



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 10:40 PM EDT

PDB ID : 3JQZ
Title : Crystal Structure of Human serum albumin complexed with Lidocaine
Authors : Hein, K.L.; Kragh-Hansen, U.; Morth, J.P.; Nissen, P.
Deposited on : 2009-09-08
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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

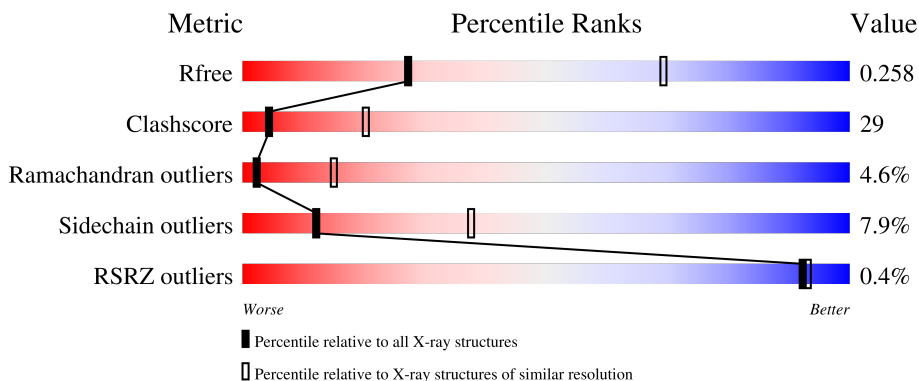
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	585	 45% 46% 7% ..
1	B	585	 % 48% 43% 7% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LQZ	A	586	-	-	X	-

2 Entry composition [i](#)

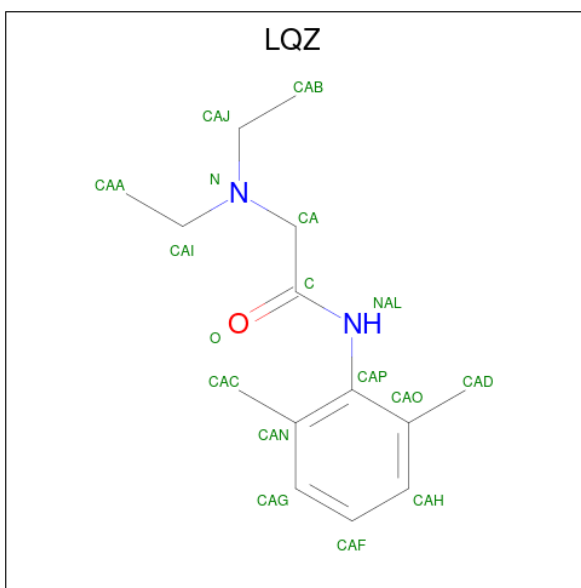
There are 2 unique types of molecules in this entry. The entry contains 9279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

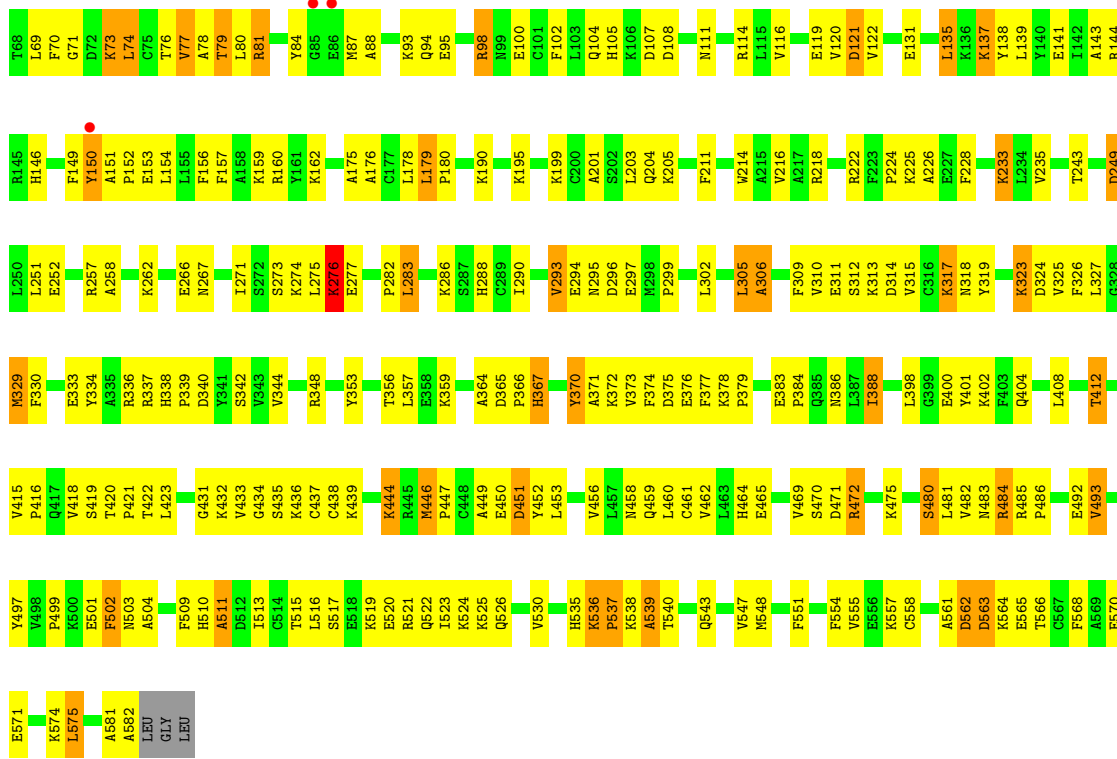
- Molecule 1 is a protein called Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	582	Total 4631	C 2922	N 783	O 885	S 41	0	0	0
1	B	582	Total 4631	C 2922	N 783	O 885	S 41	0	0	0

- Molecule 2 is 2-(diethylamino)-N-(2,6-dimethylphenyl)ethanamide (three-letter code: LQZ) (formula: C₁₄H₂₂N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 17	C 14	N 2	O 1	0	0



4 Data and refinement statistics i

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	168.48Å 168.48Å 97.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.93 – 3.30 44.93 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.93-3.30) 99.9 (44.93-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.32Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.220 , 0.268 0.213 , 0.258	Depositor DCC
R_{free} test set	1054 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	115.0	Xtrriage
Anisotropy	0.080	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 91.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.044 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9279	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LQZ

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	0.27	2/4721 (0.0%)	0.43	1/6368 (0.0%)
1	B	0.22	0/4721	0.40	0/6368
All	All	0.25	2/9442 (0.0%)	0.41	1/12736 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	ASN	C-N	6.13	1.48	1.34
1	A	182	LEU	C-N	-5.64	1.21	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ASN	O-C-N	-6.61	112.12	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ASN	Mainchain

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	4631	0	4552	287	0
1	B	4631	0	4552	255	0
2	A	17	0	22	8	0
All	All	9279	0	9126	534	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 (534) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LEU:HD22	1:B:180:PRO:HD3	1.37	1.03
1:A:77:VAL:HG23	1:A:78:ALA:H	1.34	0.91
1:B:348:ARG:HG3	1:B:482:VAL:HG12	1.54	0.90
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.54	0.88
1:A:276:LYS:HD2	1:A:277:GLU:H	1.37	0.88
1:A:47:THR:HG22	1:A:51:LYS:HE3	1.56	0.87
1:A:517:SER:HB3	1:A:520:GLU:HG2	1.54	0.87
1:A:464:HIS:HE1	1:A:470:SER:H	1.20	0.86
1:B:27:PHE:HE1	1:B:42:LEU:HB3	1.41	0.86
1:A:408:LEU:O	1:A:412:THR:HB	1.75	0.86
1:B:408:LEU:O	1:B:412:THR:HB	1.76	0.86
1:A:93:LYS:HB3	1:A:97:GLU:HB3	1.56	0.85
1:A:150:TYR:HB3	1:A:153:GLU:HB2	1.60	0.84
1:B:517:SER:HB3	1:B:520:GLU:HG2	1.59	0.83
1:A:120:VAL:HG11	1:A:175:ALA:HA	1.61	0.82
1:A:436:LYS:HD2	1:A:452:TYR:CE1	2.15	0.80
1:B:27:PHE:CE1	1:B:42:LEU:HB3	2.17	0.79
1:B:6:GLU:HA	1:B:9:HIS:HB3	1.65	0.79
1:B:179:LEU:HD13	1:B:179:LEU:H	1.49	0.78
1:A:119:GLU:HB3	1:B:79:THR:HG21	1.65	0.78
1:B:305:LEU:HG	1:B:337:ARG:HH11	1.50	0.76
1:A:459:GLN:HA	1:A:462:VAL:HG22	1.69	0.75
1:A:378:LYS:HB2	1:A:379:PRO:HD3	1.67	0.74
1:B:302:LEU:HD22	1:B:337:ARG:HH21	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:PHE:CE2	1:B:160:ARG:HD2	2.22	0.73
1:A:524:LYS:HA	1:A:524:LYS:HE2	1.71	0.73
1:A:281:LYS:NZ	1:A:285:GLU:HB3	2.05	0.72
1:A:156:PHE:HE1	1:A:285:GLU:HG2	1.54	0.72
1:B:14:LEU:HD13	1:B:22:LEU:HD12	1.71	0.72
1:A:433:VAL:HG22	1:A:452:TYR:CE2	2.25	0.71
1:A:283:LEU:HA	1:A:286:LYS:HB2	1.73	0.71
1:B:60:GLU:HG3	1:B:61:ASN:N	2.05	0.71
1:B:510:HIS:O	1:B:513:ILE:HG12	1.91	0.71
1:A:276:LYS:HD2	1:A:277:GLU:N	2.06	0.70
1:A:31:LEU:O	1:A:33:GLN:N	2.25	0.70
1:B:150:TYR:CD1	1:B:152:PRO:HD2	2.27	0.70
1:A:22:LEU:HG	1:A:155:LEU:HD11	1.73	0.70
1:A:32:GLN:HE22	1:A:107:ASP:H	1.40	0.69
1:A:433:VAL:HG22	1:A:452:TYR:CD2	2.26	0.69
1:B:524:LYS:HE2	1:B:524:LYS:HA	1.75	0.69
1:A:352:THR:O	1:A:355:THR:HG22	1.92	0.69
1:A:74:LEU:O	1:A:77:VAL:HG22	1.92	0.69
1:A:168:CYS:O	1:A:174:LYS:HB2	1.93	0.68
1:B:436:LYS:HD2	1:B:452:TYR:CZ	2.28	0.68
1:B:84:TYR:HA	1:B:87:MET:HB3	1.74	0.67
1:A:130:ASN:HD22	1:A:133:THR:HB	1.60	0.67
1:B:203:LEU:HD21	1:B:243:THR:HG22	1.77	0.67
1:B:384:PRO:O	1:B:388:ILE:HG13	1.95	0.67
1:A:149:PHE:HD1	1:A:150:TYR:H	1.43	0.66
1:B:419:SER:O	1:B:423:LEU:HD12	1.95	0.66
1:A:356:THR:O	1:A:359:LYS:HG2	1.95	0.66
1:A:545:LYS:O	1:A:545:LYS:HG3	1.95	0.66
1:A:137:LYS:HD2	1:A:138:TYR:N	2.10	0.66
1:A:295:ASN:HD22	1:A:339:PRO:HB3	1.60	0.66
1:B:42:LEU:HD22	1:B:73:LYS:HD2	1.78	0.66
1:A:276:LYS:CD	1:A:277:GLU:H	2.09	0.65
1:B:516:LEU:HG	1:B:520:GLU:HG3	1.77	0.65
1:B:274:LYS:HA	1:B:276:LYS:HE3	1.78	0.65
1:A:307:ALA:HA	1:A:311:GLU:HB2	1.78	0.65
1:B:459:GLN:HA	1:B:462:VAL:HG22	1.78	0.65
1:A:14:LEU:HD12	1:A:15:GLY:N	2.11	0.65
1:B:370:TYR:C	1:B:372:LYS:H	1.99	0.65
1:A:10:ARG:O	1:A:14:LEU:HG	1.97	0.65
1:B:143:ALA:HB2	1:B:154:LEU:HD21	1.79	0.64
1:B:557:LYS:O	1:B:561:ALA:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LYS:HB2	1:A:98:ARG:HB3	1.78	0.64
1:A:561:ALA:HB3	1:A:564:LYS:HB2	1.81	0.63
1:B:492:GLU:HG3	1:B:493:VAL:H	1.63	0.63
1:B:93:LYS:O	1:B:98:ARG:HB2	1.98	0.63
1:B:444:LYS:HE3	1:B:444:LYS:N	2.14	0.63
1:A:156:PHE:CE1	1:A:285:GLU:HG2	2.32	0.63
1:B:42:LEU:O	1:B:46:VAL:HG23	1.99	0.63
1:A:87:MET:HE2	1:B:515:THR:HB	1.80	0.63
1:A:436:LYS:HD2	1:A:452:TYR:HE1	1.58	0.63
1:A:541:LYS:HE3	1:A:545:LYS:HB2	1.81	0.63
2:A:586:LQZ:HAC	2:A:586:LQZ:O	1.99	0.62
1:B:299:PRO:HG2	1:B:302:LEU:HD21	1.81	0.62
1:A:320:ALA:HA	1:A:323:LYS:HZ2	1.65	0.62
1:B:71:GLY:HA3	1:B:98:ARG:HE	1.63	0.62
1:B:176:ALA:O	1:B:180:PRO:HG2	1.98	0.62
1:A:12:LYS:HZ1	1:A:54:VAL:HG13	1.65	0.62
1:B:71:GLY:C	1:B:98:ARG:HH11	2.02	0.62
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.80	0.62
1:A:77:VAL:HG23	1:A:78:ALA:N	2.10	0.62
1:B:228:PHE:CE1	1:B:329:MET:HG2	2.35	0.62
1:A:31:LEU:HD12	1:A:34:CYS:SG	2.40	0.62
1:A:112:LEU:CD1	1:A:145:ARG:HG2	2.30	0.62
1:A:522:GLN:O	1:A:526:GLN:HG2	2.00	0.61
1:B:226:ALA:HB2	1:B:271:ILE:HA	1.82	0.61
1:B:14:LEU:HB3	1:B:18:ASN:HD22	1.65	0.61
1:A:134:PHE:O	1:A:137:LYS:HG3	2.00	0.61
1:B:329:MET:O	1:B:333:GLU:HG2	2.01	0.61
1:A:31:LEU:HB2	1:A:39:HIS:HE1	1.64	0.61
1:B:95:GLU:OE2	1:B:98:ARG:HD2	2.00	0.61
1:B:81:ARG:HA	1:B:84:TYR:HD1	1.65	0.61
1:B:153:GLU:O	1:B:157:PHE:HD1	1.84	0.61
1:B:348:ARG:HG3	1:B:482:VAL:CG1	2.28	0.60
1:A:429:ASN:HD22	1:A:459:GLN:NE2	1.99	0.60
1:A:333:GLU:O	1:A:336:ARG:HG2	2.02	0.60
1:B:378:LYS:HB3	1:B:379:PRO:HD3	1.83	0.60
1:B:480:SER:HB3	1:B:483:ASN:HB2	1.82	0.60
1:B:306:ALA:O	1:B:310:VAL:HG22	2.00	0.60
1:B:141:GLU:O	1:B:144:ARG:HG2	2.02	0.60
1:B:492:GLU:HG3	1:B:493:VAL:N	2.17	0.60
1:A:119:GLU:CB	1:B:79:THR:HG21	2.32	0.60
1:A:149:PHE:HD1	1:A:150:TYR:N	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:C	1:A:546:ALA:H	2.04	0.60
1:A:112:LEU:HD13	1:A:145:ARG:HG2	1.84	0.60
1:B:49:PHE:CE1	1:B:69:LEU:HD11	2.36	0.60
1:A:87:MET:HG2	1:A:105:HIS:CE1	2.37	0.59
1:A:556:GLU:HG2	1:A:556:GLU:O	2.02	0.59
1:A:268:GLN:HG2	1:A:275:LEU:HB2	1.83	0.59
1:A:530:VAL:O	1:A:534:LYS:HG3	2.02	0.59
1:A:342:SER:HB3	1:A:447:PRO:HA	1.84	0.59
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.85	0.59
1:A:419:SER:OG	1:A:421:PRO:HD2	2.02	0.58
1:B:17:GLU:H	1:B:20:LYS:HG3	1.67	0.58
1:B:39:HIS:O	1:B:43:VAL:HG23	2.02	0.58
1:A:284:LEU:HD22	1:A:284:LEU:H	1.66	0.58
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.84	0.58
1:A:48:GLU:HA	1:A:51:LYS:HD2	1.86	0.58
1:A:289:CYS:O	1:A:293:VAL:HG13	2.03	0.58
1:A:35:PRO:HG3	1:B:116:VAL:HG13	1.85	0.58
1:A:281:LYS:HZ1	1:A:285:GLU:HB3	1.68	0.58
1:A:47:THR:O	1:A:51:LYS:HG3	2.04	0.58
1:B:31:LEU:HD21	1:B:74:LEU:HD21	1.85	0.57
1:A:190:LYS:HE3	2:A:586:LQZ:CAG	2.34	0.57
1:B:311:GLU:O	1:B:315:VAL:HG23	2.05	0.57
1:B:536:LYS:HE3	1:B:536:LYS:H	1.69	0.57
1:A:6:GLU:HG3	1:A:66:LEU:HD11	1.87	0.57
1:A:286:LYS:O	1:A:290:ILE:HG12	2.05	0.57
1:A:499:PRO:HB3	1:A:535:HIS:O	2.05	0.57
1:A:533:VAL:HA	1:A:536:LYS:HZ1	1.70	0.57
1:B:23:VAL:HG12	1:B:43:VAL:HG22	1.85	0.57
1:A:320:ALA:HA	1:A:323:LYS:NZ	2.20	0.57
1:A:114:ARG:NH1	2:A:586:LQZ:HACB	2.20	0.56
1:B:276:LYS:CD	1:B:277:GLU:H	2.17	0.56
1:B:551:PHE:HA	1:B:575:LEU:HD11	1.86	0.56
1:B:561:ALA:O	1:B:563:ASP:N	2.38	0.56
1:B:310:VAL:HG23	1:B:311:GLU:CD	2.26	0.56
1:A:164:ALA:O	1:A:168:CYS:HB2	2.05	0.56
1:B:81:ARG:HA	1:B:84:TYR:CD1	2.39	0.56
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.87	0.56
1:A:372:LYS:O	1:A:375:ASP:HB2	2.06	0.56
1:A:510:HIS:O	1:A:513:ILE:HG12	2.06	0.56
1:A:581:ALA:O	1:A:582:ALA:HB3	2.05	0.56
1:B:502:PHE:HE1	1:B:504:ALA:HB2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLN:CG	1:A:275:LEU:HB2	2.35	0.56
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.88	0.56
1:A:262:LYS:O	1:A:266:GLU:HG3	2.06	0.56
1:B:344:VAL:HG12	1:B:482:VAL:HG13	1.88	0.56
1:A:216:VAL:HB	1:A:331:LEU:HD23	1.86	0.56
1:A:338:HIS:HB3	1:A:341:TYR:HB2	1.87	0.55
1:A:395:PHE:HE1	1:A:400:GLU:HA	1.70	0.55
1:A:453:LEU:HD13	1:A:485:ARG:HG3	1.88	0.55
1:B:554:PHE:CD2	1:B:575:LEU:HD12	2.41	0.55
1:A:49:PHE:HZ	1:A:61:ASN:HB2	1.72	0.55
1:A:306:ALA:HA	1:A:310:VAL:HG12	1.87	0.55
1:A:563:ASP:O	1:A:564:LYS:HD2	2.07	0.55
1:B:120:VAL:HG21	1:B:175:ALA:HB2	1.88	0.55
1:A:424:VAL:O	1:A:428:ARG:HG3	2.07	0.55
1:A:497:TYR:HD2	1:A:537:PRO:HG2	1.71	0.55
1:B:519:LYS:O	1:B:523:ILE:HG13	2.06	0.55
1:B:121:ASP:OD2	1:B:121:ASP:N	2.39	0.55
1:B:537:PRO:HB2	1:B:538:LYS:HD2	1.89	0.55
1:B:400:GLU:OE1	1:B:432:LYS:HG2	2.06	0.55
1:A:138:TYR:O	1:A:142:ILE:HD13	2.07	0.55
1:B:3:HIS:CG	1:B:9:HIS:HB2	2.42	0.55
1:A:27:PHE:HB3	1:A:39:HIS:ND1	2.22	0.55
1:A:25:ILE:HG13	1:A:139:LEU:HD11	1.90	0.54
1:A:342:SER:CB	1:A:447:PRO:HA	2.37	0.54
1:A:228:PHE:HB2	1:A:332:TYR:CE2	2.41	0.54
1:A:344:VAL:HG13	1:A:482:VAL:HG13	1.90	0.54
1:A:376:GLU:O	1:A:379:PRO:HD2	2.07	0.54
1:A:567:CYS:HA	1:A:570:GLU:HB2	1.89	0.54
1:B:204:GLN:HE21	1:B:205:LYS:NZ	2.06	0.54
1:A:464:HIS:CE1	1:A:470:SER:H	2.12	0.54
1:A:481:LEU:HD12	1:A:484:ARG:HD3	1.88	0.54
1:B:324:ASP:C	1:B:326:PHE:H	2.11	0.54
1:B:333:GLU:O	1:B:337:ARG:HG2	2.08	0.54
1:B:376:GLU:O	1:B:379:PRO:HD2	2.07	0.54
1:A:536:LYS:HE3	1:A:536:LYS:H	1.72	0.54
1:B:511:ALA:HB2	1:B:565:GLU:HG3	1.90	0.54
1:A:5:SER:HB3	1:A:57:GLU:HG3	1.90	0.54
1:A:365:ASP:OD2	1:A:368:GLU:HB2	2.08	0.54
1:B:295:ASN:HD22	1:B:339:PRO:HB3	1.72	0.54
1:A:316:CYS:HA	1:A:319:TYR:HB3	1.90	0.53
1:B:581:ALA:O	1:B:582:ALA:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PHE:HA	1:A:105:HIS:CD2	2.43	0.53
1:B:309:PHE:O	1:B:315:VAL:HG21	2.07	0.53
1:A:77:VAL:CG2	1:A:78:ALA:H	2.17	0.53
1:B:8:ALA:O	1:B:12:LYS:HG2	2.07	0.53
1:B:195:LYS:NZ	1:B:218:ARG:HH12	2.06	0.53
1:B:418:VAL:HB	1:B:423:LEU:HD11	1.90	0.53
1:B:517:SER:H	1:B:520:GLU:HG3	1.74	0.53
1:A:78:ALA:HA	1:A:81:ARG:HB2	1.91	0.53
1:A:519:LYS:O	1:A:523:ILE:HG13	2.09	0.53
1:B:2:ALA:O	1:B:3:HIS:HB2	2.09	0.53
1:B:81:ARG:HG2	1:B:84:TYR:HB2	1.90	0.53
1:B:333:GLU:O	1:B:336:ARG:HG2	2.08	0.53
1:B:225:LYS:NZ	1:B:225:LYS:HB3	2.24	0.52
1:B:353:TYR:CE2	1:B:357:LEU:HD11	2.44	0.52
1:B:61:ASN:HB3	1:B:64:LYS:HD2	1.91	0.52
1:B:305:LEU:H	1:B:337:ARG:NH1	2.07	0.52
1:B:404:GLN:HG2	1:B:431:GLY:HA3	1.90	0.52
1:B:342:SER:HB2	1:B:450:GLU:HB3	1.90	0.52
1:A:41:LYS:HD2	1:B:122:VAL:HG13	1.91	0.52
1:A:41:LYS:O	1:A:45:GLU:HB2	2.10	0.52
1:B:275:LEU:HD22	1:B:290:ILE:HD12	1.91	0.52
1:B:326:PHE:HD1	1:B:327:LEU:HD23	1.74	0.52
1:B:383:GLU:O	1:B:386:ASN:HB3	2.08	0.52
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.90	0.52
1:B:434:GLY:O	1:B:438:CYS:HB2	2.10	0.52
1:A:561:ALA:O	1:A:562:ASP:C	2.48	0.52
1:B:481:LEU:O	1:B:484:ARG:HB2	2.09	0.52
1:A:545:LYS:O	1:A:545:LYS:CG	2.57	0.51
1:B:67:HIS:CE1	1:B:251:LEU:HD12	2.45	0.51
1:A:249:ASP:HB3	1:A:252:GLU:CG	2.40	0.51
1:A:370:TYR:O	1:A:372:LYS:N	2.43	0.51
1:A:464:HIS:CE1	1:A:469:VAL:H	2.27	0.51
1:B:306:ALA:C	1:B:310:VAL:HG22	2.30	0.51
1:B:334:TYR:O	1:B:338:HIS:HD2	1.94	0.51
1:A:536:LYS:NZ	1:A:539:ALA:HB3	2.26	0.51
1:B:16:GLU:C	1:B:18:ASN:H	2.14	0.51
1:B:540:THR:HG23	1:B:543:GLN:H	1.74	0.51
1:A:86:GLU:O	1:A:87:MET:HB3	2.10	0.51
1:B:21:ALA:O	1:B:25:ILE:HG13	2.09	0.51
1:B:344:VAL:CG1	1:B:482:VAL:HG13	2.40	0.51
1:A:14:LEU:HD12	1:A:15:GLY:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLU:O	1:A:104:GLN:HG3	2.10	0.51
1:A:211:PHE:O	1:A:214:TRP:HB3	2.11	0.51
1:A:165:PHE:CE1	1:A:178:LEU:HD21	2.45	0.51
1:A:275:LEU:N	1:A:275:LEU:HD22	2.26	0.51
1:B:538:LYS:HD2	1:B:538:LYS:H	1.76	0.51
1:A:156:PHE:CZ	1:A:160:ARG:HD2	2.45	0.51
1:A:409:VAL:HG12	1:A:413:LYS:HE2	1.92	0.51
1:A:446:MET:HE2	1:A:446:MET:O	2.10	0.51
1:B:41:LYS:HE2	1:B:45:GLU:OE2	2.11	0.51
1:A:81:ARG:HH11	1:A:89:ASP:HB2	1.76	0.51
1:A:430:LEU:O	1:A:433:VAL:HG23	2.10	0.51
1:B:137:LYS:O	1:B:141:GLU:HG2	2.10	0.51
1:A:234:LEU:HD21	1:A:263:TYR:HE2	1.75	0.51
1:A:294:GLU:HG3	1:A:295:ASN:O	2.11	0.51
1:B:7:VAL:HG11	1:B:49:PHE:HE1	1.76	0.51
1:A:66:LEU:HD23	1:A:251:LEU:HD12	1.91	0.50
1:A:405:ASN:O	1:A:409:VAL:HG23	2.11	0.50
1:B:71:GLY:HA3	1:B:98:ARG:NE	2.26	0.50
1:A:567:CYS:HB2	1:A:571:GLU:HG2	1.92	0.50
1:B:418:VAL:HG12	1:B:419:SER:N	2.26	0.50
1:B:150:TYR:OH	1:B:257:ARG:HD2	2.12	0.50
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.93	0.50
1:A:59:ALA:O	1:A:60:GLU:C	2.50	0.50
1:B:536:LYS:HD2	1:B:539:ALA:HB2	1.93	0.50
1:B:257:ARG:NH2	1:B:288:HIS:HA	2.27	0.50
1:A:77:VAL:O	1:A:79:THR:HG23	2.12	0.50
1:A:87:MET:CE	1:B:515:THR:HB	2.42	0.50
1:A:523:ILE:HA	1:A:526:GLN:HG3	1.94	0.50
1:B:70:PHE:O	1:B:74:LEU:HB2	2.11	0.50
1:B:420:THR:HB	1:B:421:PRO:HD3	1.94	0.50
1:B:305:LEU:HD21	1:B:333:GLU:HB3	1.94	0.50
1:A:283:LEU:CA	1:A:286:LYS:HB2	2.42	0.49
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.93	0.49
1:A:416:PRO:HB2	1:A:497:TYR:CE1	2.46	0.49
1:B:16:GLU:HA	1:B:19:PHE:HB3	1.94	0.49
1:A:360:CYS:C	1:A:362:ALA:H	2.16	0.49
2:A:586:LQZ:HAC	2:A:586:LQZ:C	2.42	0.49
1:A:122:VAL:HG22	1:B:41:LYS:HD2	1.94	0.49
1:B:146:HIS:HB3	1:B:149:PHE:HB2	1.94	0.49
1:B:276:LYS:HD2	1:B:277:GLU:H	1.78	0.49
1:B:502:PHE:CE1	1:B:504:ALA:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:HG3	1:A:122:VAL:HG23	1.94	0.49
1:A:135:LEU:HD23	1:A:161:TYR:HD2	1.77	0.49
1:A:212:LYS:O	1:A:216:VAL:HG23	2.11	0.49
1:A:353:TYR:CZ	1:A:357:LEU:HD11	2.48	0.49
1:B:449:ALA:O	1:B:453:LEU:HB2	2.12	0.49
1:A:42:LEU:O	1:A:46:VAL:HG23	2.12	0.49
1:A:151:ALA:CB	1:A:250:LEU:HD22	2.42	0.49
1:B:12:LYS:HA	1:B:12:LYS:HE2	1.95	0.49
1:A:575:LEU:C	1:A:575:LEU:HD23	2.33	0.49
1:A:134:PHE:O	1:A:137:LYS:HE3	2.13	0.49
1:B:249:ASP:HB3	1:B:252:GLU:CD	2.33	0.49
1:B:314:ASP:O	1:B:317:LYS:HB2	2.13	0.49
1:B:87:MET:HG3	1:B:105:HIS:NE2	2.28	0.49
1:A:150:TYR:CD1	1:A:152:PRO:HD2	2.48	0.48
1:A:257:ARG:NE	1:A:287:SER:HB3	2.28	0.48
1:B:224:PRO:CD	1:B:296:ASP:HB3	2.35	0.48
1:B:373:VAL:C	1:B:375:ASP:H	2.16	0.48
1:A:39:HIS:O	1:A:43:VAL:HG23	2.13	0.48
1:A:446:MET:HB3	1:A:447:PRO:HD3	1.95	0.48
1:A:563:ASP:C	1:A:564:LYS:HD2	2.34	0.48
1:B:447:PRO:O	1:B:451:ASP:HB2	2.13	0.48
1:A:244:GLU:HB3	1:A:249:ASP:HB2	1.96	0.48
1:B:286:LYS:O	1:B:290:ILE:HG12	2.13	0.48
1:A:333:GLU:O	1:A:337:ARG:HG2	2.14	0.48
1:B:131:GLU:O	1:B:135:LEU:HB2	2.14	0.48
1:B:323:LYS:O	1:B:326:PHE:HB3	2.14	0.48
1:B:4:LYS:HG3	1:B:5:SER:N	2.28	0.48
1:A:66:LEU:CD2	1:A:251:LEU:HD12	2.43	0.48
1:A:159:LYS:HB2	1:A:159:LYS:NZ	2.29	0.48
1:A:268:GLN:O	1:A:271:ILE:HG22	2.13	0.48
1:B:370:TYR:C	1:B:372:LYS:N	2.67	0.48
1:A:526:GLN:O	1:A:530:VAL:HG23	2.14	0.48
1:B:150:TYR:HD1	1:B:152:PRO:HD2	1.76	0.48
1:B:538:LYS:HD2	1:B:538:LYS:N	2.29	0.48
1:A:356:THR:HA	1:A:359:LYS:HE3	1.96	0.47
1:B:416:PRO:HB2	1:B:497:TYR:CE1	2.48	0.47
1:A:518:GLU:O	1:A:522:GLN:HG3	2.14	0.47
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.80	0.47
1:A:306:ALA:O	1:A:310:VAL:HG12	2.14	0.47
1:A:384:PRO:O	1:A:388:ILE:HG13	2.13	0.47
1:B:551:PHE:O	1:B:555:VAL:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PHE:CE2	1:A:288:HIS:CD2	3.02	0.47
1:A:234:LEU:HD22	1:A:260:LEU:HD11	1.96	0.47
1:B:60:GLU:CG	1:B:61:ASN:N	2.77	0.47
1:A:30:TYR:HB3	1:A:31:LEU:HD23	1.96	0.47
1:B:74:LEU:C	1:B:76:THR:H	2.17	0.47
1:B:367:HIS:HA	1:B:370:TYR:CE1	2.49	0.47
1:A:77:VAL:HA	1:B:119:GLU:OE2	2.14	0.47
1:A:151:ALA:HB2	1:A:250:LEU:HD22	1.97	0.47
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.95	0.47
1:A:281:LYS:HZ3	1:A:285:GLU:HB3	1.79	0.47
1:A:398:LEU:HD22	1:A:402:LYS:HB3	1.96	0.47
2:A:586:LQZ:O	2:A:586:LQZ:CAC	2.61	0.47
1:A:30:TYR:HE1	1:A:102:PHE:HB3	1.79	0.47
1:B:5:SER:OG	1:B:62:CYS:HB3	2.14	0.47
1:B:76:THR:C	1:B:78:ALA:H	2.19	0.47
1:A:321:GLU:O	1:A:321:GLU:HG2	2.14	0.47
1:B:7:VAL:HG21	1:B:69:LEU:HD13	1.97	0.47
1:B:340:ASP:O	1:B:447:PRO:HD3	2.14	0.47
1:B:40:VAL:HG23	1:B:41:LYS:H	1.80	0.46
1:A:149:PHE:CD1	1:A:150:TYR:N	2.82	0.46
1:A:310:VAL:HB	1:A:374:PHE:HE1	1.80	0.46
1:B:319:TYR:CE1	1:B:327:LEU:HD21	2.50	0.46
1:A:313:LYS:H	1:A:313:LYS:CD	2.28	0.46
1:B:338:HIS:N	1:B:339:PRO:HD3	2.31	0.46
1:B:433:VAL:HG22	1:B:452:TYR:HD2	1.80	0.46
1:B:456:VAL:HA	1:B:459:GLN:HG2	1.98	0.46
1:A:16:GLU:O	1:A:20:LYS:HG3	2.16	0.46
1:B:100:GLU:O	1:B:104:GLN:HG3	2.15	0.46
1:A:77:VAL:C	1:A:79:THR:H	2.19	0.46
1:A:114:ARG:HH21	1:A:114:ARG:HB2	1.80	0.46
1:A:416:PRO:O	1:A:534:LYS:HE3	2.15	0.46
1:B:262:LYS:O	1:B:266:GLU:HG3	2.16	0.46
1:A:150:TYR:HD1	1:A:152:PRO:HD2	1.80	0.46
1:A:365:ASP:N	1:A:366:PRO:HD3	2.30	0.46
1:B:80:LEU:O	1:B:81:ARG:HG3	2.16	0.46
1:B:565:GLU:N	1:B:565:GLU:OE1	2.49	0.46
1:A:41:LYS:HB2	1:B:122:VAL:HG11	1.96	0.46
1:A:458:ASN:O	1:A:462:VAL:HG13	2.15	0.46
1:A:572:GLY:O	1:A:576:VAL:HG23	2.15	0.46
1:A:8:ALA:HB1	1:A:12:LYS:HZ2	1.81	0.46
1:A:90:CYS:HG	1:A:101:CYS:HG	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:CG1	1:B:37:GLU:HB3	2.46	0.45
1:A:187:ASP:OD2	2:A:586:LQZ:HAI	2.16	0.45
1:A:313:LYS:H	1:A:313:LYS:HD3	1.81	0.45
1:B:15:GLY:O	1:B:16:GLU:O	2.35	0.45
1:A:284:LEU:HD22	1:A:284:LEU:N	2.31	0.45
1:A:5:SER:CB	1:A:57:GLU:HG3	2.45	0.45
1:A:353:TYR:CE2	1:A:357:LEU:HD11	2.51	0.45
1:B:485:ARG:N	1:B:486:PRO:CD	2.80	0.45
1:A:501:GLU:OE2	1:B:501:GLU:HB2	2.17	0.45
1:A:77:VAL:C	1:A:79:THR:N	2.70	0.45
1:A:222:ARG:HG2	1:A:223:PHE:CE1	2.52	0.45
1:A:269:ASP:C	1:A:271:ILE:H	2.20	0.45
1:A:367:HIS:CD2	1:A:368:GLU:HG3	2.52	0.45
1:A:23:VAL:O	1:A:27:PHE:HD1	2.00	0.45
1:A:90:CYS:HB2	1:A:93:LYS:HD2	1.99	0.45
1:A:312:SER:O	1:A:315:VAL:HG23	2.16	0.45
1:B:446:MET:HB3	1:B:447:PRO:HD3	1.99	0.45
1:A:17:GLU:C	1:A:19:PHE:H	2.20	0.45
1:A:206:PHE:CE2	1:A:481:LEU:HD13	2.52	0.45
1:A:334:TYR:O	1:A:338:HIS:HD2	2.00	0.45
1:A:423:LEU:O	1:A:427:SER:HB2	2.17	0.45
1:A:533:VAL:HA	1:A:536:LYS:CE	2.47	0.45
1:B:119:GLU:HA	1:B:119:GLU:OE1	2.16	0.45
1:A:150:TYR:CD2	1:A:153:GLU:HG3	2.52	0.45
1:B:365:ASP:N	1:B:366:PRO:HD3	2.31	0.45
1:B:433:VAL:HG22	1:B:452:TYR:CD2	2.52	0.45
1:B:79:THR:HB	1:B:80:LEU:H	1.56	0.44
1:B:114:ARG:O	1:B:114:ARG:HG3	2.17	0.44
1:A:152:PRO:O	1:A:155:LEU:HB2	2.17	0.44
1:A:377:PHE:CD1	1:A:377:PHE:N	2.85	0.44
1:A:18:ASN:O	1:A:22:LEU:HD12	2.16	0.44
1:A:567:CYS:O	1:A:571:GLU:N	2.49	0.44
1:B:275:LEU:O	1:B:276:LYS:C	2.56	0.44
1:B:401:TYR:HE1	1:B:522:GLN:HB3	1.81	0.44
1:A:238:LEU:HG	1:A:242:HIS:HD2	1.83	0.44
1:A:349:LEU:O	1:A:352:THR:HB	2.17	0.44
1:B:150:TYR:CZ	1:B:257:ARG:HD2	2.51	0.44
1:B:492:GLU:CG	1:B:493:VAL:H	2.30	0.44
1:A:271:ILE:O	1:A:272:SER:CB	2.66	0.44
1:A:542:GLU:CD	1:A:542:GLU:H	2.20	0.44
1:A:79:THR:C	1:A:81:ARG:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:ILE:O	1:B:521:ARG:HD3	2.17	0.44
1:B:199:LYS:HG3	1:B:211:PHE:HE1	1.82	0.44
1:B:564:LYS:HD2	1:B:566:THR:OG1	2.17	0.44
1:B:548:MET:HA	1:B:548:MET:CE	2.48	0.44
1:A:8:ALA:O	1:A:12:LYS:HD3	2.18	0.43
1:A:226:ALA:HB2	1:A:271:ILE:HA	1.99	0.43
1:B:203:LEU:HD23	1:B:203:LEU:O	2.17	0.43
1:B:211:PHE:O	1:B:214:TRP:HB3	2.18	0.43
1:B:4:LYS:NZ	1:B:58:SER:HB2	2.32	0.43
1:B:201:ALA:O	1:B:205:LYS:HG2	2.17	0.43
1:B:435:SER:O	1:B:439:LYS:HE3	2.18	0.43
1:B:439:LYS:HB2	1:B:439:LYS:NZ	2.33	0.43
1:A:67:HIS:CD2	1:A:99:ASN:ND2	2.86	0.43
1:B:370:TYR:HD1	1:B:371:ALA:H	1.65	0.43
1:B:436:LYS:HD2	1:B:452:TYR:CE1	2.53	0.43
1:B:521:ARG:O	1:B:525:LYS:HG3	2.17	0.43
1:A:34:CYS:HA	1:A:35:PRO:HD3	1.78	0.43
1:A:348:ARG:HG3	1:A:482:VAL:HG12	2.00	0.43
1:B:312:SER:O	1:B:314:ASP:N	2.51	0.43
1:B:472:ARG:H	1:B:472:ARG:HG3	1.62	0.43
1:B:509:PHE:O	1:B:568:PHE:HB3	2.19	0.43
1:A:228:PHE:HB2	1:A:332:TYR:CD2	2.54	0.43
2:A:586:LQZ:HAAC	2:A:586:LQZ:HAJA	1.73	0.43
1:B:464:HIS:CE1	1:B:469:VAL:H	2.37	0.43
1:A:120:VAL:HG13	1:A:178:LEU:HD23	2.00	0.43
1:A:377:PHE:N	1:A:377:PHE:HD1	2.15	0.43
1:B:570:GLU:O	1:B:574:LYS:HG3	2.18	0.43
1:A:221:GLN:O	1:A:224:PRO:HD3	2.19	0.43
1:A:114:ARG:HD2	1:A:186:ARG:NH2	2.34	0.43
1:A:130:ASN:HD22	1:A:133:THR:CB	2.29	0.43
1:B:435:SER:O	1:B:439:LYS:HG3	2.18	0.43
1:A:554:PHE:HE1	1:A:558:CYS:SG	2.42	0.43
1:B:258:ALA:HB1	1:B:283:LEU:HD12	2.01	0.43
1:B:436:LYS:HA	1:B:439:LYS:HE3	2.01	0.43
1:A:66:LEU:O	1:A:67:HIS:C	2.58	0.42
1:A:420:THR:HG21	1:A:531:GLU:HG2	2.00	0.42
1:A:438:CYS:HA	1:A:445:ARG:HD2	2.01	0.42
1:B:370:TYR:CD1	1:B:371:ALA:N	2.87	0.42
1:B:464:HIS:HE1	1:B:470:SER:H	1.67	0.42
1:A:46:VAL:HG12	1:A:46:VAL:O	2.19	0.42
1:A:137:LYS:HD2	1:A:137:LYS:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:PHE:CE1	1:A:400:GLU:HA	2.52	0.42
1:A:483:ASN:O	1:A:487:CYS:HB2	2.18	0.42
1:B:554:PHE:HE1	1:B:571:GLU:HB2	1.84	0.42
1:A:197:ARG:HD2	1:A:197:ARG:O	2.18	0.42
1:A:348:ARG:CG	1:A:482:VAL:HG12	2.49	0.42
1:A:551:PHE:HA	1:A:575:LEU:HD11	2.01	0.42
1:B:31:LEU:HB2	1:B:39:HIS:CE1	2.54	0.42
1:B:49:PHE:CZ	1:B:69:LEU:HD11	2.54	0.42
1:A:50:ALA:O	1:A:54:VAL:HG23	2.20	0.42
1:A:226:ALA:HB1	1:A:271:ILE:HD12	2.00	0.42
1:A:544:LEU:C	1:A:546:ALA:N	2.71	0.42
1:B:293:VAL:HG23	1:B:294:GLU:H	1.85	0.42
1:B:258:ALA:O	1:B:262:LYS:HG3	2.20	0.42
1:B:364:ALA:O	1:B:365:ASP:HB3	2.19	0.42
1:B:377:PHE:N	1:B:377:PHE:CD1	2.87	0.42
1:A:485:ARG:HD2	1:A:485:ARG:C	2.39	0.42
1:B:330:PHE:HE2	1:B:334:TYR:HD2	1.67	0.42
1:B:446:MET:CB	1:B:447:PRO:HD3	2.50	0.42
1:B:517:SER:HB3	1:B:520:GLU:CG	2.40	0.42
1:A:114:ARG:HH11	2:A:586:LQZ:HACB	1.84	0.42
1:B:84:TYR:HB3	1:B:87:MET:O	2.20	0.42
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.49	0.42
1:A:218:ARG:HG2	1:A:222:ARG:HH21	1.85	0.42
1:A:317:LYS:O	1:A:317:LYS:HD3	2.20	0.42
1:A:356:THR:HA	1:A:359:LYS:HG2	2.01	0.42
1:B:11:PHE:O	1:B:15:GLY:HA2	2.20	0.42
1:B:179:LEU:N	1:B:180:PRO:CD	2.82	0.42
1:A:430:LEU:HD23	1:A:456:VAL:HG11	2.01	0.42
1:B:309:PHE:CZ	1:B:330:PHE:HA	2.54	0.42
1:A:114:ARG:HG3	1:A:115:LEU:N	2.34	0.41
1:B:120:VAL:HG12	1:B:178:LEU:HD23	2.02	0.41
1:B:233:LYS:C	1:B:233:LYS:HD2	2.40	0.41
1:B:273:SER:O	1:B:276:LYS:HG3	2.20	0.41
1:B:471:ASP:O	1:B:475:LYS:HB2	2.19	0.41
1:B:558:CYS:HB3	1:B:568:PHE:CE2	2.55	0.41
1:A:37:GLU:HA	1:A:40:VAL:HG22	2.01	0.41
1:A:107:ASP:O	1:A:147:PRO:HG2	2.20	0.41
1:A:139:LEU:HD22	1:A:154:LEU:HG	2.01	0.41
1:A:176:ALA:O	1:A:180:PRO:HG2	2.20	0.41
1:B:31:LEU:HB2	1:B:39:HIS:HE1	1.86	0.41
1:B:48:GLU:O	1:B:52:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:VAL:HG23	1:B:235:VAL:HG21	2.02	0.41
1:B:419:SER:O	1:B:422:THR:HB	2.19	0.41
1:B:330:PHE:CD2	1:B:330:PHE:C	2.92	0.41
1:B:492:GLU:HG3	1:B:493:VAL:HG22	2.02	0.41
1:A:115:LEU:HD13	1:A:115:LEU:HA	1.76	0.41
1:A:261:ALA:HB1	1:A:286:LYS:HG2	2.03	0.41
1:A:366:PRO:O	1:A:369:CYS:HB3	2.20	0.41
1:B:370:TYR:HD1	1:B:371:ALA:N	2.18	0.41
1:B:499:PRO:HB3	1:B:535:HIS:O	2.20	0.41
1:A:13:ASP:HB2	1:A:255:ASP:OD1	2.21	0.41
1:A:139:LEU:CD2	1:A:154:LEU:HG	2.51	0.41
1:B:376:GLU:C	1:B:379:PRO:HD2	2.41	0.41
1:A:325:VAL:O	1:A:329:MET:HG3	2.20	0.41
1:A:446:MET:CB	1:A:447:PRO:HD3	2.50	0.41
1:A:435:SER:O	1:A:439:LYS:HE3	2.21	0.41
1:B:398:LEU:O	1:B:402:LYS:HB2	2.20	0.41
1:B:458:ASN:C	1:B:460:LEU:H	2.23	0.41
1:A:5:SER:HA	1:A:62:CYS:O	2.21	0.41
1:A:32:GLN:HE22	1:A:106:LYS:HA	1.85	0.41
1:A:65:SER:O	1:A:66:LEU:C	2.59	0.41
1:A:162:LYS:O	1:A:166:THR:HG23	2.20	0.41
1:A:201:ALA:O	1:A:205:LYS:HB2	2.21	0.41
1:A:330:PHE:CE2	1:A:334:TYR:HD2	2.39	0.41
1:A:408:LEU:HD11	1:A:526:GLN:HB3	2.03	0.41
1:A:447:PRO:O	1:A:448:CYS:C	2.58	0.41
1:A:581:ALA:O	1:A:582:ALA:CB	2.66	0.41
1:B:33:GLN:OE1	1:B:33:GLN:HA	2.21	0.41
1:B:190:LYS:HE3	1:B:190:LYS:HB2	1.80	0.41
1:B:484:ARG:N	1:B:486:PRO:HD2	2.35	0.41
1:A:139:LEU:HD13	1:A:139:LEU:O	2.21	0.41
1:A:313:LYS:HA	1:A:367:HIS:HB2	2.02	0.41
1:B:7:VAL:HG11	1:B:49:PHE:CE1	2.54	0.41
1:B:32:GLN:H	1:B:32:GLN:HG3	1.75	0.41
1:B:135:LEU:HD11	1:B:162:LYS:HB2	2.03	0.41
1:A:268:GLN:HE22	1:A:276:LYS:HA	1.87	0.40
1:B:87:MET:O	1:B:88:ALA:HB3	2.21	0.40
1:B:315:VAL:HG13	1:B:326:PHE:HZ	1.85	0.40
1:B:492:GLU:CG	1:B:493:VAL:N	2.83	0.40
1:B:562:ASP:O	1:B:563:ASP:HB2	2.21	0.40
1:A:71:GLY:O	1:A:74:LEU:HB2	2.21	0.40
1:A:140:TYR:O	1:A:144:ARG:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LYS:HB2	1:A:159:LYS:HZ3	1.86	0.40
1:A:271:ILE:HA	1:A:271:ILE:HD12	1.99	0.40
1:A:398:LEU:HD23	1:A:398:LEU:HA	1.96	0.40
1:A:533:VAL:HA	1:A:536:LYS:NZ	2.35	0.40
1:A:538:LYS:HD2	1:A:538:LYS:N	2.35	0.40
1:B:415:VAL:O	1:B:418:VAL:HG23	2.20	0.40
1:A:266:GLU:C	1:A:268:GLN:H	2.23	0.40
1:B:27:PHE:HZ	1:B:73:LYS:HG3	1.86	0.40
1:B:461:CYS:O	1:B:465:GLU:HB2	2.21	0.40
1:B:199:LYS:HE2	1:B:199:LYS:HB2	1.82	0.40
1:A:122:VAL:HG12	1:B:37:GLU:HB3	2.02	0.40
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.95	0.40
1:B:74:LEU:O	1:B:77:VAL:HG22	2.21	0.40
1:B:100:GLU:C	1:B:102:PHE:H	2.24	0.40
1:B:137:LYS:HD2	1:B:138:TYR:N	2.36	0.40
1:B:293:VAL:HG23	1:B:294:GLU:N	2.36	0.40
1:B:356:THR:HA	1:B:359:LYS:HE3	2.04	0.40
1:B:475:LYS:C	1:B:475:LYS:HD3	2.42	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	580/585 (99%)	468 (81%)	86 (15%)	26 (4%)	2 15
1	B	580/585 (99%)	459 (79%)	94 (16%)	27 (5%)	2 14
All	All	1160/1170 (99%)	927 (80%)	180 (16%)	53 (5%)	2 15

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	60	GLU
1	A	66	LEU
1	A	89	ASP
1	A	97	GLU
1	A	286	LYS
1	A	370	TYR
1	A	502	PHE
1	A	562	ASP
1	B	79	THR
1	B	276	LYS
1	B	325	VAL
1	B	493	VAL
1	B	502	PHE
1	B	562	ASP
1	B	563	ASP
1	A	150	TYR
1	A	272	SER
1	A	493	VAL
1	A	545	LYS
1	B	4	LYS
1	B	16	GLU
1	B	77	VAL
1	B	81	ARG
1	B	305	LEU
1	A	276	LYS
1	A	282	PRO
1	A	288	HIS
1	A	323	LYS
1	A	371	ALA
1	B	60	GLU
1	B	293	VAL
1	B	313	LYS
1	B	503	ASN
1	B	511	ALA
1	A	102	PHE
1	A	483	ASN
1	B	35	PRO
1	B	306	ALA
1	B	370	TYR
1	B	480	SER
1	B	539	ALA
1	A	77	VAL

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Mol	Chain	Res	Type
1	A	312	SER
1	B	323	LYS
1	B	437	CYS
1	A	447	PRO
1	A	482	VAL
1	B	317	LYS
1	B	537	PRO
1	B	282	PRO
1	A	303	PRO
1	A	96	PRO

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	509/511 (100%)	467 (92%)	42 (8%)	11	36
1	B	509/511 (100%)	471 (92%)	38 (8%)	13	39
All	All	1018/1022 (100%)	938 (92%)	80 (8%)	12	37

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	38	ASP
1	A	57	GLU
1	A	66	LEU
1	A	98	ARG
1	A	102	PHE
1	A	114	ARG
1	A	115	LEU
1	A	131	GLU
1	A	137	LYS
1	A	149	PHE
1	A	150	TYR
1	A	159	LYS

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Mol	Chain	Res	Type
1	A	177	CYS
1	A	186	ARG
1	A	243	THR
1	A	245	CYS
1	A	268	GLN
1	A	275	LEU
1	A	276	LYS
1	A	294	GLU
1	A	298	MET
1	A	308	ASP
1	A	313	LYS
1	A	321	GLU
1	A	334	TYR
1	A	355	THR
1	A	367	HIS
1	A	370	TYR
1	A	375	ASP
1	A	412	THR
1	A	425	GLU
1	A	445	ARG
1	A	446	MET
1	A	453	LEU
1	A	483	ASN
1	A	484	ARG
1	A	512	ASP
1	A	516	LEU
1	A	526	GLN
1	A	536	LYS
1	A	556	GLU
1	B	14	LEU
1	B	48	GLU
1	B	57	GLU
1	B	60	GLU
1	B	73	LYS
1	B	74	LEU
1	B	94	GLN
1	B	98	ARG
1	B	107	ASP
1	B	108	ASP
1	B	111	ASN
1	B	121	ASP
1	B	135	LEU

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Mol	Chain	Res	Type
1	B	137	LYS
1	B	139	LEU
1	B	150	TYR
1	B	159	LYS
1	B	179	LEU
1	B	222	ARG
1	B	233	LYS
1	B	249	ASP
1	B	267	ASN
1	B	276	LYS
1	B	283	LEU
1	B	297	GLU
1	B	318	ASN
1	B	329	MET
1	B	367	HIS
1	B	388	ILE
1	B	412	THR
1	B	444	LYS
1	B	446	MET
1	B	451	ASP
1	B	472	ARG
1	B	484	ARG
1	B	536	LYS
1	B	547	VAL
1	B	575	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	18	ASN
1	A	29	GLN
1	A	32	GLN
1	A	99	ASN
1	A	104	GLN
1	A	130	ASN
1	A	204	GLN
1	A	268	GLN
1	A	295	ASN
1	A	318	ASN
1	A	338	HIS
1	A	385	GLN

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Mol	Chain	Res	Type
1	A	459	GLN
1	A	464	HIS
1	A	483	ASN
1	A	522	GLN
1	A	535	HIS
1	B	18	ASN
1	B	29	GLN
1	B	61	ASN
1	B	67	HIS
1	B	99	ASN
1	B	104	GLN
1	B	111	ASN
1	B	204	GLN
1	B	221	GLN
1	B	242	HIS
1	B	295	ASN
1	B	318	ASN
1	B	338	HIS
1	B	367	HIS
1	B	385	GLN
1	B	459	GLN
1	B	464	HIS
1	B	483	ASN
1	B	535	HIS

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LQZ	A	586	-	17,17,17	5.98	9 (52%)	22,22,22	1.52	4 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LQZ	A	586	-	-	6/12/12/12	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	586	LQZ	CAP-CAO	13.53	1.60	1.40
2	A	586	LQZ	CAP-CAN	10.56	1.56	1.40
2	A	586	LQZ	CAF-CAG	8.78	1.57	1.38
2	A	586	LQZ	CAF-CAH	8.71	1.57	1.38
2	A	586	LQZ	CAG-CAN	7.77	1.56	1.39
2	A	586	LQZ	CAH-CAO	7.10	1.54	1.39
2	A	586	LQZ	C-NAL	5.20	1.47	1.35
2	A	586	LQZ	CAP-NAL	2.70	1.48	1.43
2	A	586	LQZ	O-C	-2.35	1.18	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	586	LQZ	CA-C-NAL	4.36	122.32	114.12
2	A	586	LQZ	O-C-NAL	-2.29	119.45	123.63
2	A	586	LQZ	CAH-CAO-CAP	2.11	120.90	117.77
2	A	586	LQZ	CAN-CAP-NAL	2.07	122.21	119.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	586	LQZ	CAN-CAP-NAL-C
2	A	586	LQZ	CAA-CAI-N-CAJ
2	A	586	LQZ	CAA-CAI-N-CA
2	A	586	LQZ	CAB-CAJ-N-CA
2	A	586	LQZ	CAB-CAJ-N-CAI
2	A	586	LQZ	CAO-CAP-NAL-C

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	586	LQZ	8	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	582/585 (99%)	-0.29	2 (0%) 94 94	75, 135, 213, 291	0
1	B	582/585 (99%)	-0.31	3 (0%) 91 91	78, 140, 213, 306	0
All	All	1164/1170 (99%)	-0.30	5 (0%) 92 93	75, 137, 213, 306	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	GLY	3.7
1	B	150	TYR	3.4
1	B	86	GLU	3.1
1	A	299	PRO	2.4
1	A	309	PHE	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LQZ	A	586	17/17	0.87	0.31	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.