WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 11:45 AM EDT

PDB ID	:	3DRS
Title	:	HIV reverse transcriptase K103N mutant in complex with inhibitor R8D
Authors	:	Yan, Y.; Prasad, S.
Deposited on	:	2008-07-11
Resolution	:	3.15 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

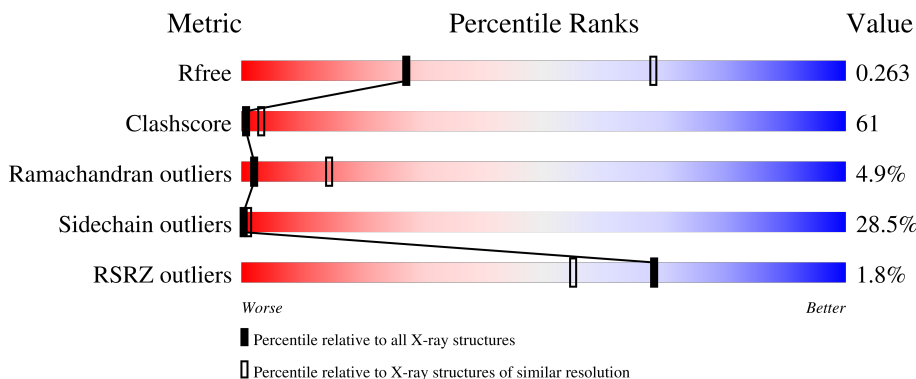|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.15 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	Percentile Ranks	Value
Rfree		0.263
Clashscore		61
Ramachandran outliers		4.9%
Sidechain outliers		28.5%
RSRZ outliers		1.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 <=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	563	% 23% 51% 21% · ·
2	B	443	2% 25% 46% 19% · 9%

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
3	R8D	A	601	-	X	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7854 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	549	4475	2891	747	829	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP P04585
A	-1	ASN	-	expression tag	UNP P04585
A	0	SER	-	expression tag	UNP P04585
A	103	ASN	LYS	engineered mutation	UNP P04585

- Molecule 2 is a protein called p66 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	405	3351	2180	555	610	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP P04585
B	-1	ASN	-	expression tag	UNP P04585
B	0	SER	-	expression tag	UNP P04585
B	103	ASN	LYS	engineered mutation	UNP P04585

- Molecule 3 is 3-chloro-5-[2-chloro-5-(1H-pyrazolo[3,4-b]pyridin-3-ylmethoxy)phenoxy]benzonitrile (three-letter code: R8D) (formula: $C_{20}H_{12}Cl_2N_4O_2$).

R8D
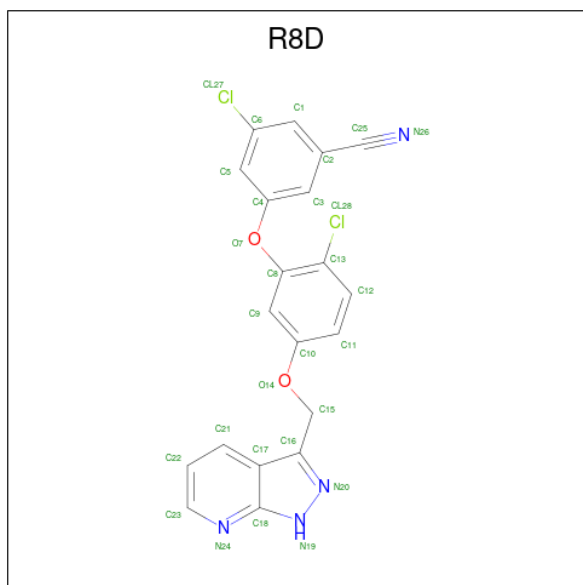
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	28	20	2	4	2	0	0

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: Reverse transcriptase/ribonuclease H
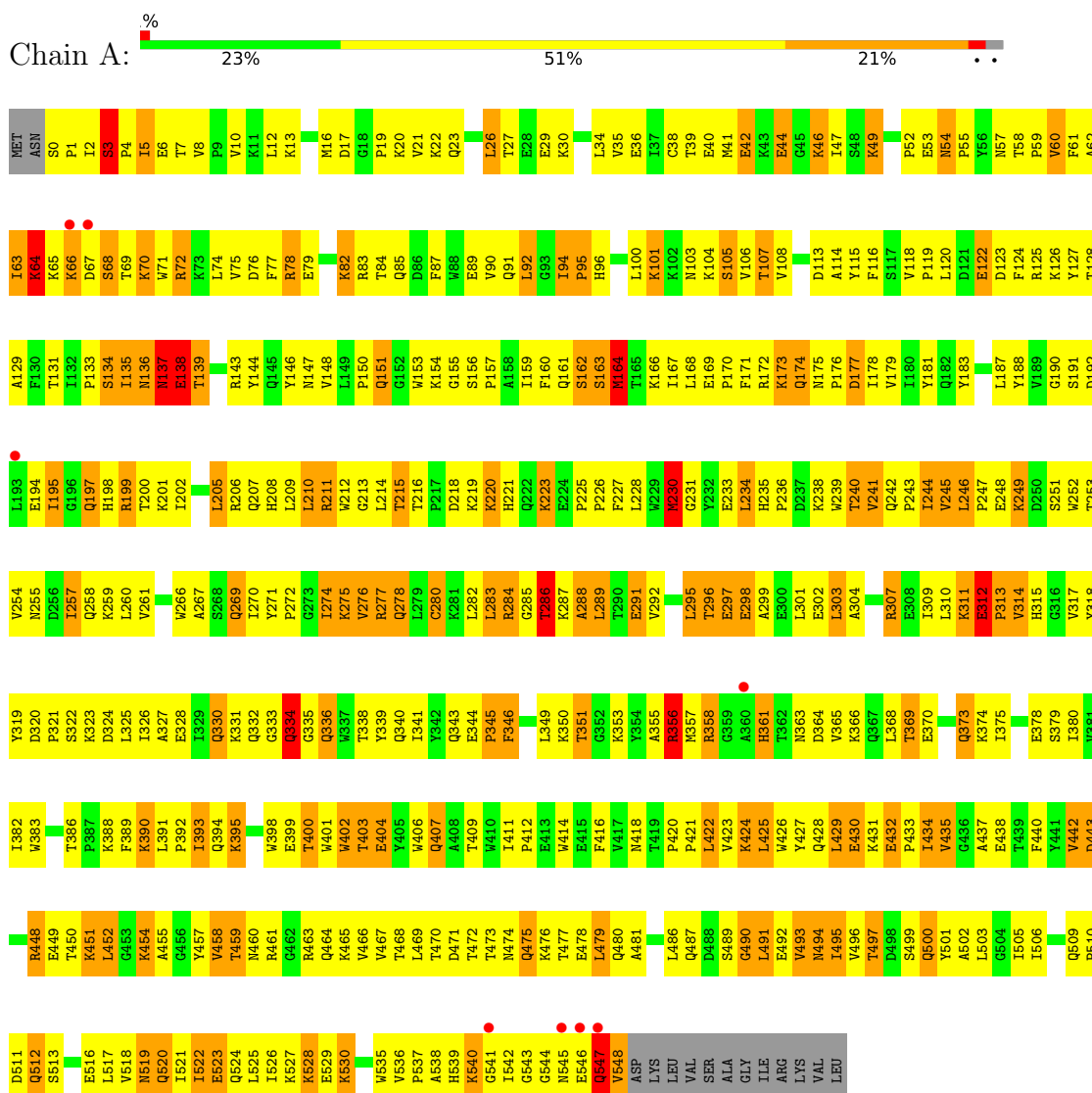
• Molecule 2: p66 RT

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	118.55Å 154.63Å 154.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.50 – 3.15 37.50 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (37.50-3.15) 99.5 (37.50-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 3.18Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.184 , 0.250 0.192 , 0.263	Depositor DCC
R_{free} test set	1255 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	68.6	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 85.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.52, < L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7854	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ 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: R8D

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	0.67	0/4592	0.89	6/6242 (0.1%)
2	B	0.67	0/3445	0.95	7/4682 (0.1%)
All	All	0.67	0/8037	0.92	13/10924 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	344	GLU	C-N-CD	-19.16	78.46	120.60
2	B	312	GLU	C-N-CD	-11.88	94.47	120.60
2	B	420	PRO	C-N-CD	-10.86	96.70	120.60
1	A	312	GLU	C-N-CD	-10.29	97.96	120.60
1	A	94	ILE	C-N-CD	-8.80	101.23	120.60
2	B	118	VAL	C-N-CD	-7.50	104.10	120.60
1	A	54	ASN	C-N-CD	-6.93	105.35	120.60
2	B	143	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	312	GLU	C-N-CA	-5.50	98.91	122.00
2	B	268	SER	N-CA-C	-5.35	96.56	111.00
1	A	536	VAL	C-N-CD	-5.29	108.97	120.60
1	A	234	LEU	CA-CB-CG	-5.23	103.28	115.30
2	B	233	GLU	N-CA-C	5.07	124.68	111.00

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	4475	0	4514	602	1
2	B	3351	0	3373	391	0
3	A	28	0	12	16	0
All	All	7854	0	7899	967	1

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 61.

All (967) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ALA:HB3	1:A:291:GLU:HB3	1.17	1.17
1:A:318:TYR:CE2	3:A:601:R8D:H15	1.82	1.14
1:A:469:LEU:HD21	1:A:480:GLN:HG2	1.32	1.12
2:B:241:VAL:HG23	2:B:243:PRO:HD3	1.16	1.08
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.41	1.02
2:B:160:PHE:HE2	2:B:164:MET:HE2	1.24	1.02
1:A:271:TYR:HB3	1:A:274:ILE:HD11	1.42	1.00
2:B:282:LEU:HD12	2:B:293:ILE:HD11	1.44	0.96
1:A:175:ASN:HB3	1:A:178:ILE:HD13	1.43	0.95
2:B:362:THR:HG23	2:B:366:LYS:HG2	1.48	0.95
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.30	0.95
1:A:442:VAL:HG12	1:A:481:ALA:HB1	1.48	0.94
2:B:298:GLU:HA	2:B:301:LEU:HG	1.49	0.94
1:A:458:VAL:HG12	1:A:548:VAL:HG13	1.50	0.94
1:A:406:TRP:CH2	1:A:407:GLN:HG3	2.03	0.94
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.50	0.93
2:B:246:LEU:HD11	2:B:310:LEU:HD23	1.49	0.93
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.51	0.92
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.52	0.91
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.51	0.91
1:A:475:GLN:HG3	1:A:501:TYR:CE2	2.06	0.90
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.07	0.90
1:A:434:ILE:HG23	1:A:530:LYS:HD3	1.55	0.90
1:A:64:LYS:NZ	1:A:69:THR:HA	1.87	0.89
2:B:125:ARG:NH1	2:B:147:ASN:HA	1.87	0.88
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.53	0.88
2:B:253:THR:O	2:B:257:ILE:HD12	1.74	0.88
1:A:181:TYR:HB2	1:A:188:TYR:HB2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TRP:CD1	1:A:295:LEU:HD21	2.09	0.88
1:A:469:LEU:CD2	1:A:480:GLN:HG2	2.04	0.88
2:B:241:VAL:CG2	2:B:243:PRO:HD3	2.03	0.88
2:B:125:ARG:HB3	2:B:146:TYR:O	1.75	0.87
1:A:5:ILE:HG22	1:A:212:TRP:CE3	2.10	0.87
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.05	0.86
1:A:434:ILE:HG13	1:A:494:ASN:HD21	1.39	0.86
1:A:107:THR:HG21	1:A:202:ILE:HD13	1.56	0.86
2:B:12:LEU:HD23	2:B:17:ASP:HA	1.57	0.85
1:A:288:ALA:CB	1:A:291:GLU:HB3	2.06	0.85
2:B:246:LEU:HD12	2:B:307:ARG:HG3	1.58	0.85
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.56	0.84
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.22	0.84
1:A:175:ASN:CB	1:A:178:ILE:HD13	2.06	0.84
1:A:448:ARG:HG2	1:A:448:ARG:HH11	1.41	0.84
1:A:100:LEU:HD22	1:A:181:TYR:HE2	1.43	0.84
1:A:85:GLN:O	1:A:154:LYS:HE2	1.78	0.84
1:A:288:ALA:HB3	1:A:291:GLU:CB	2.05	0.83
1:A:424:LYS:HE2	1:A:426:TRP:CZ2	2.13	0.83
1:A:255:ASN:HB2	1:A:289:LEU:HD13	1.58	0.83
1:A:1:PRO:O	1:A:2:ILE:HD13	1.78	0.83
1:A:175:ASN:HD21	1:A:201:LYS:NZ	1.75	0.83
2:B:87:PHE:CE2	2:B:92:LEU:HD12	2.12	0.83
1:A:162:SER:HB2	2:B:52:PRO:HG3	1.61	0.83
2:B:422:LEU:HB3	2:B:426:TRP:CZ2	2.13	0.83
1:A:2:ILE:HD11	1:A:46:LYS:NZ	1.94	0.83
1:A:175:ASN:ND2	1:A:201:LYS:NZ	2.27	0.83
1:A:311:LYS:O	1:A:312:GLU:HB3	1.79	0.83
1:A:122:GLU:HA	1:A:125:ARG:CD	2.08	0.82
1:A:134:SER:CB	1:A:139:THR:HB	2.10	0.82
2:B:298:GLU:CA	2:B:301:LEU:HG	2.08	0.82
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.61	0.81
2:B:160:PHE:CE2	2:B:164:MET:HE2	2.15	0.81
1:A:64:LYS:HZ1	1:A:69:THR:HA	1.43	0.81
1:A:175:ASN:HD21	1:A:201:LYS:HZ2	1.27	0.81
1:A:100:LEU:O	1:A:318:TYR:HB3	1.80	0.81
1:A:228:LEU:HB3	1:A:242:GLN:NE2	1.95	0.81
2:B:18:GLY:HA3	2:B:56:TYR:CE1	2.15	0.81
1:A:125:ARG:HG2	1:A:146:TYR:O	1.81	0.81
1:A:255:ASN:HB2	1:A:289:LEU:CD1	2.11	0.81
2:B:125:ARG:HH11	2:B:147:ASN:HA	1.43	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:LEU:HB3	1:A:524:GLN:HE21	1.45	0.80
1:A:76:ASP:OD2	1:A:78:ARG:HG3	1.82	0.79
2:B:277:ARG:O	2:B:281:LYS:HG3	1.82	0.79
2:B:420:PRO:HG2	2:B:423:VAL:CG2	2.12	0.79
1:A:401:TRP:HA	1:A:404:GLU:OE2	1.82	0.79
1:A:544:GLY:HA2	1:A:547:GLN:NE2	1.97	0.79
2:B:362:THR:HG22	2:B:367:GLN:HG3	1.63	0.79
1:A:258:GLN:HG3	1:A:283:LEU:HD11	1.64	0.79
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.18	0.79
1:A:460:ASN:ND2	2:B:288:ALA:HB2	1.97	0.79
1:A:493:VAL:CG2	1:A:528:LYS:HE2	2.13	0.79
2:B:241:VAL:HG23	2:B:243:PRO:CD	2.09	0.78
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.13	0.78
2:B:395:LYS:HG3	2:B:399:GLU:OE1	1.82	0.78
2:B:246:LEU:HD11	2:B:310:LEU:CD2	2.13	0.78
1:A:450:THR:OG1	1:A:452:LEU:HB2	1.83	0.77
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.64	0.77
2:B:114:ALA:CB	2:B:214:LEU:HD22	2.15	0.77
2:B:335:GLY:HA3	2:B:356:ARG:HG2	1.67	0.77
2:B:420:PRO:HG2	2:B:423:VAL:HG21	1.67	0.77
1:A:2:ILE:HD11	1:A:46:LYS:CE	2.15	0.77
1:A:271:TYR:CB	1:A:274:ILE:HD11	2.14	0.77
1:A:424:LYS:HE2	1:A:426:TRP:CH2	2.20	0.77
2:B:422:LEU:HB3	2:B:426:TRP:CE2	2.19	0.76
1:A:318:TYR:CZ	3:A:601:R8D:H15	2.20	0.76
1:A:95:PRO:HA	2:B:136:ASN:OD1	1.85	0.76
1:A:454:LYS:HZ2	1:A:468:THR:HG23	1.50	0.76
2:B:268:SER:O	2:B:270:ILE:HG22	1.85	0.76
2:B:301:LEU:O	2:B:305:GLU:HG3	1.85	0.76
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.67	0.76
1:A:3:SER:CB	1:A:5:ILE:HD12	2.14	0.76
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.15	0.76
1:A:220:LYS:HE3	1:A:221:HIS:CE1	2.21	0.76
1:A:356:ARG:CZ	1:A:358:ARG:HD2	2.16	0.75
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.21	0.75
1:A:460:ASN:HA	2:B:286:THR:OG1	1.87	0.75
1:A:320:ASP:OD2	1:A:323:LYS:HE3	1.85	0.75
2:B:303:LEU:O	2:B:307:ARG:HB2	1.85	0.75
1:A:366:LYS:O	1:A:370:GLU:HG3	1.87	0.74
1:A:522:ILE:O	1:A:526:ILE:HG13	1.87	0.74
2:B:104:LYS:HD3	2:B:192:ASP:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.67	0.74
1:A:435:VAL:HG22	2:B:290:THR:OG1	1.87	0.74
1:A:64:LYS:HZ1	1:A:69:THR:HG23	1.51	0.74
1:A:276:VAL:O	1:A:280:CYS:HB2	1.88	0.74
1:A:520:GLN:O	1:A:523:GLU:HG3	1.87	0.74
2:B:116:PHE:HA	2:B:148:VAL:HG21	1.68	0.74
2:B:425:LEU:HD23	2:B:425:LEU:H	1.53	0.74
1:A:3:SER:OG	1:A:5:ILE:HD12	1.86	0.73
2:B:422:LEU:HD13	2:B:426:TRP:CZ2	2.23	0.73
1:A:234:LEU:O	3:A:601:R8D:H21	1.89	0.73
2:B:298:GLU:HA	2:B:301:LEU:CG	2.19	0.73
1:A:244:ILE:HD12	1:A:267:ALA:HB2	1.69	0.73
1:A:434:ILE:HG13	1:A:494:ASN:ND2	2.03	0.73
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.69	0.73
2:B:332:GLN:HA	2:B:332:GLN:OE1	1.87	0.73
2:B:257:ILE:O	2:B:261:VAL:HG12	1.89	0.73
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.71	0.73
2:B:65:LYS:HE2	2:B:72:ARG:CZ	2.19	0.73
2:B:243:PRO:HB3	2:B:311:LYS:HA	1.71	0.73
1:A:105:SER:HB2	1:A:198:HIS:CE1	2.23	0.72
2:B:246:LEU:CD1	2:B:310:LEU:HD23	2.19	0.72
1:A:271:TYR:CD1	1:A:310:LEU:HD23	2.23	0.72
1:A:454:LYS:NZ	1:A:468:THR:HG23	2.03	0.72
2:B:27:THR:OG1	2:B:30:LYS:HD3	1.89	0.72
2:B:114:ALA:CA	2:B:214:LEU:HD22	2.20	0.72
1:A:27:THR:OG1	1:A:30:LYS:HG3	1.90	0.72
2:B:33:ALA:O	2:B:37:ILE:HD12	1.90	0.72
1:A:100:LEU:HD22	1:A:181:TYR:CE2	2.24	0.72
1:A:437:ALA:HB1	1:A:492:GLU:O	1.90	0.72
1:A:521:ILE:O	1:A:525:LEU:HG	1.90	0.72
1:A:79:GLU:HG3	1:A:83:ARG:NE	2.02	0.71
1:A:331:LYS:HE3	1:A:364:ASP:OD1	1.90	0.71
1:A:211:ARG:O	1:A:211:ARG:HD3	1.90	0.71
1:A:169:GLU:N	1:A:170:PRO:HD2	2.03	0.71
1:A:270:ILE:O	1:A:272:PRO:HD3	1.89	0.71
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.26	0.71
1:A:356:ARG:NH2	1:A:358:ARG:HD2	2.05	0.71
1:A:226:PRO:HG3	1:A:235:HIS:HD2	1.55	0.70
1:A:502:ALA:O	1:A:506:ILE:HD12	1.91	0.70
1:A:540:LYS:CB	1:A:542:ILE:HD13	2.21	0.70
1:A:218:ASP:OD2	1:A:221:HIS:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ARG:HH12	2:B:409:THR:CG2	2.03	0.70
2:B:354:TYR:HB2	2:B:374:LYS:NZ	2.05	0.70
1:A:108:VAL:HB	1:A:223:LYS:HG3	1.74	0.70
2:B:301:LEU:N	2:B:301:LEU:HD23	2.07	0.70
1:A:277:ARG:NH1	1:A:334:GLN:HB2	2.06	0.70
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.73	0.70
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.22	0.70
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.24	0.70
1:A:41:MET:HB3	1:A:47:ILE:HG12	1.72	0.70
1:A:54:ASN:O	1:A:143:ARG:NH2	2.25	0.70
1:A:3:SER:HB3	1:A:5:ILE:HD12	1.71	0.70
1:A:156:SER:N	1:A:157:PRO:HD2	2.07	0.70
1:A:104:LYS:HG3	1:A:192:ASP:HA	1.74	0.69
1:A:284:ARG:HH11	1:A:285:GLY:HA3	1.57	0.69
1:A:171:PHE:CD2	1:A:205:LEU:HD23	2.26	0.69
2:B:122:GLU:HA	2:B:125:ARG:HE	1.58	0.69
2:B:283:LEU:HA	2:B:287:LYS:HE2	1.73	0.69
1:A:424:LYS:HE2	1:A:426:TRP:CE2	2.26	0.69
1:A:298:GLU:OE2	1:A:298:GLU:N	2.21	0.69
2:B:87:PHE:CZ	2:B:92:LEU:HD12	2.27	0.69
2:B:279:LEU:O	2:B:282:LEU:HB2	1.91	0.69
1:A:5:ILE:HG22	1:A:212:TRP:CZ3	2.27	0.69
1:A:162:SER:CB	2:B:52:PRO:HG3	2.23	0.69
1:A:238:LYS:HB3	1:A:315:HIS:HD2	1.58	0.69
2:B:116:PHE:HD2	2:B:148:VAL:CG2	2.06	0.69
2:B:66:LYS:CA	2:B:407:GLN:HE22	2.04	0.68
1:A:104:LYS:HG3	1:A:192:ASP:CA	2.23	0.68
1:A:175:ASN:CA	1:A:178:ILE:HD13	2.23	0.68
1:A:358:ARG:NH1	2:B:396:GLU:OE1	2.26	0.68
1:A:516:GLU:O	1:A:520:GLN:HG2	1.93	0.68
1:A:298:GLU:HA	1:A:301:LEU:HD12	1.74	0.68
1:A:266:TRP:O	1:A:269:GLN:NE2	2.27	0.68
2:B:260:LEU:HD13	2:B:260:LEU:O	1.93	0.68
2:B:299:ALA:O	2:B:303:LEU:HD23	1.93	0.68
1:A:317:VAL:HG23	1:A:318:TYR:N	2.08	0.68
1:A:230:MET:HA	1:A:230:MET:HE2	1.75	0.68
2:B:253:THR:HG23	2:B:289:LEU:O	1.94	0.68
1:A:105:SER:HB2	1:A:198:HIS:ND1	2.08	0.68
1:A:399:GLU:HG3	1:A:400:THR:N	2.09	0.68
1:A:175:ASN:ND2	1:A:201:LYS:HD2	2.09	0.68
1:A:363:ASN:HA	1:A:511:ASP:OD2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.74	0.67
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.25	0.67
1:A:518:VAL:O	1:A:522:ILE:HD12	1.94	0.67
2:B:362:THR:HG21	2:B:367:GLN:HG3	1.74	0.67
1:A:20:LYS:HE2	1:A:55:PRO:HB2	1.76	0.67
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.29	0.67
2:B:13:LYS:O	2:B:16:MET:HE2	1.94	0.67
2:B:175:ASN:ND2	2:B:201:LYS:HE3	2.09	0.67
2:B:257:ILE:HG22	2:B:283:LEU:CD1	2.24	0.67
2:B:278:GLN:HA	2:B:281:LYS:HD2	1.76	0.67
1:A:175:ASN:N	1:A:176:PRO:HD3	2.08	0.67
1:A:458:VAL:CG1	1:A:548:VAL:HG22	2.23	0.67
1:A:434:ILE:CG1	1:A:494:ASN:HD21	2.08	0.67
2:B:72:ARG:HH12	2:B:409:THR:HG22	1.59	0.67
1:A:258:GLN:HG3	1:A:283:LEU:CD1	2.24	0.67
1:A:538:ALA:O	1:A:539:HIS:HB2	1.95	0.67
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.25	0.67
1:A:538:ALA:HA	1:A:545:ASN:OD1	1.94	0.66
2:B:64:LYS:NZ	2:B:69:THR:O	2.27	0.66
1:A:399:GLU:O	1:A:403:THR:HB	1.95	0.66
2:B:86:ASP:HA	2:B:90:VAL:CG2	2.24	0.66
2:B:301:LEU:O	2:B:305:GLU:N	2.28	0.66
1:A:107:THR:HB	1:A:202:ILE:HD11	1.78	0.66
2:B:422:LEU:HA	2:B:425:LEU:HD21	1.76	0.66
1:A:178:ILE:N	1:A:178:ILE:HD12	2.10	0.66
2:B:278:GLN:O	2:B:281:LYS:HB2	1.96	0.66
2:B:344:GLU:HB3	2:B:345:PRO:HD2	1.77	0.66
2:B:266:TRP:HE1	2:B:346:PHE:HE2	1.42	0.66
2:B:209:LEU:HD12	2:B:214:LEU:HD12	1.76	0.66
2:B:302:GLU:O	2:B:306:ASN:HB2	1.96	0.66
1:A:44:GLU:HB3	1:A:46:LYS:HE3	1.78	0.65
1:A:175:ASN:HD21	1:A:201:LYS:HD2	1.61	0.65
2:B:366:LYS:O	2:B:370:GLU:HG3	1.96	0.65
1:A:77:PHE:CE2	1:A:150:PRO:HB2	2.32	0.65
1:A:13:LYS:O	1:A:16:MET:HB2	1.97	0.65
2:B:253:THR:HG22	2:B:256:ASP:H	1.59	0.65
1:A:400:THR:HG22	1:A:401:TRP:N	2.10	0.65
1:A:403:THR:HG22	1:A:404:GLU:N	2.10	0.65
1:A:486:LEU:CB	1:A:524:GLN:HE21	2.08	0.65
1:A:490:GLY:O	1:A:492:GLU:N	2.28	0.65
2:B:66:LYS:H	2:B:407:GLN:NE2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:GLU:HB3	2:B:170:PRO:CD	2.26	0.65
1:A:395:LYS:HD3	1:A:414:TRP:CH2	2.32	0.65
2:B:261:VAL:O	2:B:265:ASN:HB3	1.96	0.65
1:A:91:GLN:HE21	2:B:137:ASN:HB3	1.62	0.64
2:B:396:GLU:O	2:B:400:THR:HG22	1.97	0.64
1:A:10:VAL:HG11	1:A:153:TRP:CH2	2.32	0.64
1:A:104:LYS:CG	1:A:192:ASP:HA	2.27	0.64
1:A:298:GLU:H	1:A:298:GLU:CD	2.01	0.64
1:A:365:VAL:O	1:A:369:THR:HG23	1.97	0.64
2:B:282:LEU:CD1	2:B:293:ILE:HD11	2.25	0.64
2:B:293:ILE:HD12	2:B:294:PRO:O	1.97	0.64
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.33	0.64
1:A:443:ASP:HB2	1:A:548:VAL:HB	1.80	0.64
1:A:458:VAL:CG1	1:A:548:VAL:HG13	2.25	0.64
2:B:142:ILE:HG22	2:B:144:TYR:CE2	2.33	0.64
2:B:195:ILE:HD12	2:B:195:ILE:O	1.97	0.64
2:B:92:LEU:HB3	2:B:158:ALA:HB1	1.80	0.64
2:B:246:LEU:HD12	2:B:307:ARG:CG	2.27	0.64
2:B:66:LYS:HA	2:B:407:GLN:HE22	1.63	0.64
2:B:118:VAL:O	2:B:148:VAL:HB	1.98	0.64
2:B:283:LEU:HA	2:B:287:LYS:CE	2.28	0.64
1:A:79:GLU:CG	1:A:83:ARG:HH21	2.11	0.63
1:A:2:ILE:HD11	1:A:46:LYS:HE2	1.80	0.63
1:A:464:GLN:HG2	1:A:465:LYS:H	1.63	0.63
1:A:540:LYS:O	1:A:542:ILE:N	2.30	0.63
2:B:65:LYS:HB2	2:B:65:LYS:NZ	2.13	0.63
2:B:82:LYS:HE3	2:B:413:GLU:OE2	1.97	0.63
2:B:180:ILE:HG13	2:B:189:VAL:HG13	1.80	0.63
1:A:434:ILE:CG2	1:A:530:LYS:HD3	2.27	0.63
1:A:458:VAL:CG2	2:B:286:THR:HG21	2.29	0.63
1:A:540:LYS:HB3	1:A:542:ILE:HD13	1.79	0.63
2:B:162:SER:O	2:B:166:LYS:HE2	1.97	0.63
1:A:65:LYS:HB3	1:A:65:LYS:HZ3	1.63	0.63
1:A:171:PHE:O	1:A:175:ASN:HB2	1.99	0.63
1:A:500:GLN:HG2	2:B:421:PRO:HG2	1.79	0.63
2:B:306:ASN:HD22	2:B:309:ILE:HD12	1.63	0.63
2:B:388:LYS:HE3	2:B:415:GLU:HG3	1.79	0.63
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.81	0.63
2:B:116:PHE:HZ	2:B:151:GLN:HG3	1.61	0.63
2:B:125:ARG:HD2	2:B:146:TYR:O	1.98	0.63
1:A:296:THR:HG23	1:A:299:ALA:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LEU:HB3	1:A:529:GLU:HB2	1.80	0.63
2:B:268:SER:O	2:B:269:GLN:HG3	1.99	0.63
1:A:1:PRO:HB2	1:A:213:GLY:HA2	1.80	0.63
2:B:111:VAL:HG21	2:B:187:LEU:HD22	1.79	0.62
2:B:284:ARG:HH11	2:B:284:ARG:HB2	1.63	0.62
2:B:267:ALA:O	2:B:271:TYR:HB2	1.99	0.62
2:B:268:SER:C	2:B:269:GLN:HG3	2.18	0.62
1:A:12:LEU:HD23	1:A:124:PHE:CE1	2.35	0.62
1:A:458:VAL:HG12	1:A:548:VAL:CG1	2.28	0.62
1:A:544:GLY:O	1:A:547:GLN:HB2	2.00	0.62
2:B:255:ASN:O	2:B:259:LYS:HG3	1.98	0.62
2:B:298:GLU:C	2:B:301:LEU:HG	2.20	0.62
1:A:466:VAL:HG12	1:A:467:VAL:H	1.64	0.62
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.80	0.62
2:B:282:LEU:O	2:B:287:LYS:NZ	2.30	0.62
1:A:500:GLN:HG3	2:B:422:LEU:CD1	2.28	0.62
1:A:448:ARG:HH11	1:A:448:ARG:CG	2.12	0.62
1:A:23:GLN:OE1	1:A:60:VAL:HG23	1.99	0.62
1:A:195:ILE:O	1:A:198:HIS:HB3	1.99	0.62
1:A:406:TRP:HZ2	2:B:418:ASN:OD1	1.82	0.62
1:A:460:ASN:HD21	2:B:288:ALA:HB2	1.64	0.62
1:A:466:VAL:HG12	1:A:467:VAL:N	2.14	0.62
2:B:354:TYR:HD2	2:B:374:LYS:HE3	1.64	0.62
2:B:388:LYS:HE3	2:B:415:GLU:CG	2.29	0.62
1:A:307:ARG:O	1:A:311:LYS:HD2	1.98	0.61
1:A:346:PHE:N	1:A:346:PHE:CD1	2.66	0.61
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.35	0.61
1:A:106:VAL:HG13	1:A:227:PHE:HE2	1.63	0.61
2:B:114:ALA:HA	2:B:214:LEU:HD22	1.80	0.61
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.82	0.61
1:A:175:ASN:HD21	1:A:201:LYS:CD	2.12	0.61
1:A:500:GLN:HG3	2:B:422:LEU:HD11	1.82	0.61
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.65	0.61
2:B:254:VAL:HB	2:B:289:LEU:HA	1.82	0.61
1:A:406:TRP:CZ2	2:B:418:ASN:HA	2.36	0.61
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.35	0.61
2:B:120:LEU:HD22	2:B:121:ASP:N	2.14	0.61
1:A:297:GLU:O	1:A:301:LEU:HG	2.01	0.61
2:B:122:GLU:HA	2:B:125:ARG:NE	2.15	0.61
1:A:1:PRO:C	1:A:2:ILE:HD13	2.20	0.60
1:A:380:ILE:HD11	1:A:386:THR:CG2	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:HG23	1:A:199:ARG:NE	2.16	0.60
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.82	0.60
1:A:104:LYS:HG3	1:A:192:ASP:C	2.22	0.60
2:B:270:ILE:HG23	2:B:271:TYR:H	1.66	0.60
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.82	0.60
1:A:199:ARG:HG3	1:A:219:LYS:HE3	1.83	0.60
1:A:277:ARG:HH11	1:A:334:GLN:HE21	1.48	0.60
1:A:479:LEU:CD2	1:A:501:TYR:HE2	2.14	0.60
1:A:58:THR:HG23	1:A:76:ASP:O	2.02	0.60
1:A:318:TYR:CZ	3:A:601:R8D:C15	2.84	0.60
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.01	0.60
1:A:295:LEU:HD23	1:A:295:LEU:H	1.66	0.60
1:A:497:THR:O	1:A:535:TRP:HA	2.01	0.60
1:A:2:ILE:HD11	1:A:46:LYS:HZ1	1.66	0.59
2:B:72:ARG:HG3	2:B:73:LYS:N	2.17	0.59
2:B:205:LEU:O	2:B:209:LEU:HD22	2.01	0.59
1:A:540:LYS:HB3	1:A:542:ILE:CD1	2.33	0.59
1:A:177:ASP:OD2	1:A:177:ASP:N	2.36	0.59
1:A:208:HIS:O	1:A:212:TRP:HD1	1.84	0.59
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.85	0.59
2:B:66:LYS:N	2:B:407:GLN:NE2	2.50	0.59
2:B:301:LEU:C	2:B:305:GLU:HG3	2.22	0.59
1:A:301:LEU:O	1:A:304:ALA:HB3	2.02	0.59
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.49	0.59
1:A:401:TRP:HB2	1:A:425:LEU:HD21	1.84	0.59
1:A:500:GLN:HG2	2:B:421:PRO:CG	2.32	0.59
1:A:400:THR:O	1:A:404:GLU:HG3	2.03	0.59
1:A:520:GLN:HA	1:A:523:GLU:CG	2.32	0.59
1:A:325:LEU:HD11	1:A:383:TRP:CD2	2.38	0.59
2:B:297:GLU:HA	2:B:300:GLU:HB2	1.83	0.59
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.38	0.59
1:A:175:ASN:ND2	1:A:201:LYS:HZ2	1.92	0.59
1:A:194:GLU:O	1:A:197:GLN:HG2	2.03	0.59
1:A:278:GLN:HG3	1:A:298:GLU:CB	2.33	0.59
1:A:325:LEU:O	1:A:326:ILE:HD13	2.03	0.59
2:B:175:ASN:HB3	2:B:178:ILE:HG13	1.83	0.59
1:A:3:SER:HB3	1:A:5:ILE:CD1	2.33	0.59
2:B:283:LEU:HD23	2:B:287:LYS:HE3	1.85	0.59
1:A:64:LYS:HZ1	1:A:69:THR:CA	2.16	0.58
1:A:449:GLU:O	1:A:451:LYS:HE2	2.03	0.58
1:A:3:SER:OG	1:A:5:ILE:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LYS:HE2	1:A:71:TRP:O	2.02	0.58
1:A:324:ASP:HB3	1:A:388:LYS:CE	2.33	0.58
1:A:491:LEU:H	1:A:491:LEU:CD1	2.16	0.58
1:A:245:VAL:HG22	1:A:245:VAL:O	2.04	0.58
1:A:312:GLU:HG2	1:A:313:PRO:N	2.19	0.58
2:B:267:ALA:O	2:B:270:ILE:HG23	2.03	0.58
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.68	0.58
2:B:354:TYR:HB2	2:B:374:LYS:HZ2	1.68	0.58
1:A:122:GLU:CA	1:A:125:ARG:HD2	2.27	0.58
2:B:382:ILE:HG22	2:B:383:TRP:CG	2.39	0.58
2:B:305:GLU:O	2:B:309:ILE:HG13	2.04	0.58
1:A:5:ILE:HG22	1:A:212:TRP:HE3	1.67	0.57
1:A:107:THR:HG21	1:A:202:ILE:CD1	2.30	0.57
1:A:333:GLY:O	1:A:335:GLY:N	2.37	0.57
1:A:406:TRP:CE3	1:A:407:GLN:HA	2.39	0.57
1:A:454:LYS:HA	1:A:467:VAL:O	2.04	0.57
1:A:101:LYS:CD	1:A:321:PRO:HG3	2.35	0.57
1:A:209:LEU:HD13	1:A:216:THR:HG21	1.85	0.57
1:A:432:GLU:OE1	1:A:432:GLU:HA	2.04	0.57
1:A:535:TRP:CZ3	1:A:537:PRO:HD3	2.38	0.57
2:B:175:ASN:N	2:B:176:PRO:HD3	2.18	0.57
1:A:122:GLU:HA	1:A:125:ARG:NE	2.19	0.57
1:A:244:ILE:HD12	1:A:267:ALA:CB	2.35	0.57
2:B:293:ILE:HG13	2:B:293:ILE:O	2.02	0.57
2:B:322:SER:O	2:B:323:LYS:HG2	2.04	0.57
1:A:460:ASN:HB2	2:B:286:THR:O	2.05	0.57
2:B:13:LYS:O	2:B:16:MET:HG2	2.04	0.57
2:B:114:ALA:HA	2:B:214:LEU:CD2	2.35	0.57
2:B:271:TYR:O	2:B:274:ILE:HG12	2.04	0.57
1:A:12:LEU:HD23	1:A:124:PHE:HE1	1.69	0.57
1:A:380:ILE:CD1	1:A:386:THR:HG22	2.32	0.57
1:A:540:LYS:HB2	1:A:542:ILE:HD13	1.86	0.57
1:A:443:ASP:CB	1:A:548:VAL:HB	2.33	0.57
2:B:154:LYS:HA	2:B:184:MET:HE3	1.85	0.57
2:B:374:LYS:O	2:B:378:GLU:HG3	2.04	0.57
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.85	0.57
1:A:487:GLN:HA	1:A:524:GLN:HE22	1.69	0.57
2:B:284:ARG:HB2	2:B:284:ARG:NH1	2.19	0.57
1:A:228:LEU:HB3	1:A:242:GLN:HE22	1.66	0.57
1:A:65:LYS:HD3	1:A:70:LYS:HG2	1.86	0.56
1:A:64:LYS:HZ1	1:A:69:THR:CG2	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ASP:OD2	1:A:388:LYS:NZ	2.34	0.56
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.39	0.56
1:A:455:ALA:HB3	1:A:469:LEU:HD11	1.86	0.56
2:B:174:GLN:C	2:B:176:PRO:HD3	2.25	0.56
1:A:209:LEU:CD1	1:A:216:THR:HG21	2.35	0.56
1:A:332:GLN:HG3	1:A:338:THR:HG22	1.86	0.56
2:B:194:GLU:OE1	2:B:197:GLN:N	2.36	0.56
2:B:270:ILE:O	2:B:272:PRO:HD3	2.06	0.56
2:B:284:ARG:N	2:B:287:LYS:HE2	2.21	0.56
2:B:314:VAL:HB	2:B:317:VAL:HG23	1.87	0.56
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.33	0.56
1:A:339:TYR:CG	1:A:375:ILE:CD1	2.88	0.56
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.41	0.56
2:B:63:ILE:HD13	2:B:74:LEU:HD13	1.86	0.56
2:B:378:GLU:O	2:B:382:ILE:HD12	2.06	0.56
1:A:91:GLN:NE2	2:B:137:ASN:HB3	2.20	0.56
1:A:395:LYS:CD	1:A:414:TRP:CZ2	2.88	0.56
1:A:425:LEU:HD23	1:A:428:GLN:NE2	2.20	0.56
2:B:5:ILE:HG23	2:B:6:GLU:OE1	2.06	0.56
1:A:332:GLN:HG3	1:A:338:THR:CG2	2.35	0.56
2:B:373:GLN:HE22	2:B:407:GLN:H	1.53	0.56
1:A:175:ASN:HD21	1:A:201:LYS:CE	2.17	0.56
2:B:425:LEU:HA	2:B:428:GLN:HB2	1.87	0.56
1:A:424:LYS:HE2	1:A:426:TRP:CZ3	2.40	0.55
1:A:238:LYS:HD2	1:A:315:HIS:CD2	2.42	0.55
1:A:478:GLU:OE1	1:A:499:SER:HB2	2.07	0.55
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.42	0.55
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.88	0.55
2:B:116:PHE:HD2	2:B:148:VAL:HG21	1.69	0.55
1:A:277:ARG:CZ	1:A:334:GLN:HB2	2.37	0.55
2:B:247:PRO:O	2:B:307:ARG:NH1	2.30	0.55
1:A:89:GLU:HB3	1:A:92:LEU:HD11	1.88	0.55
1:A:135:ILE:O	1:A:136:ASN:HB2	2.06	0.55
1:A:420:PRO:HA	1:A:421:PRO:C	2.27	0.55
2:B:393:ILE:HD11	2:B:397:THR:HG22	1.88	0.55
1:A:65:LYS:HD3	1:A:70:LYS:CG	2.36	0.55
1:A:164:MET:O	1:A:168:LEU:HD12	2.06	0.55
2:B:96:HIS:HE1	2:B:381:VAL:O	1.89	0.55
2:B:422:LEU:HB3	2:B:426:TRP:CH2	2.41	0.55
2:B:312:GLU:HB3	2:B:313:PRO:HD2	1.89	0.55
2:B:369:THR:HG22	2:B:370:GLU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:THR:HG23	2:B:254:VAL:N	2.21	0.54
2:B:116:PHE:HA	2:B:148:VAL:CG2	2.36	0.54
2:B:354:TYR:HB2	2:B:374:LYS:HZ1	1.73	0.54
2:B:330:GLN:HE22	2:B:340:GLN:HE22	1.54	0.54
1:A:173:LYS:HA	1:A:173:LYS:CE	2.37	0.54
2:B:122:GLU:HG2	2:B:125:ARG:NH2	2.23	0.54
2:B:301:LEU:O	2:B:304:ALA:HB3	2.07	0.54
1:A:433:PRO:HG3	2:B:255:ASN:ND2	2.22	0.54
1:A:101:LYS:HD2	1:A:321:PRO:HG3	1.89	0.54
2:B:284:ARG:H	2:B:287:LYS:CE	2.20	0.54
2:B:285:GLY:O	2:B:287:LYS:HG2	2.07	0.54
1:A:52:PRO:HD2	1:A:53:GLU:OE2	2.07	0.54
1:A:220:LYS:HE3	1:A:221:HIS:ND1	2.23	0.54
1:A:442:VAL:CG2	1:A:495:ILE:HG23	2.37	0.54
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.43	0.54
2:B:425:LEU:HG	2:B:426:TRP:N	2.23	0.54
2:B:278:GLN:O	2:B:282:LEU:HD23	2.07	0.54
1:A:219:LYS:O	1:A:220:LYS:HD2	2.07	0.54
1:A:369:THR:HG21	1:A:398:TRP:CH2	2.43	0.54
2:B:354:TYR:CB	2:B:374:LYS:HZ1	2.21	0.54
2:B:79:GLU:O	2:B:83:ARG:HG2	2.08	0.54
1:A:164:MET:SD	1:A:168:LEU:HD11	2.48	0.53
1:A:464:GLN:HG2	1:A:465:LYS:N	2.23	0.53
2:B:253:THR:CG2	2:B:255:ASN:HB3	2.38	0.53
2:B:254:VAL:HG21	2:B:288:ALA:O	2.08	0.53
2:B:270:ILE:HG23	2:B:271:TYR:N	2.22	0.53
1:A:226:PRO:HG3	1:A:235:HIS:CD2	2.41	0.53
1:A:283:LEU:N	1:A:283:LEU:HD23	2.21	0.53
2:B:276:VAL:HG22	2:B:279:LEU:HB2	1.91	0.53
2:B:80:LEU:O	2:B:80:LEU:HD22	2.08	0.53
1:A:355:ALA:O	1:A:356:ARG:O	2.26	0.53
1:A:520:GLN:HA	1:A:523:GLU:HG3	1.91	0.53
1:A:175:ASN:C	1:A:178:ILE:HD13	2.29	0.53
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.43	0.53
2:B:270:ILE:HG13	2:B:346:PHE:O	2.08	0.53
2:B:263:LYS:O	2:B:266:TRP:HE3	1.90	0.53
1:A:69:THR:O	1:A:69:THR:HG22	2.08	0.53
1:A:238:LYS:CB	1:A:315:HIS:HD2	2.22	0.53
1:A:402:TRP:CG	1:A:403:THR:N	2.75	0.53
1:A:271:TYR:CZ	1:A:314:VAL:HG23	2.44	0.53
1:A:317:VAL:CG2	1:A:318:TYR:N	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:GLU:O	2:B:301:LEU:HG	2.08	0.53
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.44	0.53
1:A:42:GLU:OE2	1:A:49:LYS:HE3	2.08	0.53
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.07	0.53
2:B:88:TRP:CZ3	2:B:89:GLU:HB2	2.44	0.53
2:B:330:GLN:NE2	2:B:340:GLN:HE22	2.07	0.53
1:A:64:LYS:HE2	1:A:69:THR:C	2.29	0.52
1:A:228:LEU:HB3	1:A:242:GLN:HE21	1.73	0.52
1:A:278:GLN:N	1:A:302:GLU:OE1	2.42	0.52
1:A:291:GLU:HG3	1:A:291:GLU:O	2.09	0.52
2:B:284:ARG:H	2:B:287:LYS:HE2	1.74	0.52
1:A:13:LYS:HB2	1:A:16:MET:SD	2.49	0.52
1:A:295:LEU:HD23	1:A:295:LEU:N	2.24	0.52
1:A:65:LYS:HZ2	1:A:68:SER:CB	2.22	0.52
1:A:241:VAL:HG12	1:A:266:TRP:NE1	2.24	0.52
1:A:276:VAL:O	1:A:276:VAL:HG12	2.09	0.52
1:A:311:LYS:O	1:A:312:GLU:OE2	2.28	0.52
1:A:458:VAL:HG13	1:A:548:VAL:HG22	1.91	0.52
1:A:475:GLN:HG3	1:A:501:TYR:CZ	2.44	0.52
2:B:116:PHE:HZ	2:B:151:GLN:CG	2.21	0.52
1:A:171:PHE:CE2	1:A:205:LEU:HD23	2.45	0.52
1:A:236:PRO:HA	3:A:601:R8D:C17	2.39	0.52
1:A:246:LEU:N	1:A:246:LEU:HD23	2.24	0.52
1:A:296:THR:HG23	1:A:299:ALA:CB	2.39	0.52
1:A:320:ASP:O	1:A:343:GLN:NE2	2.42	0.52
1:A:2:ILE:HG22	1:A:2:ILE:O	2.09	0.52
1:A:135:ILE:O	1:A:138:GLU:OE2	2.27	0.52
1:A:546:GLU:HG2	1:A:547:GLN:HE21	1.72	0.52
2:B:88:TRP:CE3	2:B:89:GLU:HB2	2.43	0.52
1:A:60:VAL:HG13	1:A:75:VAL:HG22	1.92	0.52
1:A:438:GLU:O	1:A:494:ASN:HB2	2.10	0.52
1:A:5:ILE:HD11	1:A:119:PRO:HG2	1.92	0.52
1:A:324:ASP:CG	1:A:388:LYS:HE2	2.30	0.52
1:A:403:THR:CG2	1:A:404:GLU:N	2.73	0.52
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.08	0.52
1:A:53:GLU:HG2	1:A:54:ASN:N	2.24	0.52
1:A:406:TRP:CE3	1:A:407:GLN:CA	2.93	0.52
1:A:411:ILE:HG22	1:A:412:PRO:O	2.10	0.52
1:A:429:LEU:HD21	1:A:506:ILE:HG22	1.92	0.52
1:A:493:VAL:HG21	1:A:528:LYS:HE2	1.90	0.52
1:A:459:THR:CG2	1:A:463:ARG:HB3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:VAL:O	2:B:265:ASN:N	2.26	0.52
2:B:266:TRP:NE1	2:B:346:PHE:CE2	2.77	0.52
1:A:252:TRP:CG	1:A:295:LEU:HD21	2.45	0.52
1:A:438:GLU:HG3	1:A:461:ARG:HG3	1.91	0.52
2:B:131:THR:HG22	2:B:132:ILE:N	2.24	0.52
2:B:271:TYR:HB3	2:B:274:ILE:HD11	1.92	0.52
1:A:188:TYR:CD2	3:A:601:R8D:C25	2.93	0.51
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.40	0.51
2:B:297:GLU:N	2:B:298:GLU:OE2	2.43	0.51
1:A:65:LYS:CD	1:A:70:LYS:HG2	2.39	0.51
1:A:79:GLU:OE1	1:A:82:LYS:HE2	2.10	0.51
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.09	0.51
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.46	0.51
2:B:379:SER:OG	2:B:387:PRO:HD3	2.09	0.51
1:A:17:ASP:O	1:A:83:ARG:HD3	2.09	0.51
1:A:65:LYS:HD2	1:A:72:ARG:HD2	1.92	0.51
1:A:289:LEU:HD13	1:A:289:LEU:O	2.09	0.51
1:A:527:LYS:O	1:A:528:LYS:O	2.28	0.51
2:B:306:ASN:O	2:B:309:ILE:N	2.43	0.51
1:A:94:ILE:HB	1:A:95:PRO:HD2	1.93	0.51
1:A:330:GLN:HE22	1:A:340:GLN:NE2	2.08	0.51
2:B:120:LEU:HD22	2:B:121:ASP:H	1.74	0.51
1:A:134:SER:HB2	1:A:139:THR:HB	1.90	0.51
1:A:181:TYR:HD2	3:A:601:R8D:H5	1.76	0.51
1:A:284:ARG:NH1	1:A:285:GLY:HA3	2.23	0.51
1:A:296:THR:CG2	1:A:299:ALA:HB2	2.40	0.51
1:A:458:VAL:O	1:A:458:VAL:HG22	2.10	0.51
1:A:168:LEU:C	1:A:170:PRO:HD2	2.29	0.51
1:A:175:ASN:ND2	1:A:201:LYS:HZ1	2.08	0.51
1:A:459:THR:HG21	1:A:463:ARG:HB3	1.92	0.51
1:A:278:GLN:HG3	1:A:298:GLU:HB3	1.93	0.51
1:A:311:LYS:O	1:A:312:GLU:CB	2.56	0.51
1:A:346:PHE:N	1:A:346:PHE:HD1	2.08	0.51
2:B:266:TRP:NE1	2:B:346:PHE:HE2	2.08	0.51
1:A:173:LYS:HA	1:A:173:LYS:HE3	1.92	0.51
1:A:254:VAL:HG21	1:A:288:ALA:O	2.11	0.51
1:A:137:ASN:O	1:A:138:GLU:O	2.28	0.50
2:B:154:LYS:HG3	2:B:184:MET:HE1	1.93	0.50
2:B:354:TYR:HA	2:B:374:LYS:HZ1	1.76	0.50
1:A:120:LEU:HD21	1:A:128:THR:HG21	1.93	0.50
1:A:206:ARG:NH2	1:A:218:ASP:N	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLN:NE2	1:A:338:THR:HG23	2.26	0.50
2:B:18:GLY:HA3	2:B:56:TYR:CD1	2.47	0.50
2:B:87:PHE:O	2:B:91:GLN:HB3	2.12	0.50
1:A:324:ASP:O	1:A:343:GLN:HG2	2.11	0.50
2:B:66:LYS:O	2:B:67:ASP:HB2	2.09	0.50
2:B:154:LYS:HA	2:B:184:MET:CE	2.41	0.50
2:B:195:ILE:HG23	2:B:196:GLY:N	2.26	0.50
2:B:306:ASN:O	2:B:310:LEU:N	2.35	0.50
2:B:88:TRP:CZ2	2:B:154:LYS:HD3	2.47	0.50
2:B:142:ILE:CG2	2:B:144:TYR:CE2	2.95	0.50
1:A:2:ILE:CD1	1:A:46:LYS:HE2	2.41	0.50
1:A:228:LEU:N	1:A:228:LEU:CD1	2.74	0.50
1:A:393:ILE:O	1:A:416:PHE:HD1	1.95	0.50
1:A:432:GLU:OE1	1:A:433:PRO:HD3	2.12	0.50
1:A:231:GLY:O	1:A:242:GLN:N	2.45	0.50
1:A:391:LEU:HB3	1:A:392:PRO:HD2	1.93	0.50
2:B:50:ILE:CG2	2:B:145:GLN:HB3	2.32	0.50
1:A:233:GLU:O	1:A:234:LEU:HD23	2.12	0.50
1:A:448:ARG:HG2	1:A:448:ARG:NH1	2.21	0.50
1:A:35:VAL:O	1:A:39:THR:HG23	2.12	0.50
1:A:101:LYS:CE	1:A:321:PRO:HG3	2.41	0.50
1:A:324:ASP:HB3	1:A:388:LYS:HE2	1.93	0.50
2:B:254:VAL:O	2:B:257:ILE:N	2.37	0.50
1:A:101:LYS:HD3	1:A:321:PRO:HD3	1.93	0.49
2:B:125:ARG:NH1	2:B:147:ASN:HD22	2.11	0.49
1:A:200:THR:HG22	1:A:201:LYS:N	2.26	0.49
2:B:196:GLY:HA2	2:B:199:ARG:HG3	1.93	0.49
2:B:276:VAL:HG22	2:B:279:LEU:CB	2.42	0.49
1:A:325:LEU:C	1:A:326:ILE:HD13	2.32	0.49
2:B:320:ASP:O	2:B:343:GLN:NE2	2.45	0.49
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.93	0.49
1:A:65:LYS:HB3	1:A:65:LYS:NZ	2.28	0.49
1:A:66:LYS:O	1:A:67:ASP:HB3	2.12	0.49
1:A:167:ILE:O	1:A:208:HIS:NE2	2.38	0.49
1:A:174:GLN:O	1:A:175:ASN:OD1	2.31	0.49
2:B:159:ILE:HG22	2:B:160:PHE:N	2.27	0.49
2:B:247:PRO:C	2:B:307:ARG:HH12	2.14	0.49
2:B:422:LEU:O	2:B:425:LEU:HD23	2.13	0.49
1:A:278:GLN:HB3	1:A:299:ALA:HA	1.94	0.49
1:A:511:ASP:OD2	1:A:512:GLN:HG2	2.11	0.49
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:LEU:CB	2:B:426:TRP:CH2	2.96	0.49
1:A:13:LYS:HG3	1:A:84:THR:O	2.12	0.49
1:A:100:LEU:CD2	1:A:181:TYR:CE2	2.95	0.49
1:A:230:MET:HE2	1:A:230:MET:CA	2.42	0.49
1:A:430:GLU:CD	1:A:530:LYS:HG2	2.34	0.49
1:A:477:THR:O	1:A:480:GLN:HB3	2.13	0.49
2:B:66:LYS:N	2:B:407:GLN:HE22	2.11	0.49
2:B:74:LEU:HD21	2:B:411:ILE:HD11	1.94	0.49
1:A:79:GLU:HG2	1:A:83:ARG:HH21	1.78	0.49
1:A:5:ILE:HD11	1:A:119:PRO:CG	2.43	0.48
2:B:66:LYS:CA	2:B:407:GLN:NE2	2.75	0.48
2:B:154:LYS:HG3	2:B:184:MET:CE	2.42	0.48
1:A:175:ASN:ND2	1:A:201:LYS:CE	2.76	0.48
1:A:195:ILE:CG2	1:A:199:ARG:NE	2.76	0.48
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.94	0.48
1:A:361:HIS:HB3	1:A:513:SER:HB2	1.93	0.48
2:B:172:ARG:HH21	2:B:180:ILE:HB	1.78	0.48
1:A:77:PHE:HE2	1:A:150:PRO:HB2	1.77	0.48
1:A:101:LYS:O	3:A:601:R8D:H11	2.13	0.48
1:A:120:LEU:O	1:A:125:ARG:NE	2.43	0.48
1:A:219:LYS:C	1:A:221:HIS:H	2.16	0.48
1:A:339:TYR:CD1	1:A:375:ILE:CD1	2.96	0.48
2:B:85:GLN:O	2:B:85:GLN:HG2	2.13	0.48
2:B:254:VAL:HG13	2:B:283:LEU:HD21	1.94	0.48
1:A:399:GLU:CG	1:A:400:THR:N	2.77	0.48
1:A:47:ILE:HG22	1:A:146:TYR:HA	1.96	0.48
1:A:125:ARG:NH1	1:A:147:ASN:HD22	2.12	0.48
1:A:199:ARG:H	1:A:199:ARG:HD2	1.79	0.48
1:A:339:TYR:CD1	1:A:375:ILE:HD11	2.49	0.48
1:A:424:LYS:HE2	1:A:426:TRP:CD2	2.49	0.48
2:B:63:ILE:CD1	2:B:74:LEU:HD13	2.43	0.48
2:B:204:GLU:O	2:B:207:GLN:HB2	2.14	0.48
1:A:63:ILE:CG1	1:A:74:LEU:CD1	2.91	0.48
1:A:202:ILE:O	1:A:206:ARG:HG3	2.13	0.48
2:B:254:VAL:HG13	2:B:283:LEU:CD2	2.44	0.48
1:A:230:MET:CA	1:A:230:MET:CE	2.91	0.48
1:A:320:ASP:C	1:A:322:SER:H	2.17	0.48
1:A:411:ILE:CG2	1:A:414:TRP:CD1	2.96	0.48
1:A:491:LEU:CD1	1:A:491:LEU:N	2.76	0.48
1:A:517:LEU:HA	1:A:520:GLN:HG3	1.95	0.48
2:B:72:ARG:NH1	2:B:409:THR:HG22	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TYR:CE2	3:A:601:R8D:C25	2.96	0.48
1:A:427:TYR:O	1:A:428:GLN:HG2	2.14	0.48
1:A:443:ASP:O	1:A:481:ALA:HB2	2.14	0.48
1:A:476:LYS:O	1:A:480:GLN:HB2	2.14	0.48
1:A:116:PHE:HD1	1:A:148:VAL:CG2	2.27	0.47
1:A:318:TYR:CD2	3:A:601:R8D:H15	2.42	0.47
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.49	0.47
1:A:349:LEU:HA	1:A:349:LEU:HD12	1.59	0.47
2:B:234:LEU:O	2:B:236:PRO:HD3	2.14	0.47
1:A:226:PRO:O	1:A:228:LEU:HD13	2.13	0.47
1:A:378:GLU:O	1:A:382:ILE:HG13	2.14	0.47
2:B:7:THR:CG2	2:B:119:PRO:HB2	2.45	0.47
2:B:283:LEU:HD23	2:B:287:LYS:CE	2.43	0.47
1:A:479:LEU:HD22	1:A:501:TYR:HE2	1.77	0.47
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.47	0.47
2:B:211:ARG:N	2:B:211:ARG:CD	2.76	0.47
2:B:393:ILE:CG2	2:B:398:TRP:HB2	2.44	0.47
1:A:283:LEU:HD22	1:A:283:LEU:HA	1.62	0.47
1:A:435:VAL:HG22	2:B:290:THR:CB	2.44	0.47
1:A:175:ASN:N	1:A:176:PRO:CD	2.76	0.47
2:B:10:VAL:HB	2:B:124:PHE:CD1	2.50	0.47
2:B:195:ILE:CG2	2:B:196:GLY:N	2.77	0.47
2:B:286:THR:OG1	2:B:286:THR:O	2.32	0.47
2:B:396:GLU:O	2:B:400:THR:CG2	2.63	0.47
2:B:420:PRO:CG	2:B:423:VAL:HG21	2.43	0.47
1:A:210:LEU:C	1:A:212:TRP:H	2.18	0.47
1:A:398:TRP:CZ2	1:A:411:ILE:HD12	2.49	0.47
2:B:105:SER:O	2:B:190:GLY:HA2	2.15	0.47
2:B:195:ILE:O	2:B:199:ARG:HG2	2.13	0.47
2:B:214:LEU:H	2:B:214:LEU:HD23	1.79	0.47
2:B:279:LEU:HD23	2:B:302:GLU:OE1	2.15	0.47
1:A:215:THR:O	1:A:215:THR:OG1	2.32	0.47
2:B:164:MET:O	2:B:164:MET:HG3	2.14	0.47
2:B:271:TYR:HE2	2:B:314:VAL:HA	1.79	0.47
1:A:220:LYS:HD3	1:A:221:HIS:CG	2.50	0.47
2:B:194:GLU:HB3	2:B:197:GLN:HB2	1.97	0.47
2:B:244:ILE:HD13	2:B:266:TRP:CH2	2.50	0.47
1:A:13:LYS:HE2	1:A:84:THR:O	2.15	0.47
1:A:509:GLN:N	1:A:510:PRO:HD3	2.30	0.47
2:B:44:GLU:O	2:B:46:LYS:HE2	2.15	0.47
2:B:214:LEU:HD23	2:B:214:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.65	0.46
1:A:458:VAL:HG11	1:A:548:VAL:HG22	1.95	0.46
2:B:148:VAL:HG23	2:B:149:LEU:N	2.29	0.46
1:A:475:GLN:CG	1:A:501:TYR:CZ	2.98	0.46
2:B:50:ILE:HD12	2:B:54:ASN:HB3	1.96	0.46
1:A:175:ASN:HB3	1:A:178:ILE:CD1	2.31	0.46
1:A:287:LYS:HB2	1:A:291:GLU:OE2	2.14	0.46
1:A:466:VAL:CG1	1:A:467:VAL:H	2.27	0.46
1:A:466:VAL:O	1:A:467:VAL:HG23	2.15	0.46
2:B:195:ILE:HD13	2:B:195:ILE:HA	1.80	0.46
2:B:344:GLU:O	2:B:347:LYS:HB2	2.15	0.46
1:A:188:TYR:CD2	3:A:601:R8D:C2	2.98	0.46
1:A:500:GLN:CG	2:B:422:LEU:HG	2.45	0.46
2:B:138:GLU:HB3	2:B:139:THR:HG23	1.97	0.46
2:B:284:ARG:NH1	2:B:284:ARG:CB	2.79	0.46
1:A:54:ASN:HA	1:A:55:PRO:HD3	1.73	0.46
1:A:183:TYR:HB3	1:A:188:TYR:HE1	1.80	0.46
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.45	0.46
2:B:13:LYS:HA	2:B:14:PRO:HD2	1.48	0.46
2:B:271:TYR:HD2	2:B:272:PRO:HD2	1.81	0.46
2:B:422:LEU:CD1	2:B:426:TRP:CH2	2.99	0.46
2:B:254:VAL:CG1	2:B:283:LEU:HD21	2.46	0.46
2:B:382:ILE:CG2	2:B:383:TRP:CD2	2.99	0.46
1:A:64:LYS:HZ3	1:A:69:THR:HA	1.79	0.46
1:A:435:VAL:HA	2:B:290:THR:HG21	1.97	0.46
2:B:164:MET:HA	2:B:167:ILE:HD12	1.98	0.46
2:B:320:ASP:OD1	2:B:321:PRO:HD2	2.16	0.46
1:A:325:LEU:HD22	1:A:341:ILE:CG2	2.46	0.46
2:B:72:ARG:HH12	2:B:409:THR:HG21	1.78	0.46
1:A:448:ARG:CG	1:A:448:ARG:NH1	2.75	0.46
1:A:115:TYR:HB2	1:A:151:GLN:NE2	2.30	0.46
1:A:134:SER:OG	1:A:139:THR:HB	2.16	0.46
1:A:178:ILE:N	1:A:178:ILE:CD1	2.79	0.46
1:A:199:ARG:HG2	1:A:199:ARG:NH1	2.31	0.46
1:A:418:ASN:O	1:A:420:PRO:HD3	2.16	0.46
1:A:425:LEU:HD12	1:A:425:LEU:HA	1.54	0.46
1:A:442:VAL:HG21	1:A:495:ILE:HG23	1.97	0.46
2:B:118:VAL:HA	2:B:119:PRO:HD2	1.67	0.46
1:A:2:ILE:CD1	1:A:46:LYS:NZ	2.73	0.45
1:A:65:LYS:NZ	1:A:68:SER:CB	2.78	0.45
1:A:175:ASN:ND2	1:A:201:LYS:CD	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:CE	1:A:61:PHE:CE1	2.98	0.45
1:A:127:TYR:C	1:A:129:ALA:H	2.19	0.45
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.32	0.45
1:A:327:ALA:O	1:A:389:PHE:HA	2.16	0.45
1:A:402:TRP:CD1	1:A:402:TRP:C	2.85	0.45
1:A:540:LYS:CD	1:A:540:LYS:N	2.80	0.45
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.96	0.45
2:B:183:TYR:OH	2:B:386:THR:HG23	2.16	0.45
2:B:301:LEU:O	2:B:304:ALA:N	2.49	0.45
1:A:0:SER:HB2	1:A:1:PRO:CD	2.46	0.45
1:A:103:ASN:O	3:A:601:R8D:N19	2.46	0.45
1:A:325:LEU:HD22	1:A:341:ILE:HG21	1.98	0.45
1:A:70:LYS:O	1:A:70:LYS:HG3	2.12	0.45
1:A:406:TRP:CE3	1:A:407:GLN:N	2.84	0.45
1:A:411:ILE:HG22	1:A:414:TRP:CD1	2.51	0.45
2:B:312:GLU:CB	2:B:313:PRO:HD2	2.43	0.45
1:A:26:LEU:HB2	1:A:133:PRO:HG2	1.99	0.45
1:A:63:ILE:HG12	1:A:74:LEU:HD11	1.98	0.45
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.98	0.45
1:A:65:LYS:NZ	1:A:68:SER:HB2	2.31	0.45
1:A:195:ILE:O	1:A:199:ARG:HD2	2.16	0.45
1:A:339:TYR:O	1:A:340:GLN:HG3	2.15	0.45
1:A:519:ASN:O	1:A:522:ILE:HB	2.17	0.45
2:B:382:ILE:HG21	2:B:383:TRP:CE2	2.51	0.45
1:A:64:LYS:NZ	1:A:69:THR:HG23	2.27	0.45
1:A:84:THR:HG22	1:A:85:GLN:N	2.31	0.45
1:A:286:THR:HG23	1:A:287:LYS:O	2.17	0.45
1:A:340:GLN:HA	1:A:351:THR:HA	1.99	0.45
2:B:242:GLN:HB2	2:B:352:GLY:HA2	1.99	0.45
1:A:255:ASN:HB2	1:A:289:LEU:HD11	1.97	0.45
1:A:418:ASN:C	1:A:420:PRO:HD3	2.36	0.45
1:A:422:LEU:HD12	1:A:422:LEU:HA	1.54	0.45
1:A:253:THR:O	1:A:257:ILE:HG12	2.17	0.45
1:A:324:ASP:CB	1:A:388:LYS:HE2	2.47	0.45
1:A:442:VAL:HG13	1:A:457:TYR:HB3	1.98	0.45
1:A:491:LEU:O	1:A:492:GLU:HG3	2.17	0.45
2:B:116:PHE:CD2	2:B:148:VAL:HG21	2.50	0.45
1:A:209:LEU:HD13	1:A:216:THR:CG2	2.45	0.45
1:A:220:LYS:CE	1:A:221:HIS:CE1	2.98	0.45
1:A:522:ILE:HG23	1:A:526:ILE:HD11	1.99	0.45
2:B:60:VAL:CG2	2:B:73:LYS:HD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HG12	1:A:74:LEU:CD1	2.47	0.44
1:A:244:ILE:HG22	1:A:246:LEU:CD2	2.46	0.44
1:A:319:TYR:CE1	1:A:343:GLN:NE2	2.85	0.44
2:B:125:ARG:H	2:B:125:ARG:HG2	1.50	0.44
2:B:12:LEU:HD22	2:B:127:TYR:CZ	2.53	0.44
2:B:65:LYS:NZ	2:B:65:LYS:CB	2.79	0.44
2:B:89:GLU:O	2:B:89:GLU:HG2	2.17	0.44
2:B:116:PHE:CZ	2:B:151:GLN:CG	2.95	0.44
2:B:255:ASN:HA	2:B:258:GLN:HG3	1.98	0.44
2:B:425:LEU:C	2:B:427:TYR:N	2.70	0.44
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.99	0.44
1:A:406:TRP:CD2	1:A:407:GLN:N	2.85	0.44
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.99	0.44
2:B:66:LYS:HE2	2:B:67:ASP:OD2	2.16	0.44
1:A:324:ASP:CB	1:A:388:LYS:CE	2.95	0.44
1:A:425:LEU:HD23	1:A:428:GLN:HE22	1.82	0.44
1:A:466:VAL:CG1	1:A:467:VAL:N	2.80	0.44
2:B:13:LYS:CB	2:B:16:MET:HE2	2.47	0.44
2:B:314:VAL:HB	2:B:317:VAL:CG2	2.46	0.44
1:A:181:TYR:CD2	3:A:601:R8D:H5	2.51	0.44
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.38	0.44
1:A:490:GLY:O	1:A:528:LYS:HE3	2.18	0.44
2:B:422:LEU:HD13	2:B:426:TRP:CH2	2.52	0.44
1:A:236:PRO:HA	3:A:601:R8D:C18	2.48	0.44
1:A:442:VAL:HG11	1:A:481:ALA:C	2.37	0.44
2:B:175:ASN:HD21	2:B:201:LYS:HZ1	1.66	0.44
1:A:228:LEU:CB	1:A:242:GLN:HE21	2.30	0.44
1:A:253:THR:HG22	1:A:292:VAL:CG2	2.40	0.44
1:A:326:ILE:HD12	1:A:388:LYS:HB2	2.00	0.44
1:A:434:ILE:CB	1:A:494:ASN:HD21	2.30	0.44
1:A:106:VAL:HG12	3:A:601:R8D:N24	2.33	0.44
1:A:326:ILE:HD11	1:A:388:LYS:HE3	2.00	0.44
1:A:406:TRP:CZ3	1:A:407:GLN:CG	3.01	0.44
2:B:160:PHE:CE2	2:B:164:MET:CE	2.94	0.44
2:B:276:VAL:CG2	2:B:279:LEU:HB2	2.48	0.44
1:A:92:LEU:HA	1:A:92:LEU:HD13	1.63	0.43
2:B:153:TRP:CE2	2:B:155:GLY:HA3	2.54	0.43
2:B:253:THR:HG22	2:B:255:ASN:HB3	2.00	0.43
1:A:54:ASN:HB3	1:A:143:ARG:NH2	2.33	0.43
1:A:63:ILE:CG1	1:A:74:LEU:HD11	2.47	0.43
1:A:440:PHE:CE1	1:A:489:SER:CB	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:LYS:HB3	2:B:259:LYS:HE3	1.60	0.43
1:A:30:LYS:HE2	1:A:61:PHE:CZ	2.53	0.43
1:A:174:GLN:H	1:A:174:GLN:HG2	1.57	0.43
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.53	0.43
1:A:63:ILE:HG13	1:A:74:LEU:HD12	2.00	0.43
1:A:175:ASN:O	1:A:178:ILE:HD13	2.18	0.43
1:A:393:ILE:HG12	1:A:394:GLN:N	2.33	0.43
1:A:472:THR:HB	1:A:473:THR:H	1.55	0.43
2:B:80:LEU:HD22	2:B:84:THR:HG23	1.99	0.43
1:A:10:VAL:HG11	1:A:153:TRP:HH2	1.82	0.43
1:A:270:ILE:HA	1:A:351:THR:HG23	1.99	0.43
1:A:275:LYS:HZ3	1:A:275:LYS:HG3	1.75	0.43
2:B:8:VAL:HA	2:B:9:PRO:HD2	1.61	0.43
2:B:115:TYR:N	2:B:115:TYR:CD1	2.83	0.43
2:B:98:ALA:O	2:B:101:LYS:NZ	2.31	0.43
1:A:150:PRO:HG2	1:A:153:TRP:CB	2.49	0.43
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.51	0.43
2:B:40:GLU:OE2	2:B:40:GLU:HA	2.14	0.43
1:A:179:VAL:HG12	1:A:190:GLY:O	2.19	0.43
1:A:459:THR:HG23	1:A:463:ARG:O	2.19	0.43
2:B:9:PRO:HA	2:B:121:ASP:OD1	2.18	0.43
2:B:312:GLU:HA	2:B:313:PRO:HD3	1.71	0.43
1:A:375:ILE:O	1:A:378:GLU:HB3	2.19	0.43
1:A:120:LEU:CD2	1:A:128:THR:HG21	2.49	0.42
2:B:100:LEU:CD2	2:B:181:TYR:HB3	2.49	0.42
2:B:175:ASN:HD21	2:B:201:LYS:HE3	1.82	0.42
2:B:279:LEU:HD21	2:B:303:LEU:CD2	2.49	0.42
2:B:422:LEU:CB	2:B:426:TRP:CZ2	2.95	0.42
1:A:479:LEU:CD2	1:A:501:TYR:CE2	2.99	0.42
2:B:382:ILE:CG2	2:B:383:TRP:CE2	3.02	0.42
2:B:398:TRP:CG	2:B:416:PHE:HE1	2.37	0.42
1:A:107:THR:CB	1:A:202:ILE:HD11	2.48	0.42
1:A:432:GLU:HA	1:A:433:PRO:HD3	1.79	0.42
1:A:464:GLN:CG	1:A:465:LYS:N	2.83	0.42
1:A:500:GLN:OE1	2:B:422:LEU:HG	2.19	0.42
2:B:320:ASP:HA	2:B:321:PRO:HD3	1.92	0.42
2:B:393:ILE:HG12	2:B:394:GLN:H	1.83	0.42
1:A:54:ASN:OD1	1:A:55:PRO:HD2	2.19	0.42
1:A:134:SER:OG	1:A:139:THR:O	2.37	0.42
1:A:225:PRO:HA	1:A:226:PRO:C	2.40	0.42
1:A:296:THR:HG23	1:A:299:ALA:HB2	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:HD22	1:A:452:LEU:HA	1.73	0.42
2:B:28:GLU:HG2	2:B:32:LYS:HE2	2.00	0.42
2:B:295:LEU:HD23	2:B:300:GLU:OE1	2.19	0.42
2:B:354:TYR:CB	2:B:374:LYS:NZ	2.79	0.42
1:A:72:ARG:HE	1:A:72:ARG:HB3	1.54	0.42
1:A:296:THR:CG2	1:A:299:ALA:CB	2.98	0.42
1:A:65:LYS:CG	1:A:72:ARG:HD2	2.48	0.42
1:A:303:LEU:O	1:A:307:ARG:HG3	2.20	0.42
1:A:491:LEU:N	1:A:491:LEU:HD12	2.34	0.42
2:B:395:LYS:O	2:B:399:GLU:N	2.48	0.42
1:A:424:LYS:CE	1:A:426:TRP:CE2	3.00	0.42
1:A:442:VAL:HG21	1:A:495:ILE:CG2	2.49	0.42
1:A:473:THR:OG1	1:A:476:LYS:HD3	2.19	0.42
1:A:474:ASN:O	1:A:475:GLN:C	2.56	0.42
2:B:180:ILE:CG1	2:B:189:VAL:HG13	2.49	0.42
2:B:376:THR:HB	2:B:410:TRP:CH2	2.55	0.42
1:A:8:VAL:HG21	2:B:52:PRO:HG2	2.02	0.42
1:A:195:ILE:CG2	1:A:199:ARG:CZ	2.97	0.42
1:A:288:ALA:HB3	1:A:291:GLU:H	1.85	0.42
2:B:87:PHE:CZ	2:B:92:LEU:CD1	2.99	0.42
2:B:354:TYR:CA	2:B:374:LYS:HZ1	2.33	0.42
2:B:373:GLN:NE2	2:B:408:ALA:H	2.18	0.42
1:A:96:HIS:N	2:B:136:ASN:OD1	2.46	0.42
1:A:319:TYR:CZ	1:A:321:PRO:HA	2.55	0.42
1:A:373:GLN:N	1:A:373:GLN:HE21	2.18	0.42
1:A:475:GLN:HG3	1:A:501:TYR:CD2	2.51	0.42
2:B:46:LYS:H	2:B:46:LYS:HG2	1.54	0.42
2:B:72:ARG:NH1	2:B:72:ARG:HG2	2.35	0.42
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.32	0.42
2:B:376:THR:HG23	2:B:386:THR:HB	2.01	0.42
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.89	0.42
1:A:228:LEU:CB	1:A:242:GLN:NE2	2.76	0.42
1:A:19:PRO:HB3	1:A:79:GLU:HB3	2.00	0.41
1:A:66:LYS:O	1:A:67:ASP:CB	2.68	0.41
1:A:220:LYS:HD3	1:A:221:HIS:N	2.35	0.41
1:A:223:LYS:H	1:A:223:LYS:HG2	1.48	0.41
1:A:235:HIS:CB	1:A:236:PRO:CD	2.94	0.41
2:B:320:ASP:OD1	2:B:322:SER:OG	2.29	0.41
1:A:163:SER:O	1:A:166:LYS:N	2.53	0.41
1:A:249:LYS:HB2	1:A:249:LYS:HE2	1.69	0.41
1:A:424:LYS:HE2	1:A:426:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:GLY:CA	2:B:56:TYR:CE1	2.98	0.41
2:B:83:ARG:HG2	2:B:83:ARG:H	1.44	0.41
2:B:253:THR:CG2	2:B:255:ASN:CB	2.97	0.41
2:B:306:ASN:HD22	2:B:309:ILE:CD1	2.32	0.41
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.55	0.41
2:B:373:GLN:NE2	2:B:407:GLN:H	2.19	0.41
2:B:422:LEU:CD1	2:B:426:TRP:CZ2	2.99	0.41
1:A:30:LYS:CD	1:A:61:PHE:CE1	3.03	0.41
1:A:63:ILE:CG1	1:A:74:LEU:HD12	2.50	0.41
1:A:197:GLN:HA	1:A:200:THR:HB	2.03	0.41
1:A:373:GLN:CA	1:A:373:GLN:NE2	2.83	0.41
1:A:432:GLU:HG3	1:A:433:PRO:HD2	2.02	0.41
1:A:486:LEU:O	1:A:528:LYS:NZ	2.49	0.41
1:A:191:SER:OG	1:A:198:HIS:CD2	2.74	0.41
1:A:239:TRP:C	1:A:240:THR:HG22	2.41	0.41
2:B:80:LEU:HD13	2:B:153:TRP:CD1	2.55	0.41
2:B:349:LEU:HB3	2:B:383:TRP:CZ2	2.55	0.41
2:B:391:LEU:HA	2:B:392:PRO:HD3	1.68	0.41
2:B:393:ILE:HG21	2:B:398:TRP:HB2	2.01	0.41
1:A:164:MET:O	1:A:164:MET:SD	2.79	0.41
1:A:320:ASP:O	1:A:322:SER:N	2.53	0.41
1:A:479:LEU:HD21	1:A:501:TYR:CE2	2.55	0.41
2:B:80:LEU:HA	2:B:80:LEU:HD23	1.80	0.41
2:B:329:ILE:HA	2:B:338:THR:O	2.20	0.41
2:B:122:GLU:HG2	2:B:125:ARG:HH21	1.86	0.41
2:B:310:LEU:HD12	2:B:310:LEU:HA	1.71	0.41
1:A:287:LYS:O	1:A:288:ALA:O	2.38	0.41
1:A:411:ILE:HA	1:A:412:PRO:HD2	1.87	0.41
2:B:13:LYS:HD2	2:B:85:GLN:N	2.36	0.41
2:B:330:GLN:CD	2:B:340:GLN:HE22	2.24	0.41
2:B:376:THR:CG2	2:B:386:THR:HB	2.51	0.41
2:B:63:ILE:HD13	2:B:74:LEU:HB2	2.03	0.41
2:B:125:ARG:O	2:B:145:GLN:HG3	2.20	0.41
2:B:150:PRO:HD2	2:B:153:TRP:HE3	1.86	0.41
2:B:246:LEU:CD1	2:B:307:ARG:HG3	2.39	0.41
1:A:0:SER:CB	1:A:1:PRO:CD	2.98	0.41
1:A:10:VAL:HG13	1:A:87:PHE:CZ	2.56	0.41
1:A:107:THR:CG2	1:A:202:ILE:CD1	2.97	0.41
1:A:171:PHE:O	1:A:171:PHE:CD1	2.74	0.41
1:A:356:ARG:NH2	1:A:358:ARG:CD	2.79	0.41
1:A:411:ILE:HG21	1:A:414:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LYS:O	2:B:65:LYS:HB2	2.20	0.41
2:B:168:LEU:HA	2:B:168:LEU:HD23	1.74	0.41
2:B:252:TRP:HB3	2:B:257:ILE:HD11	2.02	0.41
2:B:260:LEU:CD1	2:B:264:LEU:CD1	2.98	0.41
2:B:344:GLU:CB	2:B:345:PRO:HD2	2.38	0.41
2:B:369:THR:O	2:B:373:GLN:HG3	2.21	0.41
2:B:382:ILE:HG22	2:B:383:TRP:CD1	2.56	0.41
1:A:63:ILE:HD12	1:A:72:ARG:HG3	2.03	0.41
1:A:210:LEU:C	1:A:212:TRP:N	2.73	0.41
1:A:395:LYS:CD	1:A:414:TRP:CH2	3.02	0.41
2:B:128:THR:OG1	2:B:146:TYR:HB2	2.21	0.41
1:A:169:GLU:N	1:A:170:PRO:CD	2.77	0.40
2:B:393:ILE:HD11	2:B:397:THR:CG2	2.50	0.40
1:A:64:LYS:HB3	1:A:65:LYS:H	1.62	0.40
1:A:179:VAL:O	1:A:179:VAL:HG13	2.20	0.40
1:A:231:GLY:O	1:A:242:GLN:HB2	2.22	0.40
1:A:245:VAL:O	1:A:247:PRO:HD3	2.21	0.40
1:A:282:LEU:HD21	1:A:296:THR:HG22	2.03	0.40
2:B:203:GLU:OE1	2:B:206:ARG:NH1	2.54	0.40
2:B:271:TYR:CE2	2:B:314:VAL:HA	2.56	0.40
2:B:46:LYS:HA	2:B:148:VAL:HG13	2.02	0.40
2:B:209:LEU:HB3	2:B:214:LEU:O	2.21	0.40
1:A:4:PRO:HG2	1:A:212:TRP:CE3	2.56	0.40
1:A:64:LYS:HD3	1:A:64:LYS:HA	1.69	0.40
1:A:124:PHE:O	1:A:127:TYR:HD1	2.05	0.40
1:A:155:GLY:O	1:A:159:ILE:HD12	2.22	0.40
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.61	0.40
1:A:235:HIS:O	3:A:601:R8D:C21	2.69	0.40
2:B:260:LEU:CD1	2:B:264:LEU:HD11	2.51	0.40
1:A:96:HIS:HB3	1:A:382:ILE:HD13	2.03	0.40
1:A:289:LEU:HD13	1:A:289:LEU:C	2.41	0.40
1:A:369:THR:HG21	1:A:398:TRP:HH2	1.87	0.40
2:B:64:LYS:O	2:B:65:LYS:CB	2.70	0.40
2:B:195:ILE:O	2:B:199:ARG:CG	2.70	0.40
2:B:271:TYR:HA	2:B:272:PRO:HD2	1.81	0.40
2:B:298:GLU:CD	2:B:298:GLU:N	2.74	0.40
2:B:328:GLU:O	2:B:339:TYR:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:NH2	1:A:448:ARG:NH2[3_555]	1.54	0.66

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	547/563 (97%)	427 (78%)	91 (17%)	29 (5%)	2	13
2	B	399/443 (90%)	338 (85%)	44 (11%)	17 (4%)	2	17
All	All	946/1006 (94%)	765 (81%)	135 (14%)	46 (5%)	2	14

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	138	GLU
1	A	195	ILE
1	A	230	MET
1	A	286	THR
1	A	288	ALA
1	A	312	GLU
1	A	313	PRO
1	A	334	GLN
1	A	345	PRO
1	A	356	ARG
1	A	491	LEU
1	A	528	LYS
2	B	241	VAL
2	B	345	PRO
1	A	64	LYS
1	A	136	ASN
1	A	243	PRO
1	A	541	GLY
1	A	543	GLY

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Mol	Chain	Res	Type
2	B	14	PRO
2	B	160	PHE
2	B	270	ILE
2	B	282	LEU
2	B	304	ALA
2	B	313	PRO
1	A	3	SER
1	A	78	ARG
1	A	163	SER
2	B	66	LYS
2	B	125	ARG
2	B	137	ASN
2	B	240	THR
2	B	251	SER
1	A	137	ASN
1	A	164	MET
1	A	547	GLN
2	B	402	TRP
1	A	139	THR
2	B	276	VAL
1	A	346	PHE
2	B	161	GLN
2	B	237	ASP
1	A	490	GLY
1	A	95	PRO
1	A	276	VAL

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	491/503 (98%)	344 (70%)	147 (30%)	0	1
2	B	369/403 (92%)	271 (73%)	98 (27%)	0	2
All	All	860/906 (95%)	615 (72%)	245 (28%)	0	1

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	22	LYS
1	A	26	LEU
1	A	29	GLU
1	A	36	GLU
1	A	40	GLU
1	A	42	GLU
1	A	44	GLU
1	A	46	LYS
1	A	49	LYS
1	A	60	VAL
1	A	63	ILE
1	A	64	LYS
1	A	66	LYS
1	A	68	SER
1	A	70	LYS
1	A	72	ARG
1	A	82	LYS
1	A	92	LEU
1	A	101	LYS
1	A	105	SER
1	A	107	THR
1	A	113	ASP
1	A	118	VAL
1	A	122	GLU
1	A	123	ASP
1	A	126	LYS
1	A	134	SER
1	A	135	ILE
1	A	137	ASN
1	A	138	GLU
1	A	151	GLN
1	A	161	GLN
1	A	162	SER
1	A	164	MET
1	A	172	ARG
1	A	173	LYS
1	A	174	GLN
1	A	177	ASP
1	A	197	GLN

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Mol	Chain	Res	Type
1	A	199	ARG
1	A	205	LEU
1	A	207	GLN
1	A	210	LEU
1	A	211	ARG
1	A	215	THR
1	A	220	LYS
1	A	223	LYS
1	A	230	MET
1	A	240	THR
1	A	241	VAL
1	A	244	ILE
1	A	245	VAL
1	A	246	LEU
1	A	248	GLU
1	A	249	LYS
1	A	251	SER
1	A	257	ILE
1	A	259	LYS
1	A	260	LEU
1	A	269	GLN
1	A	274	ILE
1	A	275	LYS
1	A	277	ARG
1	A	278	GLN
1	A	280	CYS
1	A	283	LEU
1	A	284	ARG
1	A	286	THR
1	A	289	LEU
1	A	291	GLU
1	A	295	LEU
1	A	296	THR
1	A	297	GLU
1	A	298	GLU
1	A	303	LEU
1	A	307	ARG
1	A	309	ILE
1	A	311	LYS
1	A	312	GLU
1	A	314	VAL
1	A	330	GLN

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Mol	Chain	Res	Type
1	A	334	GLN
1	A	336	GLN
1	A	344	GLU
1	A	345	PRO
1	A	350	LYS
1	A	351	THR
1	A	353	LYS
1	A	356	ARG
1	A	357	MET
1	A	358	ARG
1	A	361	HIS
1	A	368	LEU
1	A	369	THR
1	A	373	GLN
1	A	374	LYS
1	A	379	SER
1	A	390	LYS
1	A	393	ILE
1	A	395	LYS
1	A	400	THR
1	A	402	TRP
1	A	403	THR
1	A	404	GLU
1	A	407	GLN
1	A	409	THR
1	A	422	LEU
1	A	424	LYS
1	A	425	LEU
1	A	429	LEU
1	A	430	GLU
1	A	431	LYS
1	A	432	GLU
1	A	434	ILE
1	A	435	VAL
1	A	442	VAL
1	A	443	ASP
1	A	448	ARG
1	A	451	LYS
1	A	452	LEU
1	A	454	LYS
1	A	458	VAL
1	A	459	THR

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Mol	Chain	Res	Type
1	A	470	THR
1	A	471	ASP
1	A	475	GLN
1	A	479	LEU
1	A	493	VAL
1	A	494	ASN
1	A	495	ILE
1	A	496	VAL
1	A	497	THR
1	A	500	GLN
1	A	503	LEU
1	A	512	GLN
1	A	519	ASN
1	A	520	GLN
1	A	522	ILE
1	A	523	GLU
1	A	530	LYS
1	A	540	LYS
1	A	547	GLN
1	A	548	VAL
2	B	6	GLU
2	B	8	VAL
2	B	10	VAL
2	B	11	LYS
2	B	26	LEU
2	B	29	GLU
2	B	30	LYS
2	B	35	VAL
2	B	40	GLU
2	B	44	GLU
2	B	46	LYS
2	B	48	SER
2	B	63	ILE
2	B	64	LYS
2	B	65	LYS
2	B	66	LYS
2	B	67	ASP
2	B	68	SER
2	B	72	ARG
2	B	73	LYS
2	B	80	LEU
2	B	90	VAL

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Mol	Chain	Res	Type
2	B	91	GLN
2	B	101	LYS
2	B	104	LYS
2	B	111	VAL
2	B	120	LEU
2	B	125	ARG
2	B	126	LYS
2	B	134	SER
2	B	138	GLU
2	B	145	GLN
2	B	148	VAL
2	B	163	SER
2	B	173	LYS
2	B	178	ILE
2	B	182	GLN
2	B	184	MET
2	B	195	ILE
2	B	199	ARG
2	B	201	LYS
2	B	202	ILE
2	B	205	LEU
2	B	206	ARG
2	B	209	LEU
2	B	211	ARG
2	B	214	LEU
2	B	234	LEU
2	B	240	THR
2	B	245	VAL
2	B	248	GLU
2	B	249	LYS
2	B	251	SER
2	B	253	THR
2	B	258	GLN
2	B	259	LYS
2	B	260	LEU
2	B	261	VAL
2	B	265	ASN
2	B	266	TRP
2	B	268	SER
2	B	269	GLN
2	B	271	TYR
2	B	275	LYS

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Mol	Chain	Res	Type
2	B	276	VAL
2	B	277	ARG
2	B	286	THR
2	B	287	LYS
2	B	289	LEU
2	B	290	THR
2	B	291	GLU
2	B	293	ILE
2	B	295	LEU
2	B	297	GLU
2	B	298	GLU
2	B	300	GLU
2	B	301	LEU
2	B	303	LEU
2	B	305	GLU
2	B	310	LEU
2	B	311	LYS
2	B	314	VAL
2	B	334	GLN
2	B	336	GLN
2	B	347	LYS
2	B	349	LEU
2	B	353	LYS
2	B	356	ARG
2	B	369	THR
2	B	374	LYS
2	B	390	LYS
2	B	394	GLN
2	B	395	LYS
2	B	399	GLU
2	B	400	THR
2	B	403	THR
2	B	414	TRP
2	B	419	THR

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	57	ASN
1	A	91	GLN
1	A	137	ASN
1	A	147	ASN

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Mol	Chain	Res	Type
1	A	175	ASN
1	A	198	HIS
1	A	242	GLN
1	A	258	GLN
1	A	315	HIS
1	A	330	GLN
1	A	332	GLN
1	A	334	GLN
1	A	340	GLN
1	A	460	ASN
1	A	474	ASN
1	A	494	ASN
1	A	524	GLN
2	B	96	HIS
2	B	103	ASN
2	B	147	ASN
2	B	161	GLN
2	B	175	ASN
2	B	255	ASN
2	B	258	GLN
2	B	306	ASN
2	B	330	GLN
2	B	336	GLN
2	B	340	GLN
2	B	367	GLN
2	B	373	GLN
2	B	407	GLN
2	B	428	GLN

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 ⓘ

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	#$|Z| > 2$
3	R8D	A	601	-	30,31,31	2.61	15 (50%)	34,43,43	3.33	17 (50%)

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
3	R8D	A	601	-	-	4/9/11/11	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	R8D	C2-C25	-6.14	1.30	1.44
3	A	601	R8D	C5-C4	-4.23	1.31	1.38
3	A	601	R8D	C6-CL27	-4.23	1.65	1.74
3	A	601	R8D	C18-N24	4.16	1.42	1.37
3	A	601	R8D	C25-N26	3.90	1.23	1.14
3	A	601	R8D	O7-C4	-3.86	1.31	1.39
3	A	601	R8D	C13-CL28	3.37	1.81	1.73
3	A	601	R8D	C22-C21	3.22	1.44	1.36
3	A	601	R8D	N19-N20	3.15	1.43	1.37
3	A	601	R8D	C23-N24	2.93	1.38	1.32
3	A	601	R8D	C18-N19	2.87	1.39	1.34
3	A	601	R8D	C8-C13	-2.75	1.34	1.39
3	A	601	R8D	O7-C8	-2.67	1.33	1.39
3	A	601	R8D	C5-C6	-2.45	1.34	1.38
3	A	601	R8D	C9-C10	2.31	1.43	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	R8D	C1-C6-C5	8.12	131.76	121.66
3	A	601	R8D	C5-C6-CL27	-6.77	110.69	119.15
3	A	601	R8D	C23-N24-C18	6.02	124.02	116.60
3	A	601	R8D	O7-C8-C13	-5.72	106.05	119.58
3	A	601	R8D	C4-C5-C6	-5.44	111.80	118.14
3	A	601	R8D	C2-C1-C6	-5.35	114.78	119.13
3	A	601	R8D	C8-C13-CL28	-4.54	114.09	119.43
3	A	601	R8D	C9-C8-C13	4.26	125.14	119.26
3	A	601	R8D	C8-O7-C4	3.85	127.61	118.00
3	A	601	R8D	C2-C3-C4	3.74	123.99	119.36
3	A	601	R8D	C22-C23-N24	-3.65	118.35	123.94
3	A	601	R8D	C12-C13-CL28	3.35	125.13	118.41
3	A	601	R8D	C8-C9-C10	-3.19	113.44	119.05
3	A	601	R8D	C1-C2-C3	-2.68	115.44	119.71
3	A	601	R8D	O7-C8-C9	2.37	128.78	121.80
3	A	601	R8D	C1-C2-C25	2.06	122.28	119.54
3	A	601	R8D	C3-C2-C25	2.02	122.23	119.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	R8D	C11-C10-O14-C15
3	A	601	R8D	C9-C10-O14-C15
3	A	601	R8D	C16-C15-O14-C10
3	A	601	R8D	C13-C8-O7-C4

There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	R8D	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
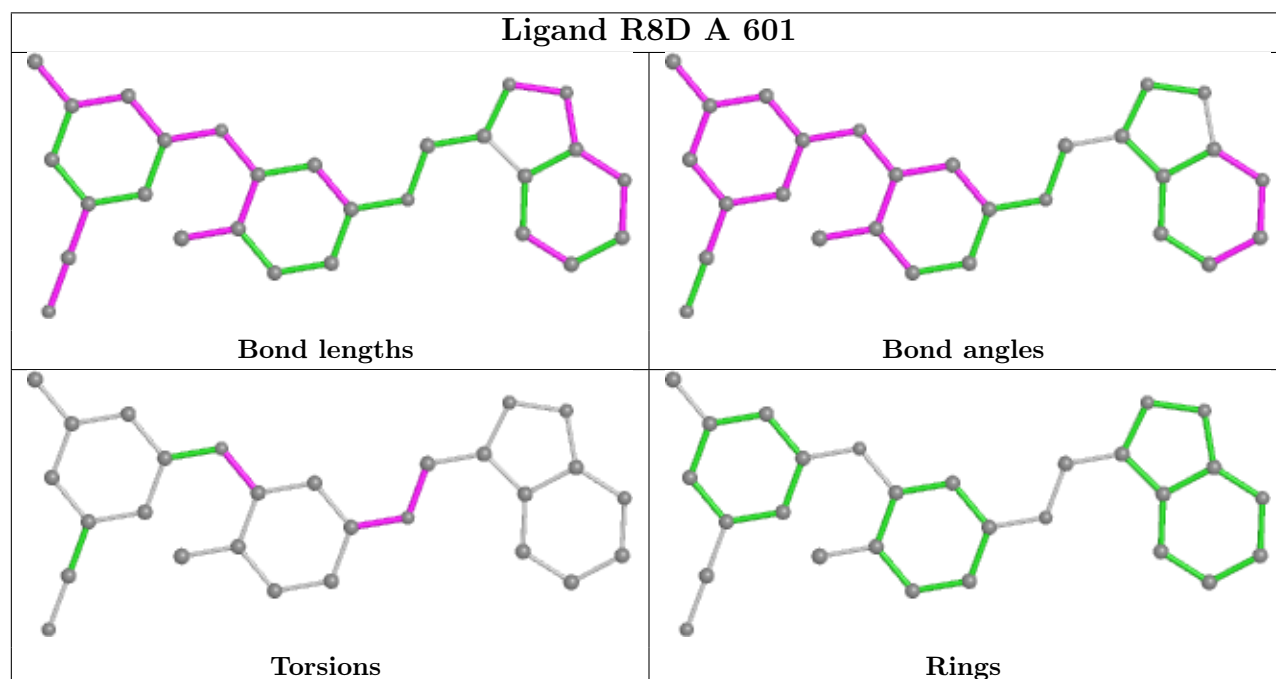
5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	549/563 (97%)	-0.18	8 (1%)	73	61	26, 58, 95, 145	0
2	B	405/443 (91%)	-0.16	9 (2%)	62	47	23, 51, 107, 124	0
All	All	954/1006 (94%)	-0.17	17 (1%)	68	55	23, 56, 105, 145	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	252	TRP	4.6
1	A	546	GLU	3.8
1	A	360	ALA	3.0
2	B	90	VAL	3.0
2	B	362	THR	3.0
1	A	67	ASP	2.9
2	B	277	ARG	2.7
2	B	361	HIS	2.7
2	B	269	GLN	2.6
1	A	66	LYS	2.6
1	A	193	LEU	2.6
2	B	297	GLU	2.3
1	A	545	ASN	2.3
2	B	251	SER	2.1
1	A	541	GLY	2.1
1	A	547	GLN	2.1
2	B	298	GLU	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ
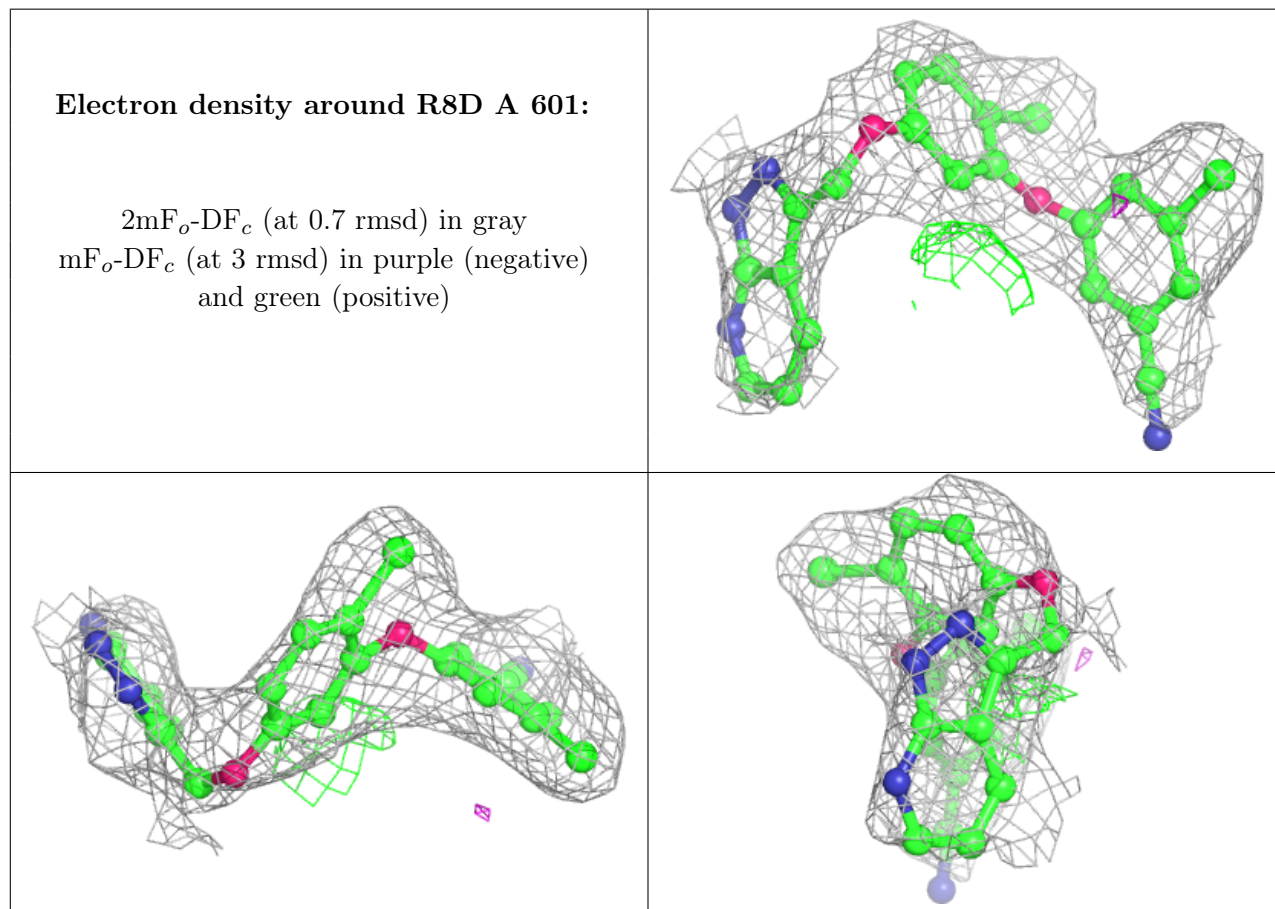
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	R8D	A	601	28/28	0.92	0.30	64,69,79,79	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around R8D A 601:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.