



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:44 PM UTC

PDB ID : 7CX1 / pdb_00007cx1
Title : Crystal structure of a tyrosine decarboxylase from *Enterococcus faecalis* in complex with the cofactor PLP and inhibitor methyl-tyrosine
Authors : Yu, X.; Gong, M.; Huang, J.; Liu, W.; Chen, C.; Guo, R.
Deposited on : 2020-09-01
Resolution : 2.54 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

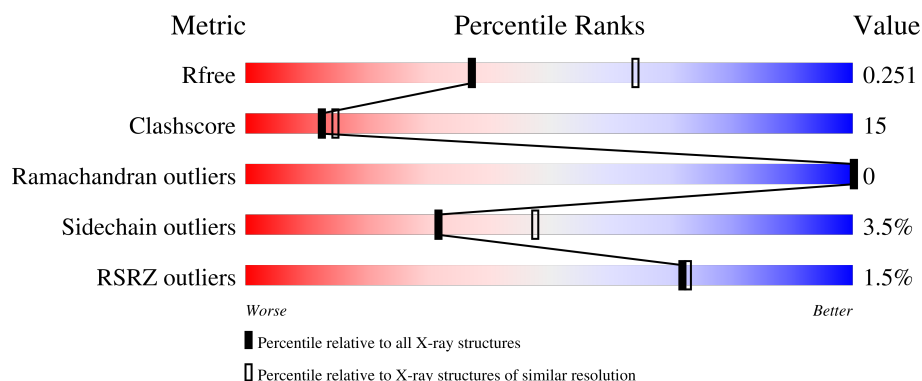
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	620	69% 27% .. 3%
1	B	620	64% 31% ..
1	C	620	66% 28% 5% 3%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14498 atoms, of which 60 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.

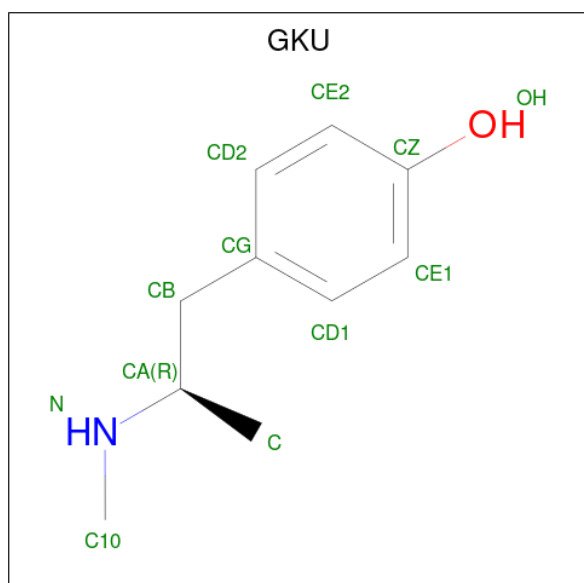
- Molecule 1 is a protein called Decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	P	S	0	0	0
			4749	3030	786	911	1	21			
1	B	603	Total	C	N	O	P	S	0	0	0
			4787	3058	792	915	1	21			
1	C	590	Total	C	N	O	P	S	0	0	0
			4649	2969	770	888	1	21			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	LYS	GLU	conflict	UNP Q8KXD2
B	62	LYS	GLU	conflict	UNP Q8KXD2
C	62	LYS	GLU	conflict	UNP Q8KXD2

- Molecule 2 is 4-[(2R)-2-(methylamino)propyl]phenol (CCD ID: GKU) (formula: C₁₀H₁₅NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			27	10	15	1	1		
2	B	1	Total	C	H	N	O	0	0
			27	10	15	1	1		
2	B	1	Total	C	H	N	O	0	0
			27	10	15	1	1		
2	C	1	Total	C	H	N	O	0	0
			27	10	15	1	1		

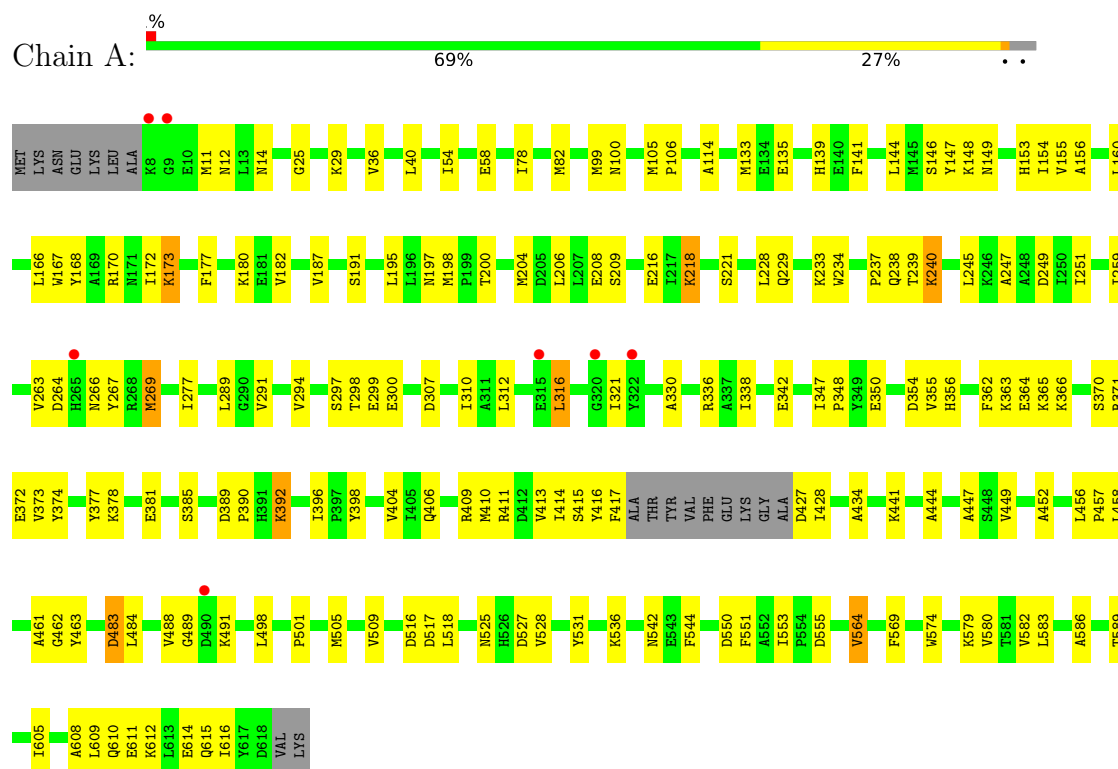
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total	O	0	0
			78	78		
3	B	62	Total	O	0	0
			62	62		
3	C	65	Total	O	0	0
			65	65		

3 Residue-property plots [i](#)

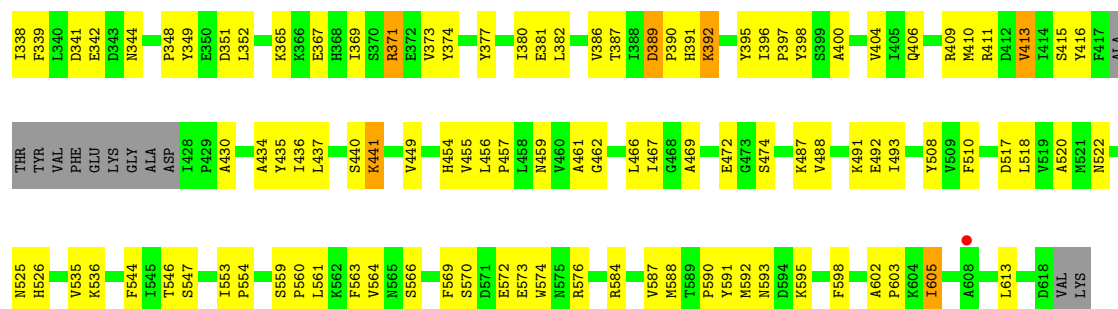
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

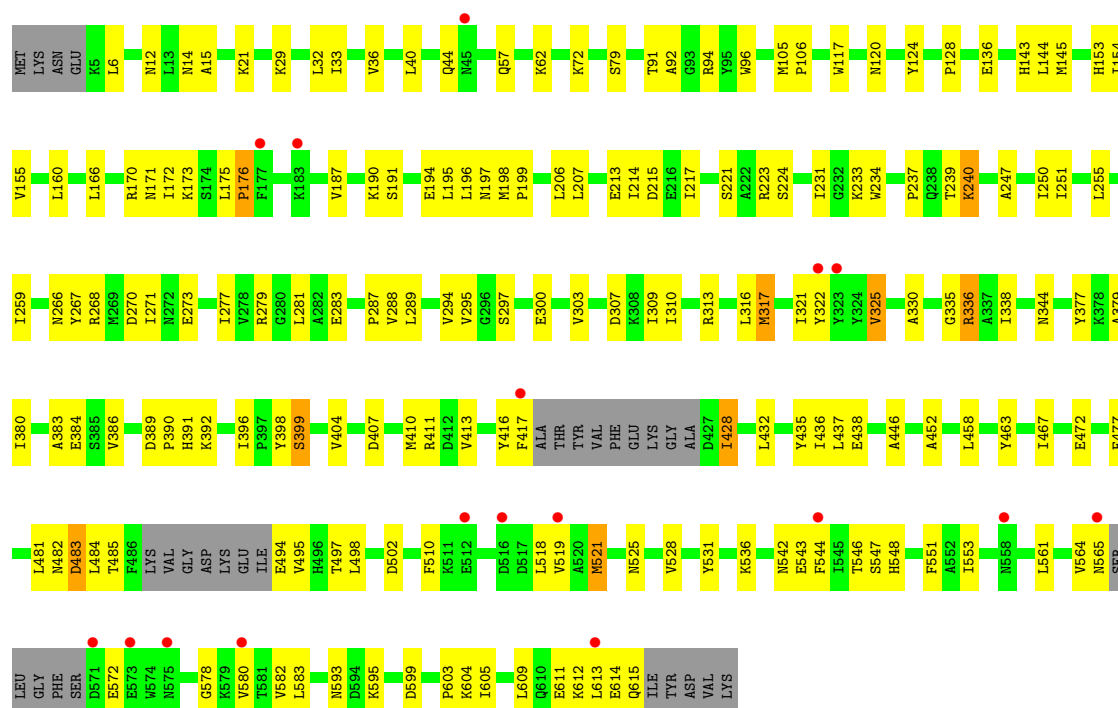


• Molecule 1: Decarboxylase





● Molecule 1: Decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.49Å 131.49Å 385.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.85 – 2.54 24.85 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.85-2.54) 99.5 (24.85-2.54)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.53Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.210 , 0.253 0.227 , 0.251	Depositor DCC
R_{free} test set	3300 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14498	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: GKU, LLP

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	0.57	0/4842	0.88	9/6580 (0.1%)
1	B	0.74	0/4880	1.13	13/6623 (0.2%)
1	C	0.56	0/4738	0.89	6/6436 (0.1%)
All	All	0.63	0/14460	0.97	28/19639 (0.1%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	ASP	CB-CA-C	8.00	117.75	109.83
1	B	371	ARG	N-CA-C	-7.64	103.42	112.89
1	C	428	ILE	N-CA-C	7.38	114.98	108.63
1	C	283	GLU	CA-C-N	-6.78	111.80	122.65
1	C	283	GLU	C-N-CA	-6.78	111.80	122.65
1	A	363	LYS	CA-C-N	-6.71	112.87	122.94
1	A	363	LYS	C-N-CA	-6.71	112.87	122.94
1	A	362	PHE	CA-C-N	-6.56	112.32	122.49
1	A	362	PHE	C-N-CA	-6.56	112.32	122.49
1	A	148	LYS	N-CA-C	-6.37	98.89	109.46
1	C	62	LYS	CG-CD-CE	-6.24	96.95	111.30
1	B	455	VAL	N-CA-C	-6.06	105.82	111.45
1	B	491	LYS	N-CA-C	5.98	118.04	110.33
1	B	430	ALA	N-CA-C	-5.82	106.01	113.23
1	B	341	ASP	CA-CB-CG	5.72	118.32	112.60
1	C	572	GLU	N-CA-C	-5.72	105.13	111.36
1	B	389	ASP	CB-CA-C	-5.66	103.89	110.17
1	A	266	ASN	N-CA-C	-5.61	105.79	113.30
1	B	454	HIS	CB-CA-C	5.55	119.32	109.65
1	A	516	ASP	N-CA-C	-5.53	106.42	112.72
1	C	239	THR	N-CA-C	-5.50	106.45	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	THR	N-CA-C	-5.49	107.15	112.97
1	B	249	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	267	TYR	CB-CA-C	5.40	120.17	111.36
1	B	272	ASN	N-CA-C	-5.36	105.52	111.36
1	B	254	GLY	CA-C-O	-5.29	118.58	122.23
1	A	517	ASP	CB-CA-C	5.29	119.53	110.81
1	B	253	ILE	N-CA-C	-5.09	105.58	110.72

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	4749	0	4503	133	0
1	B	4787	0	4592	152	0
1	C	4649	0	4415	166	0
2	A	12	15	0	1	0
2	B	24	30	0	1	0
2	C	12	15	0	0	0
3	A	78	0	0	2	0
3	B	62	0	0	1	0
3	C	65	0	0	2	0
All	All	14438	60	13510	425	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 15.

All (425) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LEU:HD21	1:C:438:GLU:HA	1.41	1.02
1:A:154:ILE:O	1:A:441:LYS:HE2	1.63	0.98
1:A:133:MET:CE	1:A:447:ALA:HA	1.95	0.96
1:C:531:TYR:HB3	1:C:612:LYS:HG3	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:LYS:HD2	1:C:259:ILE:HD11	1.54	0.89
1:B:547:SER:OG	1:B:584:ARG:HB2	1.75	0.85
1:C:207:LEU:HG	1:C:214:ILE:CD1	2.07	0.84
1:A:364:GLU:OE2	1:A:366:LYS:HD2	1.82	0.79
1:B:141:PHE:HB3	1:B:404:VAL:HG22	1.63	0.79
1:B:160:LEU:CD2	1:C:438:GLU:HA	2.12	0.78
1:A:297:SER:OG	1:A:300:GLU:HG2	1.83	0.77
1:B:96:TRP:O	1:B:546:THR:HG23	1.85	0.76
1:C:303:VAL:HG23	1:C:502:ASP:HB3	1.68	0.75
1:B:335:GLY:HA2	1:B:467:ILE:HD13	1.67	0.75
1:C:214:ILE:HG23	1:C:215:ASP:OD1	1.86	0.75
1:B:153:HIS:CE1	1:B:155:VAL:HG22	2.22	0.74
1:A:204:MET:HE3	1:A:204:MET:HA	1.68	0.74
1:A:350:GLU:H	1:A:350:GLU:CD	1.94	0.74
1:A:610:GLN:O	1:A:614:GLU:HG3	1.89	0.72
1:A:525:ASN:HA	1:A:528:VAL:HG22	1.69	0.72
1:B:240:LYS:HE3	1:B:245:LEU:HD21	1.72	0.72
1:B:573:GLU:HA	1:B:576:ARG:HG2	1.69	0.72
1:B:563:PHE:O	1:B:566:SER:HB3	1.90	0.71
1:C:191:SER:OG	1:C:194:GLU:HG3	1.91	0.71
1:A:233:LYS:HB3	1:A:259:ILE:HD12	1.72	0.71
1:C:173:LYS:HD2	1:C:289:LEU:HA	1.72	0.71
1:C:611:GLU:HG2	1:C:612:LYS:N	2.05	0.71
1:A:172:ILE:CD1	1:A:413:VAL:HG11	2.21	0.70
1:B:210:ALA:O	1:B:214:ILE:HG13	1.92	0.70
1:B:85:HIS:HB3	1:C:128:PRO:HB2	1.73	0.70
1:B:160:LEU:HD21	1:C:438:GLU:CA	2.21	0.69
1:B:602:ALA:HB3	1:B:603:PRO:HD3	1.75	0.69
1:C:172:ILE:HG13	1:C:413:VAL:HG11	1.75	0.69
1:C:335:GLY:HA2	1:C:467:ILE:HD13	1.73	0.69
1:B:544:PHE:HD2	1:B:605:ILE:HD12	1.58	0.69
1:C:531:TYR:HB3	1:C:612:LYS:CG	2.23	0.68
1:A:167:TRP:CH2	1:A:414:ILE:HG23	2.28	0.68
1:A:133:MET:HE1	1:A:447:ALA:CB	2.24	0.67
1:A:146:SER:OG	1:A:336:ARG:NH2	2.27	0.67
1:A:133:MET:HE1	1:A:447:ALA:HA	1.76	0.66
1:C:437:LEU:O	1:C:437:LEU:HD23	1.95	0.66
1:C:295:VAL:HG21	1:C:380:ILE:HD11	1.75	0.66
1:A:208:GLU:HG3	1:A:409:ARG:HD2	1.78	0.66
1:C:207:LEU:HG	1:C:214:ILE:HD11	1.76	0.66
1:C:94:ARG:NH2	1:C:604:LYS:HD2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ILE:HD13	1:A:413:VAL:HG11	1.79	0.65
1:C:615:GLN:O	1:C:615:GLN:HG2	1.96	0.65
1:C:544:PHE:CD2	1:C:605:ILE:HG23	2.32	0.65
1:C:153:HIS:CE1	1:C:155:VAL:HG22	2.32	0.65
1:C:198:MET:HE1	1:C:206:LEU:HD12	1.79	0.65
1:C:484:LEU:HD23	1:C:495:VAL:HG21	1.79	0.65
1:B:53:VAL:HG21	1:C:92:ALA:CB	2.27	0.64
1:B:85:HIS:O	1:C:128:PRO:HD2	1.97	0.64
1:A:168:TYR:O	1:A:172:ILE:HG12	1.98	0.63
1:A:170:ARG:HE	1:A:251:ILE:HG13	1.63	0.63
1:C:198:MET:HE1	1:C:206:LEU:CD1	2.29	0.63
1:A:364:GLU:OE2	1:A:366:LYS:CD	2.46	0.63
1:C:166:LEU:HD13	1:C:234:TRP:CE2	2.34	0.62
1:B:11:MET:HE3	1:B:456:LEU:HD23	1.81	0.62
1:B:335:GLY:O	1:B:338:ILE:HG12	1.99	0.62
1:B:349:TYR:HA	1:B:352:LEU:HD13	1.82	0.62
1:C:546:THR:HG22	1:C:547:SER:N	2.14	0.62
1:A:413:VAL:HG23	1:A:414:ILE:HG13	1.83	0.61
1:A:153:HIS:CE1	1:A:155:VAL:HG22	2.35	0.61
1:B:171:ASN:HB3	1:B:413:VAL:HG13	1.81	0.61
1:C:531:TYR:CB	1:C:612:LYS:HG3	2.25	0.61
1:A:233:LYS:HD2	1:A:259:ILE:HD11	1.83	0.60
1:C:386:VAL:HB	1:C:404:VAL:CG1	2.31	0.60
1:C:277:ILE:O	1:C:281:LEU:HD13	2.00	0.60
1:A:229:GLN:NE2	3:A:801:HOH:O	2.33	0.60
1:B:559:SER:OG	1:B:560:PRO:HD3	2.01	0.60
1:C:303:VAL:HG23	1:C:502:ASP:CB	2.32	0.60
1:C:437:LEU:HD23	1:C:437:LEU:C	2.27	0.60
1:C:611:GLU:O	1:C:612:LYS:HB3	1.99	0.60
1:A:427:ASP:OD1	1:A:428:ILE:N	2.32	0.60
1:A:564:VAL:HG13	1:A:569:PHE:HB2	1.83	0.59
1:A:342:GLU:OE2	1:A:461:ALA:HB2	2.02	0.59
1:C:294:VAL:HG11	1:C:297:SER:HA	1.85	0.59
1:A:527:ASP:HB3	1:A:616:ILE:HD13	1.83	0.59
1:B:187:VAL:HB	1:B:195:LEU:HD21	1.85	0.59
1:B:546:THR:HG22	1:B:547:SER:N	2.19	0.58
1:C:237:PRO:HG2	1:C:294:VAL:HG23	1.84	0.58
1:C:432:LEU:O	1:C:432:LEU:HD12	2.03	0.58
1:C:96:TRP:O	1:C:546:THR:HG23	2.03	0.58
1:C:384:GLU:HB3	1:C:410:MET:HE1	1.84	0.58
1:B:369:ILE:HG23	1:B:373:VAL:CG2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:CD2	1:C:214:ILE:HD11	2.33	0.58
1:C:297:SER:OG	1:C:300:GLU:HG2	2.03	0.58
1:A:233:LYS:CB	1:A:259:ILE:HD12	2.33	0.58
1:B:410:MET:O	1:B:413:VAL:HB	2.03	0.58
1:C:279:ARG:HG2	1:C:279:ARG:HH11	1.69	0.57
1:B:145:MET:HE3	1:B:386:VAL:HG11	1.86	0.57
1:B:546:THR:HG22	1:B:547:SER:H	1.69	0.57
1:B:32:LEU:HD11	1:B:112:ASN:HD22	1.70	0.57
1:B:172:ILE:HD13	1:B:413:VAL:HG21	1.86	0.57
1:A:133:MET:HE2	1:A:447:ALA:HA	1.83	0.57
1:B:46:TYR:CE2	1:C:91:THR:HG21	2.40	0.57
1:C:176:PRO:HB3	1:C:195:LEU:HB3	1.87	0.56
1:A:198:MET:HE1	1:A:206:LEU:HD12	1.87	0.56
1:B:211:GLU:HA	1:B:214:ILE:HD11	1.85	0.56
1:C:153:HIS:CD2	1:C:436:ILE:HG22	2.39	0.56
1:A:269:MET:HE1	1:A:291:VAL:HG13	1.88	0.56
1:C:124:TYR:CE1	1:C:428:ILE:HD13	2.40	0.56
1:A:612:LYS:O	1:A:616:ILE:HG13	2.05	0.56
1:B:170:ARG:HD3	1:B:251:ILE:HG13	1.86	0.56
1:B:437:LEU:HD23	1:C:160:LEU:HD21	1.88	0.56
1:B:153:HIS:CD2	1:B:436:ILE:HG22	2.41	0.56
1:B:411:ARG:HG3	1:B:435:TYR:CD2	2.41	0.56
1:C:542:ASN:O	1:C:543:GLU:HB2	2.05	0.56
1:B:145:MET:CE	1:B:386:VAL:HG11	2.36	0.55
1:A:133:MET:CE	1:A:447:ALA:CA	2.77	0.55
1:B:487:LYS:HG2	1:B:492:GLU:HG2	1.87	0.55
1:C:336:ARG:HG3	1:C:377:TYR:HD2	1.71	0.55
1:B:313:ARG:HD2	1:B:322:TYR:CE1	2.40	0.55
1:B:250:ILE:O	1:C:251:ILE:HA	2.07	0.55
1:A:336:ARG:HH12	1:A:378:LYS:HA	1.73	0.55
1:B:46:TYR:HE2	1:C:91:THR:HG21	1.72	0.55
1:B:369:ILE:HG23	1:B:373:VAL:HG23	1.89	0.54
1:C:544:PHE:CE2	1:C:605:ILE:HG23	2.42	0.54
1:B:147:TYR:CD2	1:B:406:GLN:HA	2.42	0.54
1:B:411:ARG:HG3	1:B:435:TYR:HD2	1.72	0.54
1:A:133:MET:HE1	1:A:447:ALA:CA	2.35	0.54
1:B:338:ILE:HD11	1:B:339:PHE:CZ	2.43	0.54
1:C:477:PHE:CE2	1:C:481:LEU:HD11	2.42	0.54
1:B:29:LYS:HG2	1:C:33:ILE:HD12	1.89	0.54
1:C:325:VAL:HG13	1:C:383:ALA:HA	1.89	0.54
1:A:172:ILE:HD11	1:A:413:VAL:HG11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:TYR:O	1:B:172:ILE:HG12	2.08	0.54
1:B:416:TYR:O	1:B:434:ALA:HB1	2.07	0.54
1:C:207:LEU:CG	1:C:214:ILE:HD11	2.36	0.54
1:B:270:ASP:HB3	1:B:273:GLU:HB2	1.89	0.54
1:B:316:LEU:HB3	1:B:321:ILE:HB	1.91	0.53
1:C:390:PRO:HB3	1:C:396:ILE:HD13	1.91	0.53
1:B:335:GLY:HA2	1:B:467:ILE:HG21	1.89	0.53
1:A:167:TRP:CE3	1:A:414:ILE:HD13	2.43	0.53
1:C:72:LYS:HE2	3:C:859:HOH:O	2.07	0.53
1:A:173:LYS:HG3	1:A:289:LEU:HD12	1.91	0.53
1:B:522:ASN:O	1:B:526:HIS:HB2	2.09	0.53
1:C:510:PHE:HZ	1:C:609:LEU:HD13	1.74	0.53
1:A:182:VAL:HG11	1:A:216:GLU:HB3	1.90	0.53
1:B:570:SER:HB2	1:B:573:GLU:H	1.73	0.53
1:A:527:ASP:CB	1:A:616:ILE:HD13	2.39	0.52
1:C:553:ILE:HD12	1:C:578:GLY:HA2	1.91	0.52
1:A:25:GLY:O	1:A:29:LYS:HG3	2.08	0.52
1:A:416:TYR:O	1:A:434:ALA:HB1	2.10	0.52
1:B:113:PHE:HE2	1:C:79:SER:HA	1.74	0.52
1:B:592:MET:HB3	1:B:598:PHE:HD1	1.75	0.52
1:C:143:HIS:HB3	1:C:344:ASN:ND2	2.25	0.52
1:B:488:VAL:HG11	1:B:613:LEU:HB3	1.91	0.51
1:C:279:ARG:HG2	1:C:279:ARG:NH1	2.23	0.51
1:A:501:PRO:HB3	1:A:505:MET:O	2.11	0.51
1:B:295:VAL:HG21	1:B:380:ILE:HD11	1.93	0.51
1:C:595:LYS:HE2	1:C:599:ASP:OD1	2.09	0.51
1:C:57:GLN:CD	1:C:57:GLN:H	2.18	0.51
1:C:561:LEU:HA	1:C:564:VAL:HG22	1.93	0.51
1:A:114:ALA:CB	1:A:444:ALA:HA	2.41	0.51
1:A:389:ASP:OD2	1:A:392:LLP:HE2	2.10	0.51
1:B:396:ILE:HG23	1:B:397:PRO:HD2	1.93	0.51
1:A:370:SER:HB3	1:A:372:GLU:OE2	2.11	0.51
1:B:55:SER:O	1:B:59:ARG:HG3	2.10	0.51
1:A:550:ASP:CG	1:A:579:LYS:HE2	2.36	0.51
1:B:237:PRO:HG2	1:B:294:VAL:HG23	1.93	0.51
1:B:389:ASP:OD2	1:B:392:LLP:HE3	2.11	0.51
1:C:144:LEU:HD13	1:C:458:LEU:HB3	1.92	0.51
1:C:166:LEU:HD13	1:C:234:TRP:CZ2	2.46	0.50
1:C:482:ASN:OD1	1:C:497:THR:HG23	2.10	0.50
1:C:498:LEU:HD21	1:C:551:PHE:HE2	1.76	0.50
1:A:518:LEU:HD23	1:A:518:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:PHE:HB2	1:C:580:VAL:HG13	1.92	0.50
1:B:298:THR:HG22	1:B:392:LLP:C3	2.42	0.50
1:C:207:LEU:HG	1:C:214:ILE:HD12	1.90	0.50
1:B:508:TYR:OH	1:B:546:THR:HG21	2.11	0.50
1:B:561:LEU:HD12	1:B:564:VAL:CG2	2.41	0.50
1:A:238:GLN:HG2	1:A:263:VAL:HG13	1.92	0.50
1:A:336:ARG:NH1	1:A:377:TYR:O	2.45	0.50
1:C:145:MET:HG3	1:C:404:VAL:HG11	1.94	0.50
1:A:542:ASN:OD1	1:A:612:LYS:NZ	2.33	0.50
1:A:415:SER:HA	1:A:434:ALA:O	2.12	0.49
1:B:166:LEU:HG	1:B:251:ILE:HG21	1.94	0.49
1:C:458:LEU:HD23	1:C:463:TYR:CD2	2.46	0.49
1:A:167:TRP:CZ3	1:A:414:ILE:CG2	2.96	0.49
1:C:531:TYR:HE1	1:C:536:LYS:HZ2	1.58	0.49
1:C:611:GLU:HG2	1:C:612:LYS:H	1.73	0.49
1:A:167:TRP:CZ3	1:A:414:ILE:HG23	2.46	0.49
1:A:330:ALA:O	1:A:389:ASP:HB2	2.11	0.49
1:B:141:PHE:HB3	1:B:404:VAL:CG2	2.40	0.49
1:C:335:GLY:CA	1:C:467:ILE:HD13	2.42	0.49
1:A:233:LYS:HB3	1:A:259:ILE:CD1	2.43	0.49
1:A:544:PHE:CD1	1:A:605:ILE:HG23	2.48	0.49
1:B:99:MET:HE2	1:B:331:TYR:CG	2.48	0.49
1:C:268:ARG:NH2	1:C:502:ASP:OD1	2.46	0.49
1:B:33:ILE:HD12	1:C:29:LYS:HG2	1.94	0.48
1:C:525:ASN:HA	1:C:528:VAL:HG22	1.94	0.48
1:B:78:ILE:O	1:B:82:MET:HG2	2.13	0.48
1:B:145:MET:HE3	1:B:386:VAL:CG1	2.43	0.48
1:B:295:VAL:HG23	1:B:327:VAL:HG13	1.93	0.48
1:A:267:TYR:OH	1:A:498:LEU:HD11	2.13	0.48
1:C:36:VAL:O	1:C:40:LEU:HG	2.13	0.48
1:C:173:LYS:HE3	1:C:288:VAL:O	2.13	0.48
1:C:564:VAL:O	1:C:565:ASN:C	2.57	0.48
1:C:611:GLU:CG	1:C:612:LYS:N	2.75	0.48
1:B:84:THR:HG22	1:B:85:HIS:CE1	2.48	0.48
1:B:561:LEU:HA	1:B:564:VAL:HG22	1.94	0.48
1:B:573:GLU:OE2	1:B:576:ARG:HD3	2.14	0.48
1:C:170:ARG:HA	1:C:289:LEU:HD11	1.95	0.48
1:A:168:TYR:OH	1:A:411:ARG:HA	2.14	0.48
1:B:113:PHE:CE2	1:C:79:SER:HA	2.48	0.48
1:B:472:GLU:HB3	1:B:593:ASN:HB2	1.96	0.48
1:C:599:ASP:O	1:C:603:PRO:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ASP:OD2	1:A:579:LYS:HE2	2.13	0.48
1:B:335:GLY:CA	1:B:467:ILE:HD13	2.40	0.48
1:C:213:GLU:O	1:C:217:ILE:HG13	2.14	0.48
1:C:510:PHE:CZ	1:C:609:LEU:HD13	2.49	0.48
1:A:528:VAL:CG2	1:A:583:LEU:HD11	2.44	0.47
1:B:70:HIS:CG	1:C:6:LEU:HD11	2.50	0.47
1:B:488:VAL:HG22	1:B:493:ILE:HG12	1.97	0.47
1:C:166:LEU:HG	1:C:251:ILE:HG21	1.96	0.47
1:A:135:GLU:OE2	1:A:139:HIS:NE2	2.46	0.47
1:C:32:LEU:O	1:C:36:VAL:HG23	2.14	0.47
1:C:546:THR:HG22	1:C:547:SER:O	2.14	0.47
1:C:483:ASP:OD1	1:C:483:ASP:N	2.47	0.47
1:A:154:ILE:C	1:A:441:LYS:HE2	2.38	0.47
1:A:336:ARG:NH1	1:A:378:LYS:HA	2.29	0.47
1:B:21:LYS:HD3	1:C:44:GLN:HA	1.96	0.47
1:B:223:ARG:HB3	1:C:255:LEU:CD2	2.44	0.47
1:B:371:ARG:HA	1:B:374:TYR:HB3	1.96	0.47
1:A:133:MET:HE1	1:A:447:ALA:HB2	1.97	0.47
1:A:170:ARG:HD2	1:A:228:LEU:HD22	1.96	0.47
1:A:509:VAL:HG12	1:A:582:VAL:HA	1.97	0.47
1:A:608:ALA:O	1:A:612:LYS:HG3	2.14	0.47
1:B:518:LEU:HD13	1:B:569:PHE:CE2	2.49	0.47
1:B:336:ARG:NH1	1:B:377:TYR:O	2.47	0.47
1:C:166:LEU:HD23	1:C:247:ALA:HB1	1.97	0.46
1:C:221:SER:OG	1:C:223:ARG:HD3	2.14	0.46
1:B:338:ILE:CD1	1:B:369:ILE:HD13	2.45	0.46
1:B:546:THR:HG22	1:B:584:ARG:O	2.15	0.46
1:A:277:ILE:HA	3:A:832:HOH:O	2.14	0.46
1:A:156:ALA:HB3	1:A:160:LEU:HD12	1.98	0.46
1:A:237:PRO:HG2	1:A:294:VAL:HG13	1.98	0.46
1:B:68:VAL:HG23	1:C:15:ALA:HB1	1.98	0.46
1:B:391:HIS:HA	1:B:396:ILE:O	2.15	0.46
1:C:531:TYR:HE1	1:C:536:LYS:NZ	2.13	0.46
1:A:240:LYS:HZ1	1:A:245:LEU:HD11	1.79	0.46
1:A:509:VAL:CG1	1:A:582:VAL:HG12	2.46	0.46
1:A:528:VAL:HG21	1:A:583:LEU:HD11	1.98	0.46
1:C:171:ASN:HB3	1:C:413:VAL:CG1	2.46	0.46
1:B:395:TYR:CD2	1:B:466:LEU:HD21	2.50	0.46
1:A:428:ILE:HG23	1:A:428:ILE:O	2.15	0.46
1:B:143:HIS:HB3	1:B:344:ASN:ND2	2.31	0.46
1:B:175:LEU:HD11	1:B:413:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:TYR:CE2	1:C:498:LEU:HD21	2.51	0.46
1:A:12:ASN:OD1	1:A:14:ASN:HB2	2.15	0.46
1:C:542:ASN:O	1:C:543:GLU:CB	2.64	0.46
1:C:199:PRO:HA	1:C:322:TYR:CD1	2.51	0.45
1:C:271:ILE:CD1	1:C:309:ILE:HG12	2.46	0.45
1:C:316:LEU:HB3	1:C:321:ILE:HB	1.97	0.45
1:A:187:VAL:HB	1:A:195:LEU:HD21	1.98	0.45
1:A:354:ASP:OD1	1:A:365:LYS:NZ	2.41	0.45
1:A:172:ILE:HG21	1:A:200:THR:HG23	1.98	0.45
1:C:614:GLU:O	1:C:615:GLN:C	2.58	0.45
1:A:297:SER:HG	1:A:300:GLU:HG2	1.78	0.45
1:C:143:HIS:HB3	1:C:344:ASN:HD21	1.81	0.45
1:B:457:PRO:HD2	1:B:462:GLY:HA3	1.99	0.45
1:A:141:PHE:HB3	1:A:404:VAL:HG22	1.98	0.45
1:C:196:LEU:HD13	1:C:287:PRO:HG3	1.98	0.45
1:C:452:ALA:HB1	1:C:463:TYR:OH	2.17	0.45
1:A:197:ASN:OD1	1:A:321:ILE:HA	2.16	0.45
1:A:416:TYR:O	1:A:417:PHE:CD1	2.70	0.45
1:B:469:ALA:HA	1:B:593:ASN:CB	2.47	0.45
1:A:348:PRO:CB	1:A:350:GLU:OE2	2.65	0.45
1:A:611:GLU:O	1:A:615:GLN:HG3	2.17	0.45
1:B:127:SER:HB3	1:B:130:THR:OG1	2.16	0.45
1:B:145:MET:HE3	1:B:386:VAL:CB	2.47	0.45
1:C:96:TRP:CZ2	1:C:605:ILE:HD11	2.52	0.45
1:C:154:ILE:CD1	1:C:446:ALA:HA	2.46	0.45
1:C:237:PRO:O	1:C:240:LYS:HB3	2.16	0.45
1:C:330:ALA:O	1:C:389:ASP:HB2	2.17	0.45
1:A:166:LEU:HD21	1:A:234:TRP:CD2	2.52	0.44
1:B:36:VAL:O	1:B:40:LEU:HG	2.16	0.44
1:B:249:ASP:OD1	1:C:170:ARG:NH2	2.46	0.44
1:C:303:VAL:CG2	1:C:502:ASP:HB3	2.42	0.44
1:C:153:HIS:NE2	1:C:436:ILE:HG22	2.33	0.44
1:A:191:SER:O	1:A:195:LEU:HG	2.18	0.44
1:B:251:ILE:HA	1:C:250:ILE:O	2.17	0.44
1:C:207:LEU:CG	1:C:214:ILE:CD1	2.88	0.44
1:C:391:HIS:HA	1:C:396:ILE:O	2.18	0.44
1:C:609:LEU:HD23	1:C:609:LEU:HA	1.74	0.44
1:A:381:GLU:O	1:A:381:GLU:HG2	2.17	0.44
1:B:47:MET:HG3	1:C:94:ARG:CD	2.47	0.44
1:B:517:ASP:HB3	1:B:520:ALA:HB3	2.00	0.44
1:C:335:GLY:HA2	1:C:467:ILE:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:ASN:C	1:C:483:ASP:OD1	2.60	0.44
1:A:99:MET:HE2	2:A:701:GKU:N	2.33	0.44
1:A:489:GLY:C	1:A:491:LYS:H	2.25	0.44
1:B:57:GLN:H	1:B:57:GLN:CD	2.25	0.44
1:C:12:ASN:OD1	1:C:14:ASN:HB2	2.18	0.44
1:C:266:ASN:HB3	1:C:268:ARG:HH11	1.82	0.44
1:C:611:GLU:O	1:C:613:LEU:N	2.46	0.44
1:A:372:GLU:CD	1:A:372:GLU:H	2.26	0.44
1:B:147:TYR:CG	1:B:406:GLN:HA	2.53	0.44
1:C:173:LYS:HD3	1:C:231:ILE:O	2.18	0.44
1:B:211:GLU:HA	1:B:214:ILE:CD1	2.46	0.44
1:B:474:SER:HA	1:B:587:VAL:HG21	1.99	0.44
1:B:39:HIS:CD2	1:B:116:LEU:HB3	2.52	0.43
1:A:105:MET:N	1:A:106:PRO:HD2	2.34	0.43
1:A:390:PRO:HB3	1:A:396:ILE:HD12	2.00	0.43
1:A:551:PHE:O	1:A:579:LYS:HA	2.18	0.43
1:B:251:ILE:HA	1:B:251:ILE:HD12	1.81	0.43
1:C:546:THR:CG2	1:C:547:SER:N	2.81	0.43
1:A:78:ILE:O	1:A:82:MET:HG2	2.18	0.43
1:B:441:LYS:HB2	1:B:441:LYS:HE3	1.51	0.43
1:B:310:ILE:HD13	1:B:325:VAL:HG21	1.98	0.43
1:A:147:TYR:CG	1:A:406:GLN:HA	2.54	0.43
1:B:396:ILE:HG21	1:B:449:VAL:HG22	2.01	0.43
1:A:36:VAL:O	1:A:40:LEU:HG	2.18	0.43
1:B:561:LEU:HD13	1:B:574:TRP:CD1	2.54	0.43
1:C:521:MET:HE2	1:C:521:MET:HB3	1.68	0.43
1:C:544:PHE:CE1	1:C:546:THR:OG1	2.71	0.43
1:B:32:LEU:HD11	1:B:112:ASN:ND2	2.33	0.43
1:A:144:LEU:HD13	1:A:458:LEU:HB3	2.01	0.43
1:A:149:ASN:CG	1:A:149:ASN:O	2.61	0.43
1:C:105:MET:N	1:C:106:PRO:HD2	2.34	0.43
1:C:207:LEU:HD21	1:C:214:ILE:HD11	2.00	0.43
1:C:546:THR:HG22	1:C:547:SER:H	1.82	0.43
1:C:611:GLU:O	1:C:612:LYS:CB	2.64	0.43
1:A:370:SER:HB2	1:A:373:VAL:H	1.84	0.42
1:B:33:ILE:HD13	1:B:33:ILE:HA	1.83	0.42
1:C:270:ASP:HB3	1:C:273:GLU:HB2	2.00	0.42
1:C:317:MET:HE2	1:C:317:MET:HB2	1.72	0.42
1:C:398:TYR:HA	1:C:399:SER:HA	1.80	0.42
1:A:54:ILE:HG23	1:A:58:GLU:HG2	2.01	0.42
1:A:146:SER:HB2	1:A:381:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:TYR:CD2	1:A:406:GLN:HA	2.54	0.42
1:A:348:PRO:HB3	1:A:350:GLU:OE2	2.20	0.42
1:A:531:TYR:CZ	1:A:536:LYS:HD3	2.53	0.42
1:B:348:PRO:HB2	1:B:351:ASP:OD2	2.19	0.42
1:B:398:TYR:CZ	1:C:120:ASN:HB2	2.54	0.42
1:C:187:VAL:HB	1:C:195:LEU:HD21	2.02	0.42
1:C:482:ASN:OD1	1:C:497:THR:CG2	2.67	0.42
1:C:197:ASN:OD1	1:C:321:ILE:HA	2.20	0.42
1:C:531:TYR:CD1	1:C:536:LYS:HG3	2.53	0.42
1:A:347:ILE:HD13	1:A:355:VAL:HG11	2.00	0.42
1:A:385:SER:HA	1:A:404:VAL:O	2.20	0.42
1:A:457:PRO:HD2	1:A:462:GLY:HA3	2.02	0.42
1:A:589:THR:O	1:A:589:THR:HG23	2.20	0.42
1:B:46:TYR:O	1:C:21:LYS:NZ	2.46	0.42
1:B:109:LEU:HD12	1:B:109:LEU:HA	1.91	0.42
1:B:122:VAL:HB	1:B:440:SER:HA	2.01	0.42
1:B:595:LYS:O	1:B:595:LYS:HG3	2.19	0.42
1:C:472:GLU:HG2	1:C:593:ASN:O	2.19	0.42
1:B:238:GLN:HG2	1:B:263:VAL:HG13	2.02	0.42
1:C:386:VAL:HB	1:C:404:VAL:HG12	2.02	0.42
1:C:411:ARG:HG3	1:C:435:TYR:HD1	1.84	0.42
1:A:218:LYS:HB3	1:A:218:LYS:HE3	1.83	0.42
1:A:452:ALA:HB1	1:A:463:TYR:OH	2.20	0.42
1:C:548:HIS:HB2	1:C:583:LEU:HD23	2.02	0.42
1:A:100:ASN:ND2	1:A:398:TYR:OH	2.48	0.42
1:A:298:THR:HG22	1:A:299:GLU:OE2	2.20	0.42
1:B:381:GLU:HG3	1:B:382:LEU:HD22	2.02	0.42
1:C:390:PRO:HB3	1:C:396:ILE:CD1	2.50	0.42
1:A:153:HIS:ND1	1:A:154:ILE:O	2.50	0.42
1:A:249:ASP:C	1:A:249:ASP:OD1	2.63	0.42
1:A:312:LEU:HG	1:A:316:LEU:HD22	2.02	0.42
1:A:525:ASN:HA	1:A:528:VAL:CG2	2.44	0.42
1:B:154:ILE:O	1:B:441:LYS:NZ	2.53	0.42
1:B:369:ILE:CG2	1:B:373:VAL:HG23	2.50	0.42
1:B:590:PRO:HD2	1:B:591:TYR:CD2	2.54	0.42
1:A:338:ILE:HG12	1:A:356:HIS:CE1	2.55	0.41
1:A:505:MET:HG3	1:A:586:ALA:HA	2.01	0.41
1:B:143:HIS:HB3	1:B:344:ASN:HD21	1.84	0.41
1:B:342:GLU:HG3	3:B:1210:HOH:O	2.20	0.41
1:B:588:MET:HE2	1:B:588:MET:HB3	1.89	0.41
1:B:173:LYS:HG3	1:B:289:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:VAL:O	1:B:488:VAL:HG23	2.19	0.41
1:C:485:THR:HG22	1:C:494:GLU:HB2	2.02	0.41
1:A:11:MET:SD	1:A:456:LEU:HD23	2.60	0.41
1:B:570:SER:C	1:B:572:GLU:N	2.75	0.41
1:C:170:ARG:NH2	1:C:171:ASN:OD1	2.49	0.41
1:C:297:SER:HG	1:C:300:GLU:HG2	1.83	0.41
1:C:307:ASP:HA	1:C:379:ALA:CB	2.50	0.41
1:C:411:ARG:HG3	1:C:435:TYR:CD1	2.55	0.41
1:A:371:ARG:O	1:A:371:ARG:HG2	2.19	0.41
1:A:551:PHE:HB2	1:A:580:VAL:CG1	2.49	0.41
1:A:553:ILE:HG12	1:A:574:TRP:CZ2	2.55	0.41
1:B:561:LEU:HD13	1:B:574:TRP:CG	2.56	0.41
1:C:33:ILE:HD13	1:C:33:ILE:HA	1.90	0.41
1:C:416:TYR:O	1:C:417:PHE:CD1	2.73	0.41
1:B:81:ARG:HH22	1:C:136:GLU:CD	2.29	0.41
1:B:86:SER:HB3	1:C:117:TRP:CD1	2.56	0.41
1:B:415:SER:HA	1:B:434:ALA:O	2.21	0.41
1:B:459:ASN:OD1	1:B:461:ALA:HB3	2.20	0.41
1:B:544:PHE:CE1	1:B:546:THR:OG1	2.74	0.41
1:C:313:ARG:NH1	1:C:325:VAL:HG12	2.35	0.41
1:C:407:ASP:O	1:C:410:MET:HB2	2.20	0.41
1:B:338:ILE:HD12	1:B:369:ILE:HD13	2.03	0.41
1:A:166:LEU:HD12	1:A:247:ALA:HB1	2.03	0.41
1:A:371:ARG:HA	1:A:374:TYR:HB3	2.02	0.41
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.89	0.41
1:B:265:HIS:CD2	1:B:265:HIS:H	2.39	0.41
1:C:172:ILE:CG1	1:C:413:VAL:HG21	2.51	0.41
1:A:146:SER:CB	1:A:336:ARG:NH2	2.84	0.41
1:B:82:MET:HE3	1:B:82:MET:HB3	1.75	0.41
1:A:99:MET:SD	1:A:392:LLP:HD2	2.60	0.41
1:A:410:MET:O	1:A:413:VAL:HG22	2.21	0.41
1:A:564:VAL:HG11	1:A:574:TRP:HB2	2.02	0.41
1:B:119:GLY:HA3	1:B:127:SER:HB2	2.03	0.41
1:B:159:SER:HB3	3:C:840:HOH:O	2.21	0.41
1:B:535:VAL:HG12	1:B:536:LYS:HG3	2.03	0.41
1:A:396:ILE:HD13	1:A:449:VAL:HG22	2.03	0.40
1:B:100:ASN:ND2	2:B:1101:GKU:OH	2.48	0.40
1:B:163:LEU:HG	1:B:437:LEU:HD11	2.02	0.40
1:B:254:GLY:HA3	1:C:224:SER:O	2.20	0.40
1:A:544:PHE:CE2	1:A:609:LEU:HD21	2.56	0.40
1:B:390:PRO:HD2	1:B:400:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:THR:CG2	1:B:584:ARG:O	2.69	0.40
1:C:96:TRP:O	1:C:546:THR:HA	2.21	0.40
1:C:498:LEU:HD13	1:C:582:VAL:HG11	2.04	0.40
1:A:238:GLN:HG3	1:A:239:THR:HG23	2.03	0.40
1:B:208:GLU:HG3	1:B:409:ARG:HD2	2.03	0.40
1:B:510:PHE:N	1:B:525:ASN:OD1	2.34	0.40
1:B:559:SER:N	1:B:560:PRO:CD	2.84	0.40
1:A:307:ASP:OD1	1:A:307:ASP:N	2.54	0.40
1:B:196:LEU:HD13	1:B:196:LEU:HA	1.92	0.40
1:C:175:LEU:HD23	1:C:175:LEU:HA	1.90	0.40
1:B:553:ILE:HB	1:B:554:PRO:HD3	2.04	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	597/620 (96%)	561 (94%)	36 (6%)	0	100	100
1	B	598/620 (96%)	572 (96%)	26 (4%)	0	100	100
1	C	581/620 (94%)	547 (94%)	34 (6%)	0	100	100
All	All	1776/1860 (96%)	1680 (95%)	96 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	493/524 (94%)	477 (97%)	16 (3%)	34	51
1	B	502/524 (96%)	479 (95%)	23 (5%)	24	36
1	C	481/524 (92%)	468 (97%)	13 (3%)	39	58
All	All	1476/1572 (94%)	1424 (96%)	52 (4%)	32	48

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	LYS
1	A	177	PHE
1	A	180	LYS
1	A	209	SER
1	A	218	LYS
1	A	221	SER
1	A	240	LYS
1	A	264	ASP
1	A	269	MET
1	A	310	ILE
1	A	316	LEU
1	A	483	ASP
1	A	484	LEU
1	A	488	VAL
1	A	555	ASP
1	A	564	VAL
1	B	66	LYS
1	B	103	THR
1	B	108	LEU
1	B	109	LEU
1	B	115	MET
1	B	131	SER
1	B	137	VAL
1	B	177	PHE
1	B	190	LYS
1	B	196	LEU
1	B	201	LYS
1	B	209	SER
1	B	218	LYS
1	B	231	ILE
1	B	251	ILE
1	B	259	ILE

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Mol	Chain	Res	Type
1	B	271	ILE
1	B	365	LYS
1	B	367	GLU
1	B	387	THR
1	B	413	VAL
1	B	441	LYS
1	B	605	ILE
1	C	176	PRO
1	C	190	LYS
1	C	240	LYS
1	C	310	ILE
1	C	317	MET
1	C	325	VAL
1	C	336	ARG
1	C	338	ILE
1	C	399	SER
1	C	483	ASP
1	C	518	LEU
1	C	519	VAL
1	C	521	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	HIS
1	A	265	HIS
1	A	406	GLN
1	A	515	ASN
1	A	575	ASN
1	A	610	GLN
1	A	615	GLN
1	B	26	GLN
1	B	76	ASN
1	B	85	HIS
1	B	149	ASN
1	B	227	HIS
1	B	257	GLN
1	B	265	HIS
1	B	353	GLN
1	B	476	HIS
1	B	526	HIS
1	C	85	HIS

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Mol	Chain	Res	Type
1	C	132	GLN
1	C	220	HIS
1	C	479	ASN
1	C	565	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	LLP	B	392	1	23,24,25	0.69	0	25,32,34	0.85	1 (4%)
1	LLP	A	392	1	23,24,25	0.73	0	25,32,34	0.91	1 (4%)
1	LLP	C	392	1	23,24,25	0.60	0	25,32,34	0.84	1 (4%)

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
1	LLP	B	392	1	-	6/16/17/19	0/1/1/1
1	LLP	A	392	1	-	6/16/17/19	0/1/1/1
1	LLP	C	392	1	-	2/16/17/19	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	392	LLP	OP4-C5'-C5	2.98	114.94	109.36
1	A	392	LLP	OP4-C5'-C5	2.84	114.68	109.36
1	B	392	LLP	OP4-C5'-C5	2.60	114.22	109.36

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	392	LLP	C4-C4'-NZ-CE
1	A	392	LLP	N-CA-CB-CG
1	A	392	LLP	C-CA-CB-CG
1	A	392	LLP	O-C-CA-CB
1	B	392	LLP	C4-C4'-NZ-CE
1	B	392	LLP	O-C-CA-CB
1	C	392	LLP	O-C-CA-CB
1	C	392	LLP	C4-C4'-NZ-CE
1	A	392	LLP	CG-CD-CE-NZ
1	B	392	LLP	CE-CD-CG-CB
1	A	392	LLP	CE-CD-CG-CB
1	B	392	LLP	CA-CB-CG-CD
1	B	392	LLP	CG-CD-CE-NZ
1	B	392	LLP	C5'-OP4-P-OP2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	392	LLP	2	0
1	A	392	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GKU	B	1102	-	12,12,12	1.06	1 (8%)	14,15,15	1.13	1 (7%)
2	GKU	B	1101	-	12,12,12	1.11	1 (8%)	14,15,15	1.84	2 (14%)
2	GKU	C	701	-	12,12,12	0.90	1 (8%)	14,15,15	0.95	1 (7%)
2	GKU	A	701	-	12,12,12	0.75	1 (8%)	14,15,15	1.58	3 (21%)

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	GKU	B	1102	-	-	2/6/6/6	0/1/1/1
2	GKU	B	1101	-	-	2/6/6/6	0/1/1/1
2	GKU	C	701	-	-	2/6/6/6	0/1/1/1
2	GKU	A	701	-	-	2/6/6/6	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1102	GKU	OH-CZ	2.72	1.43	1.37
2	B	1101	GKU	OH-CZ	2.38	1.42	1.37
2	C	701	GKU	OH-CZ	2.24	1.42	1.37
2	A	701	GKU	OH-CZ	2.04	1.41	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	GKU	C10-N-CA	-5.18	108.20	114.39
2	B	1101	GKU	C-CA-CB	-3.89	104.53	111.89
2	B	1102	GKU	C10-N-CA	-3.57	110.12	114.39
2	A	701	GKU	C10-N-CA	-2.92	110.90	114.39
2	A	701	GKU	CB-CA-N	2.86	118.65	110.49
2	A	701	GKU	C-CA-CB	-2.72	106.75	111.89
2	C	701	GKU	C10-N-CA	-2.56	111.33	114.39

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GKU	C-CA-N-C10
2	A	701	GKU	CB-CA-N-C10
2	B	1102	GKU	CB-CA-N-C10
2	C	701	GKU	CB-CA-N-C10
2	B	1102	GKU	C-CA-N-C10
2	C	701	GKU	C-CA-N-C10
2	B	1101	GKU	CB-CA-N-C10
2	B	1101	GKU	C-CA-N-C10

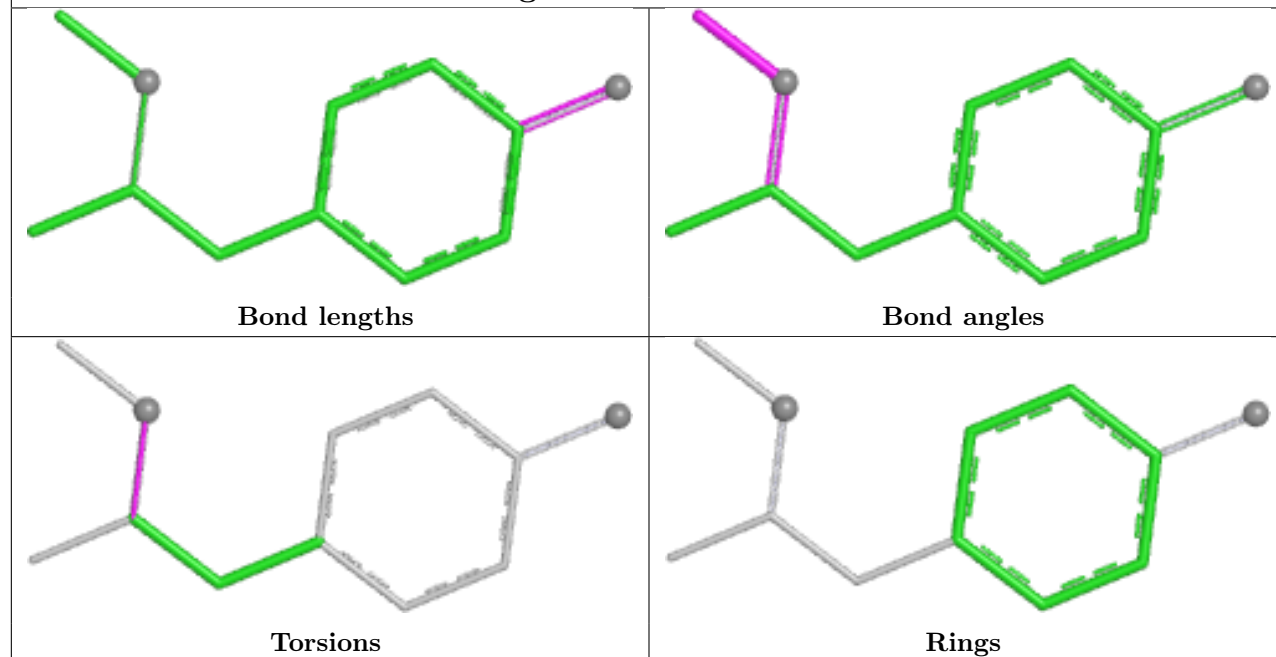
There are no ring outliers.

2 monomers are involved in 2 short contacts:

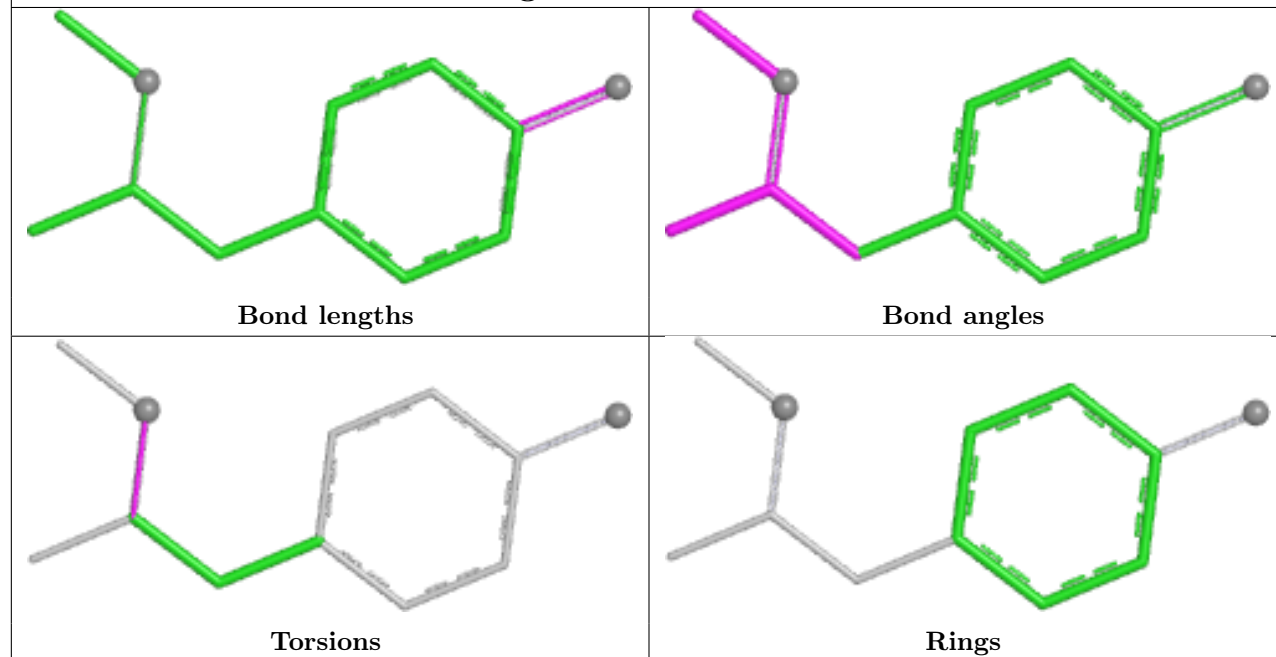
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	GKU	1	0
2	A	701	GKU	1	0

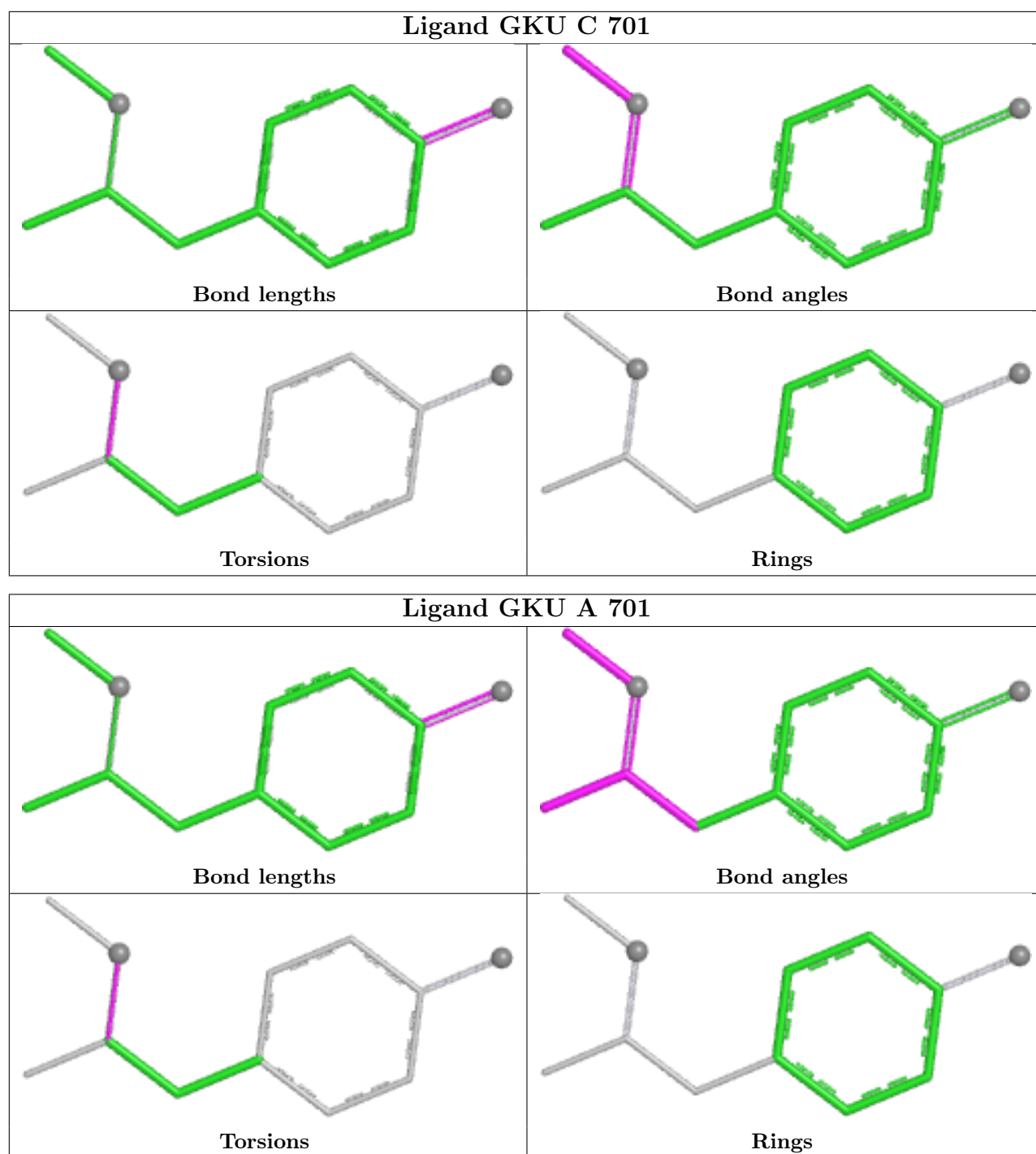
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GKU B 1102



Ligand GKU B 1101





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	601/620 (96%)	0.14	7 (1%) 76 77	25, 44, 71, 86	0
1	B	602/620 (97%)	0.23	3 (0%) 87 89	27, 50, 70, 87	0
1	C	589/620 (95%)	0.24	17 (2%) 53 55	27, 48, 81, 89	0
All	All	1792/1860 (96%)	0.20	27 (1%) 72 73	25, 48, 75, 89	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	TYR	3.3
1	C	575	ASN	3.0
1	C	516	ASP	2.8
1	C	322	TYR	2.8
1	C	512	GLU	2.8
1	C	565	ASN	2.7
1	A	315	GLU	2.5
1	A	490	ASP	2.5
1	C	558	ASN	2.5
1	C	573	GLU	2.4
1	C	417	PHE	2.4
1	C	580	VAL	2.4
1	A	265	HIS	2.4
1	C	45	ASN	2.3
1	C	613	LEU	2.3
1	B	230	ALA	2.2
1	A	9	GLY	2.2
1	B	191	SER	2.2
1	B	608	ALA	2.2
1	A	8	LYS	2.2
1	C	183	LYS	2.2
1	C	571	ASP	2.2
1	A	320	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	323	TYR	2.1
1	C	177	PHE	2.1
1	C	519	VAL	2.1
1	C	544	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	C	392	24/25	0.91	0.11	34,41,46,48	0
1	LLP	B	392	24/25	0.92	0.10	33,40,45,46	0
1	LLP	A	392	24/25	0.93	0.09	32,40,43,43	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

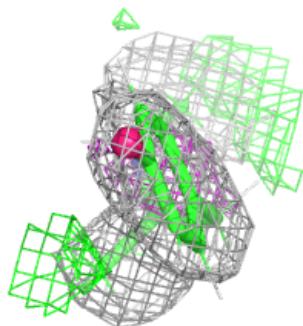
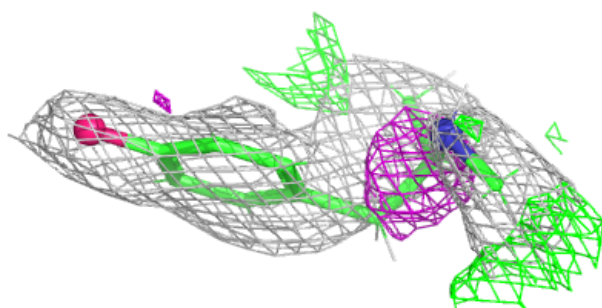
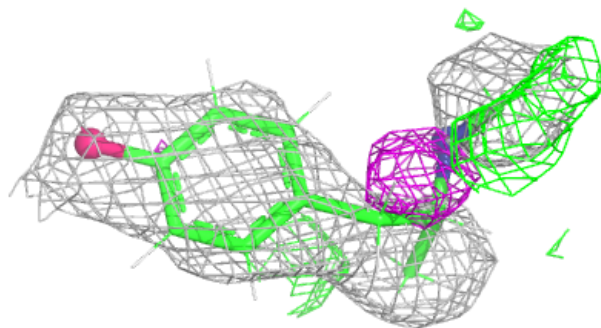
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GKU	B	1101	12/12	0.62	0.16	45,55,60,65	0
2	GKU	B	1102	12/12	0.69	0.14	39,52,64,71	0
2	GKU	A	701	12/12	0.73	0.14	41,51,59,70	0
2	GKU	C	701	12/12	0.77	0.13	42,55,64,69	0

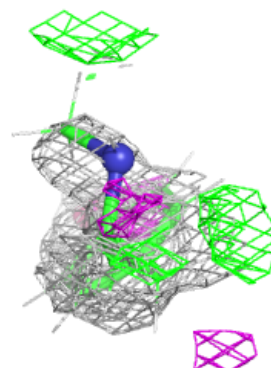
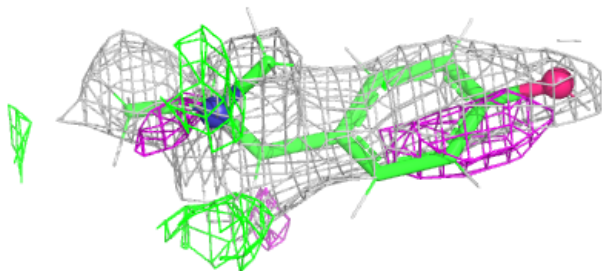
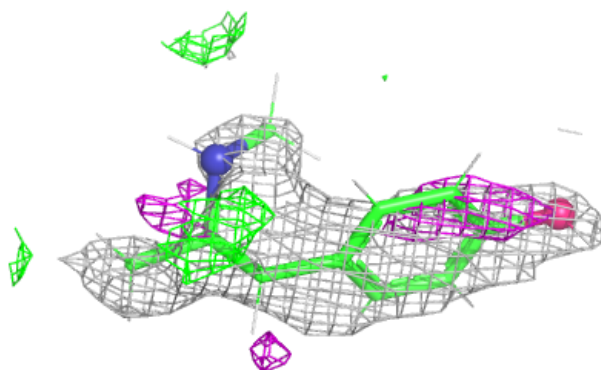
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GKU B 1101:

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

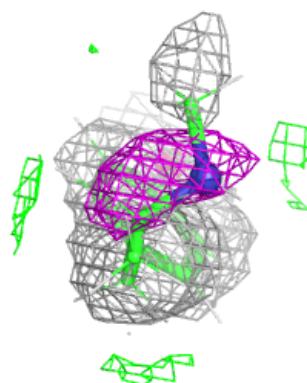
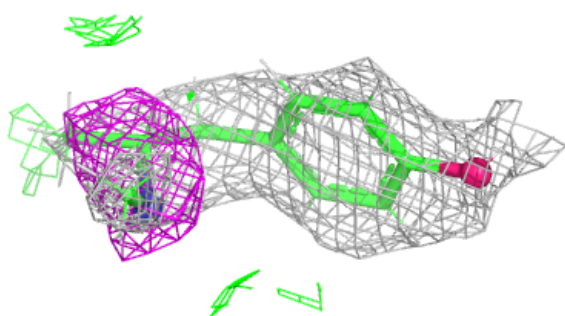
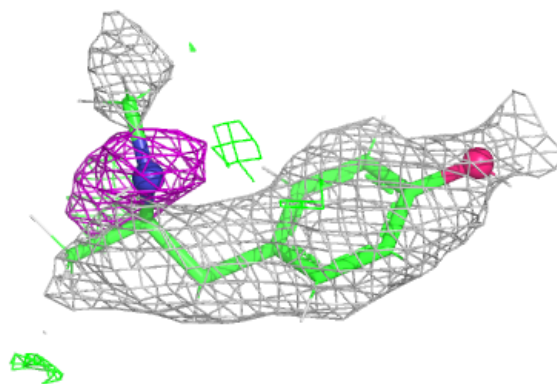
**Electron density around GKU B 1102:**

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

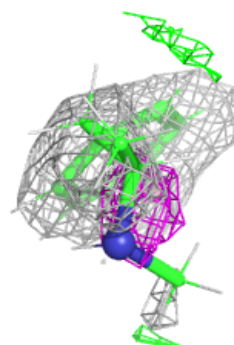
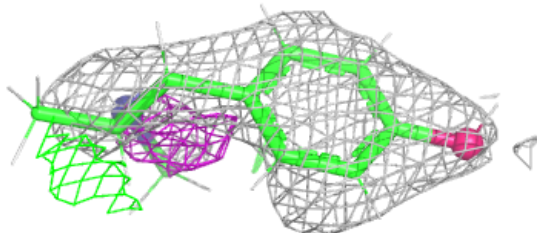
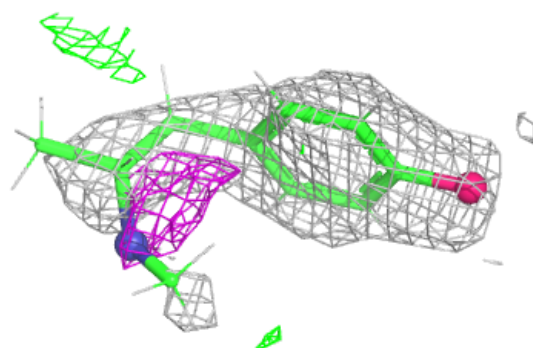


Electron density around GKU A 701:

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

**Electron density around GKU C 701:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.