



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:29 PM UTC

PDB ID : 3AQK / pdb_00003aak
Title : Structure of bacterial protein (apo form I)
Authors : Toh, Y.; Takeshita, D.; Tomita, K.
Deposited on : 2010-11-09
Resolution : 3.65 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

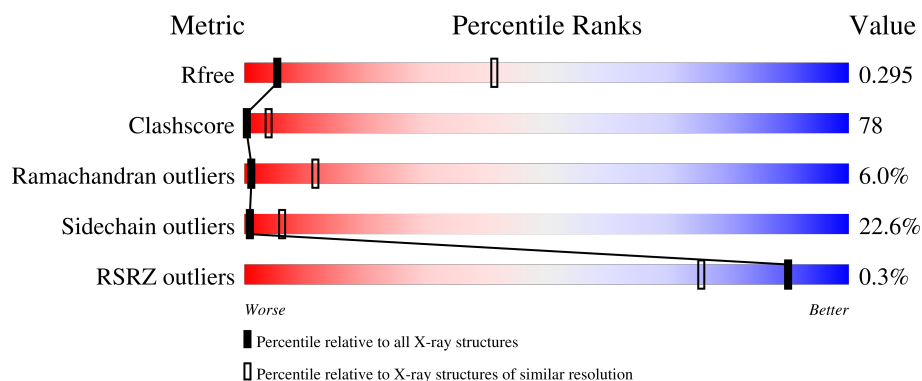
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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	414	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3185 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 Poly(A) polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3185	2034	570	567	14			

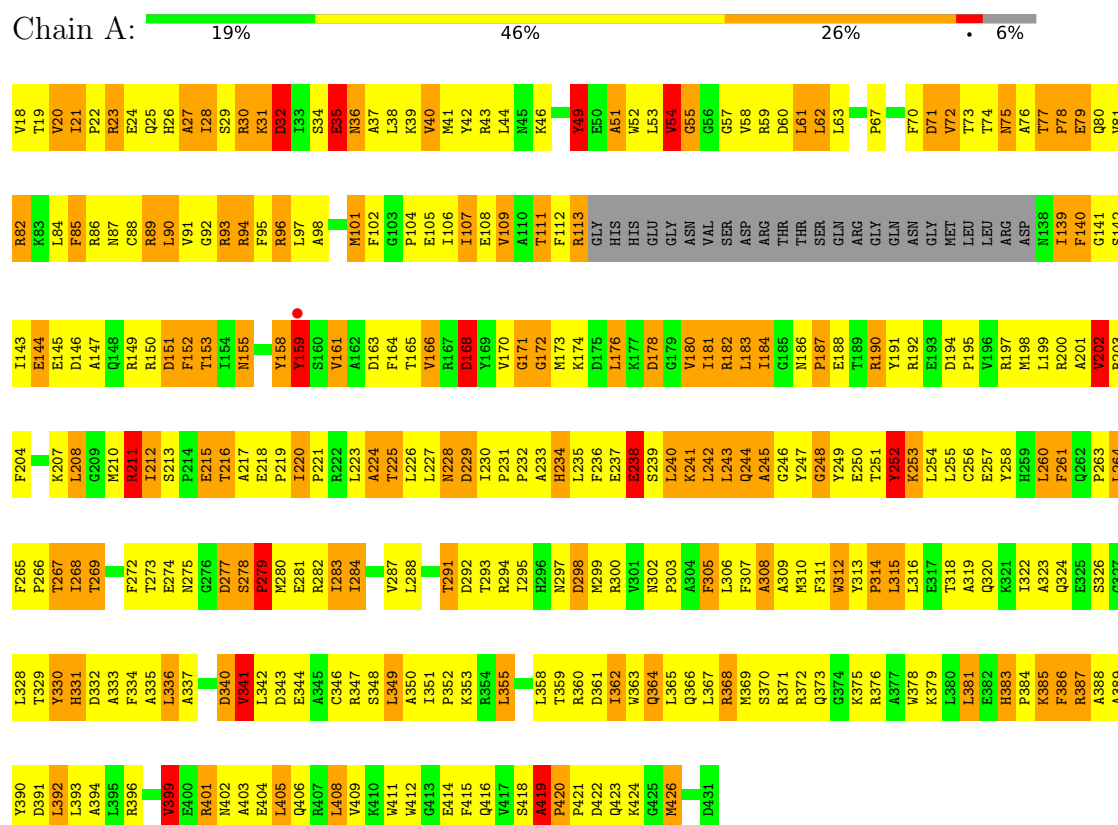
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	HIS	ARG	engineered mutation	UNP C9QS13

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: Poly(A) polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	130.85Å 130.85Å 149.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 3.65 29.97 – 3.65	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.97-3.65) 98.6 (29.97-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 3.67Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.279 , 0.295 0.279 , 0.295	Depositor DCC
R_{free} test set	457 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	116.5	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 97.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3185	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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

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	0.79	2/3255 (0.1%)	1.42	61/4399 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	THR	CA-CB	5.78	1.61	1.53
1	A	426	MET	SD-CE	-5.47	1.65	1.79

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ASN	N-CA-C	-13.83	95.81	111.71
1	A	183	LEU	N-CA-C	-11.09	95.58	110.55
1	A	151	ASP	N-CA-C	10.82	126.64	113.12
1	A	279	PRO	N-CA-C	-9.40	93.11	112.47
1	A	234	HIS	N-CA-C	-9.30	100.25	111.69
1	A	31	LYS	N-CA-C	-9.04	101.35	112.38
1	A	32	ASP	N-CA-C	8.82	121.69	111.11
1	A	211	ARG	N-CA-C	8.43	121.94	110.55
1	A	35	GLU	N-CA-C	8.43	128.75	110.80
1	A	54	VAL	N-CA-C	8.11	118.42	108.53
1	A	405	LEU	N-CA-C	-8.05	101.10	112.13
1	A	386	PHE	N-CA-C	7.97	119.66	110.97
1	A	21	ILE	CA-C-N	7.92	128.22	119.90
1	A	21	ILE	C-N-CA	7.92	128.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	GLN	N-CA-C	-7.80	102.59	113.20
1	A	182	ARG	N-CA-C	7.80	121.12	108.34
1	A	104	PRO	N-CA-C	-7.70	106.67	114.68
1	A	159	TYR	N-CA-C	7.54	119.85	108.46
1	A	158	TYR	N-CA-C	7.32	121.59	109.95
1	A	153	THR	N-CA-C	7.20	119.75	111.11
1	A	144	GLU	N-CA-C	-7.14	103.50	111.71
1	A	139	ILE	CB-CA-C	-7.08	104.83	111.06
1	A	220	ILE	N-CA-C	7.05	124.11	108.88
1	A	82	ARG	N-CA-C	-6.95	103.76	111.82
1	A	245	ALA	N-CA-C	-6.83	104.15	113.30
1	A	419	ALA	N-CA-C	-6.71	94.97	109.81
1	A	77	THR	CA-C-N	6.71	128.22	119.84
1	A	77	THR	C-N-CA	6.71	128.22	119.84
1	A	330	TYR	N-CA-C	6.53	118.08	110.97
1	A	261	PHE	N-CA-C	-6.35	104.27	111.07
1	A	341	VAL	N-CA-C	-6.25	103.28	111.09
1	A	181	ILE	N-CA-C	6.25	117.14	108.89
1	A	101	MET	N-CA-C	6.24	119.99	109.76
1	A	246	GLY	N-CA-C	-6.20	106.69	115.30
1	A	86	ARG	N-CA-C	-6.18	104.84	112.38
1	A	253	LYS	N-CA-C	-6.17	103.86	111.33
1	A	61	LEU	N-CA-C	6.13	118.76	111.71
1	A	399	VAL	N-CA-C	-6.12	104.66	110.42
1	A	49	TYR	N-CA-C	6.09	118.56	110.53
1	A	383	HIS	CA-C-N	6.04	127.39	119.84
1	A	383	HIS	C-N-CA	6.04	127.39	119.84
1	A	217	ALA	N-CA-C	6.01	119.08	111.69
1	A	278	SER	CA-C-N	-5.98	112.37	119.84
1	A	278	SER	C-N-CA	-5.98	112.37	119.84
1	A	152	PHE	N-CA-C	5.69	118.50	109.50
1	A	161	VAL	N-CA-C	-5.59	104.10	111.09
1	A	96	ARG	CB-CA-C	-5.58	110.12	116.54
1	A	268	ILE	CB-CA-C	-5.57	102.15	111.29
1	A	260	LEU	N-CA-C	-5.44	106.78	113.41
1	A	51	ALA	N-CA-C	5.39	117.76	109.07
1	A	368	ARG	N-CA-C	-5.38	107.26	113.88
1	A	240	LEU	N-CA-C	-5.36	104.48	111.02
1	A	353	LYS	N-CA-C	-5.35	105.56	111.71
1	A	238	GLU	N-CA-C	-5.25	106.84	113.20
1	A	305	PHE	N-CA-C	5.24	116.68	111.07
1	A	141	GLY	N-CA-C	5.23	117.25	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	ALA	N-CA-C	-5.22	106.02	112.38
1	A	351	ILE	N-CA-C	5.20	113.60	107.77
1	A	202	VAL	N-CA-C	-5.19	105.65	110.53
1	A	168	ASP	N-CA-C	5.17	117.56	108.56
1	A	369	MET	N-CA-C	-5.17	106.81	113.01

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3185	0	3213	500	0
All	All	3185	0	3213	500	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 78.

All (500) 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:243:LEU:HD23	1:A:243:LEU:H	1.04	1.14
1:A:52:TRP:CE3	1:A:159:TYR:HA	1.85	1.11
1:A:36:ASN:HB3	1:A:102:PHE:CE2	1.84	1.11
1:A:36:ASN:HB3	1:A:102:PHE:HE2	0.99	1.10
1:A:308:ALA:HB2	1:A:359:THR:HG23	1.09	1.07
1:A:184:ILE:HG23	1:A:190:ARG:HH12	1.20	1.06
1:A:53:LEU:HD12	1:A:54:VAL:H	1.21	1.01
1:A:250:GLU:O	1:A:253:LYS:HG2	1.59	1.01
1:A:306:LEU:HD23	1:A:306:LEU:O	1.59	1.00
1:A:402:ASN:OD1	1:A:405:LEU:HG	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD11	1:A:67:PRO:HG3	1.48	0.94
1:A:243:LEU:H	1:A:243:LEU:CD2	1.80	0.94
1:A:337:ALA:O	1:A:341:VAL:HG23	1.68	0.93
1:A:53:LEU:HD12	1:A:54:VAL:N	1.82	0.93
1:A:232:PRO:HB2	1:A:350:ALA:H	1.31	0.93
1:A:308:ALA:CB	1:A:359:THR:HG23	1.99	0.93
1:A:183:LEU:HD23	1:A:184:ILE:H	1.33	0.93
1:A:250:GLU:OE1	1:A:253:LYS:HD3	1.69	0.92
1:A:186:ASN:O	1:A:190:ARG:HG2	1.68	0.92
1:A:336:LEU:HD22	1:A:336:LEU:H	1.35	0.91
1:A:59:ARG:HG2	1:A:60:ASP:N	1.85	0.90
1:A:143:ILE:HD11	1:A:158:TYR:CD2	2.07	0.90
1:A:186:ASN:OD1	1:A:187:PRO:HD2	1.72	0.89
1:A:93:ARG:H	1:A:93:ARG:HD3	1.38	0.88
1:A:187:PRO:HB2	1:A:219:PRO:HG2	1.56	0.88
1:A:59:ARG:HG2	1:A:60:ASP:H	1.39	0.88
1:A:52:TRP:HE3	1:A:159:TYR:HA	1.39	0.88
1:A:308:ALA:HB2	1:A:359:THR:CG2	2.02	0.87
1:A:102:PHE:HB2	1:A:105:GLU:O	1.75	0.87
1:A:142:SER:O	1:A:145:GLU:HB3	1.74	0.86
1:A:243:LEU:HD23	1:A:243:LEU:N	1.89	0.85
1:A:112:PHE:CE2	1:A:143:ILE:HG13	2.10	0.85
1:A:208:LEU:N	1:A:208:LEU:HD12	1.92	0.85
1:A:306:LEU:O	1:A:309:ALA:HB3	1.78	0.84
1:A:420:PRO:N	1:A:421:PRO:HD3	1.93	0.83
1:A:266:PRO:HG2	1:A:267:THR:H	1.45	0.81
1:A:36:ASN:CB	1:A:102:PHE:HE2	1.90	0.81
1:A:183:LEU:HD23	1:A:184:ILE:N	1.94	0.81
1:A:168:ASP:OD2	1:A:173:MET:HG2	1.80	0.81
1:A:208:LEU:HD12	1:A:208:LEU:H	1.45	0.81
1:A:419:ALA:HB3	1:A:421:PRO:CD	2.11	0.80
1:A:393:LEU:HG	1:A:409:VAL:HG22	1.64	0.80
1:A:421:PRO:HD2	1:A:422:ASP:H	1.46	0.80
1:A:52:TRP:O	1:A:73:THR:HG22	1.82	0.79
1:A:238:GLU:O	1:A:242:LEU:HD23	1.81	0.79
1:A:191:TYR:CD1	1:A:198:MET:HG3	2.18	0.78
1:A:342:LEU:O	1:A:346:CYS:HB2	1.83	0.78
1:A:153:THR:OG1	1:A:182:ARG:HB2	1.84	0.77
1:A:233:ALA:HB2	1:A:350:ALA:HB3	1.66	0.77
1:A:28:ILE:HG12	1:A:30:ARG:HG2	1.66	0.77
1:A:306:LEU:HD23	1:A:306:LEU:C	2.08	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLN:OE1	1:A:376:ARG:HB2	1.85	0.76
1:A:386:PHE:C	1:A:386:PHE:CD2	2.64	0.76
1:A:284:ILE:HA	1:A:287:VAL:CG1	2.16	0.76
1:A:52:TRP:CZ3	1:A:159:TYR:HA	2.22	0.75
1:A:392:LEU:C	1:A:392:LEU:HD23	2.12	0.75
1:A:243:LEU:C	1:A:245:ALA:H	1.95	0.75
1:A:58:VAL:HG23	1:A:59:ARG:N	2.00	0.75
1:A:49:TYR:CG	1:A:76:ALA:HB2	2.22	0.74
1:A:82:ARG:HD3	1:A:82:ARG:O	1.87	0.74
1:A:232:PRO:HB2	1:A:350:ALA:N	2.02	0.73
1:A:208:LEU:HB2	1:A:210:MET:HG2	1.71	0.73
1:A:223:LEU:O	1:A:224:ALA:C	2.32	0.72
1:A:306:LEU:HD21	1:A:310:MET:CE	2.19	0.72
1:A:306:LEU:HD21	1:A:310:MET:HE3	1.70	0.72
1:A:250:GLU:HA	1:A:253:LYS:HD3	1.72	0.72
1:A:140:PHE:HD1	1:A:140:PHE:H	1.34	0.71
1:A:419:ALA:CB	1:A:421:PRO:HD3	2.19	0.71
1:A:278:SER:HB3	1:A:281:GLU:HG3	1.72	0.71
1:A:302:ASN:OD1	1:A:303:PRO:HD2	1.91	0.71
1:A:77:THR:HG23	1:A:78:PRO:HD2	1.71	0.71
1:A:278:SER:HB3	1:A:281:GLU:CG	2.21	0.70
1:A:420:PRO:N	1:A:421:PRO:CD	2.53	0.70
1:A:26:HIS:O	1:A:27:ALA:C	2.35	0.70
1:A:419:ALA:HB3	1:A:421:PRO:HD3	1.73	0.70
1:A:72:VAL:HG22	1:A:109:VAL:HA	1.73	0.70
1:A:203:ARG:NH1	1:A:238:GLU:OE1	2.25	0.70
1:A:365:LEU:HD12	1:A:389:ALA:HB2	1.73	0.69
1:A:93:ARG:HD3	1:A:93:ARG:N	2.07	0.69
1:A:170:VAL:HG12	1:A:171:GLY:N	2.07	0.69
1:A:184:ILE:HG23	1:A:190:ARG:NH1	2.02	0.69
1:A:227:LEU:HA	1:A:230:ILE:HD12	1.74	0.69
1:A:49:TYR:CD1	1:A:76:ALA:HB2	2.28	0.69
1:A:49:TYR:HB3	1:A:75:ASN:ND2	2.08	0.69
1:A:284:ILE:HA	1:A:287:VAL:HG12	1.73	0.69
1:A:313:TYR:HB2	1:A:314:PRO:HD3	1.75	0.68
1:A:36:ASN:CB	1:A:102:PHE:CE2	2.71	0.67
1:A:190:ARG:HH21	1:A:197:ARG:NH2	1.92	0.67
1:A:38:LEU:HA	1:A:41:MET:HE2	1.76	0.67
1:A:402:ASN:HD22	1:A:403:ALA:N	1.93	0.67
1:A:220:ILE:HD12	1:A:220:ILE:H	1.60	0.67
1:A:190:ARG:O	1:A:197:ARG:HD2	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HD21	1:A:408:LEU:HD12	1.77	0.66
1:A:306:LEU:HD21	1:A:310:MET:SD	2.34	0.66
1:A:28:ILE:O	1:A:30:ARG:HG3	1.95	0.66
1:A:312:TRP:NE1	1:A:396:ARG:HD2	2.11	0.66
1:A:181:ILE:HB	1:A:212:ILE:HA	1.77	0.66
1:A:363:TRP:O	1:A:366:GLN:N	2.28	0.66
1:A:49:TYR:OH	1:A:80:GLN:HB3	1.96	0.65
1:A:194:ASP:O	1:A:197:ARG:HG3	1.96	0.65
1:A:393:LEU:HG	1:A:409:VAL:CG2	2.26	0.65
1:A:381:LEU:HD13	1:A:381:LEU:O	1.97	0.65
1:A:93:ARG:O	1:A:94:ARG:HB3	1.95	0.65
1:A:408:LEU:HD13	1:A:408:LEU:C	2.21	0.65
1:A:170:VAL:HG12	1:A:171:GLY:H	1.59	0.65
1:A:101:MET:HG3	1:A:106:ILE:HD11	1.77	0.65
1:A:420:PRO:O	1:A:424:LYS:HB2	1.97	0.65
1:A:72:VAL:CG2	1:A:109:VAL:HG13	2.27	0.65
1:A:392:LEU:HD23	1:A:393:LEU:N	2.11	0.65
1:A:208:LEU:CB	1:A:210:MET:HG2	2.27	0.64
1:A:153:THR:HG23	1:A:182:ARG:HB3	1.78	0.64
1:A:306:LEU:CD2	1:A:310:MET:SD	2.86	0.64
1:A:361:ASP:O	1:A:365:LEU:HG	1.98	0.64
1:A:421:PRO:CD	1:A:422:ASP:H	2.11	0.64
1:A:96:ARG:HH22	1:A:140:PHE:HB3	1.61	0.64
1:A:418:SER:HB3	1:A:423:GLN:HG3	1.78	0.64
1:A:63:LEU:HD21	1:A:176:LEU:CD1	2.28	0.64
1:A:52:TRP:CE3	1:A:159:TYR:CA	2.72	0.63
1:A:267:THR:HG23	1:A:344:GLU:OE1	1.97	0.63
1:A:59:ARG:CG	1:A:60:ASP:N	2.61	0.63
1:A:198:MET:HG2	1:A:220:ILE:HG12	1.81	0.63
1:A:403:ALA:HA	1:A:406:GLN:HG2	1.79	0.63
1:A:280:MET:HA	1:A:313:TYR:HD2	1.64	0.63
1:A:415:PHE:CD2	1:A:415:PHE:O	2.52	0.63
1:A:280:MET:HG3	1:A:314:PRO:HD3	1.82	0.62
1:A:305:PHE:HD1	1:A:388:ALA:HB1	1.63	0.62
1:A:297:ASN:O	1:A:299:MET:HG3	2.00	0.62
1:A:22:PRO:HA	1:A:165:THR:HG22	1.81	0.62
1:A:32:ASP:OD2	1:A:32:ASP:N	2.31	0.62
1:A:112:PHE:CE2	1:A:143:ILE:CG1	2.83	0.62
1:A:153:THR:CG2	1:A:182:ARG:HB3	2.30	0.62
1:A:58:VAL:CG2	1:A:59:ARG:N	2.63	0.62
1:A:77:THR:C	1:A:79:GLU:H	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASP:OD1	1:A:282:ARG:HD2	1.99	0.62
1:A:295:ILE:C	1:A:297:ASN:H	2.06	0.62
1:A:311:PHE:O	1:A:312:TRP:C	2.43	0.62
1:A:30:ARG:C	1:A:32:ASP:N	2.55	0.61
1:A:53:LEU:HD13	1:A:71:ASP:O	2.00	0.61
1:A:266:PRO:CG	1:A:267:THR:H	2.13	0.61
1:A:360:ARG:O	1:A:364:GLN:HG3	2.01	0.61
1:A:198:MET:HG2	1:A:220:ILE:CG1	2.30	0.61
1:A:340:ASP:N	1:A:340:ASP:OD2	2.33	0.61
1:A:23:ARG:HA	1:A:164:PHE:O	2.01	0.61
1:A:72:VAL:HG21	1:A:109:VAL:HG13	1.83	0.61
1:A:140:PHE:CD1	1:A:140:PHE:N	2.69	0.61
1:A:44:LEU:HD23	1:A:84:LEU:CD2	2.31	0.61
1:A:63:LEU:CD2	1:A:176:LEU:HD11	2.31	0.61
1:A:91:VAL:HG12	1:A:92:GLY:N	2.15	0.61
1:A:36:ASN:O	1:A:39:LYS:CB	2.49	0.60
1:A:58:VAL:HG23	1:A:59:ARG:H	1.65	0.60
1:A:368:ARG:HH12	1:A:379:LYS:HZ1	1.48	0.60
1:A:386:PHE:HD2	1:A:387:ARG:N	2.00	0.60
1:A:368:ARG:HH12	1:A:379:LYS:NZ	1.98	0.60
1:A:415:PHE:HB2	1:A:426:MET:SD	2.42	0.60
1:A:203:ARG:HD3	1:A:242:LEU:HD22	1.83	0.60
1:A:208:LEU:HB2	1:A:210:MET:CG	2.31	0.60
1:A:52:TRP:HE3	1:A:159:TYR:CA	2.10	0.59
1:A:181:ILE:HD13	1:A:210:MET:HE2	1.84	0.59
1:A:63:LEU:HD21	1:A:176:LEU:HD13	1.83	0.59
1:A:142:SER:O	1:A:145:GLU:CB	2.48	0.59
1:A:215:GLU:HG3	1:A:216:THR:N	2.17	0.59
1:A:280:MET:HA	1:A:313:TYR:CD2	2.37	0.59
1:A:408:LEU:HD13	1:A:408:LEU:O	2.01	0.59
1:A:402:ASN:ND2	1:A:403:ALA:N	2.51	0.59
1:A:168:ASP:CG	1:A:173:MET:HG2	2.27	0.59
1:A:219:PRO:O	1:A:223:LEU:HD13	2.04	0.58
1:A:151:ASP:HB3	1:A:152:PHE:CE2	2.38	0.58
1:A:359:THR:HA	1:A:362:ILE:HG13	1.85	0.58
1:A:88:CYS:O	1:A:90:LEU:N	2.31	0.58
1:A:392:LEU:CD2	1:A:393:LEU:N	2.66	0.58
1:A:180:VAL:HA	1:A:211:ARG:O	2.04	0.58
1:A:363:TRP:O	1:A:365:LEU:N	2.36	0.58
1:A:58:VAL:CG2	1:A:59:ARG:H	2.15	0.58
1:A:261:PHE:CE2	1:A:265:PHE:HB2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:PHE:CD2	1:A:143:ILE:HA	2.39	0.58
1:A:306:LEU:C	1:A:306:LEU:CD2	2.76	0.58
1:A:188:GLU:OE2	1:A:192:ARG:NH2	2.28	0.58
1:A:250:GLU:OE1	1:A:253:LYS:CD	2.46	0.58
1:A:208:LEU:N	1:A:208:LEU:CD1	2.63	0.57
1:A:59:ARG:HD2	1:A:155:ASN:ND2	2.20	0.57
1:A:243:LEU:C	1:A:245:ALA:N	2.63	0.57
1:A:75:ASN:ND2	1:A:75:ASN:H	2.01	0.57
1:A:223:LEU:H	1:A:223:LEU:HD12	1.70	0.57
1:A:223:LEU:HD12	1:A:223:LEU:N	2.19	0.57
1:A:322:ILE:CG1	1:A:323:ALA:N	2.68	0.57
1:A:53:LEU:CD1	1:A:71:ASP:O	2.53	0.57
1:A:58:VAL:HG12	1:A:159:TYR:HE2	1.70	0.57
1:A:295:ILE:C	1:A:297:ASN:N	2.60	0.57
1:A:297:ASN:O	1:A:299:MET:N	2.38	0.57
1:A:232:PRO:CB	1:A:349:LEU:HA	2.35	0.57
1:A:283:ILE:HD13	1:A:283:ILE:C	2.29	0.57
1:A:208:LEU:C	1:A:210:MET:H	2.13	0.56
1:A:219:PRO:C	1:A:223:LEU:HD13	2.29	0.56
1:A:337:ALA:O	1:A:341:VAL:CG2	2.48	0.56
1:A:38:LEU:HD23	1:A:38:LEU:C	2.29	0.56
1:A:144:GLU:O	1:A:147:ALA:HB3	2.04	0.56
1:A:163:ASP:O	1:A:165:THR:HG23	2.04	0.56
1:A:305:PHE:CD1	1:A:388:ALA:HB1	2.41	0.56
1:A:254:LEU:O	1:A:258:TYR:HD2	1.89	0.56
1:A:315:LEU:O	1:A:318:THR:HB	2.06	0.56
1:A:30:ARG:C	1:A:32:ASP:H	2.14	0.56
1:A:62:LEU:HB3	1:A:176:LEU:HD21	1.86	0.56
1:A:343:ASP:O	1:A:347:ARG:HB2	2.05	0.56
1:A:244:GLN:HE22	1:A:303:PRO:HA	1.70	0.56
1:A:94:ARG:NH1	1:A:97:LEU:CD2	2.69	0.55
1:A:153:THR:HG22	1:A:170:VAL:HG11	1.87	0.55
1:A:153:THR:CG2	1:A:182:ARG:CB	2.84	0.55
1:A:200:ARG:HB3	1:A:204:PHE:HE2	1.72	0.55
1:A:243:LEU:HA	1:A:248:GLY:HA2	1.89	0.55
1:A:313:TYR:O	1:A:316:LEU:N	2.39	0.55
1:A:418:SER:CB	1:A:423:GLN:HG3	2.37	0.55
1:A:36:ASN:O	1:A:39:LYS:HB2	2.06	0.55
1:A:207:LYS:HD2	1:A:247:TYR:CE2	2.42	0.55
1:A:220:ILE:O	1:A:221:PRO:C	2.48	0.55
1:A:230:ILE:HB	1:A:235:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:THR:O	1:A:255:LEU:HD12	2.07	0.55
1:A:352:PRO:HB2	1:A:355:LEU:HD23	1.88	0.55
1:A:386:PHE:C	1:A:386:PHE:HD2	2.15	0.55
1:A:93:ARG:O	1:A:94:ARG:CB	2.55	0.55
1:A:170:VAL:C	1:A:172:GLY:H	2.13	0.55
1:A:238:GLU:O	1:A:242:LEU:CD2	2.52	0.55
1:A:392:LEU:C	1:A:392:LEU:CD2	2.78	0.55
1:A:142:SER:O	1:A:145:GLU:N	2.39	0.54
1:A:199:LEU:HD23	1:A:260:LEU:HD13	1.88	0.54
1:A:367:LEU:HD22	1:A:367:LEU:N	2.23	0.54
1:A:195:PRO:HB2	1:A:230:ILE:HD11	1.89	0.54
1:A:79:GLU:OE1	1:A:79:GLU:HA	2.07	0.54
1:A:82:ARG:HD3	1:A:82:ARG:C	2.32	0.54
1:A:243:LEU:CD2	1:A:243:LEU:N	2.56	0.54
1:A:140:PHE:HD1	1:A:140:PHE:N	2.04	0.54
1:A:336:LEU:HD13	1:A:336:LEU:N	2.21	0.54
1:A:27:ALA:O	1:A:29:SER:N	2.41	0.54
1:A:181:ILE:O	1:A:213:SER:HB2	2.08	0.54
1:A:78:PRO:HD3	1:A:111:THR:OG1	2.08	0.54
1:A:183:LEU:HB2	1:A:216:THR:HG23	1.90	0.54
1:A:371:ARG:HB3	1:A:373:GLN:HE21	1.73	0.53
1:A:190:ARG:HH21	1:A:197:ARG:HH22	1.53	0.53
1:A:392:LEU:HD21	1:A:396:ARG:HD3	1.90	0.53
1:A:96:ARG:HD2	1:A:111:THR:HB	1.90	0.53
1:A:113:ARG:O	1:A:145:GLU:HG3	2.08	0.53
1:A:181:ILE:CD1	1:A:210:MET:HE2	2.39	0.53
1:A:73:THR:HG23	1:A:73:THR:O	2.09	0.53
1:A:243:LEU:CB	1:A:248:GLY:HA2	2.39	0.53
1:A:198:MET:SD	1:A:220:ILE:HG23	2.49	0.53
1:A:280:MET:O	1:A:283:ILE:HG22	2.10	0.53
1:A:378:TRP:CZ3	1:A:423:GLN:OE1	2.62	0.53
1:A:35:GLU:C	1:A:37:ALA:N	2.64	0.52
1:A:21:ILE:CG2	1:A:26:HIS:HB3	2.40	0.52
1:A:188:GLU:O	1:A:192:ARG:HG3	2.09	0.52
1:A:419:ALA:C	1:A:421:PRO:HD3	2.34	0.52
1:A:187:PRO:CB	1:A:219:PRO:HG2	2.35	0.52
1:A:233:ALA:HA	1:A:236:PHE:HB3	1.91	0.52
1:A:393:LEU:HD12	1:A:393:LEU:O	2.09	0.52
1:A:280:MET:C	1:A:283:ILE:HG22	2.35	0.52
1:A:176:LEU:HD12	1:A:176:LEU:O	2.10	0.52
1:A:330:TYR:O	1:A:331:HIS:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD23	1:A:84:LEU:HD21	1.91	0.52
1:A:52:TRP:HE3	1:A:159:TYR:N	2.08	0.52
1:A:203:ARG:NH1	1:A:241:LYS:HB3	2.25	0.52
1:A:408:LEU:C	1:A:408:LEU:CD1	2.83	0.52
1:A:342:LEU:O	1:A:346:CYS:N	2.34	0.51
1:A:365:LEU:C	1:A:367:LEU:N	2.67	0.51
1:A:113:ARG:H	1:A:146:ASP:HB2	1.75	0.51
1:A:383:HIS:CE1	1:A:384:PRO:HG2	2.46	0.51
1:A:421:PRO:CD	1:A:422:ASP:N	2.73	0.51
1:A:161:VAL:O	1:A:164:PHE:CE1	2.64	0.51
1:A:191:TYR:HB3	1:A:198:MET:HE2	1.93	0.51
1:A:63:LEU:N	1:A:63:LEU:HD22	2.25	0.51
1:A:336:LEU:HD22	1:A:336:LEU:N	2.17	0.51
1:A:419:ALA:O	1:A:423:GLN:HG3	2.10	0.51
1:A:42:TYR:CE1	1:A:161:VAL:HG21	2.45	0.51
1:A:419:ALA:C	1:A:421:PRO:CD	2.84	0.51
1:A:241:LYS:O	1:A:245:ALA:HB2	2.10	0.51
1:A:294:ARG:HG3	1:A:299:MET:HE3	1.92	0.51
1:A:93:ARG:N	1:A:93:ARG:CD	2.71	0.51
1:A:386:PHE:O	1:A:387:ARG:C	2.53	0.51
1:A:388:ALA:O	1:A:389:ALA:C	2.53	0.51
1:A:279:PRO:O	1:A:280:MET:C	2.54	0.50
1:A:320:GLN:O	1:A:323:ALA:HB3	2.12	0.50
1:A:18:VAL:HG13	1:A:18:VAL:O	2.11	0.50
1:A:20:VAL:HG22	1:A:21:ILE:N	2.26	0.50
1:A:176:LEU:HD12	1:A:176:LEU:C	2.36	0.50
1:A:266:PRO:HG3	1:A:348:SER:OG	2.12	0.50
1:A:96:ARG:HD2	1:A:111:THR:CB	2.42	0.50
1:A:40:VAL:HG23	1:A:85:PHE:HE2	1.76	0.50
1:A:143:ILE:HG23	1:A:144:GLU:N	2.26	0.50
1:A:174:LYS:HG2	1:A:178:ASP:OD2	2.12	0.50
1:A:223:LEU:H	1:A:223:LEU:CD1	2.25	0.50
1:A:315:LEU:HG	1:A:316:LEU:N	2.23	0.50
1:A:405:LEU:O	1:A:408:LEU:N	2.45	0.50
1:A:72:VAL:HG13	1:A:108:GLU:O	2.12	0.49
1:A:170:VAL:CG1	1:A:171:GLY:N	2.75	0.49
1:A:236:PHE:O	1:A:236:PHE:CD1	2.65	0.49
1:A:313:TYR:O	1:A:314:PRO:C	2.53	0.49
1:A:336:LEU:O	1:A:337:ALA:C	2.54	0.49
1:A:21:ILE:HG23	1:A:25:GLN:OE1	2.12	0.49
1:A:264:LEU:HB2	1:A:265:PHE:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:THR:O	1:A:79:GLU:N	2.45	0.49
1:A:187:PRO:HG2	1:A:188:GLU:H	1.77	0.49
1:A:381:LEU:HD13	1:A:381:LEU:C	2.37	0.49
1:A:77:THR:C	1:A:79:GLU:N	2.70	0.49
1:A:322:ILE:HD11	1:A:333:ALA:O	2.11	0.49
1:A:319:ALA:O	1:A:322:ILE:HG12	2.13	0.49
1:A:112:PHE:HE2	1:A:143:ILE:HG13	1.71	0.49
1:A:218:GLU:O	1:A:221:PRO:HD2	2.13	0.49
1:A:307:PHE:O	1:A:311:PHE:HD2	1.96	0.49
1:A:334:PHE:O	1:A:337:ALA:HB3	2.13	0.49
1:A:183:LEU:HB2	1:A:216:THR:CG2	2.43	0.48
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.58	0.48
1:A:312:TRP:HA	1:A:312:TRP:CE3	2.48	0.48
1:A:267:THR:HG23	1:A:344:GLU:CD	2.38	0.48
1:A:348:SER:C	1:A:349:LEU:HD23	2.39	0.48
1:A:77:THR:CG2	1:A:78:PRO:HD2	2.41	0.48
1:A:224:ALA:O	1:A:227:LEU:HG	2.13	0.48
1:A:44:LEU:HD12	1:A:51:ALA:HB2	1.96	0.48
1:A:27:ALA:O	1:A:28:ILE:C	2.56	0.48
1:A:200:ARG:O	1:A:203:ARG:HB3	2.13	0.48
1:A:274:GLU:O	1:A:275:ASN:C	2.56	0.48
1:A:312:TRP:HE1	1:A:396:ARG:HD2	1.75	0.48
1:A:318:THR:HG22	1:A:319:ALA:N	2.27	0.48
1:A:61:LEU:CD1	1:A:67:PRO:HG3	2.34	0.48
1:A:318:THR:O	1:A:319:ALA:C	2.57	0.48
1:A:233:ALA:O	1:A:237:GLU:HG3	2.14	0.47
1:A:236:PHE:O	1:A:239:SER:OG	2.31	0.47
1:A:334:PHE:O	1:A:337:ALA:N	2.47	0.47
1:A:265:PHE:CD1	1:A:268:ILE:HD12	2.49	0.47
1:A:236:PHE:CD1	1:A:236:PHE:C	2.92	0.47
1:A:243:LEU:CA	1:A:248:GLY:HA2	2.43	0.47
1:A:283:ILE:O	1:A:287:VAL:HG12	2.13	0.47
1:A:315:LEU:O	1:A:315:LEU:HD12	2.14	0.47
1:A:159:TYR:N	1:A:159:TYR:HD2	2.12	0.47
1:A:163:ASP:N	1:A:163:ASP:OD1	2.47	0.47
1:A:202:VAL:HG12	1:A:254:LEU:HD23	1.97	0.47
1:A:208:LEU:C	1:A:210:MET:N	2.73	0.47
1:A:383:HIS:CE1	1:A:385:LYS:H	2.32	0.47
1:A:85:PHE:CD1	1:A:85:PHE:N	2.82	0.47
1:A:322:ILE:HG13	1:A:323:ALA:N	2.30	0.47
1:A:402:ASN:ND2	1:A:402:ASN:C	2.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TYR:C	1:A:252:TYR:CD2	2.92	0.47
1:A:415:PHE:CD2	1:A:415:PHE:C	2.92	0.47
1:A:159:TYR:N	1:A:159:TYR:CD2	2.83	0.47
1:A:159:TYR:HB3	1:A:166:VAL:HA	1.97	0.47
1:A:227:LEU:HD12	1:A:263:PRO:HG3	1.97	0.47
1:A:376:ARG:O	1:A:379:LYS:HB3	2.15	0.47
1:A:21:ILE:HG21	1:A:26:HIS:HB3	1.96	0.46
1:A:54:VAL:HA	1:A:58:VAL:HG11	1.96	0.46
1:A:106:ILE:C	1:A:107:ILE:HD13	2.40	0.46
1:A:278:SER:HB3	1:A:281:GLU:CB	2.45	0.46
1:A:227:LEU:O	1:A:229:ASP:N	2.48	0.46
1:A:313:TYR:HB2	1:A:314:PRO:CD	2.43	0.46
1:A:393:LEU:HA	1:A:396:ARG:HB3	1.97	0.46
1:A:67:PRO:HG2	1:A:70:PHE:CZ	2.50	0.46
1:A:91:VAL:CG1	1:A:92:GLY:N	2.78	0.46
1:A:96:ARG:NH1	1:A:112:PHE:O	2.48	0.46
1:A:204:PHE:O	1:A:208:LEU:CD1	2.63	0.46
1:A:170:VAL:CG1	1:A:171:GLY:H	2.26	0.46
1:A:20:VAL:C	1:A:21:ILE:HD12	2.40	0.46
1:A:84:LEU:HG	1:A:85:PHE:CE1	2.51	0.46
1:A:152:PHE:N	1:A:152:PHE:CD2	2.83	0.46
1:A:283:ILE:HG23	1:A:284:ILE:N	2.30	0.46
1:A:280:MET:HG3	1:A:313:TYR:HB2	1.98	0.46
1:A:98:ALA:O	1:A:109:VAL:HG23	2.15	0.46
1:A:143:ILE:CG2	1:A:144:GLU:N	2.79	0.46
1:A:307:PHE:C	1:A:309:ALA:N	2.73	0.46
1:A:22:PRO:O	1:A:23:ARG:C	2.59	0.46
1:A:146:ASP:O	1:A:146:ASP:CG	2.59	0.46
1:A:240:LEU:O	1:A:241:LYS:C	2.58	0.46
1:A:77:THR:HG23	1:A:78:PRO:CD	2.44	0.45
1:A:363:TRP:C	1:A:365:LEU:N	2.72	0.45
1:A:414:GLU:HB2	1:A:426:MET:HE1	1.98	0.45
1:A:26:HIS:O	1:A:26:HIS:CD2	2.69	0.45
1:A:402:ASN:HD22	1:A:403:ALA:H	1.60	0.45
1:A:31:LYS:HG2	1:A:38:LEU:HD11	1.98	0.45
1:A:55:GLY:CA	1:A:58:VAL:HG22	2.46	0.45
1:A:61:LEU:HD11	1:A:67:PRO:CG	2.32	0.45
1:A:187:PRO:O	1:A:191:TYR:CD2	2.69	0.45
1:A:219:PRO:O	1:A:223:LEU:CD1	2.63	0.45
1:A:284:ILE:CA	1:A:287:VAL:HG12	2.45	0.45
1:A:44:LEU:HD23	1:A:84:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:MET:O	1:A:284:ILE:HG13	2.16	0.45
1:A:342:LEU:O	1:A:346:CYS:CB	2.60	0.45
1:A:28:ILE:HG12	1:A:30:ARG:CG	2.40	0.45
1:A:291:THR:O	1:A:292:ASP:C	2.59	0.45
1:A:297:ASN:O	1:A:298:ASP:C	2.60	0.45
1:A:106:ILE:CG2	1:A:107:ILE:N	2.80	0.45
1:A:306:LEU:C	1:A:309:ALA:HB3	2.40	0.45
1:A:368:ARG:NH1	1:A:379:LYS:NZ	2.62	0.45
1:A:198:MET:HG2	1:A:220:ILE:HG13	1.98	0.45
1:A:150:ARG:O	1:A:184:ILE:HG21	2.17	0.45
1:A:249:TYR:HD1	1:A:250:GLU:OE2	1.99	0.45
1:A:257:GLU:O	1:A:257:GLU:HG2	2.17	0.45
1:A:26:HIS:CD2	1:A:29:SER:OG	2.70	0.44
1:A:40:VAL:CG2	1:A:85:PHE:CE2	3.00	0.44
1:A:244:GLN:HE22	1:A:303:PRO:CA	2.29	0.44
1:A:95:PHE:O	1:A:96:ARG:C	2.60	0.44
1:A:368:ARG:C	1:A:370:SER:N	2.75	0.44
1:A:375:LYS:O	1:A:375:LYS:HG2	2.16	0.44
1:A:151:ASP:CB	1:A:152:PHE:CD2	3.00	0.44
1:A:237:GLU:C	1:A:239:SER:H	2.25	0.44
1:A:264:LEU:O	1:A:349:LEU:HD21	2.18	0.44
1:A:203:ARG:NH1	1:A:241:LYS:HD3	2.32	0.44
1:A:268:ILE:O	1:A:269:THR:C	2.61	0.44
1:A:67:PRO:HB2	1:A:70:PHE:CE1	2.53	0.44
1:A:200:ARG:O	1:A:204:PHE:CD2	2.71	0.44
1:A:371:ARG:O	1:A:372:ARG:C	2.60	0.44
1:A:204:PHE:O	1:A:208:LEU:HD13	2.18	0.44
1:A:208:LEU:H	1:A:208:LEU:CD1	2.22	0.44
1:A:21:ILE:HA	1:A:22:PRO:HD3	1.67	0.44
1:A:227:LEU:HA	1:A:230:ILE:CD1	2.44	0.44
1:A:392:LEU:HD23	1:A:393:LEU:CA	2.48	0.44
1:A:183:LEU:HD11	1:A:190:ARG:HB2	2.00	0.44
1:A:203:ARG:CD	1:A:242:LEU:HD22	2.46	0.44
1:A:231:PRO:HG2	1:A:234:HIS:HB2	2.00	0.44
1:A:367:LEU:N	1:A:367:LEU:CD2	2.80	0.44
1:A:62:LEU:HD13	1:A:62:LEU:O	2.18	0.43
1:A:143:ILE:HD11	1:A:158:TYR:CE2	2.52	0.43
1:A:183:LEU:CD2	1:A:184:ILE:N	2.75	0.43
1:A:198:MET:O	1:A:201:ALA:HB3	2.18	0.43
1:A:85:PHE:C	1:A:87:ASN:N	2.76	0.43
1:A:240:LEU:O	1:A:242:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:LEU:O	1:A:368:ARG:N	2.38	0.43
1:A:366:GLN:OE1	1:A:392:LEU:HD22	2.18	0.43
1:A:96:ARG:O	1:A:97:LEU:C	2.61	0.43
1:A:113:ARG:HA	1:A:140:PHE:HA	2.00	0.43
1:A:153:THR:HB	1:A:172:GLY:HA2	2.00	0.43
1:A:170:VAL:C	1:A:172:GLY:N	2.77	0.43
1:A:381:LEU:C	1:A:381:LEU:CD1	2.91	0.43
1:A:186:ASN:O	1:A:187:PRO:C	2.59	0.43
1:A:391:ASP:O	1:A:394:ALA:HB3	2.18	0.43
1:A:94:ARG:NH1	1:A:97:LEU:HD23	2.32	0.43
1:A:158:TYR:O	1:A:166:VAL:HA	2.18	0.43
1:A:181:ILE:CB	1:A:212:ILE:HA	2.46	0.43
1:A:151:ASP:C	1:A:152:PHE:CD2	2.97	0.43
1:A:415:PHE:O	1:A:415:PHE:CG	2.71	0.43
1:A:61:LEU:HD21	1:A:67:PRO:HG3	2.01	0.43
1:A:208:LEU:O	1:A:210:MET:N	2.41	0.43
1:A:239:SER:O	1:A:243:LEU:HD23	2.19	0.42
1:A:411:TRP:HZ3	1:A:412:TRP:CE2	2.37	0.42
1:A:191:TYR:O	1:A:195:PRO:N	2.52	0.42
1:A:227:LEU:HD11	1:A:260:LEU:HD22	2.00	0.42
1:A:390:TYR:O	1:A:391:ASP:C	2.62	0.42
1:A:213:SER:HB3	1:A:216:THR:OG1	2.18	0.42
1:A:280:MET:CA	1:A:283:ILE:HG22	2.49	0.42
1:A:363:TRP:O	1:A:364:GLN:C	2.62	0.42
1:A:399:VAL:C	1:A:401:ARG:N	2.76	0.42
1:A:42:TYR:HB3	1:A:46:LYS:NZ	2.34	0.42
1:A:365:LEU:C	1:A:367:LEU:H	2.28	0.42
1:A:405:LEU:O	1:A:406:GLN:C	2.62	0.42
1:A:40:VAL:HG23	1:A:85:PHE:CE2	2.55	0.42
1:A:203:ARG:NH1	1:A:238:GLU:CD	2.77	0.42
1:A:268:ILE:HG22	1:A:272:PHE:HE2	1.83	0.42
1:A:278:SER:OG	1:A:279:PRO:CD	2.67	0.42
1:A:94:ARG:HG2	1:A:95:PHE:N	2.35	0.42
1:A:44:LEU:CD2	1:A:84:LEU:HD23	2.49	0.42
1:A:199:LEU:O	1:A:200:ARG:C	2.63	0.42
1:A:227:LEU:HG	1:A:227:LEU:H	1.66	0.42
1:A:328:LEU:HD12	1:A:328:LEU:HA	1.91	0.42
1:A:218:GLU:C	1:A:218:GLU:CD	2.88	0.42
1:A:153:THR:HG23	1:A:182:ARG:CB	2.44	0.41
1:A:187:PRO:O	1:A:188:GLU:C	2.62	0.41
1:A:223:LEU:N	1:A:223:LEU:CD1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLN:C	1:A:326:SER:H	2.28	0.41
1:A:334:PHE:O	1:A:335:ALA:C	2.63	0.41
1:A:366:GLN:OE1	1:A:396:ARG:NH1	2.53	0.41
1:A:272:PHE:CD2	1:A:280:MET:HE1	2.55	0.41
1:A:284:ILE:HG13	1:A:284:ILE:H	1.57	0.41
1:A:43:ARG:O	1:A:43:ARG:HG2	2.20	0.41
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.93	0.41
1:A:378:TRP:CH2	1:A:423:GLN:OE1	2.74	0.41
1:A:79:GLU:C	1:A:81:VAL:N	2.78	0.41
1:A:244:GLN:HE22	1:A:303:PRO:HB3	1.85	0.41
1:A:57:GLY:HA2	1:A:67:PRO:HB3	2.03	0.41
1:A:332:ASP:O	1:A:333:ALA:C	2.63	0.41
1:A:181:ILE:CG1	1:A:212:ILE:HA	2.51	0.40
1:A:200:ARG:HB3	1:A:204:PHE:CE2	2.55	0.40
1:A:220:ILE:O	1:A:224:ALA:HB2	2.20	0.40
1:A:244:GLN:HE22	1:A:303:PRO:CB	2.34	0.40
1:A:28:ILE:O	1:A:28:ILE:HG23	2.21	0.40
1:A:227:LEU:O	1:A:228:ASN:C	2.64	0.40
1:A:239:SER:O	1:A:240:LEU:C	2.63	0.40
1:A:220:ILE:O	1:A:224:ALA:N	2.42	0.40
1:A:376:ARG:N	1:A:376:ARG:CD	2.83	0.40
1:A:386:PHE:CD2	1:A:387:ARG:N	2.82	0.40
1:A:386:PHE:HD2	1:A:387:ARG:HA	1.87	0.40
1:A:411:TRP:CE3	1:A:412:TRP:CD1	3.09	0.40
1:A:38:LEU:HD23	1:A:38:LEU:O	2.22	0.40
1:A:77:THR:HG22	1:A:79:GLU:H	1.85	0.40
1:A:89:ARG:CB	1:A:101:MET:HE2	2.51	0.40
1:A:151:ASP:HB3	1:A:152:PHE:CD2	2.57	0.40
1:A:203:ARG:NH1	1:A:241:LYS:CD	2.84	0.40
1:A:239:SER:O	1:A:242:LEU:HB2	2.22	0.40
1:A:280:MET:O	1:A:283:ILE:CG2	2.69	0.40
1:A:315:LEU:HB2	1:A:341:VAL:HG21	2.03	0.40
1:A:40:VAL:CG1	1:A:41:MET:N	2.83	0.40
1:A:72:VAL:HG13	1:A:72:VAL:H	1.62	0.40
1:A:74:THR:O	1:A:111:THR:HG23	2.21	0.40
1:A:195:PRO:O	1:A:198:MET:HB2	2.21	0.40
1:A:203:ARG:HH12	1:A:241:LYS:CD	2.35	0.40
1:A:366:GLN:NE2	1:A:392:LEU:HD13	2.37	0.40
1:A:419:ALA:HB3	1:A:421:PRO:HD2	1.97	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	386/414 (93%)	288 (75%)	75 (19%)	23 (6%)	1	12

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	28	ILE
1	A	89	ARG
1	A	94	ARG
1	A	224	ALA
1	A	228	ASN
1	A	298	ASP
1	A	364	GLN
1	A	55	GLY
1	A	225	THR
1	A	248	GLY
1	A	279	PRO
1	A	78	PRO
1	A	27	ALA
1	A	190	ARG
1	A	241	LYS
1	A	312	TRP
1	A	30	ARG
1	A	187	PRO
1	A	419	ALA
1	A	172	GLY
1	A	20	VAL
1	A	171	GLY

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	337/357 (94%)	261 (77%)	76 (23%)	1 6

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	32	ASP
1	A	34	SER
1	A	35	GLU
1	A	40	VAL
1	A	49	TYR
1	A	54	VAL
1	A	62	LEU
1	A	71	ASP
1	A	72	VAL
1	A	75	ASN
1	A	79	GLU
1	A	85	PHE
1	A	90	LEU
1	A	93	ARG
1	A	107	ILE
1	A	109	VAL
1	A	111	THR
1	A	113	ARG
1	A	139	ILE
1	A	140	PHE
1	A	149	ARG
1	A	155	ASN
1	A	159	TYR
1	A	166	VAL
1	A	168	ASP
1	A	176	LEU
1	A	178	ASP
1	A	180	VAL
1	A	184	ILE

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Mol	Chain	Res	Type
1	A	202	VAL
1	A	208	LEU
1	A	211	ARG
1	A	212	ILE
1	A	215	GLU
1	A	216	THR
1	A	225	THR
1	A	226	LEU
1	A	229	ASP
1	A	238	GLU
1	A	242	LEU
1	A	243	LEU
1	A	252	TYR
1	A	256	CYS
1	A	264	LEU
1	A	267	THR
1	A	269	THR
1	A	273	THR
1	A	277	ASP
1	A	283	ILE
1	A	284	ILE
1	A	288	LEU
1	A	291	THR
1	A	293	THR
1	A	300	ARG
1	A	314	PRO
1	A	315	LEU
1	A	329	THR
1	A	331	HIS
1	A	336	LEU
1	A	340	ASP
1	A	341	VAL
1	A	349	LEU
1	A	355	LEU
1	A	358	LEU
1	A	362	ILE
1	A	381	LEU
1	A	385	LYS
1	A	387	ARG
1	A	392	LEU
1	A	399	VAL
1	A	401	ARG

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Mol	Chain	Res	Type
1	A	404	GLU
1	A	408	LEU
1	A	416	GLN
1	A	420	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	75	ASN
1	A	148	GLN
1	A	155	ASN
1	A	244	GLN
1	A	275	ASN
1	A	364	GLN
1	A	402	ASN
1	A	416	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	390/414 (94%)	-0.39	1 (0%)	90 75	94, 141, 194, 203	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	TYR	2.9

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.