



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:11 am BST

PDB ID : 5DQQ
Title : Structure, inhibition and regulation of two-pore channel TPC1 from *Arabidopsis thaliana*
Authors : Kintzer, A.F.; Stroud, R.M.
Deposited on : 2015-09-15
Resolution : 2.87 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

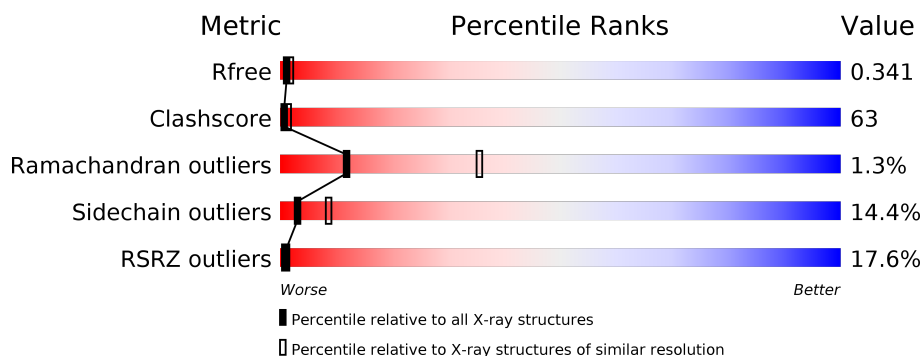
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	723	<div> <div>16%</div> <div>27%</div> <div>53%</div> <div>10%</div> <div>10%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5402 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 Two pore calcium channel protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	649	5282	3498	820	941	23	0	0	0

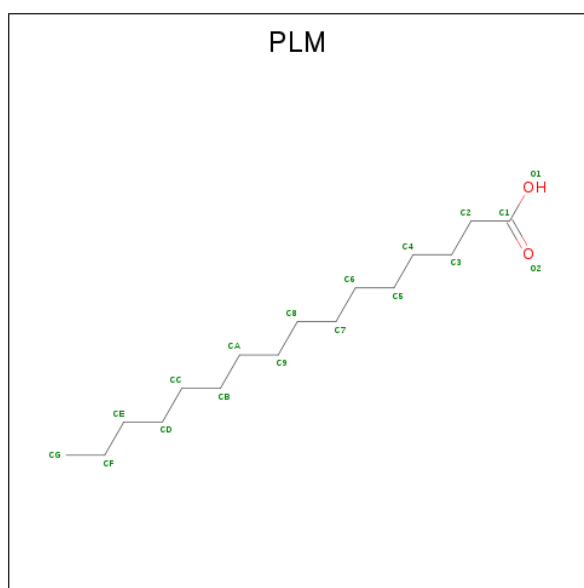
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	initiating methionine	UNP Q94KI8

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

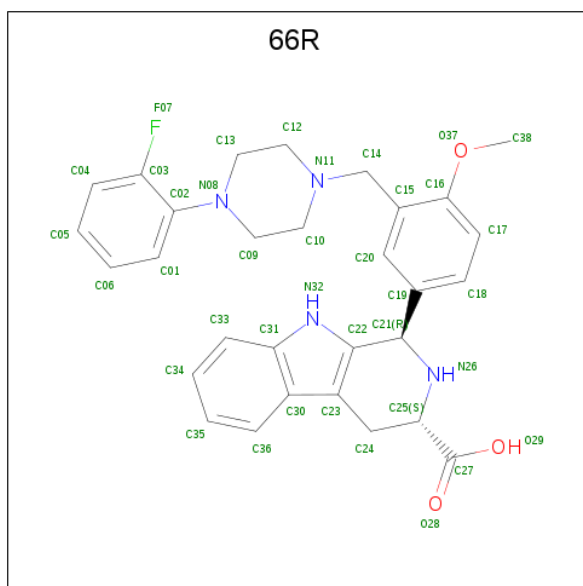
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Ca	0	0
			7	7		

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	16	2		

- Molecule 4 is trans-Ned 19 (three-letter code: 66R) (formula: $C_{30}H_{31}FN_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			38	30	1	4	3		

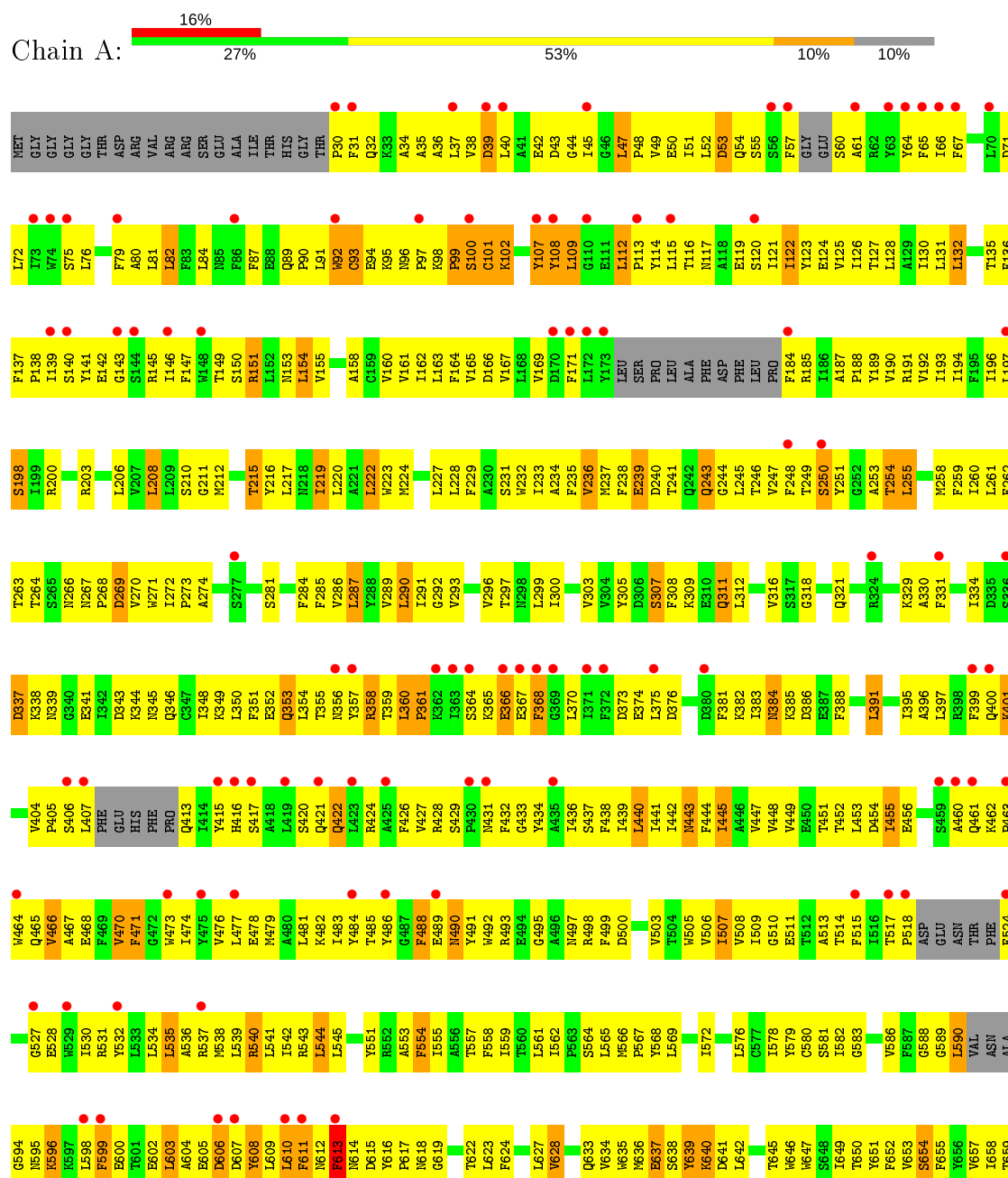
- Molecule 5 is water.

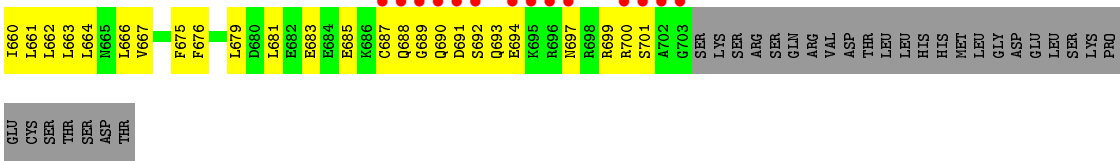
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	57	Total	O	0	0
			57	57		

3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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: Two pore calcium channel protein 1





GLU
CYS
SER
THR
SER
ASP
THR

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.18Å 154.81Å 219.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.70 – 2.87 38.70 – 2.87	Depositor EDS
% Data completeness (in resolution range)	61.3 (38.70-2.87) 61.3 (38.70-2.87)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.81 (at 2.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.297 , 0.339 0.298 , 0.341	Depositor DCC
R_{free} test set	1052 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 103.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.036 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	5402	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, CA, 66R

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	0.31	0/5412	0.47	0/7353

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5282	0	5246	670	0
2	A	7	0	0	0	0
3	A	18	0	31	1	0
4	A	38	0	0	0	0
5	A	57	0	0	6	0
All	All	5402	0	5277	670	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 63.

All (670) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ASN:O	1:A:599:PHE:HB2	1.34	1.27
1:A:31:PHE:HB2	1:A:60:SER:HA	1.20	1.19
1:A:603:LEU:HD21	1:A:638:SER:HB3	1.24	1.19
1:A:417:SER:O	1:A:421:GLN:HB2	1.41	1.17
1:A:603:LEU:HD13	1:A:606:ASP:HB2	1.28	1.15
1:A:603:LEU:HD12	1:A:610:LEU:CB	1.79	1.13
1:A:603:LEU:CD1	1:A:610:LEU:HB2	1.83	1.07
1:A:603:LEU:CD2	1:A:638:SER:HB3	1.87	1.02
1:A:290:LEU:HD22	1:A:291:ILE:HD12	1.41	1.02
1:A:602:GLU:O	1:A:603:LEU:HD23	1.62	0.99
1:A:440:LEU:HD11	1:A:541:LEU:HD13	1.44	0.98
1:A:89:GLN:OE1	1:A:581:SER:OG	1.80	0.98
1:A:603:LEU:HD12	1:A:610:LEU:HB2	0.98	0.96
1:A:603:LEU:HB3	1:A:607:ASP:N	1.81	0.96
1:A:272:ILE:HG23	1:A:273:PRO:HD3	1.49	0.95
1:A:442:ILE:HG23	1:A:471:PHE:HZ	1.28	0.95
1:A:396:ALA:O	1:A:400:GLN:HB3	1.68	0.93
1:A:590:LEU:HD12	1:A:595:ASN:HA	1.50	0.93
1:A:606:ASP:O	1:A:610:LEU:N	2.02	0.92
1:A:38:VAL:HG22	1:A:350:LEU:HD12	1.52	0.92
1:A:524:PHE:O	1:A:528:GLU:N	2.04	0.90
1:A:503:VAL:O	1:A:506:VAL:HG12	1.72	0.90
1:A:267:ASN:HB3	1:A:268:PRO:HD3	1.53	0.90
1:A:188:PRO:HA	1:A:191:ARG:HD2	1.52	0.89
1:A:603:LEU:HD22	1:A:606:ASP:CG	1.93	0.89
1:A:442:ILE:HG23	1:A:471:PHE:CZ	2.07	0.89
1:A:55:SER:HA	1:A:64:TYR:CD1	2.08	0.89
1:A:357:TYR:HB3	1:A:358:ARG:HE	1.37	0.89
1:A:503:VAL:HG12	1:A:537:ARG:HH21	1.37	0.88
1:A:462:LYS:O	1:A:465:GLN:HG2	1.74	0.87
1:A:32:GLN:HB2	1:A:35:ALA:CB	2.04	0.87
1:A:250:SER:OG	1:A:251:TYR:N	2.07	0.87
1:A:634:VAL:O	1:A:638:SER:OG	1.92	0.87
1:A:579:TYR:HA	1:A:582:ILE:HD12	1.56	0.86
1:A:34:ALA:HB1	1:A:353:GLN:OE1	1.75	0.86
1:A:107:TYR:CE1	1:A:596:LYS:HE2	2.11	0.86
1:A:513:ALA:O	1:A:517:THR:OG1	1.94	0.85
1:A:164:PHE:O	1:A:167:VAL:HG12	1.77	0.85
1:A:590:LEU:HG	1:A:642:LEU:HG	1.56	0.85
1:A:232:TRP:O	1:A:236:VAL:HG12	1.77	0.85
1:A:482:LYS:HE3	1:A:491:TYR:HE1	1.41	0.85
1:A:503:VAL:HB	1:A:537:ARG:HD3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:TYR:HH	1:A:654:SER:HG	1.06	0.84
1:A:603:LEU:CD1	1:A:606:ASP:HB2	2.07	0.83
1:A:479:MET:O	1:A:483:ILE:HG22	1.79	0.83
1:A:102:LYS:O	1:A:108:TYR:OH	1.95	0.83
1:A:312:LEU:O	1:A:316:VAL:HG22	1.78	0.83
1:A:360:LEU:HD12	1:A:360:LEU:H	1.42	0.83
1:A:507:ILE:HG13	1:A:537:ARG:HH22	1.42	0.82
1:A:150:SER:OG	1:A:153:ASN:OD1	1.97	0.82
1:A:45:ILE:HD13	1:A:396:ALA:HB2	1.61	0.82
1:A:90:PRO:HA	1:A:616:TYR:HD2	1.43	0.82
1:A:128:LEU:HD11	1:A:164:PHE:HA	1.61	0.82
1:A:603:LEU:HD21	1:A:638:SER:CB	2.08	0.81
1:A:420:SER:HB3	1:A:484:TYR:OH	1.81	0.81
1:A:67:PHE:CD1	1:A:140:SER:HB2	2.16	0.80
1:A:467:ALA:O	1:A:470:VAL:HG12	1.80	0.80
1:A:365:LYS:O	1:A:368:PHE:HB2	1.80	0.80
1:A:43:ASP:O	1:A:48:PRO:HD2	1.81	0.80
1:A:102:LYS:NZ	5:A:901:HOH:O	2.13	0.80
1:A:427:VAL:HG11	1:A:485:THR:CB	2.12	0.80
1:A:400:GLN:O	1:A:401:LYS:HG3	1.80	0.80
1:A:444:PHE:O	1:A:448:VAL:HG13	1.82	0.80
1:A:427:VAL:HG11	1:A:485:THR:HB	1.64	0.80
1:A:158:ALA:O	1:A:161:VAL:HG12	1.82	0.79
1:A:188:PRO:HA	1:A:191:ARG:CD	2.11	0.79
1:A:588:GLY:O	1:A:614:ASN:ND2	2.15	0.79
1:A:250:SER:O	1:A:254:THR:N	2.09	0.79
1:A:79:PHE:HA	1:A:82:LEU:CD1	2.11	0.79
1:A:426:PHE:O	1:A:429:SER:OG	2.00	0.78
1:A:31:PHE:HB2	1:A:60:SER:CA	2.10	0.78
1:A:445:ILE:O	1:A:448:VAL:HG22	1.84	0.78
1:A:272:ILE:CG2	1:A:273:PRO:HD3	2.13	0.78
1:A:454:ASP:HA	1:A:461:GLN:OE1	1.83	0.78
1:A:655:PHE:O	1:A:659:THR:HG22	1.84	0.77
1:A:359:THR:HG21	1:A:400:GLN:HA	1.66	0.77
1:A:132:LEU:HD21	1:A:160:VAL:HG13	1.66	0.77
1:A:359:THR:O	1:A:361:PRO:HD3	1.84	0.77
1:A:112:LEU:HD22	1:A:113:PRO:HD3	1.66	0.76
1:A:499:PHE:O	1:A:503:VAL:HG23	1.86	0.76
1:A:161:VAL:O	1:A:165:VAL:HG12	1.86	0.76
1:A:228:LEU:O	1:A:251:TYR:OH	2.03	0.76
1:A:603:LEU:HD13	1:A:606:ASP:CB	2.12	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD23	1:A:330:ALA:HB2	1.67	0.75
1:A:128:LEU:HD11	1:A:164:PHE:CA	2.16	0.75
1:A:604:ALA:N	1:A:606:ASP:OD2	2.18	0.75
1:A:67:PHE:HB2	1:A:141:TYR:HB3	1.69	0.75
1:A:664:LEU:O	1:A:667:VAL:HG22	1.87	0.75
1:A:596:LYS:HZ2	1:A:596:LYS:N	1.84	0.75
1:A:90:PRO:HA	1:A:616:TYR:CD2	2.21	0.75
1:A:94:GLU:OE1	1:A:96:ASN:ND2	2.20	0.75
1:A:344:LYS:O	1:A:348:ILE:HG23	1.87	0.74
1:A:348:ILE:HG22	1:A:368:PHE:HE2	1.52	0.74
1:A:396:ALA:HA	1:A:400:GLN:CB	2.17	0.74
1:A:688:GLN:HG2	1:A:689:GLY:H	1.53	0.74
1:A:445:ILE:O	1:A:449:VAL:HG23	1.87	0.74
1:A:32:GLN:HB2	1:A:35:ALA:HB2	1.70	0.74
1:A:116:THR:O	1:A:120:SER:N	2.21	0.73
1:A:235:PHE:HB2	1:A:254:THR:HG21	1.68	0.73
1:A:353:GLN:O	1:A:357:TYR:HB2	1.88	0.73
1:A:505:TRP:O	1:A:509:ILE:HG22	1.88	0.73
1:A:603:LEU:HD22	1:A:606:ASP:OD1	1.88	0.73
1:A:579:TYR:O	1:A:651:TYR:OH	2.03	0.73
1:A:107:TYR:HE1	1:A:596:LYS:HE2	1.53	0.73
1:A:568:TYR:O	1:A:572:ILE:HG22	1.87	0.73
1:A:193:ILE:O	1:A:196:ILE:HG12	1.89	0.73
1:A:49:VAL:HB	1:A:200:ARG:HH12	1.53	0.73
1:A:375:LEU:HG	1:A:376:ASP:OD1	1.89	0.73
1:A:165:VAL:O	1:A:169:VAL:HG23	1.89	0.73
1:A:404:VAL:HG12	1:A:405:PRO:O	1.90	0.72
1:A:646:TRP:O	1:A:649:ILE:HG12	1.89	0.72
1:A:95:LYS:NZ	1:A:184:PHE:O	2.23	0.72
1:A:32:GLN:HB2	1:A:35:ALA:HB3	1.69	0.72
1:A:359:THR:HG22	1:A:401:LYS:H	1.55	0.71
1:A:131:LEU:O	1:A:135:THR:HG23	1.89	0.71
1:A:553:ALA:O	1:A:557:THR:OG1	2.08	0.71
1:A:31:PHE:CB	1:A:60:SER:HA	2.11	0.71
1:A:212:MET:HB2	1:A:307:SER:HB2	1.73	0.71
1:A:511:GLU:OE2	1:A:531:ARG:NH1	2.23	0.71
1:A:269:ASP:O	1:A:272:ILE:HG22	1.91	0.70
1:A:481:LEU:HD12	1:A:482:LYS:N	2.05	0.70
1:A:557:THR:O	1:A:561:LEU:HB2	1.89	0.70
1:A:612:ASN:HB3	1:A:618:ASN:HD22	1.56	0.70
1:A:443:ASN:O	1:A:447:VAL:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:PHE:O	1:A:562:ILE:HG13	1.92	0.70
1:A:82:LEU:HD23	1:A:198:SER:OG	1.91	0.70
1:A:31:PHE:CE1	1:A:36:ALA:HB2	2.26	0.70
1:A:594:GLY:HA3	1:A:598:LEU:HG	1.71	0.70
1:A:453:LEU:HB3	1:A:461:GLN:HB3	1.73	0.70
1:A:121:ILE:O	1:A:125:VAL:HG23	1.92	0.70
1:A:514:THR:O	1:A:518:PRO:HD3	1.92	0.70
1:A:45:ILE:CD1	1:A:396:ALA:HB2	2.22	0.69
1:A:536:ALA:O	1:A:539:LEU:HB2	1.92	0.69
1:A:603:LEU:HB3	1:A:607:ASP:CA	2.23	0.69
1:A:351:PHE:O	1:A:355:THR:HG22	1.91	0.69
1:A:188:PRO:HA	1:A:191:ARG:HG3	1.75	0.69
1:A:49:VAL:HB	1:A:200:ARG:NH1	2.08	0.69
1:A:263:THR:O	1:A:264:THR:OG1	2.08	0.69
1:A:123:TYR:O	1:A:127:THR:HG23	1.93	0.69
1:A:542:ILE:HG21	5:A:953:HOH:O	1.92	0.69
1:A:112:LEU:HD13	1:A:113:PRO:HD2	1.75	0.68
1:A:192:VAL:O	1:A:196:ILE:HG23	1.93	0.68
1:A:424:ARG:O	1:A:427:VAL:HG12	1.93	0.68
1:A:478:GLU:OE2	1:A:482:LYS:NZ	2.19	0.68
1:A:122:ILE:O	1:A:126:ILE:HG13	1.93	0.68
1:A:367:GLU:HA	1:A:370:LEU:HG	1.74	0.68
1:A:493:ARG:O	1:A:498:ARG:NH1	2.27	0.68
1:A:95:LYS:HZ3	1:A:184:PHE:HB2	1.56	0.68
1:A:404:VAL:HG22	1:A:490:ASN:ND2	2.08	0.68
1:A:507:ILE:HG13	1:A:537:ARG:NH2	2.08	0.68
1:A:427:VAL:HG11	1:A:485:THR:CG2	2.23	0.68
1:A:561:LEU:HD22	1:A:565:LEU:HG	1.74	0.68
1:A:359:THR:CG2	1:A:400:GLN:HA	2.23	0.68
1:A:72:LEU:O	1:A:75:SER:OG	2.05	0.68
1:A:337:ASP:N	1:A:337:ASP:OD1	2.24	0.67
1:A:590:LEU:CD1	1:A:595:ASN:HA	2.24	0.67
1:A:212:MET:HE2	1:A:308:PHE:HA	1.76	0.67
1:A:606:ASP:N	1:A:606:ASP:OD2	2.27	0.67
1:A:112:LEU:HD22	1:A:113:PRO:CD	2.25	0.67
1:A:605:GLU:HG3	1:A:606:ASP:N	2.09	0.67
1:A:121:ILE:CD1	1:A:171:PHE:HA	2.25	0.67
1:A:32:GLN:OE1	1:A:35:ALA:HB2	1.95	0.67
1:A:235:PHE:HD1	1:A:247:VAL:HG11	1.60	0.67
1:A:249:THR:HB	1:A:253:ALA:HB2	1.77	0.67
1:A:637:GLU:O	1:A:640:LYS:NZ	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HG11	1:A:354:LEU:HA	1.76	0.67
1:A:289:VAL:O	1:A:293:VAL:HG23	1.95	0.66
1:A:404:VAL:HA	1:A:490:ASN:HD21	1.59	0.66
1:A:109:LEU:HD13	1:A:611:PHE:O	1.95	0.66
1:A:128:LEU:HG	1:A:163:LEU:HD23	1.75	0.66
1:A:79:PHE:HA	1:A:82:LEU:HD11	1.77	0.66
1:A:694:GLU:HA	1:A:694:GLU:OE1	1.95	0.66
1:A:79:PHE:O	1:A:82:LEU:HD12	1.96	0.66
1:A:93:CYS:HB2	1:A:115:LEU:O	1.96	0.66
1:A:128:LEU:CD1	1:A:164:PHE:HA	2.24	0.66
1:A:184:PHE:HA	5:A:918:HOH:O	1.96	0.66
1:A:442:ILE:HA	1:A:445:ILE:HD11	1.78	0.66
1:A:139:ILE:HG12	1:A:147:PHE:CB	2.27	0.65
1:A:238:PHE:HD1	1:A:241:THR:HG21	1.61	0.65
1:A:245:LEU:HD23	1:A:246:THR:H	1.61	0.65
1:A:117:ASN:HA	1:A:120:SER:HB3	1.78	0.65
1:A:473:TRP:O	1:A:476:VAL:HG12	1.96	0.65
1:A:188:PRO:HA	1:A:191:ARG:CG	2.25	0.65
1:A:61:ALA:CB	1:A:65:PHE:HD2	2.10	0.65
1:A:406:SER:O	1:A:407:LEU:HB2	1.96	0.65
1:A:615:ASP:OD1	1:A:617:PRO:HD2	1.97	0.65
1:A:243:GLN:NE2	1:A:274:ALA:HB2	2.12	0.65
1:A:433:GLY:O	1:A:436:ILE:HG13	1.97	0.65
1:A:505:TRP:HA	1:A:508:VAL:HG22	1.78	0.65
1:A:647:TRP:O	1:A:650:THR:HG23	1.96	0.65
1:A:395:ILE:O	1:A:400:GLN:N	2.30	0.64
1:A:590:LEU:HG	1:A:642:LEU:CG	2.26	0.64
1:A:290:LEU:HD22	1:A:291:ILE:CD1	2.22	0.64
1:A:555:ILE:O	1:A:559:ILE:HG13	1.97	0.64
1:A:624:PHE:O	1:A:628:VAL:HG13	1.97	0.64
1:A:473:TRP:HA	1:A:476:VAL:HG12	1.80	0.64
1:A:37:LEU:CD1	1:A:334:ILE:HB	2.27	0.64
1:A:427:VAL:HG11	1:A:485:THR:HG21	1.80	0.64
1:A:693:GLN:NE2	5:A:902:HOH:O	2.17	0.64
1:A:530:ILE:HG23	1:A:531:ARG:HG2	1.78	0.64
1:A:35:ALA:HA	1:A:353:GLN:HE22	1.64	0.63
1:A:603:LEU:HD13	1:A:606:ASP:C	2.18	0.63
1:A:603:LEU:HD22	1:A:606:ASP:CB	2.28	0.63
1:A:141:TYR:CD2	1:A:142:GLU:HG3	2.34	0.63
1:A:535:LEU:O	1:A:535:LEU:HD12	1.98	0.63
1:A:95:LYS:NZ	1:A:184:PHE:HB2	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LEU:HD21	1:A:541:LEU:HD13	1.80	0.63
1:A:688:GLN:HG2	1:A:689:GLY:N	2.13	0.62
1:A:384:ASN:OD1	1:A:384:ASN:N	2.32	0.62
1:A:640:LYS:HB3	1:A:640:LYS:NZ	2.15	0.62
1:A:131:LEU:HD21	1:A:194:ILE:HD11	1.82	0.62
1:A:228:LEU:HD12	1:A:255:LEU:CD1	2.30	0.62
1:A:396:ALA:HA	1:A:400:GLN:HB3	1.80	0.62
1:A:500:ASP:OD2	1:A:540:ARG:NH1	2.33	0.62
1:A:47:LEU:N	1:A:48:PRO:HD2	2.15	0.62
1:A:440:LEU:CD1	1:A:541:LEU:HD13	2.25	0.62
1:A:243:GLN:HE21	1:A:274:ALA:HB2	1.65	0.61
1:A:139:ILE:HG12	1:A:147:PHE:CG	2.35	0.61
1:A:100:SER:CB	1:A:101:CYS:HA	2.30	0.61
1:A:38:VAL:CG1	1:A:354:LEU:HA	2.30	0.61
1:A:511:GLU:CD	1:A:531:ARG:HH11	2.04	0.61
1:A:602:GLU:CB	1:A:642:LEU:HD11	2.31	0.61
1:A:98:LYS:HD2	1:A:98:LYS:N	2.14	0.61
1:A:612:ASN:CB	1:A:618:ASN:HD22	2.14	0.61
1:A:191:ARG:O	1:A:194:ILE:HG22	2.01	0.61
1:A:659:THR:HG23	1:A:660:ILE:CD1	2.30	0.61
1:A:122:ILE:HG13	1:A:123:TYR:N	2.15	0.60
1:A:602:GLU:C	1:A:603:LEU:HD23	2.21	0.60
1:A:596:LYS:CE	1:A:596:LYS:HA	2.17	0.60
1:A:285:PHE:O	1:A:289:VAL:HG23	2.01	0.60
1:A:359:THR:HG21	1:A:400:GLN:CA	2.32	0.60
1:A:137:PHE:N	1:A:138:PRO:HD2	2.16	0.60
1:A:131:LEU:HD21	1:A:194:ILE:CD1	2.32	0.60
1:A:659:THR:HG23	1:A:660:ILE:HD13	1.83	0.60
1:A:249:THR:HB	1:A:253:ALA:CB	2.32	0.60
1:A:211:GLY:HA3	1:A:311:GLN:HE21	1.67	0.60
1:A:331:PHE:CE1	1:A:385:LYS:HB2	2.37	0.59
1:A:492:TRP:CE3	1:A:498:ARG:HD3	2.37	0.59
1:A:344:LYS:HB2	1:A:381:PHE:CB	2.32	0.59
1:A:53:ASP:O	1:A:329:LYS:NZ	2.30	0.59
1:A:331:PHE:O	1:A:334:ILE:HG22	2.02	0.59
1:A:428:ARG:HG2	1:A:486:TYR:CE1	2.37	0.59
1:A:503:VAL:HG12	1:A:537:ARG:NH2	2.12	0.59
1:A:603:LEU:CD2	1:A:638:SER:CB	2.75	0.59
1:A:515:PHE:O	1:A:518:PRO:HD2	2.03	0.59
1:A:232:TRP:HB2	1:A:251:TYR:HE1	1.67	0.59
1:A:44:GLY:O	1:A:47:LEU:HD23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:HD2	5:A:901:HOH:O	2.02	0.59
1:A:138:PRO:HG2	1:A:147:PHE:CE2	2.38	0.59
1:A:396:ALA:HA	1:A:400:GLN:HB2	1.83	0.59
1:A:136:PHE:C	1:A:138:PRO:HD2	2.22	0.59
1:A:633:GLN:N	1:A:633:GLN:OE1	2.28	0.59
1:A:692:SER:OG	1:A:697:ASN:HB2	2.03	0.59
1:A:35:ALA:HA	1:A:353:GLN:NE2	2.18	0.58
1:A:640:LYS:HD2	1:A:646:TRP:CZ3	2.38	0.58
1:A:396:ALA:C	1:A:400:GLN:HB3	2.23	0.58
1:A:511:GLU:HA	1:A:531:ARG:NH1	2.18	0.58
1:A:38:VAL:CG2	1:A:350:LEU:HD12	2.28	0.58
1:A:260:ILE:O	1:A:263:THR:OG1	2.16	0.58
1:A:619:GLY:HA2	1:A:622:THR:HG22	1.84	0.58
1:A:128:LEU:HD22	1:A:164:PHE:HD2	1.69	0.58
1:A:244:GLY:O	1:A:248:PHE:N	2.37	0.58
1:A:234:ALA:HB2	1:A:284:PHE:CZ	2.39	0.58
1:A:337:ASP:O	1:A:338:LYS:HB2	2.04	0.58
1:A:360:LEU:N	1:A:360:LEU:HD12	2.17	0.58
1:A:39:ASP:OD1	1:A:39:ASP:N	2.36	0.58
1:A:34:ALA:C	1:A:353:GLN:HE22	2.07	0.58
1:A:31:PHE:CZ	1:A:36:ALA:HB2	2.39	0.58
1:A:373:ASP:OD1	1:A:374:GLU:N	2.36	0.58
1:A:448:VAL:O	1:A:452:THR:HG22	2.03	0.58
1:A:700:ARG:HG2	1:A:700:ARG:O	2.04	0.58
1:A:260:ILE:HG22	1:A:266:ASN:OD1	2.04	0.57
1:A:135:THR:HG21	1:A:160:VAL:HG21	1.85	0.57
1:A:564:SER:O	1:A:567:PRO:HD2	2.05	0.57
1:A:505:TRP:O	1:A:508:VAL:HG22	2.03	0.57
1:A:357:TYR:HD2	1:A:358:ARG:HH21	1.53	0.57
1:A:238:PHE:CD1	1:A:241:THR:HG21	2.39	0.57
1:A:212:MET:CB	1:A:307:SER:HB2	2.34	0.57
1:A:247:VAL:O	1:A:247:VAL:HG12	2.05	0.57
1:A:269:ASP:N	1:A:269:ASP:OD1	2.37	0.57
1:A:292:GLY:O	1:A:297:THR:OG1	2.18	0.57
1:A:151:ARG:O	1:A:155:VAL:HG23	2.04	0.57
1:A:286:VAL:HG23	1:A:287:LEU:N	2.19	0.57
1:A:349:LYS:O	1:A:353:GLN:HG3	2.05	0.57
1:A:38:VAL:HG22	1:A:350:LEU:CD1	2.31	0.57
1:A:80:ALA:O	1:A:84:LEU:HG	2.05	0.57
1:A:566:MET:N	1:A:567:PRO:HD2	2.20	0.57
1:A:259:PHE:O	1:A:262:PHE:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ILE:HG23	1:A:399:PHE:HB2	1.87	0.56
1:A:404:VAL:HG13	1:A:490:ASN:ND2	2.20	0.56
1:A:536:ALA:O	1:A:539:LEU:N	2.37	0.56
1:A:211:GLY:HA3	1:A:311:GLN:NE2	2.20	0.56
1:A:596:LYS:CE	1:A:596:LYS:CA	2.80	0.56
1:A:440:LEU:C	1:A:440:LEU:HD12	2.25	0.56
1:A:404:VAL:CA	1:A:490:ASN:HD21	2.18	0.56
1:A:143:GLY:HA3	1:A:146:ILE:HD12	1.86	0.56
1:A:247:VAL:HG12	1:A:250:SER:HA	1.87	0.56
1:A:482:LYS:HE3	1:A:491:TYR:CE1	2.31	0.56
1:A:139:ILE:HD11	1:A:147:PHE:CD1	2.41	0.56
1:A:349:LYS:HG3	1:A:350:LEU:N	2.21	0.56
1:A:37:LEU:HD23	1:A:37:LEU:N	2.20	0.56
1:A:438:PHE:HA	1:A:441:ILE:HD12	1.87	0.56
1:A:558:PHE:CE1	1:A:562:ILE:HD11	2.41	0.56
1:A:432:PHE:CZ	1:A:481:LEU:HD11	2.40	0.56
1:A:645:THR:HG22	5:A:940:HOH:O	2.03	0.56
1:A:228:LEU:HD12	1:A:255:LEU:HD11	1.88	0.56
1:A:38:VAL:HG13	1:A:354:LEU:HB2	1.88	0.56
1:A:422:GLN:O	1:A:426:PHE:HD2	1.87	0.56
1:A:477:LEU:HG	1:A:481:LEU:HD23	1.88	0.56
1:A:637:GLU:O	1:A:640:LYS:HB3	2.05	0.56
1:A:145:ARG:O	1:A:149:THR:HG22	2.05	0.56
1:A:535:LEU:HD13	1:A:538:MET:HE2	1.86	0.56
1:A:594:GLY:CA	1:A:598:LEU:HG	2.36	0.56
1:A:188:PRO:CA	1:A:191:ARG:HD2	2.31	0.55
1:A:132:LEU:HD23	1:A:132:LEU:N	2.20	0.55
1:A:404:VAL:CB	1:A:490:ASN:HD21	2.18	0.55
1:A:132:LEU:HD21	1:A:160:VAL:CG1	2.36	0.55
1:A:331:PHE:HB2	1:A:388:PHE:CD2	2.42	0.55
1:A:439:ILE:O	1:A:442:ILE:HG22	2.06	0.55
1:A:38:VAL:HG11	1:A:354:LEU:CA	2.36	0.55
1:A:558:PHE:HE1	1:A:562:ILE:HD11	1.71	0.55
1:A:72:LEU:O	1:A:75:SER:N	2.36	0.55
1:A:76:LEU:O	1:A:79:PHE:HB2	2.06	0.55
1:A:437:SER:O	1:A:441:ILE:HG13	2.07	0.55
1:A:360:LEU:HD11	1:A:401:LYS:HB2	1.89	0.55
1:A:360:LEU:HD13	1:A:360:LEU:O	2.06	0.55
1:A:503:VAL:HG11	1:A:537:ARG:HG3	1.87	0.55
1:A:38:VAL:HG21	1:A:353:GLN:HB2	1.88	0.55
1:A:404:VAL:HG13	1:A:490:ASN:HD21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLU:OE2	1:A:615:ASP:HA	2.07	0.55
1:A:453:LEU:HD12	1:A:461:GLN:HA	1.89	0.54
1:A:71:ASP:HB2	1:A:137:PHE:HE2	1.72	0.54
1:A:200:ARG:HG2	1:A:203:ARG:NH1	2.21	0.54
1:A:299:LEU:O	1:A:303:VAL:HG23	2.07	0.54
1:A:507:ILE:CD1	1:A:537:ARG:HH12	2.18	0.54
1:A:603:LEU:HD22	1:A:606:ASP:HB2	1.88	0.54
1:A:49:VAL:O	1:A:50:GLU:HG3	2.07	0.54
1:A:235:PHE:CB	1:A:254:THR:HG21	2.38	0.54
1:A:42:GLU:HB2	1:A:358:ARG:HG3	1.89	0.54
1:A:615:ASP:HB3	1:A:618:ASN:HB2	1.88	0.54
1:A:76:LEU:HA	1:A:79:PHE:HD2	1.73	0.54
1:A:232:TRP:CA	1:A:251:TYR:HE1	2.21	0.54
1:A:35:ALA:CA	1:A:353:GLN:HE22	2.21	0.54
1:A:396:ALA:CA	1:A:400:GLN:HB3	2.38	0.54
1:A:208:LEU:HG	1:A:311:GLN:HB3	1.89	0.54
1:A:219:ILE:O	1:A:219:ILE:HD12	2.08	0.54
1:A:224:MET:SD	1:A:228:LEU:HD13	2.48	0.54
1:A:47:LEU:N	1:A:48:PRO:CD	2.71	0.54
1:A:616:TYR:HB3	1:A:617:PRO:HD3	1.89	0.54
1:A:417:SER:O	1:A:421:GLN:CB	2.35	0.54
1:A:453:LEU:CD1	1:A:461:GLN:HA	2.37	0.54
1:A:619:GLY:O	1:A:622:THR:HG22	2.09	0.54
1:A:590:LEU:HG	1:A:642:LEU:CD2	2.38	0.54
1:A:216:TYR:O	1:A:219:ILE:HG22	2.08	0.53
1:A:37:LEU:HD12	1:A:334:ILE:HB	1.91	0.53
1:A:507:ILE:CG1	1:A:537:ARG:HH22	2.17	0.53
1:A:94:GLU:HB2	1:A:97:PRO:HG2	1.90	0.53
1:A:94:GLU:O	1:A:98:LYS:HD3	2.08	0.53
1:A:267:ASN:CB	1:A:268:PRO:HD3	2.33	0.53
1:A:596:LYS:HZ2	1:A:596:LYS:CA	2.21	0.53
1:A:222:LEU:O	1:A:222:LEU:HD12	2.08	0.53
1:A:271:TRP:HB3	1:A:285:PHE:CE1	2.44	0.53
1:A:345:ASN:O	1:A:348:ILE:HG12	2.09	0.53
1:A:611:PHE:CG	1:A:611:PHE:O	2.61	0.53
1:A:81:LEU:HD22	1:A:130:ILE:HG22	1.90	0.53
1:A:287:LEU:CD2	1:A:291:ILE:HD13	2.38	0.53
1:A:535:LEU:CD1	1:A:538:MET:HE2	2.39	0.53
1:A:690:GLN:HA	1:A:690:GLN:NE2	2.24	0.52
1:A:447:VAL:HA	1:A:468:GLU:OE2	2.08	0.52
1:A:100:SER:HB2	1:A:101:CYS:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:LEU:HD11	1:A:627:LEU:HD22	1.91	0.52
1:A:650:THR:O	1:A:654:SER:N	2.36	0.52
1:A:527:GLY:HA2	1:A:530:ILE:HG22	1.92	0.52
1:A:359:THR:CG2	1:A:401:LYS:H	2.21	0.52
1:A:640:LYS:HD2	1:A:646:TRP:CE3	2.45	0.52
1:A:216:TYR:CD2	1:A:662:LEU:HD13	2.44	0.52
1:A:96:ASN:CG	1:A:97:PRO:HD3	2.29	0.52
1:A:128:LEU:O	1:A:132:LEU:HG	2.09	0.52
1:A:300:ILE:HG21	1:A:661:LEU:HD22	1.91	0.52
1:A:507:ILE:HD12	1:A:537:ARG:HH12	1.74	0.52
1:A:542:ILE:O	1:A:545:LEU:HD12	2.10	0.52
1:A:606:ASP:HB3	1:A:634:VAL:HB	1.92	0.52
1:A:609:LEU:HD12	1:A:634:VAL:HG21	1.90	0.52
1:A:112:LEU:HB3	1:A:113:PRO:HD2	1.91	0.52
1:A:107:TYR:OH	1:A:596:LYS:HG2	2.09	0.52
1:A:334:ILE:HD12	1:A:350:LEU:HD22	1.91	0.52
1:A:404:VAL:HG22	1:A:490:ASN:HD21	1.73	0.52
1:A:250:SER:O	1:A:254:THR:HB	2.08	0.52
1:A:79:PHE:CA	1:A:82:LEU:CD1	2.87	0.52
1:A:473:TRP:O	1:A:476:VAL:CG1	2.57	0.51
1:A:554:PHE:CD2	1:A:554:PHE:N	2.78	0.51
1:A:128:LEU:HD23	1:A:132:LEU:HG	1.91	0.51
1:A:200:ARG:HG2	1:A:203:ARG:HH12	1.74	0.51
1:A:355:THR:OG1	1:A:361:PRO:HD2	2.11	0.51
1:A:45:ILE:HD13	1:A:396:ALA:CB	2.38	0.51
1:A:453:LEU:HD13	1:A:460:ALA:C	2.31	0.51
1:A:557:THR:CG2	1:A:675:PHE:HA	2.40	0.51
1:A:699:ARG:O	1:A:700:ARG:HB3	2.10	0.51
1:A:128:LEU:HD23	1:A:128:LEU:O	2.10	0.51
1:A:146:ILE:HA	1:A:149:THR:HG22	1.91	0.51
1:A:241:THR:HG23	1:A:243:GLN:H	1.76	0.51
1:A:440:LEU:HD11	1:A:541:LEU:CD1	2.29	0.51
1:A:557:THR:HG21	1:A:675:PHE:HA	1.91	0.51
1:A:491:TYR:O	1:A:497:ASN:HB2	2.10	0.51
1:A:143:GLY:HA3	1:A:146:ILE:CD1	2.40	0.51
1:A:334:ILE:HD11	1:A:349:LYS:HZ1	1.75	0.51
1:A:527:GLY:HA2	1:A:530:ILE:CG2	2.40	0.51
1:A:89:GLN:N	1:A:90:PRO:HD2	2.26	0.51
1:A:35:ALA:N	1:A:353:GLN:HE22	2.08	0.51
1:A:432:PHE:HZ	1:A:481:LEU:HD11	1.75	0.51
1:A:463:PRO:O	1:A:466:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HG13	1:A:545:LEU:HD13	1.92	0.51
1:A:194:ILE:O	1:A:198:SER:HB2	2.11	0.51
1:A:212:MET:CE	1:A:308:PHE:HA	2.41	0.51
1:A:348:ILE:HG22	1:A:368:PHE:CE2	2.38	0.51
1:A:375:LEU:HD11	1:A:699:ARG:NH1	2.26	0.51
1:A:460:ALA:O	1:A:463:PRO:HD2	2.10	0.50
1:A:554:PHE:H	1:A:554:PHE:HD2	1.58	0.50
1:A:551:TYR:O	1:A:555:ILE:HG12	2.12	0.50
1:A:112:LEU:CB	1:A:113:PRO:HD2	2.41	0.50
1:A:544:LEU:C	1:A:544:LEU:HD23	2.32	0.50
1:A:42:GLU:HA	1:A:42:GLU:OE1	2.11	0.50
1:A:154:LEU:C	1:A:154:LEU:HD12	2.32	0.50
1:A:437:SER:O	1:A:440:LEU:HG	2.12	0.50
1:A:272:ILE:HG23	1:A:273:PRO:CD	2.32	0.50
1:A:107:TYR:CZ	1:A:596:LYS:HE2	2.45	0.50
1:A:453:LEU:CB	1:A:461:GLN:HB3	2.41	0.50
1:A:490:ASN:N	1:A:490:ASN:OD1	2.40	0.49
1:A:636:MET:HG3	1:A:652:PHE:HB2	1.93	0.49
1:A:107:TYR:OH	1:A:596:LYS:CE	2.60	0.49
1:A:190:VAL:O	1:A:194:ILE:HB	2.12	0.49
1:A:239:GLU:HG3	1:A:240:ASP:N	2.28	0.49
1:A:666:LEU:HD23	1:A:666:LEU:C	2.32	0.49
1:A:266:ASN:ND2	1:A:270:VAL:HB	2.26	0.49
1:A:433:GLY:HA2	1:A:436:ILE:HD11	1.95	0.49
1:A:137:PHE:N	1:A:138:PRO:CD	2.76	0.49
1:A:231:SER:OG	1:A:255:LEU:HA	2.13	0.49
1:A:285:PHE:O	1:A:289:VAL:N	2.30	0.49
1:A:596:LYS:O	1:A:600:GLU:HG2	2.12	0.49
1:A:113:PRO:O	1:A:114:TYR:HB2	2.13	0.49
1:A:212:MET:HB2	1:A:307:SER:CB	2.41	0.49
1:A:247:VAL:CG1	1:A:250:SER:HA	2.43	0.49
1:A:580:CYS:HB3	1:A:616:TYR:HE1	1.78	0.49
1:A:287:LEU:HD23	1:A:291:ILE:HD13	1.95	0.48
1:A:31:PHE:HE2	1:A:57:PHE:CE1	2.30	0.48
1:A:339:ASN:OD1	1:A:339:ASN:N	2.46	0.48
1:A:61:ALA:HA	1:A:65:PHE:CD2	2.48	0.48
1:A:557:THR:HG21	1:A:675:PHE:HB2	1.95	0.48
1:A:291:ILE:O	1:A:296:VAL:HG23	2.13	0.48
1:A:594:GLY:O	1:A:598:LEU:N	2.42	0.48
1:A:636:MET:CE	1:A:653:VAL:HG23	2.43	0.48
1:A:375:LEU:O	1:A:700:ARG:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLU:OE1	1:A:382:LYS:HB3	2.14	0.48
1:A:569:LEU:O	1:A:572:ILE:HG23	2.14	0.48
1:A:619:GLY:HA2	1:A:622:THR:CG2	2.44	0.48
1:A:121:ILE:HD13	1:A:171:PHE:HA	1.95	0.48
1:A:569:LEU:HA	1:A:572:ILE:CG2	2.43	0.48
1:A:286:VAL:HG23	1:A:287:LEU:H	1.79	0.47
1:A:296:VAL:O	1:A:300:ILE:HG13	2.14	0.47
1:A:427:VAL:CG1	1:A:485:THR:HG21	2.43	0.47
1:A:87:PHE:O	1:A:90:PRO:HG2	2.14	0.47
1:A:232:TRP:CB	1:A:251:TYR:HE1	2.27	0.47
1:A:595:ASN:HB3	1:A:596:LYS:HZ1	1.79	0.47
1:A:508:VAL:HG23	1:A:509:ILE:N	2.29	0.47
1:A:596:LYS:HZ2	1:A:596:LYS:CB	2.26	0.47
1:A:615:ASP:OD1	1:A:616:TYR:N	2.47	0.47
1:A:91:LEU:O	1:A:115:LEU:HB2	2.14	0.47
1:A:147:PHE:CE2	1:A:153:ASN:HB3	2.50	0.47
1:A:261:LEU:HD11	1:A:267:ASN:HD22	1.78	0.47
1:A:440:LEU:HD21	1:A:541:LEU:CD1	2.44	0.47
1:A:590:LEU:O	1:A:614:ASN:OD1	2.32	0.47
1:A:71:ASP:HB2	1:A:137:PHE:CE2	2.48	0.47
1:A:456:GLU:OE1	1:A:456:GLU:HA	2.13	0.47
1:A:535:LEU:HD13	1:A:538:MET:CE	2.44	0.47
1:A:503:VAL:CG1	1:A:537:ARG:HH21	2.17	0.47
1:A:606:ASP:O	1:A:609:LEU:N	2.47	0.47
1:A:404:VAL:HA	1:A:490:ASN:ND2	2.28	0.47
1:A:675:PHE:CE2	1:A:679:LEU:HD11	2.50	0.47
1:A:700:ARG:O	1:A:701:SER:HB2	2.14	0.47
1:A:30:PRO:O	1:A:60:SER:HB3	2.14	0.47
1:A:511:GLU:HA	1:A:531:ARG:HH12	1.79	0.47
1:A:61:ALA:HA	1:A:65:PHE:HD2	1.79	0.47
1:A:112:LEU:CD1	1:A:113:PRO:HD2	2.45	0.47
1:A:594:GLY:O	1:A:598:LEU:HB2	2.15	0.47
1:A:428:ARG:HG2	1:A:486:TYR:HE1	1.77	0.47
1:A:128:LEU:HD11	1:A:164:PHE:N	2.30	0.47
1:A:359:THR:HG21	1:A:400:GLN:HG2	1.97	0.47
1:A:449:VAL:HG11	1:A:464:TRP:CZ3	2.50	0.47
1:A:462:LYS:N	1:A:463:PRO:HD2	2.30	0.47
1:A:164:PHE:HA	1:A:167:VAL:HG12	1.97	0.47
1:A:489:GLU:OE1	1:A:489:GLU:HA	2.14	0.47
1:A:116:THR:OG1	1:A:119:GLU:HG3	2.14	0.46
1:A:162:ILE:O	1:A:165:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:LYS:HB3	1:A:640:LYS:HZ3	1.79	0.46
1:A:492:TRP:CD2	1:A:498:ARG:HD3	2.50	0.46
1:A:582:ILE:O	1:A:586:VAL:HG23	2.15	0.46
1:A:580:CYS:HB3	1:A:616:TYR:CE1	2.51	0.46
1:A:138:PRO:HB2	1:A:142:GLU:OE2	2.15	0.46
1:A:366:GLU:HG3	1:A:366:GLU:H	1.34	0.46
1:A:619:GLY:CA	1:A:622:THR:HG22	2.45	0.46
1:A:348:ILE:HG13	1:A:349:LYS:N	2.30	0.46
1:A:359:THR:HG21	1:A:400:GLN:CB	2.46	0.46
1:A:658:ILE:O	1:A:662:LEU:HB3	2.15	0.46
1:A:67:PHE:HB3	1:A:140:SER:OG	2.15	0.46
1:A:92:TRP:CZ3	1:A:188:PRO:HG3	2.51	0.46
1:A:528:GLU:O	1:A:532:TYR:HD1	1.99	0.46
1:A:543:ARG:HD2	1:A:559:ILE:HD13	1.96	0.46
1:A:572:ILE:HD11	1:A:627:LEU:HD11	1.97	0.46
1:A:359:THR:CB	1:A:400:GLN:HA	2.46	0.46
1:A:433:GLY:HA2	1:A:436:ILE:CG1	2.45	0.46
1:A:404:VAL:CG1	1:A:490:ASN:HD21	2.29	0.46
1:A:590:LEU:N	1:A:590:LEU:HD13	2.31	0.46
1:A:353:GLN:HG3	1:A:353:GLN:H	1.40	0.46
1:A:663:LEU:O	1:A:666:LEU:HB3	2.15	0.46
1:A:100:SER:HB2	1:A:101:CYS:CA	2.46	0.46
1:A:87:PHE:C	1:A:90:PRO:HD2	2.37	0.46
1:A:462:LYS:O	1:A:466:VAL:HG23	2.16	0.45
1:A:535:LEU:O	1:A:538:MET:HG3	2.16	0.45
1:A:557:THR:HG21	1:A:675:PHE:CA	2.46	0.45
1:A:112:LEU:HB2	1:A:617:PRO:HG2	1.99	0.45
1:A:220:LEU:HD11	1:A:657:VAL:CG1	2.45	0.45
1:A:603:LEU:HG	1:A:610:LEU:HD23	1.97	0.45
1:A:61:ALA:CA	1:A:65:PHE:HD2	2.29	0.45
1:A:397:LEU:HD12	1:A:397:LEU:HA	1.65	0.45
1:A:439:ILE:HA	1:A:442:ILE:HG22	1.98	0.45
1:A:488:PHE:HD1	1:A:489:GLU:N	2.15	0.45
1:A:530:ILE:O	1:A:534:LEU:HD23	2.16	0.45
1:A:635:TRP:HB3	1:A:652:PHE:HE2	1.81	0.45
1:A:96:ASN:N	1:A:97:PRO:CD	2.79	0.45
1:A:286:VAL:CG2	1:A:287:LEU:N	2.79	0.45
1:A:223:TRP:CZ2	1:A:227:LEU:HD11	2.51	0.45
1:A:413:GLN:O	1:A:415:TYR:HD1	1.99	0.45
1:A:61:ALA:O	1:A:65:PHE:HB3	2.16	0.45
1:A:151:ARG:O	1:A:154:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:GLU:CG	1:A:531:ARG:HH11	2.30	0.45
1:A:37:LEU:HD13	1:A:330:ALA:O	2.17	0.45
1:A:462:LYS:HD2	1:A:465:GLN:OE1	2.17	0.45
1:A:489:GLU:O	1:A:493:ARG:HG3	2.16	0.45
1:A:422:GLN:O	1:A:426:PHE:CD2	2.68	0.45
1:A:482:LYS:HG2	1:A:491:TYR:CE1	2.52	0.45
1:A:517:THR:N	1:A:518:PRO:CD	2.79	0.45
1:A:146:ILE:O	1:A:149:THR:HG22	2.17	0.44
1:A:239:GLU:HG3	1:A:240:ASP:OD1	2.18	0.44
1:A:391:LEU:O	1:A:395:ILE:HG13	2.16	0.44
1:A:595:ASN:OD1	1:A:596:LYS:HE3	2.17	0.44
1:A:238:PHE:O	1:A:241:THR:HG22	2.17	0.44
1:A:290:LEU:HD23	1:A:291:ILE:N	2.33	0.44
1:A:96:ASN:O	1:A:99:PRO:HD2	2.16	0.44
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.83	0.44
1:A:449:VAL:O	1:A:452:THR:HG22	2.17	0.44
1:A:37:LEU:CD1	1:A:334:ILE:CB	2.95	0.44
1:A:76:LEU:HA	1:A:79:PHE:CD2	2.51	0.44
1:A:433:GLY:HA2	1:A:436:ILE:HG12	1.99	0.44
1:A:596:LYS:HD3	1:A:596:LYS:HA	1.41	0.44
1:A:583:GLY:HA3	1:A:613:PHE:CE1	2.53	0.44
1:A:305:TYR:HE1	1:A:309:LYS:HE2	1.82	0.44
1:A:334:ILE:CD1	1:A:350:LEU:HD22	2.48	0.44
1:A:352:GLU:O	1:A:355:THR:CG2	2.66	0.44
1:A:404:VAL:CG2	1:A:490:ASN:HD21	2.30	0.44
1:A:495:GLY:HA2	1:A:498:ARG:CZ	2.48	0.44
1:A:51:ILE:O	1:A:51:ILE:HG22	2.17	0.44
1:A:619:GLY:C	1:A:622:THR:HG22	2.38	0.44
1:A:79:PHE:HA	1:A:82:LEU:HD12	1.98	0.44
1:A:141:TYR:CE2	1:A:142:GLU:HG3	2.53	0.43
1:A:38:VAL:CG1	1:A:354:LEU:CA	2.95	0.43
1:A:603:LEU:CD2	1:A:606:ASP:HB2	2.48	0.43
1:A:608:TYR:HD1	1:A:608:TYR:HA	1.65	0.43
1:A:166:ASP:OD2	1:A:187:ALA:HB2	2.18	0.43
1:A:578:ILE:O	1:A:582:ILE:HG13	2.18	0.43
1:A:596:LYS:NZ	1:A:596:LYS:CB	2.80	0.43
1:A:352:GLU:O	1:A:355:THR:HG22	2.19	0.43
1:A:439:ILE:HG21	1:A:474:ILE:HG21	2.01	0.43
1:A:652:PHE:N	1:A:652:PHE:CD1	2.85	0.43
1:A:132:LEU:CD2	1:A:160:VAL:CG1	2.96	0.43
1:A:431:ASN:HA	1:A:434:TYR:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:ILE:HD11	1:A:627:LEU:HD21	2.01	0.43
1:A:154:LEU:HD12	1:A:155:VAL:N	2.33	0.43
1:A:233:ILE:HA	1:A:236:VAL:CG1	2.49	0.43
1:A:258:MET:HA	1:A:258:MET:CE	2.49	0.43
1:A:358:ARG:HD3	1:A:358:ARG:HA	1.54	0.43
1:A:534:LEU:HD22	1:A:534:LEU:N	2.33	0.43
1:A:543:ARG:CD	1:A:559:ILE:HD13	2.49	0.43
1:A:681:LEU:O	1:A:685:GLU:HG3	2.18	0.43
1:A:355:THR:HG23	1:A:356:ASN:N	2.34	0.43
1:A:64:TYR:CD1	1:A:64:TYR:N	2.86	0.43
1:A:217:LEU:HA	1:A:217:LEU:HD23	1.78	0.43
1:A:267:ASN:HB3	1:A:268:PRO:CD	2.36	0.43
1:A:120:SER:O	1:A:124:GLU:HG3	2.19	0.43
1:A:503:VAL:HG11	1:A:537:ARG:CG	2.48	0.43
1:A:543:ARG:H	1:A:543:ARG:HG2	1.61	0.43
1:A:589:GLY:C	1:A:590:LEU:HD22	2.39	0.43
1:A:676:PHE:HD1	1:A:679:LEU:HD12	1.84	0.43
1:A:231:SER:HA	1:A:258:MET:HG3	2.00	0.43
1:A:360:LEU:CD1	1:A:360:LEU:H	2.20	0.43
1:A:463:PRO:HG2	1:A:464:TRP:HD1	1.84	0.43
1:A:95:LYS:HA	1:A:95:LYS:HD3	1.74	0.43
1:A:107:TYR:CE1	1:A:596:LYS:CE	2.94	0.42
1:A:208:LEU:HD21	1:A:308:PHE:CD1	2.54	0.42
1:A:453:LEU:HD13	1:A:461:GLN:N	2.34	0.42
1:A:359:THR:HG22	1:A:401:LYS:N	2.28	0.42
1:A:365:LYS:HD3	1:A:367:GLU:HG3	1.99	0.42
1:A:52:LEU:HD11	1:A:141:TYR:O	2.19	0.42
1:A:132:LEU:HA	1:A:132:LEU:HD22	1.76	0.42
1:A:38:VAL:HG21	1:A:353:GLN:CD	2.40	0.42
1:A:594:GLY:HA3	1:A:598:LEU:CG	2.44	0.42
1:A:128:LEU:CD2	1:A:164:PHE:HD2	2.32	0.42
1:A:451:THR:O	1:A:455:ILE:HG23	2.19	0.42
1:A:79:PHE:CA	1:A:82:LEU:HD12	2.49	0.42
1:A:139:ILE:CG1	1:A:147:PHE:CG	3.01	0.42
1:A:244:GLY:O	1:A:248:PHE:CA	2.68	0.42
1:A:590:LEU:C	1:A:614:ASN:OD1	2.58	0.42
1:A:622:THR:HG23	1:A:623:LEU:N	2.33	0.42
1:A:235:PHE:HD1	1:A:247:VAL:CG1	2.31	0.42
1:A:346:GLN:O	1:A:349:LYS:HG2	2.19	0.42
1:A:503:VAL:CG1	1:A:534:LEU:HD12	2.50	0.42
1:A:490:ASN:O	1:A:493:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:TRP:O	1:A:639:TYR:HB2	2.20	0.42
1:A:187:ALA:O	1:A:190:VAL:HG22	2.20	0.42
1:A:233:ILE:O	1:A:236:VAL:HG13	2.20	0.42
1:A:595:ASN:O	1:A:599:PHE:CB	2.30	0.42
1:A:38:VAL:HG11	1:A:354:LEU:N	2.35	0.41
1:A:286:VAL:CG2	1:A:287:LEU:H	2.31	0.41
1:A:318:GLY:HA2	1:A:321:GLN:CD	2.40	0.41
1:A:442:ILE:HA	1:A:445:ILE:CD1	2.48	0.41
1:A:146:ILE:HA	1:A:149:THR:CG2	2.50	0.41
1:A:232:TRP:HB2	1:A:251:TYR:CE1	2.52	0.41
1:A:212:MET:O	1:A:215:THR:HG23	2.20	0.41
1:A:229:PHE:O	1:A:233:ILE:HG22	2.21	0.41
1:A:468:GLU:O	1:A:471:PHE:HB2	2.21	0.41
1:A:700:ARG:O	1:A:701:SER:CB	2.68	0.41
1:A:143:GLY:HA3	1:A:146:ILE:CG1	2.51	0.41
1:A:187:ALA:N	1:A:188:PRO:CD	2.84	0.41
1:A:128:LEU:HD13	1:A:167:VAL:HG11	2.03	0.41
1:A:193:ILE:HA	1:A:196:ILE:CD1	2.51	0.41
1:A:232:TRP:CA	1:A:251:TYR:CE1	3.03	0.41
1:A:473:TRP:O	1:A:474:ILE:C	2.59	0.41
1:A:510:GLY:C	1:A:531:ARG:NH1	2.74	0.41
1:A:596:LYS:HE3	1:A:596:LYS:HA	1.97	0.41
1:A:605:GLU:CG	1:A:606:ASP:N	2.81	0.41
1:A:603:LEU:O	1:A:607:ASP:HB2	2.21	0.41
1:A:613:PHE:H	1:A:618:ASN:HB3	1.84	0.41
1:A:71:ASP:OD1	1:A:71:ASP:O	2.38	0.41
1:A:237:MET:CE	3:A:808:PLM:H81	2.51	0.41
1:A:238:PHE:C	1:A:241:THR:HG22	2.40	0.41
1:A:373:ASP:OD1	1:A:373:ASP:C	2.59	0.41
1:A:112:LEU:CG	1:A:113:PRO:HD2	2.51	0.41
1:A:146:ILE:CA	1:A:149:THR:HG22	2.51	0.41
1:A:270:VAL:CG1	1:A:271:TRP:HD1	2.34	0.41
1:A:355:THR:OG1	1:A:361:PRO:CD	2.69	0.41
1:A:474:ILE:O	1:A:477:LEU:HB3	2.21	0.41
1:A:650:THR:O	1:A:651:TYR:C	2.59	0.41
1:A:603:LEU:CB	1:A:607:ASP:HB2	2.51	0.41
1:A:90:PRO:CA	1:A:616:TYR:HD2	2.25	0.41
1:A:82:LEU:HD23	1:A:198:SER:CB	2.51	0.41
1:A:189:TYR:HD1	1:A:189:TYR:H	1.69	0.40
1:A:299:LEU:HD12	1:A:299:LEU:C	2.41	0.40
1:A:530:ILE:HG23	1:A:531:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PHE:CD1	1:A:60:SER:O	2.74	0.40
1:A:243:GLN:O	1:A:247:VAL:HG23	2.21	0.40
1:A:112:LEU:CB	1:A:113:PRO:CD	2.99	0.40
1:A:290:LEU:CD2	1:A:291:ILE:HD12	2.31	0.40
1:A:212:MET:HE1	1:A:308:PHE:HB2	2.02	0.40
1:A:482:LYS:HA	1:A:485:THR:OG1	2.21	0.40
1:A:557:THR:HG21	1:A:675:PHE:CB	2.50	0.40
1:A:79:PHE:C	1:A:82:LEU:HD12	2.41	0.40
1:A:135:THR:O	1:A:138:PRO:HD2	2.22	0.40
1:A:555:ILE:HG22	1:A:559:ILE:HD11	2.04	0.40
1:A:143:GLY:HA3	1:A:146:ILE:HG13	2.03	0.40
1:A:258:MET:HA	1:A:258:MET:HE2	2.02	0.40
1:A:609:LEU:C	1:A:611:PHE:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	637/723 (88%)	585 (92%)	44 (7%)	8 (1%)	12	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	361	PRO
1	A	401	LYS
1	A	108	TYR
1	A	422	GLN
1	A	613	PHE
1	A	290	LEU
1	A	99	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	570/647 (88%)	488 (86%)	82 (14%)	3 8

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	53	ASP
1	A	54	GLN
1	A	66	ILE
1	A	82	LEU
1	A	92	TRP
1	A	93	CYS
1	A	100	SER
1	A	101	CYS
1	A	102	LYS
1	A	107	TYR
1	A	109	LEU
1	A	112	LEU
1	A	122	ILE
1	A	132	LEU
1	A	151	ARG
1	A	154	LEU
1	A	185	ARG
1	A	197	LEU
1	A	198	SER
1	A	206	LEU
1	A	208	LEU
1	A	210	SER
1	A	215	THR
1	A	219	ILE
1	A	222	LEU
1	A	236	VAL
1	A	239	GLU
1	A	243	GLN
1	A	250	SER

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Mol	Chain	Res	Type
1	A	254	THR
1	A	255	LEU
1	A	269	ASP
1	A	281	SER
1	A	287	LEU
1	A	307	SER
1	A	311	GLN
1	A	337	ASP
1	A	343	ASP
1	A	353	GLN
1	A	358	ARG
1	A	360	LEU
1	A	364	SER
1	A	366	GLU
1	A	368	PHE
1	A	383	ILE
1	A	384	ASN
1	A	386	ASP
1	A	391	LEU
1	A	416	HIS
1	A	440	LEU
1	A	443	ASN
1	A	445	ILE
1	A	455	ILE
1	A	466	VAL
1	A	470	VAL
1	A	471	PHE
1	A	488	PHE
1	A	490	ASN
1	A	507	ILE
1	A	535	LEU
1	A	540	ARG
1	A	544	LEU
1	A	554	PHE
1	A	590	LEU
1	A	596	LYS
1	A	599	PHE
1	A	603	LEU
1	A	606	ASP
1	A	608	TYR
1	A	610	LEU
1	A	611	PHE

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Mol	Chain	Res	Type
1	A	613	PHE
1	A	628	VAL
1	A	637	GLU
1	A	639	TYR
1	A	640	LYS
1	A	641	ASP
1	A	654	SER
1	A	683	GLU
1	A	687	CYS
1	A	691	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	GLN
1	A	267	ASN
1	A	353	GLN
1	A	443	ASN
1	A	618	ASN
1	A	631	ASN
1	A	688	GLN
1	A	690	GLN
1	A	693	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 for Mogul analysis.

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	PLM	A	808	-	14,17,17	0.29	0	13,17,17	0.27	0
4	66R	A	809	-	36,43,43	2.46	10 (27%)	46,62,62	1.51	7 (15%)

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	PLM	A	808	-	-	8/13/15/15	-
4	66R	A	809	-	-	4/14/40/40	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	809	66R	C14-N11	-8.73	1.30	1.47
4	A	809	66R	C02-N08	5.01	1.52	1.41
4	A	809	66R	C14-C15	4.93	1.59	1.51
4	A	809	66R	C23-C22	-4.13	1.32	1.39
4	A	809	66R	C25-N26	3.91	1.51	1.46
4	A	809	66R	C10-N11	-3.12	1.38	1.46
4	A	809	66R	C12-N11	-3.05	1.38	1.46
4	A	809	66R	C30-C31	-2.83	1.35	1.42
4	A	809	66R	O37-C16	2.80	1.41	1.37
4	A	809	66R	C19-C21	2.33	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	809	66R	F07-C03-C02	4.45	122.47	118.42
4	A	809	66R	C13-N08-C02	3.32	124.14	116.27
4	A	809	66R	O37-C16-C15	2.94	120.07	115.97
4	A	809	66R	C03-C02-N08	2.74	123.72	120.47
4	A	809	66R	C01-C02-N08	-2.53	118.27	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	809	66R	O37-C16-C17	-2.35	120.35	124.37
4	A	809	66R	C13-N08-C09	-2.19	106.67	111.52

There are no chirality outliers.

All (12) torsion outliers are listed below:

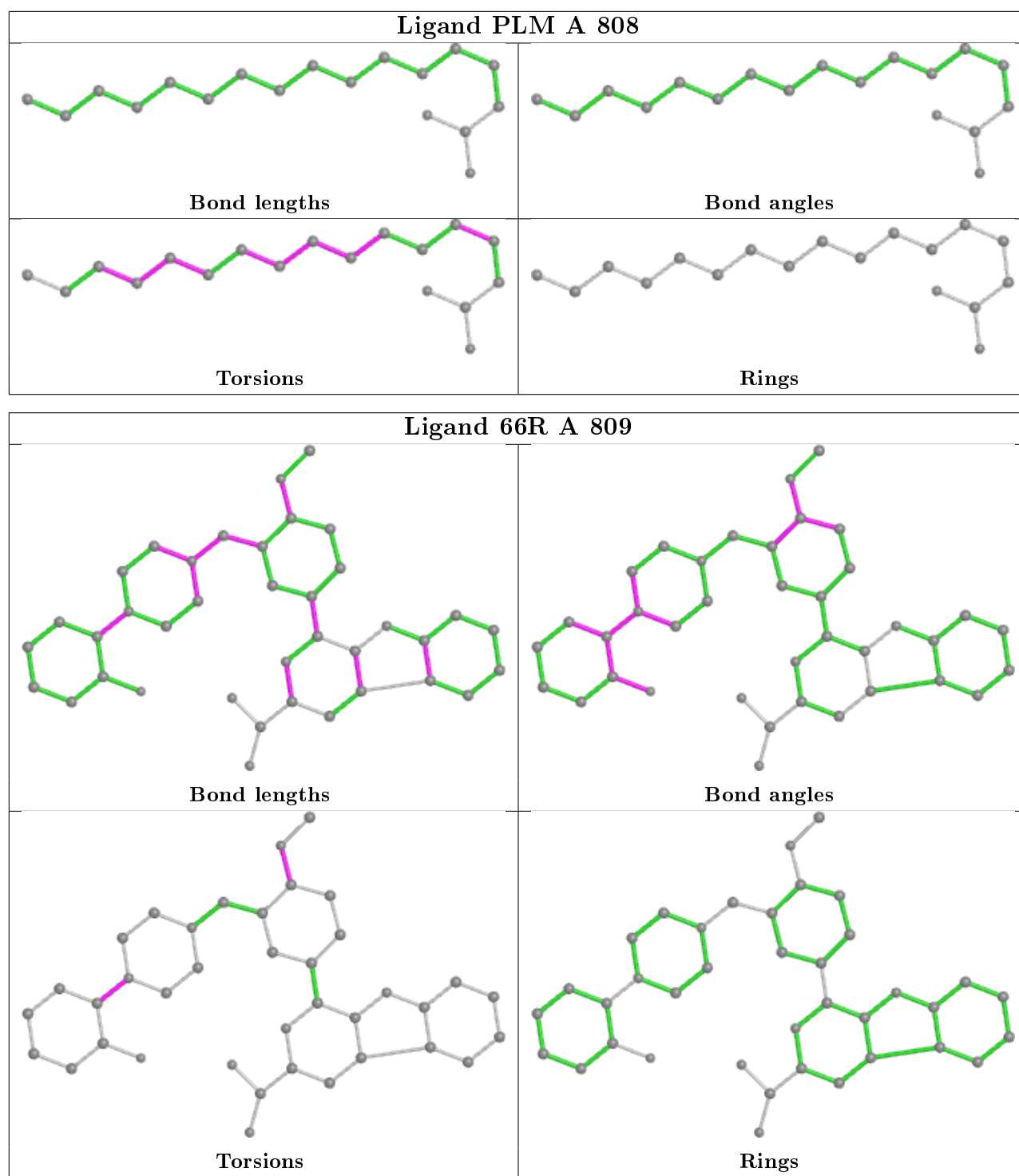
Mol	Chain	Res	Type	Atoms
4	A	809	66R	C01-C02-N08-C13
4	A	809	66R	C17-C16-O37-C38
4	A	809	66R	C03-C02-N08-C13
4	A	809	66R	C15-C16-O37-C38
3	A	808	PLM	C8-C9-CA-CB
3	A	808	PLM	CA-CB-CC-CD
3	A	808	PLM	CC-CD-CE-CF
3	A	808	PLM	C5-C6-C7-C8
3	A	808	PLM	C6-C7-C8-C9
3	A	808	PLM	C2-C3-C4-C5
3	A	808	PLM	C7-C8-C9-CA
3	A	808	PLM	CB-CC-CD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	808	PLM	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 ⓘ

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(Å ²)	Q<0.9
1	A	649/723 (89%)	1.06	114 (17%) 1 1	39, 103, 201, 344	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	PHE	12.0
1	A	696	ARG	9.9
1	A	56	SER	9.9
1	A	170	ASP	8.7
1	A	517	THR	8.5
1	A	399	PHE	8.5
1	A	74	TRP	8.4
1	A	702	ALA	7.0
1	A	173	TYR	6.9
1	A	701	SER	6.9
1	A	473	TRP	6.6
1	A	65	PHE	6.5
1	A	368	PHE	6.2
1	A	687	CYS	6.2
1	A	691	ASP	6.0
1	A	31	PHE	5.8
1	A	363	ILE	5.8
1	A	461	GLN	5.5
1	A	39	ASP	5.3
1	A	380	ASP	5.2
1	A	248	PHE	5.2
1	A	97	PRO	5.1
1	A	184	PHE	5.0
1	A	610	LEU	5.0
1	A	529	TRP	4.9
1	A	703	GLY	4.9
1	A	171	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	364	SER	4.8
1	A	475	TYR	4.6
1	A	356	ASN	4.6
1	A	108	TYR	4.6
1	A	172	LEU	4.5
1	A	460	ALA	4.5
1	A	64	TYR	4.5
1	A	406	SER	4.5
1	A	120	SER	4.5
1	A	100	SER	4.4
1	A	367	GLU	4.2
1	A	527	GLY	4.1
1	A	144	SER	4.1
1	A	423	LEU	4.1
1	A	607	ASP	4.0
1	A	63	TYR	3.9
1	A	435	ALA	3.9
1	A	477	LEU	3.9
1	A	518	PRO	3.9
1	A	419	LEU	3.9
1	A	692	SER	3.9
1	A	371	ILE	3.8
1	A	697	ASN	3.8
1	A	537	ARG	3.8
1	A	366	GLU	3.7
1	A	700	ARG	3.5
1	A	695	LYS	3.5
1	A	415	TYR	3.5
1	A	148	TRP	3.5
1	A	67	PHE	3.5
1	A	73	ILE	3.4
1	A	139	ILE	3.4
1	A	689	GLY	3.3
1	A	690	GLN	3.3
1	A	688	GLN	3.3
1	A	92	TRP	3.2
1	A	30	PRO	3.1
1	A	357	TYR	3.1
1	A	37	LEU	3.0
1	A	70	LEU	3.0
1	A	372	PHE	2.9
1	A	140	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	2.9
1	A	694	GLU	2.8
1	A	459	SER	2.8
1	A	75	SER	2.8
1	A	336	SER	2.8
1	A	524	PHE	2.7
1	A	484	TYR	2.7
1	A	464	TRP	2.7
1	A	107	TYR	2.7
1	A	331	PHE	2.6
1	A	416	HIS	2.6
1	A	375	LEU	2.6
1	A	431	ASN	2.6
1	A	197	LEU	2.6
1	A	143	GLY	2.6
1	A	599	PHE	2.5
1	A	489	GLU	2.5
1	A	362	LYS	2.5
1	A	86	PHE	2.5
1	A	606	ASP	2.4
1	A	407	LEU	2.4
1	A	417	SER	2.4
1	A	66	ILE	2.4
1	A	532	TYR	2.4
1	A	61	ALA	2.4
1	A	613	PHE	2.3
1	A	515	PHE	2.3
1	A	40	LEU	2.3
1	A	611	PHE	2.3
1	A	486	TYR	2.3
1	A	79	PHE	2.2
1	A	425	ALA	2.2
1	A	400	GLN	2.2
1	A	324	ARG	2.2
1	A	277	SER	2.2
1	A	45	ILE	2.2
1	A	110	GLY	2.2
1	A	369	GLY	2.2
1	A	113	PRO	2.2
1	A	598	LEU	2.2
1	A	146	ILE	2.1
1	A	430	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	250	SER	2.0
1	A	421	GLN	2.0
1	A	463	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

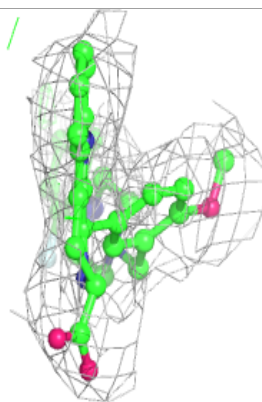
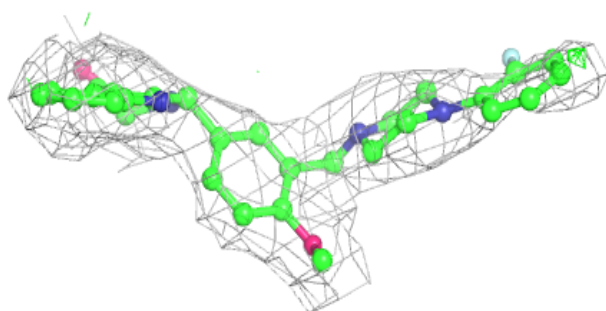
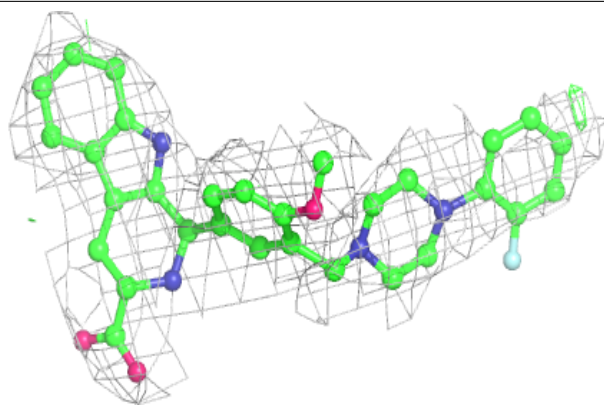
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	802	1/1	0.22	0.28	154,154,154,154	0
4	66R	A	809	38/38	0.74	0.27	109,137,162,185	0
2	CA	A	807	1/1	0.76	0.11	140,140,140,140	0
2	CA	A	801	1/1	0.80	0.26	117,117,117,117	0
3	PLM	A	808	18/18	0.87	0.26	54,86,138,183	0
2	CA	A	805	1/1	0.88	0.12	153,153,153,153	0
2	CA	A	803	1/1	0.91	0.11	57,57,57,57	0
2	CA	A	806	1/1	0.91	0.12	147,147,147,147	0
2	CA	A	804	1/1	0.92	0.07	112,112,112,112	0

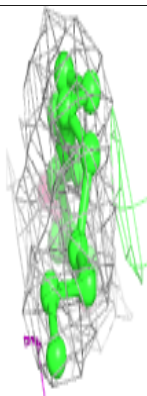
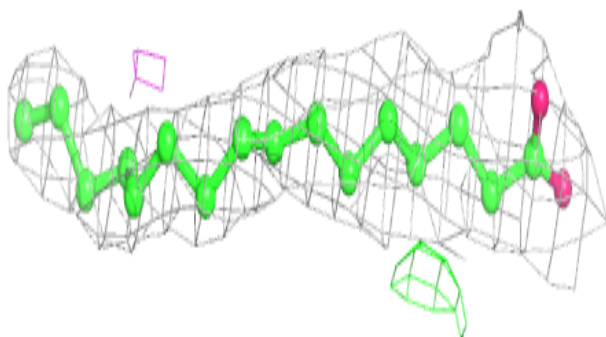
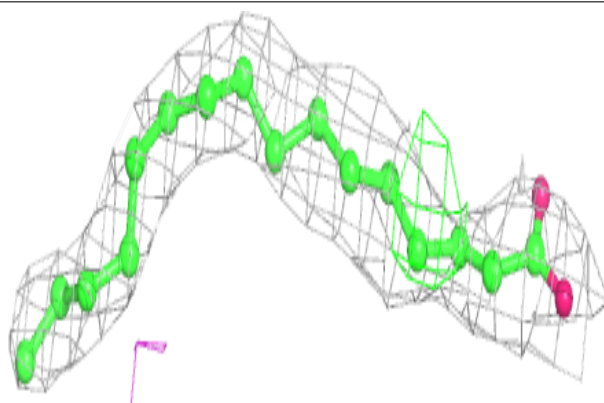
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 66R A 809:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PLM A 808:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.