35	0.56
1:A:31:GLN:O	1:A:33:GLU:N	2.39	0.56
1:A:407:LEU:C	1:A:408:ILE:HD12	2.31	0.56
1:A:570:ARG:HG3	1:A:574:LEU:HG	1.86	0.56
1:A:93:ASN:ND2	1:A:93:ASN:C	2.64	0.56
1:A:280:PRO:O	1:A:281:GLY:C	2.47	0.56
1:A:361:VAL:O	1:A:364:LYS:HG3	2.05	0.56
1:A:145:VAL:C	1:A:146:LEU:HD23	2.30	0.56
1:A:360:SER:HB3	1:A:364:LYS:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:GLU:OE2	1:A:457:LEU:HD13	2.06	0.56
1:A:165:PRO:C	1:A:167:GLU:N	2.64	0.56
1:A:119:TYR:O	1:A:123:ARG:HB3	2.06	0.56
1:A:400:ARG:HA	1:A:402:GLU:OE1	2.05	0.55
1:A:167:GLU:CD	1:A:171:THR:HB	2.30	0.55
1:A:506:ILE:HD11	1:A:690:LEU:HD22	1.88	0.55
1:A:119:TYR:O	1:A:123:ARG:N	2.39	0.55
1:A:184:ARG:HE	1:A:193:VAL:HG11	1.71	0.55
1:A:407:LEU:O	1:A:411:ILE:HG12	2.07	0.55
1:A:429:LYS:O	1:A:430:VAL:HG23	2.06	0.55
1:A:73:SER:C	1:A:75:GLY:N	2.63	0.55
1:A:82:ARG:HD3	1:A:82:ARG:O	2.07	0.55
1:A:463:ASN:HD22	1:A:463:ASN:N	2.03	0.55
1:A:328:LYS:HE3	1:A:342:LEU:HB3	1.90	0.54
1:A:400:ARG:HG2	1:A:400:ARG:HH11	1.71	0.54
1:A:189:GLY:C	1:A:190:ILE:HD12	2.32	0.54
1:A:277:ARG:HB2	2:A:733:HOH:O	2.07	0.54
1:A:443:LYS:NZ	1:A:453:SER:O	2.41	0.54
1:A:506:ILE:CD1	1:A:690:LEU:HD22	2.36	0.54
1:A:506:ILE:CG1	1:A:690:LEU:HD22	2.37	0.54
1:A:431:ASP:HB3	1:A:434:LYS:O	2.07	0.54
1:A:633:VAL:HG12	1:A:633:VAL:O	2.07	0.54
1:A:429:LYS:O	1:A:430:VAL:CB	2.56	0.54
1:A:533:LEU:HD21	1:A:689:MET:HG3	1.89	0.54
1:A:511:LYS:HG2	1:A:541:GLU:HG2	1.90	0.54
1:A:166:PHE:N	1:A:166:PHE:CD2	2.56	0.53
1:A:355:GLU:CD	1:A:414:ILE:HD13	2.33	0.53
1:A:579:VAL:O	1:A:583:LYS:HG3	2.08	0.53
1:A:406:LYS:HZ2	1:A:406:LYS:HB2	1.73	0.53
1:A:195:ARG:HG3	1:A:195:ARG:HH11	1.73	0.53
1:A:402:GLU:O	1:A:406:LYS:N	2.41	0.53
1:A:515:ALA:HB3	1:A:543:LEU:HD11	1.89	0.53
1:A:574:LEU:HB2	1:A:597:GLU:CG	2.39	0.53
1:A:31:GLN:HB3	1:A:34:LYS:HD3	1.91	0.53
1:A:333:ILE:O	1:A:333:ILE:HG12	2.08	0.53
1:A:660:LEU:O	1:A:663:THR:HB	2.08	0.53
1:A:666:ASN:ND2	1:A:673:ILE:HG21	2.23	0.53
1:A:105:LEU:HD13	1:A:111:LYS:HD2	1.89	0.53
1:A:690:LEU:O	1:A:691:ARG:HD2	2.08	0.53
1:A:350:ASP:OD1	1:A:351:VAL:HG23	2.09	0.53
1:A:473:VAL:O	1:A:476:GLN:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:THR:CG2	1:A:687:LYS:N	2.72	0.53
1:A:123:ARG:CA	1:A:126:ILE:HD12	2.32	0.53
1:A:332:VAL:O	1:A:334:THR:HG23	2.08	0.52
1:A:408:ILE:O	1:A:412:ASN:HB2	2.09	0.52
1:A:46:THR:HG22	1:A:48:LEU:H	1.74	0.52
1:A:544:THR:HG23	1:A:548:ILE:HD13	1.91	0.52
1:A:408:ILE:O	1:A:409:PRO:C	2.52	0.52
1:A:478:LEU:HB3	1:A:483:ASN:O	2.10	0.52
1:A:62:LYS:H	1:A:62:LYS:CD	2.22	0.52
1:A:128:VAL:CG2	1:A:275:ILE:HG13	2.40	0.52
1:A:283:ARG:O	1:A:287:ILE:HG23	2.09	0.52
1:A:403:ALA:HB2	1:A:436:PHE:CZ	2.45	0.52
1:A:539:PHE:C	1:A:539:PHE:CD2	2.86	0.52
1:A:93:ASN:ND2	1:A:96:GLU:HG3	2.24	0.52
1:A:114:PHE:HA	1:A:293:ARG:NH1	2.24	0.52
1:A:162:ARG:C	1:A:163:ILE:HD12	2.35	0.52
1:A:610:GLU:HB3	1:A:613:ILE:HG23	1.92	0.52
1:A:686:THR:HG23	1:A:687:LYS:N	2.24	0.52
1:A:164:GLN:HB3	1:A:257:PRO:O	2.10	0.51
1:A:399:THR:CG2	1:A:400:ARG:H	2.17	0.51
1:A:46:THR:HG22	1:A:48:LEU:N	2.26	0.51
1:A:399:THR:HG23	1:A:400:ARG:N	2.22	0.51
1:A:126:ILE:O	1:A:137:LEU:HB2	2.10	0.51
1:A:187:PRO:CB	1:A:190:ILE:HD13	2.40	0.51
1:A:398:GLN:O	1:A:398:GLN:CG	2.59	0.51
1:A:429:LYS:O	1:A:430:VAL:HB	2.11	0.51
1:A:120:LYS:HG3	1:A:121:LYS:H	1.75	0.51
1:A:202:ALA:HA	1:A:241:LEU:HD12	1.92	0.51
1:A:444:ARG:O	1:A:448:LYS:HG3	2.11	0.51
1:A:159:LEU:HD22	1:A:287:ILE:CG2	2.37	0.51
1:A:614:LYS:HZ2	1:A:663:THR:HG21	1.75	0.51
1:A:369:LYS:HE2	1:A:458:ASN:OD1	2.11	0.51
1:A:108:THR:HG22	1:A:110:VAL:HB	1.92	0.50
1:A:501:ILE:HG22	1:A:519:THR:HG23	1.93	0.50
1:A:110:VAL:HG13	1:A:111:LYS:N	2.26	0.50
1:A:364:LYS:H	1:A:364:LYS:CE	2.23	0.50
1:A:187:PRO:HA	1:A:255:LEU:HD23	1.93	0.50
1:A:511:LYS:CG	1:A:541:GLU:HG2	2.40	0.50
1:A:412:ASN:O	1:A:414:ILE:N	2.44	0.50
1:A:532:TYR:HD1	1:A:699:GLU:HB3	1.75	0.50
1:A:259:LEU:CD2	1:A:433:TYR:HA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASN:HD21	1:A:96:GLU:N	2.03	0.50
1:A:132:ASN:O	1:A:133:ARG:CB	2.60	0.50
1:A:41:ARG:HD2	1:A:72:LEU:HA	1.93	0.50
1:A:561:LYS:O	1:A:562:LYS:C	2.55	0.50
1:A:24:PHE:HE2	1:A:68:LEU:HG	1.75	0.50
1:A:400:ARG:HG2	1:A:400:ARG:NH1	2.27	0.50
1:A:528:LEU:HD22	1:A:703:MET:HG3	1.92	0.49
1:A:62:LYS:H	1:A:62:LYS:HE2	1.76	0.49
1:A:126:ILE:CD1	1:A:127:THR:HG23	2.42	0.49
1:A:187:PRO:HB2	1:A:190:ILE:HD13	1.94	0.49
1:A:683:ASP:HA	1:A:686:THR:HG22	1.94	0.49
1:A:5:ALA:CB	1:A:608:SER:HB2	2.42	0.49
1:A:689:MET:HB3	1:A:696:ILE:HD11	1.95	0.49
1:A:149:GLU:CD	1:A:619:LYS:HD3	2.38	0.49
1:A:278:MET:HB2	1:A:282:LYS:NZ	2.28	0.49
1:A:403:ALA:HB2	1:A:436:PHE:HZ	1.78	0.49
1:A:463:ASN:N	1:A:463:ASN:ND2	2.61	0.49
1:A:12:ILE:HD11	1:A:101:PHE:CE2	2.47	0.49
1:A:137:LEU:HD12	1:A:163:ILE:HG13	1.95	0.49
1:A:173:LEU:CD1	1:A:199:VAL:HG11	2.41	0.49
1:A:293:ARG:O	1:A:294:TYR:C	2.55	0.49
1:A:179:ASN:HB3	1:A:180:PRO:C	2.38	0.48
1:A:610:GLU:HB3	1:A:613:ILE:CG2	2.43	0.48
1:A:681:TYR:CE2	1:A:684:LYS:HD3	2.48	0.48
1:A:693:ILE:O	1:A:695:PRO:HD3	2.13	0.48
1:A:111:LYS:HG2	1:A:294:TYR:OH	2.13	0.48
1:A:473:VAL:O	1:A:474:ALA:C	2.56	0.48
1:A:157:LEU:HD12	1:A:158:ASP:N	2.28	0.48
1:A:187:PRO:HA	1:A:254:ILE:O	2.13	0.48
1:A:329:ASN:OD1	1:A:331:LYS:HB3	2.13	0.48
1:A:599:ILE:N	1:A:599:ILE:HD12	2.29	0.48
1:A:106:THR:O	1:A:109:LYS:HD2	2.13	0.48
1:A:276:VAL:HG13	1:A:278:MET:HG2	1.94	0.48
1:A:612:PHE:HA	1:A:631:ASN:OD1	2.14	0.48
1:A:114:PHE:HD2	1:A:115:ILE:HD12	1.78	0.48
1:A:411:ILE:HG22	1:A:449:LYS:NZ	2.23	0.48
1:A:430:VAL:O	1:A:432:PRO:HD3	2.13	0.48
1:A:170:GLN:HB2	1:A:252:ALA:C	2.38	0.48
1:A:58:TRP:CD1	1:A:58:TRP:N	2.82	0.48
1:A:183:ILE:O	1:A:185:VAL:HG13	2.14	0.48
1:A:406:LYS:C	1:A:409:PRO:HD2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:O	1:A:3:LYS:HG2	2.14	0.47
1:A:319:LYS:HD2	1:A:319:LYS:N	2.30	0.47
1:A:362:TYR:O	1:A:364:LYS:HE2	2.15	0.47
1:A:523:ASN:OD1	1:A:523:ASN:C	2.58	0.47
1:A:30:ILE:HG22	1:A:35:LEU:HD21	1.95	0.47
1:A:122:PHE:O	1:A:124:ASP:N	2.47	0.47
1:A:406:LYS:CA	1:A:409:PRO:HD2	2.43	0.47
1:A:278:MET:HB2	1:A:282:LYS:HZ1	1.78	0.47
1:A:400:ARG:HA	1:A:400:ARG:HD3	1.43	0.47
1:A:506:ILE:HG12	1:A:690:LEU:HD13	1.96	0.47
1:A:637:THR:HG23	1:A:637:THR:O	2.15	0.47
1:A:659:ILE:CG2	1:A:676:PRO:HG3	2.41	0.47
1:A:313:LYS:CE	1:A:619:LYS:H	2.27	0.47
1:A:117:ASP:OD1	1:A:120:LYS:HD3	2.14	0.47
1:A:397:ALA:HB3	1:A:402:GLU:HG3	1.96	0.47
1:A:120:LYS:C	1:A:122:PHE:H	2.22	0.47
1:A:31:GLN:CB	1:A:34:LYS:HD3	2.45	0.46
1:A:687:LYS:HB2	1:A:687:LYS:HZ2	1.79	0.46
1:A:225:ALA:O	1:A:228:GLU:HB2	2.15	0.46
1:A:368:ARG:HG3	1:A:368:ARG:NH1	2.30	0.46
1:A:15:ARG:HE	1:A:15:ARG:HB2	1.35	0.46
1:A:570:ARG:HH21	1:A:578:GLU:CD	2.22	0.46
1:A:669:SER:O	1:A:670:PHE:CD1	2.68	0.46
1:A:360:SER:OG	1:A:369:LYS:NZ	2.49	0.46
1:A:408:ILE:N	1:A:408:ILE:CD1	2.78	0.46
1:A:200:PHE:HE2	1:A:243:VAL:HG13	1.81	0.46
1:A:511:LYS:HD3	1:A:541:GLU:HG2	1.96	0.46
1:A:685:ILE:HD11	1:A:705:TRP:HB3	1.97	0.46
1:A:179:ASN:OD1	1:A:434:LYS:HD3	2.15	0.46
1:A:397:ALA:HB1	1:A:401:GLU:HG2	1.97	0.46
1:A:466:LEU:O	1:A:466:LEU:HG	2.15	0.46
1:A:592:SER:O	1:A:593:LEU:HD12	2.15	0.46
1:A:599:ILE:HB	1:A:642:LYS:HB3	1.97	0.46
1:A:684:LYS:O	1:A:688:LEU:HB2	2.16	0.46
1:A:402:GLU:O	1:A:406:LYS:HB2	2.16	0.46
1:A:30:ILE:C	1:A:32:LYS:N	2.74	0.45
1:A:230:LEU:O	1:A:236:ARG:NH2	2.49	0.45
1:A:357:ILE:HB	1:A:422:VAL:HG22	1.98	0.45
1:A:406:LYS:O	1:A:408:ILE:N	2.49	0.45
1:A:683:ASP:O	1:A:687:LYS:CB	2.65	0.45
1:A:9:LEU:HD13	1:A:154:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PHE:O	1:A:47:GLY:N	2.46	0.45
1:A:406:LYS:HB2	1:A:406:LYS:NZ	2.30	0.45
1:A:276:VAL:HG11	1:A:278:MET:HE3	1.98	0.45
1:A:59:CYS:O	1:A:61:GLY:N	2.45	0.45
1:A:465:ASN:O	1:A:469:VAL:HG23	2.15	0.45
1:A:46:THR:HG22	1:A:48:LEU:CB	2.45	0.45
1:A:429:LYS:O	1:A:430:VAL:CG2	2.65	0.45
1:A:64:GLU:HA	1:A:82:ARG:HH12	1.82	0.45
1:A:683:ASP:O	1:A:687:LYS:HB2	2.17	0.45
1:A:1:MET:HG2	1:A:2:GLY:N	2.30	0.45
1:A:410:VAL:O	1:A:412:ASN:N	2.50	0.45
1:A:419:LEU:HD12	1:A:452:PRO:O	2.16	0.45
1:A:639:GLN:O	1:A:639:GLN:HG3	2.17	0.45
1:A:159:LEU:O	1:A:283:ARG:NH1	2.50	0.45
1:A:344:ARG:HD3	1:A:344:ARG:HA	1.83	0.45
1:A:412:ASN:CG	1:A:413:LYS:N	2.71	0.45
1:A:356:ILE:CD1	1:A:373:LEU:HD11	2.46	0.45
1:A:62:LYS:HE2	1:A:62:LYS:N	2.32	0.45
1:A:396:LEU:O	1:A:397:ALA:HB2	2.17	0.45
1:A:408:ILE:O	1:A:412:ASN:CB	2.65	0.45
1:A:131:LYS:HD3	1:A:131:LYS:C	2.43	0.44
1:A:403:ALA:CB	1:A:436:PHE:HZ	2.30	0.44
1:A:104:PHE:HB3	1:A:298:LEU:CD2	2.47	0.44
1:A:335:ASN:C	1:A:335:ASN:ND2	2.73	0.44
1:A:429:LYS:C	1:A:430:VAL:HG23	2.42	0.44
1:A:162:ARG:NH1	1:A:186:LYS:NZ	2.66	0.44
1:A:277:ARG:HG3	1:A:277:ARG:HH11	1.81	0.44
1:A:403:ALA:O	1:A:407:LEU:HB2	2.18	0.44
1:A:406:LYS:NZ	1:A:438:LEU:HD22	2.32	0.44
1:A:577:ASP:OD1	1:A:577:ASP:N	2.44	0.44
1:A:143:GLU:CD	1:A:143:GLU:N	2.76	0.44
1:A:172:LEU:CD2	1:A:175:ARG:HH11	2.30	0.44
1:A:235:LEU:O	1:A:237:GLU:N	2.50	0.44
1:A:556:GLU:OE2	1:A:589:TYR:HE2	2.00	0.44
1:A:364:LYS:C	1:A:364:LYS:HD2	2.42	0.44
1:A:3:LYS:HD2	1:A:610:GLU:HA	1.99	0.43
1:A:323:LEU:HD12	1:A:323:LEU:C	2.42	0.43
1:A:113:LYS:O	1:A:116:SER:HB3	2.17	0.43
1:A:402:GLU:CD	1:A:402:GLU:H	2.26	0.43
1:A:104:PHE:HB3	1:A:298:LEU:HD21	2.00	0.43
1:A:108:THR:O	1:A:109:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HB	1:A:137:LEU:HB3	2.01	0.43
1:A:282:LYS:O	1:A:286:LEU:N	2.49	0.43
1:A:484:ILE:O	1:A:484:ILE:HG13	2.17	0.43
1:A:632:GLN:O	1:A:632:GLN:HG3	2.19	0.43
1:A:105:LEU:HD11	1:A:143:GLU:HG2	1.99	0.43
1:A:123:ARG:HA	1:A:126:ILE:HG23	2.00	0.43
1:A:278:MET:HE2	1:A:278:MET:HA	2.00	0.43
1:A:468:PHE:O	1:A:472:ASN:HB2	2.18	0.43
1:A:556:GLU:C	1:A:558:LEU:H	2.26	0.43
1:A:163:ILE:HD12	1:A:163:ILE:N	2.34	0.43
1:A:169:LEU:HD21	1:A:242:VAL:HG21	1.99	0.43
1:A:313:LYS:HE2	1:A:619:LYS:H	1.83	0.43
1:A:332:VAL:O	1:A:334:THR:N	2.51	0.43
1:A:594:GLU:OE1	1:A:650:LEU:HG	2.18	0.43
1:A:150:GLU:HG3	1:A:152:TYR:HE2	1.83	0.43
1:A:184:ARG:HE	1:A:193:VAL:CG1	2.31	0.43
1:A:216:ARG:NH1	1:A:509:ASP:OD2	2.52	0.43
1:A:274:ASP:O	1:A:275:ILE:HD13	2.18	0.43
1:A:683:ASP:CA	1:A:686:THR:HG22	2.48	0.43
1:A:179:ASN:CB	1:A:180:PRO:CA	2.88	0.43
1:A:415:LYS:O	1:A:416:ASP:O	2.37	0.43
1:A:48:LEU:O	1:A:49:PRO:C	2.60	0.43
1:A:111:LYS:O	1:A:115:ILE:HD13	2.18	0.43
1:A:322:VAL:HG12	1:A:488:LEU:HD23	2.00	0.42
1:A:511:LYS:CD	1:A:541:GLU:HG2	2.49	0.42
1:A:106:THR:C	1:A:108:THR:N	2.75	0.42
1:A:353:SER:HB2	1:A:390:LYS:HD3	2.01	0.42
1:A:412:ASN:C	1:A:414:ILE:N	2.77	0.42
1:A:327:GLY:O	1:A:328:LYS:C	2.61	0.42
1:A:50:THR:HG22	1:A:51:PHE:N	2.34	0.42
1:A:70:LEU:HG	1:A:78:VAL:HG13	2.02	0.42
1:A:145:VAL:O	1:A:146:LEU:HD23	2.19	0.42
1:A:620:LEU:HD12	1:A:620:LEU:HA	1.76	0.42
1:A:23:VAL:HA	1:A:57:PHE:O	2.20	0.42
1:A:120:LYS:CE	1:A:121:LYS:HE3	2.50	0.42
1:A:379:PHE:HE2	1:A:474:ALA:CB	2.32	0.42
1:A:83:VAL:O	1:A:84:GLY:O	2.38	0.42
1:A:200:PHE:HD1	1:A:201:LYS:O	2.03	0.42
1:A:30:ILE:O	1:A:32:LYS:HG3	2.19	0.42
1:A:487:LYS:HE2	1:A:525:LYS:CB	2.50	0.42
1:A:32:LYS:O	1:A:35:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:THR:HG22	1:A:110:VAL:N	2.22	0.42
1:A:477:VAL:O	1:A:478:LEU:C	2.61	0.42
1:A:219:HIS:O	1:A:220:LYS:C	2.62	0.42
1:A:502:ASP:OD2	1:A:502:ASP:C	2.63	0.42
1:A:190:ILE:HG13	1:A:219:HIS:CG	2.55	0.41
1:A:501:ILE:CG2	1:A:519:THR:HG23	2.50	0.41
1:A:523:ASN:HD21	1:A:527:GLU:HB2	1.83	0.41
1:A:105:LEU:HD13	1:A:111:LYS:CD	2.49	0.41
1:A:167:GLU:O	1:A:256:LYS:HG2	2.21	0.41
1:A:197:GLN:HB2	1:A:243:VAL:O	2.19	0.41
1:A:683:ASP:HA	1:A:686:THR:CG2	2.51	0.41
1:A:411:ILE:CG2	1:A:449:LYS:HZ3	2.24	0.41
1:A:103:ASP:O	1:A:106:THR:N	2.45	0.41
1:A:128:VAL:HG21	1:A:275:ILE:HG13	2.02	0.41
1:A:169:LEU:CD2	1:A:242:VAL:HG21	2.51	0.41
1:A:366:GLU:OE2	1:A:366:GLU:N	2.52	0.41
1:A:487:LYS:HD2	1:A:527:GLU:HG3	2.01	0.41
1:A:224:LYS:O	1:A:228:GLU:HG2	2.20	0.41
1:A:544:THR:O	1:A:548:ILE:HD13	2.21	0.41
1:A:214:MET:HE3	1:A:230:LEU:HD23	2.02	0.41
1:A:399:THR:OG1	1:A:400:ARG:N	2.51	0.41
1:A:532:TYR:CE2	1:A:534:THR:HG21	2.56	0.41
1:A:37:LYS:HD3	1:A:37:LYS:HA	1.99	0.41
1:A:207:GLU:HG3	1:A:208:GLU:N	2.35	0.41
1:A:226:TRP:HA	1:A:226:TRP:CE3	2.56	0.41
1:A:335:ASN:C	1:A:335:ASN:HD22	2.28	0.41
1:A:195:ARG:HH11	1:A:195:ARG:CG	2.33	0.41
1:A:413:LYS:O	1:A:413:LYS:HG2	2.19	0.41
1:A:575:TYR:CD1	1:A:575:TYR:N	2.89	0.41
1:A:104:PHE:C	1:A:106:THR:N	2.76	0.40
1:A:208:GLU:H	1:A:208:GLU:HG2	1.36	0.40
1:A:516:VAL:HG22	1:A:535:SER:HB3	2.03	0.40
1:A:38:VAL:HG22	1:A:72:LEU:HD21	2.03	0.40
1:A:180:PRO:O	1:A:183:ILE:HG13	2.21	0.40
1:A:353:SER:CB	1:A:390:LYS:HD3	2.51	0.40
1:A:487:LYS:HE2	1:A:525:LYS:HB3	2.02	0.40
1:A:96:GLU:O	1:A:97:CYS:C	2.64	0.40
1:A:289:TYR:O	1:A:292:ARG:N	2.54	0.40
1:A:74:ASN:O	1:A:74:ASN:OD1	2.39	0.40
1:A:190:ILE:HG22	1:A:191:ASP:N	2.37	0.40
1:A:574:LEU:H	1:A:597:GLU:CD	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:SER:O	1:A:149:GLU:C	2.65	0.40
1:A:413:LYS:O	1:A:415:LYS:N	2.54	0.40
1:A:584:LYS:O	1:A:587:GLU:HB3	2.20	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	680/706 (96%)	526 (77%)	114 (17%)	40 (6%)	1 10

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	132	ASN
1	A	399	THR
1	A	416	ASP
1	A	430	VAL
1	A	513	VAL
1	A	571	ASP
1	A	621	SER
1	A	622	GLU
1	A	4	GLU
1	A	65	LYS
1	A	66	ASP
1	A	67	THR
1	A	72	LEU
1	A	84	GLY
1	A	90	GLY
1	A	121	LYS
1	A	125	LYS

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Mol	Chain	Res	Type
1	A	182	ARG
1	A	188	ILE
1	A	212	LEU
1	A	236	ARG
1	A	278	MET
1	A	410	VAL
1	A	411	ILE
1	A	413	LYS
1	A	572	GLY
1	A	179	ASN
1	A	31	GLN
1	A	223	LYS
1	A	60	ALA
1	A	123	ARG
1	A	150	GLU
1	A	221	SER
1	A	228	GLU
1	A	362	TYR
1	A	408	ILE
1	A	432	PRO
1	A	635	GLU
1	A	180	PRO

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	631/647 (98%)	583 (92%)	48 (8%)	12	42

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	15	ARG
1	A	62	LYS
1	A	63	VAL

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Mol	Chain	Res	Type
1	A	70	LEU
1	A	78	VAL
1	A	93	ASN
1	A	108	THR
1	A	112	ASP
1	A	126	ILE
1	A	131	LYS
1	A	147	LYS
1	A	164	GLN
1	A	166	PHE
1	A	195	ARG
1	A	208	GLU
1	A	277	ARG
1	A	284	LEU
1	A	323	LEU
1	A	333	ILE
1	A	347	VAL
1	A	363	LYS
1	A	364	LYS
1	A	365	LEU
1	A	366	GLU
1	A	373	LEU
1	A	380	LEU
1	A	400	ARG
1	A	406	LYS
1	A	413	LYS
1	A	414	ILE
1	A	416	ASP
1	A	417	VAL
1	A	437	LEU
1	A	466	LEU
1	A	476	GLN
1	A	494	LYS
1	A	539	PHE
1	A	561	LYS
1	A	620	LEU
1	A	634	TYR
1	A	635	GLU
1	A	652	VAL
1	A	663	THR
1	A	683	ASP
1	A	687	LYS

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Mol	Chain	Res	Type
1	A	696	ILE
1	A	706	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	98	GLN
1	A	132	ASN
1	A	164	GLN
1	A	285	ASN
1	A	335	ASN
1	A	382	ASN
1	A	463	ASN
1	A	476	GLN
1	A	639	GLN
1	A	658	GLN
1	A	671	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	690/706 (97%)	-0.22	3 (0%) 88 79	16, 56, 131, 179	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	436	PHE	2.9
1	A	243	VAL	2.4
1	A	637	THR	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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.