



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 03:13 AM JST

PDB ID : 7EKU
Title : Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme (W958A)
Authors : Shen, M.; Xiang, S.
Deposited on : 2021-04-06
Resolution : 3.10 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 : 2.36
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) : 2.36

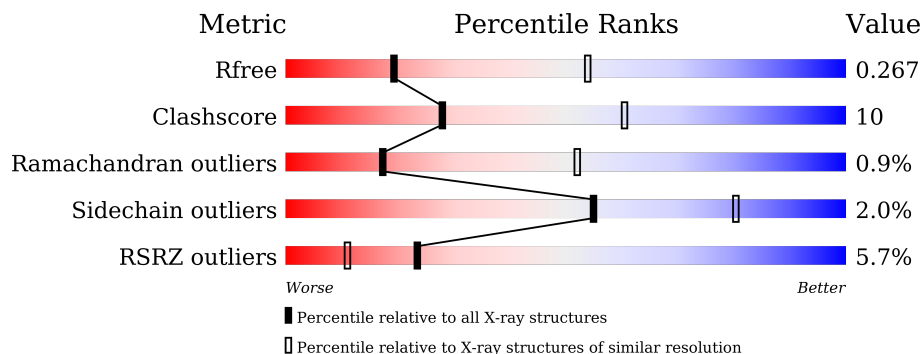
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	1536	
1	B	1536	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 24309 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 4-alpha-glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1525	12260	7817	2063	2328	52	0	0	0
1	B	1498	12049	7690	2028	2279	52	0	0	0

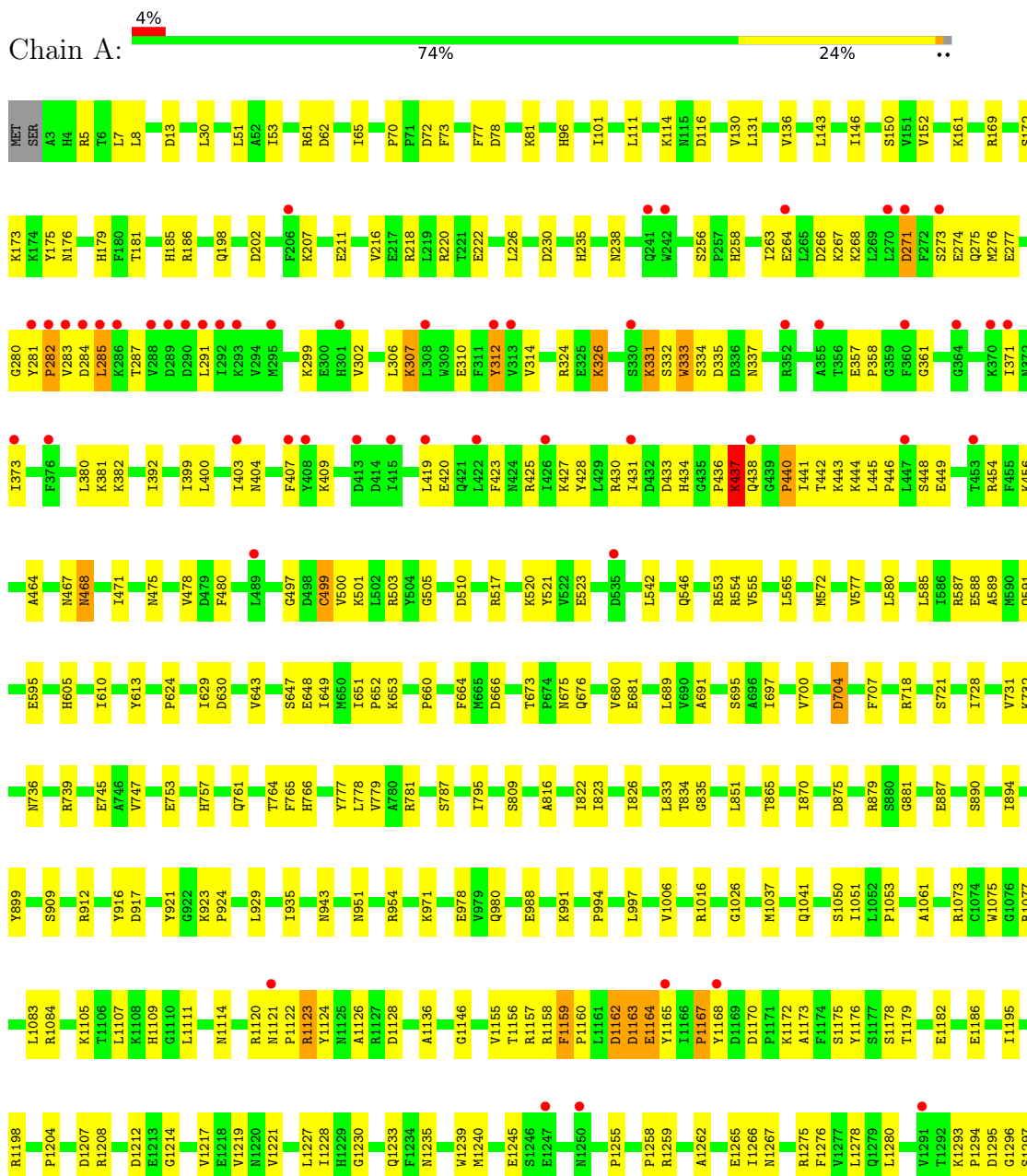
There are 18 discrepancies between the modelled and reference sequences:

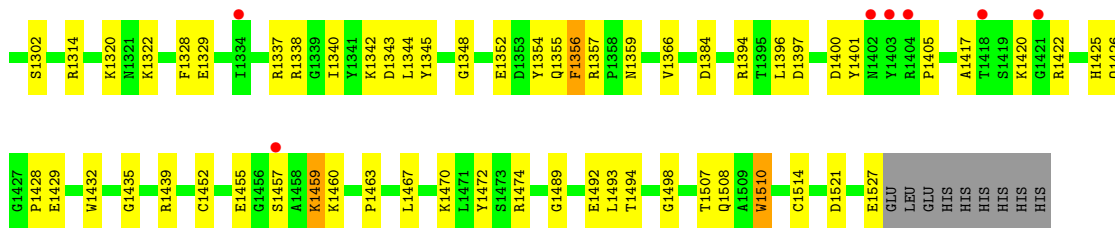
Chain	Residue	Modelled	Actual	Comment	Reference
A	958	ALA	TRP	engineered mutation	UNP Q6FSK0
A	1529	LEU	-	expression tag	UNP Q6FSK0
A	1530	GLU	-	expression tag	UNP Q6FSK0
A	1531	HIS	-	expression tag	UNP Q6FSK0
A	1532	HIS	-	expression tag	UNP Q6FSK0
A	1533	HIS	-	expression tag	UNP Q6FSK0
A	1534	HIS	-	expression tag	UNP Q6FSK0
A	1535	HIS	-	expression tag	UNP Q6FSK0
A	1536	HIS	-	expression tag	UNP Q6FSK0
B	958	ALA	TRP	engineered mutation	UNP Q6FSK0
B	1529	LEU	-	expression tag	UNP Q6FSK0
B	1530	GLU	-	expression tag	UNP Q6FSK0
B	1531	HIS	-	expression tag	UNP Q6FSK0
B	1532	HIS	-	expression tag	UNP Q6FSK0
B	1533	HIS	-	expression tag	UNP Q6FSK0
B	1534	HIS	-	expression tag	UNP Q6FSK0
B	1535	HIS	-	expression tag	UNP Q6FSK0
B	1536	HIS	-	expression tag	UNP Q6FSK0

3 Residue-property plots

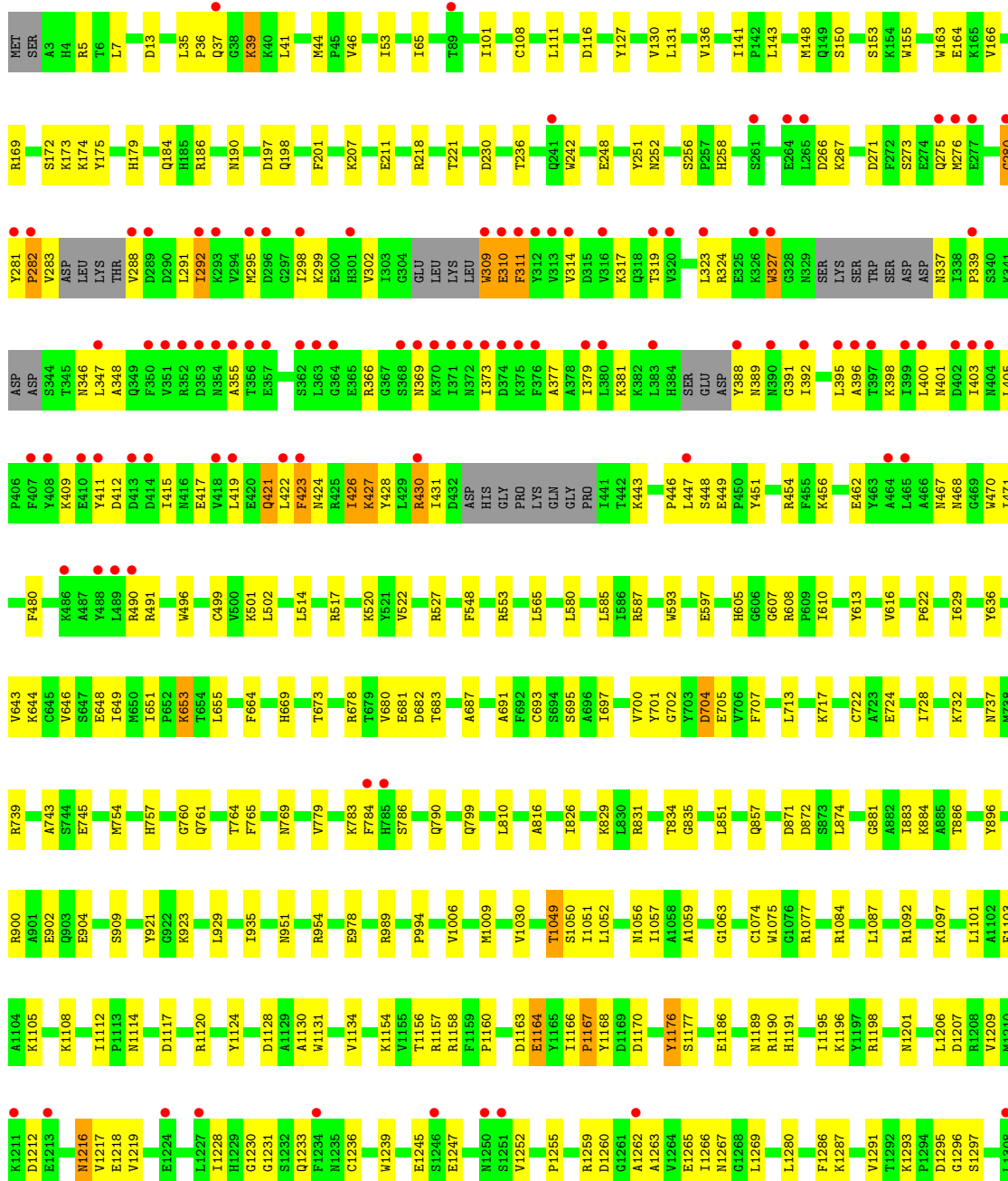
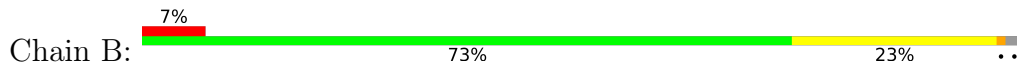
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 4-alpha-glucanotransferase





• Molecule 1: 4-alpha-glucanotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	160.22Å 200.65Å 259.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.80 – 3.10 48.02 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.80-3.10) 100.0 (48.02-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.231 , 0.273 0.227 , 0.267	Depositor DCC
R_{free} test set	2713 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å ²)	91.1	Xtrriage
Anisotropy	0.227	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24309	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/12569	0.50	0/17043
1	B	0.26	0/12347	0.51	0/16733
All	All	0.26	0/24916	0.50	0/33776

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	12260	0	11949	242	0
1	B	12049	0	11752	235	0
All	All	24309	0	23701	476	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 10.

All (476) 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:8:LEU:HB2	1:A:652:PRO:HG2	1.62	0.82
1:A:1262:ALA:HB3	1:A:1345:TYR:HB3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ASN:HB3	1:A:501:LYS:HB2	1.63	0.79
1:A:1077:ARG:HH21	1:A:1128:ASP:HB2	1.48	0.78
1:A:198:GLN:HG2	1:A:517:ARG:HH21	1.48	0.77
1:B:421:GLN:HB3	1:B:491:ARG:HB3	1.68	0.75
1:B:426:ILE:HG22	1:B:430:ARG:HB3	1.66	0.75
1:B:816:ALA:HB2	1:B:826:ILE:HG12	1.69	0.74
1:B:266:ASP:HB3	1:B:454:ARG:HH22	1.52	0.73
1:B:173:LYS:HE2	1:B:175:TYR:HE2	1.55	0.72
1:B:1189:ASN:HA	1:B:1291:VAL:HG23	1.73	0.71
1:B:1239:TRP:NE1	1:B:1359:ASN:OD1	2.21	0.70
1:B:468:ASN:HB3	1:B:501:LYS:HB2	1.73	0.69
1:B:1198:ARG:HG2	1:B:1216:ASN:HB3	1.75	0.68
1:A:1463:PRO:HB3	1:A:1467:LEU:HD23	1.75	0.68
1:B:1355:GLN:OE1	1:B:1357:ARG:NH1	2.27	0.68
1:B:451:TYR:CZ	1:B:491:ARG:HD2	2.28	0.67
1:B:309:TRP:O	1:B:311:PHE:N	2.27	0.67
1:A:1320:LYS:HA	1:A:1338:ARG:HB3	1.77	0.67
1:A:430:ARG:NH1	1:A:446:PRO:O	2.26	0.67
1:B:5:ARG:HA	1:B:643:VAL:HG22	1.78	0.66
1:B:1262:ALA:HB3	1:B:1345:TYR:HB3	1.78	0.66
1:B:1154:LYS:HE2	1:B:1177:SER:HB2	1.78	0.66
1:A:1107:LEU:HB3	1:A:1157:ARG:HH12	1.60	0.66
1:A:1198:ARG:NH2	1:A:1212:ASP:O	2.29	0.65
1:A:333:TRP:HZ3	1:A:337:ASN:HB2	1.61	0.65
1:A:425:ARG:NH2	1:A:449:GLU:OE2	2.30	0.65
1:A:761:GLN:NE2	1:A:787:SER:OG	2.30	0.64
1:B:131:LEU:HD13	1:B:143:LEU:HD22	1.79	0.64
1:B:678:ARG:NH1	1:B:682:ASP:OD2	2.28	0.64
1:A:1198:ARG:NH2	1:A:1212:ASP:OD1	2.28	0.64
1:A:1396:LEU:HD21	1:A:1400:ASP:HB3	1.79	0.64
1:A:1357:ARG:NH2	1:A:1426:GLN:OE1	2.31	0.64
1:A:169:ARG:NH1	1:A:721:SER:O	2.31	0.63
1:A:1107:LEU:HB3	1:A:1157:ARG:NH1	2.13	0.63
1:B:412:ASP:HA	1:B:415:ILE:HG12	1.80	0.63
1:B:324:ARG:HH22	1:B:392:ILE:HG22	1.64	0.63
1:A:331:LYS:HB2	1:A:381:LYS:HD2	1.80	0.63
1:A:1107:LEU:HD23	1:A:1157:ARG:HH12	1.64	0.62
1:B:1166:ILE:HD12	1:B:1166:ILE:H	1.64	0.62
1:B:1452:CYS:HB3	1:B:1467:LEU:HD22	1.82	0.62
1:B:1158:ARG:HH21	1:B:1168:TYR:HB2	1.65	0.62
1:A:283:VAL:HG22	1:A:440:PRO:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1195:ILE:HD11	1:A:1219:VAL:HB	1.82	0.61
1:B:164:GLU:OE2	1:B:218:ARG:NH1	2.32	0.61
1:B:1167:PRO:HB2	1:B:1170:ASP:HB2	1.82	0.61
1:A:361:GLY:HA2	1:A:407:PHE:HE1	1.65	0.61
1:B:267:LYS:NZ	1:B:271:ASP:OD2	2.32	0.61
1:B:702:GLY:HA2	1:B:705:GLU:HB2	1.81	0.61
1:A:1396:LEU:HD13	1:A:1426:GLN:HB3	1.81	0.61
1:A:1489:GLY:HA3	1:A:1507:THR:HG23	1.81	0.60
1:A:588:GLU:HB2	1:A:591:GLN:HG2	1.83	0.60
1:A:779:VAL:HG11	1:A:851:LEU:HD11	1.83	0.60
1:A:816:ALA:HB2	1:A:826:ILE:HG12	1.83	0.60
1:A:1219:VAL:HG22	1:A:1230:GLY:HA3	1.83	0.60
1:A:1259:ARG:NH2	1:A:1265:GLU:OE2	2.35	0.60
1:A:1452:CYS:HB3	1:A:1467:LEU:HB2	1.83	0.60
1:B:169:ARG:NE	1:B:701:TYR:OH	2.31	0.60
1:B:871:ASP:OD1	1:B:872:ASP:N	2.35	0.60
1:A:1167:PRO:HB2	1:A:1170:ASP:HB2	1.84	0.60
1:B:1195:ILE:HD11	1:B:1219:VAL:HB	1.82	0.60
1:A:1400:ASP:OD1	1:A:1401:TYR:N	2.35	0.60
1:B:1431:VAL:HG21	1:B:1491:ALA:O	2.01	0.60
1:B:1219:VAL:HG22	1:B:1230:GLY:HA3	1.84	0.59
1:B:1158:ARG:HH22	1:B:1166:ILE:HG23	1.67	0.59
1:A:1314:ARG:NH1	1:A:1329:GLU:OE2	2.34	0.59
1:A:1322:LYS:H	1:A:1322:LYS:HD2	1.68	0.59
1:B:1295:ASP:OD1	1:B:1296:GLY:N	2.35	0.59
1:A:766:HIS:NE2	1:A:865:THR:HG21	2.17	0.59
1:A:1114:ASN:HB2	1:A:1126:ALA:HB2	1.86	0.58
1:B:1233:GLN:OE1	1:B:1349:LYS:NZ	2.35	0.58
1:A:1170:ASP:HB3	1:A:1172:LYS:HG2	1.86	0.58
1:B:248:GLU:HA	1:B:252:ASN:HD21	1.69	0.58
1:B:426:ILE:HG21	1:B:447:LEU:HD11	1.84	0.58
1:A:1295:ASP:OD1	1:A:1296:GLY:N	2.37	0.58
1:B:680:VAL:HG11	1:B:826:ILE:HD12	1.85	0.58
1:B:1259:ARG:NH1	1:B:1265:GLU:OE2	2.35	0.58
1:B:377:ALA:HB1	1:B:381:LYS:HE2	1.85	0.57
1:B:53:ILE:HD11	1:B:65:ILE:HD11	1.85	0.57
1:A:1053:PRO:HB3	1:A:1120:ARG:HG3	1.85	0.57
1:B:673:THR:HG21	1:B:707:PHE:O	2.04	0.57
1:B:1398:PRO:HA	1:B:1403:TYR:CG	2.40	0.57
1:A:5:ARG:HA	1:A:643:VAL:HG12	1.85	0.57
1:A:53:ILE:HD11	1:A:65:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1293:LYS:HD3	1:B:1297:SER:HB3	1.86	0.57
1:B:1435:GLY:HA3	1:B:1514:CYS:HB3	1.87	0.57
1:A:503:ARG:NH2	1:A:510:ASP:O	2.35	0.57
1:B:1049:THR:HG22	1:B:1050:SER:H	1.68	0.57
1:A:471:ILE:HD11	1:A:480:PHE:HB3	1.87	0.57
1:B:309:TRP:HB2	1:B:411:TYR:CE1	2.39	0.57
1:B:468:ASN:HB3	1:B:501:LYS:HD2	1.87	0.57
1:A:1394:ARG:HG2	1:A:1429:GLU:HG2	1.87	0.56
1:B:467:ASN:HA	1:B:501:LYS:H	1.68	0.56
1:B:704:ASP:OD2	1:B:732:LYS:HG3	2.04	0.56
1:A:433:ASP:OD1	1:A:434:HIS:N	2.37	0.56
1:B:430:ARG:HG2	1:B:431:ILE:HG23	1.88	0.56
1:A:77:PHE:O	1:A:554:ARG:NH1	2.39	0.56
1:B:1084:ARG:NH2	1:B:1521:ASP:OD1	2.39	0.56
1:A:333:TRP:O	1:A:335:ASP:N	2.39	0.56
1:B:553:ARG:NH2	1:B:580:LEU:O	2.39	0.56
1:A:1259:ARG:NH1	1:A:1343:ASP:OD1	2.39	0.55
1:B:929:LEU:HD22	1:B:1006:VAL:HG13	1.86	0.55
1:A:691:ALA:HA	1:A:697:ILE:HG21	1.88	0.55
1:A:704:ASP:OD2	1:A:732:LYS:HG3	2.06	0.55
1:B:1342:LYS:HB2	1:B:1353:ASP:O	2.06	0.55
1:A:420:GLU:HG3	1:A:423:PHE:HE2	1.70	0.55
1:B:35:LEU:HD21	1:B:41:LEU:HD23	1.88	0.55
1:A:186:ARG:NH2	1:A:202:ASP:OD2	2.39	0.55
1:A:468:ASN:HD22	1:A:468:ASN:H	1.54	0.55
1:A:695:SER:O	1:A:739:ARG:NH2	2.40	0.55
1:A:263:ILE:HD13	1:A:464:ALA:HB3	1.89	0.55
1:B:348:ALA:HB1	1:B:403:ILE:HG12	1.89	0.55
1:A:78:ASP:HB3	1:A:81:LYS:HB3	1.88	0.54
1:A:273:SER:O	1:A:441:ILE:HD12	2.08	0.54
1:A:7:LEU:HD22	1:A:653:LYS:HB3	1.90	0.54
1:A:870:ILE:HD11	1:A:997:LEU:HD13	1.89	0.54
1:A:1384:ASP:OD1	1:A:1474:ARG:NH1	2.40	0.54
1:B:426:ILE:HG21	1:B:447:LEU:HD21	1.88	0.54
1:B:629:ILE:HG21	1:B:883:ILE:HD13	1.89	0.54
1:A:680:VAL:HG11	1:A:826:ILE:HD12	1.89	0.54
1:A:1343:ASP:CG	1:A:1357:ARG:HD2	2.28	0.54
1:A:1123:ARG:NH2	1:A:1207:ASP:HB2	2.22	0.54
1:A:1157:ARG:HD3	1:A:1176:TYR:CE1	2.43	0.54
1:B:471:ILE:HD11	1:B:480:PHE:HB3	1.89	0.54
1:A:444:LYS:HG2	1:A:445:LEU:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1221:VAL:HG22	1:A:1228:ILE:HG12	1.90	0.54
1:A:1428:PRO:HB3	1:A:1493:LEU:HD21	1.89	0.53
1:B:443:LYS:HA	1:B:446:PRO:HG3	1.90	0.53
1:B:520:LYS:HZ1	1:B:527:ARG:HH22	1.56	0.53
1:B:39:LYS:HD3	1:B:44:MET:HE1	1.89	0.53
1:A:291:LEU:HD21	1:A:423:PHE:HB2	1.90	0.53
1:A:218:ARG:HG2	1:A:222:GLU:HG3	1.89	0.53
1:A:400:LEU:O	1:A:404:ASN:ND2	2.41	0.53
1:B:921:TYR:HE2	1:B:935:ILE:HD13	1.74	0.53
1:A:442:THR:HG22	1:A:443:LYS:H	1.74	0.53
1:A:1214:GLY:O	1:A:1235:ASN:ND2	2.41	0.53
1:B:339:PRO:HG2	1:B:347:LEU:HA	1.90	0.53
1:A:721:SER:HA	1:A:822:ILE:HD11	1.90	0.53
1:A:1275:ARG:NH2	1:A:1366:VAL:O	2.41	0.52
1:B:1508:GLN:HG2	1:B:1510:TRP:HE1	1.74	0.52
1:A:565:LEU:HB3	1:A:585:LEU:HD22	1.91	0.52
1:B:37:GLN:O	1:B:39:LYS:HD2	2.08	0.52
1:B:1394:ARG:HG2	1:B:1429:GLU:HG2	1.91	0.52
1:A:131:LEU:HD13	1:A:143:LEU:HD13	1.91	0.52
1:B:622:PRO:HG3	1:B:1030:VAL:HG22	1.91	0.52
1:A:1417:ALA:O	1:A:1422:ARG:HB2	2.08	0.52
1:B:323:LEU:O	1:B:327:TRP:N	2.39	0.52
1:B:608:ARG:NH2	1:B:613:TYR:O	2.42	0.52
1:B:207:LYS:N	1:B:211:GLU:OE1	2.42	0.52
1:B:427:LYS:HA	1:B:431:ILE:HG13	1.92	0.52
1:A:834:THR:HG22	1:A:835:GLY:H	1.74	0.52
1:A:917:ASP:HA	1:A:923:LYS:HG2	1.92	0.52
1:B:426:ILE:HB	1:B:430:ARG:CZ	2.39	0.52
1:A:647:SER:OG	1:A:648:GLU:N	2.39	0.52
1:A:1158:ARG:HA	1:A:1173:ALA:O	2.10	0.52
1:B:283:VAL:HA	1:B:288:VAL:HG22	1.91	0.52
1:A:267:LYS:O	1:A:271:ASP:HB3	2.10	0.52
1:A:238:ASN:ND2	1:A:497:GLY:O	2.42	0.52
1:B:256:SER:HB2	1:B:258:HIS:CE1	2.45	0.52
1:B:757:HIS:HB3	1:B:764:THR:HB	1.92	0.52
1:A:427:LYS:O	1:A:431:ILE:N	2.43	0.51
1:B:902:GLU:OE2	1:B:923:LYS:NZ	2.30	0.51
1:A:101:ILE:HG21	1:A:130:VAL:HG21	1.92	0.51
1:B:1463:PRO:HD3	1:B:1526:TYR:CD1	2.45	0.51
1:B:198:GLN:OE1	1:B:517:ARG:NE	2.38	0.51
1:B:728:ILE:HD11	1:B:810:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:HG2	1:A:114:LYS:HB3	1.93	0.51
1:A:1158:ARG:O	1:A:1159:PHE:HD2	1.93	0.51
1:A:266:ASP:HB3	1:A:454:ARG:HH22	1.74	0.51
1:B:1157:ARG:NH2	1:B:1186:GLU:OE2	2.42	0.51
1:B:276:MET:O	1:B:280:GLY:N	2.44	0.51
1:A:307:LYS:HE3	1:A:310:GLU:HB2	1.92	0.51
1:A:1314:ARG:HA	1:A:1328:PHE:HD1	1.75	0.51
1:B:1108:LYS:HB3	1:B:1124:TYR:CE2	2.45	0.51
1:B:295:MET:HA	1:B:298:ILE:HD12	1.93	0.51
1:B:1428:PRO:HB3	1:B:1493:LEU:HD21	1.93	0.51
1:A:256:SER:HB2	1:A:258:HIS:CE1	2.46	0.51
1:A:1239:TRP:HE1	1:A:1359:ASN:ND2	2.08	0.51
1:A:1337:ARG:HB2	1:A:1340:ILE:HD12	1.92	0.51
1:B:687:ALA:HB1	1:B:732:LYS:HE3	1.93	0.51
1:A:314:VAL:HG11	1:A:371:ILE:HD13	1.92	0.50
1:A:553:ARG:NH2	1:A:580:LEU:O	2.44	0.50
1:A:1083:LEU:HD22	1:A:1136:ALA:HB1	1.93	0.50
1:B:311:PHE:O	1:B:369:ASN:ND2	2.43	0.50
1:B:1260:ASP:OD1	1:B:1260:ASP:N	2.44	0.50
1:A:1156:THR:HG22	1:A:1158:ARG:HG2	1.94	0.50
1:B:951:ASN:OD1	1:B:954:ARG:NH2	2.44	0.50
1:B:169:ARG:O	1:B:172:SER:OG	2.27	0.50
1:B:587:ARG:HG3	1:B:605:HIS:NE2	2.27	0.50
1:A:284:ASP:HB3	1:A:440:PRO:HB3	1.93	0.50
1:A:152:VAL:HA	1:A:181:THR:OG1	2.12	0.50
1:A:542:LEU:O	1:A:546:GLN:HG3	2.12	0.50
1:A:1492:GLU:HB2	1:A:1508:GLN:HB2	1.94	0.50
1:A:1493:LEU:HD23	1:A:1494:THR:N	2.26	0.50
1:B:179:HIS:NE2	1:B:230:ASP:OD2	2.40	0.50
1:A:436:PRO:O	1:A:437:LYS:HB2	2.12	0.50
1:A:1240:MET:HB2	1:A:1259:ARG:HD3	1.92	0.50
1:A:326:LYS:HG2	1:A:373:ILE:HG22	1.92	0.50
1:A:1435:GLY:HA3	1:A:1514:CYS:HB3	1.94	0.50
1:B:1263:ALA:O	1:B:1267:ASN:ND2	2.44	0.50
1:B:46:VAL:N	1:B:101:ILE:O	2.45	0.50
1:B:456:LYS:HG2	1:B:462:GLU:HB3	1.94	0.50
1:A:1508:GLN:HG2	1:A:1510:TRP:HE1	1.76	0.49
1:A:1352:GLU:HA	1:A:1355:GLN:HG3	1.94	0.49
1:B:355:ALA:HB2	1:B:379:ILE:HD12	1.93	0.49
1:B:1166:ILE:HD11	1:B:1201:ASN:OD1	2.12	0.49
1:A:887:GLU:O	1:A:1016:ARG:NH1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:LYS:HA	1:A:1175:SER:HB2	1.93	0.49
1:A:1356:PHE:HB3	1:A:1397:ASP:HB2	1.95	0.49
1:A:30:LEU:HD13	1:A:130:VAL:HG22	1.94	0.49
1:B:309:TRP:HB2	1:B:411:TYR:HE1	1.77	0.49
1:A:875:ASP:OD1	1:A:879:ARG:NH1	2.44	0.49
1:B:874:LEU:HD13	1:B:989:ARG:HD2	1.95	0.49
1:B:1105:LYS:HE2	1:B:1156:THR:O	2.13	0.49
1:A:179:HIS:NE2	1:A:230:ASP:OD1	2.42	0.49
1:A:284:ASP:HB2	1:A:438:GLN:HG3	1.93	0.49
1:A:673:THR:HG21	1:A:707:PHE:O	2.13	0.49
1:A:1157:ARG:NH2	1:A:1186:GLU:OE2	2.45	0.49
1:B:396:ALA:O	1:B:400:LEU:HG	2.12	0.49
1:A:1455:GLU:HG2	1:A:1459:LYS:HE2	1.95	0.49
1:B:430:ARG:HE	1:B:431:ILE:HG12	1.78	0.48
1:A:62:ASP:HB2	1:A:114:LYS:HB2	1.95	0.48
1:B:1103:PHE:O	1:B:1112:ILE:HD11	2.14	0.48
1:A:152:VAL:HG22	1:A:181:THR:HG21	1.95	0.48
1:A:649:ILE:HG22	1:A:651:ILE:HG13	1.95	0.48
1:A:757:HIS:HB3	1:A:764:THR:HB	1.94	0.48
1:B:174:LYS:HG3	1:B:737:ASN:ND2	2.28	0.48
1:B:310:GLU:HG3	1:B:366:ARG:HH21	1.79	0.48
1:B:467:ASN:HB2	1:B:499:CYS:O	2.13	0.48
1:B:1196:LYS:HA	1:B:1218:GLU:OE1	2.13	0.48
1:B:1312:PHE:CG	1:B:1370:LEU:HD13	2.49	0.48
1:A:1245:GLU:HG3	1:A:1420:LYS:HB3	1.96	0.48
1:A:1405:PRO:HA	1:A:1428:PRO:HD3	1.94	0.48
1:B:565:LEU:HB3	1:B:585:LEU:HD22	1.95	0.48
1:B:896:TYR:HE1	1:B:900:ARG:HH21	1.62	0.48
1:B:520:LYS:NZ	1:B:527:ARG:HH22	2.12	0.48
1:B:13:ASP:OD2	1:B:1479:ARG:NH2	2.35	0.47
1:B:1209:VAL:HG11	1:B:1245:GLU:HG3	1.95	0.47
1:A:673:THR:HG22	1:A:675:ASN:H	1.79	0.47
1:B:783:LYS:HD3	1:B:857:GLN:CB	2.44	0.47
1:A:169:ARG:O	1:A:172:SER:OG	2.31	0.47
1:A:1105:LYS:HG2	1:A:1155:VAL:HG22	1.95	0.47
1:B:695:SER:O	1:B:739:ARG:NH2	2.47	0.47
1:B:829:LYS:HE3	1:B:831:ARG:HD3	1.97	0.47
1:A:13:ASP:OD2	1:A:1472:TYR:OH	2.31	0.47
1:B:1396:LEU:HG	1:B:1426:GLN:HB2	1.95	0.47
1:A:264:GLU:O	1:A:268:LYS:HB2	2.14	0.47
1:A:399:ILE:O	1:A:403:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:GLN:OE1	1:A:1507:THR:HG21	2.15	0.47
1:B:834:THR:HG22	1:B:835:GLY:H	1.79	0.47
1:B:1087:LEU:O	1:B:1092:ARG:N	2.48	0.47
1:B:299:LYS:HE2	1:B:419:LEU:HD22	1.95	0.47
1:B:761:GLN:HG2	1:B:790:GLN:OE1	2.15	0.47
1:B:1075:TRP:HA	1:B:1114:ASN:O	2.14	0.47
1:A:280:GLY:C	1:A:282:PRO:HD2	2.35	0.47
1:A:1239:TRP:CD2	1:A:1432:TRP:HZ2	2.33	0.47
1:B:184:GLN:HA	1:B:201:PHE:HA	1.97	0.47
1:B:491:ARG:HA	1:B:491:ARG:HD3	1.61	0.47
1:B:722:CYS:O	1:B:724:GLU:HG3	2.15	0.47
1:B:1236:CYS:SG	1:B:1255:PRO:HB3	2.54	0.47
1:B:1314:ARG:HA	1:B:1328:PHE:HD1	1.79	0.47
1:A:299:LYS:HE2	1:A:419:LEU:HD22	1.97	0.46
1:A:409:LYS:HD2	1:A:409:LYS:HA	1.62	0.46
1:B:1217:VAL:HG13	1:B:1231:GLY:HA2	1.97	0.46
1:A:673:THR:HB	1:A:676:GLN:HG3	1.96	0.46
1:B:197:ASP:OD1	1:B:517:ARG:NH2	2.48	0.46
1:B:298:ILE:O	1:B:302:VAL:HG22	2.15	0.46
1:B:1198:ARG:NH1	1:B:1212:ASP:OD1	2.48	0.46
1:A:207:LYS:HD2	1:A:207:LYS:HA	1.57	0.46
1:B:745:GLU:O	1:B:769:ASN:ND2	2.48	0.46
1:B:1438:ILE:HA	1:B:1441:TYR:HB3	1.96	0.46
1:A:681:GLU:OE1	1:A:681:GLU:N	2.44	0.46
1:A:909:SER:O	1:A:912:ARG:HG2	2.14	0.46
1:A:1061:ALA:HB2	1:A:1073:ARG:CZ	2.46	0.46
1:B:1404:ARG:HB2	1:B:1423:ASN:OD1	2.15	0.46
1:A:523:GLU:HB2	1:A:555:VAL:HG21	1.97	0.46
1:A:1265:GLU:HG2	1:A:1266:ILE:N	2.31	0.46
1:B:314:VAL:HG22	1:B:369:ASN:O	2.15	0.46
1:B:522:VAL:HG21	1:B:548:PHE:HB3	1.97	0.46
1:B:1052:LEU:HD13	1:B:1057:ILE:HD11	1.98	0.46
1:B:1463:PRO:HB3	1:B:1467:LEU:HD23	1.98	0.46
1:B:426:ILE:C	1:B:428:TYR:H	2.20	0.46
1:B:1009:MET:HE3	1:B:1009:MET:O	2.16	0.46
1:A:467:ASN:HA	1:A:500:VAL:HA	1.98	0.46
1:A:161:LYS:HD2	1:A:161:LYS:HA	1.72	0.45
1:B:610:ILE:HG13	1:B:754:MET:O	2.16	0.45
1:B:648:GLU:OE2	1:B:881:GLY:N	2.50	0.45
1:B:401:ASN:O	1:B:405:LEU:HG	2.16	0.45
1:B:681:GLU:OE1	1:B:681:GLU:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1239:TRP:CD2	1:B:1432:TRP:HZ2	2.34	0.45
1:A:150:SER:OG	1:A:700:VAL:HA	2.17	0.45
1:A:718:ARG:HB2	1:A:823:ILE:HG12	1.98	0.45
1:A:1120:ARG:HD3	1:A:1168:TYR:CZ	2.51	0.45
1:A:1293:LYS:HG3	1:A:1294:PRO:N	2.30	0.45
1:B:470:TRP:HZ3	1:B:496:TRP:NE1	2.14	0.45
1:A:916:TYR:O	1:A:924:PRO:HD2	2.16	0.45
1:A:1075:TRP:HA	1:A:1114:ASN:O	2.16	0.45
1:A:1278:LEU:HD11	1:A:1302:SER:HA	1.98	0.45
1:B:377:ALA:O	1:B:381:LYS:HG3	2.16	0.45
1:B:593:TRP:HD1	1:B:597:GLU:HG3	1.80	0.45
1:A:428:TYR:HA	1:A:433:ASP:OD1	2.16	0.45
1:B:669:HIS:N	1:B:700:VAL:HG11	2.32	0.45
1:B:691:ALA:HA	1:B:697:ILE:HG21	1.98	0.45
1:B:1269:LEU:HD23	1:B:1366:VAL:HG11	1.99	0.45
1:B:1439:ARG:HD2	1:B:1521:ASP:OD2	2.16	0.45
1:A:198:GLN:HB3	1:A:521:TYR:CG	2.52	0.45
1:A:235:HIS:HB2	1:A:499:CYS:HB2	1.98	0.45
1:A:1107:LEU:HD12	1:A:1111:LEU:O	2.17	0.45
1:A:1329:GLU:OE1	1:A:1345:TYR:OH	2.26	0.45
1:B:198:GLN:NE2	1:B:236:THR:OG1	2.49	0.45
1:A:1160:PRO:HG3	1:A:1164:GLU:HB2	1.99	0.45
1:A:587:ARG:HG3	1:A:605:HIS:CE1	2.52	0.45
1:A:1050:SER:OG	1:A:1051:ILE:N	2.50	0.44
1:B:883:ILE:HA	1:B:886:THR:HG22	1.98	0.44
1:B:1117:ASP:HB3	1:B:1120:ARG:O	2.17	0.44
1:B:1131:TRP:HA	1:B:1134:VAL:HG12	1.99	0.44
1:A:70:PRO:HG3	1:A:77:PHE:HA	1.99	0.44
1:A:146:ILE:HA	1:A:176:ASN:HD21	1.82	0.44
1:A:380:LEU:HD13	1:A:392:ILE:HG23	1.98	0.44
1:A:505:GLY:HA3	1:A:510:ASP:HB2	1.98	0.44
1:A:1122:PRO:HG2	1:A:1124:TYR:CE1	2.53	0.44
1:A:281:TYR:N	1:A:282:PRO:HD2	2.32	0.44
1:A:357:GLU:HB3	1:A:358:PRO:HD2	1.99	0.44
1:A:732:LYS:O	1:A:736:ASN:ND2	2.51	0.44
1:A:1494:THR:HG21	1:A:1498:GLY:HA2	1.99	0.44
1:B:251:TYR:HE1	1:B:501:LYS:HG2	1.80	0.44
1:B:426:ILE:CG2	1:B:447:LEU:HD11	2.47	0.44
1:A:446:PRO:HG2	1:A:448:SER:O	2.17	0.44
1:A:520:LYS:HA	1:A:523:GLU:HG2	1.98	0.44
1:A:1439:ARG:HD2	1:A:1521:ASP:OD2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1316:PHE:HA	1:B:1342:LYS:HG2	1.99	0.44
1:A:1146:GLY:HA3	1:B:221:THR:HB	2.00	0.44
1:B:502:LEU:HD13	1:B:514:LEU:HD11	2.00	0.44
1:B:1077:ARG:NH2	1:B:1128:ASP:OD1	2.49	0.44
1:B:470:TRP:HZ3	1:B:496:TRP:HE1	1.66	0.44
1:B:779:VAL:HG11	1:B:851:LEU:HD11	2.00	0.44
1:B:1112:ILE:H	1:B:1130:ALA:HB2	1.83	0.44
1:B:1131:TRP:CD1	1:B:1266:ILE:HG23	2.53	0.44
1:B:1160:PRO:HG3	1:B:1164:GLU:HB2	1.99	0.44
1:A:648:GLU:OE2	1:A:881:GLY:N	2.51	0.44
1:B:799:GLN:HB2	1:B:994:PRO:HG3	2.00	0.44
1:B:337:ASN:OD1	1:B:337:ASN:N	2.49	0.43
1:B:405:LEU:O	1:B:409:LYS:HG3	2.17	0.43
1:A:282:PRO:HB3	1:A:285:LEU:CD1	2.48	0.43
1:B:65:ILE:HG12	1:B:111:LEU:HD22	2.01	0.43
1:B:348:ALA:CB	1:B:403:ILE:HG12	2.48	0.43
1:B:683:THR:HG22	1:B:728:ILE:HG13	2.00	0.43
1:B:1154:LYS:HG2	1:B:1177:SER:HB3	2.01	0.43
1:B:1325:ASP:HB3	1:B:1330:ILE:HG21	1.99	0.43
1:A:577:VAL:HG11	1:A:660:PRO:HB3	2.00	0.43
1:A:589:ALA:HB3	1:A:666:ASP:HA	2.00	0.43
1:A:777:TYR:CE1	1:A:795:ILE:HD13	2.53	0.43
1:B:1404:ARG:O	1:B:1423:ASN:ND2	2.51	0.43
1:A:613:TYR:H	1:A:943:ASN:ND2	2.17	0.43
1:A:971:LYS:HE2	1:A:980:GLN:OE1	2.18	0.43
1:B:283:VAL:HB	1:B:288:VAL:HG13	2.01	0.43
1:B:317:LYS:HE3	1:B:317:LYS:HB3	1.88	0.43
1:B:705:GLU:OE1	1:B:705:GLU:N	2.49	0.43
1:A:430:ARG:HH21	1:A:440:PRO:HA	1.82	0.43
1:B:978:GLU:OE1	1:B:978:GLU:N	2.50	0.43
1:B:136:VAL:HB	1:B:141:ILE:HD11	2.01	0.43
1:B:678:ARG:HB3	1:B:784:PHE:HA	2.00	0.43
1:B:1490:LEU:HD13	1:B:1512:THR:HG22	2.01	0.43
1:A:173:LYS:HE3	1:A:175:TYR:HE1	1.83	0.43
1:A:1459:LYS:HA	1:A:1459:LYS:HD2	1.76	0.43
1:B:148:MET:SD	1:B:179:HIS:HB2	2.59	0.43
1:B:1050:SER:OG	1:B:1051:ILE:N	2.52	0.43
1:B:1206:LEU:HD12	1:B:1207:ASP:N	2.33	0.43
1:B:1406:TYR:O	1:B:1423:ASN:ND2	2.47	0.43
1:A:629:ILE:HG22	1:A:649:ILE:HA	2.01	0.43
1:A:1155:VAL:HG12	1:A:1178:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1314:ARG:HA	1:A:1328:PHE:CD1	2.53	0.43
1:B:101:ILE:HG21	1:B:130:VAL:HG21	1.99	0.43
1:A:890:SER:O	1:A:894:ILE:HG13	2.19	0.42
1:B:760:GLY:HA3	1:B:790:GLN:HE22	1.84	0.42
1:B:799:GLN:HG3	1:B:994:PRO:HA	2.01	0.42
1:B:1059:ALA:HB1	1:B:1074:CYS:SG	2.59	0.42
1:B:1097:LYS:O	1:B:1101:LEU:HG	2.19	0.42
1:B:1216:ASN:O	1:B:1216:ASN:ND2	2.49	0.42
1:B:1228:ILE:N	1:B:1267:ASN:OD1	2.50	0.42
1:A:312:TYR:N	1:A:312:TYR:CD1	2.86	0.42
1:A:921:TYR:HE2	1:A:935:ILE:HD13	1.85	0.42
1:A:1077:ARG:HD3	1:A:1239:TRP:HB2	2.00	0.42
1:A:1120:ARG:O	1:A:1121:ASN:HB2	2.19	0.42
1:A:1240:MET:HA	1:A:1425:HIS:CE1	2.54	0.42
1:B:607:GLY:O	1:B:754:MET:HE2	2.19	0.42
1:B:1280:LEU:HB3	1:B:1286:PHE:HB2	2.01	0.42
1:A:595:GLU:HG2	1:A:761:GLN:HA	2.01	0.42
1:A:1293:LYS:HD2	1:A:1294:PRO:HD2	2.01	0.42
1:A:1342:LYS:HE2	1:A:1354:TYR:CE1	2.54	0.42
1:A:1293:LYS:HG3	1:A:1295:ASP:H	1.84	0.42
1:A:610:ILE:HA	1:A:753:GLU:HB3	2.01	0.42
1:B:186:ARG:HD2	1:B:190:ASN:O	2.19	0.42
1:B:422:LEU:HG	1:B:491:ARG:HG2	2.02	0.42
1:A:277:GLU:HA	1:A:281:TYR:HB3	2.01	0.42
1:B:1050:SER:HB2	1:B:1056:ASN:HA	2.01	0.42
1:A:899:TYR:OH	1:A:1037:MET:HB3	2.20	0.42
1:B:166:VAL:HG22	1:B:169:ARG:NH2	2.34	0.42
1:B:616:VAL:HG12	1:B:646:VAL:HG11	2.02	0.42
1:B:1493:LEU:HB3	1:B:1504:SER:HB2	2.01	0.42
1:A:72:ASP:OD1	1:A:73:PHE:N	2.52	0.42
1:A:198:GLN:HG2	1:A:517:ARG:NH2	2.25	0.42
1:A:689:LEU:HD23	1:A:778:LEU:HD23	2.02	0.42
1:A:1084:ARG:NH2	1:A:1521:ASP:OD1	2.53	0.42
1:A:1204:PRO:O	1:A:1208:ARG:HG2	2.19	0.42
1:A:1357:ARG:NH2	1:A:1396:LEU:HD12	2.35	0.42
1:B:417:GLU:CD	1:B:490:ARG:HE	2.21	0.42
1:B:1077:ARG:HD3	1:B:1239:TRP:HB2	2.01	0.42
1:A:1470:LYS:HD2	1:A:1474:ARG:HH21	1.85	0.42
1:A:1460:LYS:HE2	1:A:1460:LYS:HB3	1.83	0.41
1:A:1508:GLN:HG2	1:A:1510:TRP:NE1	2.34	0.41
1:B:1163:ASP:OD2	1:B:1190:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1493:LEU:HD23	1:B:1494:THR:N	2.35	0.41
1:A:65:ILE:HG12	1:A:111:LEU:HD22	2.01	0.41
1:A:1233:GLN:NE2	1:A:1348:GLY:HA3	2.35	0.41
1:B:311:PHE:CZ	1:B:366:ARG:HD2	2.55	0.41
1:B:388:TYR:CG	1:B:389:ASN:N	2.88	0.41
1:B:447:LEU:HD12	1:B:447:LEU:HA	1.80	0.41
1:B:1247:GLU:HG2	1:B:1252:VAL:HG21	2.02	0.41
1:A:283:VAL:HG21	1:A:441:ILE:HG22	2.02	0.41
1:A:307:LYS:HE3	1:A:307:LYS:HB2	1.88	0.41
1:A:1221:VAL:HG13	1:A:1227:LEU:O	2.19	0.41
1:B:153:SER:HB2	1:B:163:TRP:CZ2	2.55	0.41
1:B:1317:TYR:CE2	1:B:1319:PRO:HA	2.56	0.41
1:A:745:GLU:O	1:A:747:VAL:HG23	2.20	0.41
1:B:7:LEU:HD22	1:B:653:LYS:HD2	2.02	0.41
1:B:150:SER:HB2	1:B:700:VAL:HG12	2.02	0.41
1:A:216:VAL:HG12	1:A:220:ARG:NH1	2.35	0.41
1:B:1287:LYS:HE3	1:B:1287:LYS:HB2	1.85	0.41
1:A:624:PRO:HA	1:A:1026:GLY:O	2.19	0.41
1:B:108:CYS:HB3	1:B:127:TYR:CD2	2.55	0.41
1:A:1394:ARG:NH1	1:A:1429:GLU:OE2	2.53	0.41
1:B:636:TYR:CE1	1:B:644:LYS:HA	2.55	0.41
1:A:302:VAL:O	1:A:306:LEU:HB2	2.21	0.41
1:A:728:ILE:O	1:A:731:VAL:N	2.52	0.41
1:A:809:SER:HB2	1:A:833:LEU:HD11	2.03	0.41
1:B:883:ILE:HG13	1:B:884:LYS:N	2.36	0.41
1:A:207:LYS:N	1:A:211:GLU:OE1	2.51	0.41
1:A:978:GLU:OE1	1:A:978:GLU:N	2.52	0.41
1:A:1179:THR:OG1	1:A:1182:GLU:HG2	2.20	0.41
1:B:7:LEU:HD12	1:B:655:LEU:HD13	2.03	0.41
1:B:900:ARG:NH1	1:B:904:GLU:O	2.53	0.41
1:B:1461:LEU:HA	1:B:1461:LEU:HD12	1.84	0.41
1:B:1508:GLN:HG2	1:B:1510:TRP:NE1	2.36	0.41
1:A:456:LYS:N	1:A:456:LYS:HD2	2.36	0.41
1:A:988:GLU:HA	1:A:991:LYS:HE2	2.02	0.41
1:A:1255:PRO:HB2	1:A:1258:PRO:HD3	2.03	0.41
1:A:1276:PHE:O	1:A:1280:LEU:HB2	2.21	0.41
1:B:605:HIS:O	1:B:693:CYS:HB3	2.21	0.41
1:B:900:ARG:HD3	1:B:900:ARG:HA	1.92	0.41
1:A:475:ASN:HD22	1:A:478:VAL:HG23	1.85	0.40
1:B:319:THR:HG23	1:B:373:ILE:HG12	2.02	0.40
1:B:1063:GLY:HA3	1:B:1508:GLN:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:HIS:O	1:A:434:HIS:ND1	2.55	0.40
1:A:1109:HIS:CE1	1:A:1163:ASP:HB2	2.56	0.40
1:B:717:LYS:HA	1:B:717:LYS:HD2	1.93	0.40
1:A:51:LEU:O	1:A:96:HIS:HA	2.21	0.40
1:A:136:VAL:HA	1:A:226:LEU:HD21	2.03	0.40
1:A:1259:ARG:HB3	1:A:1344:LEU:HD21	2.03	0.40
1:A:1457:SER:O	1:A:1460:LYS:HG2	2.22	0.40
1:B:155:TRP:CH2	1:B:713:LEU:HA	2.56	0.40
1:A:630:ASP:O	1:A:648:GLU:HG2	2.21	0.40
1:A:761:GLN:OE1	1:A:781:ARG:NH2	2.53	0.40
1:A:929:LEU:HD22	1:A:1006:VAL:HG13	2.02	0.40
1:A:951:ASN:OD1	1:A:954:ARG:NH2	2.54	0.40
1:B:281:TYR:HA	1:B:282:PRO:HD3	1.94	0.40
1:B:292:ILE:HG12	1:B:423:PHE:HE2	1.87	0.40
1:B:446:PRO:C	1:B:448:SER:H	2.25	0.40
1:B:783:LYS:HD3	1:B:857:GLN:HB3	2.02	0.40
1:B:1364:MET:HB3	1:B:1444:PHE:HE2	1.85	0.40
1:A:382:LYS:HB3	1:A:382:LYS:HE2	1.94	0.40
1:A:994:PRO:HG2	1:A:997:LEU:HD12	2.03	0.40
1:A:1228:ILE:N	1:A:1267:ASN:OD1	2.42	0.40
1:A:1295:ASP:OD1	1:A:1297:SER:N	2.50	0.40
1:B:198:GLN:HE22	1:B:242:TRP:HZ2	1.68	0.40
1:B:649:ILE:HG22	1:B:651:ILE:HG13	2.04	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	1523/1536 (99%)	1399 (92%)	115 (8%)	9 (1%)	25 59
1	B	1484/1536 (97%)	1357 (91%)	109 (7%)	18 (1%)	13 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3007/3072 (98%)	2756 (92%)	224 (7%)	27 (1%)	17 52

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	PRO
1	A	437	LYS
1	A	1164	GLU
1	A	1167	PRO
1	B	310	GLU
1	B	346	ASN
1	B	743	ALA
1	B	1167	PRO
1	A	334	SER
1	B	275	GLN
1	B	280	GLY
1	B	311	PHE
1	B	424	ASN
1	B	427	LYS
1	B	291	LEU
1	B	1176	TYR
1	A	332	SER
1	A	440	PRO
1	A	1459	LYS
1	B	36	PRO
1	B	273	SER
1	B	282	PRO
1	A	1162	ASP
1	B	1164	GLU
1	B	292	ILE
1	B	449	GLU
1	B	391	GLY

5.3.2 Protein sidechains [i](#)

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	1342/1353 (99%)	1312 (98%)	30 (2%)	52	78
1	B	1317/1353 (97%)	1294 (98%)	23 (2%)	60	83
All	All	2659/2706 (98%)	2606 (98%)	53 (2%)	55	80

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ASP
1	A	185	HIS
1	A	271	ASP
1	A	274	GLU
1	A	275	GLN
1	A	276	MET
1	A	285	LEU
1	A	287	THR
1	A	307	LYS
1	A	312	TYR
1	A	324	ARG
1	A	326	LYS
1	A	331	LYS
1	A	333	TRP
1	A	437	LYS
1	A	468	ASN
1	A	499	CYS
1	A	572	MET
1	A	664	PHE
1	A	704	ASP
1	A	765	PHE
1	A	1123	ARG
1	A	1159	PHE
1	A	1162	ASP
1	A	1163	ASP
1	A	1165	TYR
1	A	1217	VAL
1	A	1356	PHE
1	A	1510	TRP
1	A	1527	GLU
1	B	39	LYS
1	B	116	ASP
1	B	309	TRP
1	B	327	TRP
1	B	395	LEU

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Mol	Chain	Res	Type
1	B	398	LYS
1	B	421	GLN
1	B	423	PHE
1	B	426	ILE
1	B	430	ARG
1	B	653	LYS
1	B	664	PHE
1	B	704	ASP
1	B	765	PHE
1	B	786	SER
1	B	909	SER
1	B	1049	THR
1	B	1176	TYR
1	B	1191	HIS
1	B	1216	ASN
1	B	1356	PHE
1	B	1477	LYS
1	B	1510	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	468	ASN
1	A	853	GLN
1	A	1233	GLN
1	B	252	ASN
1	B	952	ASN
1	B	1235	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 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	1525/1536 (99%)	0.22	60 (3%) 39 20	43, 81, 125, 165	0
1	B	1498/1536 (97%)	0.37	111 (7%) 14 5	45, 81, 150, 170	0
All	All	3023/3072 (98%)	0.30	171 (5%) 23 11	43, 81, 143, 170	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	319	THR	5.8
1	B	395	LEU	5.5
1	B	327	TRP	5.4
1	B	323	LEU	5.2
1	A	290	ASP	4.9
1	A	281	TYR	4.7
1	B	312	TYR	4.7
1	B	314	VAL	4.6
1	B	399	ILE	4.5
1	B	383	LEU	4.3
1	B	261	SER	4.3
1	B	355	ALA	4.3
1	B	354	ASN	4.2
1	B	371	ILE	4.1
1	A	289	ASP	4.1
1	B	370	LYS	4.1
1	B	380	LEU	4.1
1	B	281	TYR	4.0
1	A	355	ALA	4.0
1	B	447	LEU	4.0
1	B	404	ASN	4.0
1	A	241	GLN	3.9
1	B	363	LEU	3.9
1	B	419	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	379	ILE	3.8
1	B	296	ASP	3.8
1	A	282	PRO	3.8
1	B	295	MET	3.7
1	A	1421	GLY	3.6
1	B	422	LEU	3.6
1	A	270	LEU	3.6
1	B	1356	PHE	3.6
1	A	438	GLN	3.5
1	B	276	MET	3.5
1	B	375	LYS	3.5
1	A	313	VAL	3.5
1	B	369	ASN	3.5
1	B	364	GLY	3.4
1	B	407	PHE	3.4
1	A	431	ILE	3.3
1	B	403	ILE	3.3
1	B	326	LYS	3.3
1	B	400	LEU	3.3
1	B	316	VAL	3.3
1	B	489	LEU	3.2
1	B	347	LEU	3.2
1	B	309	TRP	3.2
1	B	1211	LYS	3.2
1	B	275	GLN	3.2
1	B	423	PHE	3.2
1	B	1234	PHE	3.2
1	B	410	GLU	3.1
1	A	1457	SER	3.1
1	B	465	LEU	3.1
1	A	419	LEU	3.1
1	A	291	LEU	3.1
1	B	1399	SER	3.0
1	A	364	GLY	3.0
1	B	392	ILE	3.0
1	B	264	GLU	2.9
1	B	311	PHE	2.9
1	B	339	PRO	2.9
1	A	447	LEU	2.9
1	B	37	GLN	2.9
1	A	308	LEU	2.9
1	B	418	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	413	ASP	2.8
1	B	376	PHE	2.8
1	B	362	SER	2.8
1	A	293	LYS	2.8
1	B	411	TYR	2.8
1	B	277	GLU	2.8
1	B	313	VAL	2.8
1	B	1328	PHE	2.8
1	A	295	MET	2.8
1	B	486	LYS	2.8
1	B	1246	SER	2.8
1	A	1404	ARG	2.8
1	B	414	ASP	2.7
1	A	284	ASP	2.7
1	B	402	ASP	2.7
1	B	293	LYS	2.7
1	B	1308	LEU	2.7
1	A	1121	ASN	2.7
1	A	1165	TYR	2.6
1	B	282	PRO	2.6
1	B	1338	ARG	2.6
1	B	373	ILE	2.6
1	A	330	SER	2.6
1	A	1247	GLU	2.6
1	A	283	VAL	2.6
1	B	390	ASN	2.6
1	B	785	HIS	2.6
1	A	264	GLU	2.6
1	B	353	ASP	2.6
1	B	1250	ASN	2.6
1	B	464	ALA	2.5
1	A	285	LEU	2.5
1	B	1342	LYS	2.5
1	A	373	ILE	2.5
1	B	357	GLU	2.5
1	B	351	VAL	2.5
1	B	1224	GLU	2.5
1	B	265	LEU	2.4
1	B	396	ALA	2.4
1	B	350	PHE	2.4
1	B	89	THR	2.4
1	B	397	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	370	LYS	2.4
1	B	374	ASP	2.4
1	B	430	ARG	2.4
1	B	488	TYR	2.4
1	A	360	PHE	2.4
1	A	371	ILE	2.4
1	A	1291	VAL	2.4
1	B	241	GLN	2.4
1	A	407	PHE	2.4
1	B	1422	ARG	2.4
1	B	368	SER	2.4
1	A	1402	ASN	2.4
1	A	288	VAL	2.3
1	A	292	ILE	2.3
1	A	312	TYR	2.3
1	A	426	ILE	2.3
1	B	288	VAL	2.3
1	A	301	HIS	2.3
1	B	1458	ALA	2.3
1	A	352	ARG	2.3
1	B	1319	PRO	2.3
1	A	403	ILE	2.3
1	B	292	ILE	2.3
1	A	376	PHE	2.3
1	B	1213	GLU	2.3
1	A	1334	ILE	2.3
1	A	535	ASP	2.3
1	A	206	PHE	2.3
1	B	298	ILE	2.2
1	B	408	TYR	2.2
1	A	1418	THR	2.2
1	A	286	LYS	2.2
1	A	1168	TYR	2.2
1	B	1251	SER	2.2
1	B	1511	SER	2.2
1	A	1250	ASN	2.2
1	B	490	ARG	2.2
1	B	1227	LEU	2.2
1	B	301	HIS	2.2
1	A	408	TYR	2.2
1	B	372	ASN	2.2
1	B	1370	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1345	TYR	2.1
1	B	320	VAL	2.1
1	A	413	ASP	2.1
1	B	289	ASP	2.1
1	B	1262	ALA	2.1
1	A	415	ILE	2.1
1	A	422	LEU	2.1
1	B	1330	ILE	2.1
1	B	280	GLY	2.1
1	B	310	GLU	2.1
1	A	453	THR	2.1
1	A	271	ASP	2.1
1	A	1403	TYR	2.1
1	B	352	ARG	2.1
1	A	242	TRP	2.0
1	B	388	TYR	2.0
1	A	273	SER	2.0
1	A	489	LEU	2.0
1	B	356	THR	2.0
1	B	784	PHE	2.0
1	B	1382	LEU	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.