



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:04 AM UTC

PDB ID : 5DQQ / pdb_00005dqq
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

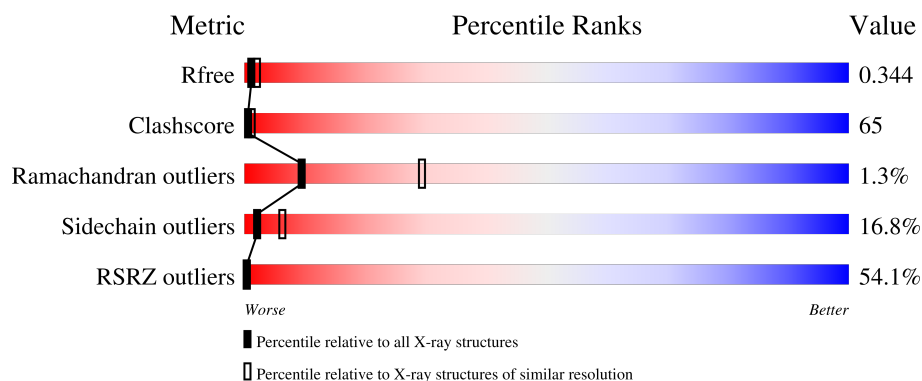
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	723	

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
1	A	649	Total	C	N	O	S	0	0	0
			5282	3498	820	941	23			

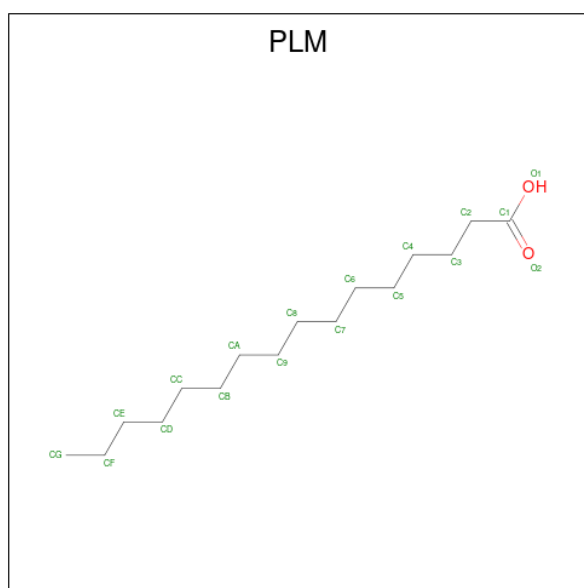
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

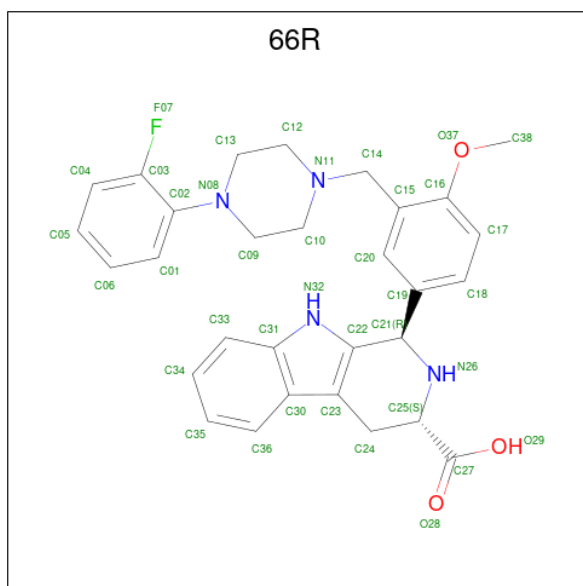
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Ca	0	0
			7	7		

- Molecule 3 is PALMITIC ACID (CCD ID: 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 (CCD ID: 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		

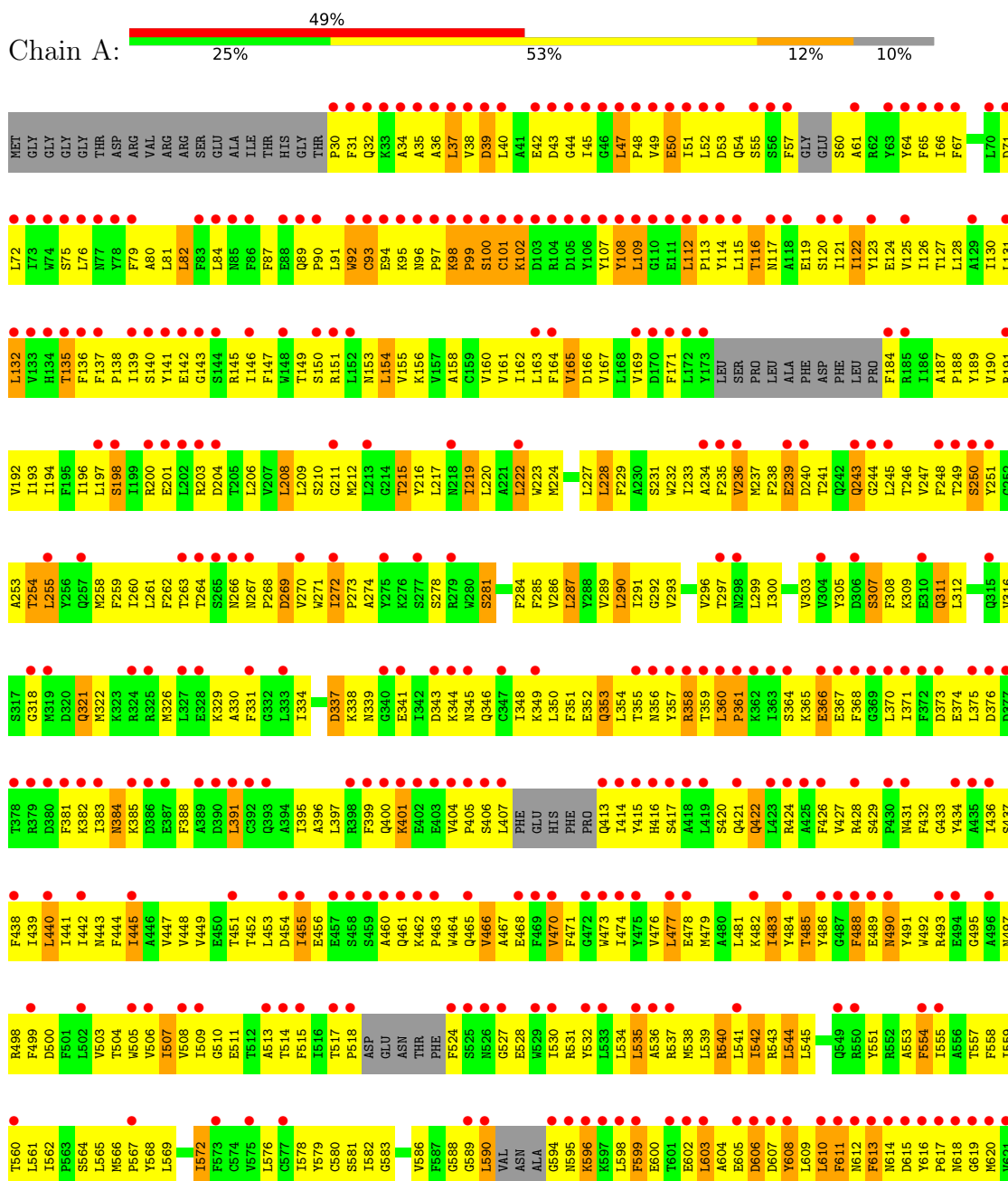
- Molecule 5 is water.

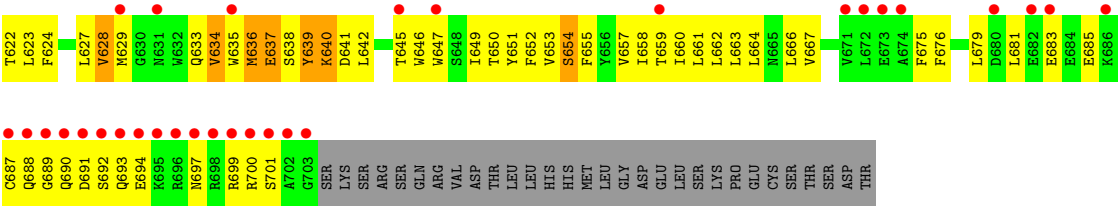
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	57	Total	O	0	0
			57	57		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Two pore calcium channel protein 1





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) 61.2 (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 , 0.344	Depositor DCC
R_{free} test set	1052 reflections (2.67%)	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)	0.29 , 116.2	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	0.83	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: CA, 66R, PLM

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	0.21	0/5412	0.45	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	688	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	688	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 65.

All (688) 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:603:LEU:HD22	1:A:606:ASP:CG	1.93	0.94
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: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:535:LEU:HD13	1:A:538:MET:HE2	1.54	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:VAL:HB	1:A:537:ARG:HD3	1.57	0.85
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:102:LYS:NZ	5:A:901:HOH:O	2.13	0.80
1:A:467:ALA:O	1:A:470:VAL:HG12	1.80	0.80
1:A:43:ASP:O	1:A:48:PRO:HD2	1.81	0.80
1:A:365:LYS:O	1:A:368:PHE:HB2	1.80	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:596:LYS:HZ2	1:A:596:LYS:N	1.80	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:579:TYR:HH	1:A:654:SER:HG	1.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:67:PHE:HB2	1:A:141:TYR:HB3	1.69	0.75
1:A:604:ALA:N	1:A:606:ASP:OD2	2.18	0.75
1:A:664:LEU:O	1:A:667:VAL:HG22	1.87	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:258:MET:HA	1:A:258:MET:HE2	1.68	0.74
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:95:LYS:NZ	1:A:184:PHE:O	2.23	0.72
1:A:646:TRP:O	1:A:649:ILE:HG12	1.89	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HD23	1:A:198:SER:OG	1.91	0.70
1:A:443:ASN:O	1:A:447:VAL:HG23	1.91	0.70
1:A:558:PHE:O	1:A:562:ILE:HG13	1.92	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:535:LEU:CD1	1:A:538:MET:HE2	2.22	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:49:VAL:HB	1:A:200:ARG:NH1	2.08	0.69
1:A:188:PRO:HA	1:A:191:ARG:HG3	1.75	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:404:VAL:HG22	1:A:490:ASN:ND2	2.08	0.68
1:A:603:LEU:HD13	1:A:606:ASP:C	2.18	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:72:LEU:O	1:A:75:SER:OG	2.05	0.68
1:A:359:THR:CG2	1:A:400:GLN:HA	2.23	0.68
1:A:337:ASP:OD1	1:A:337:ASP:N	2.24	0.67
1:A:590:LEU:CD1	1:A:595:ASN:HA	2.24	0.67
1:A:606:ASP:OD2	1:A:606:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:GLU:O	1:A:640:LYS:NZ	2.27	0.67
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:109:LEU:HD13	1:A:611:PHE:O	1.95	0.66
1:A:404:VAL:HA	1:A:490:ASN:HD21	1.59	0.66
1:A:79:PHE:HA	1:A:82:LEU:HD11	1.77	0.66
1:A:128:LEU:HG	1:A:163:LEU:HD23	1.75	0.66
1:A:79:PHE:O	1:A:82:LEU:HD12	1.96	0.66
1:A:694:GLU:OE1	1:A:694:GLU:HA	1.95	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:511:GLU:CD	1:A:531:ARG:HH11	2.04	0.66
1:A:49:VAL:HG13	1:A:322:MET:HE2	1.77	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:602:GLU:C	1:A:603:LEU:HD23	2.21	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:61:ALA:CB	1:A:65:PHE:HD2	2.10	0.65
1:A:188:PRO:HA	1:A:191:ARG:CG	2.25	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:406:SER:O	1:A:407:LEU:HB2	1.96	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:136:PHE:C	1:A:138:PRO:HD2	2.22	0.64
1:A:590:LEU:HG	1:A:642:LEU:CG	2.26	0.64
1:A:95:LYS:NZ	1:A:184:PHE:HB2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ALA:HA	1:A:353:GLN:HE22	1.64	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:396:ALA:C	1:A:400:GLN:HB3	2.23	0.63
1:A:535:LEU:HD12	1:A:535:LEU:O	1.98	0.63
1:A:440:LEU:HD21	1:A:541:LEU:HD13	1.80	0.63
1:A:34:ALA:C	1:A:353:GLN:HE22	2.07	0.62
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:NZ	1:A:640:LYS:HB3	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:98:LYS:N	1:A:98:LYS:HD2	2.14	0.61
1:A:602:GLU:CB	1:A:642:LEU:HD11	2.31	0.61
1:A:212:MET:HE2	1:A:308:PHE:HA	1.83	0.61
1:A:440:LEU:C	1:A:440:LEU:HD12	2.25	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:596:LYS:HA	1:A:596:LYS:CE	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:131:LEU:HD21	1:A:194:ILE:CD1	2.32	0.60
1:A:137:PHE:N	1:A:138:PRO:HD2	2.16	0.60
1:A:659:THR:HG23	1:A:660:ILE:HD13	1.83	0.60
1:A:211:GLY:HA3	1:A:311:GLN:HE21	1.67	0.60
1:A:249:THR:HB	1:A:253:ALA:CB	2.32	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:53:ASP:O	1:A:329:LYS:NZ	2.30	0.59
1:A:344:LYS:HB2	1:A:381:PHE:CB	2.32	0.59
1:A:331:PHE:O	1:A:334:ILE:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:633:GLN:OE1	1:A:633:GLN:N	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: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:39:ASP:OD1	1:A:39:ASP:N	2.36	0.58
1:A:234:ALA:HB2	1:A:284:PHE:CZ	2.39	0.58
1:A:360:LEU:HD12	1:A:360:LEU:N	2.17	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:O	1:A:700:ARG:HG2	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:212:MET:CB	1:A:307:SER:HB2	2.34	0.57
1:A:238:PHE:CD1	1:A:241:THR:HG21	2.39	0.57
1:A:247:VAL:HG12	1:A:247:VAL:O	2.05	0.57
1:A:269:ASP:OD1	1:A:269:ASP:N	2.37	0.57
1:A:292:GLY:O	1:A:297:THR:OG1	2.18	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:96:ASN:CG	1:A:97:PRO:HD3	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LYS:O	1:A:353:GLN:HG3	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
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:404:VAL:CA	1:A:490:ASN:HD21	2.18	0.56
1:A:596:LYS:CE	1:A:596:LYS:CA	2.80	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:37:LEU:N	1:A:37:LEU:HD23	2.20	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:438:PHE:HA	1:A:441:ILE:HD12	1.87	0.56
1:A:453:LEU:HD13	1:A:460:ALA:C	2.31	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:337:ASP:O	1:A:338:LYS:HB2	2.04	0.56
1:A:579:TYR:OH	1:A:654:SER:OG	1.98	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:594:GLY:CA	1:A:598:LEU:HG	2.36	0.56
1:A:95:LYS:HZ1	1:A:184:PHE:HB2	1.70	0.55
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: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:558:PHE:HE1	1:A:562:ILE:HD11	1.71	0.55
1:A:437:SER:O	1:A:441:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:LEU:HD11	1:A:401:LYS:HB2	1.89	0.55
1:A:544:LEU:C	1:A:544:LEU:HD23	2.32	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:94:GLU:OE2	1:A:615:ASP:HA	2.07	0.55
1:A:154:LEU:C	1:A:154:LEU:HD12	2.32	0.55
1:A:404:VAL:HG13	1:A:490:ASN:HD21	1.72	0.55
1:A:71:ASP:HB2	1:A:137:PHE:HE2	1.72	0.54
1:A:453:LEU:HD12	1:A:461:GLN:HA	1.89	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:42:GLU:HB2	1:A:358:ARG:HG3	1.89	0.54
1:A:76:LEU:HA	1:A:79:PHE:HD2	1.73	0.54
1:A:235:PHE:CB	1:A:254:THR:HG21	2.38	0.54
1:A:615:ASP:HB3	1:A:618:ASN:HB2	1.88	0.54
1:A:35:ALA:CA	1:A:353:GLN:HE22	2.21	0.54
1:A:232:TRP:CA	1:A:251:TYR:HE1	2.21	0.54
1:A:396:ALA:CA	1:A:400:GLN:HB3	2.38	0.54
1:A:666:LEU:HD23	1:A:666:LEU:C	2.32	0.54
1:A:208:LEU:HG	1:A:311:GLN:HB3	1.89	0.54
1:A:219:ILE:HD12	1:A:219:ILE:O	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:590:LEU:HG	1:A:642:LEU:CD2	2.38	0.54
1:A:619:GLY:O	1:A:622:THR:HG22	2.09	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: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:507:ILE:CG1	1:A:537:ARG:HH22	2.17	0.53
1:A:267:ASN:CB	1:A:268:PRO:HD3	2.33	0.53
1:A:222:LEU:HD12	1:A:222:LEU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:PHE:O	1:A:611:PHE:CG	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: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
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:216:TYR:CD2	1:A:662:LEU:HD13	2.44	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: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:79:PHE:CA	1:A:82:LEU:CD1	2.87	0.52
1:A:250:SER:O	1:A:254:THR:HB	2.08	0.52
1:A:473:TRP:O	1:A:476:VAL:CG1	2.57	0.51
1:A:554:PHE:N	1:A:554:PHE:CD2	2.78	0.51
1:A:45:ILE:HD13	1:A:396:ALA:CB	2.38	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:444:PHE:HA	1:A:538:MET:HE1	1.92	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:O	1:A:128:LEU:HD23	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:89:GLN:N	1:A:90:PRO:HD2	2.26	0.51
1:A:143:GLY:HA3	1:A:146:ILE:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ILE:HD11	1:A:349:LYS:HZ2	1.75	0.51
1:A:527:GLY:HA2	1:A:530:ILE:CG2	2.40	0.51
1:A:580:CYS:HB2	1:A:620:MET:HE1	1.92	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
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:87:PHE:C	1:A:90:PRO:HD2	2.37	0.50
1:A:460:ALA:O	1:A:463:PRO:HD2	2.10	0.50
1:A:551:TYR:O	1:A:555:ILE:HG12	2.12	0.50
1:A:554:PHE:H	1:A:554:PHE:HD2	1.58	0.50
1:A:580:CYS:CB	1:A:620:MET:HE1	2.41	0.50
1:A:35:ALA:N	1:A:353:GLN:HE22	2.08	0.50
1:A:112:LEU:CB	1:A:113:PRO:HD2	2.41	0.50
1:A:42:GLU:HA	1:A:42:GLU:OE1	2.11	0.50
1:A:437:SER:O	1:A:440:LEU:HG	2.12	0.50
1:A:107:TYR:CZ	1:A:596:LYS:HE2	2.45	0.50
1:A:272:ILE:HG23	1:A:273:PRO:CD	2.32	0.50
1:A:453:LEU:CB	1:A:461:GLN:HB3	2.41	0.50
1:A:490:ASN:OD1	1:A:490:ASN:N	2.40	0.49
1:A:553:ALA:O	1:A:557:THR:OG1	2.08	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: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:619:GLY:C	1:A:622:THR:HG22	2.38	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ALA:HA	1:A:65:PHE:CD2	2.48	0.48
1:A:339:ASN:OD1	1:A:339:ASN:N	2.46	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:375:LEU:O	1:A:700:ARG:HD2	2.14	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: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:87:PHE:O	1:A:90:PRO:HG2	2.14	0.47
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:232:TRP:CB	1:A:251:TYR:HE1	2.27	0.47
1:A:589:GLY:C	1:A:590:LEU:HD22	2.39	0.47
1:A:91:LEU:O	1:A:115:LEU:HB2	2.14	0.47
1:A:508:VAL:HG23	1:A:509:ILE:N	2.29	0.47
1:A:615:ASP:OD1	1:A:616:TYR:N	2.47	0.47
1:A:71:ASP:HB2	1:A:137:PHE:CE2	2.48	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:456:GLU:OE1	1:A:456:GLU:HA	2.13	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:38:VAL:HG21	1:A:353:GLN:CD	2.40	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: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:511:GLU:HA	1:A:531:ARG:HH12	1.79	0.47
1:A:594:GLY:O	1:A:598:LEU:HB2	2.15	0.47
1:A:636:MET:HE2	1:A:653:VAL:HG23	1.96	0.47
1:A:428:ARG:HG2	1:A:486:TYR:HE1	1.77	0.47
1:A:590:LEU:C	1:A:614:ASN:OD1	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:212:MET:HE1	1:A:308:PHE:HB2	1.96	0.46
1:A:492:TRP:CD2	1:A:498:ARG:HD3	2.50	0.46
1:A:580:CYS:HB3	1:A:616:TYR:CE1	2.51	0.46
1:A:582:ILE:O	1:A:586:VAL:HG23	2.15	0.46
1:A:138:PRO:HB2	1:A:142:GLU:OE2	2.15	0.46
1:A:366:GLU:H	1:A:366:GLU:HG3	1.34	0.46
1:A:619:GLY:CA	1:A:622:THR:HG22	2.45	0.46
1:A:359:THR:HG21	1:A:400:GLN:CB	2.46	0.46
1:A:596:LYS:HZ2	1:A:596:LYS:CA	2.27	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:318:GLY:HA2	1:A:321:GLN:CD	2.40	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:404:VAL:CG1	1:A:490:ASN:HD21	2.29	0.46
1:A:433:GLY:HA2	1:A:436:ILE:CG1	2.45	0.46
1:A:590:LEU:N	1:A:590:LEU:HD13	2.31	0.46
1:A:238:PHE:C	1:A:241:THR:HG22	2.40	0.46
1:A:353:GLN:HG3	1:A:353:GLN:H	1.40	0.46
1:A:473:TRP:O	1:A:474:ILE:C	2.59	0.46
1:A:510:GLY:C	1:A:531:ARG:NH1	2.74	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:278:SER:O	1:A:281:SER:OG	2.29	0.45
1:A:348:ILE:HG13	1:A:349:LYS:N	2.30	0.45
1:A:373:ASP:OD1	1:A:373:ASP:C	2.59	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HD11	1:A:657:VAL:CG1	2.45	0.45
1:A:650:THR:O	1:A:651:TYR:C	2.59	0.45
1:A:43:ASP:C	1:A:326:MET:HE1	2.41	0.45
1:A:61:ALA:CA	1:A:65:PHE:HD2	2.29	0.45
1:A:603:LEU:HG	1:A:610:LEU:HD23	1.97	0.45
1:A:96:ASN:N	1:A:97:PRO:CD	2.79	0.45
1:A:299:LEU:HD12	1:A:299:LEU:C	2.41	0.45
1:A:397:LEU:HA	1:A:397:LEU:HD12	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:286:VAL:CG2	1:A:287:LEU:N	2.79	0.45
1:A:61:ALA:O	1:A:65:PHE:HB3	2.16	0.45
1:A:79:PHE:C	1:A:82:LEU:HD12	2.41	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:151:ARG:O	1:A:154:LEU:HG	2.16	0.45
1:A:511:GLU:CG	1:A:531:ARG:HH11	2.30	0.45
1:A:609:LEU:C	1:A:611:PHE:H	2.25	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:96:ASN:O	1:A:99:PRO:HD2	2.16	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: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:583:GLY:HA3	1:A:613:PHE:CE1	2.53	0.44
1:A:596:LYS:HA	1:A:596:LYS:HD3	1.41	0.44
1:A:305:TYR:HE1	1:A:309:LYS:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:595:ASN:C	1:A:596:LYS:HZ2	2.25	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:CB	1:A:596:LYS:NZ	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:CD1	1:A:652:PHE:N	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
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:358:ARG:HA	1:A:358:ARG:HD3	1.54	0.43
1:A:534:LEU:N	1:A:534:LEU:HD22	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:64:TYR:CD1	1:A:64:TYR:N	2.86	0.43
1:A:355:THR:HG23	1:A:356:ASN:N	2.34	0.43
1:A:94:GLU:C	1:A:97:PRO:HD2	2.44	0.43
1:A:217:LEU:HD23	1:A:217:LEU:HA	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:676:PHE:HD1	1:A:679:LEU:HD12	1.84	0.43
1:A:95:LYS:HD3	1:A:95:LYS:HA	1.74	0.43
1:A:231:SER:HA	1:A:258:MET:HG3	2.00	0.43
1:A:263:THR:CG2	1:A:629:MET:HE1	2.49	0.43
1:A:360:LEU:H	1:A:360:LEU:CD1	2.20	0.43
1:A:463:PRO:HG2	1:A:464:TRP:HD1	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LEU:HD13	1:A:461:GLN:N	2.34	0.42
1:A:52:LEU:HD11	1:A:141:TYR:O	2.19	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:51:ILE:HG22	1:A:51:ILE:O	2.17	0.42
1:A:132:LEU:HD22	1:A:132:LEU:HA	1.76	0.42
1:A:594:GLY:HA3	1:A:598:LEU:CG	2.44	0.42
1:A:79:PHE:CA	1:A:82:LEU:HD12	2.49	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: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:622:THR:HG23	1:A:623:LEU:N	2.33	0.42
1:A:228:LEU:C	1:A:251:TYR:OH	2.62	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
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:535:LEU:HD12	1:A:535:LEU:C	2.44	0.41
1:A:38:VAL:CG2	1:A:353:GLN:CD	2.94	0.41
1:A:286:VAL:CG2	1:A:287:LEU:H	2.31	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:290:LEU:HD23	1:A:290:LEU:C	2.45	0.41
1:A:413:GLN:C	1:A:414:ILE:HG13	2.45	0.41
1:A:464:TRP:CD1	1:A:464:TRP:H	2.37	0.41
1:A:468:GLU:O	1:A:471:PHE:HB2	2.21	0.41
1:A:500:ASP:CG	1:A:540:ARG:NH1	2.79	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:620:MET:CA	1:A:620:MET:HE2	2.49	0.41
1:A:128:LEU:HD13	1:A:167:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:596:LYS:HA	1:A:596:LYS:HE3	1.97	0.41
1:A:605:GLU:CG	1:A:606:ASP:N	2.81	0.41
1:A:71:ASP:O	1:A:71:ASP:OD1	2.38	0.41
1:A:237:MET:CE	3:A:808:PLM:H81	2.51	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: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:629:MET:HE3	1:A:629:MET:HB3	1.91	0.41
1:A:82:LEU:HD23	1:A:198:SER:CB	2.51	0.41
1:A:90:PRO:CA	1:A:616:TYR:HD2	2.25	0.41
1:A:603:LEU:CB	1:A:607:ASP:HB2	2.51	0.41
1:A:640:LYS:HB3	1:A:640:LYS:HZ2	1.86	0.41
1:A:31:PHE:CD1	1:A:60:SER:O	2.74	0.40
1:A:189:TYR:H	1:A:189:TYR:HD1	1.69	0.40
1:A:530:ILE:HG23	1:A:531:ARG:HH21	1.86	0.40
1:A:72:LEU:C	1:A:75:SER:H	2.27	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: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: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:473:TRP:C	1:A:476:VAL:HG12	2.47	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	637/723 (88%)	585 (92%)	44 (7%)	8 (1%)	9	29

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%)	474 (83%)	96 (17%)	2	6

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	39	ASP
1	A	50	GLU
1	A	54	GLN
1	A	66	ILE
1	A	82	LEU
1	A	92	TRP
1	A	93	CYS
1	A	98	LYS
1	A	100	SER
1	A	101	CYS

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Mol	Chain	Res	Type
1	A	102	LYS
1	A	109	LEU
1	A	112	LEU
1	A	116	THR
1	A	122	ILE
1	A	132	LEU
1	A	135	THR
1	A	154	LEU
1	A	156	LYS
1	A	165	VAL
1	A	197	LEU
1	A	198	SER
1	A	201	GLU
1	A	204	ASP
1	A	206	LEU
1	A	208	LEU
1	A	209	LEU
1	A	210	SER
1	A	215	THR
1	A	219	ILE
1	A	222	LEU
1	A	228	LEU
1	A	236	VAL
1	A	239	GLU
1	A	243	GLN
1	A	250	SER
1	A	254	THR
1	A	255	LEU
1	A	269	ASP
1	A	272	ILE
1	A	281	SER
1	A	287	LEU
1	A	307	SER
1	A	311	GLN
1	A	321	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

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Mol	Chain	Res	Type
1	A	371	ILE
1	A	383	ILE
1	A	384	ASN
1	A	391	LEU
1	A	416	HIS
1	A	440	LEU
1	A	445	ILE
1	A	455	ILE
1	A	466	VAL
1	A	470	VAL
1	A	477	LEU
1	A	483	ILE
1	A	485	THR
1	A	488	PHE
1	A	490	ASN
1	A	504	THR
1	A	507	ILE
1	A	535	LEU
1	A	540	ARG
1	A	542	ILE
1	A	544	LEU
1	A	554	PHE
1	A	560	THR
1	A	572	ILE
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
1	A	628	VAL
1	A	634	VAL
1	A	636	MET
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

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Mol	Chain	Res	Type
1	A	691	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	218	ASN
1	A	243	GLN
1	A	267	ASN
1	A	353	GLN
1	A	393	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 oligosaccharides 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	-	17,17,17	0.61	0	17,17,17	0.64	0
4	66R	A	809	-	42,43,43	2.42	13 (30%)	57,62,62	1.66	11 (19%)

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	-	-	8/15/15/15	-
4	66R	A	809	-	-	10/18/40/40	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	809	66R	C14-N11	-8.82	1.30	1.47
4	A	809	66R	C30-C31	-5.11	1.35	1.41
4	A	809	66R	C02-N08	5.04	1.52	1.41
4	A	809	66R	C14-C15	4.70	1.59	1.51
4	A	809	66R	C25-N26	3.57	1.51	1.47
4	A	809	66R	C10-N11	-3.18	1.38	1.46
4	A	809	66R	C12-N11	-3.11	1.38	1.46
4	A	809	66R	C22-C23	-2.91	1.32	1.36
4	A	809	66R	C33-C31	2.85	1.44	1.39
4	A	809	66R	O37-C16	2.74	1.41	1.37
4	A	809	66R	C36-C30	2.27	1.43	1.39
4	A	809	66R	C30-C23	2.16	1.48	1.44
4	A	809	66R	C31-N32	-2.00	1.35	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	809	66R	C25-C24-C23	5.25	113.92	108.24
4	A	809	66R	F07-C03-C02	4.30	122.47	118.37
4	A	809	66R	C13-N08-C02	3.35	124.14	116.19
4	A	809	66R	C03-C02-N08	2.83	123.72	120.42
4	A	809	66R	O37-C16-C15	2.76	120.07	115.96
4	A	809	66R	C01-C02-N08	-2.65	118.27	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	809	66R	O37-C16-C17	-2.34	120.35	124.30
4	A	809	66R	C24-C23-C30	2.28	133.97	130.85
4	A	809	66R	C33-C31-C30	-2.22	120.04	122.19
4	A	809	66R	C13-N08-C09	-2.17	106.67	111.57
4	A	809	66R	O29-C27-C25	2.02	120.36	113.51

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	809	66R	N26-C25-C27-O29
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
4	A	809	66R	N26-C25-C27-O28
3	A	808	PLM	C6-C7-C8-C9
3	A	808	PLM	C2-C3-C4-C5
4	A	809	66R	C24-C25-C27-O28
4	A	809	66R	C24-C25-C27-O29
3	A	808	PLM	C7-C8-C9-CA
4	A	809	66R	C18-C19-C21-C22
4	A	809	66R	C20-C19-C21-C22
3	A	808	PLM	CB-CC-CD-CE

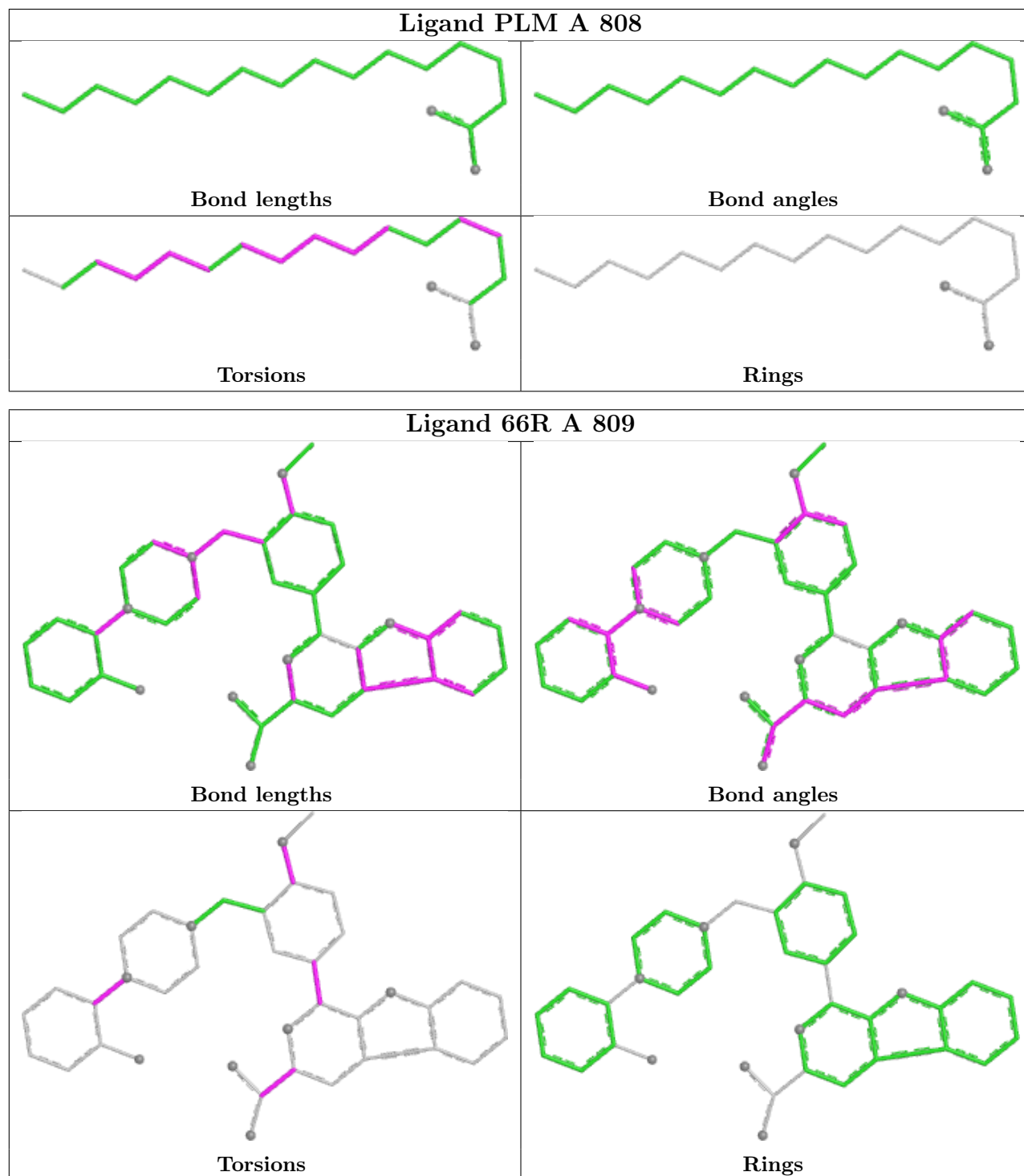
There are no ring outliers.

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%)	2.47	351 (54%) 0 0	39, 103, 201, 344	0

All (351) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	TRP	11.1
1	A	39	ASP	10.7
1	A	380	ASP	10.5
1	A	57	PHE	9.8
1	A	184	PHE	9.7
1	A	529	TRP	9.4
1	A	110	GLY	9.2
1	A	356	ASN	8.4
1	A	607	ASP	8.4
1	A	473	TRP	7.9
1	A	417	SER	7.9
1	A	65	PHE	7.7
1	A	107	TYR	7.7
1	A	248	PHE	7.6
1	A	73	ILE	7.3
1	A	687	CYS	7.1
1	A	537	ARG	7.0
1	A	170	ASP	6.8
1	A	415	TYR	6.7
1	A	379	ARG	6.6
1	A	399	PHE	6.6
1	A	691	ASP	6.5
1	A	113	PRO	6.4
1	A	75	SER	6.3
1	A	461	GLN	6.2
1	A	525	SER	6.1
1	A	49	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	524	PHE	5.9
1	A	277	SER	5.8
1	A	517	THR	5.7
1	A	250	SER	5.6
1	A	610	LEU	5.6
1	A	363	ILE	5.6
1	A	527	GLY	5.5
1	A	84	LEU	5.5
1	A	79	PHE	5.5
1	A	86	PHE	5.5
1	A	235	PHE	5.5
1	A	97	PRO	5.5
1	A	696	ARG	5.5
1	A	117	ASN	5.5
1	A	112	LEU	5.4
1	A	423	LEU	5.4
1	A	47	LEU	5.4
1	A	108	TYR	5.3
1	A	46	GLY	5.2
1	A	403	GLU	5.2
1	A	31	PHE	5.2
1	A	387	GLU	5.2
1	A	70	LEU	5.2
1	A	357	TYR	5.1
1	A	381	PHE	5.1
1	A	105	ASP	5.1
1	A	35	ALA	5.1
1	A	416	HIS	5.0
1	A	475	TYR	5.0
1	A	458	SER	5.0
1	A	51	ILE	5.0
1	A	404	VAL	5.0
1	A	50	GLU	4.9
1	A	111	GLU	4.8
1	A	375	LEU	4.8
1	A	518	PRO	4.8
1	A	606	ASP	4.8
1	A	67	PHE	4.8
1	A	462	LYS	4.7
1	A	421	GLN	4.7
1	A	197	LEU	4.7
1	A	171	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	324	ARG	4.6
1	A	418	ALA	4.6
1	A	306	ASP	4.6
1	A	63	TYR	4.6
1	A	364	SER	4.6
1	A	368	PHE	4.5
1	A	382	LYS	4.5
1	A	267	ASN	4.5
1	A	426	PHE	4.4
1	A	692	SER	4.4
1	A	489	GLU	4.4
1	A	99	PRO	4.4
1	A	526	ASN	4.3
1	A	106	TYR	4.3
1	A	76	LEU	4.3
1	A	341	GLU	4.3
1	A	549	GLN	4.3
1	A	689	GLY	4.2
1	A	66	ILE	4.2
1	A	608	TYR	4.2
1	A	595	ASN	4.1
1	A	36	ALA	4.1
1	A	95	LYS	4.0
1	A	468	GLU	4.0
1	A	490	ASN	4.0
1	A	605	GLU	4.0
1	A	611	PHE	4.0
1	A	144	SER	3.9
1	A	602	GLU	3.9
1	A	347	CYS	3.9
1	A	148	TRP	3.9
1	A	200	ARG	3.9
1	A	419	LEU	3.8
1	A	402	GLU	3.8
1	A	92	TRP	3.8
1	A	45	ILE	3.8
1	A	64	TYR	3.8
1	A	72	LEU	3.8
1	A	360	LEU	3.8
1	A	613	PHE	3.8
1	A	115	LEU	3.8
1	A	425	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	702	ALA	3.8
1	A	401	LYS	3.7
1	A	391	LEU	3.7
1	A	434	TYR	3.7
1	A	239	GLU	3.7
1	A	40	LEU	3.7
1	A	333	LEU	3.7
1	A	440	LEU	3.7
1	A	104	ARG	3.7
1	A	530	ILE	3.7
1	A	459	SER	3.7
1	A	406	SER	3.7
1	A	30	PRO	3.6
1	A	407	LEU	3.6
1	A	550	ARG	3.6
1	A	509	ILE	3.6
1	A	378	THR	3.6
1	A	249	THR	3.6
1	A	514	THR	3.6
1	A	614	ASN	3.6
1	A	697	ASN	3.6
1	A	430	PRO	3.6
1	A	598	LEU	3.6
1	A	151	ARG	3.5
1	A	245	LEU	3.5
1	A	376	ASP	3.5
1	A	96	ASN	3.5
1	A	362	LYS	3.5
1	A	103	ASP	3.5
1	A	484	TYR	3.5
1	A	137	PHE	3.5
1	A	37	LEU	3.5
1	A	48	PRO	3.5
1	A	594	GLY	3.4
1	A	703	GLY	3.4
1	A	173	TYR	3.4
1	A	77	ASN	3.4
1	A	597	LYS	3.4
1	A	366	GLU	3.4
1	A	414	ILE	3.3
1	A	695	LYS	3.3
1	A	536	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	393	GLN	3.3
1	A	469	PHE	3.3
1	A	451	THR	3.3
1	A	372	PHE	3.3
1	A	700	ARG	3.3
1	A	532	TYR	3.3
1	A	615	ASP	3.3
1	A	201	GLU	3.3
1	A	52	LEU	3.3
1	A	477	LEU	3.3
1	A	89	GLN	3.3
1	A	358	ARG	3.2
1	A	560	THR	3.2
1	A	169	VAL	3.2
1	A	343	ASP	3.2
1	A	202	LEU	3.2
1	A	38	VAL	3.2
1	A	645	THR	3.2
1	A	328	GLU	3.2
1	A	146	ILE	3.2
1	A	386	ASP	3.2
1	A	33	LYS	3.2
1	A	361	PRO	3.2
1	A	100	SER	3.1
1	A	680	ASP	3.1
1	A	88	GLU	3.1
1	A	102	LYS	3.1
1	A	513	ALA	3.1
1	A	612	ASN	3.1
1	A	120	SER	3.1
1	A	405	PRO	3.1
1	A	631	ASN	3.0
1	A	244	GLY	3.0
1	A	257	GLN	3.0
1	A	236	VAL	3.0
1	A	505	TRP	3.0
1	A	140	SER	3.0
1	A	465	GLN	3.0
1	A	508	VAL	3.0
1	A	599	PHE	3.0
1	A	555	ILE	3.0
1	A	701	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	494	GLU	3.0
1	A	541	LEU	3.0
1	A	118	ALA	3.0
1	A	554	PHE	3.0
1	A	698	ARG	2.9
1	A	647	TRP	2.9
1	A	123	TYR	2.9
1	A	218	ASN	2.9
1	A	454	ASP	2.9
1	A	133	VAL	2.9
1	A	686	LYS	2.9
1	A	392	CYS	2.9
1	A	43	ASP	2.9
1	A	204	ASP	2.8
1	A	55	SER	2.8
1	A	56	SER	2.8
1	A	109	LEU	2.8
1	A	132	LEU	2.8
1	A	319	MET	2.8
1	A	94	GLU	2.8
1	A	699	ARG	2.8
1	A	345	ASN	2.8
1	A	152	LEU	2.8
1	A	463	PRO	2.8
1	A	438	PHE	2.8
1	A	370	LEU	2.8
1	A	344	LYS	2.8
1	A	279	ARG	2.8
1	A	621	VAL	2.8
1	A	78	TYR	2.8
1	A	114	TYR	2.8
1	A	618	ASN	2.8
1	A	472	GLY	2.8
1	A	93	CYS	2.7
1	A	141	TYR	2.7
1	A	264	THR	2.7
1	A	367	GLU	2.7
1	A	431	ASN	2.7
1	A	383	ILE	2.7
1	A	486	TYR	2.7
1	A	90	PRO	2.7
1	A	71	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	222	LEU	2.7
1	A	460	ALA	2.6
1	A	377	ASP	2.6
1	A	61	ALA	2.6
1	A	400	GLN	2.6
1	A	478	GLU	2.6
1	A	390	ASP	2.6
1	A	629	MET	2.6
1	A	385	LYS	2.6
1	A	125	VAL	2.6
1	A	172	LEU	2.6
1	A	435	ALA	2.6
1	A	493	ARG	2.6
1	A	589	GLY	2.6
1	A	690	GLN	2.6
1	A	496	ALA	2.6
1	A	198	SER	2.5
1	A	620	MET	2.5
1	A	53	ASP	2.5
1	A	136	PHE	2.5
1	A	533	LEU	2.5
1	A	251	TYR	2.5
1	A	457	GLU	2.5
1	A	191	ARG	2.5
1	A	577	CYS	2.5
1	A	596	LYS	2.5
1	A	327	LEU	2.5
1	A	455	ILE	2.5
1	A	575	VAL	2.5
1	A	131	LEU	2.4
1	A	603	LEU	2.4
1	A	436	ILE	2.4
1	A	487	GLY	2.4
1	A	265	SER	2.4
1	A	304	VAL	2.4
1	A	506	VAL	2.4
1	A	150	SER	2.4
1	A	203	ARG	2.4
1	A	98	LYS	2.4
1	A	683	GLU	2.4
1	A	672	LEU	2.4
1	A	139	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	331	PHE	2.4
1	A	389	ALA	2.4
1	A	32	GLN	2.4
1	A	601	THR	2.4
1	A	693	GLN	2.4
1	A	424	ARG	2.3
1	A	482	LYS	2.3
1	A	243	GLN	2.3
1	A	134	HIS	2.3
1	A	470	VAL	2.3
1	A	688	GLN	2.3
1	A	502	LEU	2.3
1	A	135	THR	2.3
1	A	371	ILE	2.3
1	A	211	GLY	2.3
1	A	619	GLY	2.3
1	A	515	PHE	2.3
1	A	349	LYS	2.3
1	A	185	ARG	2.3
1	A	270	VAL	2.3
1	A	617	PRO	2.3
1	A	573	PHE	2.2
1	A	240	ASP	2.2
1	A	659	THR	2.2
1	A	143	GLY	2.2
1	A	318	GLY	2.2
1	A	164	PHE	2.2
1	A	673	GLU	2.2
1	A	674	ALA	2.2
1	A	298	ASN	2.2
1	A	315	GLN	2.2
1	A	359	THR	2.2
1	A	83	PHE	2.2
1	A	234	ALA	2.2
1	A	682	GLU	2.2
1	A	85	ASN	2.2
1	A	355	THR	2.2
1	A	255	LEU	2.2
1	A	34	ALA	2.2
1	A	297	THR	2.2
1	A	101	CYS	2.2
1	A	488	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	616	TYR	2.2
1	A	163	LEU	2.2
1	A	42	GLU	2.2
1	A	373	ASP	2.1
1	A	590	LEU	2.1
1	A	44	GLY	2.1
1	A	263	THR	2.1
1	A	325	ARG	2.1
1	A	428	ARG	2.1
1	A	413	GLN	2.1
1	A	266	ASN	2.1
1	A	121	ILE	2.1
1	A	275	TYR	2.1
1	A	310	GLU	2.1
1	A	442	ILE	2.1
1	A	567	PRO	2.1
1	A	535	LEU	2.1
1	A	369	GLY	2.1
1	A	499	PHE	2.1
1	A	398	ARG	2.1
1	A	129	ALA	2.1
1	A	272	ILE	2.1
1	A	474	ILE	2.1
1	A	635	TRP	2.1
1	A	142	GLU	2.1
1	A	694	GLU	2.1
1	A	671	VAL	2.0
1	A	213	LEU	2.0
1	A	340	GLY	2.0
1	A	445	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

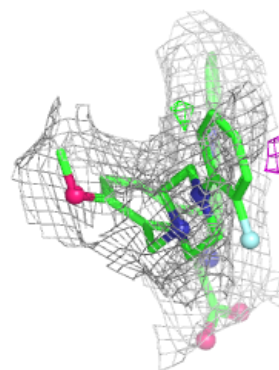
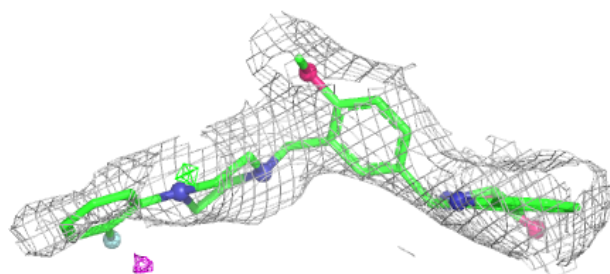
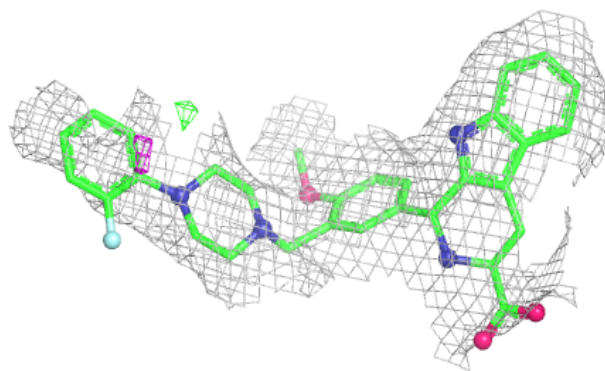
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	66R	A	809	38/38	0.80	0.25	109,137,162,185	0
2	CA	A	802	1/1	0.81	0.12	154,154,154,154	0
3	PLM	A	808	18/18	0.83	0.19	54,86,138,183	0
2	CA	A	807	1/1	0.84	0.13	140,140,140,140	0
2	CA	A	804	1/1	0.85	0.09	112,112,112,112	0
2	CA	A	801	1/1	0.88	0.20	117,117,117,117	0
2	CA	A	806	1/1	0.93	0.10	147,147,147,147	0
2	CA	A	803	1/1	0.94	0.15	57,57,57,57	0
2	CA	A	805	1/1	0.94	0.18	153,153,153,153	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.

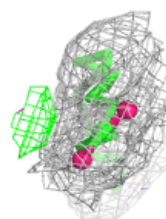
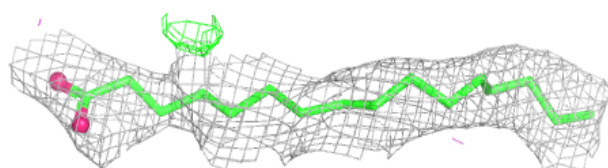
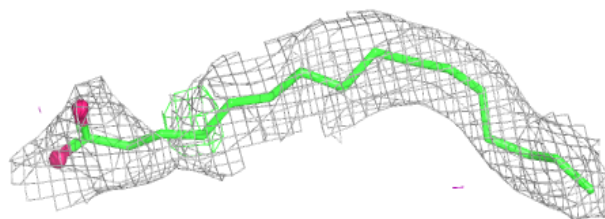
Electron density around 66R A 809:

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.