



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:37 PM UTC

PDB ID : 1QVB / pdb_00001qvb
Title : CRYSTAL STRUCTURE OF THE BETA-GLYCOSIDASE FROM THE HYPER-
THERMOPHILE THERMOSPHERA AGGREGANS
Authors : Chi, Y.-I.; Martinez-Cruz, L.A.; Swanson, R.V.; Robertson, D.E.; Kim, S.-H.
Deposited on : 1999-07-07
Resolution : 2.40 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

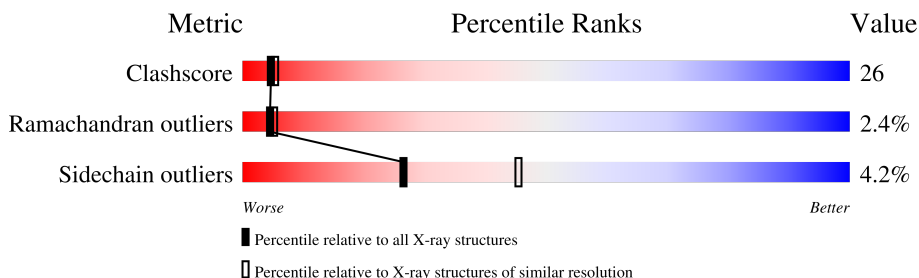
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	481	 62% 32% 6%
1	B	481	 62% 33% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8295 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 BETA-GLYCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3928	2549	659	707	13			
1	B	481	Total	C	N	O	S	0	0	0
			3928	2549	659	707	13			

- Molecule 2 is water.

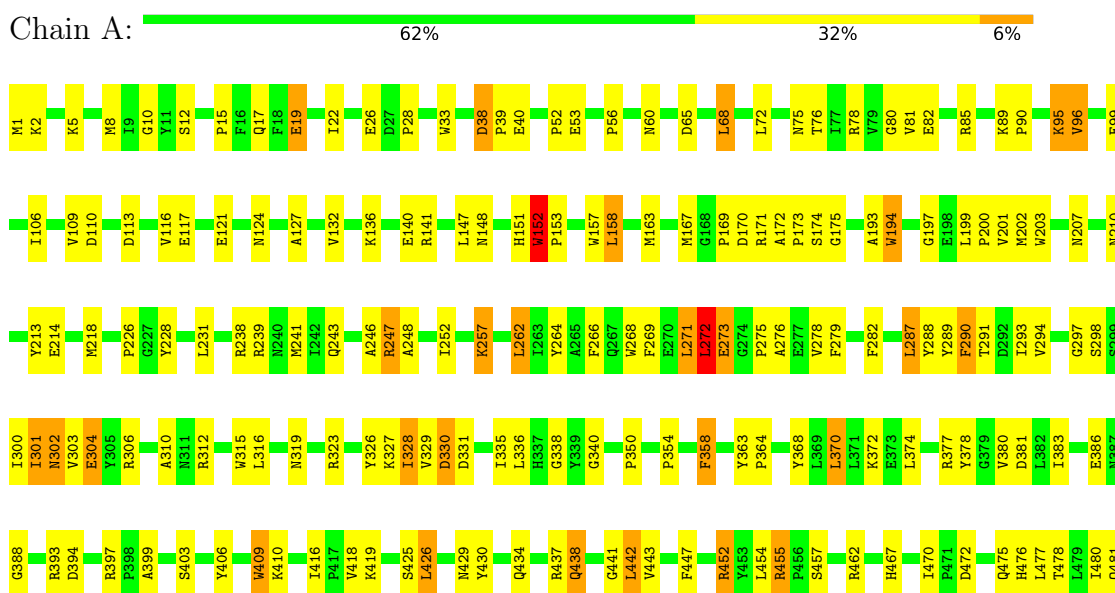
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	234	Total	O	0	0
			234	234		
2	B	205	Total	O	0	0
			205	205		

3 Residue-property plots

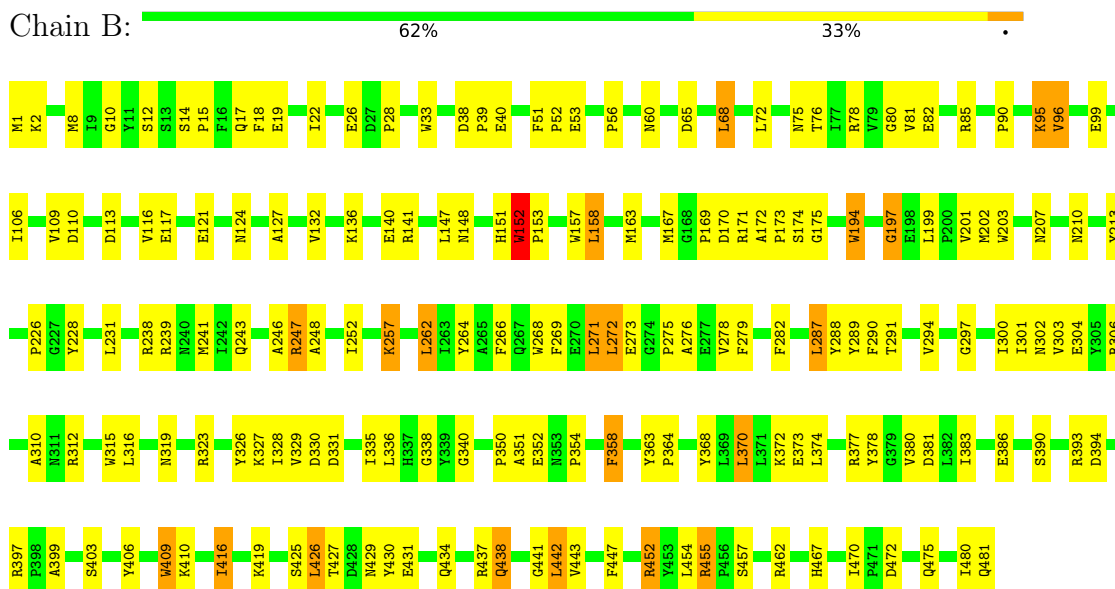
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: BETA-GLYCOSIDASE



• Molecule 1: BETA-GLYCOSIDASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.51Å 102.22Å 95.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	93.7 (20.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.210 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8295	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

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	0.42	0/4053	1.01	18/5514 (0.3%)
1	B	0.41	0/4053	1.01	13/5514 (0.2%)
All	All	0.42	0/8106	1.01	31/11028 (0.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	LEU	N-CA-C	-10.83	99.46	112.89
1	B	442	LEU	N-CA-C	-10.69	99.64	112.89
1	A	174	SER	N-CA-C	9.12	122.64	112.97
1	B	174	SER	N-CA-C	8.44	121.92	112.97
1	A	19	GLU	N-CA-C	6.98	118.58	110.97
1	B	455	ARG	N-CA-C	-6.95	101.04	110.36
1	B	19	GLU	N-CA-C	6.73	118.31	110.97
1	B	426	LEU	N-CA-C	-6.69	103.46	111.69
1	A	455	ARG	N-CA-C	-6.61	101.16	110.29
1	A	426	LEU	N-CA-C	-6.52	103.67	111.69
1	A	441	GLY	N-CA-C	6.41	119.30	111.93
1	B	152	TRP	N-CA-C	6.15	123.39	109.81
1	A	331	ASP	N-CA-C	-6.01	105.27	114.16
1	A	152	TRP	N-CA-C	5.93	122.92	109.81
1	B	331	ASP	N-CA-C	-5.72	105.69	114.16
1	B	199	LEU	N-CA-C	5.72	120.27	112.55
1	A	89	LYS	CA-C-N	5.66	125.59	119.76
1	A	89	LYS	C-N-CA	5.66	125.59	119.76
1	B	141	ARG	N-CA-C	-5.66	106.15	113.16
1	B	173	PRO	N-CA-C	-5.63	100.87	112.47
1	A	38	ASP	CA-C-N	5.45	124.64	118.97
1	A	38	ASP	C-N-CA	5.45	124.64	118.97
1	B	441	GLY	N-CA-C	5.43	119.14	112.14
1	A	199	LEU	N-CA-C	5.37	119.47	112.17
1	B	197	GLY	N-CA-C	5.33	120.36	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	PRO	N-CA-C	-5.29	101.57	112.47
1	A	478	THR	N-CA-C	-5.21	106.71	113.16
1	A	141	ARG	N-CA-C	-5.19	106.72	113.16
1	A	419	LYS	N-CA-C	5.11	119.38	113.20
1	B	419	LYS	N-CA-C	5.08	119.35	113.20
1	A	200	PRO	N-CA-C	5.05	119.24	111.57

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	3928	0	3808	204	0
1	B	3928	0	3808	209	0
2	A	234	0	0	5	0
2	B	205	0	0	3	0
All	All	8295	0	7616	400	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (400) 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:8:MET:HB3	1:B:76:THR:HG21	1.34	1.08
1:A:8:MET:HB3	1:A:76:THR:HG21	1.30	1.08
1:B:480:ILE:HG22	1:B:481:GLN:H	1.16	1.07
1:B:1:MET:HE2	1:B:475:GLN:HE22	1.16	1.07
1:A:480:ILE:HG22	1:A:481:GLN:H	1.16	1.06
1:A:278:VAL:HG11	1:A:329:VAL:HG13	1.40	1.01
1:A:1:MET:HE2	1:A:475:GLN:HE22	1.21	1.01
1:B:278:VAL:HG11	1:B:329:VAL:HG13	1.41	1.00
1:A:1:MET:HE3	1:A:470:ILE:HD12	1.53	0.91
1:A:327:LYS:HD2	1:A:336:LEU:HD21	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LYS:HD2	1:B:336:LEU:HD21	1.61	0.83
1:B:480:ILE:HG22	1:B:481:GLN:N	1.94	0.82
1:B:1:MET:HE3	1:B:470:ILE:HD12	1.60	0.81
1:A:480:ILE:HG22	1:A:481:GLN:N	1.95	0.81
1:A:171:ARG:HH11	1:B:171:ARG:HH11	1.27	0.81
1:B:163:MET:HE2	1:B:171:ARG:O	1.82	0.80
1:B:327:LYS:HD2	1:B:336:LEU:CD2	2.12	0.80
1:A:327:LYS:HD2	1:A:336:LEU:CD2	2.12	0.79
1:A:163:MET:HE2	1:A:171:ARG:O	1.83	0.79
1:A:96:VAL:HG13	1:A:110:ASP:O	1.83	0.78
1:A:201:VAL:HG23	1:A:202:MET:HG3	1.66	0.77
1:B:81:VAL:HG23	1:B:147:LEU:HD11	1.66	0.77
1:A:278:VAL:CG1	1:A:329:VAL:HG13	2.15	0.76
1:B:96:VAL:HG13	1:B:110:ASP:O	1.85	0.76
1:A:266:PHE:HD2	1:A:287:LEU:HD21	1.51	0.75
1:B:278:VAL:CG1	1:B:329:VAL:HG13	2.16	0.75
1:A:213:TYR:HD2	1:A:241:MET:CE	2.00	0.74
1:B:434:GLN:NE2	1:B:437:ARG:HE	1.85	0.74
1:B:480:ILE:CG2	1:B:481:GLN:H	1.99	0.74
1:B:201:VAL:HG23	1:B:202:MET:HG3	1.70	0.73
1:B:213:TYR:HD2	1:B:241:MET:CE	2.01	0.73
1:A:452:ARG:HD2	1:A:452:ARG:N	2.04	0.72
1:B:266:PHE:HD2	1:B:287:LEU:HD21	1.53	0.72
1:B:158:LEU:HD22	1:B:175:GLY:HA2	1.69	0.72
1:B:272:LEU:HD22	1:B:272:LEU:H	1.55	0.72
1:A:272:LEU:H	1:A:272:LEU:HD22	1.55	0.71
1:B:272:LEU:HD21	1:B:328:ILE:N	2.05	0.71
1:A:81:VAL:HG23	1:A:147:LEU:HD11	1.71	0.71
1:B:452:ARG:N	1:B:452:ARG:HD2	2.05	0.70
1:A:480:ILE:CG2	1:A:481:GLN:H	2.00	0.70
1:A:272:LEU:HD21	1:A:328:ILE:N	2.06	0.70
1:A:158:LEU:HD22	1:A:175:GLY:HA2	1.73	0.69
1:A:213:TYR:HD2	1:A:241:MET:HE3	1.57	0.69
1:A:22:ILE:HB	1:A:60:ASN:ND2	2.09	0.68
1:B:213:TYR:HD2	1:B:241:MET:HE3	1.57	0.68
1:A:434:GLN:NE2	1:A:437:ARG:HE	1.92	0.68
1:A:65:ASP:OD1	1:A:452:ARG:NH1	2.29	0.66
1:B:163:MET:HG2	1:B:172:ALA:HB2	1.76	0.66
1:A:40:GLU:HG2	1:B:231:LEU:HG	1.77	0.66
1:A:171:ARG:NH1	1:B:171:ARG:HH11	1.94	0.65
1:A:136:LYS:O	1:A:140:GLU:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:ASP:HA	1:B:475:GLN:HG2	1.78	0.65
1:A:300:ILE:O	1:A:300:ILE:HD12	1.97	0.65
1:B:272:LEU:HD21	1:B:328:ILE:H	1.62	0.65
1:A:319:ASN:CG	1:A:386:GLU:HB2	2.22	0.64
1:A:472:ASP:HA	1:A:475:GLN:HG2	1.80	0.64
1:A:272:LEU:HD21	1:A:328:ILE:H	1.63	0.64
1:A:15:PRO:CB	1:A:82:GLU:HG2	2.28	0.63
1:B:243:GLN:HE21	1:B:306:ARG:HH22	1.46	0.63
1:B:319:ASN:CG	1:B:386:GLU:HB2	2.24	0.63
1:A:171:ARG:HH11	1:B:171:ARG:NH1	1.95	0.63
1:A:243:GLN:HE21	1:A:306:ARG:HH22	1.46	0.63
1:B:275:PRO:HB2	1:B:329:VAL:HG23	1.80	0.63
1:A:163:MET:HG2	1:A:172:ALA:HB2	1.80	0.62
1:A:275:PRO:HB2	1:A:329:VAL:HG23	1.81	0.62
1:B:22:ILE:HB	1:B:60:ASN:ND2	2.14	0.62
1:B:354:PRO:HG3	1:B:481:GLN:HB2	1.80	0.62
1:A:302:ASN:OD1	1:A:304:GLU:HB2	1.98	0.62
1:A:354:PRO:HG3	1:A:481:GLN:HB2	1.80	0.62
1:B:75:ASN:OD1	1:B:76:THR:HG22	2.00	0.62
1:A:287:LEU:HD23	1:A:287:LEU:O	1.99	0.62
1:B:8:MET:CB	1:B:76:THR:HG21	2.21	0.61
1:B:15:PRO:CB	1:B:82:GLU:HG2	2.31	0.61
1:B:300:ILE:HD12	1:B:300:ILE:O	2.00	0.61
1:B:275:PRO:HB2	1:B:329:VAL:CG2	2.31	0.61
1:A:275:PRO:HB2	1:A:329:VAL:CG2	2.31	0.60
1:A:368:TYR:CZ	1:A:372:LYS:HD2	2.36	0.60
1:A:8:MET:CB	1:A:76:THR:HG21	2.20	0.60
1:B:65:ASP:OD1	1:B:452:ARG:NH1	2.34	0.60
1:B:302:ASN:OD1	1:B:304:GLU:HB2	2.00	0.60
1:B:1:MET:HE2	1:B:475:GLN:NE2	2.01	0.60
1:A:323:ARG:HD3	1:A:363:TYR:CE2	2.37	0.60
1:A:210:ASN:HA	1:A:213:TYR:CZ	2.37	0.59
1:A:1:MET:HE1	1:A:406:TYR:CD1	2.38	0.59
1:A:151:HIS:O	1:A:153:PRO:HD3	2.03	0.59
1:B:416:ILE:N	1:B:416:ILE:HD12	2.17	0.59
1:A:289:TYR:O	1:A:290:PHE:HB2	2.02	0.59
1:B:136:LYS:O	1:B:140:GLU:HG3	2.03	0.59
1:B:238:ARG:HD3	1:B:289:TYR:HE2	1.68	0.59
1:B:289:TYR:O	1:B:290:PHE:HB2	2.02	0.58
1:A:388:GLY:HA3	2:A:1365:HOH:O	2.03	0.58
1:A:106:ILE:H	1:A:243:GLN:HE22	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:PRO:HA	1:A:33:TRP:CG	2.40	0.57
1:A:78:ARG:NH2	1:A:207:ASN:OD1	2.36	0.57
1:A:416:ILE:HD12	1:A:416:ILE:N	2.19	0.57
1:B:1:MET:HE1	1:B:406:TYR:CD1	2.40	0.57
1:B:90:PRO:HG3	1:B:157:TRP:CB	2.34	0.57
1:A:2:LYS:O	1:A:409:TRP:HZ3	1.88	0.57
1:B:90:PRO:HG3	1:B:157:TRP:HB2	1.86	0.57
1:A:171:ARG:NH1	1:B:171:ARG:HD2	2.20	0.56
1:A:238:ARG:HD2	2:A:1339:HOH:O	2.04	0.56
1:A:171:ARG:HD2	1:B:171:ARG:NH1	2.20	0.56
1:A:279:PHE:O	1:A:282:PHE:HB3	2.05	0.56
1:B:106:ILE:H	1:B:243:GLN:HE22	1.52	0.56
1:B:124:ASN:HD22	1:B:127:ALA:HB2	1.70	0.56
1:A:397:ARG:HD3	1:A:442:LEU:HD23	1.88	0.56
1:A:276:ALA:HB3	1:A:278:VAL:HG12	1.88	0.56
1:B:2:LYS:O	1:B:409:TRP:HZ3	1.89	0.55
1:A:210:ASN:HA	1:A:213:TYR:CE2	2.41	0.55
1:A:12:SER:OG	1:A:78:ARG:HD3	2.07	0.55
1:A:15:PRO:HB2	1:A:82:GLU:HG2	1.88	0.55
1:B:15:PRO:HB2	1:B:82:GLU:HG2	1.87	0.55
1:B:78:ARG:NH2	1:B:207:ASN:OD1	2.39	0.55
1:B:262:LEU:C	1:B:262:LEU:HD23	2.31	0.55
1:B:109:VAL:CG2	1:B:247:ARG:HG2	2.36	0.55
1:A:358:PHE:CE2	1:A:438:GLN:HG2	2.40	0.55
1:B:158:LEU:CD2	1:B:175:GLY:HA2	2.37	0.55
1:B:279:PHE:O	1:B:282:PHE:HB3	2.07	0.55
1:B:323:ARG:HD3	1:B:363:TYR:CE2	2.42	0.55
1:B:368:TYR:CZ	1:B:372:LYS:HD2	2.41	0.54
1:A:262:LEU:C	1:A:262:LEU:HD23	2.31	0.54
1:B:257:LYS:HB3	1:B:257:LYS:HZ2	1.72	0.54
1:B:269:PHE:CD1	1:B:287:LEU:HD12	2.42	0.54
1:B:287:LEU:O	1:B:287:LEU:HD23	2.07	0.54
1:A:75:ASN:OD1	1:A:76:THR:HG22	2.07	0.54
1:A:475:GLN:HE21	1:A:475:GLN:HA	1.72	0.54
1:B:28:PRO:HA	1:B:33:TRP:CG	2.43	0.54
1:A:90:PRO:HG3	1:A:157:TRP:HB2	1.89	0.54
1:A:472:ASP:O	1:A:475:GLN:HG2	2.07	0.54
1:B:117:GLU:O	1:B:121:GLU:HG3	2.07	0.54
1:A:90:PRO:HG3	1:A:157:TRP:CB	2.38	0.54
1:A:167:MET:HE3	1:A:171:ARG:CZ	2.38	0.53
1:A:272:LEU:HB2	1:A:275:PRO:HD3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:HIS:O	1:B:153:PRO:HD3	2.08	0.53
1:A:269:PHE:CD1	1:A:287:LEU:HD12	2.43	0.53
1:B:276:ALA:HB3	1:B:278:VAL:HG12	1.90	0.53
1:A:289:TYR:CZ	1:A:293:ILE:HD11	2.43	0.53
1:B:272:LEU:HD21	1:B:327:LYS:HA	1.90	0.53
1:B:358:PHE:CE2	1:B:438:GLN:HG2	2.44	0.53
1:A:287:LEU:HD23	1:A:287:LEU:C	2.34	0.53
1:B:210:ASN:HA	1:B:213:TYR:CZ	2.43	0.53
1:A:272:LEU:HD21	1:A:327:LYS:HA	1.91	0.53
1:B:213:TYR:CD2	1:B:241:MET:HE3	2.43	0.52
1:B:158:LEU:HD23	1:B:158:LEU:O	2.09	0.52
1:A:136:LYS:HG2	1:A:140:GLU:CD	2.34	0.52
1:A:231:LEU:HG	1:B:40:GLU:HG2	1.92	0.52
1:B:287:LEU:HD23	1:B:287:LEU:C	2.35	0.52
1:B:287:LEU:HD22	1:B:288:TYR:CE2	2.45	0.52
1:B:272:LEU:HB2	1:B:275:PRO:HD3	1.90	0.52
1:A:213:TYR:CD2	1:A:241:MET:HE3	2.42	0.52
1:B:213:TYR:HD2	1:B:241:MET:HE1	1.74	0.52
1:B:287:LEU:HD22	1:B:288:TYR:CD2	2.44	0.52
1:B:289:TYR:O	1:B:290:PHE:CB	2.58	0.52
1:B:467:HIS:O	1:B:467:HIS:ND1	2.42	0.52
1:B:264:TYR:HB3	1:B:266:PHE:CE1	2.45	0.52
1:B:109:VAL:HG23	1:B:247:ARG:HG2	1.92	0.52
1:B:248:ALA:O	1:B:252:ILE:HG13	2.10	0.51
1:A:171:ARG:CZ	1:B:171:ARG:HD2	2.40	0.51
1:B:2:LYS:HE2	1:B:467:HIS:CE1	2.46	0.51
1:B:167:MET:HE3	1:B:171:ARG:CZ	2.40	0.51
1:B:472:ASP:HA	1:B:475:GLN:CG	2.41	0.51
1:A:248:ALA:O	1:A:252:ILE:HG13	2.11	0.51
1:A:257:LYS:HZ2	1:A:257:LYS:HB3	1.76	0.51
1:B:297:GLY:HA3	1:B:310:ALA:HB2	1.92	0.51
1:A:289:TYR:O	1:A:290:PHE:CB	2.58	0.51
1:B:151:HIS:O	1:B:152:TRP:HB2	2.11	0.51
1:B:82:GLU:HB2	1:B:85:ARG:HG3	1.92	0.51
1:B:136:LYS:HG2	1:B:140:GLU:CD	2.36	0.51
1:A:52:PRO:HD2	1:A:53:GLU:OE2	2.11	0.50
1:B:2:LYS:HG2	1:B:467:HIS:CE1	2.47	0.50
1:A:472:ASP:HA	1:A:475:GLN:CG	2.42	0.50
1:B:210:ASN:HA	1:B:213:TYR:CE2	2.46	0.50
1:B:238:ARG:HD3	1:B:289:TYR:CE2	2.46	0.50
1:A:213:TYR:HD2	1:A:241:MET:HE1	1.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LYS:HG2	1:A:467:HIS:CE1	2.47	0.50
1:A:117:GLU:O	1:A:121:GLU:HG3	2.11	0.50
1:B:315:TRP:HA	1:B:380:VAL:CG1	2.42	0.50
1:A:56:PRO:O	1:A:452:ARG:NH2	2.44	0.50
1:A:394:ASP:HB2	1:A:455:ARG:HD3	1.94	0.50
1:B:434:GLN:NE2	1:B:437:ARG:NE	2.59	0.50
1:A:56:PRO:HD3	1:A:447:PHE:HE2	1.76	0.50
1:A:171:ARG:HD2	1:B:171:ARG:CZ	2.42	0.50
1:B:475:GLN:HE21	1:B:475:GLN:HA	1.77	0.50
1:A:109:VAL:CG2	1:A:247:ARG:HG2	2.42	0.49
1:A:315:TRP:HA	1:A:380:VAL:CG1	2.41	0.49
1:A:326:TYR:CE2	1:A:335:ILE:HG23	2.46	0.49
1:B:80:GLY:HA2	1:B:148:ASN:O	2.12	0.49
1:B:397:ARG:HD3	1:B:442:LEU:HD23	1.94	0.49
1:A:2:LYS:HE2	1:A:467:HIS:CE1	2.48	0.49
1:A:82:GLU:HB2	1:A:85:ARG:HG3	1.92	0.49
1:A:257:LYS:HA	1:A:257:LYS:HZ3	1.77	0.49
1:A:158:LEU:HD23	1:A:158:LEU:O	2.12	0.49
1:B:56:PRO:HD3	1:B:447:PHE:HE2	1.77	0.49
1:B:26:GLU:CD	1:B:26:GLU:H	2.20	0.49
1:A:15:PRO:HB3	1:A:82:GLU:HG2	1.93	0.49
1:A:323:ARG:HD3	1:A:363:TYR:CD2	2.47	0.49
1:A:327:LYS:HD2	1:A:336:LEU:HD23	1.93	0.49
1:A:197:GLY:HA2	1:A:203:TRP:CZ2	2.48	0.49
1:B:12:SER:OG	1:B:78:ARG:HD3	2.13	0.49
1:B:327:LYS:HD2	1:B:336:LEU:HD23	1.91	0.49
1:A:106:ILE:H	1:A:243:GLN:NE2	2.10	0.49
1:A:264:TYR:HB3	1:A:266:PHE:CE1	2.48	0.49
1:B:197:GLY:HA2	1:B:203:TRP:CZ2	2.48	0.49
1:B:124:ASN:HD22	1:B:127:ALA:CB	2.26	0.49
1:B:303:VAL:HG23	1:B:304:GLU:N	2.28	0.49
1:A:80:GLY:HA2	1:A:148:ASN:O	2.13	0.49
1:A:480:ILE:HA	2:A:1048:HOH:O	2.13	0.48
1:B:106:ILE:H	1:B:243:GLN:NE2	2.11	0.48
1:A:238:ARG:HD3	1:A:289:TYR:HE2	1.77	0.48
1:A:287:LEU:C	1:A:287:LEU:CD2	2.86	0.48
1:B:52:PRO:HD2	1:B:53:GLU:OE2	2.13	0.48
1:B:393:ARG:HG2	1:B:393:ARG:HH11	1.78	0.48
1:B:452:ARG:NH2	2:B:1391:HOH:O	2.44	0.48
1:A:152:TRP:HB2	1:A:153:PRO:HD3	1.93	0.48
1:A:266:PHE:CD2	1:A:287:LEU:HD21	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PRO:HD3	1:B:228:TYR:CZ	2.48	0.48
1:A:151:HIS:O	1:A:152:TRP:HB2	2.12	0.48
1:A:338:GLY:O	1:A:350:PRO:HD3	2.13	0.48
1:A:247:ARG:HE	1:A:247:ARG:HA	1.78	0.48
1:A:370:LEU:HD22	1:A:374:LEU:CD1	2.44	0.48
1:B:124:ASN:ND2	1:B:127:ALA:HB2	2.29	0.48
1:A:113:ASP:O	1:A:117:GLU:HG3	2.14	0.48
1:A:467:HIS:O	1:A:467:HIS:ND1	2.46	0.48
1:A:358:PHE:CD2	1:A:438:GLN:HG2	2.49	0.48
1:B:113:ASP:O	1:B:117:GLU:HG3	2.14	0.48
1:A:124:ASN:HD22	1:A:127:ALA:HB2	1.78	0.47
1:B:434:GLN:HE21	1:B:437:ARG:HE	1.60	0.47
1:A:197:GLY:HA2	1:A:203:TRP:HZ2	1.78	0.47
1:B:197:GLY:HA2	1:B:203:TRP:HZ2	1.78	0.47
1:B:399:ALA:HB3	1:B:481:GLN:HG2	1.95	0.47
1:B:288:TYR:OH	1:B:373:GLU:OE2	2.28	0.47
1:B:303:VAL:O	1:B:304:GLU:C	2.56	0.47
1:B:472:ASP:O	1:B:475:GLN:HG2	2.15	0.47
1:A:26:GLU:H	1:A:26:GLU:CD	2.23	0.47
1:A:399:ALA:HB3	1:A:481:GLN:HG2	1.96	0.47
1:B:272:LEU:CD2	1:B:327:LYS:HA	2.45	0.47
1:B:338:GLY:O	1:B:350:PRO:HD3	2.15	0.47
1:A:95:LYS:O	1:A:96:VAL:HB	2.15	0.47
1:A:287:LEU:HD22	1:A:288:TYR:CD2	2.50	0.47
1:A:297:GLY:HA3	1:A:310:ALA:HB2	1.96	0.47
1:A:303:VAL:O	1:A:304:GLU:C	2.57	0.47
1:A:393:ARG:HG2	1:A:393:ARG:HH11	1.80	0.47
1:B:14:SER:HB3	1:B:151:HIS:CE1	2.49	0.47
1:B:326:TYR:CE2	1:B:335:ILE:HG23	2.48	0.47
1:B:95:LYS:O	1:B:96:VAL:HB	2.15	0.47
1:B:152:TRP:HB2	1:B:153:PRO:HD3	1.96	0.47
1:B:287:LEU:C	1:B:287:LEU:CD2	2.87	0.47
1:A:247:ARG:HA	1:A:247:ARG:NE	2.30	0.47
1:A:303:VAL:HG23	1:A:304:GLU:N	2.29	0.47
1:B:434:GLN:HE21	1:B:437:ARG:NE	2.13	0.47
1:A:287:LEU:HD22	1:A:288:TYR:CE2	2.50	0.47
1:B:380:VAL:HG12	1:B:381:ASP:N	2.29	0.47
1:A:171:ARG:NH2	1:B:170:ASP:OD1	2.48	0.46
1:A:271:LEU:HD13	1:A:275:PRO:HG3	1.97	0.46
1:B:275:PRO:O	1:B:276:ALA:HB2	2.14	0.46
1:B:323:ARG:HD3	1:B:363:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:O	1:A:462:ARG:HA	2.14	0.46
1:A:272:LEU:CD2	1:A:327:LYS:HA	2.45	0.46
1:B:290:PHE:O	1:B:294:VAL:HG22	2.14	0.46
1:A:271:LEU:HD22	1:A:275:PRO:HG3	1.98	0.46
1:B:377:ARG:HD3	1:B:378:TYR:CZ	2.50	0.46
1:A:109:VAL:HG23	1:A:247:ARG:HG2	1.98	0.46
1:B:15:PRO:HB3	1:B:82:GLU:HG2	1.98	0.46
1:B:271:LEU:HD22	1:B:275:PRO:HG3	1.97	0.46
1:B:462:ARG:HD2	2:B:1125:HOH:O	2.15	0.46
1:B:268:TRP:O	1:B:323:ARG:HB2	2.16	0.46
1:A:291:THR:HA	1:A:294:VAL:HG22	1.97	0.45
1:B:431:GLU:HG3	1:B:431:GLU:O	2.17	0.45
1:A:8:MET:HE1	1:A:383:ILE:CD1	2.47	0.45
1:B:81:VAL:CG2	1:B:147:LEU:HD11	2.41	0.45
1:A:171:ARG:NH1	1:B:171:ARG:CD	2.79	0.45
1:A:443:VAL:HG11	1:A:452:ARG:HB3	1.97	0.45
1:A:170:ASP:OD1	1:B:171:ARG:NH2	2.49	0.45
1:B:394:ASP:HB2	1:B:455:ARG:HD3	1.99	0.45
1:A:169:PRO:HD3	1:A:228:TYR:CZ	2.51	0.45
1:B:17:GLN:HB3	1:B:429:ASN:HD22	1.81	0.45
1:B:364:PRO:CB	1:B:403:SER:HB3	2.47	0.45
1:A:1:MET:HE1	1:A:406:TYR:HD1	1.81	0.45
1:A:214:GLU:O	1:A:218:MET:HB2	2.17	0.45
1:A:275:PRO:O	1:A:276:ALA:HB2	2.15	0.45
1:A:238:ARG:HD3	1:A:289:TYR:CE2	2.51	0.45
1:A:329:VAL:O	1:A:330:ASP:C	2.60	0.45
1:B:257:LYS:HA	1:B:257:LYS:HZ3	1.82	0.45
1:A:68:LEU:HD21	1:A:454:LEU:HD21	1.99	0.45
1:B:291:THR:HA	1:B:294:VAL:HG22	1.98	0.45
1:A:171:ARG:CD	1:B:171:ARG:NH1	2.80	0.45
1:A:246:ALA:HA	1:A:312:ARG:HD3	1.99	0.45
1:B:12:SER:CB	1:B:78:ARG:HD3	2.47	0.45
1:B:18:PHE:O	1:B:56:PRO:HG2	2.16	0.45
1:A:269:PHE:HB3	1:A:279:PHE:CZ	2.51	0.45
1:B:51:PHE:HB3	1:B:53:GLU:OE2	2.16	0.45
1:B:167:MET:O	1:B:171:ARG:HD3	2.16	0.44
1:A:213:TYR:CD2	1:A:241:MET:CE	2.91	0.44
1:A:290:PHE:O	1:A:294:VAL:HG22	2.16	0.44
1:B:271:LEU:HD13	1:B:275:PRO:HG3	1.99	0.44
1:B:416:ILE:N	1:B:416:ILE:CD1	2.81	0.44
1:B:399:ALA:HB3	1:B:481:GLN:CG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:MET:HE1	1:A:383:ILE:HD13	1.98	0.44
1:A:1:MET:HE3	1:A:470:ILE:CD1	2.35	0.44
1:A:472:ASP:CA	1:A:475:GLN:HG2	2.47	0.44
1:B:266:PHE:HB2	1:B:370:LEU:HD11	2.00	0.44
1:B:329:VAL:O	1:B:330:ASP:C	2.61	0.44
1:A:82:GLU:OE2	1:A:82:GLU:HA	2.17	0.44
1:A:82:GLU:CB	1:A:85:ARG:HG3	2.48	0.44
1:B:300:ILE:O	1:B:301:ILE:C	2.61	0.44
1:B:323:ARG:O	1:B:340:GLY:HA3	2.18	0.44
1:B:358:PHE:CD2	1:B:438:GLN:HG2	2.53	0.44
1:B:364:PRO:HB3	1:B:403:SER:HB3	1.99	0.43
1:B:443:VAL:HG11	1:B:452:ARG:HB3	1.99	0.43
1:B:472:ASP:CA	1:B:475:GLN:HG2	2.46	0.43
1:B:8:MET:HE1	1:B:383:ILE:CD1	2.49	0.43
1:B:247:ARG:HA	1:B:247:ARG:NE	2.32	0.43
1:A:10:GLY:HA3	1:A:76:THR:O	2.19	0.43
1:A:434:GLN:HE21	1:A:437:ARG:HE	1.66	0.43
1:B:425:SER:HB3	1:B:427:THR:O	2.18	0.43
1:A:300:ILE:O	1:A:301:ILE:C	2.62	0.43
1:A:399:ALA:HB3	1:A:481:GLN:CG	2.49	0.43
1:B:116:VAL:HG11	1:B:194:TRP:CG	2.54	0.43
1:B:56:PRO:O	1:B:452:ARG:NH2	2.52	0.43
1:B:72:LEU:HD12	1:B:426:LEU:HD11	1.99	0.43
1:B:239:ARG:HG3	1:B:239:ARG:HH11	1.83	0.43
1:B:239:ARG:HH12	1:B:306:ARG:NH1	2.16	0.43
1:B:390:SER:OG	1:B:438:GLN:HG3	2.19	0.43
1:A:15:PRO:O	1:A:19:GLU:HG3	2.19	0.43
1:A:257:LYS:HA	1:A:257:LYS:NZ	2.33	0.43
1:B:15:PRO:HD2	2:B:1110:HOH:O	2.19	0.43
1:B:246:ALA:HA	1:B:312:ARG:HD3	2.01	0.43
1:A:124:ASN:ND2	1:A:127:ALA:HB2	2.33	0.43
1:A:17:GLN:HB3	1:A:429:ASN:HD22	1.84	0.42
1:A:213:TYR:CD2	1:A:241:MET:HE1	2.54	0.42
1:B:272:LEU:H	1:B:272:LEU:CD2	2.29	0.42
1:A:167:MET:O	1:A:171:ARG:HD3	2.18	0.42
1:A:268:TRP:O	1:A:323:ARG:HB2	2.19	0.42
1:B:266:PHE:CD2	1:B:287:LEU:HD21	2.42	0.42
1:B:315:TRP:HA	1:B:380:VAL:HG12	2.00	0.42
1:A:380:VAL:HG12	1:A:381:ASP:N	2.34	0.42
1:B:257:LYS:HA	1:B:257:LYS:NZ	2.35	0.42
1:A:409:TRP:CD1	1:A:410:LYS:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLN:HA	1:A:475:GLN:NE2	2.34	0.42
1:A:12:SER:CB	1:A:78:ARG:HD3	2.49	0.42
1:A:15:PRO:HD2	2:A:1042:HOH:O	2.20	0.42
1:A:416:ILE:N	1:A:416:ILE:CD1	2.83	0.42
1:B:152:TRP:CD1	1:B:152:TRP:N	2.85	0.42
1:B:239:ARG:HH12	1:B:306:ARG:HH12	1.68	0.42
1:B:273:GLU:C	1:B:275:PRO:HD2	2.44	0.42
1:A:475:GLN:HE21	1:A:475:GLN:CA	2.29	0.42
1:B:213:TYR:CZ	1:B:238:ARG:HG3	2.55	0.42
1:A:266:PHE:HB2	1:A:370:LEU:HD11	2.02	0.42
1:B:52:PRO:HG3	1:B:430:TYR:CE2	2.55	0.42
1:B:68:LEU:HD21	1:B:454:LEU:HD21	2.02	0.42
1:B:247:ARG:HA	1:B:247:ARG:HE	1.85	0.42
1:A:116:VAL:HG11	1:A:194:TRP:CG	2.55	0.42
1:B:273:GLU:O	1:B:275:PRO:HD2	2.19	0.42
1:B:370:LEU:HD22	1:B:374:LEU:CD1	2.50	0.42
1:A:2:LYS:O	1:A:409:TRP:CZ3	2.72	0.41
1:B:380:VAL:CG1	1:B:381:ASP:N	2.82	0.41
1:B:475:GLN:NE2	1:B:475:GLN:HA	2.35	0.41
1:A:239:ARG:HH12	1:A:306:ARG:HH12	1.69	0.41
1:A:38:ASP:HA	1:A:39:PRO:HD3	1.84	0.41
1:A:158:LEU:CD2	1:A:175:GLY:HA2	2.47	0.41
1:A:315:TRP:HA	1:A:380:VAL:HG12	2.01	0.41
1:A:377:ARG:HD3	1:A:378:TYR:CZ	2.55	0.41
1:B:28:PRO:HA	1:B:33:TRP:CD1	2.55	0.41
1:B:213:TYR:HB3	1:B:241:MET:HE1	2.03	0.41
1:B:393:ARG:HG2	1:B:393:ARG:NH1	2.35	0.41
1:A:298:SER:HB3	1:A:304:GLU:O	2.20	0.41
1:A:416:ILE:HG22	1:A:418:VAL:HG23	2.03	0.41
1:B:397:ARG:HD2	1:B:457:SER:OG	2.20	0.41
1:B:409:TRP:CD1	1:B:410:LYS:N	2.87	0.41
1:A:239:ARG:HH12	1:A:306:ARG:NH1	2.17	0.41
1:A:272:LEU:H	1:A:272:LEU:CD2	2.29	0.41
1:A:28:PRO:HA	1:A:33:TRP:CD1	2.55	0.41
1:A:72:LEU:HD12	1:A:426:LEU:HD11	2.02	0.41
1:A:364:PRO:CB	1:A:403:SER:HB3	2.50	0.41
1:B:82:GLU:OE2	1:B:82:GLU:HA	2.20	0.41
1:A:5:LYS:HE3	1:A:5:LYS:HB2	1.93	0.41
1:A:273:GLU:C	1:A:275:PRO:HD2	2.45	0.41
1:B:72:LEU:O	1:B:462:ARG:HA	2.19	0.41
1:B:10:GLY:HA3	1:B:76:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:TYR:CD2	1:B:241:MET:HE1	2.55	0.41
1:A:399:ALA:CB	1:A:481:GLN:HG2	2.51	0.41
1:A:462:ARG:HD2	2:A:1380:HOH:O	2.21	0.41
1:B:1:MET:HE1	1:B:406:TYR:HD1	1.85	0.41
1:B:132:VAL:O	1:B:136:LYS:HB2	2.21	0.41
1:B:351:ALA:O	1:B:352:GLU:HB2	2.19	0.41
1:B:1:MET:HE3	1:B:470:ILE:CD1	2.43	0.41
1:B:2:LYS:HG2	1:B:467:HIS:HE1	1.85	0.41
1:B:403:SER:O	1:B:406:TYR:HB3	2.21	0.41
1:A:239:ARG:HH11	1:A:239:ARG:HG3	1.85	0.40
1:A:476:HIS:CE1	1:A:477:LEU:HG	2.56	0.40
1:B:269:PHE:HB3	1:B:279:PHE:CZ	2.56	0.40
1:A:81:VAL:CG2	1:A:147:LEU:HD11	2.47	0.40
1:A:152:TRP:N	1:A:152:TRP:CD1	2.86	0.40
1:A:193:ALA:HA	1:A:203:TRP:CH2	2.57	0.40
1:A:323:ARG:O	1:A:340:GLY:HA3	2.21	0.40
1:B:38:ASP:HA	1:B:39:PRO:HD3	1.83	0.40
1:A:132:VAL:O	1:A:136:LYS:HB2	2.20	0.40
1:B:8:MET:HE1	1:B:383:ILE:HD13	2.03	0.40
1:A:52:PRO:HG3	1:A:430:TYR:CE2	2.56	0.40
1:A:397:ARG:HD2	1:A:457:SER:OG	2.21	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	405/481 (84%)	371 (92%)	22 (5%)	12 (3%)	3	3
1	B	226/481 (47%)	216 (96%)	7 (3%)	3 (1%)	9	14
All	All	631/962 (66%)	587 (93%)	29 (5%)	15 (2%)	4	5

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	TRP
1	A	273	GLU
1	A	290	PHE
1	B	152	TRP
1	A	95	LYS
1	A	272	LEU
1	A	302	ASN
1	A	328	ILE
1	B	95	LYS
1	A	425	SER
1	A	96	VAL
1	A	301	ILE
1	B	96	VAL
1	A	304	GLU
1	A	330	ASP

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	417/417 (100%)	400 (96%)	17 (4%)	27	46
1	B	417/417 (100%)	399 (96%)	18 (4%)	26	44
All	All	834/834 (100%)	799 (96%)	35 (4%)	26	45

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LEU
1	A	99	GLU
1	A	158	LEU
1	A	194	TRP
1	A	226	PRO
1	A	247	ARG
1	A	257	LYS
1	A	262	LEU

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Mol	Chain	Res	Type
1	A	271	LEU
1	A	272	LEU
1	A	287	LEU
1	A	316	LEU
1	A	358	PHE
1	A	370	LEU
1	A	409	TRP
1	A	438	GLN
1	A	452	ARG
1	B	68	LEU
1	B	99	GLU
1	B	158	LEU
1	B	194	TRP
1	B	226	PRO
1	B	247	ARG
1	B	257	LYS
1	B	262	LEU
1	B	271	LEU
1	B	272	LEU
1	B	287	LEU
1	B	316	LEU
1	B	358	PHE
1	B	370	LEU
1	B	409	TRP
1	B	416	ILE
1	B	438	GLN
1	B	452	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	124	ASN
1	A	129	ASN
1	A	243	GLN
1	A	429	ASN
1	A	434	GLN
1	A	468	ASN
1	A	475	GLN
1	B	54	ASN
1	B	124	ASN
1	B	129	ASN

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Mol	Chain	Res	Type
1	B	130	HIS
1	B	243	GLN
1	B	251	ASN
1	B	387	ASN
1	B	429	ASN
1	B	434	GLN
1	B	468	ASN
1	B	475	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.