



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:38 PM UTC

PDB ID : 7VT9 / pdb_00007vt9
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

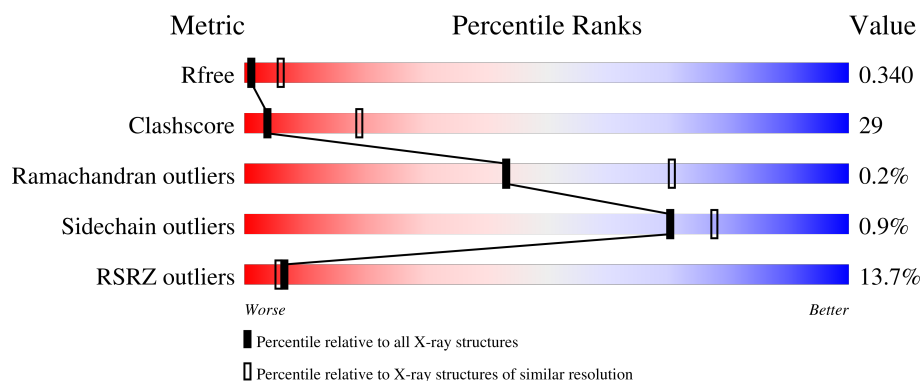
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	14% 50% 46% ..
1	B	615	13% 45% 52% ..

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

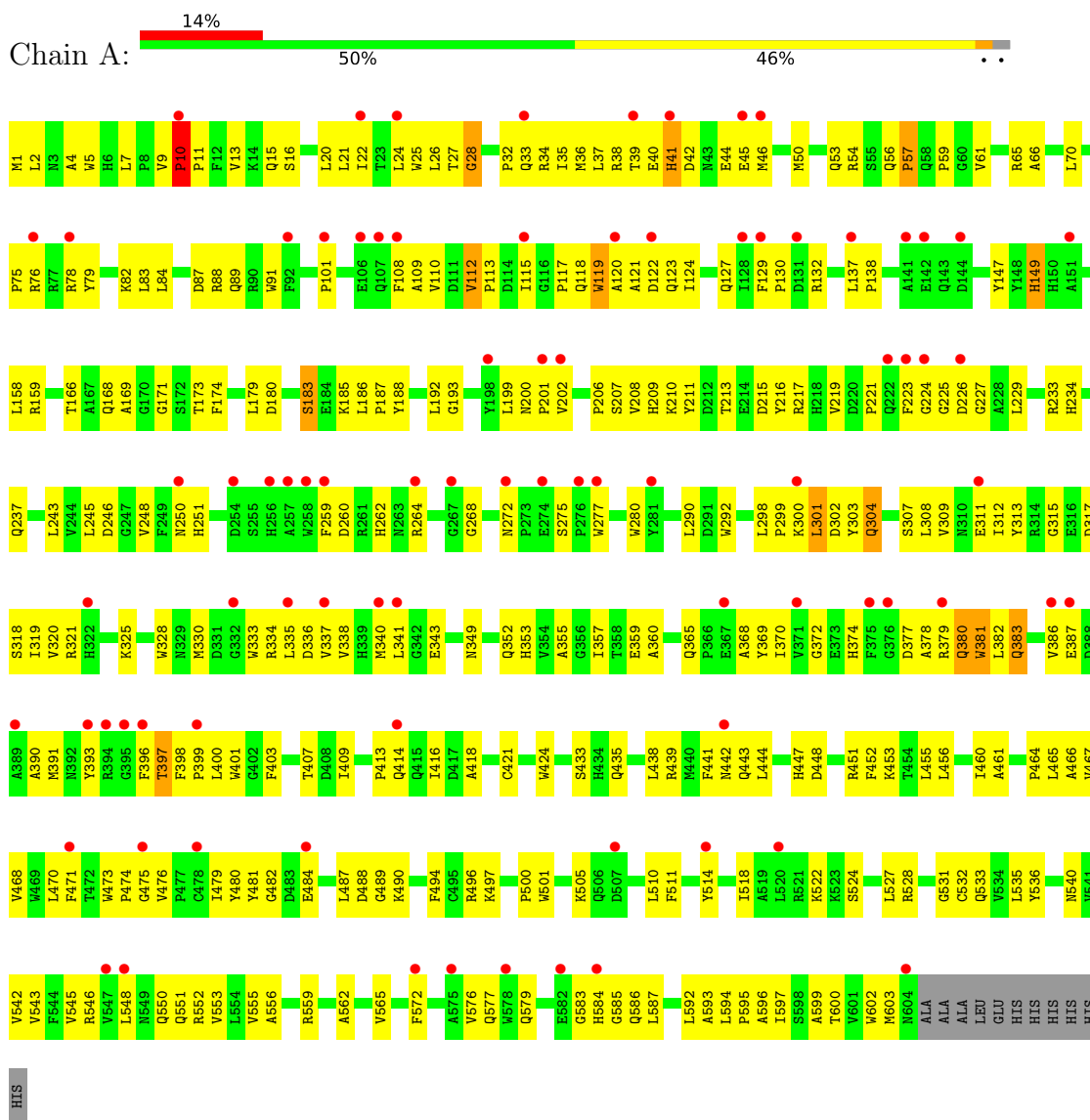
- Molecule 2 is water.

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

3 Residue-property plots

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) 98.1 (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 0.302 , 0.340	Depositor DCC
R_{free} test set	1992 reflections (4.65%)	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)	0.36 , 98.8	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	0.87	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	0.79	0/5029	1.16	26/6846 (0.4%)
1	B	0.78	0/5029	1.14	14/6846 (0.2%)
All	All	0.78	0/10058	1.15	40/13692 (0.3%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	TRP	N-CA-C	-11.51	97.02	111.75
1	B	286	ASP	N-CA-C	-9.75	102.63	112.97
1	A	119	TRP	N-CA-C	-8.90	98.84	110.33
1	B	75	PRO	N-CA-C	7.79	126.40	113.78
1	A	226	ASP	N-CA-C	-7.66	103.03	112.38
1	A	121	ALA	N-CA-C	-7.60	103.11	113.30
1	B	75	PRO	CB-CA-C	-7.09	101.21	113.20
1	A	275	SER	N-CA-C	-7.07	100.66	109.64
1	A	312	ILE	CA-C-N	-6.59	108.95	121.54
1	A	312	ILE	C-N-CA	-6.59	108.95	121.54
1	A	57	PRO	CB-CA-C	-6.28	103.08	113.06
1	B	550	GLN	N-CA-C	6.19	120.03	112.23
1	A	41	HIS	N-CA-C	-6.16	97.67	110.80
1	A	57	PRO	N-CA-C	6.00	122.04	113.47
1	B	208	VAL	N-CA-C	-6.00	107.08	112.12
1	A	129	PHE	CB-CA-C	5.93	115.78	110.44
1	A	147	TYR	CA-CB-CG	5.90	124.52	113.90
1	A	28	GLY	N-CA-C	5.78	118.38	110.69
1	A	183	SER	N-CA-C	-5.62	105.92	112.89
1	A	180	ASP	N-CA-C	-5.57	106.33	113.23
1	B	549	ASN	N-CA-C	-5.57	98.94	110.80
1	A	10	PRO	N-CA-C	5.56	117.48	110.70
1	B	385	ASP	CA-C-N	-5.54	113.54	121.52
1	B	385	ASP	C-N-CA	-5.54	113.54	121.52
1	B	255	SER	CA-C-N	5.52	128.94	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	SER	C-N-CA	5.52	128.94	120.82
1	A	117	PRO	N-CA-C	-5.46	101.21	112.47
1	A	379	ARG	CA-C-N	5.29	128.36	120.31
1	A	379	ARG	C-N-CA	5.29	128.36	120.31
1	B	313	TYR	N-CA-C	5.29	120.21	113.18
1	A	380	GLN	N-CA-C	5.28	117.94	111.82
1	A	448	ASP	N-CA-C	-5.13	106.71	113.17
1	A	119	TRP	CA-C-O	-5.12	116.25	122.03
1	A	149	HIS	CA-C-O	-5.11	116.49	122.37
1	B	242	ARG	O-C-N	-5.08	117.29	123.29
1	A	304	GLN	N-CA-C	-5.05	105.85	111.36
1	A	383	GLN	CA-CB-CG	5.03	124.16	114.10
1	B	583	GLY	CA-C-O	-5.02	118.22	122.29
1	B	130	PRO	N-CA-CB	-5.02	97.98	103.25
1	A	301	LEU	N-CA-CB	5.00	118.42	110.57

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	4880	4672	4672	273	0
1	B	4880	4672	4672	285	0
2	A	1	0	0	0	0
All	All	9761	9344	9344	549	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 29.

All (549) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:HB2	1:B:340:MET:HE2	1.59	0.85
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:328:TRP:HB3	1:B:330:MET:HE2	1.81	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:10:PRO:O	1:A:11:PRO:C	2.41	0.62
1:A:192:LEU:HD13	1:A:511:PHE:CZ	2.35	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:A:479:ILE:HG21	1:A:484:GLU:CD	2.26	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
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:41:HIS:CB	1:A:46:MET:HE3	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ALA:HB2	1:A:596:ALA:N	2.18	0.58
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:328:TRP:HB3	1:A:330:MET:HE2	1.85	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: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:A:550:GLN:C	1:A:552:ARG:NH1	2.64	0.56
1:B:124:ILE:HG23	1:B:477:PRO:HG2	1.88	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:373:GLU:CD	1:B:375:PHE:HE1	2.15	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:11:PRO:HD3	1:A:548:LEU:C	2.32	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:435:GLN:CD	1:A:435:GLN:H	2.16	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:A:424:TRP:C	1:A:424:TRP:CD1	2.86	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:C	1:A:399:PRO:HD2	2.32	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
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:A:380:GLN:C	1:A:382:LEU:N	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:PHE:HB2	1:B:92:PHE:HB3	1.91	0.52
1:A:41:HIS:HB3	1:A:46:MET:HE3	1.90	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:548:LEU:O	1:B:549:ASN:C	2.53	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:202:VAL:O	1:A:219:VAL:HG13	2.11	0.51
1:A:341:LEU:HD23	1:A:341:LEU:C	2.36	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:254:ASP:CG	1:B:297:SER:HA	2.37	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: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:285:ASP:C	1:B:287:GLY:H	2.21	0.49
1:B:594:LEU:HD22	1:B:598:SER:OG	2.12	0.49
1:A:44:GLU:O	1:A:45:GLU:C	2.54	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:B:19:GLN:CD	1:B:67:ALA:HB1	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ALA:O	1:A:359:GLU:HG3	2.12	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:O	1:A:381:TRP:C	2.55	0.48
1:B:321:ARG:HB3	1:B:364:THR:OG1	2.13	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:118:GLN:C	1:B:120:ALA:H	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLN:C	1:A:119:TRP:O	2.51	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:225:GLY:C	1:A:227:GLY:N	2.68	0.47
1:A:418:ALA:HB1	1:A:542:VAL:HG22	1.96	0.47
1:A:451:ARG:HG3	1:A:488:ASP:C	2.40	0.47
1:A:545:VAL:HA	1:A:553:VAL:O	2.14	0.47
1:A:551:GLN:HE21	1:A:603:MET:HE3	1.80	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: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:262:HIS:C	1:A:264:ARG:N	2.72	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:438:LEU:C	1:A:475:GLY:HA2	2.41	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:514:TYR:C	1:A:518:ILE:HD12	2.41	0.45
1:A:380:GLN:CA	1:A:383:GLN:HG2	2.45	0.45
1:B:37:LEU:CD2	1:B:66:ALA:HB3	2.46	0.45
1:A:211:TYR:OH	1:A:246:ASP:OD2	2.29	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:B:581:LYS:HE3	1:B:603:MET:HE2	1.97	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:321:ARG:HH22	1:B:363:GLU:CD	2.25	0.45
1:B:337:VAL:O	1:B:337:VAL:CG2	2.62	0.45
1:B:418:ALA:HB1	1:B:542:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:488:ASP:N	1:A:488:ASP:OD1	2.49	0.45
1:B:514:TYR:O	1:B:515:GLN:C	2.60	0.45
1:A:234:HIS:HA	1:A:237:GLN:CD	2.41	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: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:B:412:ASP:O	1:B:413:PRO:C	2.59	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:303:TYR:CZ	1:B:341:LEU:HD11	2.53	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: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:219:VAL:HB	1:B:225:GLY:C	2.43	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:B:465:LEU:HA	1:B:599:ALA:HB2	2.00	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:192:LEU:HD21	1:A:484:GLU:CD	2.43	0.43
1:A:336:ASP:O	1:A:337:VAL:C	2.61	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:204:LYS:HD2	1:B:221:PRO:HD3	1.99	0.43
1:A:207:SER:HG	1:A:209:HIS:CE1	2.37	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: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:B:286:ASP:C	1:B:288:THR:H	2.27	0.43
1:A:75:PRO:CB	1:A:113:PRO:HD2	2.49	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
1:B:46:MET:HB3	1:B:46:MET:HE2	1.67	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: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:369:TYR:C	1:A:370:ILE:HD13	2.44	0.42
1:A:173:THR:O	1:A:208:VAL:HG21	2.18	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:B:398:PHE:O	1:B:399:PRO:C	2.62	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:53:GLN:O	1:A:54:ARG:C	2.63	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:C	1:B:493:PRO:HD2	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLY:HA2	1:A:497:LYS:NZ	2.35	0.41
1:B:493:PRO:HG2	1:B:494:PHE:CZ	2.55	0.41
1:A:374:HIS:HE2	1:A:381:TRP:CG	2.38	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:A:424:TRP:C	1:A:424:TRP:HD1	2.29	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:O	1:B:214:GLU:HG2	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: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:292:TRP:CD1	1:A:340:MET:HE1	2.56	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:287:GLY:O	1:B:288:THR:C	2.64	0.41
1:B:384:ALA:CB	1:B:386:VAL:HG13	2.51	0.41
1:B:480:TYR:O	1:B:481:TYR:C	2.63	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: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:118:GLN:C	1:B:120:ALA:N	2.79	0.40
1:A:109:ALA:C	1:A:110:VAL:HG23	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:328:TRP:CD1	1:B:328:TRP:N	2.88	0.40
1:A:188:TYR:CD1	1:A:188:TYR:C	2.98	0.40
1:A:200:ASN:HB3	1:A:201:PRO:CD	2.52	0.40
1:B:1:MET:O	1:B:2:LEU:C	2.64	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:182:ILE:HG21	1:B:232:LEU:HD21	2.04	0.40
1:B:425:MET:HE2	1:B:425:MET:HB3	1.86	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%)	43	71
1	B	602/615 (98%)	531 (88%)	69 (12%)	2 (0%)	36	65
All	All	1204/1230 (98%)	1051 (87%)	150 (12%)	3 (0%)	43	71

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%)	505 (99%)	3 (1%)	78	81
1	B	508/516 (98%)	502 (99%)	6 (1%)	63	75
All	All	1016/1032 (98%)	1007 (99%)	9 (1%)	70	78

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PRO
1	A	112	VAL
1	A	334	ARG
1	B	58	GLN
1	B	130	PRO
1	B	366	PRO
1	B	449	THR
1	B	476	VAL
1	B	600	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	352	GLN
1	A	515	GLN
1	B	3	ASN
1	B	123	GLN
1	B	222	GLN
1	B	365	GLN
1	B	491	ASN
1	B	584	HIS
1	B	604	ASN

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

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%)	0.98	84 (13%) 6 5	46, 97, 136, 201	0
1	B	604/615 (98%)	1.00	81 (13%) 7 6	39, 93, 143, 204	0
All	All	1208/1230 (98%)	0.99	165 (13%) 6 5	39, 95, 139, 204	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	PHE	8.0
1	A	484	GLU	7.4
1	A	335	LEU	5.8
1	B	483	ASP	5.4
1	B	295	TYR	4.9
1	B	223	PHE	4.9
1	B	361	ALA	4.8
1	B	211	TYR	4.8
1	B	410	SER	4.7
1	B	222	GLN	4.7
1	B	333	TRP	4.5
1	B	358	THR	4.5
1	A	222	GLN	4.2
1	A	340	MET	4.2
1	A	548	LEU	4.2
1	B	25	TRP	4.1
1	A	311	GLU	3.9
1	B	277	TRP	3.9
1	B	38	ARG	3.8
1	A	276	PRO	3.8
1	A	106	GLU	3.8
1	A	257	ALA	3.8
1	B	200	ASN	3.8
1	A	578	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	492	ASP	3.7
1	A	376	GLY	3.7
1	B	411	TYR	3.7
1	A	131	ASP	3.7
1	A	258	TRP	3.6
1	B	488	ASP	3.6
1	B	202	VAL	3.6
1	B	264	ARG	3.5
1	B	475	GLY	3.5
1	A	386	VAL	3.5
1	A	604	ASN	3.5
1	B	144	ASP	3.5
1	A	226	ASP	3.4
1	A	393	TYR	3.4
1	B	224	GLY	3.4
1	A	256	HIS	3.4
1	A	46	MET	3.3
1	A	10	PRO	3.3
1	B	206	PRO	3.3
1	B	357	ILE	3.2
1	A	572	PHE	3.2
1	A	584	HIS	3.2
1	A	442	ASN	3.2
1	B	74	GLN	3.2
1	A	201	PRO	3.2
1	A	396	PHE	3.2
1	A	379	ARG	3.2
1	B	225	GLY	3.2
1	B	276	PRO	3.2
1	B	53	GLN	3.2
1	A	367	GLU	3.1
1	B	337	VAL	3.1
1	B	584	HIS	3.1
1	A	115	ILE	3.0
1	B	400	LEU	3.0
1	A	41	HIS	3.0
1	A	78	ARG	3.0
1	A	198	TYR	3.0
1	B	336	ASP	3.0
1	B	109	ALA	2.9
1	A	267	GLY	2.9
1	B	213	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	115	ILE	2.9
1	B	290	LEU	2.9
1	B	480	TYR	2.9
1	A	76	ARG	2.9
1	B	156	ILE	2.9
1	A	272	ASN	2.8
1	B	230	LEU	2.8
1	B	479	ILE	2.8
1	A	337	VAL	2.8
1	A	274	GLU	2.8
1	B	559	ARG	2.8
1	A	322	HIS	2.7
1	B	266	THR	2.7
1	B	342	GLY	2.7
1	B	389	ALA	2.7
1	B	576	VAL	2.7
1	A	582	GLU	2.7
1	A	24	LEU	2.7
1	B	215	ASP	2.7
1	B	396	PHE	2.6
1	A	478	CYS	2.6
1	A	341	LEU	2.6
1	B	14	LYS	2.6
1	A	259	PHE	2.6
1	A	389	ALA	2.6
1	B	604	ASN	2.6
1	A	141	ALA	2.5
1	B	265	GLY	2.5
1	B	161	TRP	2.5
1	A	264	ARG	2.5
1	A	394	ARG	2.5
1	A	520	LEU	2.5
1	B	143	GLN	2.5
1	A	137	LEU	2.5
1	B	335	LEU	2.5
1	A	144	ASP	2.4
1	A	300	LYS	2.4
1	B	137	LEU	2.4
1	A	120	ALA	2.4
1	A	471	PHE	2.4
1	A	101	PRO	2.4
1	A	202	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	547	VAL	2.4
1	B	188	TYR	2.4
1	B	320	VAL	2.4
1	A	92	PHE	2.4
1	B	412	ASP	2.4
1	B	339	HIS	2.4
1	A	277	TRP	2.4
1	B	247	GLY	2.4
1	B	351	MET	2.4
1	A	375	PHE	2.3
1	A	371	VAL	2.3
1	B	157	ILE	2.3
1	A	332	GLY	2.3
1	B	381	TRP	2.3
1	B	172	SER	2.3
1	A	224	GLY	2.3
1	A	395	GLY	2.3
1	B	390	ALA	2.3
1	A	39	THR	2.3
1	A	33	GLN	2.3
1	B	370	ILE	2.2
1	B	243	LEU	2.2
1	B	578	TRP	2.2
1	A	108	PHE	2.2
1	B	494	PHE	2.2
1	A	250	ASN	2.2
1	A	254	ASP	2.2
1	A	575	ALA	2.2
1	B	409	ILE	2.2
1	B	317	ASP	2.2
1	B	448	ASP	2.2
1	A	151	ALA	2.2
1	A	22	ILE	2.1
1	A	142	GLU	2.1
1	A	122	ASP	2.1
1	A	507	ASP	2.1
1	A	128	ILE	2.1
1	A	281	TYR	2.1
1	B	37	LEU	2.1
1	B	334	ARG	2.1
1	B	408	ASP	2.1
1	A	514	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	475	GLY	2.1
1	A	129	PHE	2.1
1	B	29	GLU	2.1
1	B	117	PRO	2.1
1	B	359	GLU	2.1
1	B	147	TYR	2.1
1	A	107	GLN	2.1
1	B	534	VAL	2.0
1	B	67	ALA	2.0
1	B	481	TYR	2.0
1	A	414	GLN	2.0
1	A	399	PRO	2.0
1	B	210	LYS	2.0
1	A	45	GLU	2.0
1	A	387	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.