



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:37 PM UTC

PDB ID : 3DSL / pdb_00003dsl
Title : The Three-dimensional Structure of Bothropasin, the Main Hemorrhagic Factor from Bothrops jararaca venom.
Authors : Muniz, J.R.C.; Ambrosio, A.; Selistre-de-Araujo, H.S.; Oliva, G.; Garratt, R.C.; Souza, D.H.F.
Deposited on : 2008-07-13
Resolution : 2.70 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

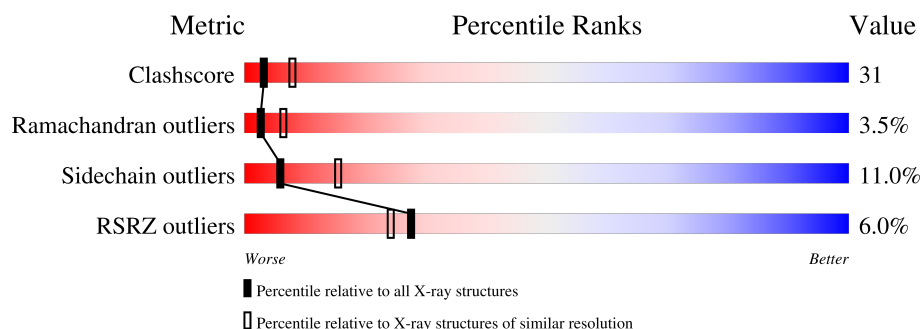
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	419	3% 53% 38% 8% .
1	B	419	9% 44% 45% 9% .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6675 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 Zinc metalloproteinase-disintegrin bothropasin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3219	1998	543	631	47			
1	B	412	Total	C	N	O	S	0	0	0
			3190	1981	538	624	47			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		

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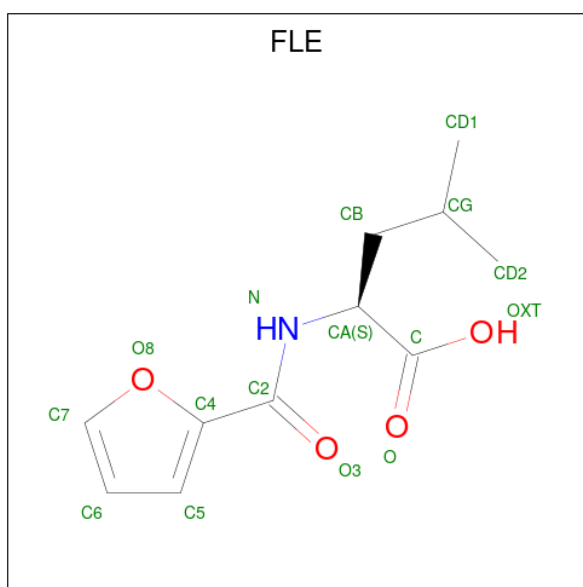
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

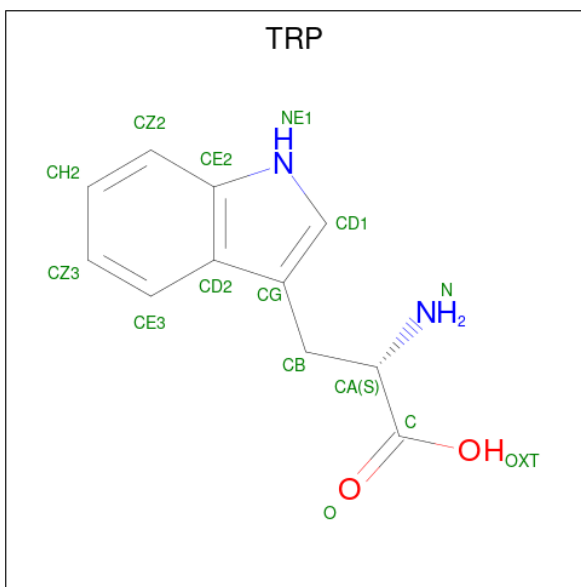
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is FUROYL-LEUCINE (CCD ID: FLE) (formula: C₁₁H₁₅NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	11	1	3		
5	A	1	Total	C	N	O	0	0
			15	11	1	3		

- Molecule 6 is TRYPTOPHAN (CCD ID: TRP) (formula: C₁₁H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			15	11	2	2		
6	A	1	Total	C	N	O	0	0
			15	11	2	2		

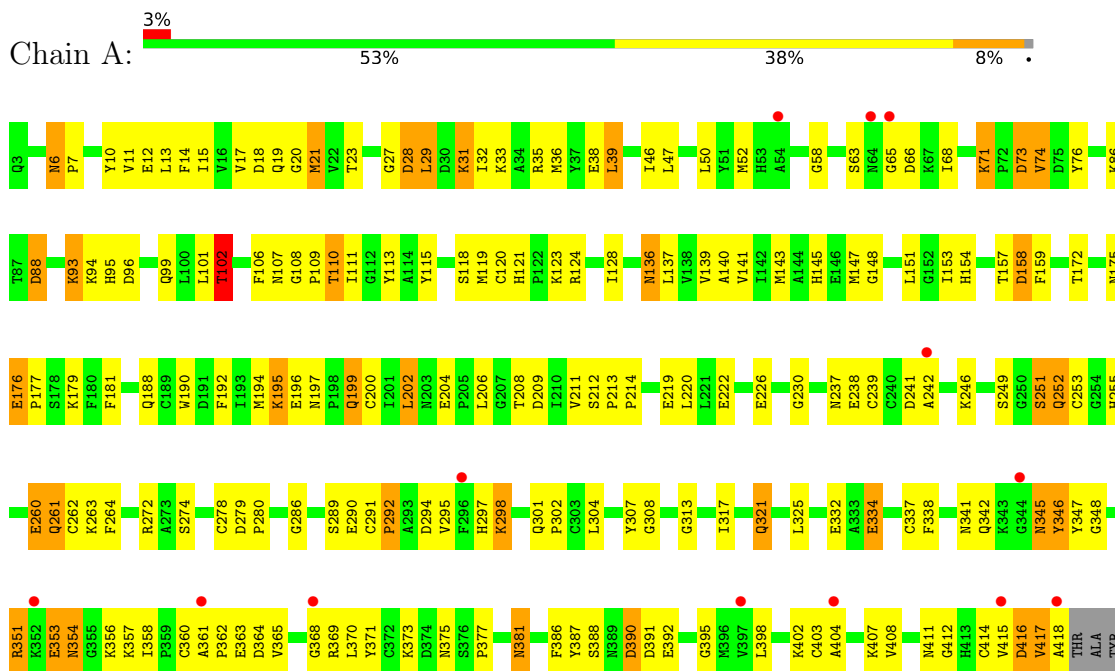
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	113	Total	O	0	0
			113	113		
7	B	71	Total	O	0	0
			71	71		

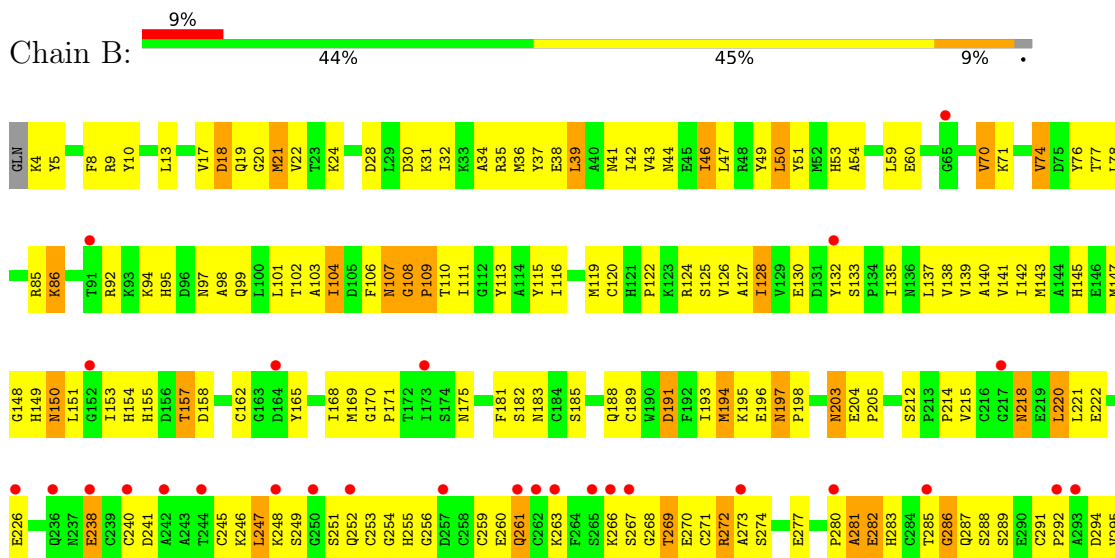
3 Residue-property plots

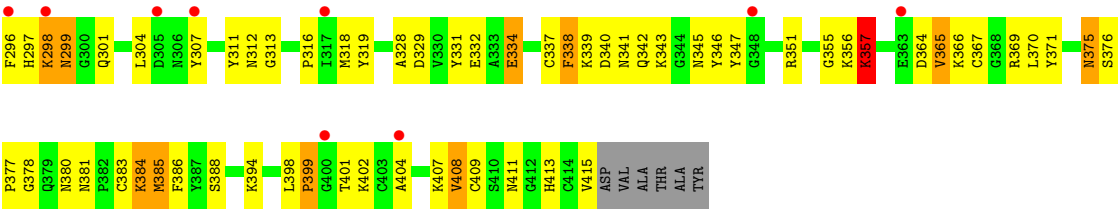
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Zinc metalloproteinase-disintegrin bothropasin



- Molecule 1: Zinc metalloproteinase-disintegrin bothropasin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.76Å 100.27Å 133.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.44 – 2.70 30.44 – 2.70	Depositor EDS
% Data completeness (in resolution range)	88.9 (30.44-2.70) 91.9 (30.44-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.210 , 0.294 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 84.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6675	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.10% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FLE, ZN, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/3294	0.96	14/4458 (0.3%)
1	B	0.59	1/3265 (0.0%)	0.92	8/4418 (0.2%)
All	All	0.55	1/6559 (0.0%)	0.94	22/8876 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	355	GLY	C-N	-19.41	1.05	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	GLU	CA-C-N	8.21	128.85	120.14
1	A	176	GLU	C-N-CA	8.21	128.85	120.14
1	A	6	ASN	CA-C-N	7.69	127.34	119.19
1	A	6	ASN	C-N-CA	7.69	127.34	119.19
1	B	355	GLY	O-C-N	7.25	131.91	122.42
1	A	291	CYS	CA-C-N	6.28	127.69	119.84
1	A	291	CYS	C-N-CA	6.28	127.69	119.84
1	B	355	GLY	CA-C-N	-6.13	113.52	122.65
1	B	355	GLY	C-N-CA	-6.13	113.52	122.65
1	A	381	ASN	CA-C-N	6.12	127.50	119.84
1	A	381	ASN	C-N-CA	6.12	127.50	119.84
1	B	357	LYS	N-CA-C	5.93	118.92	109.24
1	A	390	ASP	N-CA-C	-5.87	106.12	113.28
1	B	355	GLY	N-CA-C	-5.65	107.87	115.21
1	B	133	SER	N-CA-C	5.58	115.30	108.11
1	A	286	GLY	N-CA-C	-5.57	107.97	115.21
1	A	158	ASP	CB-CA-C	-5.50	110.21	116.54
1	A	71	LYS	CA-C-N	5.37	125.44	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	LYS	C-N-CA	5.37	125.44	119.32
1	A	102	THR	N-CA-C	5.22	117.18	108.99
1	B	286	GLY	N-CA-C	-5.07	101.16	113.18
1	B	142	ILE	CB-CA-C	-5.00	105.39	112.14

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	3219	0	2997	173	0
1	B	3190	0	2971	221	0
2	A	14	0	13	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	30	0	28	3	0
6	A	30	0	20	1	0
7	A	113	0	0	3	0
7	B	71	0	0	7	0
All	All	6675	0	6029	388	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 31.

All (388) 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:B:357:LYS:HD3	1:B:357:LYS:N	1.52	1.13
1:A:353:GLU:OE1	1:A:353:GLU:HA	1.42	1.06
1:A:121:HIS:CD2	1:A:123:LYS:H	1.76	1.03
1:B:39:LEU:HG	1:B:143:MET:HE1	1.41	1.02
1:A:121:HIS:HD2	1:A:123:LYS:H	1.01	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LYS:HD3	1:B:357:LYS:H	1.12	0.99
1:B:357:LYS:H	1:B:357:LYS:CD	1.69	0.99
1:B:139:VAL:HG12	1:B:143:MET:HE2	1.48	0.96
1:A:351:ARG:HD3	1:A:412:GLY:HA3	1.50	0.94
1:B:106:PHE:CZ	1:B:128:ILE:HD11	2.03	0.93
1:B:155:HIS:CD2	1:B:171:PRO:HA	2.06	0.91
1:A:334:GLU:CD	1:A:334:GLU:H	1.84	0.86
1:B:140:ALA:HA	1:B:143:MET:HE3	1.55	0.86
1:B:247:LEU:HB3	1:B:251:SER:HB2	1.60	0.83
1:A:417:VAL:HG13	1:A:418:ALA:H	1.43	0.83
1:B:226:GLU:HB2	1:B:246:LYS:HA	1.61	0.80
1:B:215:VAL:HB	1:B:218:ASN:OD1	1.82	0.79
1:A:121:HIS:HD2	1:A:123:LYS:N	1.78	0.78
1:B:248:LYS:HE3	1:B:249:SER:H	1.49	0.77
1:B:154:HIS:HB2	1:B:188:GLN:HE22	1.48	0.77
1:B:286:GLY:C	1:B:288:SER:H	1.94	0.76
1:B:203:ASN:N	1:B:203:ASN:HD22	1.84	0.76
1:B:194:MET:HA	1:B:194:MET:HE2	1.69	0.75
1:A:21:MET:HE2	1:A:101:LEU:HB3	1.68	0.74
1:A:86:LYS:HD2	1:A:123:LYS:HB2	1.70	0.73
1:A:345:ASN:H	1:A:345:ASN:HD22	1.37	0.73
1:A:11:VAL:HG21	1:A:147:MET:HE3	1.71	0.72
1:A:17:VAL:HG13	1:A:21:MET:HE3	1.71	0.72
1:B:370:LEU:HD12	1:B:371:TYR:H	1.52	0.72
1:A:298:LYS:H	1:A:298:LYS:HD2	1.53	0.72
1:B:218:ASN:C	1:B:218:ASN:HD22	1.96	0.72
1:A:370:LEU:HD12	1:A:371:TYR:H	1.54	0.71
1:B:338:PHE:CD2	1:B:366:LYS:HA	2.26	0.71
1:A:298:LYS:H	1:A:298:LYS:CD	2.04	0.71
1:A:93:LYS:HD3	1:A:94:LYS:N	2.07	0.70
1:B:338:PHE:O	1:B:365:VAL:HG22	1.91	0.70
1:A:377:PRO:HB3	1:B:113:TYR:CZ	2.27	0.70
1:B:218:ASN:ND2	1:B:220:LEU:H	1.91	0.69
1:B:226:GLU:HG3	1:B:246:LYS:HD3	1.75	0.69
1:B:18:ASP:O	1:B:22:VAL:HG23	1.94	0.68
1:A:356:LYS:HD3	1:A:356:LYS:N	2.08	0.68
1:B:39:LEU:CG	1:B:143:MET:HE1	2.20	0.68
1:B:44:ASN:HD22	1:B:54:ALA:H	1.41	0.68
1:A:18:ASP:OD1	1:A:21:MET:HB2	1.93	0.68
1:B:99:GLN:HE22	1:B:143:MET:HG2	1.59	0.68
1:A:136:ASN:ND2	1:A:136:ASN:H	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:HG22	1:A:181:PHE:HE2	1.59	0.67
1:B:21:MET:HE2	1:B:101:LEU:HB3	1.76	0.67
1:A:353:GLU:OE1	1:A:353:GLU:CA	2.30	0.67
1:B:39:LEU:HG	1:B:143:MET:CE	2.22	0.65
1:B:341:ASN:HD21	1:B:369:ARG:HB3	1.61	0.65
1:B:370:LEU:HD12	1:B:371:TYR:N	2.12	0.65
1:A:121:HIS:CD2	1:A:124:ARG:H	2.15	0.64
1:A:260:GLU:O	1:A:261:GLN:C	2.40	0.64
1:A:308:GLY:HA2	1:A:402:LYS:HG3	1.80	0.64
1:A:73:ASP:OD2	1:A:76:TYR:HB3	1.98	0.63
1:A:417:VAL:HG13	1:A:418:ALA:N	2.12	0.63
1:B:218:ASN:ND2	1:B:220:LEU:HB2	2.14	0.63
1:A:194:MET:C	1:A:195:LYS:HD3	2.25	0.62
1:A:206:LEU:O	1:A:209:ASP:HB2	2.00	0.62
1:B:255:HIS:CG	1:B:256:GLY:N	2.67	0.62
1:A:195:LYS:HD3	1:A:195:LYS:N	2.14	0.62
1:A:220:LEU:O	1:A:222:GLU:HG3	1.99	0.62
1:B:299:ASN:HD22	1:B:299:ASN:H	1.47	0.62
1:B:364:ASP:O	1:B:367:CYS:HB2	2.00	0.62
1:A:272:ARG:HD2	1:A:294:ASP:OD2	2.00	0.61
1:B:319:TYR:HE1	1:B:331:TYR:CD2	2.17	0.61
1:A:351:ARG:CG	1:A:351:ARG:HH11	2.14	0.61
1:A:345:ASN:H	1:A:345:ASN:ND2	1.99	0.61
1:B:319:TYR:HE1	1:B:331:TYR:HD2	1.45	0.61
1:A:46:ILE:HG22	1:A:181:PHE:CE2	2.36	0.61
1:B:44:ASN:HD21	1:B:53:HIS:CD2	2.19	0.60
1:B:297:HIS:ND1	1:B:301:GLN:OE1	2.31	0.60
1:A:88:ASP:OD2	1:A:88:ASP:C	2.44	0.60
1:A:363:GLU:OE2	1:A:414:CYS:HB3	2.02	0.60
1:A:252:GLN:NE2	1:A:264:PHE:H	1.99	0.60
1:B:78:LEU:HD22	1:B:113:TYR:CD2	2.37	0.60
1:B:135:ILE:HG22	1:B:138:VAL:H	1.65	0.60
1:A:113:TYR:CZ	1:B:377:PRO:HB3	2.37	0.60
1:A:101:LEU:N	1:A:101:LEU:HD12	2.17	0.59
1:B:8:PHE:O	1:B:9:ARG:HD3	2.02	0.59
1:B:238:GLU:CD	1:B:238:GLU:H	2.10	0.59
1:B:241:ASP:HB2	1:B:248:LYS:HG2	1.85	0.59
1:A:369:ARG:HD3	1:A:395:GLY:O	2.03	0.59
1:B:381:ASN:ND2	1:B:384:LYS:HB2	2.18	0.59
1:A:278:CYS:O	1:A:313:GLY:HA2	2.03	0.59
1:B:59:LEU:HD12	1:B:60:GLU:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ASP:OD1	1:B:343:LYS:HD2	2.03	0.59
1:A:280:PRO:HG3	1:A:297:HIS:CE1	2.38	0.58
1:B:282:GLU:OE1	1:B:294:ASP:OD1	2.21	0.58
1:A:416:ASP:HB2	7:A:598:HOH:O	2.04	0.58
1:B:140:ALA:HA	1:B:143:MET:CE	2.28	0.58
1:B:155:HIS:HD2	1:B:171:PRO:HA	1.60	0.58
1:A:31:LYS:HB3	1:A:31:LYS:HZ3	1.68	0.58
1:B:271:CYS:SG	1:B:292:PRO:HD2	2.44	0.58
1:A:115:TYR:CE1	1:B:378:GLY:HA3	2.39	0.58
1:A:370:LEU:HD12	1:A:371:TYR:N	2.18	0.58
1:A:31:LYS:HB3	1:A:31:LYS:NZ	2.18	0.58
1:A:14:PHE:CE1	1:A:58:GLY:HA3	2.39	0.58
1:A:341:ASN:HB3	1:A:360:CYS:SG	2.44	0.57
1:A:15:ILE:HG23	1:A:101:LEU:HD13	1.86	0.57
1:B:34:ALA:O	1:B:38:GLU:HG3	2.04	0.57
1:A:73:ASP:OD2	1:A:73:ASP:O	2.22	0.57
1:B:189:CYS:O	1:B:193:ILE:HG13	2.05	0.57
1:B:299:ASN:HD22	1:B:299:ASN:N	2.01	0.57
1:B:280:PRO:O	1:B:282:GLU:N	2.37	0.57
1:A:107:ASN:O	1:A:110:THR:HG22	2.05	0.56
1:B:319:TYR:CE1	1:B:331:TYR:HD2	2.21	0.56
1:A:47:LEU:CD1	1:A:147:MET:HE2	2.35	0.56
1:A:36:MET:SD	1:A:101:LEU:HD22	2.46	0.56
1:B:272:ARG:HG3	1:B:273:ALA:N	2.20	0.56
1:A:136:ASN:H	1:A:136:ASN:HD22	1.53	0.56
1:A:377:PRO:HB3	1:B:113:TYR:CE2	2.40	0.56
1:A:381:ASN:ND2	1:A:381:ASN:C	2.62	0.56
1:B:42:ILE:O	1:B:46:ILE:HG13	2.05	0.56
1:A:321:GLN:O	1:A:325:LEU:HD23	2.06	0.56
1:B:74:VAL:HG13	1:B:106:PHE:CG	2.41	0.56
1:B:119:MET:O	1:B:120:CYS:HB2	2.05	0.56
1:B:296:PHE:O	1:B:297:HIS:HD2	1.89	0.56
1:B:204:GLU:OE2	1:B:255:HIS:HE1	1.90	0.55
1:B:408:VAL:CG1	1:B:409:CYS:N	2.69	0.55
1:B:404:ALA:HB3	1:B:407:LYS:HB2	1.88	0.55
1:B:386:PHE:CE2	1:B:394:LYS:HD3	2.42	0.55
1:B:267:SER:C	1:B:269:THR:H	2.15	0.55
1:A:10:TYR:CZ	1:A:204:GLU:HG3	2.41	0.55
1:B:398:LEU:HD23	7:B:486:HOH:O	2.07	0.55
1:A:297:HIS:HB3	1:A:301:GLN:NE2	2.22	0.55
1:A:342:GLN:HE22	1:A:362:PRO:HG3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HD21	1:B:181:PHE:CD2	2.42	0.54
1:A:280:PRO:HD2	1:A:295:VAL:O	2.07	0.54
1:A:19:GLN:HE21	1:A:65:GLY:HA2	1.73	0.54
1:B:20:GLY:C	1:B:103:ALA:HB3	2.33	0.54
1:B:106:PHE:CE2	1:B:128:ILE:HD11	2.42	0.54
1:B:107:ASN:O	1:B:108:GLY:C	2.49	0.54
1:B:272:ARG:HD2	1:B:294:ASP:CG	2.33	0.53
1:B:140:ALA:O	1:B:143:MET:HB2	2.09	0.53
1:B:203:ASN:HD22	1:B:203:ASN:H	1.56	0.53
5:A:506:FLE:C7	1:B:111:ILE:HD11	2.39	0.53
1:A:74:VAL:HG13	1:A:113:TYR:CD2	2.42	0.53
1:A:148:GLY:CA	1:A:153:ILE:HD12	2.39	0.53
1:B:35:ARG:HH22	1:B:139:VAL:HG21	1.73	0.53
1:B:411:ASN:HB3	7:B:460:HOH:O	2.08	0.53
1:B:115:TYR:CD1	1:B:124:ARG:HG2	2.44	0.53
1:B:409:CYS:HA	1:B:413:HIS:O	2.08	0.53
1:B:282:GLU:CD	1:B:294:ASP:HA	2.34	0.52
1:A:304:LEU:HD13	1:A:317:ILE:HD13	1.91	0.52
1:A:415:VAL:HG22	1:A:416:ASP:H	1.75	0.52
1:A:356:LYS:HD3	1:A:356:LYS:H	1.74	0.52
1:B:272:ARG:CZ	1:B:272:ARG:HB2	2.39	0.52
1:A:252:GLN:HE22	1:A:264:PHE:H	1.57	0.52
1:A:118:SER:O	1:A:119:MET:C	2.51	0.52
1:B:85:ARG:NH2	1:B:125:SER:HB3	2.25	0.52
1:A:357:LYS:HE2	1:A:392:GLU:OE1	2.10	0.51
1:A:204:GLU:OE2	1:A:255:HIS:NE2	2.37	0.51
1:A:99:GLN:HE22	1:A:143:MET:HB3	1.75	0.51
1:B:218:ASN:HD22	1:B:220:LEU:H	1.55	0.51
1:B:346:TYR:CZ	1:B:347:TYR:HD2	2.27	0.51
1:B:104:ILE:O	1:B:104:ILE:HG13	2.09	0.51
1:B:398:LEU:HD13	1:B:399:PRO:HD2	1.93	0.51
1:A:73:ASP:OD2	1:A:73:ASP:C	2.54	0.51
1:A:13:LEU:HD12	1:A:14:PHE:H	1.76	0.51
1:B:19:GLN:O	1:B:20:GLY:C	2.52	0.51
1:A:356:LYS:N	1:A:356:LYS:CD	2.74	0.51
1:B:407:LYS:O	1:B:408:VAL:HG23	2.10	0.51
1:A:136:ASN:ND2	1:A:136:ASN:N	2.58	0.50
1:A:226:GLU:HG3	1:A:246:LYS:HA	1.92	0.50
1:B:99:GLN:NE2	1:B:143:MET:HG2	2.26	0.50
1:B:280:PRO:HG3	1:B:297:HIS:CD2	2.46	0.50
1:B:318:MET:HB3	1:B:332:GLU:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:TYR:HA	7:B:488:HOH:O	2.10	0.50
1:A:407:LYS:HG2	1:A:415:VAL:O	2.12	0.50
1:B:39:LEU:HB3	1:B:143:MET:HE1	1.94	0.50
1:A:190:TRP:O	1:A:194:MET:HG2	2.12	0.50
1:B:85:ARG:HG3	1:B:126:VAL:CG1	2.41	0.50
1:A:47:LEU:HD11	1:A:147:MET:HE2	1.94	0.50
1:A:308:GLY:HA2	1:A:402:LYS:CG	2.41	0.50
1:B:70:VAL:HG23	1:B:104:ILE:CD1	2.42	0.50
1:B:357:LYS:H	1:B:357:LYS:CE	2.24	0.50
1:B:402:LYS:HA	1:B:408:VAL:HG22	1.94	0.50
1:B:385:MET:SD	1:B:385:MET:C	2.95	0.49
1:A:121:HIS:HD2	1:A:124:ARG:H	1.58	0.49
1:B:267:SER:HA	1:B:285:THR:HA	1.94	0.49
1:B:311:TYR:O	1:B:313:GLY:N	2.44	0.49
1:B:338:PHE:HD2	1:B:366:LYS:HA	1.75	0.49
1:A:93:LYS:HD3	1:A:93:LYS:C	2.36	0.49
1:A:325:LEU:HD12	1:A:386:PHE:CB	2.42	0.49
1:A:345:ASN:HD22	1:A:345:ASN:N	2.00	0.49
1:A:381:ASN:C	1:A:381:ASN:HD22	2.21	0.49
1:B:375:ASN:O	1:B:376:SER:C	2.56	0.49
1:B:286:GLY:O	1:B:288:SER:N	2.44	0.49
1:A:274:SER:HA	1:A:279:ASP:OD1	2.13	0.49
1:B:203:ASN:N	1:B:203:ASN:ND2	2.57	0.49
1:A:14:PHE:CD1	1:A:58:GLY:HA3	2.47	0.49
1:A:342:GLN:NE2	1:A:362:PRO:HG3	2.28	0.49
1:B:59:LEU:HD12	1:B:60:GLU:H	1.77	0.49
1:B:70:VAL:HG23	1:B:104:ILE:HD11	1.94	0.49
1:B:168:ILE:HG21	1:B:181:PHE:CZ	2.48	0.49
1:A:194:MET:HB3	1:A:195:LYS:NZ	2.27	0.49
1:A:253:CYS:HB2	1:A:289:SER:OG	2.13	0.48
1:B:71:LYS:HD2	1:B:76:TYR:CD2	2.47	0.48
1:B:197:ASN:N	1:B:197:ASN:HD22	2.10	0.48
1:A:145:HIS:CE1	6:A:505:TRP:CE2	3.02	0.48
1:B:291:CYS:SG	1:B:292:PRO:HD2	2.54	0.48
1:B:98:ALA:HB3	1:B:126:VAL:HG12	1.96	0.48
1:B:39:LEU:CB	1:B:143:MET:HE1	2.44	0.48
1:A:345:ASN:ND2	1:A:345:ASN:N	2.60	0.48
1:B:269:THR:C	1:B:283:HIS:HB3	2.39	0.48
1:A:19:GLN:O	1:A:20:GLY:C	2.58	0.47
1:A:35:ARG:HG2	1:A:39:LEU:HD22	1.96	0.47
1:A:119:MET:O	1:A:120:CYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:VAL:HG13	1:B:106:PHE:CD1	2.49	0.47
1:B:282:GLU:OE2	1:B:294:ASP:HA	2.14	0.47
1:A:52:MET:HE2	1:A:151:LEU:CD1	2.44	0.47
1:A:159:PHE:O	2:A:501:NAG:H3	2.13	0.47
1:A:345:ASN:O	1:A:347:TYR:N	2.47	0.47
1:B:145:HIS:CE1	1:B:169:MET:HA	2.49	0.47
1:B:218:ASN:C	1:B:218:ASN:ND2	2.68	0.47
1:A:199:GLN:O	1:A:202:LEU:HB2	2.15	0.47
1:B:149:HIS:O	1:B:151:LEU:N	2.47	0.47
1:B:286:GLY:C	1:B:288:SER:N	2.61	0.47
1:A:108:GLY:N	1:A:109:PRO:HA	2.28	0.47
1:A:157:THR:O	1:A:158:ASP:C	2.57	0.47
1:B:252:GLN:HG3	1:B:263:LYS:NZ	2.29	0.47
1:B:270:GLU:HA	1:B:283:HIS:ND1	2.30	0.47
1:B:281:ALA:HB3	7:B:450:HOH:O	2.14	0.47
1:B:328:ALA:O	1:B:329:ASP:HB2	2.15	0.47
1:B:21:MET:O	1:B:24:LYS:HB3	2.15	0.47
1:B:337:CYS:C	1:B:339:LYS:H	2.22	0.47
1:B:337:CYS:O	1:B:339:LYS:N	2.48	0.47
7:A:589:HOH:O	1:B:116:ILE:HD11	2.14	0.47
1:A:139:VAL:O	1:A:143:MET:HG3	2.15	0.46
1:B:266:LYS:HA	1:B:266:LYS:HD3	1.65	0.46
1:B:281:ALA:C	1:B:282:GLU:HG3	2.40	0.46
1:B:285:THR:C	1:B:286:GLY:O	2.54	0.46
1:B:17:VAL:HG22	1:B:36:MET:HE3	1.98	0.46
1:B:157:THR:OG1	1:B:158:ASP:N	2.46	0.46
1:A:192:PHE:CD1	1:A:196:GLU:HG3	2.51	0.46
1:B:78:LEU:HD22	1:B:113:TYR:HD2	1.80	0.46
1:B:141:VAL:HG13	1:B:168:ILE:CD1	2.45	0.46
1:B:149:HIS:C	1:B:151:LEU:N	2.73	0.46
1:A:18:ASP:OD1	1:A:102:THR:HA	2.16	0.46
1:B:248:LYS:HE3	1:B:249:SER:N	2.25	0.46
1:A:137:LEU:O	1:A:141:VAL:HG23	2.15	0.46
1:A:252:GLN:NE2	1:A:264:PHE:N	2.64	0.46
1:A:321:GLN:OE1	1:A:398:LEU:HB2	2.15	0.46
1:A:251:SER:HB3	1:A:262:CYS:HB3	1.98	0.46
1:A:338:PHE:O	1:A:365:VAL:HB	2.16	0.46
1:B:337:CYS:HB3	1:B:383:CYS:HB3	1.79	0.46
1:A:29:LEU:HD11	1:A:63:SER:HB3	1.98	0.46
1:B:141:VAL:HG13	1:B:168:ILE:HD13	1.98	0.46
1:B:218:ASN:ND2	1:B:220:LEU:N	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:CG2	1:A:147:MET:HE3	2.44	0.46
1:A:175:ASN:O	1:A:177:PRO:HD3	2.16	0.46
1:A:290:GLU:O	1:A:292:PRO:HD3	2.16	0.46
1:B:147:MET:O	1:B:150:ASN:HB2	2.15	0.46
1:A:47:LEU:HD13	1:A:147:MET:HE2	1.98	0.46
1:A:46:ILE:HG12	1:A:179:LYS:HG2	1.98	0.45
1:B:107:ASN:O	1:B:109:PRO:N	2.50	0.45
1:A:28:ASP:CG	1:A:31:LYS:HB2	2.41	0.45
1:A:52:MET:HE1	1:A:151:LEU:HD21	1.99	0.45
1:A:111:ILE:HG23	5:A:504:FLE:C5	2.46	0.45
1:A:213:PRO:O	1:A:214:PRO:C	2.57	0.45
1:A:334:GLU:CD	1:A:334:GLU:N	2.64	0.45
1:B:99:GLN:HA	1:B:127:ALA:O	2.16	0.45
1:B:148:GLY:O	1:B:153:ILE:HB	2.17	0.45
1:B:108:GLY:O	1:B:109:PRO:C	2.60	0.45
1:B:154:HIS:HB2	1:B:188:GLN:NE2	2.26	0.45
1:B:74:VAL:HG11	1:B:110:THR:HG21	1.97	0.45
1:B:255:HIS:CG	1:B:256:GLY:H	2.31	0.45
1:A:74:VAL:HG23	1:A:106:PHE:CD1	2.52	0.45
1:A:417:VAL:CG1	1:A:418:ALA:H	2.20	0.45
1:B:182:SER:O	1:B:185:SER:HB2	2.17	0.45
1:B:337:CYS:C	1:B:339:LYS:N	2.73	0.45
1:A:212:SER:O	1:A:213:PRO:C	2.60	0.44
1:B:35:ARG:NH2	1:B:139:VAL:HG21	2.31	0.44
1:B:71:LYS:HD2	1:B:76:TYR:CG	2.51	0.44
1:B:86:LYS:HB2	1:B:122:PRO:O	2.17	0.44
1:B:92:ARG:HG2	1:B:92:ARG:NH2	2.33	0.44
1:B:119:MET:O	1:B:120:CYS:CB	2.65	0.44
1:A:219:GLU:O	1:A:220:LEU:HD23	2.18	0.44
5:A:506:FLE:HG	1:B:109:PRO:O	2.18	0.44
1:B:365:VAL:C	1:B:367:CYS:H	2.25	0.44
1:A:39:LEU:HD12	1:A:140:ALA:HB2	1.99	0.44
1:B:70:VAL:HG23	1:B:70:VAL:O	2.17	0.44
1:A:304:LEU:O	1:A:307:TYR:HB2	2.18	0.44
1:A:347:TYR:CD1	1:A:348:GLY:N	2.86	0.44
1:A:354:ASN:HD22	1:A:354:ASN:HA	1.56	0.44
1:B:280:PRO:HG3	1:B:297:HIS:NE2	2.33	0.44
1:A:11:VAL:HB	1:A:147:MET:HE1	1.99	0.44
1:A:12:GLU:HG3	1:A:96:ASP:OD2	2.18	0.44
1:A:176:GLU:HA	1:A:177:PRO:HD3	1.75	0.44
1:B:218:ASN:HD22	1:B:220:LEU:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ASP:OD1	1:B:241:ASP:C	2.60	0.43
1:B:5:TYR:CD1	1:B:5:TYR:C	2.96	0.43
1:B:8:PHE:C	1:B:9:ARG:HD3	2.42	0.43
1:B:162:CYS:O	1:B:165:TYR:HD2	2.01	0.43
1:B:298:LYS:HE2	1:B:298:LYS:HB3	1.86	0.43
1:B:316:PRO:HB2	1:B:401:THR:OG1	2.18	0.43
1:A:115:TYR:CD1	1:A:124:ARG:HG2	2.54	0.43
1:A:388:SER:OG	1:B:388:SER:HB2	2.18	0.43
1:B:154:HIS:H	1:B:188:GLN:NE2	2.16	0.43
1:B:194:MET:HA	1:B:194:MET:CE	2.42	0.43
1:A:346:TYR:CZ	1:A:347:TYR:HD2	2.36	0.43
1:B:94:LYS:O	1:B:95:HIS:HB3	2.18	0.43
1:A:351:ARG:NH1	1:A:351:ARG:HG2	2.33	0.43
1:B:307:TYR:O	1:B:402:LYS:HD3	2.19	0.43
1:B:260:GLU:O	1:B:261:GLN:C	2.62	0.43
1:A:154:HIS:HB2	1:A:188:GLN:HE22	1.84	0.43
1:A:252:GLN:NE2	1:A:264:PHE:CG	2.87	0.43
1:A:278:CYS:HB2	1:A:313:GLY:C	2.44	0.43
1:B:43:VAL:O	1:B:43:VAL:HG12	2.19	0.43
1:B:268:GLY:C	1:B:283:HIS:HB3	2.44	0.43
1:B:149:HIS:O	1:B:150:ASN:C	2.61	0.43
1:A:35:ARG:HG2	1:A:39:LEU:CD2	2.49	0.42
1:A:66:ASP:HB3	1:A:68:ILE:O	2.19	0.42
1:A:121:HIS:CE1	1:A:124:ARG:NH1	2.87	0.42
1:B:214:PRO:HA	1:B:222:GLU:OE1	2.19	0.42
1:A:6:ASN:HA	1:A:7:PRO:HD3	1.76	0.42
1:A:388:SER:C	1:A:390:ASP:H	2.27	0.42
1:B:37:TYR:CD2	1:B:212:SER:HB3	2.54	0.42
1:B:334:GLU:CD	1:B:334:GLU:H	2.27	0.42
1:A:341:ASN:OD1	1:A:365:VAL:O	2.37	0.42
1:B:119:MET:O	1:B:198:PRO:HB3	2.19	0.42
1:B:188:GLN:O	1:B:189:CYS:C	2.63	0.42
1:A:14:PHE:HB2	1:A:95:HIS:CD2	2.54	0.42
1:A:301:GLN:O	1:A:302:PRO:C	2.61	0.42
1:B:191:ASP:OD1	1:B:195:LYS:HE3	2.20	0.42
1:A:71:LYS:HD2	1:A:76:TYR:CD2	2.55	0.42
1:B:259:CYS:HA	1:B:263:LYS:O	2.20	0.42
1:B:408:VAL:HG13	1:B:409:CYS:H	1.84	0.42
1:A:241:ASP:O	1:A:242:ALA:C	2.63	0.42
1:B:10:TYR:CD1	1:B:205:PRO:HD2	2.55	0.42
1:B:10:TYR:CE1	1:B:204:GLU:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASN:OD1	1:A:7:PRO:HD2	2.20	0.42
1:A:148:GLY:HA2	1:A:153:ILE:HD12	2.02	0.42
1:A:347:TYR:CD1	1:A:347:TYR:C	2.98	0.42
1:B:97:ASN:HA	1:B:125:SER:O	2.20	0.42
1:B:240:CYS:HA	1:B:247:LEU:HA	2.01	0.42
1:A:32:ILE:O	1:A:33:LYS:C	2.63	0.41
1:B:44:ASN:ND2	1:B:53:HIS:CD2	2.85	0.41
1:A:346:TYR:HD1	1:A:387:TYR:CE2	2.37	0.41
1:A:351:ARG:CG	1:A:351:ARG:NH1	2.76	0.41
1:B:31:LYS:O	1:B:32:ILE:C	2.64	0.41
1:B:148:GLY:HA2	1:B:153:ILE:HD12	2.01	0.41
1:B:170:GLY:O	1:B:171:PRO:C	2.63	0.41
1:B:203:ASN:HB2	7:B:435:HOH:O	2.18	0.41
1:A:27:GLY:O	1:A:29:LEU:N	2.53	0.41
1:A:154:HIS:HD2	1:B:329:ASP:OD2	2.02	0.41
1:A:252:GLN:HE21	1:A:252:GLN:HB2	1.66	0.41
1:A:346:TYR:HA	1:A:357:LYS:NZ	2.35	0.41
1:A:368:GLY:O	1:A:369:ARG:C	2.63	0.41
1:B:226:GLU:CB	1:B:246:LYS:HA	2.41	0.41
1:B:49:TYR:C	1:B:51:TYR:H	2.28	0.41
1:B:296:PHE:O	1:B:297:HIS:CD2	2.72	0.41
1:B:356:LYS:C	1:B:357:LYS:HD3	2.32	0.41
1:B:149:HIS:C	1:B:151:LEU:H	2.29	0.41
1:B:226:GLU:HB2	1:B:245:CYS:O	2.21	0.41
1:B:139:VAL:HG12	1:B:143:MET:CE	2.34	0.41
1:B:196:GLU:O	1:B:197:ASN:C	2.64	0.41
1:B:221:LEU:HD23	1:B:255:HIS:CD2	2.56	0.41
1:A:13:LEU:HD12	1:A:14:PHE:N	2.36	0.41
1:A:101:LEU:N	1:A:101:LEU:CD1	2.83	0.41
1:B:268:GLY:O	1:B:283:HIS:ND1	2.53	0.41
1:B:345:ASN:HB2	7:B:467:HOH:O	2.21	0.41
1:B:398:LEU:HA	1:B:399:PRO:HD3	1.92	0.41
1:A:219:GLU:HG3	1:A:230:GLY:CA	2.50	0.41
1:A:375:ASN:O	1:A:377:PRO:HD3	2.20	0.41
1:B:240:CYS:SG	1:B:247:LEU:HD23	2.61	0.41
1:B:280:PRO:HD2	1:B:295:VAL:O	2.21	0.41
1:B:298:LYS:O	1:B:299:ASN:C	2.64	0.41
1:B:338:PHE:HB3	1:B:365:VAL:HG13	2.02	0.41
1:B:365:VAL:CG1	1:B:366:LYS:N	2.84	0.41
1:A:237:ASN:C	1:A:239:CYS:H	2.29	0.41
1:B:130:GLU:C	1:B:132:TYR:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:LYS:CE	1:A:404:ALA:O	2.69	0.40
1:A:402:LYS:HE2	1:A:402:LYS:HB3	1.89	0.40
1:B:44:ASN:ND2	1:B:53:HIS:HD2	2.18	0.40
1:B:218:ASN:HD21	1:B:220:LEU:HB2	1.84	0.40
1:B:183:ASN:ND2	7:B:484:HOH:O	2.48	0.40
1:B:407:LYS:HA	1:B:415:VAL:O	2.22	0.40
1:B:137:LEU:HD23	1:B:137:LEU:O	2.21	0.40
1:B:311:TYR:C	1:B:313:GLY:H	2.29	0.40
1:B:386:PHE:CD2	1:B:386:PHE:C	2.99	0.40
1:A:121:HIS:CD2	1:A:121:HIS:C	3.00	0.40
1:A:202:LEU:HD21	7:A:555:HOH:O	2.21	0.40
1:A:334:GLU:HG2	1:A:337:CYS:SG	2.62	0.40
1:A:361:ALA:O	1:A:364:ASP:N	2.55	0.40
1:B:137:LEU:HD23	1:B:137:LEU:C	2.47	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	414/419 (99%)	351 (85%)	54 (13%)	9 (2%)	5	14
1	B	410/419 (98%)	320 (78%)	70 (17%)	20 (5%)	1	3
All	All	824/838 (98%)	671 (81%)	124 (15%)	29 (4%)	3	6

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	249	SER
1	B	107	ASN
1	B	157	THR

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Mol	Chain	Res	Type
1	B	281	ALA
1	B	312	ASN
1	A	261	GLN
1	A	391	ASP
1	B	109	PRO
1	B	150	ASN
1	B	247	LEU
1	B	261	GLN
1	B	338	PHE
1	A	346	TYR
1	A	417	VAL
1	B	254	GLY
1	B	269	THR
1	A	292	PRO
1	B	304	LEU
1	B	351	ARG
1	B	399	PRO
1	A	197	ASN
1	B	28	ASP
1	B	282	GLU
1	B	298	LYS
1	A	411	ASN
1	B	46	ILE
1	B	287	GLN
1	B	108	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	361/363 (99%)	321 (89%)	40 (11%)	6	15
1	B	358/363 (99%)	319 (89%)	39 (11%)	6	16
All	All	719/726 (99%)	640 (89%)	79 (11%)	6	15

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	23	THR
1	A	29	LEU
1	A	31	LYS
1	A	38	GLU
1	A	39	LEU
1	A	50	LEU
1	A	73	ASP
1	A	74	VAL
1	A	88	ASP
1	A	93	LYS
1	A	102	THR
1	A	110	THR
1	A	128	ILE
1	A	136	ASN
1	A	172	THR
1	A	195	LYS
1	A	199	GLN
1	A	200	CYS
1	A	202	LEU
1	A	208	THR
1	A	211	VAL
1	A	238	GLU
1	A	251	SER
1	A	252	GLN
1	A	260	GLU
1	A	263	LYS
1	A	298	LYS
1	A	321	GLN
1	A	332	GLU
1	A	334	GLU
1	A	345	ASN
1	A	351	ARG
1	A	353	GLU
1	A	354	ASN
1	A	358	ILE
1	A	373	LYS
1	A	403	CYS
1	A	408	VAL
1	A	416	ASP
1	B	4	LYS
1	B	13	LEU
1	B	18	ASP

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Mol	Chain	Res	Type
1	B	21	MET
1	B	30	ASP
1	B	39	LEU
1	B	41	ASN
1	B	47	LEU
1	B	50	LEU
1	B	70	VAL
1	B	74	VAL
1	B	77	THR
1	B	86	LYS
1	B	102	THR
1	B	104	ILE
1	B	128	ILE
1	B	175	ASN
1	B	191	ASP
1	B	194	MET
1	B	197	ASN
1	B	203	ASN
1	B	218	ASN
1	B	220	LEU
1	B	238	GLU
1	B	253	CYS
1	B	272	ARG
1	B	274	SER
1	B	277	GLU
1	B	289	SER
1	B	299	ASN
1	B	334	GLU
1	B	342	GLN
1	B	357	LYS
1	B	365	VAL
1	B	375	ASN
1	B	380	ASN
1	B	384	LYS
1	B	385	MET
1	B	408	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	19	GLN

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Mol	Chain	Res	Type
1	A	26	ASN
1	A	64	ASN
1	A	99	GLN
1	A	121	HIS
1	A	150	ASN
1	A	154	HIS
1	A	188	GLN
1	A	199	GLN
1	A	237	ASN
1	A	252	GLN
1	A	297	HIS
1	A	299	ASN
1	A	301	GLN
1	A	312	ASN
1	A	341	ASN
1	A	342	GLN
1	A	345	ASN
1	A	354	ASN
1	A	375	ASN
1	A	381	ASN
1	A	393	HIS
1	B	19	GLN
1	B	44	ASN
1	B	53	HIS
1	B	79	ASN
1	B	99	GLN
1	B	150	ASN
1	B	155	HIS
1	B	188	GLN
1	B	197	ASN
1	B	218	ASN
1	B	255	HIS
1	B	261	GLN
1	B	287	GLN
1	B	299	ASN
1	B	321	GLN
1	B	341	ASN
1	B	342	GLN
1	B	393	HIS

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 ⓘ

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 for Mogul analysis.

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$
6	TRP	A	507	4,5	15,16,16	0.79	1 (6%)	18,22,22	0.79	1 (5%)
2	NAG	A	501	1	14,14,15	1.69	2 (14%)	17,19,21	2.09	5 (29%)
5	FLE	A	506	6	14,15,16	1.92	4 (28%)	18,19,21	2.07	4 (22%)
5	FLE	A	504	6	14,15,16	1.65	4 (28%)	18,19,21	3.31	6 (33%)
6	TRP	A	505	4,5	15,16,16	0.82	1 (6%)	18,22,22	0.91	1 (5%)

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
6	TRP	A	507	4,5	-	1/8/8/8	0/2/2/2
2	NAG	A	501	1	-	4/6/23/26	0/1/1/1
5	FLE	A	506	6	-	3/13/14/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FLE	A	504	6	-	2/13/14/16	0/1/1/1
6	TRP	A	505	4,5	-	2/8/8/8	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAG	C1-C2	4.48	1.58	1.52
5	A	506	FLE	C2-N	3.67	1.41	1.34
5	A	506	FLE	C4-C2	3.63	1.54	1.47
5	A	504	FLE	CB-CA	3.50	1.58	1.53
5	A	506	FLE	CB-CA	3.30	1.57	1.53
5	A	504	FLE	C2-N	3.18	1.40	1.34
5	A	504	FLE	CA-N	2.56	1.50	1.46
2	A	501	NAG	C3-C2	2.45	1.57	1.52
6	A	507	TRP	OXT-C	-2.40	1.23	1.30
5	A	506	FLE	CA-N	2.33	1.49	1.46
6	A	505	TRP	OXT-C	-2.18	1.23	1.30
5	A	504	FLE	C4-C2	2.02	1.51	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	FLE	C4-C2-N	8.67	130.58	115.73
5	A	504	FLE	CB-CA-N	6.60	120.65	110.69
5	A	506	FLE	C4-C2-N	5.74	125.56	115.73
2	A	501	NAG	C1-O5-C5	5.46	119.50	112.19
5	A	504	FLE	O3-C2-N	-4.84	114.56	123.09
5	A	504	FLE	O3-C2-C4	-4.55	113.96	121.10
5	A	504	FLE	CB-CA-C	4.50	117.91	110.99
5	A	506	FLE	O3-C2-N	-4.29	115.54	123.09
2	A	501	NAG	C1-C2-N2	3.68	116.23	110.43
6	A	505	TRP	OXT-C-O	-3.27	116.66	124.08
2	A	501	NAG	C4-C3-C2	-3.01	106.61	111.02
6	A	507	TRP	OXT-C-O	-2.89	117.53	124.08
2	A	501	NAG	C3-C4-C5	-2.66	105.41	110.23
5	A	506	FLE	O8-C4-C2	2.66	124.52	117.98
2	A	501	NAG	O5-C1-C2	-2.50	107.43	111.29
5	A	506	FLE	CB-CA-N	2.19	113.99	110.69
5	A	504	FLE	CA-N-C2	-2.03	114.58	121.93

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	FLE	N-CA-CB-CG
5	A	504	FLE	C-CA-CB-CG
5	A	506	FLE	N-CA-CB-CG
5	A	506	FLE	C-CA-CB-CG
5	A	506	FLE	O-C-CA-CB
2	A	501	NAG	O5-C5-C6-O6
2	A	501	NAG	C4-C5-C6-O6
2	A	501	NAG	C3-C2-N2-C7
2	A	501	NAG	C1-C2-N2-C7
6	A	505	TRP	CA-CB-CG-CD2
6	A	505	TRP	CA-CB-CG-CD1
6	A	507	TRP	CA-CB-CG-CD1

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	1	0
5	A	506	FLE	2	0
5	A	504	FLE	1	0
6	A	505	TRP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	355:GLY	C	356:LYS	N	1.05

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	416/419 (99%)	0.15	13 (3%)	51 48	22, 38, 78, 180	0
1	B	412/419 (98%)	0.49	37 (8%)	15 13	24, 49, 129, 235	0
All	All	828/838 (98%)	0.32	50 (6%)	27 24	22, 43, 105, 235	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	CYS	6.5
1	A	361	ALA	6.2
1	B	273	ALA	5.9
1	B	262	CYS	4.6
1	B	293	ALA	4.4
1	B	363	GLU	4.3
1	B	226	GLU	3.9
1	B	400	GLY	3.8
1	B	280	PRO	3.5
1	B	404	ALA	3.5
1	A	242	ALA	3.4
1	B	263	LYS	3.3
1	B	266	LYS	3.3
1	B	267	SER	3.3
1	A	65	GLY	3.2
1	A	296	PHE	3.2
1	B	257	ASP	3.2
1	B	164	ASP	2.9
1	B	317	ILE	2.9
1	A	368	GLY	2.8
1	B	248	LYS	2.8
1	B	152	GLY	2.7
1	B	217	GLY	2.7
1	A	404	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	54	ALA	2.7
1	B	305	ASP	2.7
1	B	244	THR	2.6
1	B	65	GLY	2.6
1	B	242	ALA	2.6
1	B	252	GLN	2.6
1	A	344	GLY	2.5
1	B	298	LYS	2.5
1	A	64	ASN	2.4
1	B	236	GLN	2.4
1	B	296	PHE	2.4
1	B	292	PRO	2.4
1	B	250	GLY	2.4
1	B	238	GLU	2.3
1	B	265	SER	2.3
1	A	418	ALA	2.3
1	B	285	THR	2.3
1	A	415	VAL	2.2
1	B	91	THR	2.1
1	B	173	ILE	2.1
1	A	352	LYS	2.1
1	A	397	VAL	2.1
1	B	261	GLN	2.0
1	B	348	GLY	2.0
1	B	132	TYR	2.0
1	B	307	TYR	2.0

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](#)

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($\text{\AA}^2$)	Q<0.9
2	NAG	A	501	14/15	0.82	0.12	42,45,52,61	0
5	FLE	A	506	15/16	0.88	0.10	42,42,42,42	0
6	TRP	A	507	15/15	0.88	0.13	53,53,53,53	0
5	FLE	A	504	15/16	0.92	0.10	24,24,24,24	0
3	CA	A	1	1/1	0.97	0.07	19,19,19,19	0
3	CA	B	423	1/1	0.97	0.04	34,34,34,34	0
6	TRP	A	505	15/15	0.97	0.06	16,16,16,16	0
3	CA	B	424	1/1	0.97	0.04	72,72,72,72	0
3	CA	A	502	1/1	0.98	0.02	34,34,34,34	0
3	CA	B	422	1/1	0.98	0.03	24,24,24,24	0
4	ZN	A	503	1/1	0.99	0.11	33,33,33,33	0
4	ZN	B	1	1/1	0.99	0.06	48,48,48,48	0
3	CA	A	2	1/1	0.99	0.05	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.