



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2022 – 02:27 PM JST

PDB ID : 7VT9
Title : CRYSTAL STRUCTURE AT 3.4 ANGSTROMS RESOLUTION OF Mal-
todextrin glucosidase, MalZ, FROM Escherichia coli
Authors : Ahn, W.-C.; Ahn, Y.; Woo, E.-J.
Deposited on : 2021-10-28
Resolution : 3.30 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

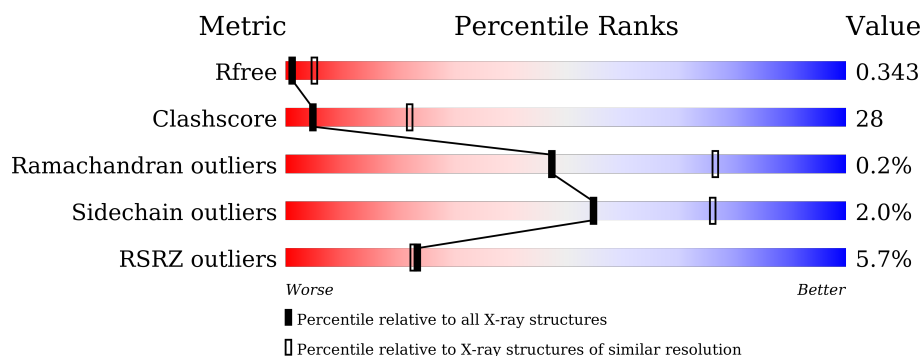
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	615	<div> <div>5%</div> <div> <div></div> <div>51%</div> <div>46%</div> <div>..</div> </div> </div>
1	B	615	<div> <div>7%</div> <div> <div></div> <div>46%</div> <div>49%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19105 atoms, of which 9344 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 Maltodextrin glucosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	604	Total	C	H	N	O	S	0	0	0
			9552	3107	4672	871	880	22			
1	B	604	Total	C	H	N	O	S	0	0	0
			9552	3107	4672	871	880	22			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	605	ALA	-	expression tag	UNP P21517
A	606	ALA	-	expression tag	UNP P21517
A	607	ALA	-	expression tag	UNP P21517
A	608	LEU	-	expression tag	UNP P21517
A	609	GLU	-	expression tag	UNP P21517
A	610	HIS	-	expression tag	UNP P21517
A	611	HIS	-	expression tag	UNP P21517
A	612	HIS	-	expression tag	UNP P21517
A	613	HIS	-	expression tag	UNP P21517
A	614	HIS	-	expression tag	UNP P21517
A	615	HIS	-	expression tag	UNP P21517
B	605	ALA	-	expression tag	UNP P21517
B	606	ALA	-	expression tag	UNP P21517
B	607	ALA	-	expression tag	UNP P21517
B	608	LEU	-	expression tag	UNP P21517
B	609	GLU	-	expression tag	UNP P21517
B	610	HIS	-	expression tag	UNP P21517
B	611	HIS	-	expression tag	UNP P21517
B	612	HIS	-	expression tag	UNP P21517
B	613	HIS	-	expression tag	UNP P21517
B	614	HIS	-	expression tag	UNP P21517
B	615	HIS	-	expression tag	UNP P21517

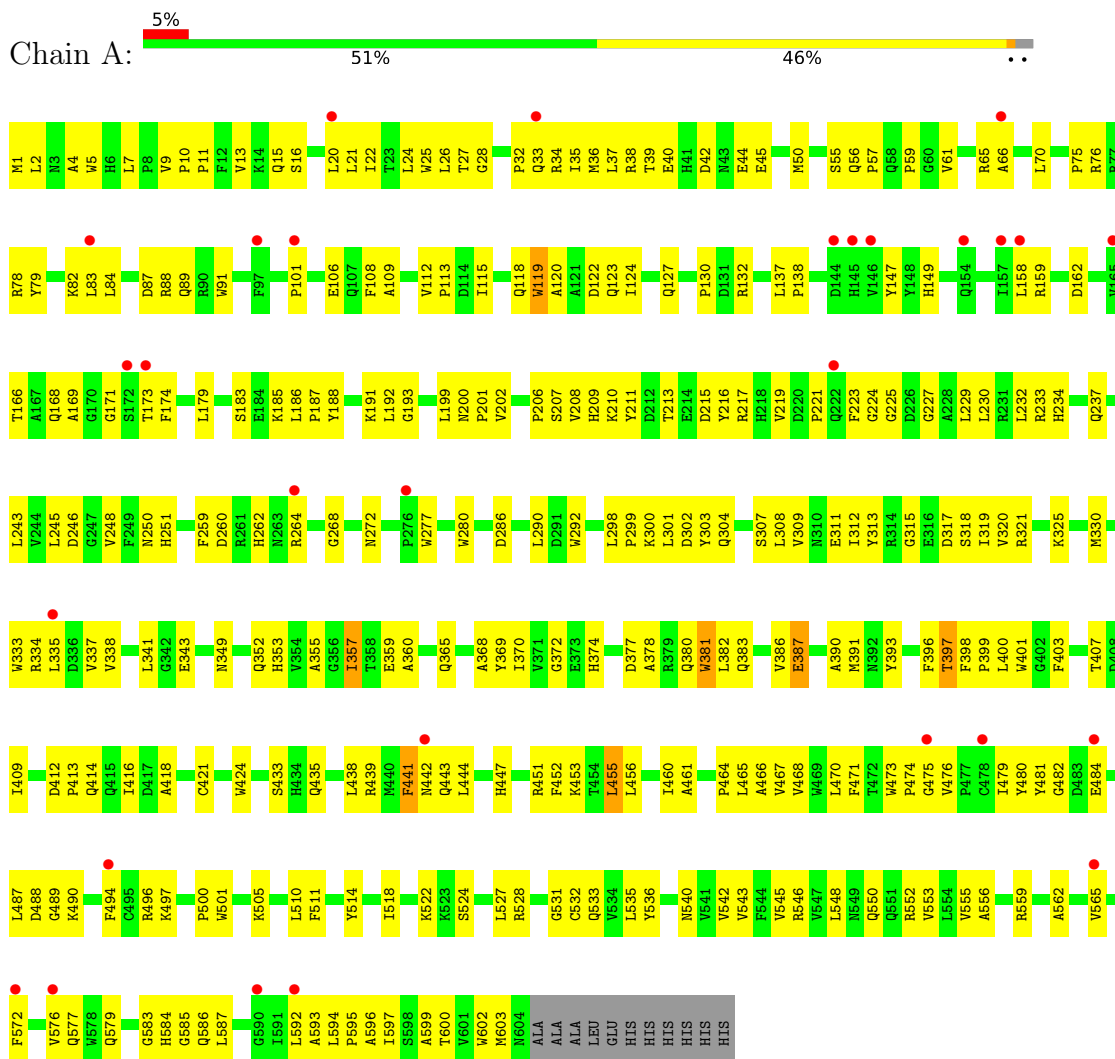
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		

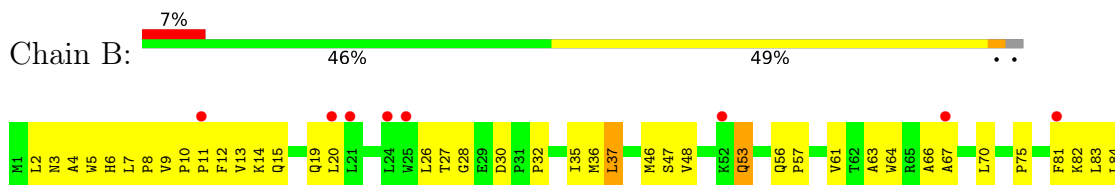
3 Residue-property plots [i](#)

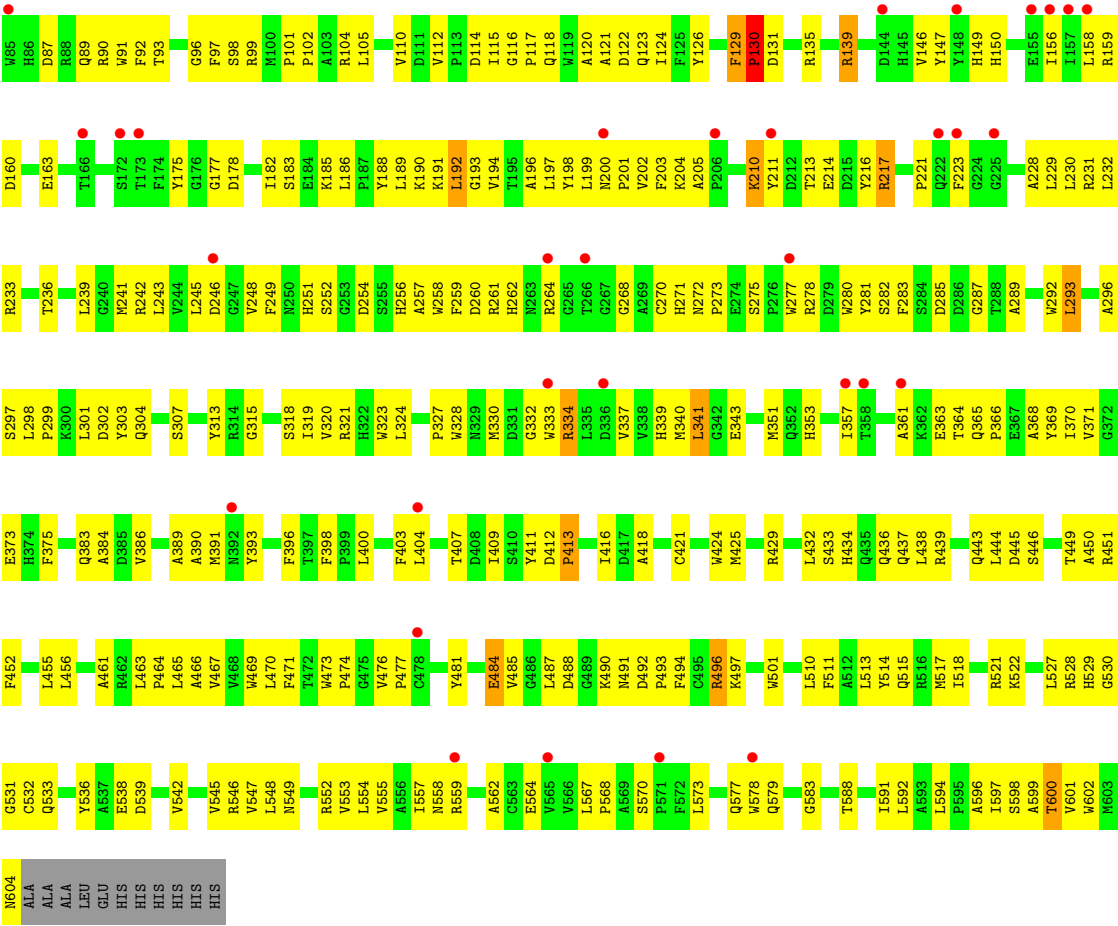
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Maltodextrin glucosidase





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	204.19Å 204.19Å 267.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.91 – 3.30 40.91 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (40.91-3.30) 98.0 (40.91-3.30)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.32Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.303 , 0.343 0.304 , 0.343	Depositor DCC
R_{free} test set	1960 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	80.2	Xtrriage
Anisotropy	0.261	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 93.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	19105	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4560e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.71	1/5029 (0.0%)	0.91	11/6846 (0.2%)
1	B	0.70	0/5029	0.92	5/6846 (0.1%)
All	All	0.70	1/10058 (0.0%)	0.91	16/13692 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	GLU	CG-CD	5.19	1.59	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	TYR	CA-CB-CG	5.86	124.52	113.40
1	B	37	LEU	CA-CB-CG	5.80	128.65	115.30
1	A	412	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	119	TRP	CB-CA-C	5.56	121.51	110.40
1	B	75	PRO	N-CA-C	5.50	126.40	112.10
1	A	191	LYS	CD-CE-NZ	5.49	124.33	111.70
1	A	455	LEU	CB-CG-CD1	-5.47	101.71	111.00
1	A	55	SER	N-CA-CB	-5.18	102.73	110.50
1	A	381	TRP	N-CA-C	-5.18	97.02	111.00
1	A	232	LEU	CA-CB-CG	5.17	127.18	115.30
1	B	293	LEU	CA-CB-CG	-5.14	103.49	115.30
1	B	341	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	B	192	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	A	312	ILE	C-N-CA	-5.10	108.95	121.70
1	A	357	ILE	CG1-CB-CG2	-5.08	100.22	111.40
1	A	230	LEU	CB-CG-CD2	-5.06	102.40	111.00

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	4880	4672	4672	261	0
1	B	4880	4672	4672	276	0
2	A	1	0	0	0	0
All	All	9761	9344	9344	527	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (527) 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:381:TRP:O	1:A:386:VAL:HG22	1.69	0.92
1:A:535:LEU:HB2	1:A:543:VAL:HG12	1.51	0.89
1:A:377:ASP:HB3	1:B:104:ARG:HB2	1.61	0.82
1:B:4:ALA:HB2	1:B:26:LEU:HD23	1.62	0.82
1:B:199:LEU:HD12	1:B:243:LEU:HD11	1.63	0.81
1:A:320:VAL:HG21	1:A:357:ILE:HG23	1.63	0.81
1:B:200:ASN:O	1:B:202:VAL:HG13	1.80	0.80
1:B:186:LEU:HD13	1:B:239:LEU:HD12	1.64	0.79
1:A:32:PRO:HG3	1:A:83:LEU:HD23	1.65	0.78
1:A:382:LEU:HD11	1:A:390:ALA:CB	2.13	0.78
1:A:382:LEU:HD11	1:A:390:ALA:HB2	1.67	0.77
1:A:109:ALA:HB3	1:A:433:SER:HA	1.67	0.77
1:B:126:TYR:HB2	1:B:194:VAL:HG11	1.67	0.76
1:B:32:PRO:HG3	1:B:83:LEU:HD23	1.67	0.76
1:B:216:TYR:HD2	1:B:319:ILE:HG21	1.51	0.75
1:B:130:PRO:HB2	1:B:223:PHE:CE2	2.22	0.75
1:B:4:ALA:HB2	1:B:26:LEU:CD2	2.17	0.74
1:B:418:ALA:HB2	1:B:539:ASP:O	1.88	0.73
1:A:391:MET:HA	1:A:441:PHE:HB3	1.71	0.72
1:B:320:VAL:HG21	1:B:357:ILE:HG23	1.71	0.72
1:B:577:GLN:HG2	1:B:579:GLN:HG2	1.72	0.72
1:A:527:LEU:HD21	1:A:553:VAL:HG11	1.72	0.71
1:B:337:VAL:HG22	1:B:337:VAL:O	1.91	0.71
1:A:333:TRP:HB2	1:A:370:ILE:HD12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:TRP:HE1	1:B:337:VAL:HG21	1.56	0.70
1:A:444:LEU:HD12	1:A:470:LEU:HD22	1.74	0.69
1:B:121:ALA:HA	1:B:476:VAL:HG12	1.74	0.69
1:A:124:ILE:HD12	1:A:471:PHE:CE2	2.28	0.69
1:B:200:ASN:HB3	1:B:201:PRO:CD	2.22	0.69
1:A:447:HIS:HB2	1:A:496:ARG:HE	1.58	0.68
1:B:57:PRO:HB2	1:B:61:VAL:HG11	1.75	0.68
1:A:465:LEU:HD21	1:A:597:ILE:O	1.94	0.68
1:A:396:PHE:O	1:A:400:LEU:HD13	1.94	0.68
1:B:487:LEU:HD11	1:B:497:LYS:HB2	1.76	0.67
1:B:369:TYR:O	1:B:370:ILE:HD13	1.94	0.67
1:B:416:ILE:HD12	1:B:421:CYS:HB2	1.75	0.67
1:A:179:LEU:HD13	1:A:229:LEU:HD13	1.76	0.67
1:B:444:LEU:HG	1:B:470:LEU:HD22	1.77	0.67
1:A:262:HIS:HB2	1:A:264:ARG:HD2	1.76	0.66
1:A:39:THR:HG22	1:A:79:TYR:HB3	1.76	0.66
1:A:380:GLN:HA	1:A:383:GLN:HG2	1.77	0.66
1:B:4:ALA:CB	1:B:26:LEU:HD23	2.26	0.65
1:B:547:VAL:HG13	1:B:552:ARG:HD3	1.77	0.65
1:B:583:GLY:HA3	1:B:600:THR:HA	1.76	0.65
1:B:200:ASN:HB3	1:B:201:PRO:HD2	1.78	0.64
1:B:425:MET:O	1:B:429:ARG:HG3	1.97	0.64
1:B:433:SER:O	1:B:437:GLN:HG3	1.98	0.64
1:A:120:ALA:HA	1:A:123:GLN:HG3	1.79	0.63
1:B:216:TYR:CD2	1:B:319:ILE:HG21	2.32	0.63
1:A:20:LEU:HB2	1:A:70:LEU:HD11	1.78	0.63
1:B:259:PHE:CD2	1:B:261:ARG:HB2	2.33	0.63
1:A:124:ILE:HD12	1:A:471:PHE:HE2	1.63	0.62
1:B:245:LEU:HG	1:B:330:MET:HG3	1.81	0.62
1:B:332:GLY:HA3	1:B:369:TYR:O	1.99	0.62
1:A:192:LEU:HD13	1:A:511:PHE:CZ	2.35	0.62
1:A:44:GLU:HB2	1:B:340:MET:HE2	1.80	0.62
1:A:213:THR:HG21	1:A:216:TYR:CZ	2.35	0.62
1:B:146:VAL:HG23	1:B:158:LEU:HD12	1.80	0.61
1:B:259:PHE:CE2	1:B:261:ARG:HB2	2.35	0.61
1:A:365:GLN:HB3	1:A:368:ALA:HB2	1.83	0.61
1:B:487:LEU:HD12	1:B:488:ASP:H	1.66	0.61
1:A:233:ARG:O	1:A:237:GLN:HG3	2.01	0.60
1:A:398:PHE:CE2	1:A:409:ILE:HD12	2.36	0.60
1:B:8:PRO:HA	1:B:13:VAL:HG21	1.84	0.60
1:B:201:PRO:HB2	1:B:210:LYS:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:GLN:HB2	1:B:343:GLU:HB3	1.85	0.59
1:A:527:LEU:HD23	1:A:546:ARG:HG3	1.84	0.59
1:B:26:LEU:HD12	1:B:64:TRP:NE1	2.17	0.59
1:A:482:GLY:HA3	1:A:487:LEU:HD23	1.84	0.59
1:A:259:PHE:O	1:A:259:PHE:CD2	2.55	0.59
1:B:105:LEU:HD13	1:B:383:GLN:HG2	1.83	0.59
1:B:283:PHE:HA	1:B:289:ALA:HA	1.85	0.58
1:B:418:ALA:CB	1:B:539:ASP:O	2.51	0.58
1:A:374:HIS:ND1	1:A:378:ALA:HB1	2.19	0.58
1:B:117:PRO:HG3	1:B:369:TYR:HD1	1.68	0.58
1:A:199:LEU:HB2	1:A:245:LEU:HD23	1.84	0.58
1:B:131:ASP:HB2	1:B:223:PHE:CE1	2.38	0.58
1:A:500:PRO:HB2	1:A:505:LYS:HB2	1.86	0.58
1:A:115:ILE:HG22	1:A:115:ILE:O	2.04	0.58
1:B:532:CYS:HB2	1:B:546:ARG:HD2	1.86	0.58
1:A:562:ALA:HB2	1:A:596:ALA:N	2.18	0.58
1:A:10:PRO:O	1:A:11:PRO:C	2.41	0.57
1:A:39:THR:HG22	1:A:79:TYR:CB	2.34	0.57
1:B:147:TYR:CZ	1:B:156:ILE:HD13	2.39	0.57
1:A:171:GLY:O	1:A:208:VAL:HG12	2.04	0.57
1:A:280:TRP:CE3	1:A:308:LEU:HD13	2.39	0.57
1:A:396:PHE:O	1:A:399:PRO:HD2	2.05	0.57
1:B:555:VAL:HG22	1:B:601:VAL:HG22	1.86	0.57
1:A:25:TRP:HE1	1:A:57:PRO:HG3	1.69	0.57
1:A:259:PHE:CD2	1:A:299:PRO:HB3	2.39	0.57
1:B:365:GLN:HB3	1:B:368:ALA:HB2	1.85	0.57
1:B:536:TYR:CE1	1:B:538:GLU:HB3	2.40	0.57
1:A:137:LEU:HG	1:A:138:PRO:HD3	1.86	0.57
1:B:82:LYS:HB2	1:B:91:TRP:CZ3	2.40	0.57
1:A:192:LEU:HB2	1:A:511:PHE:HZ	1.70	0.56
1:A:451:ARG:HG3	1:A:488:ASP:O	2.04	0.56
1:A:479:ILE:HG21	1:A:484:GLU:CD	2.26	0.56
1:A:510:LEU:HG	1:A:514:TYR:HE1	1.70	0.56
1:B:471:PHE:CE1	1:B:518:ILE:HG12	2.40	0.56
1:B:280:TRP:HE1	1:B:307:SER:HB2	1.70	0.56
1:A:101:PRO:HD2	1:B:424:TRP:CZ3	2.40	0.56
1:B:122:ASP:OD1	1:B:528:ARG:HD2	2.05	0.56
1:A:120:ALA:O	1:A:476:VAL:CG2	2.53	0.56
1:A:2:LEU:HA	1:A:28:GLY:HA3	1.86	0.56
1:A:7:LEU:HD21	1:A:533:GLN:HB2	1.88	0.56
1:B:124:ILE:HG23	1:B:477:PRO:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:O	1:B:190:LYS:HE3	2.06	0.55
1:B:416:ILE:CD1	1:B:421:CYS:HB2	2.36	0.55
1:B:445:ASP:OD2	1:B:452:PHE:HB2	2.05	0.55
1:A:9:VAL:HB	1:A:10:PRO:HD2	1.88	0.55
1:A:414:GLN:HA	1:B:89:GLN:HG2	1.88	0.55
1:B:260:ASP:HB3	1:B:268:GLY:HA3	1.88	0.55
1:A:20:LEU:HD12	1:A:21:LEU:H	1.71	0.55
1:B:292:TRP:CH2	1:B:293:LEU:HD12	2.42	0.55
1:A:211:TYR:HD1	1:A:248:VAL:HG21	1.72	0.55
1:A:119:TRP:O	1:A:120:ALA:HB3	2.07	0.55
1:B:87:ASP:N	1:B:87:ASP:OD1	2.40	0.55
1:B:216:TYR:HD1	1:B:256:HIS:HE2	1.53	0.55
1:A:374:HIS:CB	1:A:378:ALA:HB2	2.36	0.55
1:B:536:TYR:HE1	1:B:538:GLU:HB3	1.69	0.55
1:B:327:PRO:HD2	1:B:328:TRP:CD1	2.42	0.55
1:B:421:CYS:O	1:B:424:TRP:HB3	2.06	0.55
1:A:301:LEU:HB3	1:A:308:LEU:HD21	1.88	0.54
1:A:583:GLY:HA3	1:A:600:THR:HA	1.89	0.54
1:A:382:LEU:HD11	1:A:390:ALA:HB3	1.86	0.54
1:B:282:SER:OG	1:B:302:ASP:HB2	2.07	0.54
1:A:112:VAL:HB	1:A:113:PRO:HD3	1.90	0.54
1:A:251:HIS:HD2	1:A:298:LEU:HD22	1.72	0.54
1:A:424:TRP:CH2	1:B:101:PRO:HG2	2.43	0.54
1:A:464:PRO:O	1:A:468:VAL:HG23	2.08	0.54
1:B:398:PHE:CE1	1:B:409:ILE:HG13	2.43	0.54
1:B:9:VAL:HG21	1:B:531:GLY:H	1.73	0.54
1:B:130:PRO:HB2	1:B:223:PHE:CD2	2.42	0.54
1:B:600:THR:O	1:B:601:VAL:HG23	2.07	0.54
1:A:56:GLN:OE1	1:A:59:PRO:HA	2.08	0.53
1:A:555:VAL:HG12	1:A:556:ALA:N	2.22	0.53
1:B:185:LYS:HG3	1:B:501:TRP:CH2	2.44	0.53
1:A:380:GLN:HA	1:A:383:GLN:HB2	1.91	0.53
1:B:192:LEU:O	1:B:518:ILE:HD12	2.08	0.53
1:A:9:VAL:HG11	1:A:531:GLY:N	2.24	0.53
1:A:213:THR:HG21	1:A:216:TYR:CE2	2.43	0.53
1:B:600:THR:HB	1:B:602:TRP:CH2	2.44	0.53
1:A:396:PHE:O	1:A:400:LEU:CD1	2.57	0.53
1:A:127:GLN:HB3	1:A:480:TYR:HA	1.91	0.53
1:B:115:ILE:HG13	1:B:116:GLY:N	2.24	0.53
1:A:137:LEU:HD12	1:A:138:PRO:CD	2.38	0.53
1:B:409:ILE:HD12	1:B:409:ILE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:GLN:NE2	1:B:446:SER:HB3	2.24	0.53
1:B:451:ARG:NH2	1:B:487:LEU:HD23	2.24	0.53
1:A:119:TRP:CE3	1:A:120:ALA:HB2	2.44	0.52
1:B:129:PHE:CE2	1:B:496:ARG:HG2	2.42	0.52
1:B:186:LEU:HD23	1:B:189:LEU:HD12	1.91	0.52
1:B:434:HIS:HA	1:B:437:GLN:OE1	2.09	0.52
1:B:90:ARG:NH1	1:B:97:PHE:HB3	2.25	0.52
1:B:36:MET:HB3	1:B:47:SER:OG	2.09	0.52
1:A:259:PHE:O	1:A:259:PHE:CG	2.63	0.52
1:B:81:PHE:HB2	1:B:92:PHE:HB3	1.91	0.52
1:A:251:HIS:CD2	1:A:298:LEU:HD22	2.45	0.52
1:B:407:THR:HG21	1:B:455:LEU:HD13	1.91	0.52
1:B:438:LEU:HD13	1:B:529:HIS:HA	1.90	0.52
1:A:15:GLN:OE1	1:A:16:SER:N	2.42	0.52
1:A:183:SER:HA	1:A:186:LEU:HG	1.92	0.52
1:A:130:PRO:HB2	1:A:223:PHE:CE2	2.45	0.52
1:B:147:TYR:CE1	1:B:156:ILE:HD13	2.45	0.52
1:B:245:LEU:O	1:B:333:TRP:HA	2.09	0.52
1:B:251:HIS:CD2	1:B:298:LEU:HB3	2.45	0.52
1:B:412:ASP:N	1:B:413:PRO:CD	2.73	0.52
1:A:380:GLN:HA	1:A:383:GLN:CB	2.40	0.52
1:B:129:PHE:CD2	1:B:496:ARG:HG2	2.45	0.52
1:B:577:GLN:HG2	1:B:579:GLN:CG	2.39	0.52
1:B:260:ASP:OD1	1:B:262:HIS:O	2.28	0.51
1:A:292:TRP:HE1	1:A:337:VAL:HG11	1.74	0.51
1:B:463:LEU:O	1:B:467:VAL:HG23	2.11	0.51
1:A:84:LEU:HD11	1:B:411:TYR:CD2	2.45	0.51
1:B:105:LEU:HD13	1:B:383:GLN:CG	2.39	0.51
1:B:371:VAL:HG13	1:B:390:ALA:HA	1.91	0.51
1:B:93:THR:HG21	1:B:102:PRO:HB3	1.92	0.51
1:B:210:LYS:HD3	1:B:223:PHE:CE2	2.46	0.51
1:B:236:THR:O	1:B:241:MET:N	2.43	0.51
1:B:216:TYR:CB	1:B:319:ILE:HD13	2.41	0.51
1:B:487:LEU:HD12	1:B:488:ASP:N	2.25	0.51
1:A:36:MET:HB2	1:A:82:LYS:HB3	1.93	0.51
1:A:377:ASP:HB3	1:B:104:ARG:CB	2.37	0.51
1:A:550:GLN:C	1:A:552:ARG:NH1	2.64	0.51
1:A:202:VAL:O	1:A:219:VAL:HG13	2.11	0.51
1:A:484:GLU:HG3	1:A:514:TYR:CD2	2.46	0.51
1:A:24:LEU:HD12	1:A:25:TRP:H	1.75	0.51
1:A:211:TYR:HD1	1:A:248:VAL:CG2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ALA:HB1	1:A:24:LEU:HD11	1.93	0.51
1:A:465:LEU:HD11	1:A:597:ILE:HG22	1.93	0.51
1:A:562:ALA:H	1:A:596:ALA:HB2	1.76	0.50
1:A:374:HIS:CG	1:A:378:ALA:CB	2.94	0.50
1:B:261:ARG:CZ	1:B:296:ALA:HB1	2.41	0.50
1:B:149:HIS:HB2	1:B:156:ILE:HG23	1.92	0.50
1:A:174:PHE:CZ	1:A:208:VAL:HA	2.46	0.50
1:A:482:GLY:O	1:A:487:LEU:HB2	2.11	0.50
1:A:338:VAL:HG21	1:A:387:GLU:OE2	2.12	0.50
1:B:135:ARG:HD3	1:B:139:ARG:HD2	1.94	0.50
1:B:429:ARG:HB3	1:B:437:GLN:NE2	2.25	0.50
1:A:335:LEU:HD13	1:A:338:VAL:HG21	1.93	0.50
1:A:452:PHE:HE2	1:A:466:ALA:CB	2.25	0.50
1:B:6:HIS:CE1	1:B:12:PHE:HB3	2.47	0.50
1:B:373:GLU:CD	1:B:375:PHE:HE1	2.15	0.50
1:B:588:THR:HG23	1:B:591:ILE:HB	1.93	0.50
1:B:5:TRP:HZ3	1:B:27:THR:HB	1.77	0.50
1:B:465:LEU:HD13	1:B:557:ILE:HG23	1.93	0.50
1:B:35:ILE:HG23	1:B:83:LEU:HD12	1.93	0.50
1:A:587:LEU:HD13	1:A:592:LEU:HD13	1.94	0.49
1:B:48:VAL:HG12	1:B:66:ALA:HB1	1.94	0.49
1:A:320:VAL:HG21	1:A:357:ILE:CG2	2.38	0.49
1:A:401:TRP:HE3	1:A:407:THR:HG23	1.76	0.49
1:A:11:PRO:HD3	1:A:548:LEU:C	2.32	0.49
1:A:527:LEU:HD21	1:A:553:VAL:CG1	2.39	0.49
1:B:37:LEU:HD22	1:B:66:ALA:HB3	1.92	0.49
1:B:56:GLN:HB2	1:B:61:VAL:O	2.12	0.49
1:B:334:ARG:NH2	1:B:391:MET:SD	2.85	0.49
1:A:398:PHE:N	1:A:399:PRO:CD	2.76	0.49
1:B:213:THR:O	1:B:256:HIS:HD2	1.96	0.49
1:B:562:ALA:HB2	1:B:596:ALA:N	2.28	0.49
1:B:594:LEU:HD22	1:B:598:SER:OG	2.12	0.49
1:A:192:LEU:HB2	1:A:511:PHE:CZ	2.47	0.49
1:A:586:GLN:O	1:A:593:ALA:HB3	2.12	0.49
1:B:277:TRP:CD1	1:B:280:TRP:CZ3	3.00	0.49
1:A:321:ARG:O	1:A:325:LYS:HG2	2.12	0.49
1:A:435:GLN:H	1:A:435:GLN:CD	2.16	0.49
1:B:259:PHE:HB2	1:B:281:TYR:OH	2.13	0.49
1:B:521:ARG:HA	1:B:527:LEU:HD12	1.93	0.49
1:A:20:LEU:HD12	1:A:21:LEU:N	2.28	0.49
1:A:40:GLU:OE1	1:A:78:ARG:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:HB2	1:B:243:LEU:HD12	1.94	0.49
1:B:258:TRP:HA	1:B:277:TRP:CE3	2.47	0.49
1:B:557:ILE:CG2	1:B:558:ASN:N	2.76	0.49
1:A:87:ASP:OD1	1:A:88:ARG:N	2.46	0.48
1:A:321:ARG:CZ	1:A:360:ALA:HB1	2.43	0.48
1:A:349:ASN:O	1:A:352:GLN:HB3	2.13	0.48
1:A:355:ALA:O	1:A:359:GLU:HG3	2.12	0.48
1:A:424:TRP:C	1:A:424:TRP:CD1	2.86	0.48
1:A:562:ALA:N	1:A:596:ALA:HB2	2.28	0.48
1:B:315:GLY:O	1:B:318:SER:HB3	2.13	0.48
1:B:32:PRO:HG3	1:B:83:LEU:CD2	2.39	0.48
1:B:339:HIS:CD2	1:B:340:MET:HG3	2.48	0.48
1:B:384:ALA:HB3	1:B:386:VAL:HG13	1.94	0.48
1:A:380:GLN:C	1:A:382:LEU:N	2.56	0.48
1:B:321:ARG:HB3	1:B:364:THR:OG1	2.13	0.48
1:A:396:PHE:C	1:A:399:PRO:HD2	2.32	0.48
1:B:570:SER:HB3	1:B:573:LEU:HG	1.95	0.48
1:B:577:GLN:O	1:B:604:ASN:HA	2.13	0.48
1:A:200:ASN:HA	1:A:246:ASP:HB2	1.95	0.48
1:A:215:ASP:OD1	1:A:216:TYR:N	2.47	0.48
1:A:461:ALA:O	1:A:464:PRO:HD2	2.13	0.48
1:A:487:LEU:HD12	1:A:488:ASP:H	1.78	0.48
1:B:461:ALA:O	1:B:464:PRO:HD2	2.13	0.48
1:B:492:ASP:N	1:B:493:PRO:CD	2.76	0.48
1:A:221:PRO:HA	1:A:224:GLY:O	2.13	0.48
1:A:382:LEU:CD2	1:A:387:GLU:HB2	2.44	0.48
1:A:577:GLN:HG2	1:A:579:GLN:HE21	1.79	0.48
1:B:160:ASP:OD1	1:B:163:GLU:HG3	2.14	0.48
1:B:361:ALA:HB1	1:B:370:ILE:HD11	1.95	0.48
1:A:186:LEU:N	1:A:187:PRO:CD	2.76	0.48
1:B:186:LEU:HD13	1:B:239:LEU:CD1	2.39	0.48
1:A:277:TRP:HB3	1:A:280:TRP:CG	2.49	0.48
1:B:389:ALA:CB	1:B:439:ARG:O	2.61	0.48
1:A:13:VAL:CG1	1:A:20:LEU:HD11	2.44	0.48
1:A:280:TRP:CZ2	1:A:307:SER:HB2	2.48	0.48
1:A:393:TYR:HB3	1:A:398:PHE:CE2	2.49	0.48
1:A:602:TRP:O	1:A:603:MET:HB2	2.13	0.48
1:B:205:ALA:HB3	1:B:210:LYS:HG3	1.95	0.48
1:A:290:LEU:O	1:A:300:LYS:CB	2.62	0.47
1:B:104:ARG:HG2	1:B:105:LEU:HD23	1.96	0.47
1:B:270:CYS:HB3	1:B:271:HIS:CD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:TRP:CG	1:B:474:PRO:HD2	2.49	0.47
1:A:22:ILE:HG21	1:A:79:TYR:CE2	2.50	0.47
1:A:70:LEU:HD22	1:A:112:VAL:HG11	1.96	0.47
1:A:540:ASN:HB3	1:A:559:ARG:HG3	1.96	0.47
1:B:130:PRO:O	1:B:177:GLY:HA3	2.14	0.47
1:B:283:PHE:CD2	1:B:289:ALA:HB2	2.49	0.47
1:B:432:LEU:HD23	1:B:432:LEU:HA	1.57	0.47
1:A:210:LYS:HE2	1:A:223:PHE:CE1	2.49	0.47
1:A:600:THR:HG21	1:A:602:TRP:CH2	2.49	0.47
1:B:320:VAL:CG2	1:B:357:ILE:HG23	2.43	0.47
1:B:404:LEU:HD13	1:B:466:ALA:HB2	1.96	0.47
1:B:461:ALA:HB1	1:B:597:ILE:HG21	1.96	0.47
1:A:10:PRO:HA	1:A:13:VAL:O	2.13	0.47
1:A:37:LEU:HG	1:A:39:THR:HG23	1.97	0.47
1:A:217:ARG:NH1	1:A:317:ASP:O	2.43	0.47
1:A:250:ASN:CB	1:A:337:VAL:HG23	2.44	0.47
1:A:416:ILE:HD12	1:A:421:CYS:HB2	1.97	0.47
1:A:453:LYS:HA	1:A:456:LEU:HD12	1.95	0.47
1:A:576:VAL:HG13	1:A:577:GLN:HB2	1.97	0.47
1:B:56:GLN:O	1:B:56:GLN:HG2	2.14	0.47
1:B:146:VAL:HG23	1:B:158:LEU:CD1	2.43	0.47
1:A:137:LEU:CG	1:A:138:PRO:HD3	2.43	0.47
1:A:490:LYS:HG3	1:A:494:PHE:HD2	1.79	0.47
1:B:3:ASN:N	1:B:27:THR:O	2.48	0.47
1:B:292:TRP:CZ3	1:B:293:LEU:HD12	2.49	0.47
1:B:393:TYR:HB3	1:B:398:PHE:CE2	2.49	0.47
1:A:50:MET:HA	1:A:66:ALA:HB2	1.97	0.47
1:A:188:TYR:CD2	1:A:501:TRP:HZ3	2.32	0.47
1:A:418:ALA:HB1	1:A:542:VAL:HG22	1.96	0.47
1:A:545:VAL:HA	1:A:553:VAL:O	2.14	0.47
1:B:203:PHE:CZ	1:B:323:TRP:CE2	3.02	0.47
1:B:281:TYR:CE1	1:B:301:LEU:HD23	2.50	0.47
1:B:324:LEU:HD12	1:B:361:ALA:HA	1.96	0.47
1:B:548:LEU:O	1:B:549:ASN:C	2.53	0.47
1:A:369:TYR:HE1	1:A:439:ARG:HB3	1.79	0.47
1:B:217:ARG:NE	1:B:319:ILE:HG12	2.30	0.47
1:B:484:GLU:HG2	1:B:485:VAL:HG13	1.97	0.47
1:A:374:HIS:CG	1:A:378:ALA:HB2	2.48	0.47
1:A:380:GLN:HA	1:A:383:GLN:CG	2.43	0.47
1:B:203:PHE:CE1	1:B:323:TRP:CZ2	3.03	0.47
1:B:281:TYR:CD1	1:B:299:PRO:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:SER:OG	1:B:436:GLN:HG3	2.14	0.47
1:A:26:LEU:HD11	1:A:35:ILE:HD11	1.97	0.47
1:A:137:LEU:CD1	1:A:138:PRO:HD3	2.45	0.47
1:B:213:THR:HG21	1:B:216:TYR:CD1	2.50	0.47
1:B:450:ALA:CB	1:B:490:LYS:O	2.63	0.47
1:B:216:TYR:OH	1:B:248:VAL:O	2.28	0.46
1:B:510:LEU:HA	1:B:510:LEU:HD12	1.60	0.46
1:A:38:ARG:HD3	1:A:91:TRP:CH2	2.51	0.46
1:A:277:TRP:HA	1:A:280:TRP:CD1	2.50	0.46
1:A:391:MET:HB3	1:A:393:TYR:CE1	2.51	0.46
1:B:2:LEU:HD11	1:B:32:PRO:HD2	1.98	0.46
1:A:225:GLY:C	1:A:227:GLY:N	2.68	0.46
1:A:372:GLY:HA3	1:A:387:GLU:OE1	2.15	0.46
1:B:196:ALA:CB	1:B:242:ARG:HB2	2.46	0.46
1:B:201:PRO:HB2	1:B:210:LYS:CB	2.44	0.46
1:B:216:TYR:HB3	1:B:319:ILE:HD13	1.97	0.46
1:B:530:GLY:O	1:B:546:ARG:NH2	2.49	0.46
1:A:159:ARG:HH12	1:A:166:THR:HG23	1.81	0.46
1:A:21:LEU:HD13	1:A:65:ARG:HD3	1.98	0.46
1:B:150:HIS:CE1	1:B:264:ARG:NE	2.83	0.46
1:A:341:LEU:HD23	1:A:341:LEU:C	2.36	0.46
1:A:5:TRP:O	1:A:24:LEU:HD12	2.16	0.46
1:A:524:SER:O	1:A:528:ARG:NH1	2.49	0.46
1:B:229:LEU:HD23	1:B:328:TRP:CZ3	2.51	0.46
1:A:7:LEU:HD11	1:A:572:PHE:CZ	2.51	0.46
1:A:132:ARG:NH1	1:A:496:ARG:O	2.49	0.46
1:B:53:GLN:N	1:B:63:ALA:O	2.48	0.46
1:B:513:LEU:O	1:B:517:MET:HG2	2.15	0.46
1:A:40:GLU:O	1:A:42:ASP:N	2.49	0.45
1:A:119:TRP:CZ3	1:A:120:ALA:HB2	2.51	0.45
1:A:380:GLN:CA	1:A:383:GLN:HG2	2.45	0.45
1:A:488:ASP:N	1:A:488:ASP:OD1	2.49	0.45
1:B:37:LEU:CD2	1:B:66:ALA:HB3	2.46	0.45
1:A:455:LEU:HA	1:A:455:LEU:HD23	1.48	0.45
1:A:192:LEU:HD21	1:A:484:GLU:OE2	2.17	0.45
1:B:491:ASN:HB2	1:B:493:PRO:HD2	1.98	0.45
1:A:137:LEU:HD12	1:A:138:PRO:HD3	1.97	0.45
1:B:15:GLN:HA	1:B:20:LEU:HD12	1.98	0.45
1:B:193:GLY:O	1:B:522:LYS:HE3	2.17	0.45
1:B:228:ALA:HB2	1:B:231:ARG:NH2	2.32	0.45
1:B:337:VAL:O	1:B:337:VAL:CG2	2.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ALA:HB1	1:B:542:VAL:HG23	1.98	0.45
1:A:76:ARG:HG3	1:A:78:ARG:HG3	1.98	0.45
1:A:311:GLU:HG3	1:A:319:ILE:HD12	1.99	0.45
1:B:254:ASP:CG	1:B:297:SER:HA	2.37	0.45
1:B:254:ASP:N	1:B:297:SER:O	2.46	0.45
1:B:272:ASN:ND2	1:B:275:SER:HB2	2.32	0.45
1:A:453:LYS:HG3	1:A:460:ILE:HD13	1.99	0.45
1:A:535:LEU:HB2	1:A:543:VAL:CG1	2.36	0.45
1:B:545:VAL:HG22	1:B:547:VAL:HG22	1.98	0.45
1:A:168:GLN:HG2	1:A:169:ALA:N	2.31	0.45
1:A:193:GLY:HA3	1:A:518:ILE:HG21	1.98	0.45
1:A:207:SER:HG	1:A:209:HIS:CE1	2.35	0.45
1:B:188:TYR:CD2	1:B:189:LEU:HD23	2.52	0.45
1:B:313:TYR:CD1	1:B:357:ILE:CD1	2.99	0.45
1:B:521:ARG:NH1	1:B:527:LEU:O	2.50	0.45
1:A:44:GLU:O	1:A:44:GLU:HG3	2.17	0.44
1:A:199:LEU:CB	1:A:245:LEU:HD23	2.48	0.44
1:A:112:VAL:CB	1:A:113:PRO:HD3	2.47	0.44
1:B:2:LEU:HD11	1:B:32:PRO:CD	2.47	0.44
1:B:285:ASP:C	1:B:287:GLY:H	2.21	0.44
1:B:303:TYR:CZ	1:B:341:LEU:HD11	2.53	0.44
1:A:44:GLU:O	1:A:45:GLU:C	2.54	0.44
1:B:10:PRO:HB3	1:B:14:LYS:HG2	1.98	0.44
1:B:249:PHE:CE2	1:B:320:VAL:HG22	2.52	0.44
1:B:527:LEU:HD21	1:B:553:VAL:HG11	1.98	0.44
1:B:545:VAL:HG22	1:B:547:VAL:CG2	2.47	0.44
1:A:403:PHE:HB2	1:A:416:ILE:HD11	2.00	0.44
1:B:19:GLN:CD	1:B:67:ALA:HB1	2.37	0.44
1:B:126:TYR:CZ	1:B:481:TYR:HA	2.53	0.44
1:B:217:ARG:CZ	1:B:319:ILE:HG12	2.48	0.44
1:A:545:VAL:O	1:A:545:VAL:HG13	2.18	0.44
1:A:555:VAL:HG12	1:A:556:ALA:H	1.82	0.44
1:A:82:LYS:HE2	1:A:89:GLN:NE2	2.33	0.44
1:B:190:LYS:HE2	1:B:239:LEU:HD13	1.99	0.44
1:B:303:TYR:HB3	1:B:353:HIS:NE2	2.32	0.44
1:A:9:VAL:O	1:A:13:VAL:HG23	2.17	0.44
1:B:492:ASP:N	1:B:493:PRO:HD2	2.33	0.44
1:A:185:LYS:HE3	1:A:501:TRP:CE3	2.52	0.44
1:B:303:TYR:HB3	1:B:353:HIS:CD2	2.53	0.44
1:A:380:GLN:O	1:A:381:TRP:C	2.55	0.44
1:B:465:LEU:HA	1:B:599:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:TRP:HE1	1:A:27:THR:HG21	1.83	0.43
1:A:260:ASP:HB3	1:A:268:GLY:HA3	2.00	0.43
1:A:480:TYR:CE1	1:A:481:TYR:CE2	3.06	0.43
1:B:396:PHE:O	1:B:400:LEU:HD13	2.18	0.43
1:A:397:THR:HG22	1:A:401:TRP:NE1	2.33	0.43
1:B:117:PRO:HG2	1:B:439:ARG:CD	2.47	0.43
1:B:567:LEU:HA	1:B:568:PRO:HD2	1.89	0.43
1:A:84:LEU:CD1	1:B:411:TYR:CD2	3.01	0.43
1:B:118:GLN:C	1:B:120:ALA:H	2.22	0.43
1:B:204:LYS:HD2	1:B:221:PRO:HD3	1.99	0.43
1:A:584:HIS:HB2	1:A:595:PRO:HG2	2.00	0.43
1:B:196:ALA:HB2	1:B:242:ARG:HB2	2.00	0.43
1:B:246:ASP:OD1	1:B:334:ARG:O	2.36	0.43
1:A:33:GLN:HG3	1:A:34:ARG:HG2	2.01	0.43
1:A:302:ASP:OD1	1:A:304:GLN:HB2	2.18	0.43
1:A:315:GLY:O	1:A:318:SER:N	2.51	0.43
1:A:413:PRO:HB3	1:B:87:ASP:O	2.18	0.43
1:A:484:GLU:HA	1:A:514:TYR:CE1	2.53	0.43
1:B:456:LEU:HD23	1:B:456:LEU:HA	1.83	0.43
1:B:469:TRP:HD1	1:B:473:TRP:HB2	1.82	0.43
1:B:530:GLY:H	1:B:546:ARG:HH21	1.67	0.43
1:A:149:HIS:CD2	1:A:206:PRO:HB2	2.53	0.43
1:A:441:PHE:HD2	1:A:443:GLN:HE21	1.67	0.43
1:A:464:PRO:O	1:A:467:VAL:N	2.51	0.43
1:B:2:LEU:HA	1:B:28:GLY:HA3	1.99	0.43
1:B:117:PRO:HG3	1:B:369:TYR:HA	2.01	0.43
1:B:465:LEU:HD13	1:B:557:ILE:CG2	2.48	0.43
1:B:492:ASP:O	1:B:496:ARG:CD	2.67	0.43
1:A:309:VAL:HG13	1:A:313:TYR:CE2	2.53	0.43
1:B:465:LEU:HD23	1:B:599:ALA:HB2	1.99	0.43
1:B:7:LEU:HD11	1:B:533:GLN:HB2	1.99	0.43
1:B:117:PRO:HG2	1:B:439:ARG:HD2	2.01	0.43
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.87	0.43
1:A:200:ASN:HB3	1:A:201:PRO:HD2	2.00	0.43
1:A:262:HIS:C	1:A:264:ARG:N	2.72	0.43
1:A:335:LEU:HD11	1:A:370:ILE:HG22	2.01	0.43
1:B:92:PHE:HE1	1:B:96:GLY:HA2	1.83	0.43
1:A:75:PRO:CB	1:A:113:PRO:HD2	2.49	0.43
1:A:118:GLN:C	1:A:119:TRP:O	2.51	0.43
1:A:120:ALA:O	1:A:476:VAL:HG21	2.18	0.43
1:A:251:HIS:HA	1:A:301:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ARG:O	1:B:175:TYR:HA	2.19	0.43
1:B:233:ARG:HA	1:B:233:ARG:HD2	1.69	0.43
1:B:281:TYR:CE1	1:B:299:PRO:HB2	2.54	0.43
1:B:403:PHE:CZ	1:B:559:ARG:HG2	2.53	0.43
1:A:44:GLU:HB2	1:B:340:MET:CE	2.49	0.42
1:A:536:TYR:CE2	1:A:565:VAL:HG13	2.54	0.42
1:A:290:LEU:O	1:A:300:LYS:N	2.42	0.42
1:A:343:GLU:OE1	1:A:349:ASN:OD1	2.36	0.42
1:A:173:THR:O	1:A:208:VAL:HG21	2.18	0.42
1:A:451:ARG:HG3	1:A:488:ASP:C	2.40	0.42
1:B:114:ASP:OD1	1:B:115:ILE:N	2.53	0.42
1:A:313:TYR:CD2	1:A:357:ILE:HG13	2.55	0.42
1:A:424:TRP:HD1	1:A:424:TRP:O	2.02	0.42
1:A:522:LYS:O	1:A:528:ARG:NH1	2.52	0.42
1:A:536:TYR:CE2	1:A:565:VAL:CG1	3.03	0.42
1:A:13:VAL:HG13	1:A:20:LEU:HD11	2.02	0.42
1:B:11:PRO:O	1:B:14:LYS:HG3	2.19	0.42
1:A:192:LEU:HD13	1:A:511:PHE:CE1	2.54	0.42
1:A:1:MET:HG2	1:A:2:LEU:N	2.34	0.42
1:A:79:TYR:CZ	1:A:108:PHE:HB2	2.55	0.42
1:A:586:GLN:HG3	1:A:593:ALA:HB3	2.01	0.42
1:A:398:PHE:CZ	1:A:409:ILE:HG13	2.55	0.42
1:B:473:TRP:CD1	1:B:474:PRO:HD2	2.54	0.42
1:B:562:ALA:HB2	1:B:596:ALA:H	1.85	0.42
1:A:303:TYR:CB	1:A:353:HIS:CD2	3.03	0.42
1:B:98:SER:OG	1:B:99:ARG:N	2.53	0.42
1:B:178:ASP:O	1:B:182:ILE:HG13	2.20	0.42
1:B:193:GLY:HA3	1:B:518:ILE:HG21	2.02	0.42
1:B:351:MET:SD	1:B:386:VAL:HG21	2.59	0.42
1:B:491:ASN:CB	1:B:493:PRO:HD2	2.50	0.42
1:B:554:LEU:HD23	1:B:602:TRP:CE3	2.55	0.42
1:A:290:LEU:O	1:A:300:LYS:HB3	2.19	0.41
1:A:369:TYR:O	1:A:370:ILE:HD13	2.20	0.41
1:A:480:TYR:CE1	1:A:481:TYR:CD2	3.08	0.41
1:B:270:CYS:HG	1:B:271:HIS:CE1	2.38	0.41
1:A:33:GLN:HG2	1:A:84:LEU:O	2.20	0.41
1:A:586:GLN:CG	1:A:593:ALA:HB3	2.50	0.41
1:B:147:TYR:CD1	1:B:156:ILE:HG12	2.55	0.41
1:A:122:ASP:HA	1:A:528:ARG:HD2	2.02	0.41
1:A:186:LEU:HD23	1:A:186:LEU:HA	1.78	0.41
1:A:489:GLY:HA2	1:A:497:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:TYR:C	1:A:518:ILE:HD12	2.41	0.41
1:B:493:PRO:HG2	1:B:494:PHE:CZ	2.55	0.41
1:B:20:LEU:N	1:B:70:LEU:HD11	2.35	0.41
1:B:313:TYR:CD1	1:B:357:ILE:HD11	2.55	0.41
1:B:552:ARG:HB3	1:B:578:TRP:CH2	2.55	0.41
1:A:396:PHE:CG	1:A:442:ASN:HB3	2.56	0.41
1:B:117:PRO:HG3	1:B:369:TYR:CD1	2.51	0.41
1:A:233:ARG:HD3	1:A:330:MET:SD	2.61	0.41
1:B:89:GLN:O	1:B:89:GLN:HG3	2.21	0.41
1:B:110:VAL:HG12	1:B:112:VAL:HG23	2.02	0.41
1:B:213:THR:O	1:B:256:HIS:CD2	2.72	0.41
1:B:214:GLU:HG2	1:B:214:GLU:O	2.20	0.41
1:A:174:PHE:CE2	1:A:208:VAL:HA	2.56	0.41
1:A:202:VAL:O	1:A:219:VAL:HA	2.21	0.41
1:A:234:HIS:HA	1:A:237:GLN:CD	2.41	0.41
1:A:438:LEU:C	1:A:475:GLY:HA2	2.41	0.41
1:B:256:HIS:ND1	1:B:257:ALA:N	2.69	0.41
1:A:27:THR:HB	1:A:61:VAL:HG22	2.03	0.41
1:A:548:LEU:HD12	1:A:548:LEU:HA	1.98	0.41
1:B:600:THR:CG2	1:B:602:TRP:CZ2	3.04	0.41
1:A:532:CYS:HB2	1:A:546:ARG:HD2	2.02	0.41
1:B:8:PRO:HA	1:B:13:VAL:CG2	2.47	0.41
1:B:123:GLN:O	1:B:124:ILE:HD13	2.21	0.41
1:B:191:LYS:HG2	1:B:511:PHE:HZ	1.85	0.41
1:B:384:ALA:CB	1:B:386:VAL:HG13	2.51	0.41
1:A:25:TRP:NE1	1:A:57:PRO:HG3	2.34	0.41
1:A:243:LEU:HD12	1:A:243:LEU:HA	1.75	0.41
1:A:268:GLY:O	1:A:272:ASN:HB3	2.20	0.41
1:A:473:TRP:CD2	1:A:474:PRO:HD2	2.55	0.41
1:A:562:ALA:HB1	1:A:594:LEU:O	2.21	0.41
1:B:84:LEU:HD23	1:B:84:LEU:HA	1.59	0.41
1:B:313:TYR:CE1	1:B:357:ILE:HD11	2.56	0.41
1:A:369:TYR:OH	1:A:439:ARG:O	2.29	0.40
1:A:585:GLY:CA	1:A:593:ALA:O	2.69	0.40
1:B:37:LEU:HB3	1:B:48:VAL:HB	2.03	0.40
1:B:26:LEU:HD12	1:B:64:TRP:HE1	1.87	0.40
1:B:213:THR:HB	1:B:216:TYR:CE1	2.56	0.40
1:A:357:ILE:O	1:A:360:ALA:N	2.54	0.40
1:A:468:VAL:HG21	1:A:599:ALA:HB3	2.04	0.40
1:B:2:LEU:HD13	1:B:30:ASP:O	2.20	0.40
1:B:46:MET:HE2	1:B:46:MET:HB3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:TRP:CD1	1:B:280:TRP:HZ3	2.40	0.40
1:B:273:PRO:HA	1:B:278:ARG:HD3	2.03	0.40
1:B:321:ARG:HH22	1:B:363:GLU:CD	2.25	0.40
1:B:328:TRP:CD1	1:B:328:TRP:N	2.88	0.40
1:B:425:MET:HE2	1:B:473:TRP:CE2	2.55	0.40
1:A:200:ASN:HB3	1:A:201:PRO:CD	2.52	0.40
1:B:211:TYR:O	1:B:248:VAL:HG11	2.20	0.40
1:B:230:LEU:HD21	1:B:328:TRP:CD2	2.57	0.40
1:B:514:TYR:O	1:B:515:GLN:C	2.60	0.40
1:B:182:ILE:HG21	1:B:232:LEU:HD21	2.04	0.40
1:B:564:GLU:HA	1:B:592:LEU:O	2.21	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	602/615 (98%)	520 (86%)	81 (14%)	1 (0%)	47	77
1	B	602/615 (98%)	531 (88%)	69 (12%)	2 (0%)	41	71
All	All	1204/1230 (98%)	1051 (87%)	150 (12%)	3 (0%)	47	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	130	PRO
1	A	397	THR
1	B	413	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	508/516 (98%)	503 (99%)	5 (1%)	76	86
1	B	508/516 (98%)	493 (97%)	15 (3%)	41	68
All	All	1016/1032 (98%)	996 (98%)	20 (2%)	55	76

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	GLU
1	A	162	ASP
1	A	286	ASP
1	A	334	ARG
1	A	441	PHE
1	B	53	GLN
1	B	129	PHE
1	B	130	PRO
1	B	139	ARG
1	B	183	SER
1	B	198	TYR
1	B	210	LYS
1	B	217	ARG
1	B	252	SER
1	B	334	ARG
1	B	366	PRO
1	B	449	THR
1	B	484	GLU
1	B	496	ARG
1	B	600	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	443	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 monosaccharides 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

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	604/615 (98%)	0.49	29 (4%) 30 28	61, 119, 160, 226	0
1	B	604/615 (98%)	0.51	40 (6%) 18 18	58, 117, 163, 213	0
All	All	1208/1230 (98%)	0.50	69 (5%) 23 23	58, 118, 162, 226	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144	ASP	4.5
1	A	264	ARG	3.9
1	B	166	THR	3.8
1	B	156	ILE	3.7
1	B	565	VAL	3.7
1	B	25	TRP	3.4
1	A	565	VAL	3.4
1	B	157	ILE	3.2
1	A	475	GLY	3.1
1	A	144	ASP	3.0
1	A	145	HIS	3.0
1	A	572	PHE	3.0
1	A	146	VAL	3.0
1	A	154	GLN	3.0
1	B	225	GLY	2.8
1	A	576	VAL	2.8
1	B	148	TYR	2.8
1	B	21	LEU	2.8
1	B	264	ARG	2.7
1	A	335	LEU	2.7
1	B	20	LEU	2.7
1	B	336	ASP	2.7
1	B	172	SER	2.6
1	A	478	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	222	GLN	2.6
1	B	266	THR	2.6
1	B	578	TRP	2.6
1	A	442	ASN	2.6
1	B	11	PRO	2.5
1	B	173	THR	2.5
1	B	81	PHE	2.5
1	B	67	ALA	2.4
1	B	559	ARG	2.4
1	B	404	LEU	2.4
1	B	277	TRP	2.3
1	B	358	THR	2.3
1	B	52	LYS	2.3
1	B	571	PRO	2.2
1	A	494	PHE	2.2
1	B	357	ILE	2.2
1	B	158	LEU	2.2
1	A	101	PRO	2.2
1	B	206	PRO	2.2
1	A	158	LEU	2.2
1	A	484	GLU	2.2
1	A	172	SER	2.2
1	A	590	GLY	2.2
1	A	83	LEU	2.2
1	B	223	PHE	2.2
1	A	157	ILE	2.2
1	A	20	LEU	2.2
1	B	361	ALA	2.2
1	B	246	ASP	2.1
1	B	200	ASN	2.1
1	B	478	CYS	2.1
1	A	165	VAL	2.1
1	B	85	TRP	2.1
1	B	155	GLU	2.1
1	A	33	GLN	2.1
1	B	392	ASN	2.1
1	B	211	TYR	2.1
1	B	333	TRP	2.1
1	B	24	LEU	2.1
1	A	66	ALA	2.0
1	A	173	THR	2.0
1	A	592	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	97	PHE	2.0
1	A	276	PRO	2.0
1	B	222	GLN	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 monosaccharides 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.