



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:41 pm BST

PDB ID : 4LLH
Title : Substrate bound outward-open state of the symporter BetP
Authors : Perez, C.; Faust, B.; Ziegler, C.
Deposited on : 2013-07-09
Resolution : 2.80 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

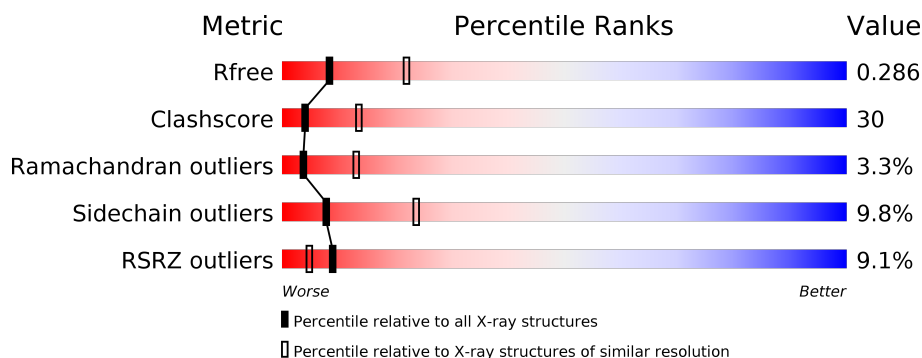
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	566	<div> <div>9%</div> <div>47%</div> <div>35%</div> <div>9%</div> <div>7%</div> </div>
1	B	566	<div> <div>9%</div> <div>40%</div> <div>40%</div> <div>6%</div> <div>13%</div> </div>
1	C	566	<div> <div>7%</div> <div>45%</div> <div>38%</div> <div>•</div> <div>13%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CM5	C	602	X	-	-	-
5	CM5	C	604	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11589 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.

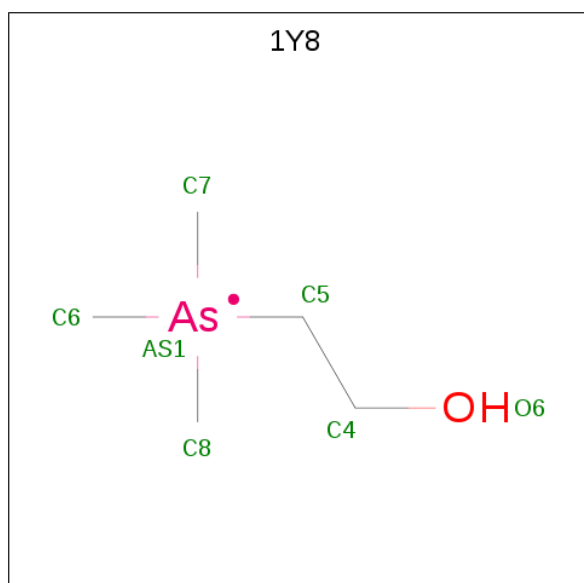
- Molecule 1 is a protein called Glycine betaine transporter BetP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			4001	2625	661	699	16			
1	B	492	Total	C	N	O	S	0	0	0
			3701	2443	590	652	16			
1	C	490	Total	C	N	O	S	0	0	0
			3704	2451	587	650	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLY	ENGINEERED MUTATION	UNP P54582
B	153	ASP	GLY	ENGINEERED MUTATION	UNP P54582
C	153	ASP	GLY	ENGINEERED MUTATION	UNP P54582

- Molecule 2 is 2-(trimethyl-lambda 5 -arsanyl)ethanol (three-letter code: 1Y8) (formula: C₅H₁₄AsO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	As	C	O	0	0
			7	1	5	1		
2	B	1	Total	As	C	O	0	0
			7	1	5	1		
2	C	1	Total	As	C	O	0	0
			7	1	5	1		

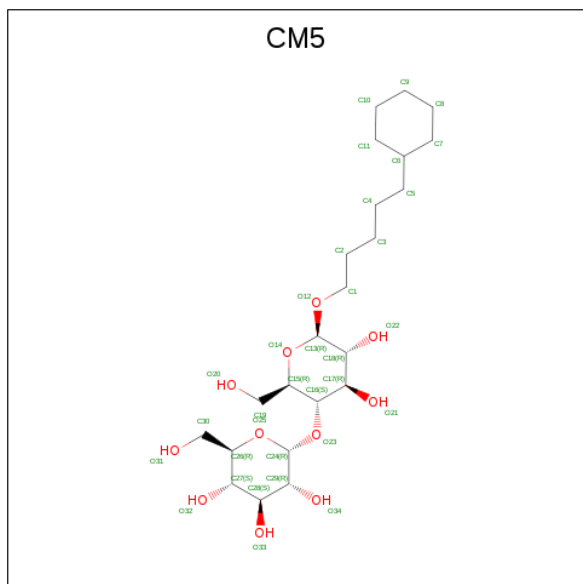
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSE (three-letter code: CM5) (formula: C₂₃H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			34	23	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			34	23	11		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total	O	0	0
			25	25		
6	B	26	Total	O	0	0
			26	26		
6	C	40	Total	O	0	0
			40	40		

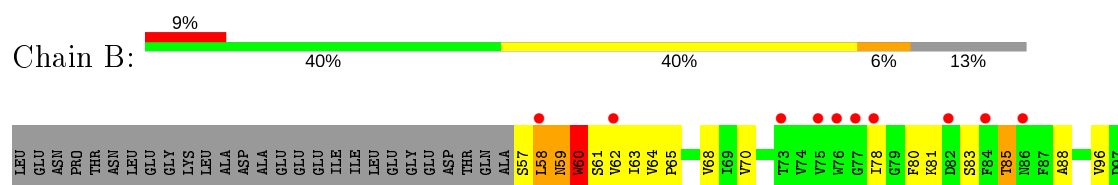
3 Residue-property plots

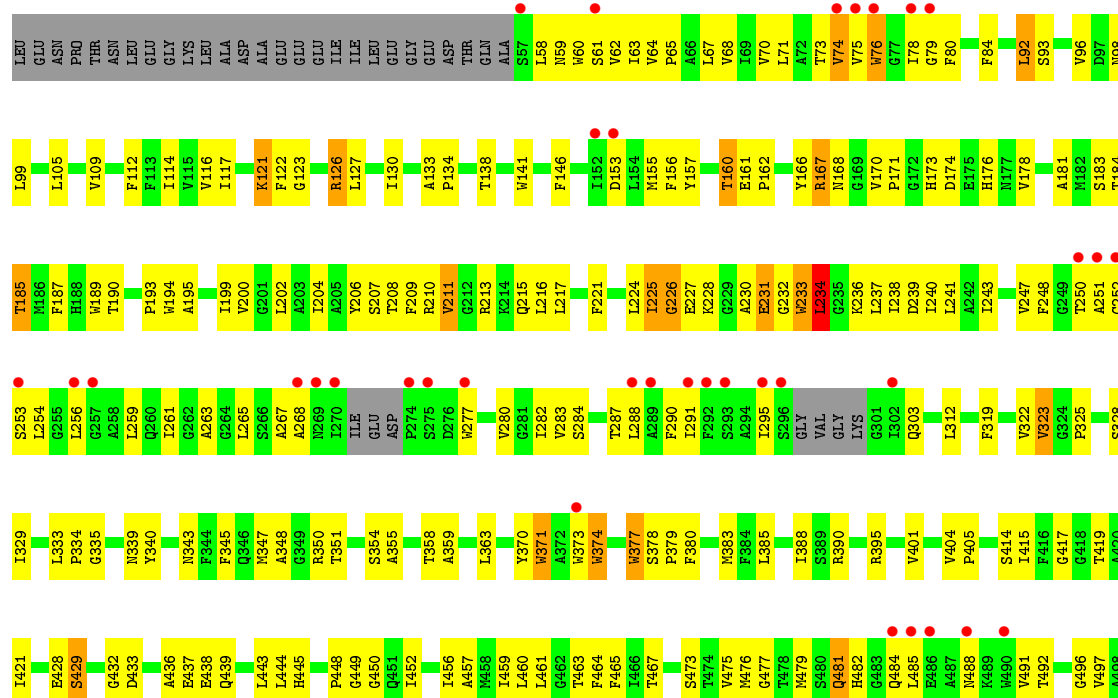
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



• Molecule 1: Glycine betaine transporter BetP







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.47Å 129.69Å 164.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.30 – 2.80 36.33 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.5 (36.30-2.80) 75.8 (36.33-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.73 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.240 , 0.290 0.237 , 0.286	Depositor DCC
R_{free} test set	2350 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 74.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	11589	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CM5, 1Y8, CL

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	0.24	0/4102	0.42	0/5584
1	B	0.24	0/3798	0.41	0/5184
1	C	0.25	0/3801	0.41	0/5186
All	All	0.24	0/11701	0.41	0/15954

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 ⓘ

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	4001	0	4032	240	0
1	B	3701	0	3723	260	0
1	C	3704	0	3730	200	0
2	A	7	0	3	0	0
2	B	7	0	3	2	0
2	C	7	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	C	1	0	0	1	0
5	C	68	0	84	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	25	0	0	3	0
6	B	26	0	0	3	0
6	C	40	0	0	5	0
All	All	11589	0	11578	693	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 30.

All (693) 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:141:TRP:HD1	1:A:388:ILE:HG22	1.30	0.94
1:A:295:ILE:HG22	1:A:296:SER:H	1.33	0.93
1:A:297:GLY:HA3	1:A:300:LYS:H	1.37	0.90
5:C:604:CM5:H17	5:C:604:CM5:H29	1.54	0.90
1:A:162:PRO:HG2	1:A:417:GLY:HA3	1.55	0.88
1:A:260:GLN:HE21	1:A:437:GLU:HG3	1.36	0.88
1:B:222:VAL:HG13	1:B:227:GLU:HA	1.56	0.87
1:C:78:ILE:HD12	1:C:79:GLY:H	1.38	0.87
1:A:160:THR:HB	1:A:439:GLN:NE2	1.89	0.86
1:A:211:VAL:HG11	1:A:213:ARG:HE	1.41	0.86
1:B:59:ASN:HA	1:B:60:TRP:CB	2.04	0.86
5:C:604:CM5:H11	5:C:604:CM5:O22	1.75	0.85
1:C:114:ILE:HD13	1:C:199:ILE:HD13	1.58	0.84
1:B:59:ASN:HA	1:B:60:TRP:CG	2.12	0.84
1:C:252:CYS:HB2	1:C:522:THR:HG21	1.59	0.82
1:A:248:PHE:HB3	1:A:522:THR:HG22	1.62	0.82
1:A:540:LEU:O	1:A:544:LEU:HB2	1.80	0.81
1:C:290:PHE:CE2	1:C:496:GLY:HA3	2.16	0.81
1:B:225:ILE:HG22	1:B:226:GLY:H	1.45	0.80
1:A:153:ASP:O	1:A:157:TYR:HB2	1.81	0.79
1:A:214:LYS:HD2	1:A:214:LYS:H	1.47	0.79
1:B:271:ILE:HG12	1:B:272:GLU:HA	1.62	0.79
1:C:64:VAL:HG13	1:C:65:PRO:HD3	1.65	0.78
1:A:305:LEU:HD12	1:A:466:ILE:HD11	1.63	0.78
1:A:329:ILE:HG21	1:A:415:ILE:HG22	1.65	0.78
1:C:237:LEU:O	1:C:240:ILE:HG22	1.84	0.78
1:A:63:ILE:HG13	1:A:495:TRP:CZ2	2.19	0.77
1:A:295:ILE:HG22	1:A:296:SER:N	1.98	0.77
1:C:225:ILE:HG23	1:C:226:GLY:H	1.47	0.77
1:C:354:SER:O	1:C:359:ALA:HB3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:TRP:CH2	1:B:389:SER:HB3	2.20	0.76
1:C:225:ILE:HG23	1:C:226:GLY:N	2.00	0.76
1:B:183:SER:OG	1:B:339:ASN:HB3	1.86	0.76
1:B:59:ASN:HA	1:B:60:TRP:CD1	2.21	0.76
1:A:63:ILE:HG13	1:A:495:TRP:HZ2	1.51	0.75
1:A:379:PRO:HG3	1:A:529:PHE:CE2	2.22	0.74
1:B:101:TRP:HA	1:B:104:ILE:HD11	1.69	0.74
1:C:232:GLY:O	1:C:236:LYS:HB3	1.87	0.74
1:B:530:LEU:O	1:B:534:ILE:HG12	1.88	0.74
1:B:162:PRO:HG2	1:B:417:GLY:HA3	1.70	0.73
1:B:70:VAL:HG23	1:B:248:PHE:CE1	2.23	0.73
1:C:225:ILE:CG2	1:C:226:GLY:H	2.01	0.73
1:B:453:MET:SD	1:B:456:ILE:HD11	2.28	0.73
5:C:604:CM5:C17	5:C:604:CM5:H29	2.18	0.72
1:B:144:MET:HG2	1:B:303:GLN:OE1	1.89	0.72
1:C:184:THR:HA	1:C:347:MET:CE	2.20	0.72
1:A:292:PHE:HA	1:A:293:SER:C	2.10	0.72
1:A:292:PHE:HA	1:A:293:SER:O	1.89	0.72
1:A:248:PHE:HB3	1:A:522:THR:CG2	2.18	0.72
1:A:332:LEU:HD13	1:B:353:MET:HG3	1.71	0.72
1:C:417:GLY:O	1:C:421:ILE:HG12	1.90	0.72
1:A:202:LEU:HD22	1:A:540:LEU:HD21	1.70	0.72
1:A:415:ILE:O	1:A:419:THR:HG23	1.91	0.71
1:B:161:GLU:HB3	1:B:162:PRO:HD3	1.71	0.71
1:C:243:ILE:O	1:C:247:VAL:HG23	1.91	0.71
1:A:527:THR:N	1:A:528:PRO:HD2	2.06	0.71
1:B:151:GLY:H	2:B:601:1Y8:H1	1.55	0.71
1:B:247:VAL:HG13	1:B:499:THR:HG22	1.72	0.71
1:B:59:ASN:CA	1:B:60:TRP:HB3	2.20	0.70
1:B:203:ALA:HA	1:B:540:LEU:HD13	1.74	0.70
1:C:64:VAL:CG1	1:C:65:PRO:HD3	2.22	0.70
1:C:67:LEU:HA	1:C:70:VAL:HG12	1.73	0.70
1:C:211:VAL:HG12	1:C:213:ARG:HG3	1.72	0.69
1:A:160:THR:HB	1:A:439:GLN:HE21	1.55	0.69
1:B:285:VAL:O	1:B:289:ALA:HB2	1.91	0.69
1:A:295:ILE:CG2	1:A:296:SER:H	2.05	0.69
1:B:141:TRP:O	1:B:145:MET:HG3	1.93	0.69
1:B:384:PHE:O	1:B:388:ILE:HG12	1.93	0.69
1:B:265:LEU:HB3	1:B:269:ASN:HB3	1.74	0.68
1:B:63:ILE:HD11	1:B:480:SER:HB2	1.74	0.68
1:B:64:VAL:HB	1:B:65:PRO:HD3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:THR:HA	1:B:466:ILE:HG22	1.75	0.68
1:C:239:ASP:O	1:C:243:ILE:HG12	1.94	0.68
1:C:343:ASN:O	1:C:347:MET:HG3	1.93	0.68
1:B:280:VAL:HG22	1:B:504:LEU:HD21	1.75	0.68
1:B:60:TRP:O	1:B:60:TRP:HD1	1.77	0.68
1:C:60:TRP:O	1:C:64:VAL:HG12	1.93	0.68
1:C:415:ILE:O	1:C:419:THR:HG23	1.94	0.68
1:B:211:VAL:HG21	1:B:213:ARG:HH21	1.57	0.67
1:B:59:ASN:HA	1:B:60:TRP:HB3	1.75	0.67
1:A:518:LEU:O	1:A:522:THR:HG23	1.94	0.67
1:C:184:THR:HA	1:C:347:MET:HE1	1.76	0.67
1:A:203:ALA:HA	1:A:540:LEU:HD23	1.76	0.67
1:C:227:GLU:C	1:C:228:LYS:HD2	2.14	0.67
1:C:457:ALA:O	1:C:461:LEU:HD13	1.95	0.67
1:A:375:ILE:HD13	1:A:530:LEU:HA	1.76	0.66
1:B:161:GLU:HG2	1:B:185:THR:HG23	1.77	0.66
1:A:211:VAL:HG11	1:A:213:ARG:NE	2.08	0.66
1:B:122:PHE:O	1:B:125:ILE:HG23	1.95	0.66
1:B:193:PRO:HB3	1:B:374:TRP:CD2	2.31	0.66
1:A:139:VAL:HG23	1:A:140:SER:H	1.61	0.65
1:A:210:ARG:HH22	1:A:549:ILE:HD12	1.62	0.65
1:C:380:PHE:HD1	1:C:475:VAL:HG21	1.61	0.65
1:B:475:VAL:O	1:B:479:MET:HG2	1.97	0.65
1:C:155:MET:HE3	1:C:464:PHE:HE2	1.62	0.64
1:A:387:ARG:C	1:A:389:SER:H	2.01	0.64
1:C:74:VAL:HG13	1:C:502:ILE:HG22	1.79	0.64
1:A:311:VAL:O	1:A:315:LEU:HB2	1.98	0.64
1:A:136:PHE:CD1	1:A:388:ILE:HA	2.33	0.64
1:A:502:ILE:HG22	1:A:506:LEU:HD23	1.80	0.64
1:C:283:VAL:O	1:C:287:THR:HG22	1.97	0.64
1:A:161:GLU:HA	1:A:164:THR:HG22	1.79	0.64
1:B:295:ILE:HG21	1:B:493:ALA:HB2	1.80	0.63
1:C:419:THR:OG1	1:C:443:LEU:HD11	1.97	0.63
1:A:583:ARG:H	1:A:583:ARG:HD3	1.62	0.63
1:B:243:ILE:O	1:B:246:THR:HG22	1.99	0.63
1:A:59:ASN:O	1:A:63:ILE:HG22	1.99	0.63
1:B:274:PRO:HB2	1:B:277:TRP:HB3	1.80	0.63
1:B:293:SER:O	1:B:302:ILE:HD12	1.98	0.63
1:B:60:TRP:CD1	1:B:60:TRP:C	2.72	0.63
1:B:213:ARG:HB3	1:B:219:SER:HB2	1.81	0.62
1:B:60:TRP:O	1:B:60:TRP:CD1	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:LYS:O	1:B:304:TYR:HB3	1.99	0.62
1:B:243:ILE:O	1:B:247:VAL:HG23	2.00	0.62
1:C:121:LYS:N	1:C:121:LYS:HD3	2.15	0.62
1:A:211:VAL:CG1	1:A:213:ARG:HE	2.13	0.62
1:C:162:PRO:CG	1:C:417:GLY:HA3	2.29	0.62
1:A:206:TYR:CE1	1:A:210:ARG:HG2	2.35	0.61
1:B:59:ASN:CA	1:B:60:TRP:CB	2.75	0.61
1:A:414:SER:O	1:A:418:GLY:HA3	2.00	0.61
1:C:183:SER:HB2	1:C:340:TYR:HA	1.81	0.61
1:B:243:ILE:HA	1:B:246:THR:HG22	1.83	0.61
1:B:85:THR:HA	1:B:517:ASN:ND2	2.15	0.61
1:A:530:LEU:O	1:A:534:ILE:HG12	2.00	0.61
1:B:196:ILE:HD11	1:B:374:TRP:CB	2.30	0.61
1:B:213:ARG:HH11	1:B:222:VAL:HB	1.66	0.61
1:C:121:LYS:H	1:C:121:LYS:CD	2.14	0.61
1:C:226:GLY:HA2	1:C:227:GLU:C	2.21	0.61
1:B:144:MET:SD	1:B:303:GLN:HA	2.40	0.60
1:C:162:PRO:HG2	1:C:417:GLY:HA3	1.82	0.60
1:C:523:ILE:O	1:C:527:THR:HG22	2.00	0.60
1:C:379:PRO:HG2	6:C:714:HOH:O	2.00	0.60
1:B:381:VAL:O	1:B:385:LEU:HG	2.01	0.60
1:A:125:ILE:O	1:A:394:ILE:HG12	2.01	0.60
1:A:387:ARG:NH1	1:A:387:ARG:HB3	2.17	0.59
1:B:196:ILE:HD11	1:B:374:TRP:HB2	1.83	0.59
1:C:527:THR:HG23	1:C:528:PRO:HD3	1.83	0.59
1:A:211:VAL:HG21	1:A:213:ARG:HH21	1.68	0.59
1:B:452:ILE:O	1:B:455:ILE:HG12	2.03	0.59
1:A:197:TYR:CE1	1:A:381:VAL:HG21	2.37	0.59
1:B:389:SER:HB2	1:B:392:ARG:HB2	1.85	0.59
1:C:284:SER:O	1:C:288:LEU:HB2	2.03	0.59
1:C:503:GLY:O	1:C:507:LEU:HD13	2.03	0.59
1:A:370:TYR:O	1:A:374:TRP:CD1	2.55	0.58
1:A:404:VAL:HB	1:A:405:PRO:HD3	1.85	0.58
1:B:224:LEU:HG	1:B:539:ALA:HB2	1.84	0.58
1:C:477:GLY:O	1:C:481:GLN:HG3	2.04	0.58
1:A:150:MET:HE2	1:A:374:TRP:HZ3	1.69	0.58
1:C:290:PHE:CZ	1:C:496:GLY:HA3	2.38	0.58
1:A:257:GLY:O	1:A:261:ILE:HG12	2.04	0.58
1:C:126:ARG:HD3	6:C:711:HOH:O	2.03	0.58
1:B:225:ILE:HG22	1:B:226:GLY:N	2.16	0.58
1:B:534:ILE:O	1:B:537:MET:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:THR:HG21	1:A:215:GLN:NE2	2.18	0.58
1:C:183:SER:HB3	1:C:339:ASN:HB3	1.86	0.57
1:A:227:GLU:O	1:A:228:LYS:HD3	2.04	0.57
1:B:290:PHE:C	1:B:292:PHE:H	2.07	0.57
1:B:290:PHE:HB3	1:B:466:ILE:HG13	1.86	0.57
1:C:475:VAL:O	1:C:479:MET:HG2	2.03	0.57
1:C:58:LEU:HA	1:C:481:GLN:HB3	1.86	0.57
1:A:60:TRP:HA	1:A:63:ILE:HG22	1.85	0.57
1:B:254:LEU:HA	1:B:465:PHE:CE1	2.40	0.57
1:B:274:PRO:HG2	1:B:278:THR:HG23	1.86	0.57
1:C:112:PHE:O	1:C:116:VAL:HG13	2.04	0.57
1:A:284:SER:HA	1:A:287:THR:HG22	1.87	0.57
1:A:85:THR:HG23	1:A:517:ASN:HD21	1.70	0.57
1:A:142:ILE:H	1:A:142:ILE:HD13	1.70	0.57
1:B:343:ASN:O	1:B:347:MET:HG2	2.03	0.57
1:B:158:GLY:HA2	1:B:413:PHE:CE1	2.40	0.57
1:C:112:PHE:HZ	1:C:345:PHE:HE1	1.53	0.57
1:B:110:PHE:CD1	1:B:196:ILE:HG22	2.39	0.57
1:C:488:ASN:HB3	1:C:491:VAL:HG12	1.86	0.57
1:A:290:PHE:C	1:A:290:PHE:CD1	2.77	0.57
1:B:70:VAL:HG21	1:B:247:VAL:HG11	1.86	0.57
1:A:409:SER:O	1:A:413:PHE:HD2	1.86	0.57
1:B:319:PHE:O	1:B:323:VAL:HG22	2.03	0.57
1:B:378:SER:OG	1:B:379:PRO:HD3	2.05	0.56
1:A:192:HIS:N	1:A:193:PRO:HD2	2.20	0.56
1:A:215:GLN:CD	1:A:387:ARG:HH22	2.07	0.56
1:A:114:ILE:HG23	1:A:199:ILE:HG12	1.86	0.56
1:A:158:GLY:HA2	1:A:413:PHE:CE1	2.40	0.56
1:B:158:GLY:HA2	1:B:413:PHE:CD1	2.41	0.56
1:B:58:LEU:O	1:B:59:ASN:C	2.43	0.56
1:C:383:MET:HG3	1:C:475:VAL:HG13	1.87	0.56
1:A:243:ILE:O	1:A:247:VAL:HG23	2.06	0.56
1:B:476:MET:HB3	1:B:495:TRP:CE3	2.41	0.56
1:A:490:TRP:HA	1:A:493:ALA:HB3	1.88	0.56
1:A:295:ILE:N	1:A:295:ILE:HD12	2.21	0.56
1:A:526:ALA:O	1:A:529:PHE:HB2	2.05	0.56
1:B:283:VAL:HG11	1:B:504:LEU:HD23	1.87	0.56
1:A:489:LYS:HG3	1:A:490:TRP:H	1.69	0.56
1:A:181:ALA:O	1:A:185:THR:HG23	2.05	0.56
1:C:64:VAL:O	1:C:68:VAL:HG23	2.06	0.56
1:A:305:LEU:CD1	1:A:466:ILE:HD11	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:PRO:HG3	1:B:529:PHE:CE2	2.41	0.56
1:A:214:LYS:HE3	1:A:228:LYS:HE2	1.87	0.56
1:A:304:TYR:CD1	1:A:305:LEU:HD22	2.41	0.55
1:A:256:LEU:HG	1:A:515:LEU:HB3	1.88	0.55
1:B:140:SER:O	1:B:144:MET:HB2	2.06	0.55
1:B:218:SER:HB3	1:B:230:ALA:HB1	1.87	0.55
1:B:370:TYR:O	1:B:374:TRP:HD1	1.89	0.55
1:C:74:VAL:HG12	1:C:505:THR:OG1	2.06	0.55
1:C:202:LEU:HD23	1:C:540:LEU:HD21	1.87	0.55
1:A:418:GLY:O	1:A:422:VAL:HG23	2.06	0.55
1:B:194:TRP:CE3	1:B:197:TYR:HD2	2.24	0.55
1:C:221:PHE:CD2	1:C:238:ILE:HD13	2.42	0.55
1:C:350:ARG:HG2	1:C:363:LEU:HD11	1.89	0.55
1:B:211:VAL:HG21	1:B:213:ARG:NH2	2.21	0.55
1:C:122:PHE:CD1	1:C:544:LEU:HB3	2.42	0.55
1:B:372:ALA:HB1	1:B:523:ILE:HG23	1.87	0.55
1:C:456:ILE:O	1:C:459:ILE:HG22	2.06	0.55
1:B:152:ILE:O	1:B:155:MET:HB2	2.07	0.55
1:B:242:ALA:O	1:B:246:THR:HB	2.07	0.55
1:C:250:THR:O	1:C:254:LEU:HG	2.07	0.55
1:C:76:TRP:O	1:C:84:PHE:HB2	2.06	0.55
1:B:351:THR:HG23	1:B:353:MET:H	1.70	0.55
1:B:129:ARG:O	1:B:130:ILE:HB	2.08	0.54
1:B:290:PHE:HB2	1:B:470:ASP:HB3	1.89	0.54
1:C:93:SER:HA	1:C:96:VAL:HG12	1.90	0.54
1:A:141:TRP:CD1	1:A:388:ILE:HG22	2.23	0.54
1:C:209:PHE:CE1	1:C:390:ARG:HB2	2.43	0.54
1:A:92:LEU:HA	1:A:95:VAL:HG22	1.90	0.54
1:C:121:LYS:H	1:C:121:LYS:HD3	1.71	0.54
1:C:225:ILE:HD11	1:C:234:LEU:HD23	1.89	0.54
1:A:423:PHE:HB3	1:A:428:GLU:O	2.08	0.54
1:B:481:GLN:NE2	1:B:491:VAL:HG11	2.22	0.54
1:C:195:ALA:O	1:C:199:ILE:HG12	2.07	0.54
1:C:333:LEU:HB2	1:C:334:PRO:CD	2.38	0.54
1:C:378:SER:N	1:C:379:PRO:HD2	2.23	0.54
1:C:485:LEU:H	1:C:485:LEU:HD12	1.72	0.54
1:B:322:VAL:HG23	1:B:323:VAL:N	2.23	0.54
1:A:262:GLY:HA2	1:A:265:LEU:HB2	1.90	0.53
1:A:76:TRP:CD1	1:A:84:PHE:HD1	2.26	0.53
1:B:257:GLY:O	1:B:261:ILE:HG12	2.08	0.53
1:C:221:PHE:CE2	1:C:536:LEU:HD13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:ALA:HA	1:B:517:ASN:HB2	1.89	0.53
1:A:204:ILE:O	1:A:208:THR:HG23	2.08	0.53
1:A:476:MET:HA	1:A:479:MET:HG2	1.89	0.53
1:C:254:LEU:HB3	1:C:465:PHE:CE1	2.43	0.53
1:A:293:SER:O	1:A:295:ILE:N	2.41	0.53
1:B:472:ALA:O	1:B:476:MET:HG3	2.07	0.53
1:C:173:HIS:HB2	6:C:730:HOH:O	2.08	0.53
1:B:274:PRO:HG2	1:B:278:THR:CG2	2.39	0.53
1:C:67:LEU:HD23	1:C:70:VAL:HG11	1.91	0.53
1:C:157:TYR:O	1:C:161:GLU:HB3	2.08	0.53
1:C:207:SER:HB3	6:C:725:HOH:O	2.09	0.53
1:C:208:THR:HG21	1:C:215:GLN:HG3	1.90	0.53
1:A:354:SER:O	1:A:359:ALA:HB3	2.09	0.53
1:B:302:ILE:HG21	1:B:384:PHE:HZ	1.74	0.53
1:B:134:PRO:HB3	1:B:392:ARG:NH1	2.24	0.53
1:C:233:TRP:H	1:C:233:TRP:HD1	1.56	0.53
1:A:477:GLY:O	1:A:481:GLN:HG2	2.09	0.52
1:A:578:LEU:HD12	1:A:581:LYS:HE3	1.92	0.52
1:C:355:ALA:O	1:C:358:THR:HB	2.08	0.52
1:B:287:THR:HA	1:B:290:PHE:CE2	2.45	0.52
1:A:260:GLN:NE2	1:A:437:GLU:HG3	2.16	0.52
1:C:329:ILE:HD11	1:C:419:THR:CG2	2.40	0.52
1:A:355:ALA:O	1:A:358:THR:HB	2.10	0.52
1:A:76:TRP:HD1	1:A:84:PHE:HD1	1.57	0.52
1:B:141:TRP:HZ3	1:B:388:ILE:HB	1.73	0.52
1:A:346:GLN:HG3	6:C:702:HOH:O	2.09	0.52
1:B:351:THR:HG23	1:B:353:MET:HB2	1.92	0.52
1:B:246:THR:OG1	1:B:380:PHE:HB3	2.10	0.52
1:B:110:PHE:CZ	1:B:534:ILE:HD13	2.44	0.52
1:C:280:VAL:HG22	1:C:504:LEU:HD11	1.91	0.52
1:A:141:TRP:HD1	1:A:388:ILE:CG2	2.13	0.52
1:C:181:ALA:O	1:C:185:THR:HG23	2.10	0.52
1:B:144:MET:HE3	1:B:303:GLN:HA	1.92	0.52
1:B:194:TRP:HB3	1:B:401:VAL:O	2.09	0.51
1:C:92:LEU:HG	1:C:93:SER:N	2.24	0.51
1:B:145:MET:CE	1:B:401:VAL:HB	2.39	0.51
1:A:404:VAL:O	1:A:408:VAL:HG13	2.10	0.51
1:B:193:PRO:O	1:B:196:ILE:HG12	2.11	0.51
1:B:276:ASP:HA	1:B:279:ILE:HB	1.92	0.51
1:A:130:ILE:HG23	1:A:131:ASP:H	1.75	0.51
1:A:252:CYS:SG	1:A:518:LEU:HD13	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:HG12	1:A:382:GLY:HA3	1.93	0.51
1:A:202:LEU:HD13	1:A:540:LEU:HD11	1.93	0.51
1:B:463:THR:HA	1:B:466:ILE:CG2	2.39	0.51
1:B:128:GLY:HA2	1:B:209:PHE:O	2.11	0.51
1:B:184:THR:HG22	1:B:188:HIS:CE1	2.45	0.51
1:A:222:VAL:N	1:A:223:PRO:CD	2.73	0.51
1:B:183:SER:HG	1:B:339:ASN:HB3	1.74	0.51
1:B:59:ASN:N	1:B:60:TRP:HB3	2.26	0.51
1:C:225:ILE:O	1:C:227:GLU:HB2	2.10	0.51
1:A:74:VAL:HG22	1:A:502:ILE:CG2	2.41	0.51
1:B:333:LEU:O	1:B:337:ILE:HG13	2.11	0.51
1:B:96:VAL:HG13	1:B:368:ILE:HG21	1.93	0.51
1:B:530:LEU:C	1:B:530:LEU:HD23	2.32	0.51
1:A:243:ILE:O	1:A:246:THR:HG22	2.11	0.51
1:A:258:ALA:CB	1:A:283:VAL:HG12	2.41	0.51
1:A:323:VAL:CG1	1:A:448:PRO:HD2	2.41	0.51
1:B:504:LEU:O	1:B:504:LEU:HD13	2.10	0.50
1:A:198:ALA:O	1:A:202:LEU:HB2	2.10	0.50
1:B:248:PHE:HB3	1:B:522:THR:OG1	2.11	0.50
1:C:130:ILE:HD12	1:C:130:ILE:H	1.77	0.50
1:A:293:SER:OG	1:A:470:ASP:HB2	2.12	0.50
1:B:208:THR:HG21	1:B:215:GLN:HA	1.93	0.50
1:A:370:TYR:O	1:A:374:TRP:HD1	1.94	0.50
1:A:387:ARG:C	1:A:388:ILE:HG13	2.31	0.50
1:B:290:PHE:HB3	1:B:466:ILE:CG1	2.41	0.50
1:C:383:MET:HG3	1:C:475:VAL:CG1	2.42	0.50
1:C:323:VAL:CG2	1:C:448:PRO:HG2	2.41	0.50
1:B:313:ALA:HA	1:B:460:LEU:HD11	1.94	0.50
1:C:519:GLN:O	1:C:523:ILE:HG13	2.12	0.50
1:A:380:PHE:CD2	1:A:380:PHE:N	2.71	0.50
1:B:219:SER:HA	1:B:222:VAL:HG23	1.94	0.50
1:A:387:ARG:HG2	1:A:388:ILE:HG13	1.94	0.50
1:A:261:ILE:HD12	1:A:461:LEU:HD13	1.92	0.50
1:C:184:THR:HA	1:C:347:MET:HE3	1.93	0.50
1:A:260:GLN:HG2	1:A:437:GLU:HG3	1.93	0.50
1:B:388:ILE:O	1:B:388:ILE:HG22	2.12	0.50
1:A:583:ARG:HD3	1:A:583:ARG:N	2.27	0.49
1:B:236:LYS:O	1:B:240:ILE:HG13	2.11	0.49
1:B:252:CYS:O	1:B:256:LEU:HB3	2.11	0.49
1:A:527:THR:N	1:A:528:PRO:CD	2.74	0.49
1:B:225:ILE:C	1:B:227:GLU:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:HIS:N	1:A:193:PRO:CD	2.75	0.49
1:B:141:TRP:HE3	1:B:388:ILE:HG22	1.75	0.49
1:C:133:ALA:HB1	1:C:134:PRO:CD	2.41	0.49
1:C:549:ILE:HG13	4:C:601:CL:CL	2.49	0.49
1:A:153:ASP:HB3	1:A:157:TYR:HD2	1.76	0.49
1:A:240:ILE:O	1:A:244:ILE:HG13	2.13	0.49
1:A:379:PRO:HG3	1:A:529:PHE:CZ	2.47	0.49
1:B:271:ILE:CG1	1:B:272:GLU:HA	2.36	0.49
1:C:167:ARG:HG3	1:C:168:ASN:N	2.28	0.49
1:A:111:VAL:O	1:A:115:VAL:HG23	2.13	0.49
1:A:243:ILE:HD13	1:A:479:MET:HG3	1.93	0.49
1:A:575:LYS:HA	1:A:578:LEU:HB3	1.94	0.49
1:A:78:ILE:HD11	1:A:506:LEU:HA	1.93	0.49
1:B:322:VAL:HG23	1:B:323:VAL:HG13	1.94	0.49
1:B:419:THR:CG2	1:B:443:LEU:HD11	2.43	0.49
1:A:258:ALA:HB1	1:A:283:VAL:HG12	1.93	0.49
1:B:327:VAL:HG11	1:C:98:ASN:HD22	1.77	0.49
1:C:256:LEU:HA	1:C:259:LEU:HG	1.95	0.49
1:C:513:ASN:O	1:C:515:LEU:N	2.45	0.49
1:C:59:ASN:O	1:C:63:ILE:HG13	2.11	0.49
1:C:71:LEU:HA	1:C:74:VAL:HG22	1.95	0.49
1:C:92:LEU:HD22	1:C:520:ASN:CG	2.33	0.49
1:A:502:ILE:O	1:A:506:LEU:HB2	2.13	0.49
1:B:222:VAL:HG13	1:B:227:GLU:CA	2.36	0.49
1:A:331:ASN:HB3	1:B:351:THR:OG1	2.13	0.49
1:C:322:VAL:HG23	1:C:323:VAL:N	2.27	0.49
1:B:140:SER:O	1:B:144:MET:HE2	2.13	0.49
1:B:182:MET:O	1:B:186:MET:HE2	2.12	0.49
1:B:341:LEU:HD23	1:C:345:PHE:CE1	2.47	0.49
1:C:444:LEU:O	1:C:450:GLY:HA3	2.13	0.49
1:B:161:GLU:OE1	1:B:366:TRP:HZ3	1.96	0.49
1:B:103:PHE:CD1	1:B:530:LEU:HD12	2.47	0.49
1:A:214:LYS:HD2	1:A:214:LYS:N	2.22	0.49
1:A:258:ALA:O	1:A:279:ILE:HD11	2.13	0.49
1:A:136:PHE:CE1	1:A:388:ILE:HA	2.48	0.48
1:A:263:ALA:HB3	1:A:437:GLU:HG2	1.95	0.48
1:B:186:MET:HE1	1:B:336:SER:HB3	1.94	0.48
1:A:209:PHE:CE2	1:A:390:ARG:HB2	2.47	0.48
1:A:397:PHE:O	1:A:401:VAL:HG23	2.14	0.48
1:C:206:TYR:CE1	1:C:210:ARG:HG2	2.48	0.48
1:C:200:VAL:HG21	1:C:378:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:VAL:HG21	1:B:378:SER:HB2	1.93	0.48
1:A:246:THR:HA	1:A:380:PHE:CE2	2.48	0.48
1:B:272:GLU:O	1:B:272:GLU:HG2	2.14	0.48
1:C:76:TRP:O	1:C:76:TRP:CG	2.66	0.48
1:A:70:VAL:HG11	1:A:247:VAL:HG11	1.95	0.48
1:A:407:GLY:O	1:A:411:VAL:HG12	2.14	0.48
1:B:334:PRO:HG2	1:C:351:THR:HG21	1.95	0.48
1:B:57:SER:HB2	1:B:482:HIS:HD2	1.77	0.48
1:A:387:ARG:O	1:A:389:SER:N	2.45	0.48
1:B:278:THR:O	1:B:282:ILE:HG12	2.14	0.48
1:B:289:ALA:HB1	1:B:466:ILE:HD12	1.95	0.48
1:B:526:ALA:O	1:B:529:PHE:HB2	2.13	0.48
1:B:106:PHE:CD1	1:B:534:ILE:HD12	2.49	0.48
1:C:166:TYR:CE1	1:C:176:HIS:HA	2.48	0.48
1:A:136:PHE:O	1:A:137:ARG:HB3	2.14	0.48
1:B:395:ARG:O	1:B:399:LEU:HG	2.14	0.48
1:C:78:ILE:HD12	1:C:79:GLY:N	2.19	0.48
1:A:138:THR:O	1:A:140:SER:N	2.46	0.48
1:A:202:LEU:HD21	1:A:394:ILE:HD12	1.94	0.48
1:A:443:LEU:C	1:A:443:LEU:HD12	2.34	0.48
1:A:64:VAL:O	1:A:68:VAL:HG13	2.14	0.48
1:A:76:TRP:O	1:A:84:PHE:HB2	2.13	0.48
1:C:404:VAL:HB	1:C:405:PRO:HD3	1.96	0.48
1:C:473:SER:HB3	1:C:492:THR:O	2.13	0.48
1:C:247:VAL:HG12	1:C:502:ILE:HD11	1.95	0.48
1:A:117:ILE:O	1:A:120:SER:HB3	2.13	0.48
1:C:253:SER:HB3	1:C:377:TRP:CH2	2.49	0.48
1:B:202:LEU:HD23	1:B:540:LEU:HD21	1.96	0.47
1:C:247:VAL:HG22	1:C:476:MET:SD	2.54	0.47
1:A:213:ARG:HH11	1:A:222:VAL:HG13	1.79	0.47
1:A:496:GLY:HA3	6:A:722:HOH:O	2.14	0.47
1:A:121:LYS:C	1:A:123:GLY:H	2.16	0.47
1:C:228:LYS:C	1:C:230:ALA:H	2.18	0.47
1:C:233:TRP:N	1:C:233:TRP:CD1	2.82	0.47
1:A:208:THR:HG21	1:A:215:GLN:HA	1.95	0.47
1:B:136:PHE:CZ	1:B:298:VAL:HG21	2.49	0.47
1:B:460:LEU:O	1:B:464:PHE:HB2	2.14	0.47
1:C:312:LEU:HB2	1:C:460:LEU:HD13	1.96	0.47
1:A:421:ILE:O	1:A:425:GLN:HG3	2.15	0.47
1:A:565:ARG:HG3	1:C:130:ILE:HB	1.96	0.47
1:B:144:MET:SD	1:B:306:SER:HB2	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:LYS:N	1:C:121:LYS:CD	2.76	0.47
1:C:58:LEU:HB3	1:C:63:ILE:CD1	2.44	0.47
1:A:160:THR:HB	1:A:439:GLN:HE22	1.74	0.47
1:A:66:ALA:O	1:A:70:VAL:HG23	2.15	0.47
1:A:112:PHE:O	1:A:116:VAL:HG13	2.14	0.47
1:A:74:VAL:HG22	1:A:502:ILE:HG23	1.97	0.47
1:B:527:THR:N	1:B:528:PRO:CD	2.77	0.47
1:C:193:PRO:HB3	1:C:374:TRP:CD1	2.50	0.47
1:C:162:PRO:HG3	1:C:417:GLY:HA3	1.96	0.47
1:B:200:VAL:O	1:B:204:ILE:HG12	2.14	0.47
1:A:304:TYR:HD1	1:A:305:LEU:HD22	1.79	0.47
1:A:441:PHE:HA	1:A:444:LEU:HD11	1.96	0.47
1:B:354:SER:O	1:B:359:ALA:HB3	2.15	0.47
1:C:537:MET:O	1:C:541:VAL:HG23	2.15	0.47
1:A:114:ILE:CG2	1:A:199:ILE:HG12	2.44	0.47
1:A:316:LEU:HA	1:A:319:PHE:HB3	1.95	0.47
1:B:392:ARG:HG3	1:B:396:GLU:OE1	2.15	0.47
1:B:320:VAL:HG22	1:B:415:ILE:CG2	2.45	0.46
1:B:508:LEU:HD13	1:B:509:SER:N	2.31	0.46
1:B:521:VAL:O	1:B:524:VAL:HG22	2.15	0.46
1:C:345:PHE:HA	1:C:348:ALA:HB3	1.96	0.46
1:B:196:ILE:HD11	1:B:374:TRP:HB3	1.96	0.46
1:A:150:MET:HE2	1:A:374:TRP:CZ3	2.49	0.46
1:A:78:ILE:HD12	1:A:78:ILE:H	1.81	0.46
1:C:122:PHE:CE1	1:C:544:LEU:HB3	2.50	0.46
1:B:113:PHE:CZ	1:B:117:ILE:HD12	2.51	0.46
1:B:404:VAL:HB	1:B:405:PRO:HD3	1.97	0.46
1:B:298:VAL:HA	1:B:302:ILE:HB	1.97	0.46
1:C:428:GLU:O	1:C:429:SER:C	2.54	0.46
1:C:59:ASN:HB2	1:C:482:HIS:CE1	2.51	0.46
1:C:67:LEU:HA	1:C:70:VAL:CG1	2.45	0.46
1:C:211:VAL:HG11	1:C:213:ARG:CZ	2.46	0.46
1:A:59:ASN:HD22	1:A:61:SER:H	1.62	0.46
1:A:538:PHE:O	1:A:542:LYS:HB2	2.16	0.46
1:B:151:GLY:H	2:B:601:1Y8:C4	2.27	0.46
1:B:520:ASN:O	1:B:524:VAL:HG13	2.16	0.46
1:A:118:ALA:HB2	1:A:398:ILE:HG21	1.98	0.46
1:B:114:ILE:HD12	1:B:402:LEU:HD22	1.97	0.46
1:B:273:ASP:O	1:B:274:PRO:C	2.54	0.46
1:C:303:GLN:H	1:C:303:GLN:CD	2.19	0.46
1:B:155:MET:HE3	1:B:460:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ILE:O	1:B:244:ILE:HG13	2.16	0.45
1:A:387:ARG:C	1:A:389:SER:N	2.68	0.45
1:B:229:GLY:C	1:B:231:GLU:H	2.19	0.45
1:B:329:ILE:HG21	1:B:415:ILE:HG12	1.98	0.45
1:A:197:TYR:CZ	1:A:381:VAL:HG21	2.51	0.45
1:A:464:PHE:HA	1:A:464:PHE:HD1	1.67	0.45
1:B:319:PHE:CE2	1:B:453:MET:HG3	2.50	0.45
1:A:121:LYS:C	1:A:123:GLY:N	2.70	0.45
1:A:329:ILE:HD13	1:A:415:ILE:HA	1.99	0.45
1:B:145:MET:HE2	1:B:401:VAL:HB	1.99	0.45
1:B:243:ILE:HA	1:B:246:THR:CG2	2.46	0.45
1:B:321:PHE:HE1	1:B:330:LEU:HD13	1.82	0.45
1:C:248:PHE:CD1	1:C:502:ILE:HD12	2.51	0.45
1:A:394:ILE:O	1:A:398:ILE:HG13	2.17	0.45
1:B:418:GLY:O	1:B:422:VAL:HG23	2.16	0.45
1:B:155:MET:HE1	1:B:460:LEU:HD13	1.98	0.45
1:B:488:ASN:O	1:B:491:VAL:HG12	2.17	0.45
1:A:274:PRO:HB2	1:A:275:SER:H	1.59	0.45
1:B:470:ASP:O	1:B:474:THR:HG23	2.16	0.45
1:C:319:PHE:CZ	1:C:323:VAL:HG11	2.52	0.45
1:C:373:TRP:CZ2	1:C:377:TRP:HZ3	2.34	0.45
1:C:216:LEU:CD2	1:C:479:MET:HA	2.47	0.45
1:A:523:ILE:O	1:A:527:THR:HG23	2.17	0.45
1:B:134:PRO:HB3	1:B:392:ARG:HH11	1.82	0.45
1:B:269:ASN:HD21	1:B:274:PRO:HD2	1.81	0.45
1:B:515:LEU:HA	1:B:515:LEU:HD12	1.81	0.45
1:B:379:PRO:HG3	1:B:529:PHE:CZ	2.52	0.45
1:C:114:ILE:HA	1:C:114:ILE:HD12	1.82	0.45
1:C:61:SER:O	1:C:65:PRO:HG2	2.16	0.45
1:C:385:LEU:HD13	1:C:401:VAL:HG11	1.99	0.45
1:B:156:PHE:HE1	1:B:260:GLN:HG2	1.81	0.45
1:C:204:ILE:O	1:C:208:THR:HG23	2.17	0.45
1:A:213:ARG:HH11	1:A:222:VAL:CG1	2.31	0.44
1:B:78:ILE:HG22	1:B:508:LEU:HD11	2.00	0.44
1:C:236:LYS:HG2	1:C:237:LEU:N	2.30	0.44
1:A:321:PHE:CZ	1:A:330:LEU:HD11	2.52	0.44
1:A:155:MET:SD	1:A:460:LEU:HD23	2.57	0.44
1:A:216:LEU:HD21	1:A:239:ASP:OD2	2.18	0.44
1:A:85:THR:HG23	1:A:517:ASN:ND2	2.31	0.44
1:B:140:SER:HA	1:B:143:SER:HB2	1.99	0.44
1:B:60:TRP:C	1:B:62:VAL:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:HA	1:A:84:PHE:HB3	1.98	0.44
1:B:226:GLY:C	1:B:228:LYS:H	2.20	0.44
1:B:59:ASN:HD22	1:B:482:HIS:CE1	2.35	0.44
1:C:189:TRP:CH2	1:C:370:TYR:CZ	3.05	0.44
1:C:329:ILE:HG23	1:C:414:SER:O	2.17	0.44
1:B:127:LEU:HD23	1:B:206:TYR:HA	1.98	0.44
1:A:473:SER:HA	1:A:476:MET:HG2	1.99	0.44
1:A:210:ARG:NH2	1:A:549:ILE:HD12	2.31	0.44
1:B:254:LEU:HG	1:B:255:GLY:N	2.33	0.44
1:B:321:PHE:CE1	1:B:330:LEU:HD13	2.53	0.44
1:B:88:ALA:HB3	1:B:517:ASN:HD22	1.82	0.44
1:A:461:LEU:HD12	1:A:462:GLY:N	2.33	0.44
1:A:493:ALA:HA	6:A:722:HOH:O	2.18	0.44
1:B:59:ASN:ND2	1:B:60:TRP:CD1	2.86	0.44
1:A:88:ALA:HB3	1:A:517:ASN:HB3	1.99	0.44
1:B:137:ARG:N	1:B:137:ARG:HD2	2.33	0.44
1:B:144:MET:CE	1:B:303:GLN:HA	2.48	0.44
1:B:330:LEU:HA	1:B:330:LEU:HD12	1.84	0.44
1:A:240:ILE:HA	1:A:243:ILE:HG22	1.99	0.43
1:A:260:GLN:HE21	1:A:437:GLU:CG	2.20	0.43
1:A:330:LEU:HD23	1:B:101:TRP:NE1	2.33	0.43
1:B:274:PRO:O	1:B:275:SER:C	2.56	0.43
1:B:373:TRP:O	1:B:376:SER:HB3	2.18	0.43
1:B:378:SER:N	1:B:379:PRO:CD	2.81	0.43
1:A:366:TRP:HE3	1:A:370:TYR:HE2	1.66	0.43
1:B:277:TRP:HE3	1:B:278:THR:HG23	1.83	0.43
1:A:318:ILE:HB	6:A:712:HOH:O	2.18	0.43
1:A:456:ILE:O	1:A:460:LEU:HB2	2.19	0.43
1:A:507:LEU:HD23	1:A:507:LEU:O	2.18	0.43
1:B:481:GLN:O	1:B:484:GLN:HG3	2.17	0.43
1:B:527:THR:N	1:B:528:PRO:HD2	2.33	0.43
1:B:529:PHE:O	1:B:532:VAL:HB	2.18	0.43
1:C:105:LEU:O	1:C:109:VAL:HG23	2.18	0.43
1:A:295:ILE:CG2	1:A:296:SER:N	2.68	0.43
1:A:504:LEU:O	1:A:508:LEU:HD23	2.18	0.43
1:A:548:VAL:HG23	1:A:549:ILE:H	1.84	0.43
1:B:188:HIS:CG	6:B:726:HOH:O	2.72	0.43
1:B:286:LEU:O	1:B:289:ALA:HB3	2.19	0.43
1:B:366:TRP:O	1:B:367:THR:C	2.56	0.43
1:B:508:LEU:HD13	1:B:509:SER:H	1.83	0.43
1:C:395:ARG:HB2	1:C:395:ARG:HE	1.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:ASN:HA	1:C:520:ASN:HB2	2.00	0.43
1:A:574:ARG:HA	1:A:574:ARG:HD3	1.83	0.43
1:A:59:ASN:HD22	1:A:59:ASN:C	2.22	0.43
1:B:70:VAL:HA	1:B:248:PHE:CZ	2.54	0.43
1:C:123:GLY:HA3	1:C:395:ARG:HE	1.83	0.43
1:A:204:ILE:HD11	1:A:217:LEU:HG	2.00	0.43
1:A:330:LEU:HB3	1:B:101:TRP:CG	2.54	0.43
1:B:156:PHE:HE1	1:B:260:GLN:CG	2.31	0.43
1:B:192:HIS:HB2	1:B:193:PRO:HD3	2.01	0.43
1:B:81:LYS:O	1:B:83:SER:N	2.49	0.43
1:C:156:PHE:CG	1:C:256:LEU:HD13	2.54	0.43
1:C:243:ILE:CD1	1:C:479:MET:HG3	2.49	0.43
1:C:62:VAL:HG13	1:C:240:ILE:HD12	2.01	0.43
1:A:261:ILE:CD1	1:A:461:LEU:HD13	2.48	0.43
1:A:387:ARG:HB3	1:A:387:ARG:HH11	1.84	0.43
1:A:462:GLY:O	1:A:466:ILE:HG23	2.19	0.43
1:B:99:LEU:HD12	1:B:527:THR:HG21	2.00	0.43
1:C:261:ILE:HB	1:C:282:ILE:HD13	2.00	0.43
1:C:71:LEU:HA	1:C:74:VAL:CG2	2.49	0.43
1:A:449:GLY:O	1:A:452:ILE:HG12	2.19	0.43
1:A:78:ILE:HD12	1:A:78:ILE:N	2.33	0.43
1:C:146:PHE:CE1	1:C:404:VAL:HG13	2.53	0.43
1:C:92:LEU:HD22	1:C:520:ASN:ND2	2.33	0.43
1:A:211:VAL:HG21	1:A:213:ARG:NH2	2.33	0.43
1:B:213:ARG:NH1	1:B:223:PRO:HD3	2.33	0.43
1:B:217:LEU:HD13	1:B:242:ALA:CB	2.48	0.43
1:B:398:ILE:C	1:B:400:GLY:H	2.22	0.43
1:C:312:LEU:HB3	1:C:460:LEU:HD22	1.99	0.43
1:C:263:ALA:HB1	1:C:438:GLU:HB3	2.00	0.43
1:B:62:VAL:C	1:B:65:PRO:HD2	2.39	0.43
1:C:73:THR:C	1:C:75:VAL:H	2.21	0.43
1:A:251:ALA:O	1:A:254:LEU:HB3	2.19	0.42
1:A:92:LEU:HD12	1:A:92:LEU:C	2.40	0.42
1:B:152:ILE:HG13	1:B:153:ASP:N	2.31	0.42
1:B:319:PHE:CZ	1:B:453:MET:HG3	2.54	0.42
1:C:194:TRP:CZ2	1:C:405:PRO:HB3	2.54	0.42
1:A:371:TRP:HA	1:A:371:TRP:CE3	2.54	0.42
1:B:139:VAL:O	1:B:140:SER:HB3	2.20	0.42
1:B:541:VAL:C	1:B:543:ASP:H	2.21	0.42
1:C:184:THR:O	1:C:187:PHE:HB3	2.19	0.42
1:A:304:TYR:O	1:A:308:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:MET:HE2	1:A:475:VAL:HG13	2.01	0.42
1:B:203:ALA:O	1:B:207:SER:HB3	2.19	0.42
1:C:291:ILE:HD11	1:C:497:VAL:HG11	2.00	0.42
1:A:103:PHE:CE1	1:A:372:ALA:HA	2.54	0.42
1:A:130:ILE:HG23	1:A:131:ASP:N	2.35	0.42
1:A:207:SER:O	1:A:211:VAL:HB	2.19	0.42
1:A:290:PHE:HB3	1:A:466:ILE:HB	2.01	0.42
1:A:399:LEU:HG	1:A:403:LEU:HD12	2.00	0.42
1:A:110:PHE:CZ	1:A:534:ILE:HD13	2.53	0.42
1:B:161:GLU:OE1	1:B:366:TRP:CZ3	2.72	0.42
1:B:185:THR:O	1:B:189:TRP:HD1	2.02	0.42
1:B:125:ILE:HD11	1:B:206:TYR:HE1	1.84	0.42
1:B:430:ILE:HG13	6:B:717:HOH:O	2.19	0.42
1:C:208:THR:CG2	1:C:215:GLN:HA	2.49	0.42
1:C:295:ILE:HG22	1:C:295:ILE:O	2.19	0.42
1:A:161:GLU:HG2	1:A:185:THR:HG22	2.01	0.42
1:A:170:VAL:HG22	1:A:362:TRP:CZ2	2.54	0.42
1:A:65:PRO:O	1:A:68:VAL:HG22	2.19	0.42
1:B:228:LYS:HA	1:B:228:LYS:HD3	1.84	0.42
1:B:70:VAL:HG21	1:B:247:VAL:CG1	2.49	0.42
1:C:463:THR:O	1:C:467:THR:HG23	2.20	0.42
1:A:353:MET:CE	1:A:353:MET:HA	2.49	0.42
1:A:435:ALA:HB3	1:A:438:GLU:HG2	2.02	0.42
1:A:248:PHE:CB	1:A:522:THR:HG22	2.40	0.42
1:B:190:THR:O	1:B:193:PRO:HD2	2.19	0.42
1:B:372:ALA:O	1:B:375:ILE:HG22	2.19	0.42
1:B:477:GLY:HA3	1:B:492:THR:HG22	2.02	0.42
1:C:226:GLY:HA2	1:C:227:GLU:O	2.20	0.42
1:A:225:ILE:HG13	1:A:230:ALA:HB2	2.02	0.42
1:C:170:VAL:HG13	1:C:171:PRO:HD2	2.01	0.42
1:C:251:ALA:HB1	1:C:502:ILE:HG13	2.01	0.42
1:C:374:TRP:HA	1:C:374:TRP:HE3	1.84	0.42
1:C:485:LEU:N	1:C:485:LEU:HD12	2.35	0.42
1:B:130:ILE:HG23	1:B:131:ASP:N	2.35	0.42
1:C:133:ALA:HB1	1:C:134:PRO:HD2	2.02	0.42
1:C:58:LEU:HB3	1:C:63:ILE:HD11	2.02	0.42
1:A:300:LYS:HG3	1:A:303:GLN:HG3	2.01	0.42
1:A:67:LEU:O	1:A:71:LEU:HG	2.20	0.42
1:B:137:ARG:NE	1:B:137:ARG:HA	2.35	0.42
1:C:325:PRO:HB2	1:C:328:SER:HB2	2.00	0.42
1:C:374:TRP:CE3	1:C:374:TRP:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:SER:C	1:A:347:MET:HE1	2.41	0.42
1:B:481:GLN:HE22	1:B:488:ASN:HB2	1.84	0.42
1:C:117:ILE:HA	1:C:117:ILE:HD13	1.94	0.42
1:C:502:ILE:HA	1:C:505:THR:HB	2.02	0.42
1:A:137:ARG:O	1:A:138:THR:O	2.38	0.41
1:B:138:THR:O	1:B:141:TRP:HB3	2.20	0.41
1:B:60:TRP:O	1:B:61:SER:HB3	2.19	0.41
1:A:490:TRP:O	1:A:491:VAL:HB	2.19	0.41
1:B:547:ASP:OD1	1:B:548:VAL:HG22	2.20	0.41
1:C:224:LEU:HD11	1:C:538:PHE:CB	2.50	0.41
1:C:256:LEU:N	1:C:518:LEU:HD21	2.35	0.41
1:C:481:GLN:NE2	1:C:484:GLN:HB2	2.35	0.41
1:A:197:TYR:HH	1:A:374:TRP:HE3	1.67	0.41
1:A:295:ILE:H	1:A:295:ILE:HD12	1.84	0.41
1:B:290:PHE:C	1:B:292:PHE:N	2.71	0.41
1:B:64:VAL:O	1:B:68:VAL:HG13	2.20	0.41
1:A:291:ILE:O	1:A:291:ILE:HG22	2.20	0.41
1:C:228:LYS:HD2	1:C:228:LYS:N	2.36	0.41
1:C:254:LEU:HD12	1:C:499:THR:HG22	2.03	0.41
1:C:58:LEU:H	1:C:58:LEU:HD12	1.86	0.41
1:C:160:THR:HG21	1:C:436:ALA:HB1	2.01	0.41
1:A:349:GLY:O	1:C:335:GLY:HA2	2.21	0.41
1:C:371:TRP:CE3	1:C:371:TRP:HA	2.56	0.41
1:C:251:ALA:CB	1:C:502:ILE:HG13	2.50	0.41
1:A:161:GLU:HA	1:A:164:THR:CG2	2.49	0.41
1:A:381:VAL:O	1:A:385:LEU:HD13	2.20	0.41
1:A:444:LEU:O	1:A:450:GLY:HA2	2.20	0.41
1:A:81:LYS:O	1:A:83:SER:N	2.53	0.41
1:B:211:VAL:HG11	1:B:213:ARG:NE	2.35	0.41
1:B:209:PHE:CD2	1:B:390:ARG:HA	2.55	0.41
1:B:247:VAL:HA	1:B:476:MET:HE3	2.03	0.41
1:C:190:THR:O	1:C:193:PRO:HG2	2.20	0.41
1:C:236:LYS:O	1:C:240:ILE:HB	2.20	0.41
1:C:536:LEU:HD12	1:C:536:LEU:HA	1.96	0.41
1:B:146:PHE:CD1	1:B:310:MET:HE1	2.56	0.41
1:B:188:HIS:CD2	6:B:726:HOH:O	2.73	0.41
1:C:380:PHE:CD1	1:C:475:VAL:HG21	2.50	0.41
1:C:210:ARG:HH22	1:C:549:ILE:HG12	1.84	0.41
1:A:305:LEU:CD2	1:A:305:LEU:N	2.83	0.41
1:A:331:ASN:OD1	1:B:101:TRP:HB3	2.20	0.41
1:B:204:ILE:HD13	1:B:220:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ARG:NH1	1:B:222:VAL:HB	2.33	0.41
1:B:290:PHE:O	1:B:291:ILE:HB	2.20	0.41
1:B:152:ILE:HG22	1:B:465:PHE:HB2	2.03	0.41
1:C:112:PHE:O	1:C:116:VAL:CG1	2.68	0.41
1:C:161:GLU:OE2	1:C:189:TRP:HZ3	2.02	0.41
1:C:449:GLY:O	1:C:452:ILE:HG12	2.20	0.41
5:C:602:CM5:H17	5:C:602:CM5:H24	1.58	0.41
1:A:132:GLU:OE2	1:A:390:ARG:HD2	2.20	0.41
1:B:171:PRO:HB3	1:B:359:ALA:HB2	2.02	0.41
1:C:267:ALA:HB1	1:C:445:HIS:NE2	2.34	0.41
1:C:347:MET:HB3	1:C:347:MET:HE2	1.81	0.41
1:C:395:ARG:HG2	5:C:602:CM5:H12	2.02	0.41
1:C:524:VAL:O	1:C:527:THR:HG23	2.21	0.41
1:B:152:ILE:CG2	1:B:465:PHE:HB2	2.51	0.41
1:A:387:ARG:HH12	1:A:485:LEU:HD22	1.86	0.41
1:B:193:PRO:HB3	1:B:374:TRP:CE3	2.55	0.41
1:B:203:ALA:HB1	1:B:536:LEU:HD11	2.03	0.41
1:B:295:ILE:C	1:B:297:GLY:H	2.23	0.41
1:B:359:ALA:O	1:B:363:LEU:HG	2.21	0.41
1:B:401:VAL:HG22	1:B:401:VAL:O	2.20	0.41
1:B:440:LEU:O	1:B:443:LEU:HB3	2.21	0.41
1:A:473:SER:HA	1:A:476:MET:SD	2.61	0.40
1:A:565:ARG:HG3	1:C:130:ILE:CG2	2.50	0.40
1:A:573:HIS:O	1:A:577:GLU:HG2	2.21	0.40
1:C:187:PHE:CB	1:C:347:MET:HE1	2.51	0.40
1:C:253:SER:CB	1:C:377:TRP:HH2	2.34	0.40
1:A:371:TRP:HA	1:A:371:TRP:HE3	1.86	0.40
1:B:254:LEU:CD2	1:B:500:ALA:HA	2.51	0.40
1:B:371:TRP:O	1:B:375:ILE:HB	2.21	0.40
1:B:57:SER:HB2	1:B:482:HIS:CD2	2.56	0.40
1:C:333:LEU:HB2	1:C:334:PRO:HD3	2.02	0.40
1:C:530:LEU:O	1:C:534:ILE:HG13	2.21	0.40
1:A:213:ARG:NH1	1:A:222:VAL:HG22	2.35	0.40
1:B:320:VAL:O	1:B:324:GLY:HA3	2.21	0.40
1:C:138:THR:O	1:C:141:TRP:HB3	2.22	0.40
1:C:161:GLU:HG2	1:C:185:THR:HB	2.03	0.40
1:C:265:LEU:C	1:C:267:ALA:H	2.24	0.40
1:A:281:GLY:O	1:A:285:VAL:HG13	2.22	0.40
1:A:378:SER:N	1:A:379:PRO:CD	2.85	0.40
1:A:580:ALA:O	1:A:583:ARG:HG3	2.21	0.40
1:B:307:ASN:O	1:B:311:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:GLY:C	1:B:434:GLY:H	2.24	0.40
1:B:453:MET:CE	1:B:456:ILE:HD11	2.52	0.40
1:B:455:ILE:HG13	1:B:456:ILE:N	2.36	0.40
1:C:225:ILE:C	1:C:227:GLU:HB2	2.42	0.40
1:C:123:GLY:HA3	1:C:395:ARG:HB2	2.04	0.40
1:A:82:ASP:O	1:A:86:ASN:N	2.45	0.40
1:C:166:TYR:CB	1:C:421:ILE:HD12	2.50	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	520/566 (92%)	445 (86%)	53 (10%)	22 (4%)	3	9
1	B	490/566 (87%)	424 (86%)	50 (10%)	16 (3%)	4	13
1	C	484/566 (86%)	429 (89%)	43 (9%)	12 (2%)	5	19
All	All	1494/1698 (88%)	1298 (87%)	146 (10%)	50 (3%)	4	13

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	ASP
1	A	138	THR
1	A	139	VAL
1	A	228	LYS
1	A	274	PRO
1	A	489	LYS
1	B	130	ILE
1	B	140	SER
1	B	271	ILE
1	B	274	PRO

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Mol	Chain	Res	Type
1	A	132	GLU
1	A	151	GLY
1	A	294	ALA
1	B	59	ASN
1	B	291	ILE
1	B	432	GLY
1	B	513	ASN
1	C	127	LEU
1	C	231	GLU
1	C	268	ALA
1	C	429	SER
1	C	432	GLY
1	C	514	ALA
1	A	82	ASP
1	A	267	ALA
1	A	276	ASP
1	A	487	ALA
1	B	404	VAL
1	A	81	LYS
1	A	130	ILE
1	A	293	SER
1	A	387	ARG
1	A	388	ILE
1	B	275	SER
1	B	301	GLY
1	C	234	LEU
1	A	157	TYR
1	A	297	GLY
1	A	448	PRO
1	A	490	TRP
1	B	302	ILE
1	C	225	ILE
1	B	60	TRP
1	B	367	THR
1	C	433	ASP
1	B	299	GLY
1	C	74	VAL
1	C	511	GLY
1	C	226	GLY
1	B	225	ILE

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	410/443 (93%)	359 (88%)	51 (12%)	4	14
1	B	381/443 (86%)	348 (91%)	33 (9%)	10	30
1	C	382/443 (86%)	351 (92%)	31 (8%)	11	33
All	All	1173/1329 (88%)	1058 (90%)	115 (10%)	8	24

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	67	LEU
1	A	137	ARG
1	A	142	ILE
1	A	150	MET
1	A	157	TYR
1	A	159	THR
1	A	160	THR
1	A	167	ARG
1	A	170	VAL
1	A	174	ASP
1	A	202	LEU
1	A	213	ARG
1	A	214	LYS
1	A	222	VAL
1	A	228	LYS
1	A	265	LEU
1	A	277	TRP
1	A	279	ILE
1	A	283	VAL
1	A	285	VAL
1	A	290	PHE
1	A	300	LYS
1	A	303	GLN
1	A	305	LEU
1	A	307	ASN

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Mol	Chain	Res	Type
1	A	316	LEU
1	A	330	LEU
1	A	332	LEU
1	A	353	MET
1	A	358	THR
1	A	371	TRP
1	A	380	PHE
1	A	381	VAL
1	A	387	ARG
1	A	390	ARG
1	A	443	LEU
1	A	444	LEU
1	A	452	ILE
1	A	456	ILE
1	A	464	PHE
1	A	488	ASN
1	A	489	LYS
1	A	502	ILE
1	A	506	LEU
1	A	512	ASP
1	A	518	LEU
1	A	529	PHE
1	A	542	LYS
1	A	548	VAL
1	A	583	ARG
1	B	58	LEU
1	B	60	TRP
1	B	80	PHE
1	B	85	THR
1	B	117	ILE
1	B	125	ILE
1	B	126	ARG
1	B	127	LEU
1	B	138	THR
1	B	144	MET
1	B	152	ILE
1	B	191	LEU
1	B	207	SER
1	B	217	LEU
1	B	260	GLN
1	B	271	ILE
1	B	273	ASP

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Mol	Chain	Res	Type
1	B	292	PHE
1	B	309	ASN
1	B	310	MET
1	B	330	LEU
1	B	341	LEU
1	B	371	TRP
1	B	392	ARG
1	B	393	SER
1	B	451	GLN
1	B	464	PHE
1	B	465	PHE
1	B	475	VAL
1	B	504	LEU
1	B	508	LEU
1	B	515	LEU
1	B	518	LEU
1	C	76	TRP
1	C	80	PHE
1	C	92	LEU
1	C	99	LEU
1	C	121	LYS
1	C	126	ARG
1	C	153	ASP
1	C	160	THR
1	C	167	ARG
1	C	174	ASP
1	C	178	VAL
1	C	185	THR
1	C	211	VAL
1	C	217	LEU
1	C	231	GLU
1	C	233	TRP
1	C	234	LEU
1	C	241	LEU
1	C	277	TRP
1	C	323	VAL
1	C	371	TRP
1	C	374	TRP
1	C	377	TRP
1	C	388	ILE
1	C	437	GLU
1	C	439	GLN

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Mol	Chain	Res	Type
1	C	481	GLN
1	C	506	LEU
1	C	527	THR
1	C	542	LYS
1	C	553	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	260	GLN
1	A	307	ASN
1	A	439	GLN
1	A	517	ASN
1	B	343	ASN
1	B	481	GLN
1	B	482	HIS
1	B	517	ASN
1	C	98	ASN
1	C	331	ASN
1	C	346	GLN
1	C	482	HIS
1	C	520	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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$
2	1Y8	B	601	-	2,6,6	0.49	0	1,8,8	1.01	0
2	1Y8	A	601	-	2,6,6	0.52	0	1,8,8	0.91	0
5	CM5	C	604	-	36,36,36	1.52	5 (13%)	49,49,49	1.57	10 (20%)
5	CM5	C	602	-	36,36,36	1.48	6 (16%)	49,49,49	1.35	6 (12%)
2	1Y8	C	603	-	2,6,6	0.50	0	1,8,8	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1Y8	B	601	-	-	0/3/4/4	-
2	1Y8	A	601	-	-	0/3/4/4	-
2	1Y8	C	603	-	-	0/3/4/4	-
5	CM5	C	602	-	4/4/11/11	14/17/65/65	0/3/3/3
5	CM5	C	604	-	6/6/11/11	14/17/65/65	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	604	CM5	C17-C18	-4.93	1.39	1.52
5	C	602	CM5	C17-C18	-4.12	1.41	1.52
5	C	602	CM5	C17-C16	-3.87	1.41	1.52
5	C	604	CM5	C17-C16	-3.77	1.42	1.52
5	C	604	CM5	C28-C27	-3.69	1.42	1.52
5	C	602	CM5	C28-C27	-3.53	1.43	1.52
5	C	602	CM5	O21-C17	2.75	1.49	1.43
5	C	604	CM5	O21-C17	2.63	1.49	1.43
5	C	604	CM5	O25-C26	2.47	1.50	1.44
5	C	602	CM5	C27-C26	-2.14	1.48	1.53
5	C	602	CM5	O25-C26	2.13	1.49	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	602	CM5	C1-O12-C13	4.51	121.33	113.84
5	C	604	CM5	C1-O12-C13	4.15	120.73	113.84
5	C	604	CM5	O14-C15-C16	3.07	116.22	109.75
5	C	604	CM5	O25-C26-C27	2.90	114.96	109.69
5	C	604	CM5	O20-C19-C15	2.88	121.16	111.29
5	C	604	CM5	C24-C29-C28	2.83	115.89	110.00
5	C	604	CM5	O12-C1-C2	2.79	119.35	109.56
5	C	602	CM5	C18-C17-C16	2.74	115.95	109.68
5	C	604	CM5	C13-O14-C15	2.65	118.88	113.69
5	C	602	CM5	O12-C1-C2	2.55	118.49	109.56
5	C	602	CM5	C13-C18-C17	2.39	114.97	110.00
5	C	604	CM5	O23-C24-C29	2.32	114.11	108.10
5	C	604	CM5	O25-C26-C30	2.31	112.19	106.44
5	C	604	CM5	O31-C30-C26	2.21	118.86	111.29
5	C	602	CM5	O14-C15-C16	2.02	114.02	109.75
5	C	602	CM5	O31-C30-C26	2.02	118.21	111.29

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	604	CM5	C18
5	C	604	CM5	C16
5	C	604	CM5	C24
5	C	604	CM5	C27
5	C	604	CM5	C13
5	C	604	CM5	C28
5	C	602	CM5	C15
5	C	602	CM5	C18
5	C	602	CM5	C28
5	C	602	CM5	C24

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	604	CM5	C2-C1-O12-C13
5	C	604	CM5	O14-C13-O12-C1
5	C	602	CM5	C2-C1-O12-C13
5	C	602	CM5	O14-C13-O12-C1
5	C	604	CM5	O25-C24-O23-C16
5	C	604	CM5	C29-C24-O23-C16
5	C	602	CM5	C17-C16-O23-C24
5	C	602	CM5	C27-C26-C30-O31
5	C	602	CM5	O14-C15-C19-O20

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Mol	Chain	Res	Type	Atoms
5	C	604	CM5	C27-C26-C30-O31
5	C	602	CM5	O25-C26-C30-O31
5	C	602	CM5	C16-C15-C19-O20
5	C	604	CM5	O25-C26-C30-O31
5	C	604	CM5	C18-C13-O12-C1
5	C	604	CM5	C2-C3-C4-C5
5	C	602	CM5	C4-C5-C6-C11
5	C	602	CM5	O12-C1-C2-C3
5	C	604	CM5	C3-C4-C5-C6
5	C	604	CM5	O12-C1-C2-C3
5	C	602	CM5	C18-C13-O12-C1
5	C	602	CM5	C29-C24-O23-C16
5	C	602	CM5	C4-C5-C6-C7
5	C	602	CM5	O25-C24-O23-C16
5	C	604	CM5	C4-C5-C6-C11
5	C	602	CM5	C2-C3-C4-C5
5	C	604	CM5	C4-C5-C6-C7
5	C	604	CM5	C17-C16-O23-C24
5	C	604	CM5	C1-C2-C3-C4

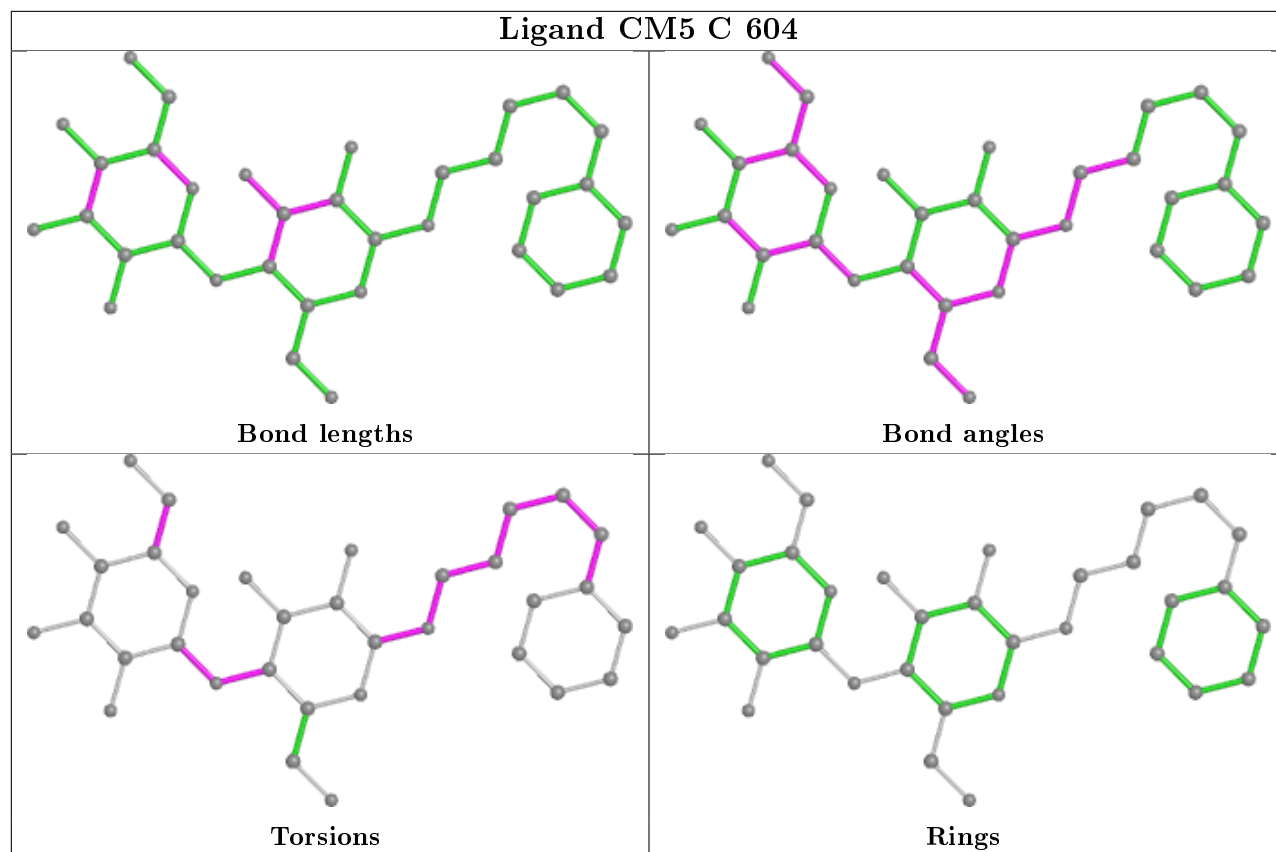
There are no ring outliers.

3 monomers are involved in 7 short contacts:

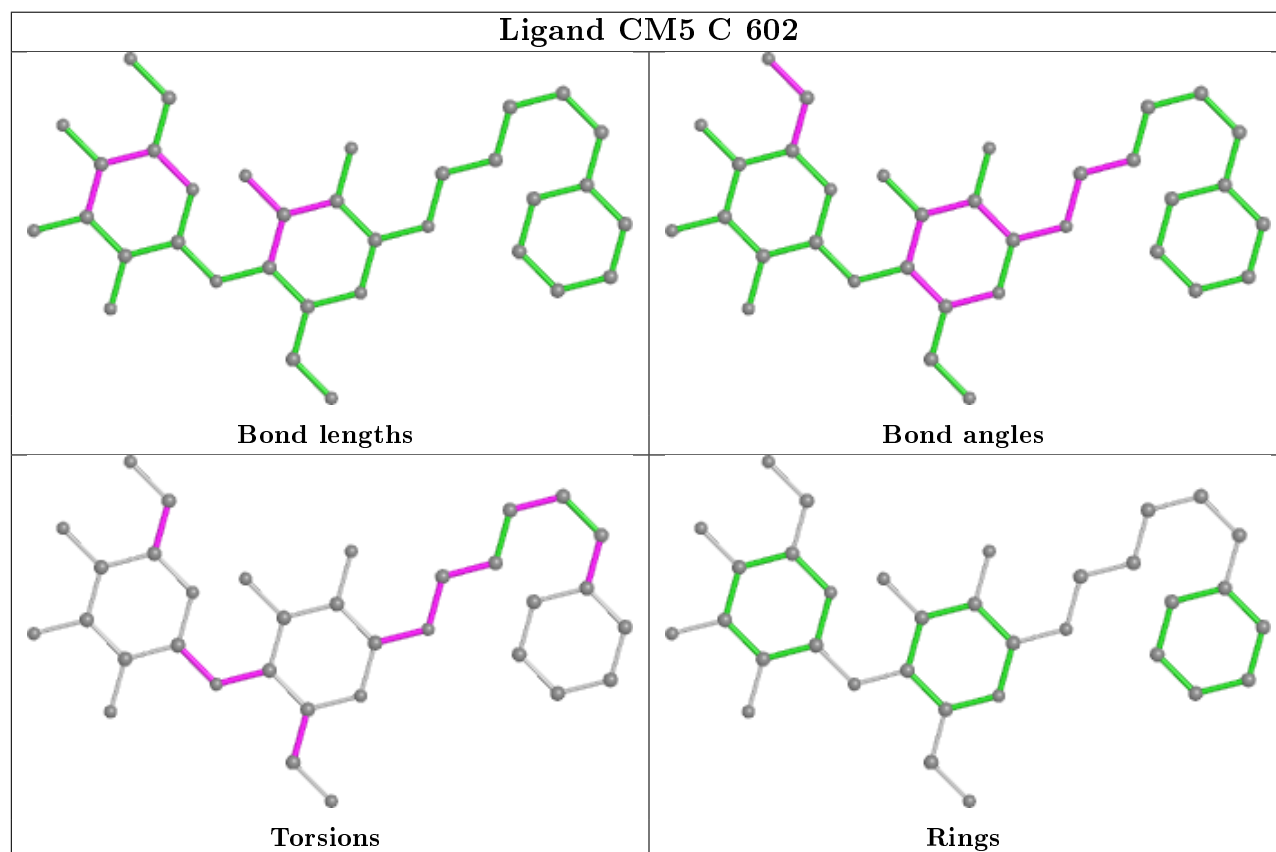
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	1Y8	2	0
5	C	604	CM5	3	0
5	C	602	CM5	2	0

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.

Ligand CM5 C 604



Ligand CM5 C 602



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	524/566 (92%)	0.31	49 (9%) 8 4	20, 68, 134, 227	0
1	B	492/566 (86%)	0.31	51 (10%) 6 3	16, 68, 151, 205	0
1	C	490/566 (86%)	0.00	37 (7%) 13 7	12, 50, 124, 192	0
All	All	1506/1698 (88%)	0.21	137 (9%) 9 5	12, 64, 136, 227	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	VAL	13.1
1	A	297	GLY	11.8
1	A	82	ASP	10.4
1	B	511	GLY	9.8
1	C	296	SER	9.4
1	B	490	TRP	8.3
1	A	486	GLU	7.3
1	A	86	ASN	7.2
1	B	488	ASN	6.8
1	A	296	SER	6.7
1	A	77	GLY	6.4
1	C	57	SER	6.2
1	B	269	ASN	6.0
1	B	226	GLY	5.9
1	C	269	ASN	5.5
1	C	292	PHE	5.5
1	C	486	GLU	5.1
1	A	83	SER	5.0
1	B	82	ASP	4.8
1	A	284	SER	4.7
1	C	288	LEU	4.3
1	B	78	ILE	4.2
1	C	293	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	487	ALA	4.0
1	C	277	TRP	4.0
1	A	81	LYS	4.0
1	B	481	GLN	4.0
1	C	484	GLN	4.0
1	B	512	ASP	3.9
1	A	299	GLY	3.9
1	A	234	LEU	3.7
1	C	488	ASN	3.7
1	B	58	LEU	3.6
1	C	253	SER	3.6
1	B	509	SER	3.6
1	A	78	ILE	3.5
1	A	277	TRP	3.5
1	A	509	SER	3.5
1	B	506	LEU	3.5
1	C	553	TYR	3.4
1	C	274	PRO	3.4
1	C	270	ILE	3.4
1	C	78	ILE	3.4
1	B	150	MET	3.3
1	A	511	GLY	3.3
1	B	377	TRP	3.3
1	C	256	LEU	3.2
1	C	291	ILE	3.2
1	B	275	SER	3.2
1	C	252	CYS	3.1
1	A	510	GLY	3.1
1	A	236	LYS	3.1
1	B	451	GLN	3.0
1	A	76	TRP	3.0
1	A	553	TYR	3.0
1	B	438	GLU	3.0
1	B	227	GLU	2.9
1	B	76	TRP	2.9
1	B	495	TRP	2.9
1	A	231	GLU	2.9
1	B	270	ILE	2.9
1	C	79	GLY	2.9
1	B	468	SER	2.8
1	B	149	GLY	2.8
1	C	152	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	275	SER	2.8
1	A	282	ILE	2.8
1	A	513	ASN	2.8
1	B	151	GLY	2.8
1	A	133	ALA	2.8
1	A	80	PHE	2.8
1	B	77	GLY	2.8
1	C	61	SER	2.7
1	A	280	VAL	2.7
1	B	84	PHE	2.7
1	A	64	VAL	2.7
1	A	237	LEU	2.7
1	B	62	VAL	2.7
1	C	250	THR	2.7
1	C	485	LEU	2.7
1	A	512	ASP	2.6
1	B	486	GLU	2.6
1	A	273	ASP	2.6
1	B	134	PRO	2.6
1	A	433	ASP	2.6
1	C	75	VAL	2.6
1	B	73	THR	2.5
1	C	153	ASP	2.5
1	B	86	ASN	2.5
1	A	506	LEU	2.5
1	A	75	VAL	2.5
1	C	74	VAL	2.5
1	A	240	ILE	2.5
1	C	550	TYR	2.5
1	A	150	MET	2.5
1	A	68	VAL	2.5
1	A	151	GLY	2.5
1	B	137	ARG	2.4
1	B	434	GLY	2.4
1	B	378	SER	2.4
1	C	302	ILE	2.4
1	A	427	GLY	2.4
1	A	281	GLY	2.4
1	A	227	GLU	2.3
1	B	389	SER	2.3
1	B	482	HIS	2.3
1	A	233	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	271	ILE	2.3
1	B	133	ALA	2.3
1	B	546	ASN	2.3
1	B	538	PHE	2.3
1	A	552	GLU	2.3
1	C	490	TRP	2.3
1	A	294	ALA	2.3
1	B	441	PHE	2.3
1	B	379	PRO	2.3
1	A	226	GLY	2.3
1	A	428	GLU	2.2
1	B	274	PRO	2.2
1	C	76	TRP	2.2
1	B	510	GLY	2.2
1	A	514	ALA	2.2
1	B	396	GLU	2.2
1	B	374	TRP	2.2
1	C	289	ALA	2.1
1	B	98	ASN	2.1
1	B	75	VAL	2.1
1	B	276	ASP	2.1
1	C	251	ALA	2.1
1	A	377	TRP	2.1
1	B	433	ASP	2.0
1	C	295	ILE	2.0
1	A	90	SER	2.0
1	B	541	VAL	2.0
1	C	257	GLY	2.0
1	C	268	ALA	2.0
1	C	373	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

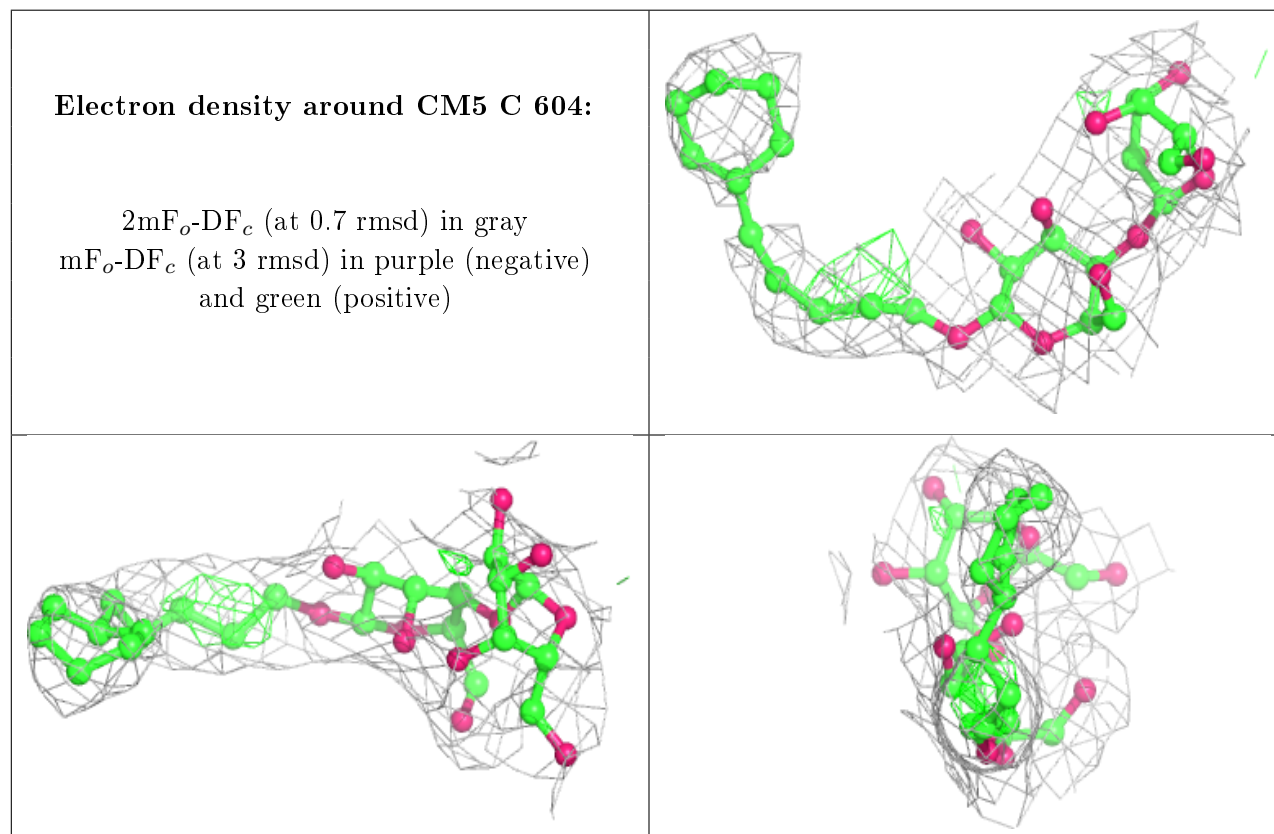
There are no carbohydrates in this entry.

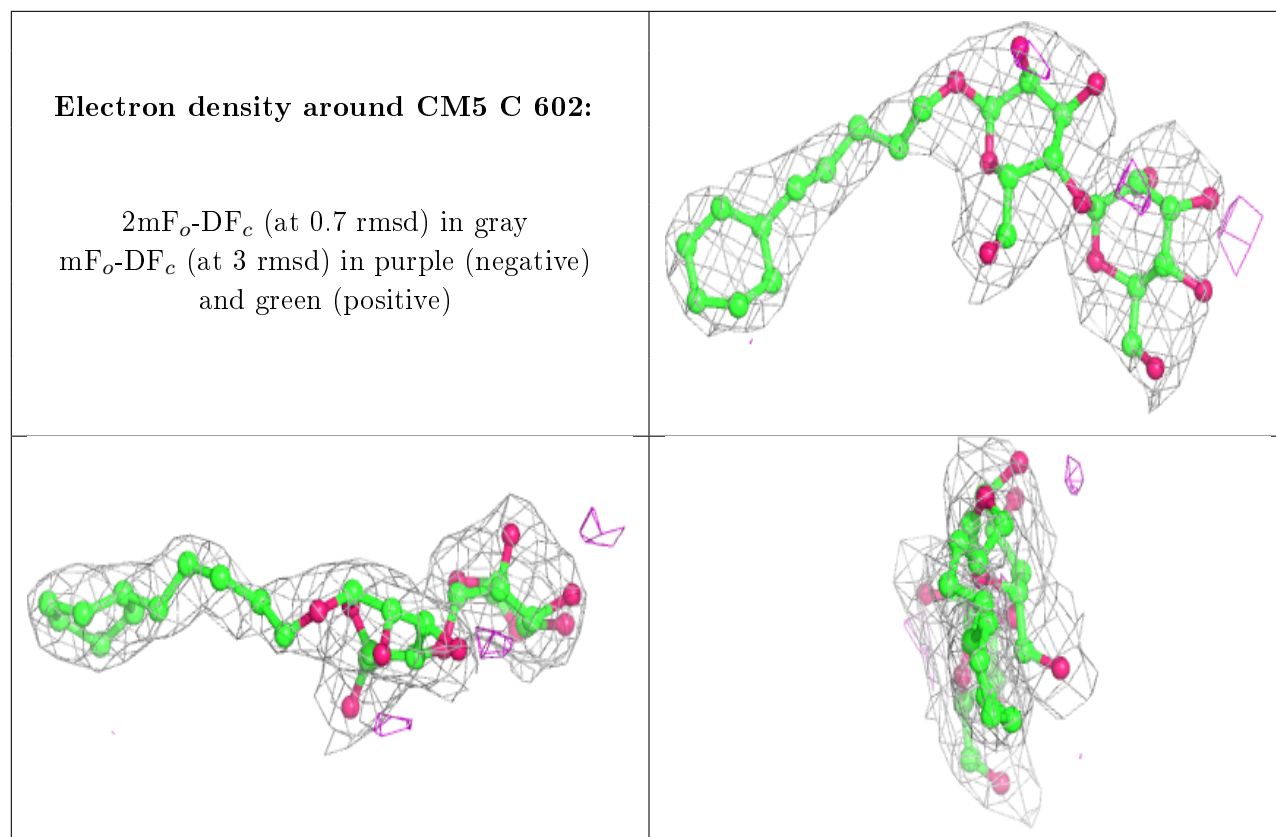
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CM5	C	604	34/34	0.77	0.23	94,126,142,144	0
3	NA	A	602	1/1	0.80	0.35	62,62,62,62	0
3	NA	B	602	1/1	0.89	1.27	96,96,96,96	0
2	1Y8	C	603	7/7	0.90	0.64	48,89,134,236	0
2	1Y8	A	601	7/7	0.95	0.27	44,95,161,167	0
5	CM5	C	602	34/34	0.95	0.27	42,67,71,71	0
2	1Y8	B	601	7/7	0.97	0.28	86,96,132,230	0
4	CL	C	601	1/1	0.98	0.06	37,37,37,37	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.