



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:53 AM UTC

PDB ID : 1E9Z / pdb_00001e9z
Title : Crystal structure of Helicobacter pylori urease
Authors : Ha, N.-C.; Oh, S.-T.; Oh, B.-H.
Deposited on : 2000-11-01
Resolution : 3.00 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

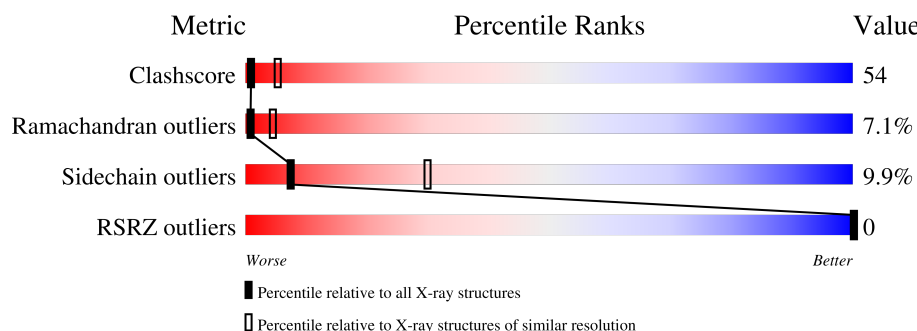
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

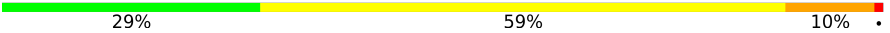
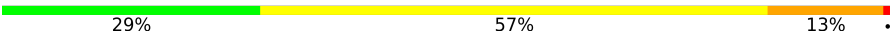
The reported resolution of this entry is 3.00 Å.

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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	238	
2	B	569	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6278 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 UREASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1864	1175	333	348	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	ALA	SER	conflict	UNP P14916

- Molecule 2 is a protein called UREASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	569	Total	C	N	O	S	0	0	0
			4334	2716	747	850	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	219	KCX	LYS	modified residue	UNP P14917
B	355	ALA	ILE	conflict	UNP P69996
B	522	VAL	ILE	conflict	UNP P69996
B	531	ASN	ASP	conflict	UNP P69996

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ni	0	0
			2	2		

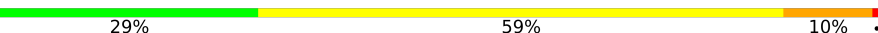
- Molecule 4 is water.

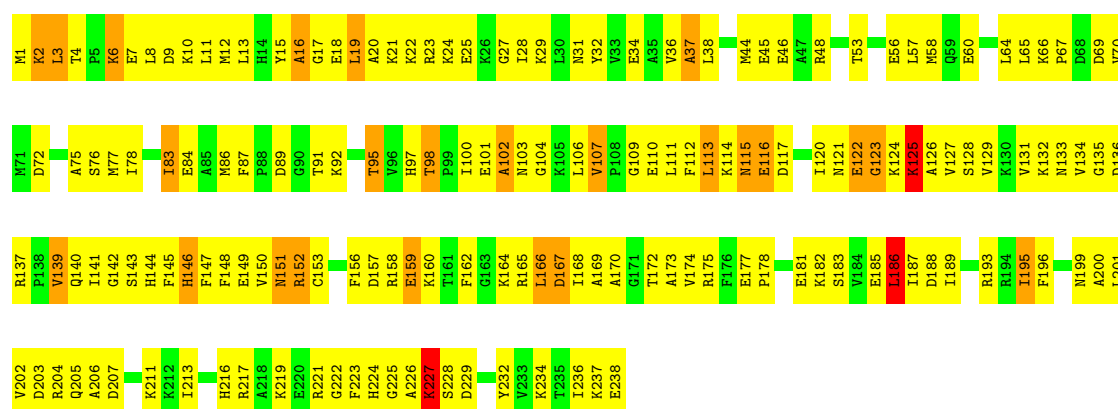
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total 8	O 8	0	0
4	B	70	Total 70	O 70	0	0

3 Residue-property plots

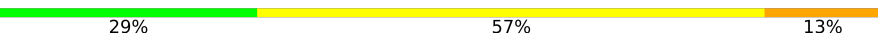
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

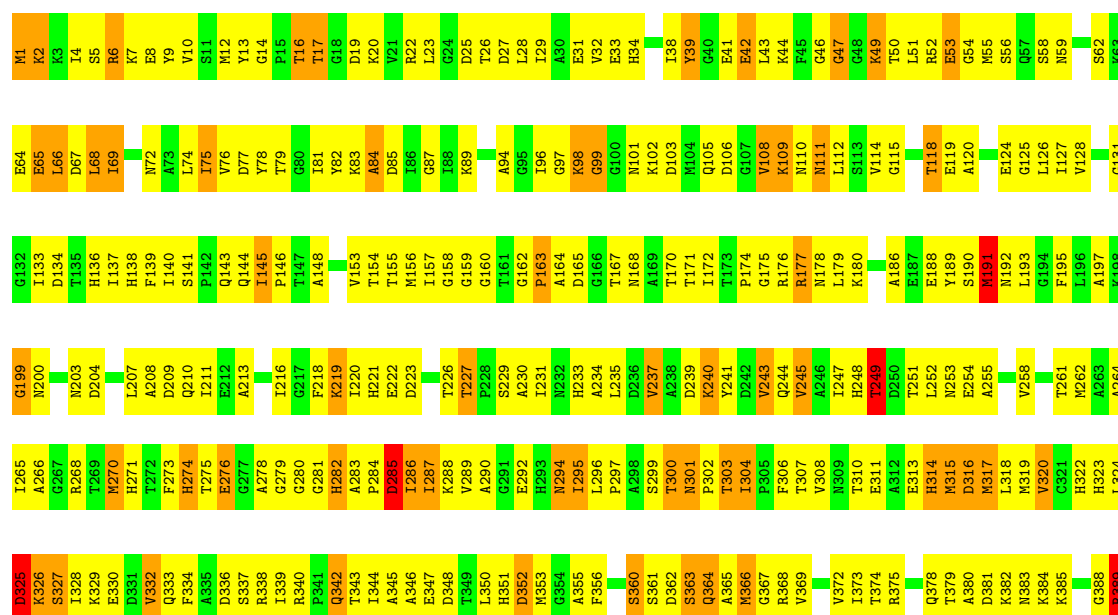
• Molecule 1: UREASE SUBUNIT ALPHA

Chain A: 



• Molecule 2: UREASE SUBUNIT BETA

Chain B: 



K390	K391	E392	K393	G394	G395	D396	N397	D398	N399	F400	R401	I402	K403	R404	Y405	L406	S407	K408	Y409	T410	I411	N412	P413	A414	I415	A416	H417	G418	I419	S420	E421	Y422	V423	G424	S425	V426	E427	V428	G429	K430	V431	A432	D433	L434	V435	L436	W437	S438	P439	A440	F441	F442	G443	V444	K445	P446	N447	M448	I449
L450	K451	F454	I455	A456	L457	S458	Q459	M460	G461	D462	A465	S466	I467	P468	T469	P470	Q471	P472	V473	Y474	Y475	R476	E477	M478	F479	A480	H481	H482	A485	K486	Y487	N490	I491	T492	F493	V494	K504	E505	E506	L507	G508	L509	E510	R511	Q512	V513	L514	P515	C519	R520	T523	K524							
K525	D526	M527	Q528	F529	N530	M531	T532	T533	A534	H535	I536	N539	F540	E541	T542	Y543	H544	W545	F546	V547	D548	G549	K550	E551	V552	T553	A557	N558	K559	V560	S561	L562	A563	Q564	L565	F566	S567	I568	F569																				

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	177.91Å 177.91Å 177.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (20.00-3.00) 95.5 (20.00-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.284 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.062 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6278	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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: KCX, NI

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	0.63	0/1892	0.99	8/2532 (0.3%)
2	B	0.70	0/4405	1.03	14/5958 (0.2%)
All	All	0.68	0/6297	1.02	22/8490 (0.3%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	189	TYR	N-CA-C	7.25	121.25	110.52
1	A	101	GLU	N-CA-C	6.37	118.62	109.14
2	B	106	ASP	N-CA-C	6.11	118.45	111.11
1	A	16	ALA	N-CA-C	-6.11	104.69	111.71
2	B	281	GLY	N-CA-C	5.94	118.15	111.85
1	A	142	GLY	N-CA-C	5.87	122.55	112.51
2	B	470	PRO	N-CA-C	5.70	119.81	111.03
1	A	139	VAL	N-CA-C	5.68	116.25	107.78
1	A	98	THR	CA-C-N	5.59	125.21	119.56
1	A	98	THR	C-N-CA	5.59	125.21	119.56
2	B	445	LYS	CA-C-N	5.55	125.45	119.85
2	B	445	LYS	C-N-CA	5.55	125.45	119.85
1	A	186	LEU	N-CA-C	5.50	117.39	108.26
2	B	295	ILE	N-CA-C	5.45	116.83	108.71
2	B	473	VAL	N-CA-C	5.40	114.14	106.53
2	B	423	VAL	N-CA-CB	-5.22	106.31	112.32
2	B	188	GLU	N-CA-C	5.21	116.96	111.28
1	A	222	GLY	N-CA-C	5.20	122.77	115.43
2	B	314	HIS	N-CA-C	5.20	117.63	111.33
2	B	199	GLY	N-CA-C	-5.19	107.88	114.16
2	B	465	ALA	N-CA-C	5.16	116.99	110.33
2	B	75	ILE	N-CA-C	5.15	116.11	108.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1864	0	1909	175	0
2	B	4334	0	4261	512	0
3	B	2	0	0	0	0
4	A	8	0	0	2	0
4	B	70	0	0	14	0
All	All	6278	0	6170	670	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 54.

All (670) 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)
2:B:52:ARG:HH21	2:B:55:MET:HE1	1.21	1.04
2:B:301:ASN:ND2	2:B:368:ARG:H	1.55	1.02
2:B:109:LYS:H	2:B:109:LYS:HE3	1.23	1.02
2:B:200:ASN:HD21	2:B:221:HIS:H	1.01	1.00
2:B:140:ILE:HD12	2:B:364:GLN:HB3	1.42	0.99
2:B:244:GLN:HE21	2:B:245:VAL:H	1.07	0.96
2:B:211:ILE:HD13	2:B:243:VAL:HG21	1.47	0.95
2:B:244:GLN:NE2	2:B:245:VAL:H	1.65	0.94
2:B:405:TYR:HA	2:B:408:LYS:HD2	1.48	0.94
2:B:286:ILE:HG23	2:B:287:ILE:H	1.32	0.94
2:B:115:GLY:H	2:B:118:THR:CG2	1.79	0.93
2:B:300:THR:HG23	2:B:301:ASN:H	1.30	0.93
2:B:165:ASP:HA	2:B:168:ASN:HD22	1.33	0.91
2:B:44:LYS:H	2:B:50:THR:CG2	1.84	0.89
1:A:67:PRO:HB2	1:A:103:ASN:HB2	1.53	0.89
2:B:20:LYS:HG2	2:B:31:GLU:HG3	1.52	0.89
2:B:156:MET:N	2:B:191:MET:HE1	1.87	0.88
2:B:109:LYS:H	2:B:109:LYS:CE	1.86	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:THR:HG21	2:B:286:ILE:HD13	1.57	0.87
2:B:318:LEU:HD21	2:B:339:ILE:HD11	1.57	0.85
2:B:299:SER:HB2	2:B:351:HIS:HE1	1.37	0.85
2:B:44:LYS:O	2:B:50:THR:HG22	1.79	0.82
2:B:301:ASN:HD22	2:B:368:ARG:H	1.26	0.82
1:A:46:GLU:HG2	1:A:57:LEU:HD21	1.62	0.81
2:B:361:SER:O	2:B:367:GLY:HA3	1.81	0.81
2:B:411:ILE:HG21	2:B:528:GLN:HG3	1.63	0.81
1:A:121:ASN:HD21	1:A:165:ARG:HH22	1.30	0.79
2:B:44:LYS:H	2:B:50:THR:HG22	1.45	0.79
2:B:315:MET:HE1	2:B:336:ASP:OD1	1.82	0.79
2:B:347:GLU:HA	2:B:350:LEU:HD12	1.63	0.79
1:A:129:VAL:O	1:A:183:SER:HA	1.83	0.79
2:B:507:LEU:HB2	2:B:509:LEU:CD2	2.12	0.79
1:A:141:ILE:O	1:A:173:ALA:HB1	1.84	0.78
2:B:287:ILE:HD11	2:B:350:LEU:HD11	1.66	0.78
1:A:124:LYS:C	1:A:125:LYS:HD3	2.09	0.78
2:B:286:ILE:HG23	2:B:287:ILE:N	1.99	0.77
1:A:125:LYS:HD3	1:A:125:LYS:N	1.99	0.77
2:B:101:ASN:ND2	2:B:103:ASP:H	1.83	0.77
2:B:422:TYR:O	2:B:431:VAL:HG22	1.85	0.77
2:B:148:ALA:HB2	2:B:369:VAL:HG22	1.65	0.77
2:B:235:LEU:CD1	2:B:265:ILE:HA	2.15	0.76
2:B:507:LEU:HB2	2:B:509:LEU:HD21	1.67	0.76
1:A:149:GLU:HG2	1:A:201:LEU:HD12	1.67	0.75
1:A:159:GLU:HG3	1:A:160:LYS:HD2	1.68	0.75
1:A:21:LYS:HG3	1:A:22:LYS:N	2.01	0.75
2:B:390:LEU:H	2:B:393:GLU:HG3	1.50	0.75
2:B:76:VAL:HG22	2:B:81:ILE:HG23	1.66	0.75
2:B:398:ASP:O	2:B:402:ILE:HG12	1.87	0.74
2:B:136:HIS:HB3	2:B:360:SER:HB3	1.69	0.74
2:B:274:HIS:CB	2:B:279:GLY:HA3	2.18	0.74
2:B:200:ASN:HD21	2:B:221:HIS:N	1.80	0.74
2:B:294:ASN:H	2:B:294:ASN:HD22	1.35	0.74
2:B:186:ALA:HB1	2:B:193:LEU:HD12	1.69	0.73
2:B:318:LEU:HB2	2:B:319:MET:HE2	1.70	0.73
2:B:294:ASN:HD22	2:B:294:ASN:N	1.84	0.73
2:B:144:GLN:HE22	2:B:364:GLN:HB2	1.52	0.73
2:B:153:VAL:HG21	4:B:2014:HOH:O	1.89	0.73
2:B:433:ASP:OD1	2:B:451:LYS:HD2	1.89	0.72
1:A:45:GLU:HG3	4:A:2003:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ASN:HB2	2:B:124:GLU:HB3	1.69	0.72
2:B:390:LEU:HD21	2:B:401:ARG:NH2	2.04	0.72
1:A:4:THR:OG1	1:A:7:GLU:HG3	1.89	0.72
1:A:66:LYS:HG2	1:A:69:ASP:CG	2.15	0.72
1:A:157:ASP:CG	1:A:160:LYS:HD3	2.15	0.71
2:B:27:ASP:N	2:B:381:ASP:OD1	2.23	0.71
2:B:448:MET:HB3	2:B:458:SER:HB2	1.71	0.71
2:B:389:ARG:HH11	2:B:389:ARG:HG3	1.56	0.71
2:B:467:ILE:HG13	2:B:470:PRO:HD3	1.72	0.71
2:B:378:GLN:O	2:B:382:LYS:HG2	1.91	0.71
2:B:390:LEU:HG	4:B:2039:HOH:O	1.91	0.71
2:B:119:GLU:HG3	2:B:120:ALA:N	2.06	0.70
1:A:1:MET:HE3	1:A:3:LEU:HD22	1.72	0.70
2:B:276:GLU:CD	2:B:278:ALA:H	2.00	0.70
2:B:66:LEU:HD21	2:B:87:GLY:HA3	1.72	0.70
1:A:109:GLY:HA2	2:B:22:ARG:O	1.92	0.70
2:B:365:ALA:O	2:B:366:MET:HB2	1.92	0.69
1:A:72:ASP:OD1	1:A:106:LEU:HB3	1.92	0.69
2:B:115:GLY:H	2:B:118:THR:HG23	1.56	0.69
2:B:444:VAL:HG11	2:B:562:LEU:HB3	1.74	0.69
1:A:67:PRO:HB2	1:A:103:ASN:CB	2.22	0.69
2:B:322:HIS:HB2	2:B:324:LEU:HG	1.73	0.69
2:B:454:PHE:HD1	2:B:480:ALA:HB2	1.58	0.69
2:B:381:ASP:HB3	2:B:382:LYS:HZ3	1.58	0.68
2:B:318:LEU:H	2:B:318:LEU:HD22	1.58	0.68
2:B:176:ARG:HD2	2:B:209:ASP:OD1	1.93	0.68
2:B:278:ALA:O	2:B:366:MET:HE1	1.93	0.68
2:B:101:ASN:C	2:B:101:ASN:HD22	2.02	0.68
1:A:46:GLU:HB3	1:A:57:LEU:HD11	1.75	0.68
1:A:132:LYS:HG3	1:A:181:GLU:HB2	1.76	0.67
1:A:87:PHE:CE2	1:A:92:LYS:HB2	2.29	0.67
2:B:397:ASN:HD22	2:B:399:ASN:H	1.42	0.67
2:B:423:VAL:HG22	4:B:2012:HOH:O	1.93	0.67
2:B:23:LEU:HD13	2:B:442:PHE:CE2	2.30	0.66
2:B:275:THR:HG21	2:B:290:ALA:HB2	1.75	0.66
2:B:467:ILE:HD12	2:B:469:THR:CG2	2.26	0.66
2:B:467:ILE:HD12	2:B:469:THR:HG23	1.76	0.66
1:A:217:ARG:O	1:A:221:ARG:HD3	1.96	0.66
2:B:144:GLN:NE2	2:B:364:GLN:HB2	2.10	0.66
2:B:235:LEU:HD11	2:B:265:ILE:HA	1.78	0.66
2:B:304:ILE:O	2:B:375:ARG:HD3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:SER:HB2	2:B:351:HIS:CE1	2.25	0.66
2:B:239:ASP:OD1	2:B:520:ARG:HG3	1.96	0.66
2:B:520:ARG:HD2	2:B:520:ARG:N	2.09	0.66
2:B:78:TYR:CE2	2:B:411:ILE:HG13	2.32	0.65
2:B:274:HIS:HB3	2:B:300:THR:HB	1.77	0.65
2:B:476:ARG:O	2:B:478:MET:HE2	1.96	0.65
2:B:534:ALA:O	2:B:536:ILE:HG22	1.96	0.65
1:A:75:ALA:HA	1:A:100:ILE:HG13	1.78	0.65
2:B:504:LYS:HA	2:B:509:LEU:HD23	1.79	0.65
2:B:176:ARG:NH1	2:B:209:ASP:OD2	2.30	0.65
2:B:374:THR:OG1	2:B:444:VAL:HG12	1.97	0.64
2:B:520:ARG:HA	2:B:520:ARG:HH11	1.62	0.64
2:B:546:PHE:CE2	2:B:551:GLU:HB2	2.33	0.64
2:B:27:ASP:HB2	2:B:385:LYS:NZ	2.12	0.64
2:B:157:ILE:HG23	2:B:216:ILE:HD11	1.78	0.64
2:B:285:ASP:HB3	2:B:288:LYS:HE3	1.79	0.64
2:B:381:ASP:HB3	2:B:382:LYS:NZ	2.12	0.64
2:B:9:TYR:CZ	2:B:13:TYR:HD2	2.15	0.64
2:B:99:GLY:HA2	2:B:108:VAL:HG23	1.79	0.64
2:B:145:ILE:HB	2:B:146:PRO:CD	2.26	0.64
2:B:361:SER:O	2:B:362:ASP:HB2	1.97	0.64
1:A:83:ILE:HD12	1:A:84:GLU:N	2.12	0.64
2:B:412:ASN:HD21	2:B:528:GLN:H	1.44	0.64
2:B:490:ASN:C	2:B:491:ILE:HD12	2.22	0.64
1:A:75:ALA:HA	1:A:100:ILE:CD1	2.28	0.64
2:B:319:MET:HG3	2:B:326:LYS:CE	2.28	0.64
2:B:444:VAL:CG1	2:B:562:LEU:HB3	2.27	0.64
2:B:98:LYS:H	2:B:109:LYS:NZ	1.95	0.64
2:B:25:ASP:OD1	2:B:561:SER:HB2	1.97	0.64
1:A:23:ARG:O	1:A:28:ILE:HG22	1.97	0.64
2:B:390:LEU:HB2	2:B:393:GLU:HG2	1.80	0.63
2:B:287:ILE:HD11	2:B:350:LEU:CD1	2.28	0.63
2:B:550:LYS:HG2	2:B:551:GLU:N	2.12	0.63
1:A:131:VAL:N	1:A:182:LYS:O	2.32	0.63
2:B:301:ASN:ND2	2:B:368:ARG:N	2.38	0.63
2:B:469:THR:N	2:B:470:PRO:HD2	2.12	0.63
2:B:66:LEU:O	2:B:118:THR:HB	1.98	0.63
2:B:115:GLY:H	2:B:118:THR:HG21	1.62	0.63
1:A:107:VAL:HG23	1:A:110:GLU:CD	2.24	0.62
2:B:539:ASN:CG	2:B:542:THR:HG22	2.24	0.62
2:B:245:VAL:HB	2:B:270:MET:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:THR:HB	2:B:381:ASP:CG	2.24	0.62
2:B:422:TYR:O	2:B:430:LYS:HB3	2.00	0.62
2:B:467:ILE:HG13	2:B:470:PRO:CD	2.28	0.62
1:A:158:ARG:HD3	1:A:224:HIS:O	1.99	0.62
2:B:98:LYS:HE3	2:B:99:GLY:O	1.99	0.62
2:B:304:ILE:HG23	2:B:379:THR:OG1	2.00	0.62
2:B:44:LYS:H	2:B:50:THR:HG21	1.61	0.62
2:B:128:VAL:HG22	2:B:436:LEU:HD22	1.82	0.62
2:B:547:VAL:C	2:B:549:GLY:H	2.08	0.61
1:A:134:VAL:O	1:A:134:VAL:HG12	1.99	0.61
1:A:167:ASP:HB2	1:A:187:ILE:HG23	1.83	0.61
2:B:318:LEU:HB3	2:B:324:LEU:HD12	1.81	0.61
2:B:381:ASP:O	2:B:385:LYS:HG2	2.00	0.61
2:B:4:ILE:HD11	2:B:8:GLU:CB	2.31	0.60
2:B:6:ARG:HH11	2:B:6:ARG:HG2	1.64	0.60
2:B:115:GLY:O	2:B:118:THR:HG23	2.01	0.60
2:B:308:VAL:HG23	2:B:557:ALA:O	2.00	0.60
2:B:423:VAL:HG22	2:B:424:GLY:H	1.66	0.60
2:B:352:ASP:OD1	2:B:383:ASN:HB3	2.01	0.60
2:B:404:ARG:CZ	4:B:2042:HOH:O	2.48	0.60
2:B:218:PHE:HB2	2:B:245:VAL:HG13	1.84	0.60
1:A:32:TYR:CD1	1:A:77:MET:HE2	2.37	0.60
1:A:115:ASN:O	1:A:116:GLU:HB2	2.00	0.60
2:B:411:ILE:HG21	2:B:528:GLN:CG	2.30	0.60
2:B:479:PHE:C	2:B:481:HIS:H	2.10	0.60
2:B:171:THR:OG1	2:B:219:KCX:HE2	2.02	0.60
2:B:271:HIS:HA	2:B:296:LEU:HB2	1.82	0.60
2:B:520:ARG:HH11	2:B:520:ARG:CG	2.14	0.60
1:A:170:ALA:HB3	2:B:42:GLU:HG2	1.83	0.60
1:A:213:ILE:HD13	1:A:238:GLU:HB3	1.83	0.60
1:A:227:LYS:HA	1:A:227:LYS:HE2	1.84	0.60
2:B:412:ASN:HD21	2:B:528:GLN:N	2.00	0.60
2:B:58:SER:HB2	2:B:101:ASN:ND2	2.17	0.60
2:B:159:GLY:H	2:B:171:THR:HB	1.67	0.60
2:B:286:ILE:CG2	2:B:287:ILE:H	2.11	0.59
2:B:43:LEU:HD22	2:B:56:SER:OG	2.02	0.59
2:B:46:GLY:HA3	2:B:49:LYS:HD3	1.84	0.59
2:B:141:SER:O	2:B:144:GLN:HG3	2.01	0.59
2:B:394:LYS:HD2	2:B:395:GLY:N	2.17	0.59
2:B:220:ILE:HB	2:B:247:ILE:HG13	1.84	0.59
2:B:261:THR:O	2:B:265:ILE:HG13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:ASN:ND2	2:B:101:ASN:C	2.58	0.59
2:B:300:THR:HG23	2:B:301:ASN:N	2.10	0.59
1:A:121:ASN:ND2	1:A:165:ARG:HH22	1.97	0.59
2:B:423:VAL:HG22	2:B:424:GLY:N	2.18	0.59
2:B:74:LEU:HD23	2:B:127:ILE:HG12	1.85	0.59
2:B:520:ARG:HA	2:B:520:ARG:NH1	2.18	0.59
2:B:6:ARG:O	2:B:7:LYS:C	2.46	0.58
2:B:319:MET:HG3	2:B:326:LYS:NZ	2.18	0.58
2:B:492:THR:HG23	2:B:513:VAL:HG22	1.85	0.58
1:A:76:SER:CB	1:A:107:VAL:HG12	2.34	0.58
2:B:288:LYS:HA	2:B:536:ILE:HG12	1.85	0.58
2:B:346:ALA:HB1	2:B:552:VAL:HG23	1.85	0.58
1:A:143:SER:O	1:A:165:ARG:HB2	2.02	0.58
2:B:38:ILE:HG22	2:B:38:ILE:O	2.04	0.58
2:B:297:PRO:HG3	2:B:524:LYS:HE3	1.85	0.58
2:B:539:ASN:O	2:B:543:TYR:HA	2.04	0.58
1:A:144:HIS:O	2:B:55:MET:HG2	2.04	0.58
1:A:221:ARG:HD2	1:A:221:ARG:N	2.19	0.58
2:B:83:LYS:O	2:B:84:ALA:HB2	2.04	0.58
2:B:180:LYS:HG3	2:B:507:LEU:HD22	1.85	0.58
2:B:62:SER:C	2:B:64:GLU:H	2.11	0.58
2:B:75:ILE:HD12	2:B:82:TYR:CE1	2.39	0.58
2:B:144:GLN:OE1	2:B:363:SER:HB2	2.04	0.58
2:B:200:ASN:ND2	2:B:221:HIS:H	1.86	0.58
2:B:334:PHE:HA	2:B:337:SER:OG	2.04	0.58
2:B:136:HIS:CB	2:B:360:SER:HB3	2.33	0.58
2:B:176:ARG:HA	2:B:179:LEU:HD12	1.85	0.58
2:B:285:ASP:O	2:B:287:ILE:HG22	2.03	0.58
2:B:240:LYS:H	2:B:240:LYS:HD2	1.69	0.57
2:B:316:ASP:O	2:B:319:MET:HG2	2.04	0.57
1:A:193:ARG:HB2	1:A:205:GLN:HE22	1.68	0.57
2:B:137:ILE:HG21	2:B:156:MET:HE2	1.86	0.57
2:B:319:MET:HG3	2:B:326:LYS:HE3	1.85	0.57
2:B:6:ARG:NH1	2:B:19:ASP:OD2	2.37	0.57
2:B:111:ASN:C	2:B:111:ASN:HD22	2.11	0.57
2:B:156:MET:H	2:B:191:MET:HE1	1.70	0.57
2:B:507:LEU:HB2	2:B:509:LEU:HD22	1.85	0.57
1:A:18:GLU:O	1:A:22:LYS:HG3	2.03	0.57
2:B:32:VAL:HG22	2:B:74:LEU:HD13	1.87	0.57
2:B:207:LEU:HD21	2:B:234:ALA:HA	1.87	0.57
2:B:380:ALA:HB2	2:B:405:TYR:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:ASN:ND2	4:B:2040:HOH:O	2.36	0.57
1:A:1:MET:HE3	1:A:3:LEU:CD2	2.34	0.57
1:A:164:LYS:HG2	1:A:188:ASP:HA	1.87	0.57
2:B:288:LYS:HA	2:B:536:ILE:CD1	2.35	0.57
2:B:75:ILE:O	2:B:81:ILE:HA	2.05	0.57
2:B:145:ILE:HB	2:B:146:PRO:HD3	1.87	0.56
2:B:220:ILE:CG2	2:B:226:THR:HG23	2.35	0.56
2:B:542:THR:O	2:B:543:TYR:HB2	2.05	0.56
1:A:122:GLU:O	1:A:123:GLY:C	2.48	0.56
2:B:26:THR:HG22	2:B:561:SER:OG	2.05	0.56
2:B:27:ASP:HB2	2:B:385:LYS:HZ1	1.71	0.56
2:B:211:ILE:CD1	2:B:243:VAL:HG21	2.28	0.56
2:B:274:HIS:HB2	2:B:279:GLY:HA3	1.86	0.56
1:A:8:LEU:H	1:A:8:LEU:HD22	1.70	0.56
2:B:158:GLY:O	2:B:195:PHE:HA	2.06	0.56
2:B:542:THR:OG1	2:B:544:HIS:ND1	2.39	0.56
2:B:66:LEU:HD23	2:B:69:ILE:HG23	1.88	0.56
2:B:109:LYS:HE3	2:B:109:LYS:N	2.08	0.56
2:B:111:ASN:C	2:B:111:ASN:ND2	2.63	0.56
2:B:46:GLY:C	2:B:49:LYS:HD3	2.31	0.56
2:B:539:ASN:OD1	2:B:541:GLU:HB2	2.06	0.56
2:B:530:ASN:H	2:B:530:ASN:HD22	1.53	0.56
1:A:32:TYR:O	1:A:36:VAL:HG23	2.05	0.55
2:B:133:ILE:HG12	2:B:155:THR:HB	1.86	0.55
2:B:285:ASP:O	2:B:287:ILE:N	2.39	0.55
1:A:31:ASN:OD1	1:A:34:GLU:HG3	2.07	0.55
2:B:4:ILE:HG12	2:B:5:SER:N	2.22	0.55
2:B:520:ARG:HG3	2:B:520:ARG:NH1	2.21	0.55
1:A:3:LEU:HD23	1:A:8:LEU:HD11	1.88	0.55
1:A:13:LEU:HB2	2:B:472:PRO:HG3	1.88	0.55
1:A:46:GLU:CG	1:A:57:LEU:HD21	2.35	0.55
2:B:286:ILE:O	2:B:288:LYS:N	2.39	0.55
1:A:177:GLU:O	1:A:178:PRO:C	2.50	0.55
2:B:302:PRO:C	2:B:304:ILE:H	2.14	0.55
2:B:316:ASP:O	2:B:318:LEU:N	2.40	0.55
1:A:45:GLU:O	1:A:48:ARG:HB3	2.06	0.55
1:A:76:SER:HB3	1:A:107:VAL:HG12	1.87	0.55
2:B:329:LYS:HB3	4:B:2031:HOH:O	2.06	0.55
2:B:191:MET:C	2:B:191:MET:HE3	2.31	0.55
2:B:394:LYS:HD2	2:B:395:GLY:H	1.72	0.55
2:B:4:ILE:HD11	2:B:8:GLU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:GLY:CA	2:B:49:LYS:HD3	2.37	0.55
2:B:249:THR:HB	2:B:282:HIS:H	1.71	0.54
2:B:454:PHE:CD1	2:B:480:ALA:HB2	2.40	0.54
2:B:542:THR:HG23	2:B:544:HIS:H	1.72	0.54
2:B:51:LEU:HA	2:B:56:SER:HB3	1.90	0.54
2:B:392:GLU:CD	2:B:392:GLU:H	2.16	0.54
1:A:78:ILE:N	1:A:78:ILE:HD12	2.23	0.54
1:A:196:PHE:HA	1:A:203:ASP:HA	1.90	0.54
2:B:262:MET:HE3	2:B:289:VAL:HG22	1.90	0.54
1:A:124:LYS:O	1:A:125:LYS:C	2.51	0.54
1:A:186:LEU:HD12	1:A:186:LEU:O	2.08	0.54
1:A:204:ARG:NH2	1:A:238:GLU:HA	2.22	0.54
2:B:328:ILE:O	2:B:332:VAL:HG22	2.08	0.54
2:B:346:ALA:O	2:B:350:LEU:HG	2.07	0.54
2:B:278:ALA:HB3	2:B:303:THR:HG21	1.90	0.53
2:B:384:LYS:O	2:B:388:GLY:N	2.36	0.53
2:B:411:ILE:O	2:B:415:ILE:HG13	2.08	0.53
2:B:134:ASP:HB2	4:B:2014:HOH:O	2.08	0.53
2:B:220:ILE:HG21	2:B:226:THR:HG23	1.89	0.53
1:A:115:ASN:O	1:A:116:GLU:CB	2.56	0.53
2:B:16:THR:OG1	2:B:17:THR:N	2.40	0.53
2:B:162:GLY:O	2:B:164:ALA:N	2.37	0.53
2:B:407:SER:HA	2:B:410:THR:OG1	2.08	0.53
2:B:306:PHE:HB3	4:B:2029:HOH:O	2.09	0.53
2:B:155:THR:C	2:B:191:MET:HE1	2.32	0.53
2:B:191:MET:O	2:B:193:LEU:HG	2.08	0.53
2:B:460:MET:HB2	2:B:478:MET:HE1	1.90	0.53
2:B:568:ILE:HG12	2:B:568:ILE:O	2.08	0.53
2:B:471:GLN:HA	2:B:473:VAL:HG23	1.90	0.53
2:B:525:LYS:HG2	4:B:2062:HOH:O	2.07	0.53
1:A:78:ILE:HG22	1:A:78:ILE:O	2.09	0.53
1:A:140:GLN:HE21	1:A:175:ARG:NH1	2.06	0.53
2:B:72:ASN:O	2:B:124:GLU:HA	2.09	0.53
1:A:66:LYS:HG2	1:A:69:ASP:OD1	2.09	0.53
1:A:156:PHE:O	1:A:225:GLY:HA3	2.09	0.53
2:B:126:LEU:CD1	2:B:126:LEU:N	2.72	0.53
2:B:345:ALA:CB	2:B:553:THR:HG23	2.39	0.53
2:B:467:ILE:CD1	2:B:469:THR:HG23	2.39	0.53
2:B:136:HIS:CE1	2:B:362:ASP:OD1	2.62	0.52
2:B:294:ASN:N	2:B:294:ASN:ND2	2.57	0.52
2:B:320:VAL:HG12	2:B:320:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:HG22	1:A:186:LEU:O	2.09	0.52
2:B:247:ILE:HB	2:B:270:MET:SD	2.50	0.52
1:A:19:LEU:HD13	2:B:568:ILE:HD11	1.92	0.52
2:B:32:VAL:HG22	2:B:74:LEU:CD1	2.38	0.52
2:B:482:HIS:O	2:B:485:ALA:HB3	2.08	0.52
1:A:110:GLU:HG2	2:B:22:ARG:HD2	1.91	0.52
1:A:195:ILE:HD13	1:A:195:ILE:N	2.25	0.52
2:B:109:LYS:C	2:B:111:ASN:N	2.68	0.52
2:B:491:ILE:HD12	2:B:491:ILE:N	2.24	0.52
2:B:26:THR:HB	2:B:381:ASP:OD1	2.10	0.52
2:B:301:ASN:HD22	2:B:368:ARG:N	2.02	0.52
2:B:233:HIS:O	2:B:237:VAL:HG12	2.10	0.52
1:A:25:GLU:C	1:A:27:GLY:H	2.18	0.51
1:A:24:LYS:O	1:A:27:GLY:N	2.39	0.51
2:B:44:LYS:N	2:B:50:THR:HG22	2.21	0.51
2:B:324:LEU:O	2:B:325:ASP:C	2.53	0.51
2:B:12:MET:HG2	2:B:13:TYR:CE1	2.45	0.51
2:B:251:THR:O	2:B:253:ASN:N	2.44	0.51
2:B:176:ARG:HH11	2:B:209:ASP:CG	2.17	0.51
2:B:447:ASN:O	2:B:459:GLN:HG2	2.09	0.51
1:A:120:ILE:HD13	1:A:169:ALA:HA	1.92	0.51
1:A:148:PHE:CD1	1:A:148:PHE:C	2.89	0.51
1:A:185:GLU:HG3	2:B:2:LYS:CE	2.41	0.51
2:B:286:ILE:O	2:B:287:ILE:C	2.54	0.51
1:A:147:PHE:O	1:A:150:VAL:HG22	2.11	0.51
2:B:339:ILE:HG22	2:B:339:ILE:O	2.09	0.51
2:B:461:GLY:O	2:B:462:ASP:C	2.54	0.51
2:B:144:GLN:O	2:B:145:ILE:C	2.53	0.51
2:B:314:HIS:O	2:B:315:MET:C	2.53	0.51
2:B:474:TYR:OH	2:B:476:ARG:NH1	2.43	0.51
2:B:85:ASP:OD2	2:B:98:LYS:O	2.29	0.50
1:A:19:LEU:CD1	2:B:568:ILE:HD11	2.42	0.50
2:B:434:LEU:HD12	2:B:450:ILE:HD11	1.93	0.50
1:A:10:LYS:HD2	1:A:44:MET:HE1	1.93	0.50
1:A:75:ALA:HA	1:A:100:ILE:CG1	2.39	0.50
2:B:1:MET:HE3	2:B:1:MET:O	2.11	0.50
2:B:69:ILE:HD13	2:B:114:VAL:CG2	2.40	0.50
2:B:164:ALA:C	2:B:168:ASN:ND2	2.70	0.50
2:B:408:LYS:HE2	2:B:530:ASN:OD1	2.11	0.50
2:B:407:SER:HA	2:B:410:THR:HG1	1.76	0.50
1:A:110:GLU:OE1	1:A:112:PHE:HE2	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:LYS:C	2:B:111:ASN:H	2.18	0.50
2:B:52:ARG:NH1	4:B:2003:HOH:O	2.44	0.50
2:B:404:ARG:O	2:B:408:LYS:HG3	2.12	0.50
1:A:102:ALA:C	1:A:104:GLY:H	2.19	0.50
2:B:28:LEU:C	2:B:29:ILE:HD12	2.37	0.50
1:A:189:ILE:O	1:A:193:ARG:HG2	2.12	0.49
1:A:87:PHE:CD2	1:A:92:LYS:HB2	2.47	0.49
2:B:186:ALA:CB	2:B:193:LEU:HD12	2.40	0.49
1:A:147:PHE:O	1:A:150:VAL:HG13	2.13	0.49
2:B:244:GLN:HE21	2:B:245:VAL:N	1.92	0.49
2:B:450:ILE:HG13	2:B:450:ILE:O	2.10	0.49
1:A:70:VAL:HG21	1:A:100:ILE:HD12	1.94	0.49
1:A:150:VAL:O	1:A:151:ASN:C	2.55	0.49
2:B:226:THR:HG22	2:B:231:ILE:HD11	1.93	0.49
1:A:116:GLU:O	2:B:6:ARG:HD2	2.12	0.49
2:B:208:ALA:HB1	2:B:241:TYR:OH	2.12	0.49
2:B:264:ALA:C	2:B:266:ALA:N	2.69	0.49
1:A:2:LYS:H	1:A:2:LYS:HD3	1.78	0.49
2:B:138:HIS:HA	2:B:171:THR:HG22	1.95	0.49
2:B:286:ILE:C	2:B:288:LYS:N	2.69	0.49
2:B:240:LYS:HD2	2:B:240:LYS:N	2.27	0.49
2:B:520:ARG:HH11	2:B:520:ARG:CA	2.23	0.49
1:A:128:SER:HB3	1:A:183:SER:OG	2.13	0.49
2:B:520:ARG:HG3	2:B:520:ARG:HH11	1.77	0.49
1:A:144:HIS:NE2	2:B:41:GLU:OE1	2.41	0.49
2:B:101:ASN:HD22	2:B:102:LYS:N	2.11	0.49
2:B:234:ALA:O	2:B:237:VAL:HG13	2.13	0.49
2:B:340:ARG:HE	2:B:343:THR:HG21	1.77	0.49
2:B:417:HIS:O	2:B:419:ILE:HG23	2.13	0.49
2:B:494:VAL:O	2:B:515:PRO:HA	2.13	0.49
1:A:144:HIS:HA	1:A:165:ARG:HD2	1.93	0.48
2:B:172:ILE:HG12	2:B:219:KCX:HB2	1.95	0.48
2:B:227:THR:O	2:B:231:ILE:HG13	2.13	0.48
2:B:448:MET:CB	2:B:458:SER:HB2	2.40	0.48
1:A:86:MET:HA	1:A:91:THR:HA	1.95	0.48
2:B:136:HIS:HB2	2:B:360:SER:OG	2.14	0.48
1:A:202:VAL:O	1:A:204:ARG:HG3	2.14	0.48
2:B:220:ILE:HG22	2:B:226:THR:OG1	2.13	0.48
1:A:232:TYR:CE1	1:A:234:LYS:HA	2.49	0.48
2:B:64:GLU:O	2:B:65:GLU:C	2.56	0.48
2:B:519:CYS:C	2:B:520:ARG:HD2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:520:ARG:HH11	2:B:520:ARG:CB	2.26	0.48
1:A:17:GLY:O	1:A:20:ALA:HB3	2.13	0.48
1:A:38:LEU:CD2	1:A:65:LEU:HD21	2.43	0.48
1:A:232:TYR:HE1	1:A:234:LYS:HA	1.78	0.48
2:B:137:ILE:HD12	2:B:156:MET:HE3	1.95	0.48
2:B:286:ILE:CG2	2:B:287:ILE:N	2.70	0.48
2:B:565:LEU:O	2:B:565:LEU:CD2	2.62	0.48
1:A:8:LEU:HD22	1:A:8:LEU:N	2.28	0.48
2:B:156:MET:HG3	2:B:191:MET:CE	2.44	0.48
2:B:268:ARG:HG2	4:B:2026:HOH:O	2.14	0.48
2:B:389:ARG:HG3	2:B:389:ARG:NH1	2.26	0.48
2:B:528:GLN:O	2:B:529:PHE:HB2	2.14	0.48
1:A:237:LYS:O	1:A:237:LYS:HG3	2.13	0.48
2:B:301:ASN:HB3	2:B:302:PRO:CD	2.44	0.48
1:A:29:LYS:HA	1:A:69:ASP:O	2.13	0.47
2:B:85:ASP:HB2	2:B:97:GLY:O	2.14	0.47
2:B:126:LEU:N	2:B:126:LEU:HD12	2.28	0.47
1:A:37:ALA:O	1:A:38:LEU:C	2.56	0.47
1:A:53:THR:OG1	1:A:56:GLU:HG3	2.13	0.47
2:B:467:ILE:O	2:B:470:PRO:HD2	2.15	0.47
1:A:226:ALA:O	1:A:227:LYS:C	2.57	0.47
2:B:53:GLU:C	2:B:55:MET:H	2.22	0.47
2:B:98:LYS:N	2:B:109:LYS:NZ	2.60	0.47
2:B:160:GLY:HA3	2:B:167:THR:HG23	1.95	0.47
1:A:1:MET:O	1:A:2:LYS:C	2.58	0.47
2:B:345:ALA:HB1	2:B:553:THR:HG23	1.97	0.47
1:A:117:ASP:OD1	2:B:5:SER:HA	2.14	0.47
1:A:133:ASN:ND2	1:A:135:GLY:H	2.13	0.47
1:A:216:HIS:O	1:A:219:LYS:HB3	2.14	0.47
2:B:547:VAL:O	2:B:549:GLY:N	2.48	0.47
2:B:274:HIS:HB3	2:B:279:GLY:HA3	1.95	0.47
2:B:338:ARG:HA	2:B:340:ARG:NH1	2.29	0.47
2:B:530:ASN:H	2:B:530:ASN:ND2	2.12	0.47
1:A:1:MET:CE	1:A:3:LEU:HD22	2.43	0.47
2:B:29:ILE:HD12	2:B:29:ILE:N	2.29	0.47
2:B:46:GLY:N	2:B:49:LYS:HB2	2.30	0.47
2:B:138:HIS:O	2:B:140:ILE:N	2.44	0.47
2:B:191:MET:O	2:B:192:ASN:C	2.57	0.47
2:B:299:SER:CB	2:B:351:HIS:HE1	2.20	0.47
2:B:319:MET:HA	2:B:324:LEU:HB2	1.96	0.47
2:B:562:LEU:HA	2:B:566:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASN:C	1:A:153:CYS:H	2.22	0.47
2:B:62:SER:HB3	2:B:110:ASN:ND2	2.30	0.47
2:B:239:ASP:HA	2:B:520:ARG:HG2	1.96	0.47
2:B:244:GLN:HG2	2:B:416:ALA:O	2.15	0.47
2:B:547:VAL:C	2:B:549:GLY:N	2.72	0.47
1:A:114:LYS:O	2:B:6:ARG:HD3	2.15	0.47
2:B:140:ILE:O	2:B:163:PRO:HD3	2.15	0.47
2:B:172:ILE:CG1	2:B:219:KCX:HB2	2.45	0.47
2:B:455:ILE:HG22	2:B:478:MET:CB	2.45	0.47
2:B:374:THR:HA	2:B:443:GLY:O	2.15	0.47
2:B:53:GLU:HG2	2:B:59:ASN:HD21	1.80	0.46
2:B:114:VAL:HA	2:B:118:THR:HG21	1.97	0.46
2:B:297:PRO:HB2	2:B:356:PHE:HD1	1.79	0.46
2:B:311:GLU:N	4:B:2030:HOH:O	2.47	0.46
2:B:460:MET:HB3	2:B:476:ARG:HB2	1.96	0.46
1:A:217:ARG:O	1:A:221:ARG:CD	2.62	0.46
2:B:23:LEU:HB3	2:B:442:PHE:CD2	2.50	0.46
2:B:285:ASP:HB3	2:B:288:LYS:CE	2.45	0.46
1:A:13:LEU:O	1:A:16:ALA:HB3	2.16	0.46
2:B:96:ILE:HG13	2:B:428:VAL:HG23	1.96	0.46
2:B:165:ASP:CA	2:B:168:ASN:HD22	2.15	0.46
2:B:384:LYS:HA	2:B:401:ARG:NH1	2.30	0.46
2:B:98:LYS:CB	2:B:109:LYS:HZ3	2.28	0.46
2:B:275:THR:HB	2:B:356:PHE:CE1	2.50	0.46
1:A:2:LYS:H	1:A:2:LYS:CD	2.27	0.46
2:B:164:ALA:O	2:B:168:ASN:ND2	2.49	0.46
2:B:4:ILE:CG1	2:B:5:SER:N	2.78	0.46
2:B:9:TYR:CE2	2:B:13:TYR:HD2	2.33	0.46
2:B:20:LYS:HE2	2:B:396:ASP:O	2.15	0.46
2:B:33:GLU:O	2:B:34:HIS:CD2	2.68	0.46
2:B:125:GLY:C	2:B:126:LEU:HD12	2.39	0.46
2:B:145:ILE:H	2:B:145:ILE:HG12	1.60	0.46
2:B:389:ARG:HH21	2:B:396:ASP:C	2.22	0.46
2:B:457:LEU:HA	2:B:478:MET:HG2	1.97	0.46
2:B:539:ASN:HB3	2:B:542:THR:HG23	1.98	0.46
2:B:222:GLU:OE1	2:B:251:THR:HB	2.16	0.46
2:B:288:LYS:HA	2:B:536:ILE:CG1	2.46	0.46
2:B:530:ASN:ND2	2:B:530:ASN:N	2.63	0.46
2:B:111:ASN:ND2	2:B:111:ASN:O	2.46	0.46
2:B:251:THR:C	2:B:253:ASN:N	2.73	0.46
2:B:285:ASP:OD1	2:B:285:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HE2	1:A:69:ASP:OD2	2.16	0.46
1:A:125:LYS:O	1:A:125:LYS:HG2	2.16	0.46
1:A:141:ILE:HD13	1:A:141:ILE:N	2.31	0.46
2:B:197:ALA:HB3	2:B:218:PHE:HD2	1.80	0.46
2:B:486:LYS:HG3	2:B:487:TYR:N	2.31	0.46
2:B:43:LEU:HA	2:B:50:THR:HG21	1.98	0.45
2:B:353:MET:HE1	2:B:552:VAL:HG11	1.98	0.45
2:B:350:LEU:HB3	2:B:355:ALA:HB3	1.99	0.45
2:B:471:GLN:HA	2:B:472:PRO:C	2.41	0.45
2:B:479:PHE:HB2	4:B:2048:HOH:O	2.16	0.45
1:A:64:LEU:O	1:A:65:LEU:HD23	2.15	0.45
1:A:185:GLU:HG3	2:B:2:LYS:HE2	1.98	0.45
2:B:283:ALA:HA	2:B:284:PRO:HA	1.75	0.45
2:B:302:PRO:HD3	2:B:367:GLY:HA2	1.98	0.45
2:B:467:ILE:HD12	2:B:469:THR:HG21	1.98	0.45
1:A:58:MET:HG3	1:A:95:THR:O	2.16	0.45
1:A:139:VAL:HG12	1:A:141:ILE:HD11	1.98	0.45
2:B:138:HIS:CD2	2:B:171:THR:CG2	3.00	0.45
2:B:177:ARG:NH1	2:B:180:LYS:HD3	2.30	0.45
2:B:314:HIS:CB	2:B:339:ILE:HD13	2.46	0.45
2:B:148:ALA:HB2	2:B:369:VAL:CG2	2.41	0.45
2:B:363:SER:CB	2:B:369:VAL:HB	2.46	0.45
1:A:23:ARG:C	1:A:28:ILE:HG22	2.42	0.45
1:A:156:PHE:CE1	1:A:158:ARG:HA	2.51	0.45
1:A:111:LEU:CD2	2:B:10:VAL:HG11	2.47	0.45
2:B:4:ILE:HD11	2:B:8:GLU:HB3	1.96	0.45
2:B:10:VAL:O	2:B:14:GLY:N	2.48	0.45
2:B:38:ILE:O	2:B:39:TYR:C	2.60	0.45
2:B:136:HIS:HB2	2:B:273:PHE:CE1	2.51	0.45
2:B:299:SER:CB	2:B:351:HIS:CE1	2.98	0.45
2:B:340:ARG:O	2:B:344:ILE:HG13	2.17	0.45
2:B:251:THR:C	2:B:253:ASN:H	2.23	0.45
2:B:405:TYR:HA	2:B:408:LYS:CD	2.34	0.45
2:B:407:SER:O	2:B:412:ASN:HB2	2.17	0.45
1:A:107:VAL:HG23	1:A:110:GLU:OE2	2.17	0.45
2:B:172:ILE:O	2:B:174:PRO:HD3	2.17	0.45
2:B:46:GLY:O	2:B:47:GLY:C	2.59	0.45
2:B:203:ASN:O	2:B:204:ASP:C	2.60	0.45
2:B:393:GLU:OE1	2:B:398:ASP:HA	2.17	0.45
1:A:6:LYS:O	1:A:9:ASP:HB2	2.17	0.44
1:A:162:PHE:CE1	1:A:211:LYS:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:GLN:O	2:B:146:PRO:HG2	2.17	0.44
2:B:289:VAL:HG12	2:B:295:ILE:HG21	1.98	0.44
1:A:219:LYS:HG2	1:A:229:ASP:OD2	2.17	0.44
2:B:9:TYR:CZ	2:B:13:TYR:CD2	3.02	0.44
2:B:361:SER:HB3	2:B:372:VAL:CG2	2.46	0.44
1:A:87:PHE:HB2	1:A:89:ASP:OD2	2.17	0.44
2:B:25:ASP:OD1	2:B:25:ASP:C	2.60	0.44
1:A:3:LEU:HD23	1:A:8:LEU:CD1	2.47	0.44
2:B:411:ILE:CG2	2:B:528:GLN:CG	2.96	0.44
2:B:422:TYR:OH	2:B:515:PRO:O	2.29	0.44
2:B:490:ASN:O	2:B:512:GLN:HB3	2.17	0.44
1:A:111:LEU:HD21	2:B:10:VAL:HG11	1.99	0.44
1:A:152:ARG:HB2	1:A:223:PHE:HA	1.99	0.44
2:B:69:ILE:HD13	2:B:114:VAL:HG21	1.99	0.44
2:B:226:THR:HG22	2:B:226:THR:O	2.17	0.44
1:A:60:GLU:O	1:A:60:GLU:HG2	2.17	0.44
2:B:325:ASP:OD1	2:B:327:SER:HB3	2.17	0.44
2:B:332:VAL:O	2:B:333:GLN:HG3	2.18	0.44
2:B:382:LYS:HE3	2:B:560:VAL:HA	1.99	0.44
2:B:550:LYS:CG	2:B:551:GLU:N	2.81	0.44
2:B:197:ALA:HB3	2:B:218:PHE:CD2	2.53	0.44
2:B:207:LEU:HD23	2:B:237:VAL:HG11	1.99	0.44
1:A:147:PHE:CE1	1:A:166:LEU:HD21	2.53	0.44
2:B:420:SER:O	2:B:430:LYS:HE2	2.18	0.44
2:B:547:VAL:HG12	2:B:552:VAL:HG13	2.00	0.44
1:A:140:GLN:HE21	1:A:175:ARG:HH11	1.64	0.44
2:B:6:ARG:HG2	2:B:6:ARG:NH1	2.32	0.44
2:B:67:ASP:OD2	2:B:89:LYS:HA	2.18	0.44
2:B:318:LEU:CD2	2:B:339:ILE:HD11	2.38	0.44
2:B:527:MET:HA	2:B:527:MET:HE2	1.99	0.44
2:B:62:SER:C	2:B:64:GLU:N	2.76	0.43
1:A:97:HIS:O	1:A:98:THR:C	2.61	0.43
2:B:136:HIS:O	2:B:362:ASP:HA	2.17	0.43
1:A:166:LEU:HD13	1:A:174:VAL:CG2	2.47	0.43
2:B:279:GLY:HA2	2:B:366:MET:CE	2.48	0.43
2:B:307:THR:H	2:B:310:THR:HG23	1.84	0.43
2:B:308:VAL:HG21	2:B:558:ASN:OD1	2.18	0.43
2:B:412:ASN:N	2:B:413:PRO:HD2	2.33	0.43
2:B:94:ALA:C	2:B:111:ASN:HD21	2.26	0.43
2:B:133:ILE:HG23	2:B:155:THR:HB	2.01	0.43
2:B:363:SER:HB3	2:B:369:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:SER:HA	2:B:439:PRO:HD2	1.78	0.43
1:A:8:LEU:H	1:A:8:LEU:CD2	2.30	0.43
1:A:150:VAL:O	1:A:158:ARG:NH2	2.49	0.43
2:B:275:THR:HB	2:B:356:PHE:HE1	1.83	0.43
2:B:144:GLN:OE1	2:B:363:SER:CB	2.67	0.43
2:B:313:GLU:HG2	2:B:317:MET:HE3	2.01	0.43
2:B:352:ASP:OD1	2:B:401:ARG:NH2	2.50	0.43
2:B:8:GLU:O	2:B:9:TYR:C	2.61	0.43
2:B:340:ARG:C	2:B:342:GLN:N	2.76	0.43
2:B:455:ILE:O	2:B:480:ALA:HB3	2.18	0.43
2:B:467:ILE:CG1	2:B:469:THR:HG23	2.49	0.43
1:A:72:ASP:O	1:A:106:LEU:HD23	2.18	0.43
2:B:406:LEU:C	2:B:408:LYS:H	2.27	0.43
2:B:49:LYS:HB3	2:B:50:THR:H	1.61	0.43
2:B:254:GLU:HG3	2:B:255:ALA:N	2.34	0.43
2:B:565:LEU:O	2:B:565:LEU:HD22	2.17	0.43
1:A:1:MET:HE3	1:A:3:LEU:HD13	2.01	0.43
1:A:12:MET:SD	1:A:12:MET:C	3.02	0.43
1:A:152:ARG:HA	1:A:223:PHE:CD2	2.54	0.43
2:B:78:TYR:CE2	2:B:79:THR:HG23	2.53	0.42
2:B:115:GLY:N	2:B:118:THR:HG23	2.27	0.42
2:B:248:HIS:CG	2:B:274:HIS:CE1	3.07	0.42
2:B:300:THR:O	2:B:301:ASN:HB2	2.18	0.42
1:A:2:LYS:HD3	1:A:2:LYS:N	2.33	0.42
1:A:38:LEU:HD23	1:A:65:LEU:HD21	2.02	0.42
1:A:144:HIS:C	2:B:55:MET:HE3	2.44	0.42
1:A:202:VAL:HG12	1:A:204:ARG:H	1.84	0.42
2:B:264:ALA:C	2:B:266:ALA:H	2.25	0.42
2:B:174:PRO:O	2:B:178:ASN:ND2	2.41	0.42
2:B:369:VAL:HG22	2:B:369:VAL:O	2.18	0.42
1:A:219:LYS:HD3	1:A:228:SER:HA	2.01	0.42
2:B:523:THR:O	2:B:526:ASP:HB2	2.18	0.42
1:A:146:HIS:HE1	1:A:202:VAL:HG21	1.85	0.42
2:B:280:GLY:HA2	2:B:338:ARG:CZ	2.50	0.42
1:A:199:ASN:O	1:A:200:ALA:HB3	2.20	0.42
2:B:219:KCX:OQ2	2:B:221:HIS:HD2	2.03	0.42
1:A:133:ASN:C	1:A:133:ASN:HD22	2.27	0.42
2:B:192:ASN:ND2	2:B:451:LYS:HE2	2.34	0.42
2:B:301:ASN:HD22	2:B:367:GLY:HA2	1.84	0.42
2:B:527:MET:O	2:B:531:ASN:HB3	2.20	0.42
1:A:126:ALA:O	1:A:127:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASP:OD1	1:A:137:ARG:NE	2.53	0.42
2:B:77:ASP:C	2:B:79:THR:N	2.77	0.42
2:B:138:HIS:CD2	2:B:171:THR:HG23	2.55	0.42
2:B:297:PRO:CG	2:B:524:LYS:HE3	2.50	0.42
2:B:362:ASP:O	2:B:363:SER:C	2.62	0.42
2:B:49:LYS:HD2	2:B:49:LYS:N	2.35	0.42
2:B:248:HIS:NE2	2:B:280:GLY:HA3	2.35	0.42
1:A:4:THR:O	1:A:7:GLU:N	2.53	0.41
1:A:112:PHE:HB2	2:B:20:LYS:HB2	2.01	0.41
1:A:114:LYS:O	1:A:114:LYS:HG3	2.20	0.41
2:B:314:HIS:O	2:B:316:ASP:N	2.53	0.41
2:B:332:VAL:O	2:B:332:VAL:HG23	2.20	0.41
1:A:106:LEU:HD12	1:A:107:VAL:H	1.84	0.41
2:B:271:HIS:CD2	2:B:271:HIS:C	2.98	0.41
2:B:348:ASP:OD1	2:B:348:ASP:N	2.48	0.41
1:A:167:ASP:OD1	1:A:167:ASP:C	2.64	0.41
2:B:134:ASP:OD1	2:B:361:SER:HB3	2.19	0.41
2:B:191:MET:HE2	2:B:191:MET:HB3	1.86	0.41
2:B:360:SER:HB3	2:B:361:SER:H	1.68	0.41
2:B:568:ILE:HG23	2:B:569:PHE:HD1	1.85	0.41
2:B:69:ILE:HD13	2:B:114:VAL:HG22	2.01	0.41
2:B:273:PHE:O	2:B:274:HIS:ND1	2.53	0.41
2:B:389:ARG:HH21	2:B:397:ASN:N	2.18	0.41
1:A:114:LYS:O	1:A:115:ASN:C	2.61	0.41
1:A:227:LYS:HG3	1:A:228:SER:H	1.86	0.41
2:B:99:GLY:HA3	2:B:112:LEU:HB3	2.02	0.41
2:B:318:LEU:H	2:B:318:LEU:CD2	2.30	0.41
1:A:166:LEU:HD13	1:A:174:VAL:HG23	2.01	0.41
2:B:211:ILE:C	2:B:213:ALA:N	2.77	0.41
1:A:10:LYS:CD	1:A:44:MET:HE1	2.51	0.41
1:A:139:VAL:HG12	1:A:141:ILE:CD1	2.51	0.41
1:A:166:LEU:O	1:A:168:ILE:HG12	2.21	0.41
1:A:236:ILE:HG12	1:A:236:ILE:O	2.21	0.41
2:B:99:GLY:N	2:B:109:LYS:HZ1	2.19	0.41
2:B:102:LYS:HA	2:B:108:VAL:CG1	2.51	0.41
1:A:11:LEU:O	1:A:15:TYR:HD2	2.03	0.41
1:A:125:LYS:N	1:A:125:LYS:CD	2.79	0.41
2:B:197:ALA:HB1	2:B:210:GLN:CD	2.46	0.41
2:B:301:ASN:HD21	2:B:368:ARG:H	1.54	0.41
1:A:91:THR:HG23	4:A:2005:HOH:O	2.20	0.41
1:A:122:GLU:HG3	1:A:123:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:SER:O	2:B:6:ARG:C	2.61	0.41
2:B:136:HIS:CE1	2:B:273:PHE:CG	3.09	0.41
2:B:175:GLY:O	2:B:179:LEU:HG	2.21	0.41
2:B:412:ASN:ND2	2:B:528:GLN:H	2.16	0.41
2:B:441:PHE:O	2:B:442:PHE:C	2.63	0.41
1:A:66:LYS:HB2	1:A:67:PRO:HD2	2.03	0.41
2:B:68:LEU:HD13	2:B:68:LEU:C	2.46	0.41
2:B:131:GLY:HA3	2:B:154:THR:HG23	2.03	0.41
2:B:199:GLY:HA3	2:B:220:ILE:HD13	2.03	0.41
2:B:229:SER:O	2:B:230:ALA:C	2.64	0.41
2:B:316:ASP:O	2:B:317:MET:C	2.63	0.41
2:B:373:ILE:HB	4:B:2036:HOH:O	2.21	0.41
1:A:46:GLU:HB3	1:A:57:LEU:CD1	2.47	0.40
1:A:145:PHE:CD2	1:A:145:PHE:C	2.99	0.40
2:B:220:ILE:HG22	2:B:226:THR:HG23	2.03	0.40
2:B:445:LYS:HA	2:B:446:PRO:HD2	1.92	0.40
2:B:469:THR:N	2:B:470:PRO:CD	2.81	0.40
1:A:122:GLU:O	1:A:124:LYS:HG2	2.21	0.40
2:B:58:SER:HB2	2:B:101:ASN:CG	2.46	0.40
2:B:109:LYS:O	2:B:111:ASN:N	2.54	0.40
2:B:221:HIS:CE1	2:B:223:ASP:OD1	2.75	0.40
2:B:466:SER:O	2:B:467:ILE:HG23	2.21	0.40
2:B:99:GLY:H	2:B:109:LYS:HZ1	1.70	0.40
2:B:124:GLU:HG2	2:B:124:GLU:O	2.22	0.40
2:B:294:ASN:H	2:B:294:ASN:ND2	2.08	0.40
2:B:441:PHE:CD1	2:B:441:PHE:N	2.89	0.40
2:B:511:ARG:O	2:B:513:VAL:HG23	2.21	0.40
1:A:219:LYS:HG2	1:A:229:ASP:CG	2.47	0.40
2:B:110:ASN:HD22	2:B:110:ASN:HA	1.69	0.40
2:B:525:LYS:HD3	2:B:531:ASN:HD22	1.86	0.40
1:A:1:MET:O	1:A:3:LEU:N	2.54	0.40
1:A:21:LYS:HG3	1:A:22:LYS:H	1.84	0.40
1:A:113:LEU:HD12	1:A:113:LEU:O	2.22	0.40
2:B:26:THR:HG22	2:B:561:SER:CB	2.52	0.40
2:B:393:GLU:CD	2:B:398:ASP:HA	2.47	0.40
2:B:479:PHE:C	2:B:481:HIS:N	2.74	0.40
2:B:533:THR:O	2:B:534:ALA:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	236/238 (99%)	183 (78%)	37 (16%)	16 (7%)	1	5
2	B	566/569 (100%)	428 (76%)	97 (17%)	41 (7%)	1	4
All	All	802/807 (99%)	611 (76%)	134 (17%)	57 (7%)	1	4

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ALA
1	A	116	GLU
1	A	125	LYS
1	A	172	THR
1	A	227	LYS
2	B	49	LYS
2	B	249	THR
2	B	285	ASP
2	B	286	ILE
2	B	300	THR
2	B	301	ASN
2	B	317	MET
1	A	2	LYS
1	A	122	GLU
1	A	123	GLY
1	A	151	ASN
1	A	167	ASP
2	B	2	LYS
2	B	47	GLY
2	B	191	MET
2	B	282	HIS
2	B	327	SER
2	B	389	ARG
2	B	462	ASP
2	B	39	TYR

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Mol	Chain	Res	Type
2	B	65	GLU
2	B	84	ALA
2	B	139	PHE
2	B	163	PRO
2	B	252	LEU
2	B	274	HIS
2	B	287	ILE
2	B	360	SER
2	B	363	SER
2	B	439	PRO
2	B	480	ALA
2	B	548	ASP
2	B	564	GLN
1	A	152	ARG
1	A	166	LEU
1	A	206	ALA
2	B	315	MET
2	B	326	LYS
2	B	366	MET
1	A	37	ALA
1	A	146	HIS
2	B	17	THR
2	B	303	THR
2	B	316	ASP
2	B	332	VAL
1	A	115	ASN
2	B	54	GLY
2	B	99	GLY
2	B	320	VAL
2	B	325	ASP
2	B	444	VAL
2	B	426	VAL

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	197/197 (100%)	184 (93%)	13 (7%)	15	46
2	B	458/458 (100%)	406 (89%)	52 (11%)	5	24
All	All	655/655 (100%)	590 (90%)	65 (10%)	7	30

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	6	LYS
1	A	19	LEU
1	A	83	ILE
1	A	95	THR
1	A	107	VAL
1	A	113	LEU
1	A	125	LYS
1	A	159	GLU
1	A	186	LEU
1	A	195	ILE
1	A	207	ASP
1	A	227	LYS
2	B	1	MET
2	B	6	ARG
2	B	16	THR
2	B	42	GLU
2	B	53	GLU
2	B	66	LEU
2	B	68	LEU
2	B	69	ILE
2	B	98	LYS
2	B	105	GLN
2	B	108	VAL
2	B	109	LYS
2	B	111	ASN
2	B	118	THR
2	B	145	ILE
2	B	170	THR
2	B	177	ARG
2	B	190	SER
2	B	191	MET
2	B	227	THR
2	B	237	VAL
2	B	240	LYS

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Mol	Chain	Res	Type
2	B	243	VAL
2	B	245	VAL
2	B	249	THR
2	B	258	VAL
2	B	270	MET
2	B	276	GLU
2	B	285	ASP
2	B	292	GLU
2	B	294	ASN
2	B	304	ILE
2	B	323	HIS
2	B	325	ASP
2	B	330	GLU
2	B	342	GLN
2	B	352	ASP
2	B	364	GLN
2	B	389	ARG
2	B	411	ILE
2	B	420	SER
2	B	435	VAL
2	B	436	LEU
2	B	457	LEU
2	B	469	THR
2	B	492	THR
2	B	506	GLU
2	B	514	LEU
2	B	520	ARG
2	B	530	ASN
2	B	536	ILE
2	B	565	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	59	GLN
1	A	121	ASN
1	A	133	ASN
1	A	140	GLN
1	A	192	ASN
1	A	205	GLN
2	B	34	HIS

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Mol	Chain	Res	Type
2	B	101	ASN
2	B	110	ASN
2	B	111	ASN
2	B	168	ASN
2	B	200	ASN
2	B	244	GLN
2	B	294	ASN
2	B	301	ASN
2	B	342	GLN
2	B	351	HIS
2	B	364	GLN
2	B	383	ASN
2	B	397	ASN
2	B	412	ASN
2	B	417	HIS
2	B	459	GLN
2	B	464	ASN
2	B	471	GLN
2	B	490	ASN
2	B	496	GLN
2	B	512	GLN
2	B	518	ASN
2	B	535	HIS
2	B	564	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	KCX	B	219	3,2	10,11,12	1.15	1 (10%)	6,12,14	1.06	1 (16%)

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	KCX	B	219	3,2	-	3/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	219	KCX	OQ1-CX	2.49	1.26	1.21

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	219	KCX	OQ1-CX-NZ	-2.07	121.77	124.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	219	KCX	OQ1-CX-NZ-CE
2	B	219	KCX	OQ2-CX-NZ-CE
2	B	219	KCX	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	219	KCX	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	238/238 (100%)	-1.83	0 100 100	6, 26, 47, 79	0
2	B	568/569 (99%)	-1.85	0 100 100	1, 13, 55, 100	0
All	All	806/807 (99%)	-1.84	0 100 100	1, 17, 50, 100	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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	KCX	B	219	12/13	0.99	0.04	18,24,39,41	0

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
3	NI	B	3001	1/1	1.00	0.05	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NI	B	3002	1/1	1.00	0.02	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.