



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:11 AM UTC

PDB ID : 4LLH / pdb_00004llh
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 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

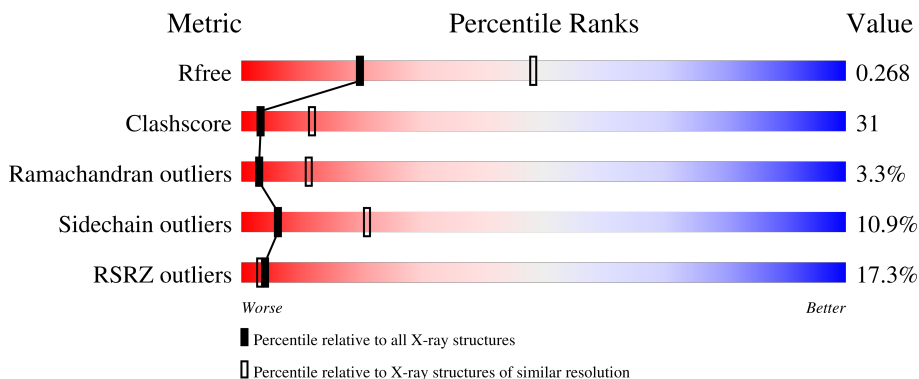
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	566	
1	B	566	
1	C	566	

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.

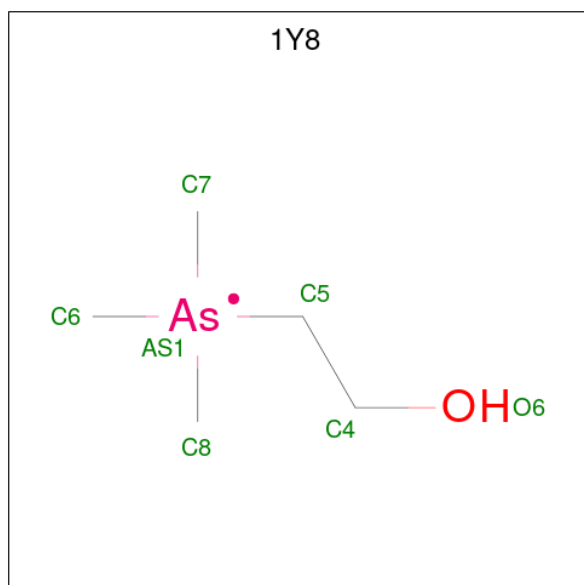
- Molecule 1 is a protein called Glycine betaine transporter BetP.

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 (CCD ID: 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		

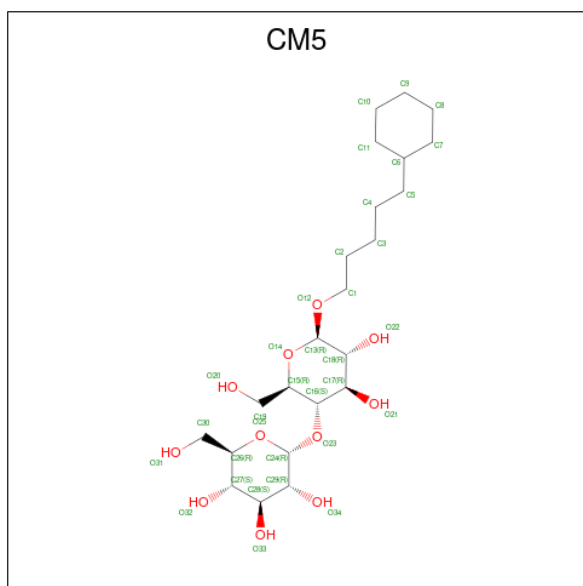
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (CCD ID: 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-MALTOSIDE (CCD ID: 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.

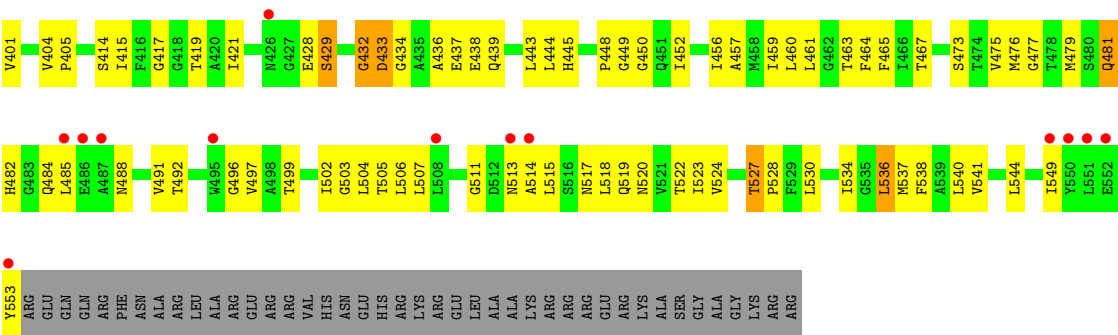
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total	O	0	0
			25	25		
6	B	26	Total	O	0	0
			26	26		
6	C	40	Total	O	0	0
			40	40		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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: 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 36.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.5 (36.30-2.80) 75.7 (36.30-2.80)	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 (Not available) , 0.268	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)	0.26 , 62.6	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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/4102	0.73	1/5584 (0.0%)
1	B	0.31	0/3798	0.72	3/5184 (0.1%)
1	C	0.33	0/3801	0.72	1/5186 (0.0%)
All	All	0.32	0/11701	0.72	5/15954 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	GLY	N-CA-C	-5.93	107.55	115.32
1	B	512	ASP	CB-CA-C	-5.17	110.59	116.54
1	C	228	LYS	CB-CA-C	-5.10	109.72	115.79
1	B	141	TRP	N-CA-C	-5.09	105.00	111.11
1	B	401	VAL	N-CA-C	-5.02	108.23	113.10

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	4001	0	4032	246	0
1	B	3701	0	3723	271	0
1	C	3704	0	3730	207	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
6	A	25	0	0	3	0
6	B	26	0	0	3	0
6	C	40	0	0	6	0
All	All	11589	0	11578	717	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 31.

All (717) 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:C:184:THR:HA	1:C:347:MET:HE1	1.30	1.09
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:O22	5:C:604:CM5:H11	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:B:476:MET:HE2	1:B:495:TRP:HE3	1.43	0.83
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:182:MET:HE3	1:C:332:LEU:HD13	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LYS:H	1:A:214:LYS:HD2	1.47	0.79
1:C:155:MET:HE3	1:C:464:PHE:HE2	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:A:292:PHE:HA	1:A:293:SER:C	2.10	0.76
1:C:354:SER:O	1:C:359:ALA:HB3	1.86	0.76
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:A:150:MET:HE2	1:A:374:TRP:HZ3	1.51	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:H29	5:C:604:CM5:C17	2.18	0.72
1:B:144:MET:HG2	1:B:303:GLN:OE1	1.89	0.72
1:A:248:PHE:HB3	1:A:522:THR:CG2	2.18	0.72
1:A:292:PHE:HA	1:A:293:SER:O	1.89	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:C:227:GLU:C	1:C:228:LYS:HD2	2.14	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:144:MET:HE3	1:B:303:GLN:NE2	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:PHE:CD1	1:B:310:MET:HE1	2.25	0.70
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:A:387:ARG:C	1:A:389:SER:H	2.01	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
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:60:TRP:HD1	1:B:60:TRP:O	1.77	0.68
1:B:280:VAL:HG22	1:B:504:LEU:HD21	1.75	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:60:TRP:CD1	1:B:60:TRP:C	2.72	0.67
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:150:MET:HE2	1:A:374:TRP:CZ3	2.29	0.67
1:A:518:LEU:O	1:A:522:THR:HG23	1.94	0.67
1:A:203:ALA:HA	1:A:540:LEU:HD23	1.76	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:186:MET:HE1	1:B:336:SER:O	1.95	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:C:226:GLY:HA2	1:C:227:GLU:C	2.21	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:74:VAL:HG13	1:C:502:ILE:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2.52	0.62
1:B:213:ARG:HB3	1:B:219:SER:HB2	1.81	0.62
1:B:300:LYS:O	1:B:304:TYR:HB3	1.99	0.62
1:B:290:PHE:C	1:B:292:PHE:H	2.07	0.62
1:B:243:ILE:O	1:B:247:VAL:HG23	2.00	0.62
1:C:121:LYS:HD3	1:C:121:LYS:N	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:A:290:PHE:CD1	1:A:290:PHE:C	2.77	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:85:THR:HA	1:B:517:ASN:ND2	2.15	0.61
1:B:243:ILE:HA	1:B:246:THR:HG22	1.83	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:475:VAL:HG23	1:B:479:MET:HE3	1.83	0.61
1:A:215:GLN:CD	1:A:387:ARG:HH22	2.07	0.61
1:B:58:LEU:O	1:B:59:ASN:C	2.43	0.61
1:C:184:THR:HA	1:C:347:MET:CE	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:476:MET:HE2	1:B:495:TRP:CE3	2.33	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:353:MET:HE3	1:A:353:MET:HA	1.85	0.58
1:A:155:MET:HE3	1:A:440:LEU:HD11	1.85	0.58
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:233:TRP:H	1:C:233:TRP:CD1	2.22	0.58
1:C:477:GLY:O	1:C:481:GLN:HG3	2.04	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
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:150:MET:HE1	1:B:374:TRP:HH2	1.69	0.57
1:B:290:PHE:HB3	1:B:466:ILE:HG13	1.86	0.57
1:C:58:LEU:HA	1:C:481:GLN:HB3	1.86	0.57
1:C:475:VAL:O	1:C:479:MET:HG2	2.03	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:85:THR:HG23	1:A:517:ASN:HD21	1.70	0.57
1:A:284:SER:HA	1:A:287:THR:HG22	1.87	0.57
1:A:142:ILE:HD13	1:A:142:ILE:H	1.70	0.57
1:B:158:GLY:HA2	1:B:413:PHE:CE1	2.40	0.57
1:B:343:ASN:O	1:B:347:MET:HG2	2.03	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:B:70:VAL:HG21	1:B:247:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:MET:HE1	1:B:401:VAL:HB	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: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: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:HD12	1:A:295:ILE:N	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
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:387:ARG:C	1:A:388:ILE:HG13	2.31	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:B:530:LEU:C	1:B:530:LEU:HD23	2.32	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:76:TRP:O	1:C:84:PHE:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:THR:O	1:C:254:LEU:HG	2.07	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:B:225:ILE:C	1:B:227:GLU:H	2.16	0.54
1:A:141:TRP:CD1	1:A:388:ILE:HG22	2.23	0.54
1:C:92:LEU:HD22	1:C:520:ASN:CG	2.33	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:HD3	1:C:121:LYS:H	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:76:TRP:CD1	1:A:84:PHE:HD1	2.26	0.53
1:A:262:GLY:HA2	1:A:265:LEU:HB2	1.90	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
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:C:473:SER:HA	1:C:476:MET:HE3	1.90	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:A:443:LEU:HD12	1:A:443:LEU:C	2.34	0.53
1:B:134:PRO:HB3	1:B:392:ARG:NH1	2.24	0.53
1:B:302:ILE:HG21	1:B:384:PHE:HZ	1.74	0.53
1:C:233:TRP:H	1:C:233:TRP:HD1	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:228:LYS:C	1:C:230:ALA:H	2.18	0.52
1:A:121:LYS:C	1:A:123:GLY:H	2.16	0.52
1:A:260:GLN:NE2	1:A:437:GLU:HG3	2.16	0.52
1:B:155:MET:HE1	1:B:460:LEU:HD13	1.91	0.52
1:C:329:ILE:HD11	1:C:419:THR:CG2	2.40	0.52
1:A:76:TRP:HD1	1:A:84:PHE:HD1	1.57	0.52
1:A:355:ALA:O	1:A:358:THR:HB	2.10	0.52
1:B:141:TRP:HZ3	1:B:388:ILE:HB	1.73	0.52
1:C:155:MET:HE3	1:C:464:PHE:CE2	2.38	0.52
1:A:346:GLN:HG3	6:C:702:HOH:O	2.09	0.52
1:B:110:PHE:CZ	1:B:534:ILE:HD13	2.44	0.52
1:B:246:THR:OG1	1:B:380:PHE:HB3	2.10	0.52
1:B:351:THR:HG23	1:B:353:MET:HB2	1.92	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:273:ASP:O	1:B:274:PRO:C	2.54	0.50
1:C:303:GLN:CD	1:C:303:GLN:H	2.19	0.50
1:A:370:TYR:O	1:A:374:TRP:HD1	1.94	0.50
1:B:290:PHE:HB3	1:B:466:ILE:CG1	2.41	0.50
1:C:323:VAL:CG2	1:C:448:PRO:HG2	2.41	0.50
1:C:383:MET:HG3	1:C:475:VAL:CG1	2.42	0.50
1:B:261:ILE:CG2	1:B:458:MET:HE1	2.40	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:N	1:A:380:PHE:CD2	2.71	0.50
1:B:219:SER:HA	1:B:222:VAL:HG23	1.94	0.50
1:B:229:GLY:C	1:B:231:GLU:H	2.19	0.50
1:A:261:ILE:HD12	1:A:461:LEU:HD13	1.92	0.50
1:A:387:ARG:HG2	1:A:388:ILE:HG13	1.94	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: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:78:ILE:HD11	1:A:506:LEU:HA	1.93	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:B:322:VAL:HG23	1:B:323:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:331:ASN:HB3	1:B:351:THR:OG1	2.13	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:C:322:VAL:HG23	1:C:323:VAL:N	2.27	0.49
1:C:428:GLU:O	1:C:429:SER:C	2.54	0.49
1:B:60:TRP:C	1:B:62:VAL:H	2.20	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:103:PHE:CD1	1:B:530:LEU:HD12	2.47	0.49
1:B:161:GLU:OE1	1:B:366:TRP:HZ3	1.96	0.49
1:B:226:GLY:C	1:B:228:LYS:H	2.20	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: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:200:VAL:HG21	1:C:378:SER:HB2	1.95	0.48
1:C:206:TYR:CE1	1:C:210:ARG:HG2	2.48	0.48
1:A:260:GLN:C	1:A:260:GLN:CD	2.81	0.48
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:B:274:PRO:O	1:B:275:SER:C	2.56	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:57:SER:HB2	1:B:482:HIS:HD2	1.77	0.48
1:B:334:PRO:HG2	1:C:351:THR:HG21	1.95	0.48
1:A:387:ARG:O	1:A:389:SER:N	2.45	0.48
1:B:106:PHE:CD1	1:B:534:ILE:HD12	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:366:TRP:O	1:B:367:THR:C	2.56	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:59:ASN:C	1:A:59:ASN:HD22	2.22	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: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:B:183:SER:HA	1:B:186:MET:HE3	1.95	0.48
1:C:247:VAL:HG12	1:C:502:ILE:HD11	1.95	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: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:B:398:ILE:C	1:B:400:GLY:H	2.22	0.47
1:A:476:MET:HE2	1:A:495:TRP:HB3	1.95	0.47
1:B:62:VAL:C	1:B:65:PRO:HD2	2.39	0.47
1:C:233:TRP:CD1	1:C:233:TRP:N	2.82	0.47
1:A:92:LEU:HD12	1:A:92:LEU:C	2.40	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
1:B:541:VAL:C	1:B:543:ASP:H	2.21	0.47
1:C:58:LEU:HB3	1:C:63:ILE:CD1	2.44	0.47
1:C:73:THR:C	1:C:75:VAL:H	2.21	0.47
1:C:121:LYS:N	1:C:121:LYS:CD	2.76	0.47
1:A:66:ALA:O	1:A:70:VAL:HG23	2.15	0.47
1:A:160:THR:HB	1:A:439:GLN:HE22	1.74	0.47
1:A:74:VAL:HG22	1:A:502:ILE:HG23	1.97	0.47
1:A:112:PHE:O	1:A:116:VAL:HG13	2.14	0.47
1:B:200:VAL:O	1:B:204:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:THR:N	1:B:528:PRO:CD	2.77	0.47
1:C:162:PRO:HG3	1:C:417:GLY:HA3	1.96	0.47
1:C:193:PRO:HB3	1:C:374:TRP:CD1	2.50	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: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:290:PHE:C	1:B:292:PHE:N	2.71	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: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:A:121:LYS:C	1:A:123:GLY:N	2.70	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:240:ILE:O	1:B:244:ILE:HG13	2.16	0.45
1:B:329:ILE:HG21	1:B:415:ILE:HG12	1.98	0.45
1:C:347:MET:HE3	6:C:739:HOH:O	2.16	0.45
1:A:197:TYR:CZ	1:A:381:VAL:HG21	2.51	0.45
1:A:464:PHE:HD1	1:A:464:PHE:HA	1.67	0.45
1:B:295:ILE:C	1:B:297:GLY:H	2.23	0.45
1:B:319:PHE:CE2	1:B:453:MET:HG3	2.50	0.45
1:A:329:ILE:HD13	1:A:415:ILE:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:432:GLY:C	1:B:434:GLY:H	2.24	0.45
1:B:470:ASP:O	1:B:474:THR:HG23	2.16	0.45
1:C:216:LEU:CD2	1:C:479:MET:HA	2.47	0.45
1:C:225:ILE:C	1:C:227:GLU:HB2	2.42	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: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:379:PRO:HG3	1:B:529:PHE:CZ	2.52	0.45
1:B:515:LEU:HA	1:B:515:LEU:HD12	1.81	0.45
1:C:61:SER:O	1:C:65:PRO:HG2	2.16	0.45
1:C:114:ILE:HD12	1:C:114:ILE:HA	1.82	0.45
1:C:265:LEU:C	1:C:267:ALA:H	2.24	0.45
1:C:385:LEU:HD13	1:C:401:VAL:HG11	1.99	0.45
1:A:260:GLN:O	1:A:261:ILE:C	2.60	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:475:VAL:HG12	1:A:479:MET:HE3	1.99	0.44
1:A:155:MET:SD	1:A:460:LEU:HD23	2.57	0.44
1:A:85:THR:HG23	1:A:517:ASN:ND2	2.31	0.44
1:A:216:LEU:HD21	1:A:239:ASP:OD2	2.18	0.44
1:B:140:SER:HA	1:B:143:SER:HB2	1.99	0.44
1:A:81:LYS:HA	1:A:84:PHE:HB3	1.98	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:210:ARG:NH2	1:A:549:ILE:HD12	2.31	0.44
1:A:473:SER:HA	1:A:476:MET:HG2	1.99	0.44
1:B:88:ALA:HB3	1:B:517:ASN:HD22	1.82	0.44
1:B:144:MET:N	1:B:144:MET:HE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:178:VAL:O	1:C:179:GLY:C	2.61	0.44
1:A:88:ALA:HB3	1:A:517:ASN:HB3	1.99	0.44
1:A:475:VAL:CG1	1:A:479:MET:HE3	2.47	0.44
1:B:137:ARG:HD2	1:B:137:ARG:N	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: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:C:225:ILE:O	1:C:226:GLY:C	2.61	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:508:LEU:HD13	1:B:509:SER:H	1.83	0.43
1:C:395:ARG:HE	1:C:395:ARG:HB2	1.43	0.43
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:B:70:VAL:HA	1:B:248:PHE:CZ	2.54	0.43
1:B:319:PHE:CB	1:B:453:MET:HE2	2.49	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:81:LYS:O	1:B:83:SER:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:301:GLY:O	1:B:302:ILE:C	2.61	0.43
1:C:62:VAL:HG13	1:C:240:ILE:HD12	2.01	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: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:71:LEU:HA	1:C:74:VAL:CG2	2.49	0.43
1:C:261:ILE:HB	1:C:282:ILE:HD13	2.00	0.43
1:A:78:ILE:HD12	1:A:78:ILE:N	2.33	0.43
1:A:449:GLY:O	1:A:452:ILE:HG12	2.19	0.43
1:C:92:LEU:HD22	1:C:520:ASN:ND2	2.33	0.43
1:C:146:PHE:CE1	1:C:404:VAL:HG13	2.53	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:C:263:ALA:HB1	1:C:438:GLU:HB3	2.00	0.43
1:C:312:LEU:HB3	1:C:460:LEU:HD22	1.99	0.43
1:C:432:GLY:C	1:C:434:GLY:H	2.27	0.43
1:A:251:ALA:O	1:A:254:LEU:HB3	2.19	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:B:508:LEU:C	1:B:508:LEU:HD22	2.44	0.42
1:C:194:TRP:CZ2	1:C:405:PRO:HB3	2.54	0.42
1:A:371:TRP:CE3	1:A:371:TRP:HA	2.54	0.42
1:B:139:VAL:O	1:B:140:SER:HB3	2.20	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
1:B:155:MET:HE3	1:B:460:LEU:HD22	2.01	0.42
1:B:203:ALA:O	1:B:207:SER:HB3	2.19	0.42
1:B:481:GLN:C	1:B:483:GLY:H	2.27	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:110:PHE:CZ	1:A:534:ILE:HD13	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ILE:HD11	1:B:206:TYR:HE1	1.84	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: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:O	1:C:295:ILE:HG22	2.19	0.42
1:A:65:PRO:O	1:A:68:VAL:HG22	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:183:SER:C	1:A:347:MET:HE1	2.44	0.42
1:B:70:VAL:HG21	1:B:247:VAL:CG1	2.49	0.42
1:B:228:LYS:HA	1:B:228:LYS:HD3	1.84	0.42
1:C:463:THR:O	1:C:467:THR:HG23	2.20	0.42
1:A:248:PHE:CB	1:A:522:THR:HG22	2.40	0.42
1:A:435:ALA:HB3	1:A:438:GLU:HG2	2.02	0.42
1:B:190:THR:O	1:B:193:PRO:HD2	2.19	0.42
1:B:261:ILE:HG23	1:B:458:MET:HE1	2.01	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:HD12	1:C:485:LEU:N	2.35	0.42
1:B:130:ILE:HG23	1:B:131:ASP:N	2.35	0.42
1:C:58:LEU:HB3	1:C:63:ILE:HD11	2.02	0.42
1:C:133:ALA:HB1	1:C:134:PRO:HD2	2.02	0.42
1:A:67:LEU:O	1:A:71:LEU:HG	2.20	0.42
1:A:300:LYS:HG3	1:A:303:GLN:HG3	2.01	0.42
1:A:488:ASN:O	1:A:489:LYS:C	2.61	0.42
1:B:137:ARG:HA	1:B:137:ARG:NE	2.35	0.42
1:B:234:LEU:O	1:B:235:GLY:C	2.62	0.42
1:C:325:PRO:HB2	1:C:328:SER:HB2	2.00	0.42
1:C:374:TRP:HA	1:C:374:TRP:CE3	2.55	0.42
1:B:481:GLN:HE22	1:B:488:ASN:HB2	1.84	0.42
1:C:117:ILE:HD13	1:C:117:ILE:HA	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:60:TRP:O	1:B:61:SER:HB3	2.19	0.41
1:B:138:THR:O	1:B:141:TRP:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:295:ILE:HD12	1:A:295:ILE:H	1.84	0.41
1:B:64:VAL:O	1:B:68:VAL:HG13	2.20	0.41
1:B:485:LEU:HD23	1:B:485:LEU:C	2.45	0.41
1:A:291:ILE:O	1:A:291:ILE:HG22	2.20	0.41
1:C:58:LEU:H	1:C:58:LEU:HD12	1.86	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:A:349:GLY:O	1:C:335:GLY:HA2	2.21	0.41
1:C:160:THR:HG21	1:C:436:ALA:HB1	2.01	0.41
1:C:251:ALA:CB	1:C:502:ILE:HG13	2.50	0.41
1:C:371:TRP:HA	1:C:371:TRP:CE3	2.56	0.41
1:A:81:LYS:O	1:A:83:SER:N	2.53	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:B:209:PHE:CD2	1:B:390:ARG:HA	2.55	0.41
1:B:211:VAL:HG11	1:B:213:ARG:NE	2.35	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:433:ASP:OD1	1:C:433:ASP:C	2.63	0.41
1:C:536:LEU:HD12	1:C:536:LEU:HA	1.96	0.41
1:B:188:HIS:CD2	6:B:726:HOH:O	2.73	0.41
1:C:210:ARG:HH22	1:C:549:ILE:HG12	1.84	0.41
1:C:380:PHE:CD1	1:C:475:VAL:HG21	2.50	0.41
1:A:305:LEU:N	1:A:305:LEU:CD2	2.83	0.41
1:A:331:ASN:OD1	1:B:101:TRP:HB3	2.20	0.41
1:A:387:ARG:C	1:A:389:SER:N	2.68	0.41
1:B:152:ILE:HG22	1:B:465:PHE:HB2	2.03	0.41
1:B:204:ILE:HD13	1:B:220:ALA:HB2	2.03	0.41
1:B:213:ARG:NH1	1:B:222:VAL:HB	2.33	0.41
1:B:225:ILE:C	1:B:227:GLU:N	2.78	0.41
1:B:290:PHE:O	1:B:291:ILE:HB	2.20	0.41
1:C:62:VAL:C	1:C:65:PRO:HD2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:152:ILE:CG2	1:B:465:PHE:HB2	2.51	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: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: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:359:ALA:O	1:B:363:LEU:HG	2.21	0.41
1:B:401:VAL:O	1:B:401:VAL:HG22	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: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:57:SER:HB2	1:B:482:HIS:CD2	2.56	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:512:ASP:CG	1:B:513:ASN:H	2.29	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:A:304:TYR:CD1	1:A:304:TYR:C	2.99	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: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
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: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

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	520/566 (92%)	445 (86%)	53 (10%)	22 (4%)	2	7
1	B	490/566 (87%)	424 (86%)	50 (10%)	16 (3%)	3	11
1	C	484/566 (86%)	429 (89%)	43 (9%)	12 (2%)	4	16
All	All	1494/1698 (88%)	1298 (87%)	146 (10%)	50 (3%)	3	11

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
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

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Mol	Chain	Res	Type
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%)	354 (86%)	56 (14%)	3	13
1	B	381/443 (86%)	341 (90%)	40 (10%)	6	22
1	C	382/443 (86%)	350 (92%)	32 (8%)	10	32
All	All	1173/1329 (88%)	1045 (89%)	128 (11%)	6	21

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	67	LEU
1	A	92	LEU
1	A	116	VAL
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	279	ILE
1	A	283	VAL
1	A	285	VAL
1	A	290	PHE
1	A	300	LYS
1	A	305	LEU
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	375	ILE
1	A	380	PHE
1	A	381	VAL
1	A	387	ARG
1	A	388	ILE
1	A	390	ARG
1	A	408	VAL
1	A	410	THR
1	A	411	VAL
1	A	415	ILE
1	A	443	LEU

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Mol	Chain	Res	Type
1	A	452	ILE
1	A	456	ILE
1	A	464	PHE
1	A	466	ILE
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	540	LEU
1	A	542	LYS
1	A	548	VAL
1	A	583	ARG
1	B	58	LEU
1	B	60	TRP
1	B	62	VAL
1	B	80	PHE
1	B	81	LYS
1	B	85	THR
1	B	95	VAL
1	B	104	ILE
1	B	117	ILE
1	B	125	ILE
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
1	B	292	PHE
1	B	302	ILE
1	B	309	ASN
1	B	310	MET
1	B	320	VAL
1	B	330	LEU
1	B	341	LEU
1	B	371	TRP
1	B	375	ILE

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Mol	Chain	Res	Type
1	B	393	SER
1	B	451	GLN
1	B	459	ILE
1	B	464	PHE
1	B	466	ILE
1	B	475	VAL
1	B	504	LEU
1	B	508	LEU
1	B	515	LEU
1	B	517	ASN
1	B	518	LEU
1	B	524	VAL
1	C	76	TRP
1	C	78	ILE
1	C	92	LEU
1	C	99	LEU
1	C	114	ILE
1	C	116	VAL
1	C	121	LYS
1	C	126	ARG
1	C	153	ASP
1	C	160	THR
1	C	167	ARG
1	C	178	VAL
1	C	185	THR
1	C	211	VAL
1	C	217	LEU
1	C	231	GLU
1	C	234	LEU
1	C	236	LYS
1	C	241	LEU
1	C	277	TRP
1	C	315	LEU
1	C	323	VAL
1	C	358	THR
1	C	371	TRP
1	C	388	ILE
1	C	437	GLU
1	C	439	GLN
1	C	481	GLN
1	C	506	LEU
1	C	527	THR

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Mol	Chain	Res	Type
1	C	536	LEU
1	C	553	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	260	GLN
1	A	439	GLN
1	A	517	ASN
1	A	556	GLN
1	A	557	GLN
1	B	269	ASN
1	B	343	ASN
1	B	426	ASN
1	B	481	GLN
1	B	482	HIS
1	B	517	ASN
1	C	98	ASN
1	C	331	ASN
1	C	451	GLN
1	C	481	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 oligosaccharides 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	A	601	-	2,6,6	0.53	0	1,8,8	0.89	0
2	1Y8	C	603	-	2,6,6	0.51	0	1,8,8	0.91	0
5	CM5	C	604	-	36,36,36	1.50	5 (13%)	49,49,49	1.58	11 (22%)
2	1Y8	B	601	-	2,6,6	0.50	0	1,8,8	0.99	0
5	CM5	C	602	-	36,36,36	1.46	6 (16%)	49,49,49	1.36	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1Y8	A	601	-	-	0/3/4/4	-
2	1Y8	C	603	-	-	0/3/4/4	-
5	CM5	C	604	-	6/6/11/11	15/17/65/65	0/3/3/3
2	1Y8	B	601	-	-	0/3/4/4	-
5	CM5	C	602	-	4/4/11/11	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	-4.84	1.39	1.52
5	C	602	CM5	C17-C18	-4.05	1.41	1.52
5	C	602	CM5	C17-C16	-3.80	1.41	1.52
5	C	604	CM5	C17-C16	-3.70	1.42	1.52
5	C	604	CM5	C28-C27	-3.62	1.42	1.52
5	C	602	CM5	C28-C27	-3.47	1.43	1.52
5	C	602	CM5	O21-C17	2.63	1.49	1.43
5	C	604	CM5	O21-C17	2.51	1.49	1.43
5	C	604	CM5	O25-C26	2.44	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	602	CM5	O25-C26	2.10	1.49	1.44
5	C	602	CM5	C27-C26	-2.10	1.48	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	602	CM5	C1-O12-C13	4.48	121.33	113.68
5	C	604	CM5	C1-O12-C13	4.13	120.73	113.68
5	C	604	CM5	O14-C15-C16	3.14	116.22	109.72
5	C	604	CM5	O12-C1-C2	2.94	119.35	109.37
5	C	604	CM5	O25-C26-C27	2.92	114.96	109.70
5	C	604	CM5	O20-C19-C15	2.89	121.16	111.33
5	C	604	CM5	C24-C29-C28	2.80	115.89	110.01
5	C	602	CM5	C18-C17-C16	2.76	115.95	109.68
5	C	602	CM5	O12-C1-C2	2.69	118.49	109.37
5	C	604	CM5	C13-O14-C15	2.64	118.88	113.72
5	C	604	CM5	O23-C24-C29	2.45	114.11	108.09
5	C	602	CM5	C13-C18-C17	2.36	114.97	110.01
5	C	604	CM5	O25-C26-C30	2.32	112.19	106.44
5	C	604	CM5	O31-C30-C26	2.21	118.86	111.33
5	C	602	CM5	O14-C15-C16	2.08	114.02	109.72
5	C	604	CM5	O12-C13-C18	2.03	111.36	108.27
5	C	602	CM5	O31-C30-C26	2.02	118.21	111.33

All (10) chirality outliers are listed below:

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

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	602	CM5	C2-C1-O12-C13

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Mol	Chain	Res	Type	Atoms
5	C	602	CM5	O14-C13-O12-C1
5	C	604	CM5	C2-C1-O12-C13
5	C	604	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
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	O12-C1-C2-C3
5	C	602	CM5	C4-C5-C6-C11
5	C	602	CM5	C18-C13-O12-C1
5	C	604	CM5	O12-C1-C2-C3
5	C	604	CM5	C3-C4-C5-C6
5	C	602	CM5	C4-C5-C6-C7
5	C	602	CM5	C29-C24-O23-C16
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	C17-C16-O23-C24
5	C	604	CM5	C4-C5-C6-C7
5	C	604	CM5	C1-C2-C3-C4
5	C	604	CM5	C15-C16-O23-C24

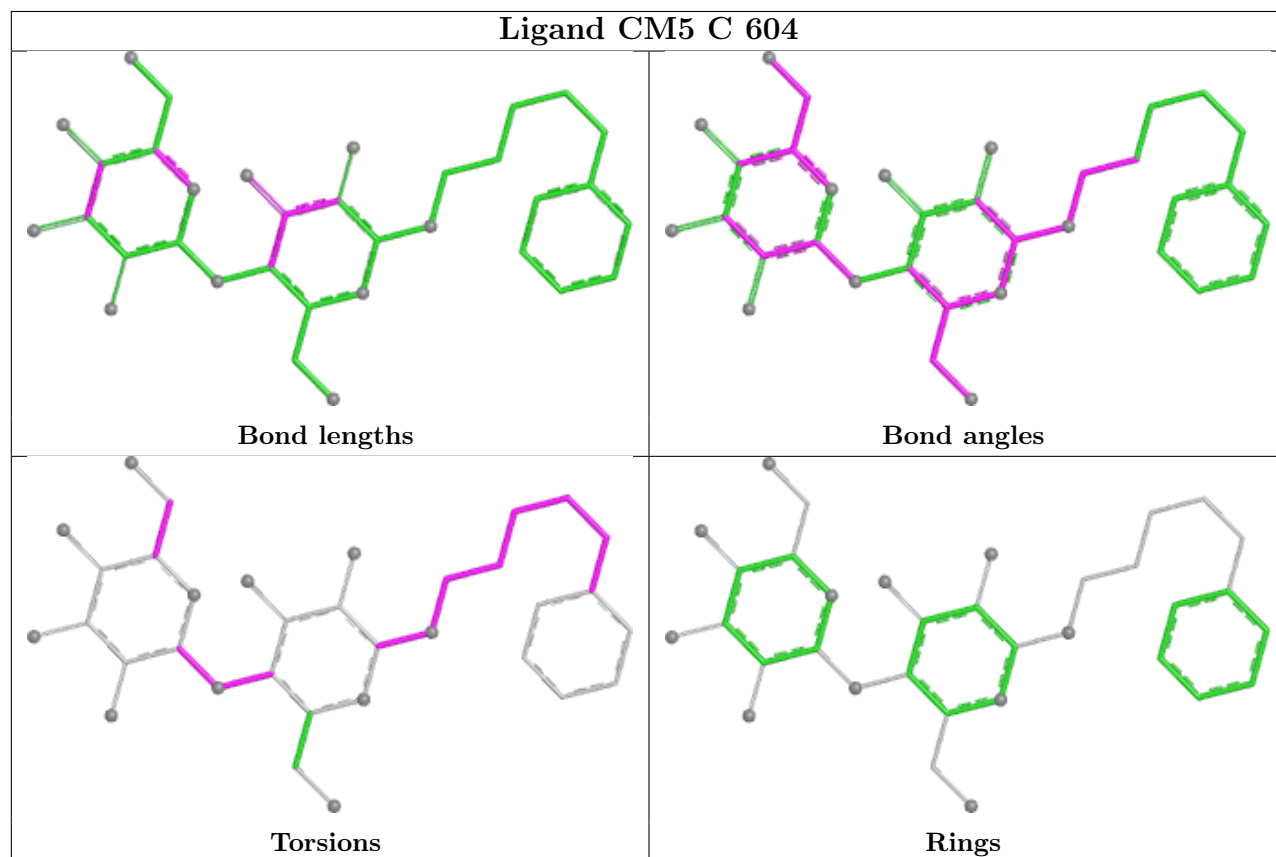
There are no ring outliers.

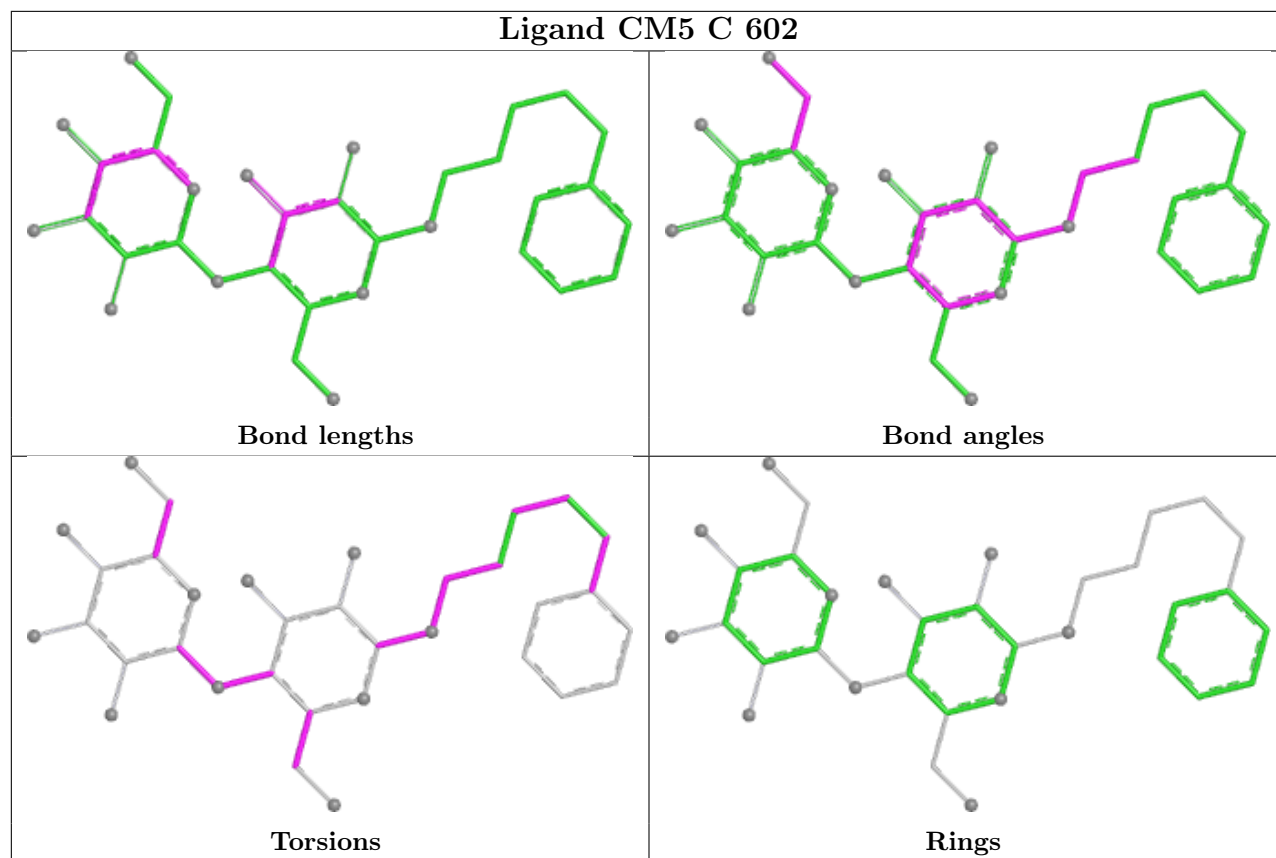
3 monomers are involved in 7 short contacts:

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





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%)	1.10	107 (20%) 3 2	20, 68, 134, 227	0
1	B	492/566 (86%)	0.93	96 (19%) 3 2	16, 68, 151, 205	0
1	C	490/566 (86%)	0.53	57 (11%) 9 7	12, 50, 124, 192	0
All	All	1506/1698 (88%)	0.86	260 (17%) 4 3	12, 64, 136, 227	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	ALA	7.9
1	A	297	GLY	7.8
1	C	229	GLY	7.8
1	C	230	ALA	7.0
1	A	298	VAL	6.4
1	A	234	LEU	6.4
1	A	86	ASN	6.1
1	A	267	ALA	5.7
1	B	488	ASN	5.7
1	B	490	TRP	5.6
1	C	227	GLU	5.6
1	A	82	ASP	5.4
1	B	130	ILE	5.4
1	C	269	ASN	5.3
1	C	274	PRO	5.3
1	A	284	SER	5.2
1	A	255	GLY	5.0
1	A	294	ALA	5.0
1	C	553	TYR	5.0
1	B	495	TRP	5.0
1	B	451	GLN	4.9
1	C	486	GLU	4.8
1	A	237	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	296	SER	4.8
1	C	292	PHE	4.7
1	C	270	ILE	4.7
1	B	215	GLN	4.6
1	B	230	ALA	4.6
1	A	512	ASP	4.5
1	A	400	GLY	4.5
1	A	309	ASN	4.5
1	B	441	PHE	4.5
1	C	288	LEU	4.5
1	B	502	ILE	4.5
1	A	295	ILE	4.4
1	C	226	GLY	4.4
1	A	486	GLU	4.4
1	B	80	PHE	4.3
1	A	487	ALA	4.2
1	B	145	MET	4.2
1	C	293	SER	4.2
1	A	304	TYR	4.2
1	C	485	LEU	4.2
1	C	302	ILE	4.2
1	C	296	SER	4.1
1	B	271	ILE	4.1
1	C	228	LYS	4.1
1	A	469	ALA	4.1
1	B	269	ASN	4.0
1	A	260	GLN	4.0
1	A	566	GLU	4.0
1	B	58	LEU	4.0
1	B	233	TRP	3.9
1	A	233	TRP	3.9
1	A	387	ARG	3.9
1	A	278	THR	3.9
1	B	277	TRP	3.8
1	A	286	LEU	3.8
1	B	497	VAL	3.7
1	A	508	LEU	3.7
1	A	251	ALA	3.7
1	A	273	ASP	3.7
1	B	542	LYS	3.7
1	B	501	ALA	3.6
1	A	89	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	156	PHE	3.6
1	B	483	GLY	3.6
1	A	231	GLU	3.6
1	B	214	LYS	3.5
1	C	256	LEU	3.5
1	C	80	PHE	3.5
1	A	277	TRP	3.5
1	A	80	PHE	3.5
1	A	509	SER	3.5
1	B	293	SER	3.5
1	C	291	ILE	3.5
1	A	490	TRP	3.4
1	C	289	ALA	3.4
1	B	434	GLY	3.4
1	B	387	ARG	3.4
1	B	396	GLU	3.4
1	A	150	MET	3.4
1	A	262	GLY	3.3
1	C	231	GLU	3.3
1	B	487	ALA	3.3
1	A	282	ILE	3.3
1	A	452	ILE	3.3
1	B	388	ILE	3.3
1	A	510	GLY	3.3
1	B	493	ALA	3.2
1	C	75	VAL	3.2
1	A	275	SER	3.2
1	A	71	LEU	3.2
1	A	259	LEU	3.2
1	B	485	LEU	3.2
1	C	57	SER	3.1
1	A	488	ASN	3.1
1	B	68	VAL	3.1
1	A	301	GLY	3.1
1	C	277	TRP	3.1
1	B	152	ILE	3.1
1	B	268	ALA	3.1
1	B	298	VAL	3.1
1	C	275	SER	3.1
1	B	60	TRP	3.0
1	B	141	TRP	3.0
1	C	276	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	485	LEU	3.0
1	A	555	GLU	3.0
1	A	497	VAL	3.0
1	B	389	SER	3.0
1	B	496	GLY	3.0
1	C	295	ILE	3.0
1	B	241	LEU	3.0
1	B	478	THR	3.0
1	A	552	GLU	3.0
1	C	514	ALA	3.0
1	A	280	VAL	3.0
1	B	234	LEU	2.9
1	C	552	GLU	2.9
1	B	300	LYS	2.9
1	B	57	SER	2.9
1	B	512	ASP	2.9
1	A	404	VAL	2.9
1	B	227	GLU	2.9
1	A	544	LEU	2.9
1	B	504	LEU	2.9
1	C	551	LEU	2.9
1	B	391	GLY	2.9
1	B	432	GLY	2.9
1	A	299	GLY	2.8
1	C	68	VAL	2.8
1	B	248	PHE	2.8
1	A	254	LEU	2.8
1	B	499	THR	2.8
1	C	58	LEU	2.8
1	A	226	GLY	2.8
1	B	137	ARG	2.8
1	B	392	ARG	2.8
1	B	445	HIS	2.8
1	B	461	LEU	2.8
1	C	61	SER	2.8
1	B	226	GLY	2.8
1	B	486	GLU	2.8
1	A	238	ILE	2.8
1	A	546	ASN	2.8
1	B	250	THR	2.8
1	B	491	VAL	2.7
1	A	288	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	310	MET	2.7
1	A	79	GLY	2.7
1	A	172	GLY	2.7
1	A	354	SER	2.7
1	B	473	SER	2.7
1	B	511	GLY	2.7
1	C	549	ILE	2.7
1	A	266	SER	2.7
1	A	346	GLN	2.7
1	B	438	GLU	2.7
1	C	74	VAL	2.7
1	A	446	ALA	2.7
1	C	76	TRP	2.7
1	A	236	LYS	2.7
1	A	152	ILE	2.6
1	A	293	SER	2.7
1	C	89	SER	2.7
1	B	510	GLY	2.6
1	C	426	ASN	2.6
1	A	215	GLN	2.6
1	A	227	GLU	2.6
1	B	509	SER	2.6
1	B	433	ASP	2.6
1	C	88	ALA	2.6
1	A	306	SER	2.6
1	A	489	LYS	2.6
1	B	228	LYS	2.6
1	B	299	GLY	2.6
1	A	315	LEU	2.6
1	A	380	PHE	2.6
1	B	59	ASN	2.5
1	C	357	GLY	2.5
1	A	279	ILE	2.5
1	A	563	LEU	2.5
1	B	291	ILE	2.5
1	B	74	VAL	2.5
1	C	258	ALA	2.5
1	B	390	ARG	2.5
1	B	506	LEU	2.5
1	A	274	PRO	2.5
1	A	545	SER	2.5
1	B	270	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	232	GLY	2.5
1	C	70	VAL	2.5
1	C	233	TRP	2.5
1	A	511	GLY	2.4
1	B	132	GLU	2.4
1	A	507	LEU	2.4
1	A	240	ILE	2.4
1	B	458	MET	2.4
1	A	153	ASP	2.4
1	A	292	PHE	2.4
1	C	361	GLU	2.4
1	B	545	SER	2.4
1	C	550	TYR	2.4
1	A	247	VAL	2.3
1	B	79	GLY	2.3
1	A	547	ASP	2.3
1	A	492	THR	2.3
1	C	287	THR	2.3
1	B	131	ASP	2.3
1	C	487	ALA	2.3
1	A	281	GLY	2.3
1	A	76	TRP	2.3
1	A	513	ASN	2.3
1	A	303	GLN	2.3
1	A	68	VAL	2.3
1	B	548	VAL	2.3
1	A	369	PHE	2.2
1	A	401	VAL	2.2
1	B	503	GLY	2.2
1	B	435	ALA	2.2
1	B	466	ILE	2.2
1	C	152	ILE	2.2
1	B	129	ARG	2.2
1	A	134	PRO	2.2
1	A	287	THR	2.2
1	B	505	THR	2.2
1	B	383	MET	2.2
1	B	216	LEU	2.2
1	A	583	ARG	2.2
1	C	301	GLY	2.2
1	C	508	LEU	2.2
1	A	135	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	75	VAL	2.2
1	B	541	VAL	2.2
1	B	492	THR	2.2
1	C	85	THR	2.2
1	B	229	GLY	2.2
1	A	252	CYS	2.2
1	A	302	ILE	2.1
1	B	292	PHE	2.1
1	C	87	PHE	2.1
1	B	104	ILE	2.1
1	B	481	GLN	2.1
1	C	513	ASN	2.1
1	B	267	ALA	2.1
1	A	451	GLN	2.1
1	B	440	LEU	2.1
1	B	380	PHE	2.1
1	C	278	THR	2.1
1	A	130	ILE	2.1
1	A	491	VAL	2.1
1	A	436	ALA	2.1
1	C	78	ILE	2.1
1	C	495	TRP	2.1
1	A	93	SER	2.0
1	B	67	LEU	2.0
1	A	216	LEU	2.0
1	A	403	LEU	2.0
1	B	455	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.

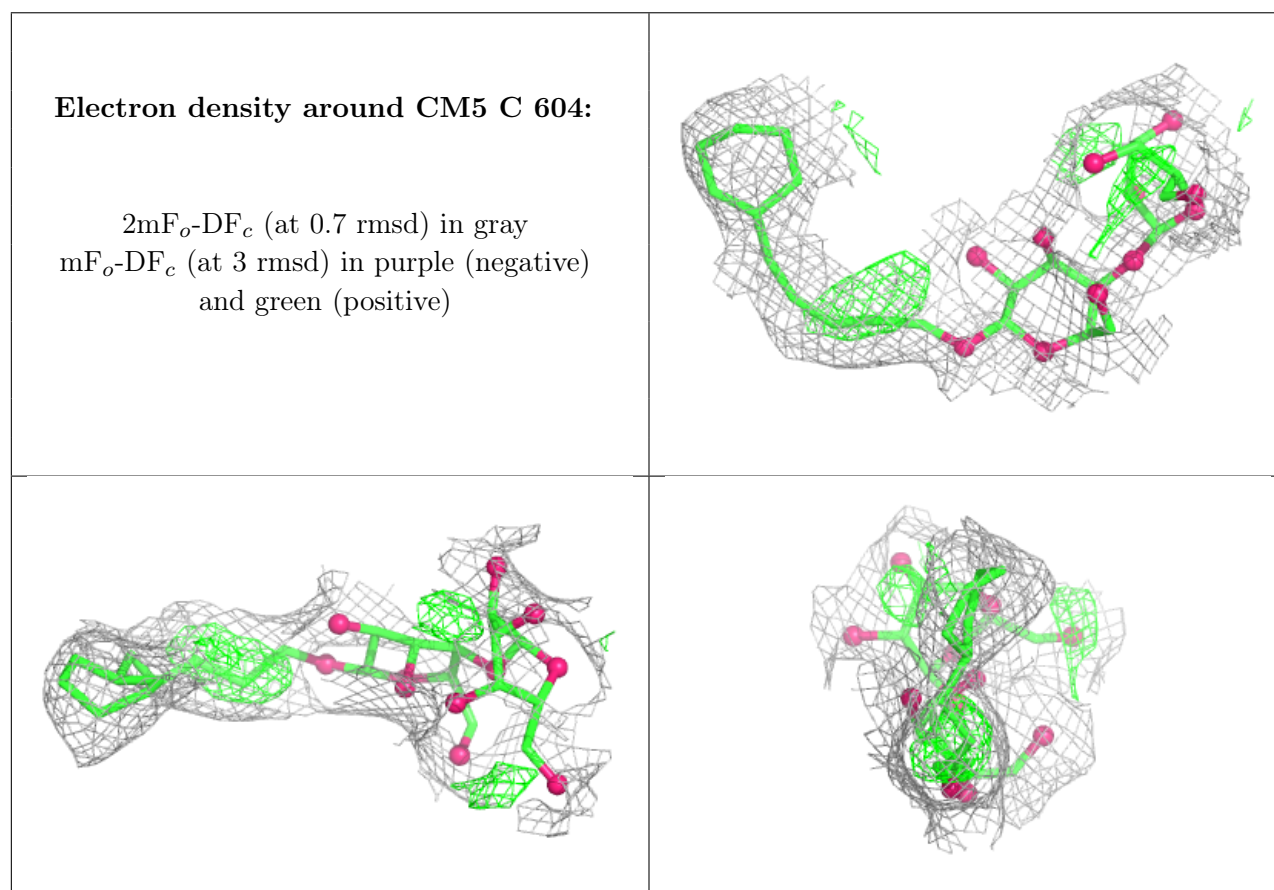
6.4 Ligands [i](#)

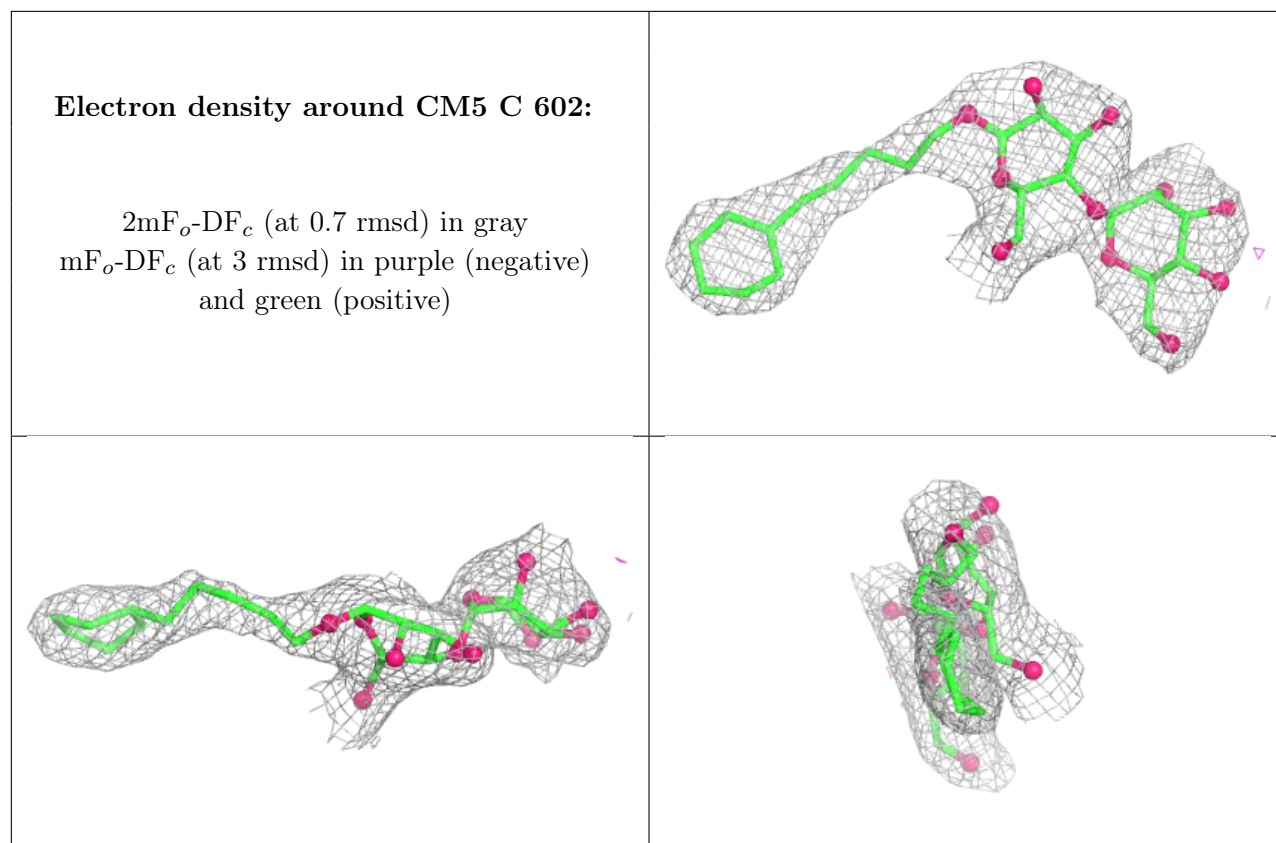
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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
5	CM5	C	604	34/34	0.73	0.19	94,126,142,144	0
3	NA	A	602	1/1	0.85	0.16	62,62,62,62	0
3	NA	B	602	1/1	0.88	0.33	96,96,96,96	0
2	1Y8	A	601	7/7	0.92	0.19	44,95,161,167	0
5	CM5	C	602	34/34	0.94	0.09	42,67,71,71	0
2	1Y8	C	603	7/7	0.94	0.18	48,89,134,236	0
2	1Y8	B	601	7/7	0.96	0.19	86,96,132,230	0
4	CL	C	601	1/1	0.98	0.04	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.