



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:53 pm BST

PDB ID : 2QE5
Title : Structure of HCV NS5B Bound to an Anthranilic Acid Inhibitor
Authors : Chopra, R.; Svenson, K.; Bard, J.
Deposited on : 2007-06-22
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

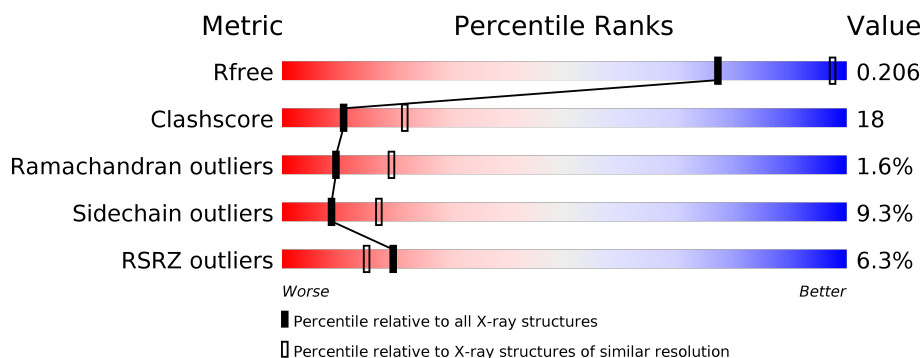
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	578	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>32%</div> <div>• •</div> </div> </div>
1	B	578	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>30%</div> <div>5%</div> <div>•</div> </div> </div>
1	C	578	<div> <div>7%</div> <div> <div></div> <div>59%</div> <div>32%</div> <div>6%</div> <div>•</div> </div> </div>
1	D	578	<div> <div>6%</div> <div> <div></div> <div>61%</div> <div>31%</div> <div>5%</div> <div>•</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17395 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4342	2740	766	805	31			
1	B	559	Total	C	N	O	S	0	0	0
			4342	2740	766	805	31			
1	C	559	Total	C	N	O	S	0	0	0
			4342	2740	766	805	31			
1	D	559	Total	C	N	O	S	0	0	0
			4342	2740	766	805	31			

There are 32 discrepancies between the modelled and reference sequences:

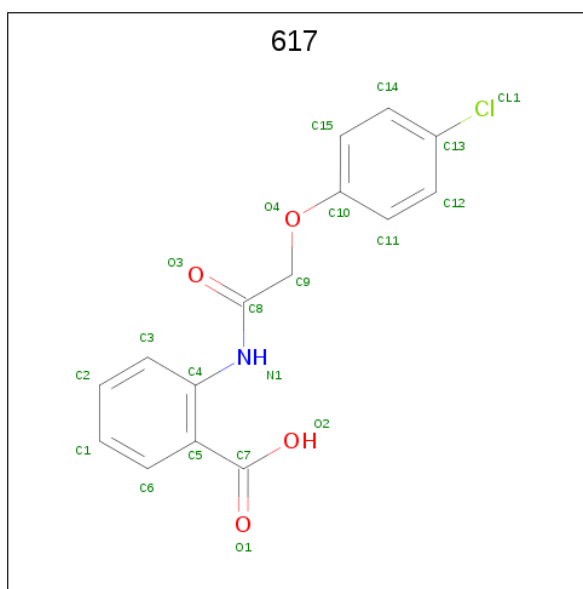
Chain	Residue	Modelled	Actual	Comment	Reference
A	571	GLY	-	EXPRESSION TAG	UNP Q99AU2
A	572	SER	-	EXPRESSION TAG	UNP Q99AU2
A	573	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	574	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	575	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	576	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	577	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	578	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	571	GLY	-	EXPRESSION TAG	UNP Q99AU2
B	572	SER	-	EXPRESSION TAG	UNP Q99AU2
B	573	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	574	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	575	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	576	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	577	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	578	HIS	-	EXPRESSION TAG	UNP Q99AU2
C	571	GLY	-	EXPRESSION TAG	UNP Q99AU2
C	572	SER	-	EXPRESSION TAG	UNP Q99AU2
C	573	HIS	-	EXPRESSION TAG	UNP Q99AU2
C	574	HIS	-	EXPRESSION TAG	UNP Q99AU2
C	575	HIS	-	EXPRESSION TAG	UNP Q99AU2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	576	HIS	-	EXPRESSION TAG	UNP Q99AU2
C	577	HIS	-	EXPRESSION TAG	UNP Q99AU2
C	578	HIS	-	EXPRESSION TAG	UNP Q99AU2
D	571	GLY	-	EXPRESSION TAG	UNP Q99AU2
D	572	SER	-	EXPRESSION TAG	UNP Q99AU2
D	573	HIS	-	EXPRESSION TAG	UNP Q99AU2
D	574	HIS	-	EXPRESSION TAG	UNP Q99AU2
D	575	HIS	-	EXPRESSION TAG	UNP Q99AU2
D	576	HIS	-	EXPRESSION TAG	UNP Q99AU2
D	577	HIS	-	EXPRESSION TAG	UNP Q99AU2
D	578	HIS	-	EXPRESSION TAG	UNP Q99AU2

- Molecule 2 is 2-[[[(4-CHLOROPHENOXY)ACETYL]AMINO}BENZOIC ACID (three-letter code: 617) (formula: C₁₅H₁₂ClNO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0
			21	15	1	1	4	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

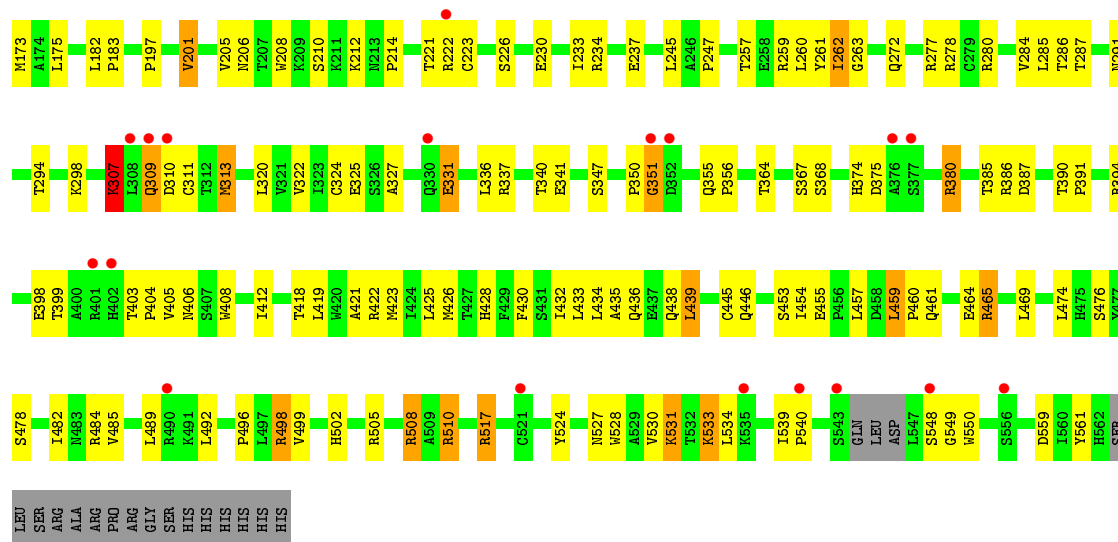
Chain A:

Chain B:

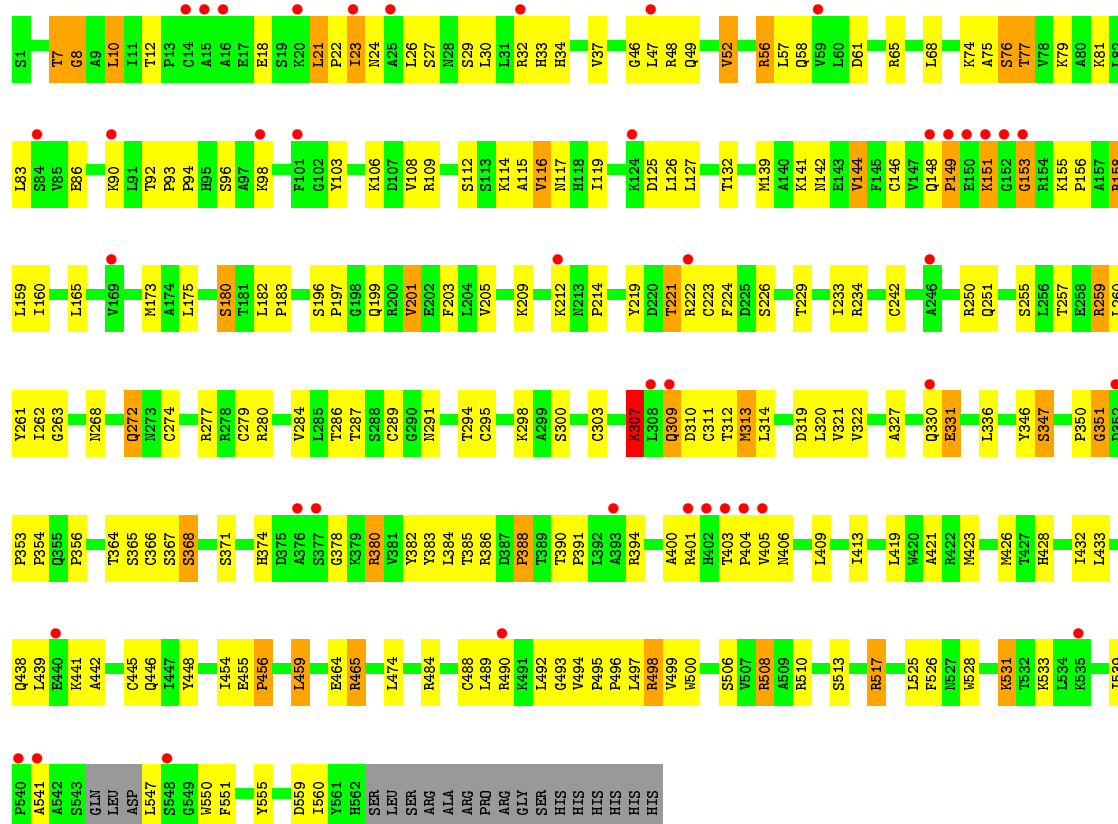
6% 62% 30% 5%

S1 L21 P22 I23 I24 A25 L26 N35 K36 V37 T40 T41 S42 R43 S44 A45 Q46 L47 R48 Q49 K50 K51 V52 R56 L57 Q58 D61 D62 H63 V64 R65 L68 K74 T77 A80 R81 L82 L83 R86

K90 L91 T92 P93 P94 R95 K98 Y103 K106 R109 S112 S113 K114 A115 N116 N117 H118 I119 K124 D125 L126 L127 E128 D129 T130 V131 T132 P133 I134 K141 V144 F145 C146 V147 Q148 P149 E150 K151 G152 G153 R154 A157 R158 G166 V169 C170 E171 F172

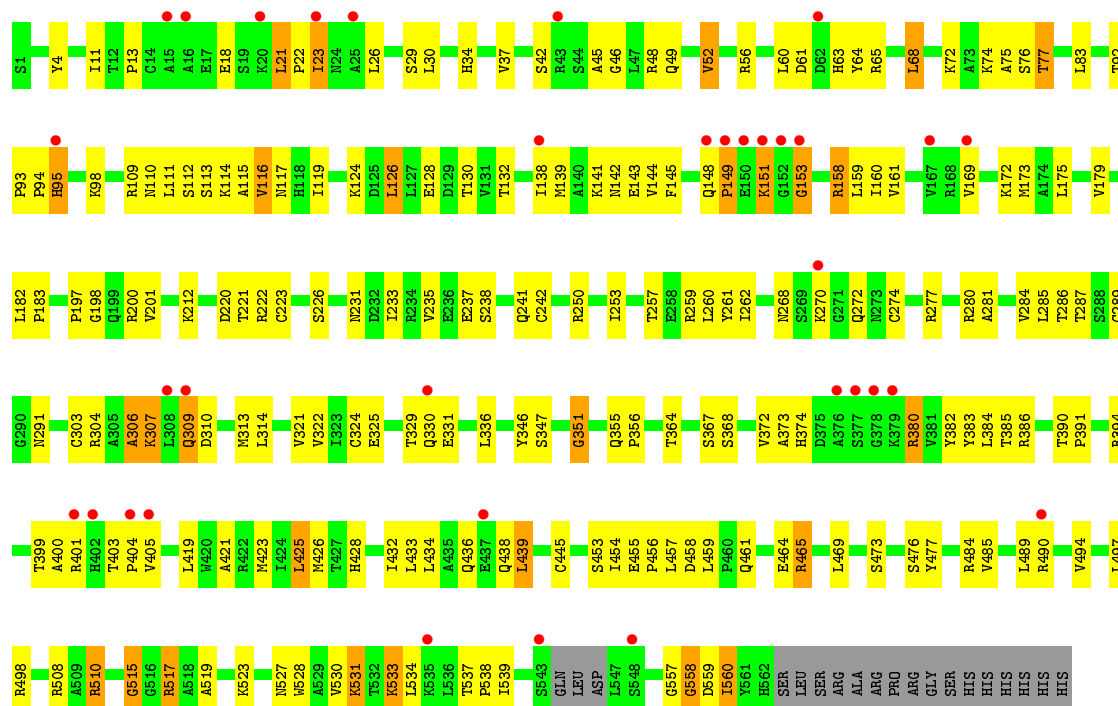


• Molecule 1: RNA-directed RNA polymerase



• Molecule 1: RNA-directed RNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.34Å 101.47Å 251.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.60 19.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	87.1 (19.93-2.60) 87.2 (19.93-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.59Å)	Xtriage
Refinement program	CNS 1.1, CNX	Depositor
R, R_{free}	0.218 , 0.225 0.204 , 0.206	Depositor DCC
R_{free} test set	3559 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.088 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17395	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.41% 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: 617

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	0.43	0/4437	0.74	2/6020 (0.0%)
1	B	0.43	0/4437	0.76	1/6020 (0.0%)
1	C	0.41	0/4437	0.73	3/6020 (0.0%)
1	D	0.43	0/4437	0.73	2/6020 (0.0%)
All	All	0.43	0/17748	0.74	8/24080 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	GLY	N-CA-C	-8.10	92.85	113.10
1	D	558	GLY	N-CA-C	-6.88	95.90	113.10
1	C	351	GLY	N-CA-C	-6.13	97.78	113.10
1	A	351	GLY	N-CA-C	-5.90	98.34	113.10
1	A	126	LEU	CA-CB-CG	5.42	127.76	115.30
1	C	312	THR	N-CA-C	-5.35	96.55	111.00
1	D	351	GLY	N-CA-C	-5.33	99.79	113.10
1	C	214	PRO	N-CA-C	5.01	125.13	112.10

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	4342	0	4363	158	0
1	B	4342	0	4363	159	0
1	C	4342	0	4363	165	0
1	D	4342	0	4363	156	0
2	A	21	0	11	1	0
3	A	6	0	0	0	0
All	All	17395	0	17463	633	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 18.

All (633) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:ARG:HG2	1:B:510:ARG:HH11	0.98	1.10
1:D:465:ARG:HG3	1:D:465:ARG:HH11	1.15	1.05
1:B:465:ARG:HH11	1:B:465:ARG:HG3	0.86	1.02
1:A:307:LYS:H	1:A:307:LYS:HD3	1.19	1.02
1:A:531:LYS:H	1:A:531:LYS:HD2	1.22	0.99
1:B:510:ARG:NH1	1:B:510:ARG:HG2	1.76	0.97
1:B:531:LYS:H	1:B:531:LYS:HD2	1.28	0.97
1:B:465:ARG:NH1	1:B:465:ARG:HG3	1.64	0.96
1:B:465:ARG:CG	1:B:465:ARG:HH11	1.79	0.94
1:A:26:LEU:HD13	1:A:432:ILE:HD12	1.47	0.94
1:C:144:VAL:HG22	1:C:394:ARG:HG2	1.48	0.94
1:A:132:THR:O	1:A:259:ARG:HD2	1.68	0.92
1:C:26:LEU:HD13	1:C:432:ILE:HD12	1.49	0.92
1:B:336:LEU:HD22	1:B:356:PRO:HD3	1.54	0.90
1:C:465:ARG:HG3	1:C:465:ARG:HH11	1.36	0.90
1:A:358:TYR:CD2	1:D:113:SER:HB2	2.07	0.89
1:C:307:LYS:HD3	1:C:307:LYS:H	1.38	0.88
1:D:48:ARG:HG2	1:D:159:LEU:HG	1.56	0.88
1:B:26:LEU:HD13	1:B:432:ILE:HD12	1.55	0.86
1:D:465:ARG:CG	1:D:465:ARG:HH11	1.89	0.85
1:D:61:ASP:O	1:D:65:ARG:HG3	1.77	0.85
1:C:465:ARG:NH1	1:C:465:ARG:HG3	1.91	0.83
1:C:46:GLY:HA2	1:C:49:GLN:HE21	1.45	0.81
1:D:465:ARG:HG3	1:D:465:ARG:NH1	1.79	0.81
1:B:40:THR:HB	1:B:157:ALA:HB2	1.62	0.81
1:B:132:THR:O	1:B:259:ARG:HD2	1.82	0.80
1:C:234:ARG:HG2	1:C:262:ILE:HD11	1.61	0.80
1:C:336:LEU:HD22	1:C:356:PRO:HD3	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLN:HG3	1:B:347:SER:HB2	1.63	0.80
1:B:510:ARG:CG	1:B:510:ARG:HH11	1.88	0.79
1:D:46:GLY:HA2	1:D:49:GLN:HE21	1.47	0.79
1:C:433:LEU:HB3	1:C:439:LEU:HD12	1.64	0.79
1:B:340:THR:HG23	1:B:350:PRO:HG3	1.65	0.79
1:C:465:ARG:CG	1:C:465:ARG:HH11	1.95	0.79
1:A:180:SER:HB3	1:A:555:TYR:OH	1.83	0.78
1:B:109:ARG:HB2	1:B:109:ARG:NH1	1.99	0.78
1:B:327:ALA:O	1:B:331:GLU:HG3	1.84	0.78
1:B:284:VAL:O	1:B:287:THR:HG22	1.84	0.77
1:C:48:ARG:HG2	1:C:159:LEU:HG	1.66	0.77
1:D:144:VAL:HG22	1:D:394:ARG:HG2	1.66	0.77
1:D:510:ARG:HH11	1:D:510:ARG:HG2	1.48	0.77
1:C:284:VAL:O	1:C:287:THR:HG22	1.85	0.77
1:A:52:VAL:HG22	1:A:226:SER:OG	1.86	0.76
1:C:212:LYS:HB2	1:C:212:LYS:NZ	2.00	0.76
1:B:212:LYS:NZ	1:B:212:LYS:HB2	2.01	0.76
1:B:74:LYS:O	1:B:77:THR:HB	1.85	0.76
1:A:233:ILE:HD13	1:A:261:TYR:O	1.87	0.75
1:D:374:HIS:ND1	1:D:476:SER:HB2	2.02	0.74
1:D:132:THR:O	1:D:259:ARG:HD2	1.86	0.74
1:C:24:ASN:HB3	1:C:27:SER:HB3	1.69	0.74
1:D:26:LEU:HD13	1:D:432:ILE:HD12	1.68	0.74
1:A:307:LYS:HD3	1:A:307:LYS:N	1.97	0.74
1:A:109:ARG:HB2	1:A:109:ARG:NH1	2.03	0.74
1:A:358:TYR:HD2	1:D:113:SER:HB2	1.53	0.73
1:D:485:VAL:O	1:D:489:LEU:HG	1.88	0.73
1:A:106:LYS:HB3	1:A:106:LYS:NZ	2.04	0.73
1:A:86:GLU:HG3	1:A:111:LEU:HD11	1.69	0.73
1:A:531:LYS:H	1:A:531:LYS:CD	1.97	0.73
1:D:531:LYS:HD2	1:D:531:LYS:H	1.53	0.73
1:A:469:LEU:HD21	1:A:538:PRO:HA	1.70	0.73
1:A:547:LEU:O	1:A:550:TRP:HB2	1.89	0.73
1:C:531:LYS:HD2	1:C:531:LYS:H	1.53	0.73
1:D:510:ARG:NH1	1:D:510:ARG:HG2	1.99	0.73
1:D:260:LEU:O	1:D:277:ARG:NH2	2.22	0.72
1:D:436:GLN:HB2	1:D:438:GLN:HG2	1.69	0.72
1:B:144:VAL:HG22	1:B:394:ARG:HG2	1.71	0.72
1:A:433:LEU:HB3	1:A:439:LEU:HD12	1.71	0.72
1:B:307:LYS:H	1:B:307:LYS:HD3	1.55	0.72
1:A:148:GLN:HB2	1:A:153:GLY:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:SER:O	1:C:116:VAL:HG13	1.90	0.72
1:A:327:ALA:O	1:A:331:GLU:HG3	1.90	0.71
1:A:517:ARG:HH11	1:A:517:ARG:CB	2.04	0.71
1:B:45:ALA:O	1:B:49:GLN:HG3	1.90	0.71
1:D:280:ARG:HD2	1:D:291:ASN:OD1	1.90	0.71
1:D:307:LYS:H	1:D:307:LYS:HD3	1.54	0.71
1:D:368:SER:HB2	1:D:385:THR:O	1.90	0.70
1:C:86:GLU:HG2	1:C:90:LYS:HE3	1.74	0.70
1:C:115:ALA:O	1:C:119:ILE:HG12	1.91	0.70
1:B:86:GLU:HG2	1:B:90:LYS:HE3	1.73	0.70
1:A:109:ARG:HB2	1:A:109:ARG:HH11	1.54	0.70
1:D:179:VAL:HG13	1:D:289:CYS:HB2	1.73	0.69
1:B:340:THR:CG2	1:B:350:PRO:HG3	2.22	0.69
1:B:510:ARG:CG	1:B:510:ARG:NH1	2.53	0.68
1:A:36:MET:HB3	1:A:147:VAL:HG22	1.73	0.68
1:B:106:LYS:HB3	1:B:106:LYS:NZ	2.08	0.68
1:A:51:LYS:HE3	1:A:156:PRO:HG3	1.74	0.68
1:B:109:ARG:CB	1:B:109:ARG:HH11	2.06	0.67
1:C:433:LEU:HB3	1:C:439:LEU:CD1	2.24	0.67
1:A:469:LEU:HD21	1:A:538:PRO:CA	2.25	0.67
1:B:496:PRO:HB2	1:B:498:ARG:HD2	1.76	0.67
1:A:336:LEU:HD22	1:A:356:PRO:HD3	1.77	0.67
1:D:52:VAL:HG22	1:D:226:SER:OG	1.95	0.67
1:B:80:ALA:HB3	1:B:245:LEU:CD2	2.26	0.66
1:B:485:VAL:O	1:B:489:LEU:HG	1.96	0.66
1:B:508:ARG:CZ	1:B:530:VAL:HG11	2.25	0.66
1:A:86:GLU:HG2	1:A:90:LYS:HE3	1.78	0.66
1:C:74:LYS:O	1:C:77:THR:HB	1.96	0.66
1:B:436:GLN:HB2	1:B:438:GLN:HG2	1.78	0.65
1:B:309:GLN:HB2	1:B:325:GLU:HB2	1.79	0.65
1:A:30:LEU:HB2	1:A:428:HIS:CD2	2.31	0.65
1:D:83:LEU:HB2	1:D:173:MET:HA	1.78	0.65
1:A:307:LYS:HB3	1:A:309:GLN:HG2	1.78	0.65
1:A:560:ILE:N	1:A:560:ILE:HD13	2.12	0.65
1:B:148:GLN:HG3	1:B:149:PRO:HD2	1.79	0.65
1:B:234:ARG:CG	1:B:262:ILE:HD11	2.27	0.64
1:C:46:GLY:HA2	1:C:49:GLN:NE2	2.12	0.64
1:D:68:LEU:HD22	1:D:72:LYS:HE3	1.78	0.64
1:D:237:GLU:HG3	1:D:257:THR:OG1	1.97	0.64
1:A:423:MET:HG2	1:A:528:TRP:CZ3	2.33	0.64
1:C:268:ASN:HB3	1:C:274:CYS:SG	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:ARG:CG	1:D:517:ARG:HH11	2.10	0.64
1:D:531:LYS:HD2	1:D:531:LYS:N	2.13	0.64
1:C:26:LEU:O	1:C:29:SER:HB3	1.98	0.64
1:D:458:ASP:HA	1:D:461:GLN:HE22	1.63	0.64
1:D:21:LEU:HD23	1:D:37:VAL:HB	1.79	0.63
1:A:237:GLU:HG3	1:A:257:THR:OG1	1.99	0.63
1:D:11:ILE:HG13	1:D:45:ALA:HB1	1.80	0.63
1:B:307:LYS:CD	1:B:307:LYS:H	2.12	0.63
1:A:48:ARG:HG2	1:A:159:LEU:HG	1.80	0.63
1:A:559:ASP:C	1:A:560:ILE:HD13	2.19	0.63
1:C:314:LEU:HB3	1:C:321:VAL:HG12	1.81	0.63
1:B:52:VAL:HG22	1:B:226:SER:OG	2.00	0.62
1:C:260:LEU:O	1:C:277:ARG:NH2	2.32	0.62
1:A:433:LEU:HB3	1:A:439:LEU:CD1	2.30	0.62
1:D:309:GLN:HB2	1:D:325:GLU:HB2	1.82	0.62
1:B:374:HIS:ND1	1:B:476:SER:HB2	2.15	0.62
1:B:531:LYS:HD2	1:B:531:LYS:N	2.09	0.62
1:C:205:VAL:O	1:C:209:LYS:HG2	2.00	0.61
1:A:150:GLU:H	1:A:150:GLU:CD	2.02	0.61
1:A:260:LEU:O	1:A:277:ARG:NH2	2.32	0.61
1:B:158:ARG:CB	1:B:158:ARG:HH11	2.14	0.61
1:C:132:THR:O	1:C:259:ARG:HD2	2.00	0.61
1:A:280:ARG:HG3	1:A:281:ALA:N	2.14	0.61
1:C:510:ARG:NH1	1:C:510:ARG:HG2	2.16	0.61
1:B:399:THR:OG1	1:B:428:HIS:HE1	1.83	0.61
1:A:523:LYS:HE2	1:A:536:LEU:HD23	1.81	0.61
1:C:405:VAL:HG11	1:C:446:GLN:HE21	1.66	0.61
1:B:368:SER:HB2	1:B:385:THR:O	2.00	0.61
1:C:139:MET:O	1:C:160:ILE:HG22	2.01	0.61
1:D:222:ARG:HG3	1:D:351:GLY:HA2	1.82	0.61
1:A:68:LEU:HD22	1:A:72:LYS:HE3	1.83	0.60
1:C:510:ARG:HG2	1:C:510:ARG:HH11	1.66	0.60
1:D:284:VAL:O	1:D:287:THR:HG22	2.00	0.60
1:B:260:LEU:O	1:B:277:ARG:NH2	2.34	0.60
1:D:74:LYS:O	1:D:77:THR:HB	2.02	0.60
1:C:76:SER:HA	1:C:242:CYS:O	2.02	0.60
1:D:517:ARG:CB	1:D:517:ARG:HH11	2.13	0.60
1:C:144:VAL:CG2	1:C:394:ARG:HG2	2.28	0.60
1:D:18:GLU:OE1	1:D:401:ARG:HD2	2.01	0.60
1:D:115:ALA:O	1:D:119:ILE:HG12	2.02	0.60
1:C:489:LEU:HD22	1:C:494:VAL:HB	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LYS:O	1:B:128:GLU:HG3	2.02	0.60
1:C:18:GLU:OE2	1:C:22:PRO:HG3	2.02	0.60
1:D:336:LEU:HD22	1:D:356:PRO:HD3	1.83	0.60
1:A:287:THR:HG23	1:A:288:SER:H	1.67	0.59
1:A:374:HIS:ND1	1:A:476:SER:HB2	2.17	0.59
1:C:313:MET:HE2	1:C:320:LEU:HD11	1.84	0.59
1:C:517:ARG:HG3	1:C:517:ARG:NH1	2.15	0.59
1:A:93:PRO:HG2	1:A:96:SER:HB2	1.84	0.59
1:C:464:GLU:OE2	1:C:539:ILE:HB	2.02	0.59
1:C:212:LYS:HB2	1:C:212:LYS:HZ2	1.66	0.59
1:A:149:PRO:HB2	1:A:150:GLU:OE1	2.03	0.59
1:D:30:LEU:O	1:D:494:VAL:HG22	2.02	0.59
1:B:83:LEU:HB2	1:B:173:MET:HA	1.85	0.58
1:A:74:LYS:O	1:A:77:THR:HB	2.03	0.58
1:D:61:ASP:HB3	1:D:63:HIS:H	1.67	0.58
1:B:93:PRO:HB3	1:B:561:TYR:HB2	1.85	0.58
1:D:148:GLN:HB3	1:D:153:GLY:HA3	1.84	0.58
1:A:280:ARG:HD2	1:A:291:ASN:OD1	2.03	0.58
1:B:230:GLU:OE2	1:B:278:ARG:HB3	2.03	0.58
1:B:433:LEU:HB3	1:B:439:LEU:CD1	2.34	0.58
1:B:524:TYR:CZ	1:B:539:ILE:HG12	2.39	0.58
1:D:141:LYS:HD2	1:D:158:ARG:NH1	2.19	0.58
1:A:83:LEU:HB2	1:A:173:MET:HA	1.85	0.58
1:C:517:ARG:HH11	1:C:517:ARG:CG	2.17	0.58
1:D:458:ASP:HA	1:D:461:GLN:NE2	2.19	0.58
1:C:21:LEU:HD23	1:C:37:VAL:HB	1.86	0.57
1:B:434:LEU:HD21	1:B:510:ARG:HB2	1.87	0.57
1:D:144:VAL:HG22	1:D:394:ARG:CG	2.34	0.57
1:B:307:LYS:HG2	1:B:311:CYS:SG	2.44	0.57
1:A:106:LYS:HZ3	1:A:106:LYS:HB3	1.68	0.57
1:C:103:TYR:HA	1:C:114:LYS:HZ1	1.68	0.57
1:C:18:GLU:OE1	1:C:401:ARG:HD2	2.03	0.57
1:A:434:LEU:HD21	1:A:510:ARG:HB2	1.87	0.57
1:B:234:ARG:HG3	1:B:262:ILE:HD11	1.87	0.57
1:A:358:TYR:CE1	1:D:117:ASN:ND2	2.72	0.57
1:C:423:MET:SD	1:C:497:LEU:HD22	2.44	0.57
1:C:413:ILE:CD1	1:C:454:ILE:HD13	2.34	0.57
1:D:314:LEU:HB3	1:D:321:VAL:CG1	2.35	0.57
1:B:222:ARG:HG3	1:B:351:GLY:HA2	1.86	0.57
1:C:83:LEU:HB2	1:C:173:MET:HA	1.87	0.57
1:D:175:LEU:HD21	1:D:253:ILE:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:LEU:HB3	1:D:439:LEU:CD1	2.34	0.57
1:C:180:SER:HB3	1:C:555:TYR:OH	2.05	0.56
1:A:284:VAL:O	1:A:287:THR:HG22	2.05	0.56
1:A:517:ARG:HB3	1:A:517:ARG:HH11	1.68	0.56
1:C:496:PRO:HD2	1:C:499:VAL:CG2	2.35	0.56
1:C:496:PRO:HG2	1:C:498:ARG:HH11	1.71	0.56
1:D:233:ILE:HD13	1:D:261:TYR:O	2.05	0.56
1:D:531:LYS:H	1:D:531:LYS:CD	2.12	0.56
1:C:146:CYS:SG	1:C:492:LEU:HD21	2.46	0.56
1:D:403:THR:HB	1:D:404:PRO:HD2	1.87	0.56
1:D:534:LEU:O	1:D:534:LEU:HD12	2.04	0.56
1:B:234:ARG:HG2	1:B:262:ILE:HD11	1.86	0.56
1:C:106:LYS:HB3	1:C:106:LYS:NZ	2.21	0.56
1:D:560:ILE:N	1:D:560:ILE:HD13	2.20	0.56
1:C:30:LEU:O	1:C:494:VAL:HG13	2.06	0.56
1:D:436:GLN:CB	1:D:438:GLN:HG2	2.36	0.56
1:A:146:CYS:SG	1:A:492:LEU:HD21	2.46	0.56
1:A:148:GLN:O	1:A:149:PRO:C	2.44	0.56
1:D:60:LEU:HD13	1:D:64:TYR:CE2	2.41	0.56
1:B:58:GLN:CG	1:B:347:SER:HB2	2.32	0.55
1:D:285:LEU:HG	1:D:285:LEU:O	2.06	0.55
1:A:223:CYS:O	1:A:227:THR:HG23	2.06	0.55
1:A:10:LEU:O	1:A:12:THR:HG23	2.07	0.55
1:A:46:GLY:HA2	1:A:49:GLN:NE2	2.22	0.55
1:A:501:ARG:HG2	1:A:501:ARG:HH11	1.71	0.55
1:D:309:GLN:HG3	1:D:324:CYS:HB2	1.87	0.55
1:D:421:ALA:HA	1:D:425:LEU:HB2	1.88	0.55
1:D:559:ASP:C	1:D:560:ILE:HD13	2.27	0.55
1:B:233:ILE:HD13	1:B:261:TYR:O	2.06	0.55
1:A:287:THR:HG23	1:A:288:SER:N	2.21	0.55
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.89	0.55
1:B:201:VAL:O	1:B:205:VAL:HG23	2.07	0.55
1:B:92:THR:O	1:B:109:ARG:NH2	2.39	0.55
1:C:517:ARG:HH11	1:C:517:ARG:HG3	1.71	0.54
1:D:145:PHE:CE2	1:D:394:ARG:NH2	2.75	0.54
1:A:197:PRO:HA	2:A:579:617:CL1	2.44	0.54
1:A:464:GLU:HG3	1:A:469:LEU:HD13	1.89	0.54
1:D:515:GLY:HA2	1:D:519:ALA:HB2	1.89	0.54
1:D:22:PRO:O	1:D:400:ALA:HB1	2.08	0.54
1:C:127:LEU:HD23	1:C:251:GLN:CG	2.37	0.54
1:A:287:THR:CG2	1:A:556:SER:O	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:ARG:NE	1:C:490:ARG:HA	2.22	0.54
1:A:534:LEU:O	1:A:534:LEU:HD12	2.08	0.54
1:A:5:THR:O	1:A:275:GLY:HA3	2.08	0.54
1:D:380:ARG:NH2	1:D:382:TYR:OH	2.34	0.54
1:A:24:ASN:HB3	1:A:27:SER:H	1.73	0.54
1:B:212:LYS:HZ2	1:B:212:LYS:HB2	1.73	0.54
1:B:464:GLU:OE2	1:B:539:ILE:HB	2.07	0.54
1:C:126:LEU:HA	1:C:259:ARG:HH21	1.73	0.53
1:C:413:ILE:HD11	1:C:454:ILE:HD13	1.89	0.53
1:A:380:ARG:NH2	1:A:382:TYR:OH	2.28	0.53
1:B:94:PRO:HD3	1:B:109:ARG:NH2	2.23	0.53
1:C:307:LYS:HG2	1:C:311:CYS:SG	2.47	0.53
1:C:75:ALA:C	1:C:77:THR:H	2.12	0.53
1:A:46:GLY:HA2	1:A:49:GLN:HE21	1.72	0.53
1:C:374:HIS:HD2	1:C:378:GLY:O	1.91	0.53
1:D:307:LYS:HG3	1:D:309:GLN:CD	2.29	0.53
1:D:30:LEU:HB2	1:D:428:HIS:CD2	2.43	0.53
1:D:231:ASN:O	1:D:235:VAL:HG23	2.09	0.53
1:A:26:LEU:HD13	1:A:432:ILE:CD1	2.29	0.53
1:A:418:THR:O	1:A:422:ARG:HG3	2.09	0.53
1:B:80:ALA:HB3	1:B:245:LEU:HD21	1.90	0.53
1:C:219:TYR:HB3	1:C:320:LEU:HD23	1.91	0.53
1:D:307:LYS:N	1:D:307:LYS:HD3	2.23	0.53
1:C:148:GLN:O	1:C:149:PRO:C	2.46	0.53
1:C:445:CYS:SG	1:C:454:ILE:HD12	2.49	0.53
1:D:510:ARG:HH11	1:D:510:ARG:CG	2.18	0.53
1:B:109:ARG:CB	1:B:109:ARG:NH1	2.66	0.52
1:B:112:SER:O	1:B:116:VAL:HG13	2.09	0.52
1:B:405:VAL:HG11	1:B:446:GLN:HE21	1.75	0.52
1:C:390:THR:HB	1:C:391:PRO:HD3	1.91	0.52
1:C:197:PRO:O	1:C:201:VAL:HG12	2.08	0.52
1:C:18:GLU:CD	1:C:22:PRO:HG3	2.29	0.52
1:C:496:PRO:HD2	1:C:499:VAL:HG21	1.92	0.52
1:C:22:PRO:O	1:C:400:ALA:HB1	2.10	0.52
1:B:109:ARG:HH11	1:B:109:ARG:HB2	1.64	0.52
1:C:234:ARG:CG	1:C:262:ILE:HD11	2.37	0.52
1:D:423:MET:HA	1:D:528:TRP:CZ2	2.44	0.52
1:D:95:HIS:CD2	1:D:95:HIS:H	2.26	0.52
1:C:280:ARG:HD2	1:C:291:ASN:OD1	2.09	0.52
1:D:212:LYS:NZ	1:D:212:LYS:HB2	2.24	0.52
1:D:95:HIS:N	1:D:95:HIS:CD2	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ARG:NH1	1:A:510:ARG:HG2	2.25	0.52
1:A:374:HIS:O	1:A:474:LEU:HA	2.10	0.52
1:B:313:MET:HE2	1:B:320:LEU:HD11	1.91	0.52
1:A:222:ARG:HG3	1:A:351:GLY:HA2	1.90	0.52
1:A:51:LYS:HE3	1:A:156:PRO:CG	2.40	0.52
1:D:423:MET:HG2	1:D:528:TRP:CZ3	2.44	0.52
1:D:434:LEU:HD21	1:D:510:ARG:HB2	1.91	0.52
1:A:119:ILE:CD1	1:A:166:GLY:HA2	2.40	0.51
1:C:108:VAL:HG21	1:C:165:LEU:HD21	1.92	0.51
1:D:175:LEU:HD13	1:D:286:THR:HG21	1.92	0.51
1:D:464:GLU:OE2	1:D:539:ILE:HB	2.10	0.51
1:A:307:LYS:H	1:A:307:LYS:CD	2.08	0.51
1:B:423:MET:HA	1:B:528:TRP:CZ2	2.45	0.51
1:D:175:LEU:HD13	1:D:286:THR:CG2	2.41	0.51
1:D:517:ARG:NH1	1:D:517:ARG:HG3	2.25	0.51
1:A:364:THR:HA	1:A:368:SER:O	2.10	0.51
1:B:119:ILE:CD1	1:B:166:GLY:HA2	2.41	0.51
1:D:48:ARG:CG	1:D:159:LEU:HG	2.36	0.51
1:D:92:THR:O	1:D:109:ARG:NH2	2.44	0.51
1:B:280:ARG:HD2	1:B:291:ASN:OD1	2.11	0.51
1:B:433:LEU:HB3	1:B:439:LEU:HD12	1.92	0.51
1:C:203:PHE:CE1	1:C:314:LEU:HD13	2.45	0.51
1:C:48:ARG:NH2	1:C:156:PRO:HG2	2.26	0.51
1:C:196:SER:OG	1:C:199:GLN:HG3	2.11	0.51
1:A:205:VAL:O	1:A:209:LYS:HG2	2.11	0.51
1:A:310:ASP:OD1	1:A:325:GLU:HG3	2.10	0.51
1:C:374:HIS:O	1:C:474:LEU:HA	2.10	0.51
1:C:498:ARG:HG2	1:C:499:VAL:N	2.24	0.51
1:D:141:LYS:CD	1:D:158:ARG:HH12	2.24	0.51
1:B:13:PRO:HD3	1:B:42:SER:OG	2.11	0.51
1:B:18:GLU:OE2	1:B:22:PRO:HG3	2.11	0.51
1:B:531:LYS:H	1:B:531:LYS:CD	2.03	0.51
1:D:75:ALA:C	1:D:77:THR:H	2.13	0.51
1:A:548:SER:C	1:A:550:TRP:H	2.15	0.50
1:A:26:LEU:O	1:A:29:SER:HB3	2.11	0.50
1:D:26:LEU:O	1:D:29:SER:HB3	2.11	0.50
1:A:22:PRO:O	1:A:400:ALA:HB1	2.10	0.50
1:B:134:ILE:HG13	1:B:259:ARG:HB3	1.94	0.50
1:C:423:MET:HG2	1:C:528:TRP:CZ3	2.47	0.50
1:B:505:ARG:CZ	1:B:531:LYS:HE2	2.42	0.50
1:B:517:ARG:HG3	1:B:517:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:PRO:O	1:D:201:VAL:HG12	2.12	0.50
1:A:307:LYS:N	1:A:307:LYS:CD	2.72	0.50
1:D:112:SER:O	1:D:116:VAL:HG13	2.11	0.50
1:C:403:THR:HB	1:C:404:PRO:HD2	1.94	0.50
1:D:490:ARG:HA	1:D:490:ARG:NE	2.25	0.50
1:D:508:ARG:CZ	1:D:530:VAL:HG11	2.42	0.50
1:A:462:ILE:O	1:A:466:LEU:HG	2.11	0.50
1:C:52:VAL:HG22	1:C:226:SER:OG	2.12	0.49
1:A:109:ARG:CB	1:A:109:ARG:HH11	2.23	0.49
1:B:307:LYS:HB3	1:B:309:GLN:HG2	1.93	0.49
1:B:47:LEU:HD12	1:B:47:LEU:N	2.27	0.49
1:C:517:ARG:CG	1:C:517:ARG:NH1	2.75	0.49
1:D:76:SER:HA	1:D:242:CYS:O	2.12	0.49
1:C:314:LEU:HB3	1:C:321:VAL:CG1	2.42	0.49
1:D:109:ARG:HB2	1:D:109:ARG:NH1	2.28	0.49
1:D:110:ASN:O	1:D:111:LEU:HB2	2.12	0.49
1:D:148:GLN:CB	1:D:153:GLY:HA3	2.41	0.49
1:A:510:ARG:HG2	1:A:510:ARG:HH11	1.77	0.49
1:B:408:TRP:HE3	1:B:412:ILE:HD12	1.77	0.49
1:A:517:ARG:CG	1:A:517:ARG:HH11	2.24	0.49
1:A:531:LYS:N	1:A:531:LYS:HD2	2.07	0.49
1:B:498:ARG:O	1:B:502:HIS:HD2	1.96	0.49
1:B:56:ARG:HD3	1:B:56:ARG:N	2.28	0.49
1:B:106:LYS:HB3	1:B:106:LYS:HZ2	1.78	0.49
1:D:124:LYS:NZ	1:D:128:GLU:OE2	2.42	0.49
1:D:268:ASN:HB3	1:D:274:CYS:SG	2.52	0.49
1:A:10:LEU:HD23	1:A:10:LEU:N	2.28	0.49
1:A:307:LYS:HG2	1:A:311:CYS:SG	2.53	0.49
1:C:388:PRO:HG2	1:C:488:CYS:SG	2.52	0.49
1:B:61:ASP:HB3	1:B:63:HIS:H	1.77	0.48
1:C:92:THR:O	1:C:109:ARG:NH2	2.46	0.48
1:B:527:ASN:O	1:B:530:VAL:HG22	2.13	0.48
1:D:517:ARG:HG3	1:D:517:ARG:HH11	1.78	0.48
1:A:385:THR:HG23	1:A:484:ARG:NH2	2.28	0.48
1:A:86:GLU:HG3	1:A:111:LEU:CD1	2.39	0.48
1:C:508:ARG:HG3	1:C:526:PHE:HB2	1.95	0.48
1:D:404:PRO:HG2	1:D:405:VAL:H	1.78	0.48
1:D:434:LEU:HD21	1:D:510:ARG:CB	2.43	0.48
1:B:172:LYS:NZ	1:B:559:ASP:HB3	2.28	0.48
1:C:175:LEU:HD13	1:C:286:THR:CG2	2.43	0.48
1:B:197:PRO:O	1:B:201:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ILE:O	1:B:435:ALA:HB3	2.14	0.48
1:C:233:ILE:HD13	1:C:261:TYR:O	2.14	0.48
1:B:46:GLY:O	1:B:50:LYS:HG2	2.14	0.48
1:C:93:PRO:HG2	1:C:96:SER:HB2	1.95	0.48
1:B:103:TYR:N	1:B:114:LYS:HZ2	2.11	0.48
1:B:148:GLN:O	1:B:149:PRO:C	2.52	0.48
1:B:80:ALA:HB3	1:B:245:LEU:HD23	1.95	0.48
1:A:390:THR:O	1:A:394:ARG:HG3	2.13	0.48
1:B:464:GLU:HG3	1:B:469:LEU:HD12	1.95	0.48
1:C:103:TYR:H	1:C:103:TYR:HD2	1.60	0.48
1:D:307:LYS:HG3	1:D:309:GLN:OE1	2.14	0.48
1:A:423:MET:HG2	1:A:528:TRP:CH2	2.48	0.47
1:B:208:TRP:CE2	1:B:214:PRO:HB2	2.49	0.47
1:B:327:ALA:O	1:B:331:GLU:CG	2.61	0.47
1:C:79:LYS:HE3	1:C:81:LYS:HE2	1.94	0.47
1:D:141:LYS:CD	1:D:158:ARG:NH1	2.77	0.47
1:B:115:ALA:O	1:B:119:ILE:HG12	2.14	0.47
1:C:23:ILE:HD12	1:C:34:HIS:CD2	2.50	0.47
1:C:7:THR:OG1	1:C:8:GLY:N	2.42	0.47
1:D:268:ASN:ND2	1:D:272:GLN:HB3	2.29	0.47
1:A:560:ILE:N	1:A:560:ILE:CD1	2.76	0.47
1:B:148:GLN:CB	1:B:153:GLY:O	2.62	0.47
1:A:408:TRP:CZ3	1:A:412:ILE:HD12	2.49	0.47
1:D:523:LYS:HG3	1:D:534:LEU:HD11	1.96	0.47
1:A:138:ILE:HD11	1:A:159:LEU:HD13	1.97	0.47
1:A:485:VAL:O	1:A:489:LEU:HG	2.13	0.47
1:C:23:ILE:HD12	1:C:34:HIS:NE2	2.29	0.47
1:B:172:LYS:HZ3	1:B:559:ASP:HB3	1.79	0.47
1:A:346:TYR:O	1:A:347:SER:HB3	2.15	0.47
1:C:309:GLN:HE22	1:C:327:ALA:HB2	1.79	0.47
1:C:222:ARG:HG3	1:C:351:GLY:HA2	1.97	0.47
1:B:478:SER:O	1:B:482:ILE:HG13	2.14	0.47
1:D:445:CYS:SG	1:D:454:ILE:HD12	2.55	0.47
1:A:100:LYS:HG3	1:A:164:ASP:OD2	2.14	0.47
1:A:46:GLY:O	1:A:50:LYS:HG2	2.15	0.47
1:C:331:GLU:N	1:C:331:GLU:OE1	2.47	0.47
1:C:148:GLN:HB2	1:C:153:GLY:O	2.15	0.47
1:C:212:LYS:CB	1:C:212:LYS:NZ	2.75	0.47
1:D:60:LEU:HD13	1:D:64:TYR:CD2	2.50	0.47
1:B:374:HIS:O	1:B:474:LEU:HA	2.14	0.46
1:B:517:ARG:HH11	1:B:517:ARG:CG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HD21	1:A:253:ILE:HG12	1.96	0.46
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.75	0.46
1:C:456:PRO:HA	1:C:459:LEU:HD22	1.97	0.46
1:C:506:SER:O	1:C:510:ARG:HG3	2.16	0.46
1:A:148:GLN:CG	1:A:149:PRO:HD2	2.46	0.46
1:A:62:ASP:OD1	1:A:65:ARG:NH1	2.48	0.46
1:B:294:THR:O	1:B:298:LYS:HG3	2.15	0.46
1:C:409:LEU:O	1:C:413:ILE:HG13	2.16	0.46
1:D:390:THR:HB	1:D:391:PRO:HD3	1.97	0.46
1:D:523:LYS:HE3	1:D:534:LEU:CD1	2.44	0.46
1:A:408:TRP:HB2	1:A:429:PHE:CE1	2.51	0.46
1:D:307:LYS:HB3	1:D:309:GLN:HG2	1.97	0.46
1:D:346:TYR:O	1:D:347:SER:HB3	2.16	0.46
1:D:527:ASN:O	1:D:533:LYS:HG2	2.15	0.46
1:C:465:ARG:CG	1:C:465:ARG:NH1	2.60	0.46
1:A:457:LEU:HD23	1:A:521:CYS:SG	2.56	0.46
1:A:540:PRO:HG2	1:A:541:ALA:H	1.80	0.46
1:A:144:VAL:CG2	1:A:394:ARG:HG2	2.45	0.46
1:B:455:GLU:OE2	1:B:517:ARG:NH2	2.47	0.46
1:D:304:ARG:C	1:D:306:ALA:H	2.19	0.46
1:D:21:LEU:HD23	1:D:37:VAL:CB	2.46	0.46
1:D:515:GLY:CA	1:D:519:ALA:HB2	2.45	0.46
1:B:367:SER:O	1:B:386:ARG:HG3	2.16	0.46
1:C:22:PRO:O	1:C:23:ILE:C	2.54	0.46
1:C:30:LEU:HB2	1:C:428:HIS:CD2	2.51	0.45
1:C:531:LYS:CD	1:C:531:LYS:H	2.20	0.45
1:A:508:ARG:O	1:A:512:LEU:HG	2.17	0.45
1:B:150:GLU:CD	1:B:150:GLU:H	2.20	0.45
1:B:158:ARG:HB2	1:B:158:ARG:HH11	1.81	0.45
1:A:331:GLU:N	1:A:331:GLU:OE1	2.48	0.45
1:B:154:ARG:HH11	1:B:154:ARG:HG3	1.82	0.45
1:C:255:SER:O	1:C:259:ARG:HG3	2.15	0.45
1:A:330:GLN:HB3	1:A:331:GLU:OE1	2.17	0.45
1:A:375:ASP:OD1	1:A:379:LYS:HB3	2.16	0.45
1:B:337:ARG:NH2	1:B:341:GLU:OE1	2.50	0.45
1:A:209:LYS:HD2	1:C:510:ARG:HH12	1.81	0.45
1:D:423:MET:SD	1:D:497:LEU:HD22	2.56	0.45
1:D:523:LYS:HE3	1:D:534:LEU:HD13	1.98	0.45
1:A:48:ARG:CG	1:A:159:LEU:HG	2.46	0.45
1:A:45:ALA:O	1:A:49:GLN:HG3	2.17	0.45
1:C:307:LYS:HG2	1:C:307:LYS:HZ3	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:TYR:CE1	1:C:551:PHE:HD2	2.35	0.45
1:D:93:PRO:HA	1:D:94:PRO:HD3	1.85	0.45
1:C:57:LEU:HD23	1:C:57:LEU:HA	1.68	0.45
1:D:307:LYS:HG3	1:D:309:GLN:CG	2.46	0.45
1:D:372:VAL:HG22	1:D:382:TYR:CD2	2.52	0.45
1:B:212:LYS:N	1:B:325:GLU:OE2	2.41	0.45
1:A:219:TYR:OH	1:A:350:PRO:HD3	2.16	0.45
1:A:401:ARG:HD3	1:A:402:HIS:N	2.31	0.45
1:A:423:MET:HA	1:A:528:TRP:CZ2	2.52	0.45
1:A:86:GLU:O	1:A:90:LYS:HG3	2.17	0.45
1:C:307:LYS:HG3	1:C:309:GLN:HG3	1.98	0.45
1:C:367:SER:HB3	1:C:386:ARG:NH1	2.32	0.45
1:D:148:GLN:O	1:D:149:PRO:C	2.55	0.45
1:D:439:LEU:HG	1:D:457:LEU:HD21	1.99	0.45
1:A:224:PHE:CZ	1:A:295:CYS:HB2	2.52	0.44
1:A:334:ALA:O	1:A:337:ARG:HB2	2.17	0.44
1:A:469:LEU:CD2	1:A:538:PRO:HA	2.44	0.44
1:B:56:ARG:NH2	1:B:278:ARG:O	2.50	0.44
1:D:233:ILE:HB	1:D:262:ILE:HD12	1.99	0.44
1:A:21:LEU:HD23	1:A:37:VAL:HB	1.99	0.44
1:C:257:THR:HG22	1:C:262:ILE:HD13	1.98	0.44
1:C:495:PRO:HG2	1:C:500:TRP:CZ2	2.52	0.44
1:D:13:PRO:HB3	1:D:42:SER:OG	2.17	0.44
1:A:385:THR:HG21	1:A:481:GLU:OE1	2.18	0.44
1:B:517:ARG:HH11	1:B:517:ARG:HG3	1.82	0.44
1:C:353:PRO:HA	1:C:354:PRO:HD2	1.74	0.44
1:C:423:MET:HA	1:C:528:TRP:CZ2	2.53	0.44
1:B:374:HIS:NE2	1:B:380:ARG:HG3	2.32	0.44
1:B:386:ARG:HG2	1:B:387:ASP:N	2.32	0.44
1:B:62:ASP:OD1	1:B:65:ARG:NH1	2.51	0.44
1:C:221:THR:HA	1:C:350:PRO:HA	2.00	0.44
1:C:268:ASN:HD21	1:C:272:GLN:HE21	1.65	0.44
1:C:492:LEU:HB2	1:C:494:VAL:HG23	1.98	0.44
1:D:143:GLU:OE2	1:D:158:ARG:CZ	2.65	0.44
1:B:94:PRO:HD3	1:B:109:ARG:HH22	1.83	0.44
1:C:219:TYR:OH	1:C:350:PRO:HD3	2.17	0.44
1:B:106:LYS:HB3	1:B:106:LYS:HZ3	1.80	0.44
1:D:464:GLU:HG3	1:D:469:LEU:HD12	2.00	0.44
1:B:141:LYS:CD	1:B:158:ARG:HH12	2.31	0.44
1:C:526:PHE:HA	1:C:528:TRP:CD1	2.53	0.44
1:B:309:GLN:CB	1:B:325:GLU:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:VAL:CG2	1:B:533:LYS:HA	2.47	0.44
1:C:183:PRO:HG3	1:C:289:CYS:SG	2.58	0.44
1:C:61:ASP:O	1:C:65:ARG:HG3	2.18	0.44
1:D:329:THR:HG22	1:D:330:GLN:N	2.32	0.44
1:B:212:LYS:HZ3	1:B:212:LYS:HB2	1.81	0.44
1:B:237:GLU:HG3	1:B:257:THR:OG1	2.18	0.44
1:C:371:SER:HB3	1:C:383:TYR:CZ	2.53	0.44
1:D:383:TYR:HH	1:D:477:TYR:HD2	1.66	0.44
1:D:421:ALA:O	1:D:426:MET:HG3	2.18	0.44
1:B:148:GLN:CG	1:B:149:PRO:HD2	2.46	0.43
1:B:263:GLY:HA3	1:B:277:ARG:O	2.17	0.43
1:B:3:SER:HB3	1:B:56:ARG:HE	1.83	0.43
1:C:250:ARG:HH11	1:C:250:ARG:HG2	1.82	0.43
1:D:124:LYS:O	1:D:128:GLU:HG3	2.18	0.43
1:D:77:THR:O	1:D:77:THR:HG23	2.18	0.43
1:A:75:ALA:C	1:A:77:THR:H	2.21	0.43
1:B:146:CYS:SG	1:B:492:LEU:HD21	2.58	0.43
1:B:68:LEU:HD22	1:B:68:LEU:O	2.18	0.43
1:A:478:SER:O	1:A:482:ILE:HG13	2.18	0.43
1:C:148:GLN:HG3	1:C:149:PRO:HD2	1.99	0.43
1:A:466:LEU:HD21	1:A:547:LEU:HD13	2.00	0.43
1:A:86:GLU:HG2	1:A:90:LYS:CE	2.45	0.43
1:C:94:PRO:HD3	1:C:109:ARG:HH22	1.84	0.43
1:D:148:GLN:HG3	1:D:149:PRO:HD2	2.00	0.43
1:D:399:THR:OG1	1:D:428:HIS:HE1	2.01	0.43
1:D:560:ILE:CD1	1:D:560:ILE:N	2.82	0.43
1:D:126:LEU:HA	1:D:259:ARG:HH21	1.84	0.43
1:D:423:MET:HA	1:D:528:TRP:CH2	2.53	0.43
1:A:388:PRO:C	1:A:391:PRO:HD2	2.39	0.43
1:C:421:ALA:O	1:C:426:MET:HG3	2.18	0.43
1:C:438:GLN:OE1	1:C:441:LYS:HD2	2.18	0.43
1:D:198:GLY:HA2	1:D:201:VAL:CG1	2.49	0.43
1:D:309:GLN:CB	1:D:325:GLU:HB2	2.47	0.43
1:D:367:SER:HB3	1:D:386:ARG:NH1	2.33	0.43
1:A:144:VAL:HG11	1:A:397:TRP:CD2	2.54	0.43
1:A:464:GLU:CD	1:A:469:LEU:HD13	2.38	0.43
1:A:71:MET:SD	1:A:297:LEU:HD13	2.58	0.43
1:A:530:VAL:O	1:A:533:LYS:HE2	2.17	0.43
1:B:430:PHE:O	1:B:434:LEU:HB2	2.19	0.43
1:C:365:SER:O	1:C:366:CYS:HB2	2.18	0.43
1:B:498:ARG:HG2	1:B:499:VAL:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ARG:CG	1:B:465:ARG:NH1	2.50	0.42
1:C:423:MET:HE1	1:C:497:LEU:HB3	2.01	0.42
1:C:58:GLN:HG3	1:C:229:THR:HG21	2.01	0.42
1:A:39:ALA:HB2	1:A:144:VAL:HG12	2.01	0.42
1:A:465:ARG:NH1	1:A:465:ARG:HG3	2.35	0.42
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.59	0.42
1:C:132:THR:O	1:C:259:ARG:HB3	2.19	0.42
1:C:56:ARG:HH21	1:C:279:CYS:HB3	1.84	0.42
1:C:56:ARG:HD3	1:C:56:ARG:N	2.34	0.42
1:D:4:TYR:CD1	1:D:52:VAL:HG13	2.54	0.42
1:A:416:ALA:N	1:A:417:PRO:CD	2.82	0.42
1:B:418:THR:O	1:B:422:ARG:HG3	2.19	0.42
1:D:182:LEU:HD23	1:D:183:PRO:N	2.34	0.42
1:A:198:GLY:O	1:A:201:VAL:HG12	2.20	0.42
1:A:469:LEU:HD21	1:A:538:PRO:N	2.34	0.42
1:B:374:HIS:HE2	1:B:380:ARG:HG3	1.83	0.42
1:C:26:LEU:HD22	1:C:432:ILE:CD1	2.49	0.42
1:D:52:VAL:HG22	1:D:226:SER:HG	1.85	0.42
1:A:307:LYS:CB	1:A:309:GLN:HG2	2.46	0.42
1:A:440:GLU:N	1:A:440:GLU:OE1	2.53	0.42
1:A:517:ARG:CG	1:A:517:ARG:NH1	2.82	0.42
1:B:21:LEU:HD23	1:B:37:VAL:HB	2.01	0.42
1:B:403:THR:HB	1:B:404:PRO:HD2	2.01	0.42
1:D:183:PRO:HG3	1:D:289:CYS:SG	2.59	0.42
1:D:439:LEU:HA	1:D:439:LEU:HD12	1.88	0.42
1:C:559:ASP:C	1:C:560:ILE:HD12	2.39	0.42
1:C:93:PRO:HA	1:C:94:PRO:HD3	1.80	0.42
1:D:557:GLY:C	1:D:558:GLY:O	2.50	0.42
1:A:501:ARG:NH1	1:A:501:ARG:HG2	2.33	0.42
1:B:285:LEU:O	1:B:285:LEU:HG	2.19	0.42
1:C:10:LEU:O	1:C:12:THR:HG23	2.20	0.42
1:C:141:LYS:CD	1:C:158:ARG:NH1	2.83	0.42
1:C:294:THR:O	1:C:298:LYS:HG3	2.19	0.42
1:C:547:LEU:O	1:C:550:TRP:HB2	2.20	0.42
1:A:314:LEU:HB3	1:A:321:VAL:HG13	2.02	0.42
1:B:141:LYS:HD2	1:B:158:ARG:NH1	2.35	0.42
1:B:421:ALA:O	1:B:426:MET:HG3	2.19	0.42
1:B:539:ILE:HA	1:B:540:PRO:HD2	1.81	0.42
1:B:175:LEU:HD13	1:B:286:THR:HG21	2.01	0.42
1:C:125:ASP:OD1	1:C:259:ARG:NH2	2.52	0.42
1:C:263:GLY:HA3	1:C:277:ARG:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:VAL:HG12	1:D:373:ALA:N	2.35	0.42
1:A:372:VAL:HG11	1:A:380:ARG:HG2	2.02	0.41
1:B:261:TYR:HE1	1:B:284:VAL:HB	1.84	0.41
1:C:307:LYS:HG3	1:C:309:GLN:CG	2.50	0.41
1:A:223:CYS:HB2	1:A:226:SER:HB2	2.02	0.41
1:B:222:ARG:O	1:B:223:CYS:C	2.58	0.41
1:D:138:ILE:HG13	1:D:161:VAL:HG22	2.02	0.41
1:B:206:ASN:O	1:B:210:SER:HB3	2.20	0.41
1:D:222:ARG:O	1:D:223:CYS:C	2.57	0.41
1:B:548:SER:C	1:B:550:TRP:H	2.23	0.41
1:C:368:SER:CB	1:C:385:THR:O	2.68	0.41
1:D:280:ARG:HG3	1:D:281:ALA:N	2.35	0.41
1:A:154:ARG:HH11	1:A:154:ARG:HG3	1.84	0.41
1:B:208:TRP:CZ2	1:B:214:PRO:HB2	2.55	0.41
1:C:346:TYR:O	1:C:347:SER:HB3	2.21	0.41
1:C:32:ARG:HB2	1:C:493:GLY:O	2.21	0.41
1:D:139:MET:HB2	1:D:160:ILE:CG2	2.50	0.41
1:B:309:GLN:H	1:B:309:GLN:HG2	1.77	0.41
1:C:203:PHE:HE1	1:C:314:LEU:HD13	1.84	0.41
1:C:224:PHE:CZ	1:C:295:CYS:HB2	2.56	0.41
1:C:18:GLU:OE1	1:C:22:PRO:HG3	2.20	0.41
1:C:380:ARG:NH2	1:C:382:TYR:OH	2.45	0.41
1:D:22:PRO:O	1:D:23:ILE:C	2.59	0.41
1:A:348:ALA:N	1:A:349:PRO:CD	2.83	0.41
1:A:30:LEU:HB2	1:A:428:HIS:NE2	2.35	0.41
1:A:556:SER:C	1:A:558:GLY:H	2.23	0.41
1:B:182:LEU:N	1:B:183:PRO:CD	2.83	0.41
1:B:398:GLU:OE2	1:B:408:TRP:HD1	2.02	0.41
1:C:148:GLN:CB	1:C:153:GLY:HA3	2.51	0.41
1:D:325:GLU:HA	1:D:325:GLU:OE1	2.21	0.41
1:A:230:GLU:OE2	1:A:278:ARG:HB3	2.21	0.41
1:B:151:LYS:HE2	1:B:151:LYS:HB3	1.64	0.41
1:A:455:GLU:HB3	1:A:458:ASP:OD2	2.20	0.41
1:B:459:LEU:N	1:B:460:PRO:CD	2.84	0.41
1:C:141:LYS:CD	1:C:158:ARG:HH12	2.33	0.41
1:C:307:LYS:HD3	1:C:307:LYS:N	2.14	0.41
1:C:442:ALA:HA	1:C:455:GLU:HA	2.02	0.41
1:C:455:GLU:OE2	1:C:517:ARG:NH2	2.47	0.41
1:A:198:GLY:HA2	1:A:201:VAL:HG12	2.02	0.41
1:C:47:LEU:CD1	1:C:47:LEU:N	2.84	0.41
1:D:404:PRO:HG2	1:D:405:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:PRO:O	1:B:23:ILE:C	2.60	0.41
1:C:223:CYS:O	1:C:224:PHE:C	2.59	0.41
1:C:233:ILE:CG2	1:C:262:ILE:HD12	2.50	0.41
1:A:540:PRO:C	1:A:542:ALA:H	2.25	0.40
1:B:309:GLN:HG3	1:B:324:CYS:HB2	2.03	0.40
1:B:331:GLU:N	1:B:331:GLU:OE1	2.53	0.40
1:B:534:LEU:C	1:B:534:LEU:HD12	2.41	0.40
1:C:300:SER:O	1:C:303:CYS:HB2	2.21	0.40
1:C:525:LEU:HB2	1:C:526:PHE:CD1	2.56	0.40
1:D:241:GLN:OE1	1:D:250:ARG:HG2	2.20	0.40
1:D:455:GLU:HA	1:D:456:PRO:HD2	1.88	0.40
1:A:111:LEU:N	1:A:111:LEU:HD23	2.35	0.40
1:B:390:THR:HB	1:B:391:PRO:HD3	2.03	0.40
1:B:47:LEU:N	1:B:47:LEU:CD1	2.84	0.40
1:C:495:PRO:HA	1:C:496:PRO:HD3	1.95	0.40
1:C:465:ARG:HB3	1:C:547:LEU:HD12	2.02	0.40
1:B:35:ASN:HD22	1:B:35:ASN:HA	1.76	0.40
1:C:455:GLU:HA	1:C:456:PRO:HD2	1.81	0.40
1:D:132:THR:O	1:D:259:ARG:CD	2.66	0.40
1:A:158:ARG:HH11	1:A:158:ARG:CB	2.35	0.40
1:A:464:GLU:CG	1:A:469:LEU:HD13	2.50	0.40
1:B:439:LEU:HB3	1:B:457:LEU:HD11	2.04	0.40
1:D:169:VAL:O	1:D:172:LYS:HB2	2.21	0.40
1:A:285:LEU:O	1:A:285:LEU:HG	2.21	0.40
1:A:172:LYS:NZ	1:A:559:ASP:HB3	2.37	0.40
1:B:47:LEU:H	1:B:47:LEU:CD1	2.35	0.40
1:B:81:LYS:HD3	1:B:81:LYS:HA	1.75	0.40
1:A:209:LYS:O	1:C:513:SER:HB3	2.22	0.40
1:D:303:CYS:SG	1:D:313:MET:CE	3.10	0.40
1:D:18:GLU:OE1	1:D:401:ARG:NH1	2.55	0.40
1:D:537:THR:O	1:D:539:ILE:N	2.55	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	555/578 (96%)	511 (92%)	36 (6%)	8 (1%)	11	22
1	B	555/578 (96%)	508 (92%)	40 (7%)	7 (1%)	12	24
1	C	555/578 (96%)	504 (91%)	39 (7%)	12 (2%)	6	12
1	D	555/578 (96%)	506 (91%)	41 (7%)	8 (1%)	11	22
All	All	2220/2312 (96%)	2029 (91%)	156 (7%)	35 (2%)	9	19

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	151	LYS
1	A	153	GLY
1	A	515	GLY
1	B	23	ILE
1	B	153	GLY
1	B	307	LYS
1	C	23	ILE
1	C	151	LYS
1	C	153	GLY
1	C	307	LYS
1	D	23	ILE
1	D	153	GLY
1	D	515	GLY
1	A	157	ALA
1	A	307	LYS
1	A	541	ALA
1	B	549	GLY
1	C	7	THR
1	D	151	LYS
1	D	538	PRO
1	A	149	PRO
1	B	149	PRO
1	B	151	LYS
1	C	8	GLY
1	C	33	HIS
1	C	541	ALA
1	D	34	HIS
1	C	76	SER
1	C	347	SER

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Mol	Chain	Res	Type
1	D	306	ALA
1	B	8	GLY
1	C	149	PRO
1	C	456	PRO
1	D	149	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	475/492 (96%)	429 (90%)	46 (10%)	8	15
1	B	475/492 (96%)	429 (90%)	46 (10%)	8	15
1	C	475/492 (96%)	432 (91%)	43 (9%)	9	18
1	D	475/492 (96%)	433 (91%)	42 (9%)	10	19
All	All	1900/1968 (96%)	1723 (91%)	177 (9%)	9	17

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	52	VAL
1	A	56	ARG
1	A	68	LEU
1	A	77	THR
1	A	95	HIS
1	A	98	LYS
1	A	113	SER
1	A	126	LEU
1	A	130	THR
1	A	143	GLU
1	A	151	LYS
1	A	158	ARG
1	A	180	SER
1	A	220	ASP
1	A	221	THR

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Mol	Chain	Res	Type
1	A	223	CYS
1	A	236	GLU
1	A	270	LYS
1	A	272	GLN
1	A	307	LYS
1	A	308	LEU
1	A	309	GLN
1	A	310	ASP
1	A	322	VAL
1	A	330	GLN
1	A	331	GLU
1	A	341	GLU
1	A	364	THR
1	A	380	ARG
1	A	384	LEU
1	A	386	ARG
1	A	387	ASP
1	A	401	ARG
1	A	406	ASN
1	A	425	LEU
1	A	453	SER
1	A	459	LEU
1	A	469	LEU
1	A	470	SER
1	A	484	ARG
1	A	498	ARG
1	A	517	ARG
1	A	531	LYS
1	A	533	LYS
1	A	560	ILE
1	B	21	LEU
1	B	42	SER
1	B	52	VAL
1	B	56	ARG
1	B	68	LEU
1	B	77	THR
1	B	95	HIS
1	B	98	LYS
1	B	117	ASN
1	B	126	LEU
1	B	130	THR
1	B	131	VAL

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Mol	Chain	Res	Type
1	B	144	VAL
1	B	150	GLU
1	B	151	LYS
1	B	158	ARG
1	B	201	VAL
1	B	221	THR
1	B	247	PRO
1	B	262	ILE
1	B	272	GLN
1	B	307	LYS
1	B	309	GLN
1	B	310	ASP
1	B	313	MET
1	B	322	VAL
1	B	331	GLU
1	B	355	GLN
1	B	364	THR
1	B	375	ASP
1	B	380	ARG
1	B	406	ASN
1	B	419	LEU
1	B	425	LEU
1	B	439	LEU
1	B	453	SER
1	B	459	LEU
1	B	461	GLN
1	B	465	ARG
1	B	484	ARG
1	B	498	ARG
1	B	508	ARG
1	B	510	ARG
1	B	517	ARG
1	B	531	LYS
1	B	533	LYS
1	C	10	LEU
1	C	21	LEU
1	C	52	VAL
1	C	56	ARG
1	C	68	LEU
1	C	77	THR
1	C	98	LYS
1	C	116	VAL

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Mol	Chain	Res	Type
1	C	117	ASN
1	C	142	ASN
1	C	144	VAL
1	C	151	LYS
1	C	155	LYS
1	C	158	ARG
1	C	180	SER
1	C	182	LEU
1	C	201	VAL
1	C	221	THR
1	C	259	ARG
1	C	272	GLN
1	C	307	LYS
1	C	309	GLN
1	C	310	ASP
1	C	313	MET
1	C	319	ASP
1	C	322	VAL
1	C	330	GLN
1	C	331	GLU
1	C	364	THR
1	C	368	SER
1	C	380	ARG
1	C	384	LEU
1	C	388	PRO
1	C	406	ASN
1	C	419	LEU
1	C	459	LEU
1	C	465	ARG
1	C	484	ARG
1	C	498	ARG
1	C	508	ARG
1	C	517	ARG
1	C	531	LYS
1	C	533	LYS
1	D	21	LEU
1	D	52	VAL
1	D	56	ARG
1	D	68	LEU
1	D	77	THR
1	D	95	HIS
1	D	98	LYS

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Mol	Chain	Res	Type
1	D	114	LYS
1	D	116	VAL
1	D	126	LEU
1	D	130	THR
1	D	142	ASN
1	D	151	LYS
1	D	158	ARG
1	D	200	ARG
1	D	220	ASP
1	D	221	THR
1	D	238	SER
1	D	270	LYS
1	D	307	LYS
1	D	309	GLN
1	D	310	ASP
1	D	322	VAL
1	D	331	GLU
1	D	355	GLN
1	D	364	THR
1	D	380	ARG
1	D	384	LEU
1	D	419	LEU
1	D	425	LEU
1	D	439	LEU
1	D	453	SER
1	D	459	LEU
1	D	465	ARG
1	D	473	SER
1	D	484	ARG
1	D	498	ARG
1	D	510	ARG
1	D	517	ARG
1	D	531	LYS
1	D	533	LYS
1	D	560	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	49	GLN
1	A	194	GLN

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Mol	Chain	Res	Type
1	A	206	ASN
1	A	272	GLN
1	A	355	GLN
1	A	428	HIS
1	A	483	ASN
1	A	502	HIS
1	B	35	ASN
1	B	142	ASN
1	B	206	ASN
1	B	272	GLN
1	B	316	ASN
1	B	355	GLN
1	B	428	HIS
1	B	446	GLN
1	B	483	ASN
1	B	502	HIS
1	C	35	ASN
1	C	49	GLN
1	C	142	ASN
1	C	206	ASN
1	C	272	GLN
1	C	309	GLN
1	C	316	ASN
1	C	355	GLN
1	C	428	HIS
1	C	446	GLN
1	C	483	ASN
1	D	35	ASN
1	D	49	GLN
1	D	95	HIS
1	D	117	ASN
1	D	142	ASN
1	D	206	ASN
1	D	272	GLN
1	D	316	ASN
1	D	355	GLN
1	D	428	HIS
1	D	461	GLN
1	D	483	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	617	A	579	-	20,22,22	2.67	7 (35%)	25,29,29	1.32	3 (12%)

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	617	A	579	-	-	0/9/13/13	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	579	617	C5-C7	8.00	1.55	1.47
2	A	579	617	C11-C10	3.64	1.45	1.38
2	A	579	617	C5-C4	3.38	1.45	1.40
2	A	579	617	C8-N1	3.03	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	579	617	C14-C13	2.82	1.43	1.38
2	A	579	617	C6-C5	2.67	1.44	1.40
2	A	579	617	C15-C10	2.37	1.43	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	579	617	O3-C8-N1	3.47	129.96	123.63
2	A	579	617	C9-C8-N1	-3.11	109.23	115.61
2	A	579	617	C9-O4-C10	2.35	121.81	117.67

There are no chirality outliers.

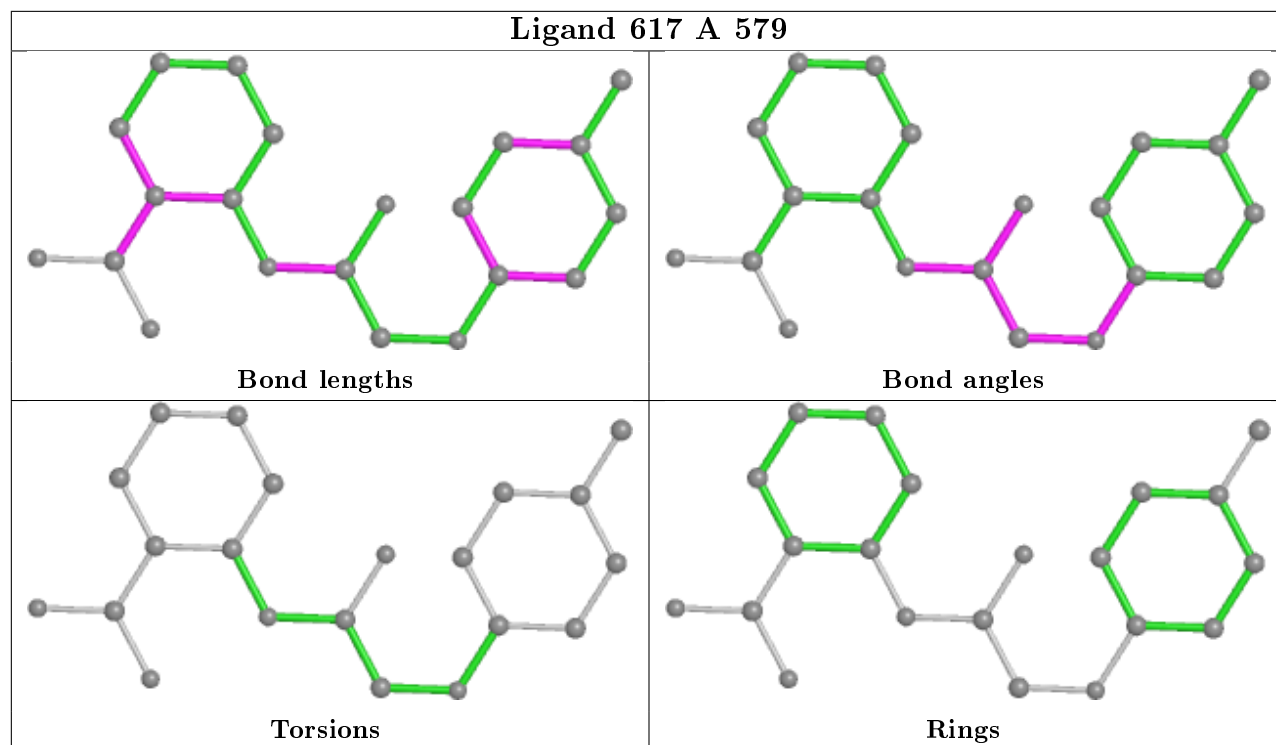
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	579	617	1	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 than 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	559/578 (96%)	0.20	30 (5%)	25	20	21, 38, 69, 126	0
1	B	559/578 (96%)	0.20	34 (6%)	21	16	22, 39, 70, 121	0
1	C	559/578 (96%)	0.27	42 (7%)	14	10	23, 42, 75, 114	0
1	D	559/578 (96%)	0.20	34 (6%)	21	16	22, 38, 70, 112	0
All	All	2236/2312 (96%)	0.22	140 (6%)	20	15	21, 39, 71, 126	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	308	LEU	10.4
1	B	149	PRO	10.3
1	A	152	GLY	10.2
1	B	151	LYS	9.1
1	A	308	LEU	8.0
1	A	153	GLY	7.6
1	C	308	LEU	7.4
1	D	151	LYS	7.3
1	D	149	PRO	6.9
1	D	308	LEU	6.8
1	C	149	PRO	6.6
1	B	152	GLY	6.6
1	A	548	SER	6.3
1	A	540	PRO	6.0
1	C	152	GLY	5.7
1	A	16	ALA	5.0
1	B	330	GLN	5.0
1	C	541	ALA	4.9
1	D	153	GLY	4.7
1	C	330	GLN	4.7
1	D	548	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	23	ILE	4.2
1	C	151	LYS	3.8
1	D	152	GLY	3.8
1	C	153	GLY	3.7
1	B	26	LEU	3.7
1	C	15	ALA	3.6
1	D	15	ALA	3.6
1	C	535	LYS	3.6
1	D	376	ALA	3.5
1	C	401	ARG	3.4
1	C	405	VAL	3.4
1	A	23	ILE	3.4
1	B	150	GLU	3.4
1	D	169	VAL	3.4
1	B	47	LEU	3.3
1	D	330	GLN	3.3
1	D	148	GLN	3.3
1	C	548	SER	3.2
1	B	540	PRO	3.2
1	D	402	HIS	3.2
1	C	402	HIS	3.1
1	B	15	ALA	3.0
1	B	543	SER	3.0
1	D	309	GLN	3.0
1	A	541	ALA	3.0
1	D	25	ALA	3.0
1	A	150	GLU	3.0
1	B	25	ALA	3.0
1	A	149	PRO	3.0
1	C	25	ALA	3.0
1	A	148	GLN	2.9
1	A	377	SER	2.9
1	C	246	ALA	2.9
1	C	16	ALA	2.9
1	C	148	GLN	2.9
1	B	352	ASP	2.9
1	B	377	SER	2.9
1	A	222	ARG	2.9
1	B	170	CYS	2.8
1	A	169	VAL	2.8
1	C	20	LYS	2.8
1	C	14	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	548	SER	2.8
1	B	169	VAL	2.7
1	A	543	SER	2.7
1	B	490	ARG	2.7
1	D	377	SER	2.7
1	C	403	THR	2.7
1	D	535	LYS	2.6
1	B	62	ASP	2.6
1	D	404	PRO	2.6
1	D	16	ALA	2.6
1	A	525	LEU	2.6
1	A	490	ARG	2.6
1	A	15	ALA	2.5
1	D	270	LYS	2.5
1	A	376	ALA	2.5
1	A	401	ARG	2.5
1	C	59	VAL	2.5
1	C	377	SER	2.5
1	C	440	GLU	2.5
1	C	32	ARG	2.5
1	B	153	GLY	2.5
1	D	405	VAL	2.5
1	C	352	ASP	2.5
1	D	378	GLY	2.4
1	B	16	ALA	2.4
1	A	35	ASN	2.4
1	D	379	LYS	2.4
1	B	310	ASP	2.4
1	C	222	ARG	2.4
1	B	376	ALA	2.4
1	B	43	ARG	2.4
1	B	309	GLN	2.3
1	C	23	ILE	2.3
1	D	62	ASP	2.3
1	A	309	GLN	2.3
1	C	540	PRO	2.3
1	D	543	SER	2.3
1	B	401	ARG	2.3
1	C	309	GLN	2.3
1	D	401	ARG	2.3
1	A	402	HIS	2.2
1	B	57	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	222	ARG	2.2
1	C	376	ALA	2.2
1	D	437	GLU	2.2
1	C	84	SER	2.2
1	B	535	LYS	2.2
1	C	404	PRO	2.2
1	D	20	LYS	2.2
1	A	20	LYS	2.2
1	A	151	LYS	2.2
1	B	521	CYS	2.2
1	A	352	ASP	2.2
1	C	101	PHE	2.2
1	C	98	LYS	2.2
1	B	351	GLY	2.1
1	B	556	SER	2.1
1	D	167	VAL	2.1
1	C	490	ARG	2.1
1	A	535	LYS	2.1
1	A	18	GLU	2.1
1	A	86	GLU	2.1
1	C	169	VAL	2.1
1	C	124	LYS	2.1
1	D	43	ARG	2.1
1	D	138	ILE	2.1
1	C	150	GLU	2.1
1	B	148	GLN	2.1
1	C	212	LYS	2.1
1	A	7	THR	2.1
1	B	402	HIS	2.0
1	C	90	LYS	2.0
1	C	47	LEU	2.0
1	D	150	GLU	2.0
1	D	490	ARG	2.0
1	C	393	ALA	2.0
1	D	95	HIS	2.0

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 [i](#)

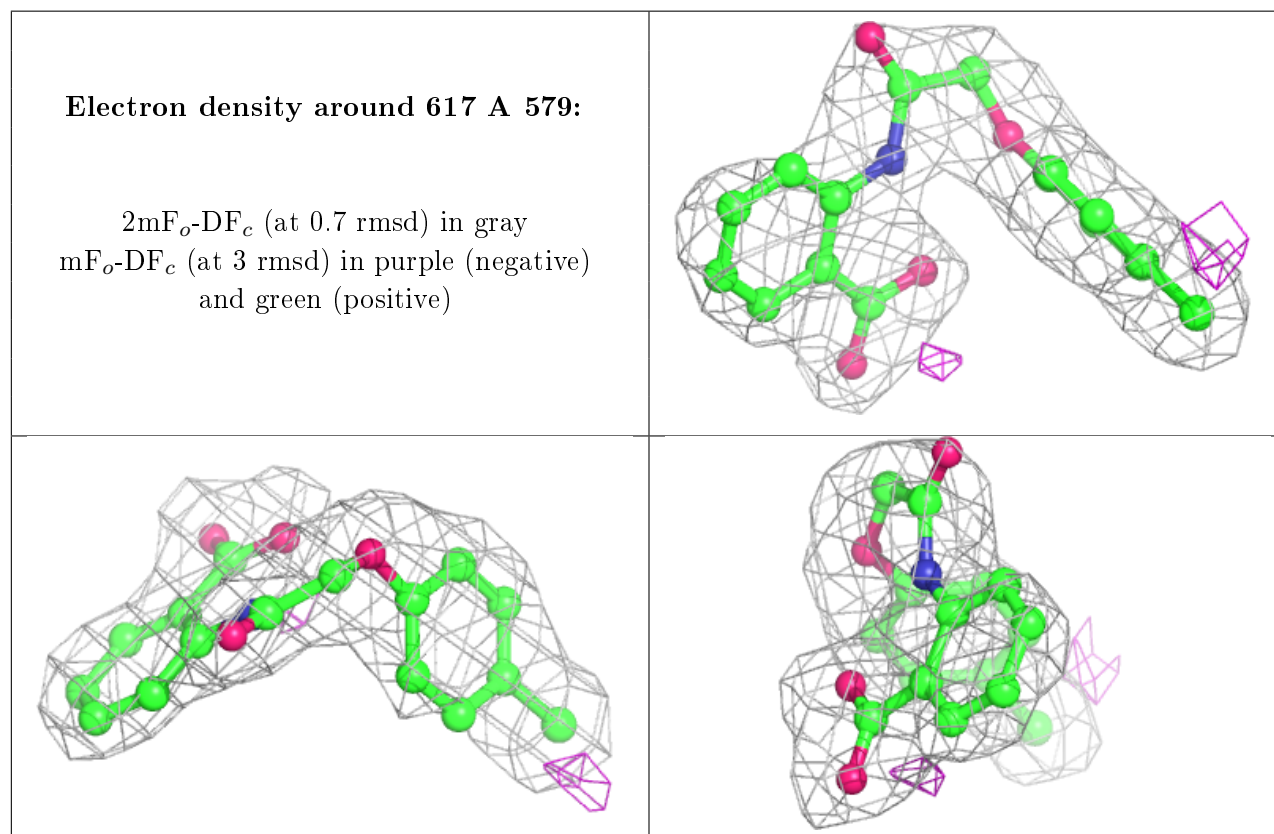
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	617	A	579	21/21	0.93	0.18	19,28,50,61	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.