



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:15 PM UTC

PDB ID : 3JQZ / pdb_00003jqz
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

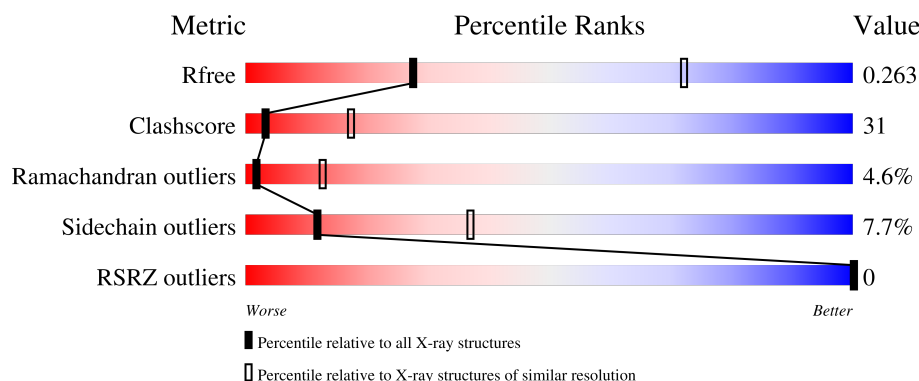
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

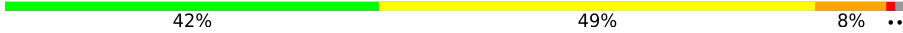
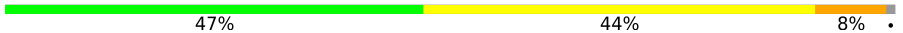
The reported resolution of this entry is 3.30 Å.

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	585	 42% 49% 8% ..
1	B	585	 47% 44% 8% .

2 Entry composition [i](#)

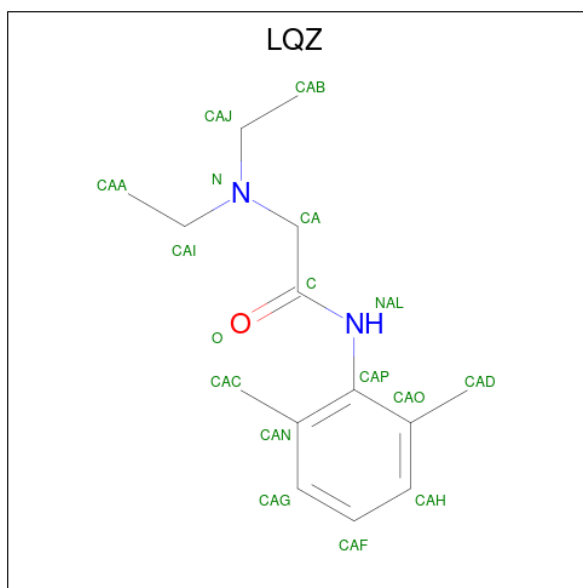
There are 2 unique types of molecules in this entry. The entry contains 9279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	582	Total	C	N	O	S	0	0	0
			4631	2922	783	885	41			
1	B	582	Total	C	N	O	S	0	0	0
			4631	2922	783	885	41			

- Molecule 2 is 2-(diethylamino)-N-(2,6-dimethylphenyl)ethanamide (CCD ID: LQZ) (formula: C₁₄H₂₂N₂O).

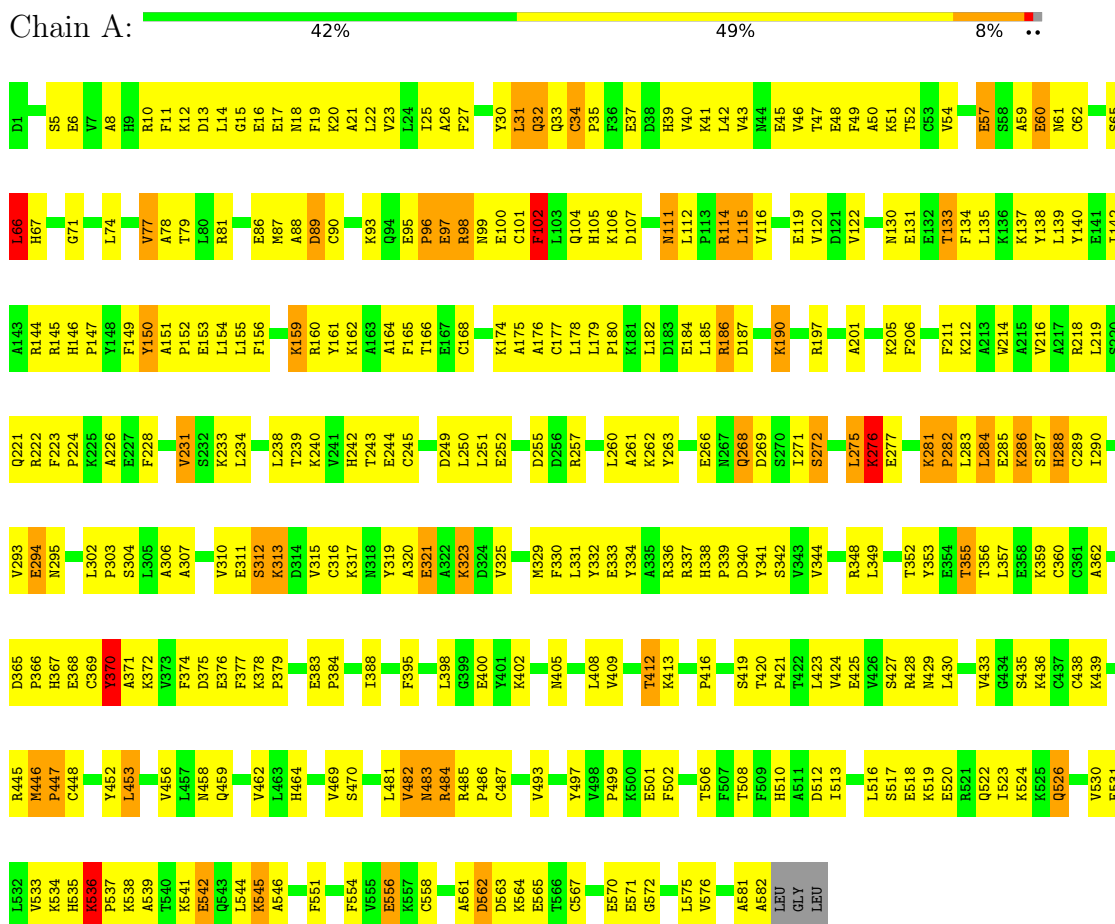


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	14	2	1		

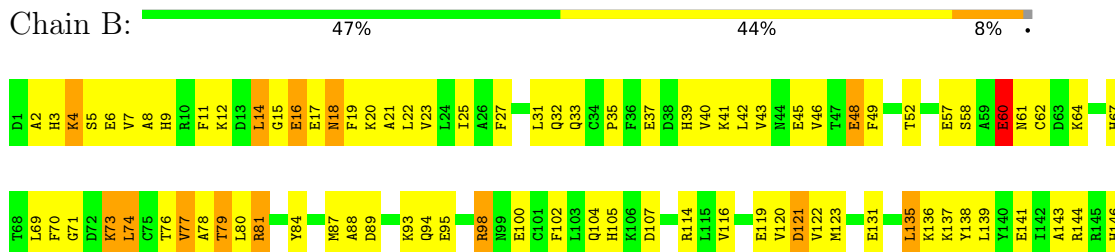
3 Residue-property plots

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: Serum albumin



• Molecule 1: Serum albumin



A561	F149	E401	K323	D249	F150
D562	Y150	K402	V325	L250	A151
D563	A151	F403	F326	L251	P152
K564	R484	Q404	L327	E252	E153
E565	R485	G328	M329	R257	L154
T566	P486	L408	F330	A258	L155
G567	E492	T412	E333	K262	F156
F568	V493	V415	Y334	A158	F157
A569	Y497	P416	A335	E266	A159
E570	V498	Q417	R337	N267	R160
K574	P499	S419	H338	Y161	Y161
L575	E501	T420	P339	I271	K162
A581	F502	P421	D340	S272	F165
LEU	N503	L423	Y341	S273	A175
GLY	A504	G431	S342	K274	A176
LEU	F509	K432	Y343	K276	C177
	H510	V433	V344	E277	L178
	A511	G434	R348	P282	L179
	D512	S435	Y353	L283	P180
	I513	K436	E354	K286	K190
	C514	C437	T355	S287	K195
	T515	C438	T356	H288	K199
	L516	K439	L357	C289	C200
	S517	E358	I290	K199	A201
	E518	K444	K359	V293	S202
	K519	R445	C360	E294	L203
	E520	M446	C361	N295	Q204
	R521	P447	A362	D296	K205
	Q522	C448	A363	E297	F211
	I523	A449	A364	N298	W214
	K524	E450	D365	P299	A215
	K525	D451	P366	L302	V216
	Q526	Y452	H367	P303	A217
	V530	L453	Y370	S304	R218
	H535	V456	A371	L305	R222
	K536	L457	K372	A306	F223
	P537	N458	V373	A307	P224
	K538	Q459	F374	D375	K225
	A539	L460	D375	F309	A226
	T540	C461	E376	V310	E227
	Q543	L463	K378	E311	F228
	V547	H464	P379	S312	K233
	N548	E465	K313	D314	L234
	F551	V469	V315	C316	V235
	F554	S470	Q385	K317	T239
	V555	D471	N386	W318	T243
	E556	R472	L387	Y319	
	K557	K475	I388	A320	
	C558	E479	L398	E321	
			G399	A322	

4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	168.48 Å 168.48 Å 97.02 Å 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 3.32 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.220 , 0.268 0.213 , 0.263	Depositor DCC
R_{free} test set	1054 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	115.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 98.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.044 for -k,-h,-l	Xtriage
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

Xtriage'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

5.1 Standard geometry

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	0.37	2/4721 (0.0%)	0.75	11/6368 (0.2%)
1	B	0.28	0/4721	0.73	4/6368 (0.1%)
All	All	0.33	2/9442 (0.0%)	0.74	15/12736 (0.1%)

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	11.11	1.48	1.32
1	A	182	LEU	C-N	-8.78	1.21	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	GLU	N-CA-C	-8.15	102.38	113.30
1	A	184	GLU	N-CA-C	-8.06	102.58	111.36
1	A	111	ASN	O-C-N	-7.95	112.12	122.61
1	B	565	GLU	N-CA-C	-7.04	104.84	113.50
1	B	18	ASN	N-CA-C	-6.09	105.89	113.38
1	A	146	HIS	CA-C-N	5.97	125.67	119.82
1	A	146	HIS	C-N-CA	5.97	125.67	119.82
1	A	281	LYS	CA-C-N	5.83	127.12	119.84
1	A	281	LYS	C-N-CA	5.83	127.12	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	ASP	N-CA-C	-5.67	105.11	113.61
1	A	34	CYS	CA-C-N	5.58	126.81	119.84
1	A	34	CYS	C-N-CA	5.58	126.81	119.84
1	B	460	LEU	N-CA-C	-5.45	107.28	114.04
1	A	536	LYS	CA-C-N	5.18	126.32	119.84
1	A	536	LYS	C-N-CA	5.18	126.32	119.84

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 ⓘ

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	302	0
1	B	4631	0	4552	272	0
2	A	17	0	22	5	0
All	All	9279	0	9126	564	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 31.

All (564) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:548:MET:HE3	1:B:548:MET:HA	1.70	0.73
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:370:TYR:C	1:B:372:LYS:H	1.99	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:B:71:GLY:C	1:B:98:ARG:HH11	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:10:ARG:O	1:A:14:LEU:HG	1.97	0.65
1:A:544:LEU:C	1:A:546:ALA:H	2.04	0.64
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
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:388:ILE:HD11	1:B:446:MET:HE3	1.81	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: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
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: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:12:LYS:HZ1	1:A:54:VAL:HG13	1.65	0.62
1:A:522:GLN:O	1:A:526:GLN:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:310:VAL:HG23	1:B:311:GLU:CD	2.26	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
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:B:324:ASP:C	1:B:326:PHE:H	2.11	0.59
1:B:123:MET:HE2	1:B:165:PHE:HZ	1.68	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:561:ALA:O	1:A:562:ASP:C	2.48	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:16:GLU:C	1:B:18:ASN:H	2.14	0.56
1:B:502:PHE:HE1	1:B:504:ALA:HB2	1.71	0.56
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:306:ALA:C	1:B:310:VAL:HG22	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:360:CYS:C	1:A:362:ALA:H	2.16	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: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:A:59:ALA:O	1:A:60:GLU:C	2.50	0.54
1:B:295:ASN:HD22	1:B:339:PRO:HB3	1.72	0.54
1:A:575:LEU:C	1:A:575:LEU:HD23	2.33	0.53
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
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:B:373:VAL:C	1:B:375:ASP:H	2.16	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:B:195:LYS:HZ1	1:B:218:ARG:HH12	1.57	0.53
1:B:249:ASP:HB3	1:B:252:GLU:CD	2.33	0.53
1:A:78:ALA:HA	1:A:81:ARG:HB2	1.91	0.53
1:A:563:ASP:C	1:A:564:LYS:HD2	2.34	0.53
1:A:519:LYS:O	1:A:523:ILE:HG13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:87:MET:HE2	1:B:515:THR:HB	1.91	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:B:74:LEU:C	1:B:76:THR:H	2.17	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:76:THR:C	1:B:78:ALA:H	2.19	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:540:THR:HG23	1:B:543:GLN:H	1.74	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
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:2:ALA:O	1:B:3:HIS:HB2	2.09	0.51
1:B:538:LYS:HD2	1:B:538:LYS:H	1.76	0.51
1:A:77:VAL:C	1:A:79:THR:H	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:86:GLU:O	1:A:87:MET:HB3	2.10	0.50
1:A:87:MET:CE	1:B:515:THR:HB	2.42	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: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: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:A:269:ASP:C	1:A:271:ILE:H	2.20	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:77:VAL:C	1:A:79:THR:N	2.70	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
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:B:275:LEU:O	1:B:276:LYS:C	2.56	0.49
1:A:90:CYS:HG	1:A:101:CYS:HG	1.58	0.49
1:A:134:PHE:O	1:A:137:LYS:HE3	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:586:LQZ:CAC	2:A:586:LQZ:O	2.61	0.48
1:A:79:THR:C	1:A:81:ARG:H	2.21	0.48
1:B:224:PRO:CD	1:B:296:ASP:HB3	2.35	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: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:A:446:MET:HE2	1:A:446:MET:O	2.14	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:17:GLU:C	1:A:19:PHE:H	2.20	0.47
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:66:LEU:O	1:A:67:HIS:C	2.58	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:A:542:GLU:CD	1:A:542:GLU:H	2.20	0.47
1:B:551:PHE:O	1:B:555:VAL:HG13	2.14	0.47
1:A:137:LYS:HD2	1:A:137:LYS:C	2.40	0.47
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:B:87:MET:HE2	1:B:105:HIS:CD2	2.50	0.47
1:A:30:TYR:HB3	1:A:31:LEU:HD23	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:TYR:C	1:B:372:LYS:N	2.67	0.47
1:A:8:ALA:HB1	1:A:12:LYS:HZ2	1.80	0.47
1:A:30:TYR:HE1	1:A:102:PHE:HB3	1.79	0.47
1:A:485:ARG:HD2	1:A:485:ARG:C	2.39	0.47
1:B:5:SER:OG	1:B:62:CYS:HB3	2.14	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:B:233:LYS:C	1:B:233:LYS:HD2	2.40	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:330:PHE:C	1:B:330:PHE:CD2	2.92	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:B:376:GLU:C	1:B:379:PRO:HD2	2.41	0.46
1:B:458:ASN:C	1:B:460:LEU:H	2.23	0.46
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:65:SER:O	1:A:66:LEU:C	2.59	0.45
1:A:284:LEU:HD22	1:A:284:LEU:N	2.31	0.45
1:A:447:PRO:O	1:A:448:CYS:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:222:ARG:HG2	1:A:223:PHE:CE1	2.52	0.45
1:A:266:GLU:C	1:A:268:GLN:H	2.23	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:100:GLU:C	1:B:102:PHE:H	2.24	0.45
1:B:446:MET:HB3	1:B:447:PRO:HD3	1.99	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: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:87:MET:O	1:A:88:ALA:C	2.60	0.44
1:A:302:LEU:C	1:A:304:SER:H	2.25	0.44
1:A:567:CYS:O	1:A:571:GLU:N	2.49	0.44
1:B:114:ARG:O	1:B:114:ARG:HG3	2.17	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:B:137:LYS:C	1:B:137:LYS:HD2	2.43	0.44
1:B:513:ILE:O	1:B:521:ARG:HD3	2.17	0.44
1:A:43:VAL:C	1:A:45:GLU:H	2.26	0.44
1:B:199:LYS:HG3	1:B:211:PHE:HE1	1.82	0.44
1:B:475:LYS:HD3	1:B:475:LYS:C	2.42	0.44
1:B:564:LYS:HD2	1:B:566:THR:OG1	2.17	0.44
1:B:304:SER:O	1:B:305:LEU:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:319:TYR:C	1:B:321:GLU:H	2.25	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:16:GLU:C	1:B:18:ASN:N	2.76	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:25:ILE:O	1:A:26:ALA:C	2.61	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:544:LEU:C	1:A:546:ALA:N	2.71	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: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:O	1:A:46:VAL:HG12	2.19	0.42
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:10:ARG:O	1:A:11:PHE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:293:VAL:HG23	1:B:294:GLU:H	1.85	0.42
1:B:324:ASP:C	1:B:326:PHE:N	2.76	0.42
1:A:231:VAL:C	1:A:233:LYS:N	2.77	0.42
1:A:286:LYS:O	1:A:287:SER:C	2.62	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:373:VAL:C	1:B:375:ASP:N	2.77	0.42
1:B:377:PHE:N	1:B:377:PHE:CD1	2.87	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:79:THR:C	1:A:81:ARG:N	2.75	0.42
1:A:185:LEU:O	1:A:186:ARG:C	2.62	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:338:HIS:C	1:A:340:ASP:H	2.27	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:317:LYS:C	1:B:319:TYR:H	2.28	0.41
1:A:21:ALA:C	1:A:23:VAL:N	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:239:THR:O	1:A:240:LYS:C	2.64	0.41
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.46	0.41
1:B:360:CYS:C	1:B:362:ALA:H	2.29	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:A:506:THR:C	1:A:508:THR:H	2.27	0.41
1:A:536:LYS:HE3	1:A:536:LYS:C	2.45	0.41
1:B:319:TYR:C	1:B:321:GLU:N	2.78	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:114:ARG:NH1	2:A:586:LQZ:CAC	2.83	0.41
1:A:139:LEU:CD2	1:A:154:LEU:HG	2.51	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:452:TYR:CD2	1:A:452:TYR:C	2.98	0.41
1:A:95:GLU:HA	1:A:96:PRO:C	2.46	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: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: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: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:446:MET:O	1:B:446:MET:HE2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:483:ASN:C	1:B:486:PRO:HD2	2.45	0.40
1:B:492:GLU:CG	1:B:493:VAL:N	2.83	0.40
1:B:536:LYS:O	1:B:537:PRO:C	2.64	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
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:B:27:PHE:HZ	1:B:73:LYS:HG3	1.86	0.40
1:B:306:ALA:O	1:B:307:ALA:C	2.65	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: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

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 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	580/585 (99%)	459 (79%)	94 (16%)	27 (5%)	2	12
All	All	1160/1170 (99%)	927 (80%)	180 (16%)	53 (5%)	2	13

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	471 (92%)	38 (8%)	12	38
1	B	509/511 (100%)	469 (92%)	40 (8%)	11	36
All	All	1018/1022 (100%)	940 (92%)	78 (8%)	12	37

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	52	THR
1	A	57	GLU
1	A	66	LEU
1	A	98	ARG
1	A	102	PHE

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Mol	Chain	Res	Type
1	A	114	ARG
1	A	115	LEU
1	A	116	VAL
1	A	131	GLU
1	A	133	THR
1	A	159	LYS
1	A	177	CYS
1	A	186	ARG
1	A	190	LYS
1	A	231	VAL
1	A	243	THR
1	A	245	CYS
1	A	268	GLN
1	A	275	LEU
1	A	276	LYS
1	A	284	LEU
1	A	294	GLU
1	A	313	LYS
1	A	321	GLU
1	A	355	THR
1	A	370	TYR
1	A	412	THR
1	A	425	GLU
1	A	446	MET
1	A	453	LEU
1	A	484	ARG
1	A	512	ASP
1	A	516	LEU
1	A	526	GLN
1	A	536	LYS
1	A	542	GLU
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	121	ASP

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Mol	Chain	Res	Type
1	B	135	LEU
1	B	136	LYS
1	B	139	LEU
1	B	150	TYR
1	B	159	LYS
1	B	179	LEU
1	B	216	VAL
1	B	222	ARG
1	B	225	LYS
1	B	239	THR
1	B	267	ASN
1	B	276	LYS
1	B	283	LEU
1	B	297	GLU
1	B	329	MET
1	B	355	THR
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	479	GLU
1	B	484	ARG
1	B	513	ILE
1	B	536	LYS
1	B	547	VAL
1	B	555	VAL
1	B	575	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	18	ASN
1	A	29	GLN
1	A	32	GLN
1	A	67	HIS
1	A	99	ASN
1	A	104	GLN
1	A	130	ASN

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Mol	Chain	Res	Type
1	A	170	GLN
1	A	204	GLN
1	A	268	GLN
1	A	295	ASN
1	A	318	ASN
1	A	338	HIS
1	A	385	GLN
1	A	458	ASN
1	A	459	GLN
1	A	464	HIS
1	A	483	ASN
1	A	522	GLN
1	A	580	GLN
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	128	HIS
1	B	204	GLN
1	B	221	GLN
1	B	242	HIS
1	B	295	ASN
1	B	338	HIS
1	B	385	GLN
1	B	417	GLN
1	B	429	ASN
1	B	464	HIS
1	B	483	ASN
1	B	503	ASN
1	B	535	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

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	6.56	9 (52%)	22,22,22	1.55	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	14.19	1.60	1.40
2	A	586	LQZ	CAP-CAN	11.07	1.56	1.40
2	A	586	LQZ	CAF-CAG	10.82	1.57	1.38
2	A	586	LQZ	CAF-CAH	10.74	1.57	1.38
2	A	586	LQZ	CAG-CAN	8.25	1.56	1.39
2	A	586	LQZ	CAH-CAO	7.55	1.54	1.39
2	A	586	LQZ	C-NAL	5.37	1.47	1.35
2	A	586	LQZ	CAP-NAL	2.79	1.48	1.43
2	A	586	LQZ	O-C	-2.41	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	4.37	122.32	114.23
2	A	586	LQZ	O-C-NAL	-2.34	119.45	123.64
2	A	586	LQZ	CAH-CAO-CAP	2.26	120.90	117.76
2	A	586	LQZ	CAN-CAP-NAL	2.16	122.21	118.99

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 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	586	LQZ	5	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%)	-0.78	0 100 100	75, 135, 213, 291	0
1	B	582/585 (99%)	-0.78	0 100 100	78, 140, 213, 306	0
All	All	1164/1170 (99%)	-0.78	0 100 100	75, 137, 213, 306	0

There are no RSRZ outliers to report.

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](#)

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(Å ²)	Q<0.9
2	LQZ	A	586	17/17	0.92	0.09	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.