



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:06 pm BST

PDB ID : 3NL5
Title : The Crystal Structure of Candida glabrata THI6, a Bifunctional Enzyme involved in Thiamin Biosynthesis of Eukaryotes
Authors : Paul, D.; Chatterjee, A.; Begley, T.P.; Ealick, S.E.
Deposited on : 2010-06-21
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

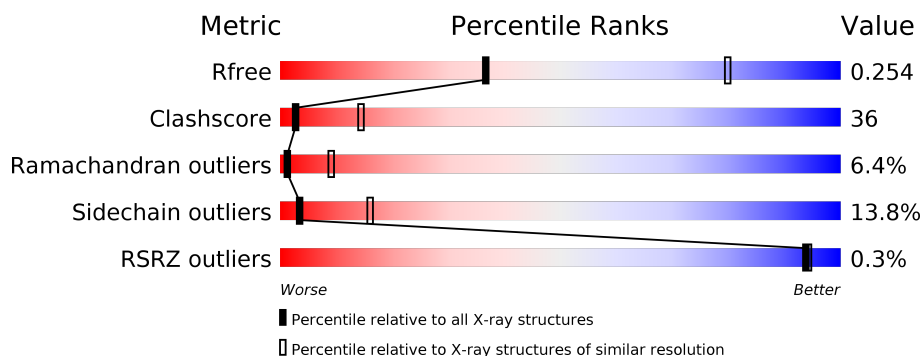
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	540	<div> <div>40%</div> <div>45%</div> <div>10%</div> <div>5%</div> </div>
1	B	540	<div> <div>40%</div> <div>45%</div> <div>9%</div> <div>6%</div> </div>
1	C	540	<div> <div>41%</div> <div>43%</div> <div>10%</div> <div>5%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TZE	B	542	-	-	X	-
4	TZE	B	543	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11543 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.

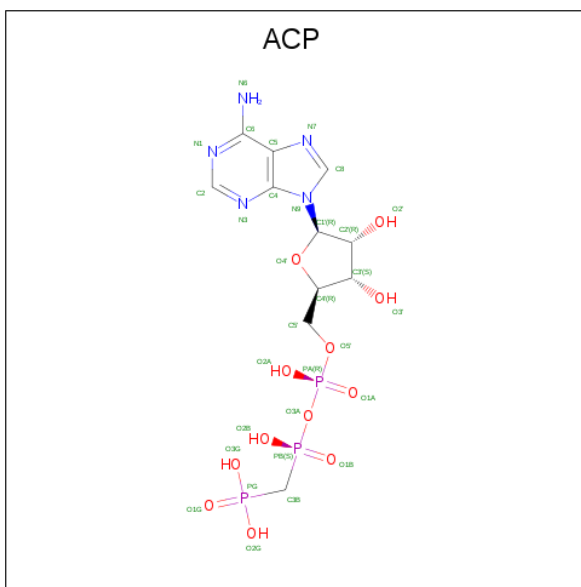
- Molecule 1 is a protein called Thiamine biosynthetic bifunctional enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			3817	2410	639	745	23			
1	B	510	Total	C	N	O	S	0	0	0
			3799	2402	632	742	23			
1	C	511	Total	C	N	O	S	0	0	0
			3804	2407	632	742	23			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

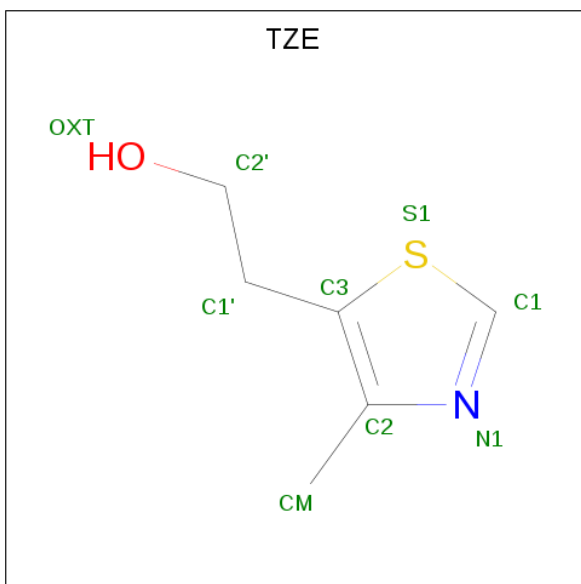
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
3	B	1	Total 31	C 11	N 5	O 12	P 3	0	0
3	C	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 4 is 2-(4-METHYL-THIAZOL-5-YL)-ETHANOL (three-letter code: TZE) (formula: C₆H₉NOS).

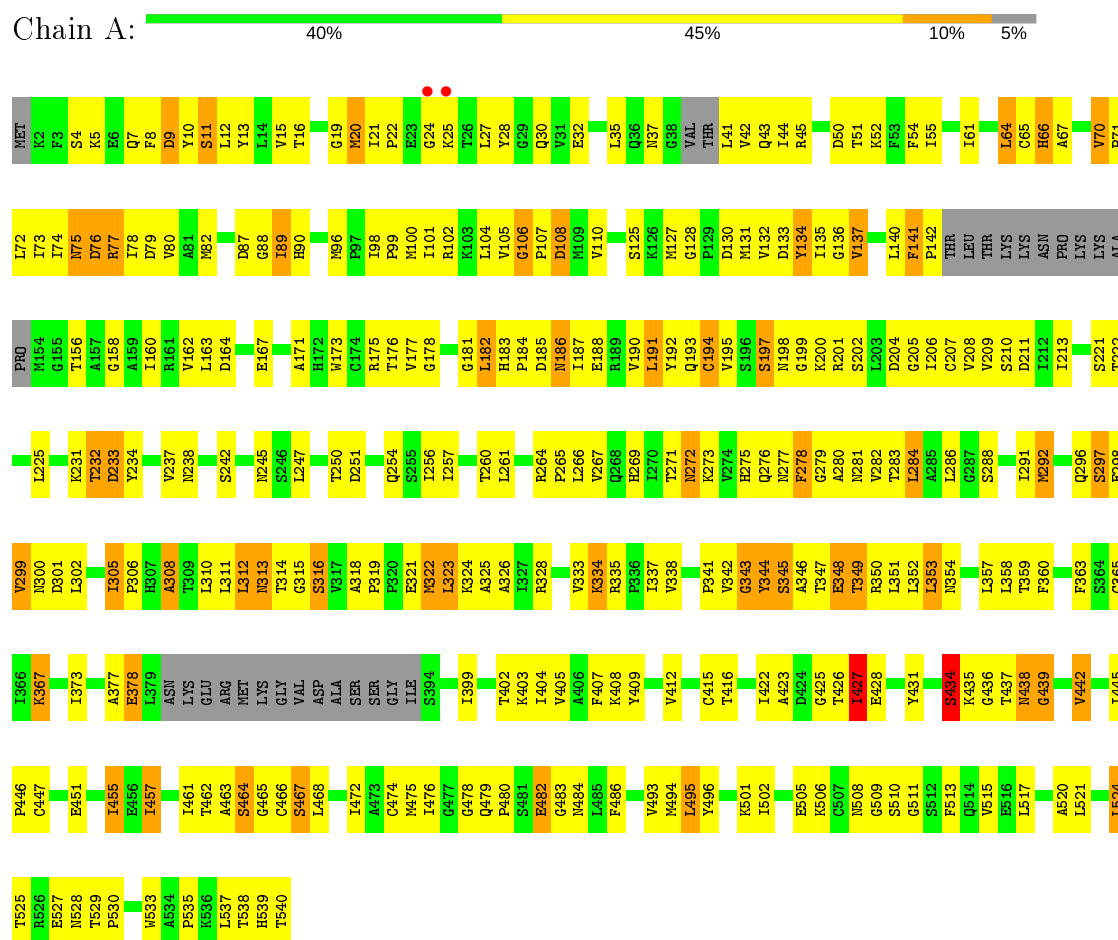


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			9	6	1	1	1		
4	B	1	Total	C	N	O	S	0	0
			9	6	1	1	1		
4	C	1	Total	C	N	O	S	0	0
			9	6	1	1	1		

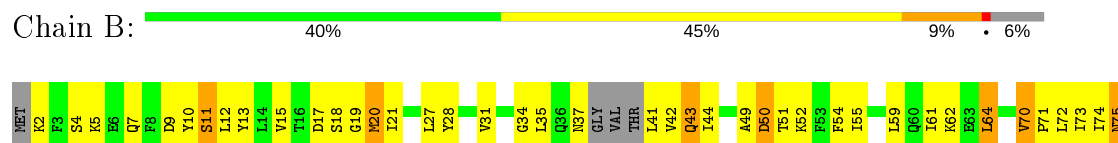
3 Residue-property plots

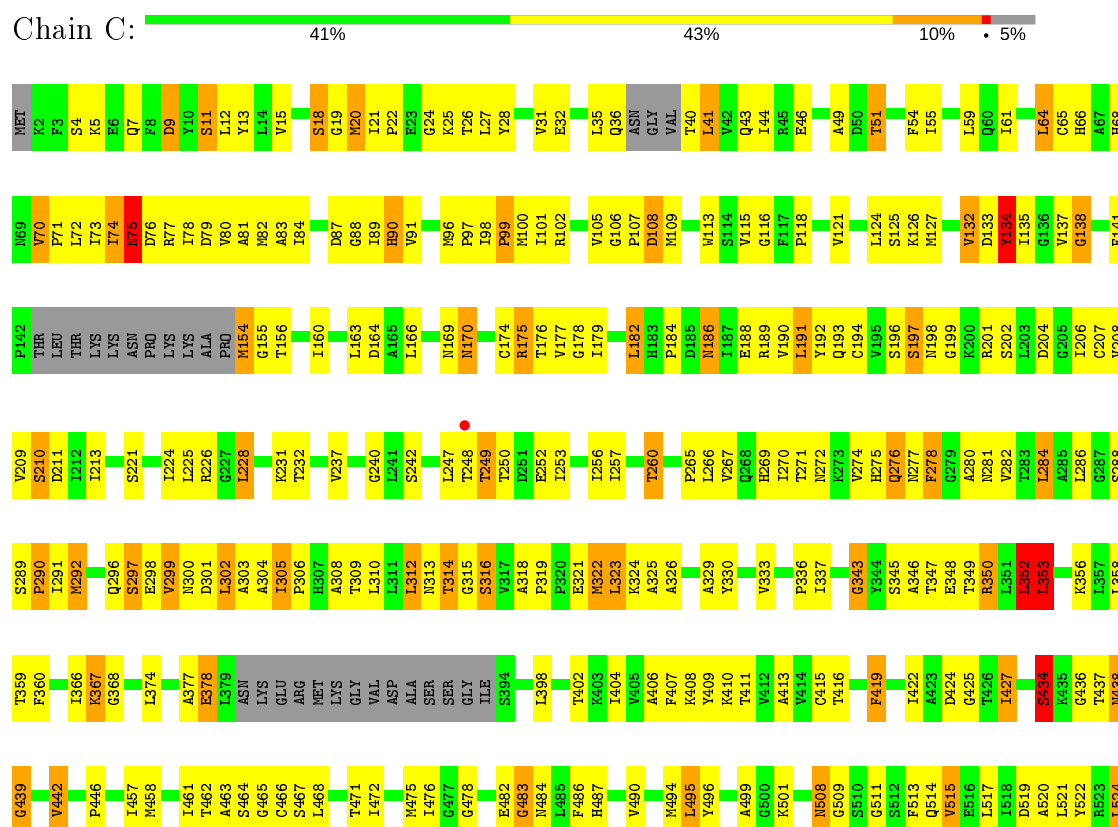
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Thiamine biosynthetic bifunctional enzyme



- Molecule 1: Thiamine biosynthetic bifunctional enzyme





T525	W533
R526	A534
E527	P535
N528	K536
T529	L537
P530	T538
	H539
	T540

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.33Å 153.93Å 108.58Å 90.00° 117.60° 90.00°	Depositor
Resolution (Å)	36.00 – 3.30 48.29 – 3.30	Depositor EDS
% Data completeness (in resolution range)	91.3 (36.00-3.30) 91.5 (48.29-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.33Å)	Xtriage
Refinement program	PHENIX ?	Depositor
R, R_{free}	0.204 , 0.243 0.200 , 0.254	Depositor DCC
R_{free} test set	1637 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11543	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: MG, ACP, TZE

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	0.46	0/3877	0.67	2/5259 (0.0%)
1	B	0.44	0/3858	0.66	2/5232 (0.0%)
1	C	0.42	0/3864	0.64	1/5242 (0.0%)
All	All	0.44	0/11599	0.66	5/15733 (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	B	434	SER	CB-CA-C	-8.55	93.85	110.10
1	A	434	SER	CB-CA-C	-8.04	94.83	110.10
1	A	435	LYS	N-CA-C	-7.37	91.10	111.00
1	C	434	SER	CB-CA-C	-6.08	98.55	110.10
1	B	435	LYS	N-CA-C	-5.12	97.18	111.00

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	3817	0	3804	274	0
1	B	3799	0	3785	288	0
1	C	3804	0	3795	276	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	31	0	14	4	0
3	B	31	0	14	8	0
3	C	31	0	14	8	0
4	B	18	0	18	17	0
4	C	9	0	9	1	0
All	All	11543	0	11453	820	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 36.

All (820) 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:272:ASN:OD1	1:B:316:SER:N	1.89	1.05
1:A:465:GLY:HA3	3:A:799:ACP:H3B2	1.36	1.02
3:B:899:ACP:O2G	4:B:542:TZE:OXT	1.82	0.97
1:A:463:ALA:O	1:A:466:CYS:N	1.98	0.96
1:B:416:THR:HB	3:B:899:ACP:H3'	1.50	0.94
1:B:59:LEU:HD21	1:B:84:ILE:HB	1.47	0.93
1:A:342:VAL:O	1:A:344:TYR:N	2.03	0.92
1:B:461:ILE:HD11	1:B:514:GLN:HG3	1.52	0.91
1:A:260:THR:HG21	1:A:475:MET:HA	1.53	0.90
1:B:101:ILE:O	1:B:105:VAL:HG22	1.73	0.89
1:A:102:ARG:HH11	1:A:107:PRO:HA	1.36	0.86
1:A:465:GLY:CA	3:A:799:ACP:H3B2	2.06	0.85
1:B:344:TYR:HA	1:B:354:ASN:ND2	1.91	0.85
1:C:407:PHE:HB3	1:C:442:VAL:HG23	1.57	0.84
1:A:44:ILE:HD12	1:A:72:LEU:HD11	1.59	0.84
1:C:266:LEU:HD11	1:C:291:ILE:HG13	1.59	0.84
1:C:75:ASN:O	1:C:77:ARG:N	2.10	0.84
1:A:195:VAL:HG12	1:A:202:SER:HB3	1.59	0.83
1:C:79:ASP:HA	1:C:82:MET:HE2	1.61	0.82
1:A:265:PRO:HD2	1:A:288:SER:HB3	1.60	0.81
1:A:322:MET:HG3	1:A:323:LEU:HD23	1.62	0.81
1:B:272:ASN:ND2	4:B:542:TZE:S1	2.54	0.81
1:A:190:VAL:O	1:A:194:CYS:HB2	1.81	0.80
1:A:461:ILE:HG23	1:A:464:SER:HB3	1.63	0.80
1:C:101:ILE:O	1:C:105:VAL:HG22	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:SER:HB3	1:B:436:GLY:HA2	1.61	0.80
1:C:472:ILE:O	1:C:476:ILE:HG13	1.82	0.80
1:B:260:THR:HG21	1:B:475:MET:HA	1.64	0.79
1:A:282:VAL:HG21	1:A:467:SER:OG	1.83	0.79
1:C:202:SER:HB3	1:C:436:GLY:HA2	1.64	0.79
1:B:89:ILE:HD11	1:B:101:ILE:HG21	1.65	0.78
1:A:35:LEU:HD22	1:A:70:VAL:HG11	1.65	0.78
1:B:247:LEU:HD21	1:B:539:HIS:CD2	2.19	0.78
1:A:310:LEU:HD23	1:A:337:ILE:HG23	1.67	0.77
1:B:296:GLN:HG3	1:B:322:MET:HB2	1.66	0.77
3:B:899:ACP:PG	4:B:542:TZE:OXT	2.43	0.77
1:B:160:ILE:HD11	1:B:193:GLN:O	1.85	0.77
1:A:342:VAL:C	1:A:344:TYR:H	1.86	0.76
1:B:81:ALA:HB1	1:B:86:ALA:HB3	1.67	0.76
1:B:41:LEU:HD12	1:B:71:PRO:HG2	1.66	0.76
1:A:344:TYR:O	1:A:345:SER:HB3	1.83	0.76
1:B:422:ILE:HD12	1:B:490:VAL:HG22	1.68	0.76
1:C:296:GLN:O	1:C:299:VAL:HG22	1.85	0.76
1:A:101:ILE:O	1:A:105:VAL:HG22	1.86	0.75
1:B:257:ILE:HD11	1:B:533:TRP:HH2	1.51	0.75
1:A:247:LEU:HD21	1:A:539:HIS:CD2	2.22	0.75
1:B:183:HIS:O	1:B:187:ILE:HG13	1.86	0.75
1:A:344:TYR:O	1:A:345:SER:CB	2.34	0.75
1:A:41:LEU:HD12	1:A:71:PRO:HG2	1.68	0.75
1:A:160:ILE:HD11	1:A:193:GLN:O	1.87	0.75
1:C:265:PRO:HD2	1:C:288:SER:HB3	1.69	0.75
1:C:406:ALA:HB2	1:C:413:ALA:HB3	1.68	0.75
1:B:74:ILE:HG13	1:B:81:ALA:HB2	1.69	0.74
1:C:468:LEU:O	1:C:472:ILE:HG13	1.86	0.74
1:B:465:GLY:H	3:B:899:ACP:H3B2	1.51	0.74
1:B:274:VAL:HG21	4:B:542:TZE:H11'	1.68	0.74
1:A:324:LYS:HB2	1:A:360:PHE:CE1	2.22	0.73
1:B:185:ASP:O	1:B:186:ASN:HB3	1.88	0.73
1:A:341:PRO:HB2	1:A:344:TYR:CB	2.17	0.73
1:A:192:TYR:CD1	1:A:234:TYR:HD2	2.06	0.73
4:B:543:TZE:H11'	1:C:274:VAL:HG21	1.70	0.73
1:B:482:GLU:CD	1:B:482:GLU:H	1.90	0.72
1:A:208:VAL:HG11	1:A:225:LEU:HD13	1.71	0.72
1:B:250:THR:HG23	1:B:530:PRO:HB2	1.71	0.72
1:B:271:THR:HA	1:B:313:ASN:HB2	1.69	0.72
1:A:404:ILE:HA	1:A:442:VAL:CG2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ILE:O	1:A:260:THR:HG23	1.89	0.71
1:A:377:ALA:O	1:A:378:GLU:HB2	1.90	0.71
1:B:278:PHE:HD2	1:B:463:ALA:HB3	1.54	0.71
1:B:353:LEU:HD12	1:B:353:LEU:O	1.90	0.71
1:C:51:THR:O	1:C:55:ILE:HG13	1.91	0.71
1:B:341:PRO:HB2	1:B:344:TYR:CB	2.21	0.71
1:C:257:ILE:HD11	1:C:533:TRP:HH2	1.55	0.71
1:C:271:THR:HA	1:C:313:ASN:HB2	1.72	0.71
1:C:324:LYS:HB2	1:C:360:PHE:CD1	2.25	0.71
1:A:276:GLN:HE22	1:A:292:MET:HG2	1.56	0.71
1:C:252:GLU:O	1:C:256:ILE:HG12	1.91	0.70
1:B:190:VAL:O	1:B:194:CYS:HB2	1.91	0.70
1:A:15:VAL:O	1:A:209:VAL:HG22	1.91	0.70
1:B:204:ASP:OD1	1:B:434:SER:HB3	1.91	0.69
1:B:437:THR:O	1:B:439:GLY:N	2.25	0.69
1:C:4:SER:OG	1:C:7:GLN:HG3	1.93	0.69
1:B:192:TYR:CD1	1:B:234:TYR:HD2	2.11	0.69
1:C:281:ASN:HA	1:C:284:LEU:CD2	2.22	0.69
1:C:437:THR:O	1:C:439:GLY:N	2.26	0.69
1:A:296:GLN:O	1:A:299:VAL:HG22	1.92	0.69
1:B:463:ALA:O	1:B:467:SER:HB2	1.93	0.69
1:B:4:SER:OG	1:B:7:GLN:HG3	1.92	0.69
1:B:407:PHE:HB3	1:B:442:VAL:HG23	1.74	0.68
1:B:59:LEU:CD2	1:B:84:ILE:HB	2.20	0.68
1:C:249:THR:HG23	1:C:252:GLU:OE1	1.92	0.68
1:B:140:LEU:HD12	1:B:182:LEU:HD11	1.75	0.68
1:C:322:MET:HG3	1:C:323:LEU:HD23	1.76	0.68
1:A:41:LEU:CD1	1:A:71:PRO:HG2	2.24	0.68
1:C:74:ILE:HG22	1:C:75:ASN:N	2.09	0.68
1:A:276:GLN:NE2	1:A:292:MET:HG2	2.09	0.67
1:B:272:ASN:OD1	1:B:316:SER:CA	2.41	0.67
1:A:231:LYS:HG2	1:A:232:THR:H	1.58	0.67
1:C:35:LEU:HD22	1:C:70:VAL:HG11	1.77	0.67
1:C:74:ILE:HG22	1:C:75:ASN:H	1.57	0.67
1:C:59:LEU:HD21	1:C:84:ILE:HB	1.77	0.67
1:C:186:ASN:O	1:C:190:VAL:HG23	1.94	0.67
1:C:260:THR:HG21	1:C:475:MET:HA	1.76	0.67
1:A:75:ASN:O	1:A:77:ARG:N	2.28	0.67
1:C:278:PHE:HD2	1:C:463:ALA:HB3	1.59	0.67
1:A:257:ILE:HD11	1:A:533:TRP:HH2	1.60	0.66
1:B:292:MET:N	4:B:543:TZE:N1	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:TYR:O	1:A:205:GLY:HA3	1.94	0.66
1:A:247:LEU:HD12	1:A:537:LEU:HG	1.77	0.66
1:B:282:VAL:HG21	1:B:467:SER:OG	1.94	0.66
1:B:520:ALA:O	1:B:524:LEU:HB2	1.94	0.66
1:C:137:VAL:CG2	1:C:178:GLY:HA2	2.25	0.66
1:A:20:MET:HG3	1:A:20:MET:O	1.96	0.66
1:A:353:LEU:O	1:A:357:LEU:HG	1.95	0.66
1:C:182:LEU:HD23	1:C:206:ILE:HG23	1.77	0.66
1:C:102:ARG:HH11	1:C:107:PRO:HA	1.60	0.66
1:A:457:ILE:HG13	1:A:457:ILE:O	1.96	0.66
1:C:190:VAL:O	1:C:194:CYS:HB2	1.95	0.66
1:B:307:HIS:HD2	1:B:477:GLY:O	1.79	0.65
1:A:343:GLY:O	1:A:345:SER:N	2.30	0.65
1:C:133:ASP:O	1:C:134:TYR:HB3	1.95	0.65
1:A:463:ALA:O	1:A:465:GLY:N	2.30	0.65
1:B:518:ILE:HG22	1:C:511:GLY:H	1.62	0.65
1:B:89:ILE:HD11	1:B:101:ILE:CG2	2.27	0.65
1:B:112:GLY:CA	1:B:134:TYR:CE2	2.80	0.65
1:C:15:VAL:HG22	1:C:43:GLN:HB3	1.78	0.65
1:B:256:ILE:O	1:B:260:THR:HG23	1.97	0.65
1:B:298:GLU:OE1	1:C:350:ARG:HD2	1.97	0.65
1:C:358:LEU:HD22	1:C:409:TYR:CD2	2.32	0.64
1:A:185:ASP:O	1:A:186:ASN:HB3	1.97	0.64
1:B:457:ILE:O	1:B:457:ILE:HG13	1.96	0.64
1:C:284:LEU:HA	1:C:288:SER:O	1.97	0.64
1:B:404:ILE:HA	1:B:442:VAL:HG22	1.80	0.64
1:B:78:ILE:HD13	1:B:96:MET:SD	2.38	0.64
1:C:74:ILE:O	1:C:75:ASN:HB2	1.97	0.64
1:C:27:LEU:HD23	1:C:61:ILE:HD11	1.79	0.64
1:C:73:ILE:HG23	1:C:88:GLY:C	2.19	0.64
1:C:89:ILE:HD11	1:C:101:ILE:HG21	1.81	0.63
1:A:202:SER:CB	1:A:436:GLY:HA2	2.29	0.63
1:A:37:ASN:HB2	1:A:222:THR:CG2	2.29	0.63
1:A:310:LEU:HD23	1:A:337:ILE:CG2	2.27	0.63
1:C:97:PRO:HB2	1:C:100:MET:HG3	1.80	0.63
1:B:265:PRO:HD2	1:B:288:SER:HB3	1.80	0.62
1:B:243:THR:HG23	1:B:446:PRO:HG3	1.81	0.62
1:A:13:TYR:CD1	1:A:41:LEU:HD23	2.34	0.62
1:A:437:THR:O	1:A:439:GLY:N	2.32	0.62
1:C:407:PHE:HE2	1:C:427:ILE:HD11	1.63	0.62
1:A:158:GLY:O	1:A:162:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:CD2	1:B:70:VAL:HG11	2.29	0.62
1:C:404:ILE:HA	1:C:442:VAL:CG2	2.28	0.62
1:C:404:ILE:HA	1:C:442:VAL:HG22	1.82	0.62
1:A:296:GLN:HG3	1:A:322:MET:HB2	1.81	0.62
1:C:137:VAL:HG22	1:C:177:VAL:O	1.99	0.62
1:C:310:LEU:HD23	1:C:337:ILE:HG23	1.80	0.62
1:C:528:ASN:O	1:C:530:PRO:HD3	2.00	0.62
1:B:281:ASN:HD21	1:C:462:THR:H	1.47	0.62
1:B:495:LEU:HD11	1:B:525:THR:HG22	1.80	0.62
1:C:160:ILE:HD11	1:C:193:GLN:O	2.00	0.62
1:C:482:GLU:H	1:C:482:GLU:CD	2.02	0.62
1:B:41:LEU:CD1	1:B:71:PRO:HG2	2.29	0.62
1:A:520:ALA:O	1:A:524:LEU:HB2	2.00	0.62
1:C:324:LYS:HB2	1:C:360:PHE:CE1	2.35	0.62
1:B:291:ILE:HA	4:B:543:TZE:N1	2.15	0.61
1:B:334:LYS:O	1:B:336:PRO:HD3	1.98	0.61
1:A:343:GLY:O	1:A:344:TYR:C	2.39	0.61
1:B:193:GLN:NE2	1:B:362:GLN:HE22	1.97	0.61
1:A:281:ASN:HA	1:A:284:LEU:CD2	2.30	0.61
1:B:133:ASP:O	1:B:134:TYR:HB3	2.00	0.61
1:B:513:PHE:CD2	1:B:513:PHE:C	2.72	0.61
1:A:100:MET:O	1:A:104:LEU:HG	2.01	0.61
1:B:343:GLY:O	1:B:344:TYR:CB	2.48	0.61
1:B:9:ASP:C	1:B:9:ASP:OD1	2.39	0.61
1:C:125:SER:C	1:C:127:MET:H	2.04	0.61
1:C:465:GLY:H	3:C:999:ACP:H3B2	1.66	0.61
1:B:310:LEU:HD13	1:B:330:TYR:CE1	2.36	0.60
1:A:204:ASP:OD1	1:A:434:SER:HB3	2.01	0.60
1:A:457:ILE:HG23	1:A:513:PHE:HE1	1.66	0.60
1:B:272:ASN:OD1	1:B:316:SER:HA	2.02	0.60
1:B:344:TYR:HA	1:B:354:ASN:HD22	1.65	0.60
1:A:528:ASN:O	1:A:530:PRO:HD3	2.01	0.60
1:A:192:TYR:HA	1:A:431:TYR:HB3	1.82	0.60
1:A:404:ILE:HA	1:A:442:VAL:HG22	1.84	0.60
1:B:249:THR:HG23	1:B:252:GLU:OE1	2.01	0.60
1:B:208:VAL:HG11	1:B:225:LEU:HD13	1.82	0.59
1:C:115:VAL:O	1:C:138:GLY:N	2.28	0.59
1:A:35:LEU:CD2	1:A:70:VAL:HG11	2.32	0.59
1:B:404:ILE:HA	1:B:442:VAL:CG2	2.32	0.59
1:A:102:ARG:NH1	1:A:107:PRO:HA	2.13	0.59
1:A:137:VAL:HG23	1:A:178:GLY:HA2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:PHE:HB3	1:A:442:VAL:HG23	1.83	0.59
1:A:457:ILE:HG12	1:A:513:PHE:HD1	1.67	0.59
1:A:472:ILE:O	1:A:476:ILE:HG13	2.03	0.59
1:B:112:GLY:HA3	1:B:134:TYR:CE2	2.38	0.59
1:C:495:LEU:HD11	1:C:525:THR:HG22	1.85	0.59
1:B:257:ILE:HG22	1:B:261:LEU:HD12	1.82	0.59
1:B:274:VAL:CG2	4:B:542:TZE:H11'	2.32	0.59
1:B:484:ASN:HD22	1:B:487:HIS:H	1.50	0.59
1:C:281:ASN:HA	1:C:284:LEU:HD21	1.85	0.59
1:A:509:GLY:HA2	1:C:522:TYR:CD2	2.38	0.59
1:A:299:VAL:HG11	1:A:326:ALA:HB2	1.85	0.59
1:A:260:THR:HA	1:A:478:GLY:HA3	1.85	0.59
1:C:267:VAL:HG12	1:C:269:HIS:CE1	2.38	0.58
1:A:202:SER:HB3	1:A:436:GLY:HA2	1.86	0.58
1:B:37:ASN:HB2	1:B:222:THR:CG2	2.33	0.58
1:C:276:GLN:HE22	1:C:292:MET:CG	2.16	0.58
1:A:24:GLY:O	1:A:25:LYS:HG3	2.04	0.58
1:A:457:ILE:HG12	1:A:513:PHE:CD1	2.38	0.58
1:C:270:ILE:CD1	1:C:310:LEU:HD11	2.34	0.58
1:B:465:GLY:H	3:B:899:ACP:C3B	2.16	0.58
1:A:342:VAL:C	1:A:344:TYR:N	2.50	0.57
1:B:74:ILE:HG22	1:B:75:ASN:H	1.68	0.57
1:C:247:LEU:HD12	1:C:537:LEU:HG	1.85	0.57
1:A:164:ASP:OD1	1:A:197:SER:HB2	2.03	0.57
1:A:462:THR:C	1:A:464:SER:H	2.07	0.57
1:B:260:THR:HA	1:B:478:GLY:HA3	1.85	0.57
1:C:9:ASP:OD2	1:C:40:THR:HG21	2.04	0.57
1:C:20:MET:O	1:C:20:MET:HG3	2.03	0.57
1:A:30:GLN:OE1	1:A:30:GLN:HA	2.04	0.57
1:C:209:VAL:HG12	1:C:210:SER:N	2.19	0.57
1:A:495:LEU:CD2	1:A:521:LEU:HD23	2.34	0.57
1:A:164:ASP:CG	1:A:197:SER:HB2	2.25	0.57
1:C:465:GLY:H	3:C:999:ACP:C3B	2.18	0.57
1:B:296:GLN:HG3	1:B:322:MET:CB	2.35	0.57
1:B:310:LEU:HD23	1:B:337:ILE:HG23	1.86	0.57
1:A:349:THR:OG1	1:C:297:SER:HB2	2.05	0.56
4:B:543:TZE:C1'	1:C:274:VAL:HG21	2.34	0.56
1:C:265:PRO:O	1:C:288:SER:HB2	2.04	0.56
1:A:463:ALA:O	1:A:464:SER:C	2.44	0.56
1:A:89:ILE:O	1:A:89:ILE:CG1	2.52	0.56
1:A:176:THR:O	1:A:204:ASP:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ASN:HA	1:B:284:LEU:CD2	2.34	0.56
1:B:528:ASN:C	1:B:530:PRO:HD3	2.26	0.56
1:B:81:ALA:HA	1:B:84:ILE:HG12	1.88	0.56
1:C:407:PHE:CB	1:C:442:VAL:HG23	2.33	0.56
1:C:65:CYS:HB3	1:C:70:VAL:O	2.04	0.56
1:A:107:PRO:O	1:A:108:ASP:HB2	2.05	0.56
1:B:247:LEU:H	1:B:247:LEU:CD2	2.19	0.56
1:C:78:ILE:HG12	1:C:89:ILE:HD12	1.87	0.56
1:C:457:ILE:HG13	1:C:457:ILE:O	2.05	0.56
1:B:358:LEU:HD23	1:B:363:PHE:HE1	1.70	0.56
1:B:522:TYR:CE1	1:B:526:ARG:NE	2.72	0.56
1:B:18:SER:O	1:B:21:ILE:HG13	2.06	0.56
1:A:9:ASP:C	1:A:9:ASP:OD1	2.45	0.56
1:B:305:ILE:HG23	1:B:306:PRO:HD2	1.88	0.56
1:B:247:LEU:HD22	1:B:247:LEU:H	1.71	0.55
4:B:543:TZE:H12'	1:C:274:VAL:HG22	1.88	0.55
1:C:407:PHE:HB3	1:C:442:VAL:CG2	2.31	0.55
1:C:406:ALA:O	1:C:425:GLY:HA3	2.06	0.55
1:A:322:MET:HG3	1:A:323:LEU:N	2.21	0.55
1:B:290:PRO:O	4:B:543:TZE:H2M	2.06	0.55
1:A:282:VAL:O	1:A:286:LEU:HG	2.05	0.55
1:C:314:THR:HG23	1:C:315:GLY:H	1.71	0.55
1:B:358:LEU:HD23	1:B:363:PHE:CE1	2.41	0.55
1:B:35:LEU:HD22	1:B:70:VAL:HG11	1.86	0.55
1:A:191:LEU:HD22	1:A:206:ILE:HD11	1.89	0.55
1:B:455:ILE:HG22	1:B:455:ILE:O	2.06	0.55
1:C:15:VAL:O	1:C:209:VAL:HG22	2.07	0.55
1:C:169:ASN:O	1:C:170:ASN:C	2.46	0.55
1:C:398:LEU:HD22	1:C:415:CYS:SG	2.47	0.55
1:B:292:MET:SD	1:B:292:MET:N	2.80	0.55
1:C:281:ASN:HA	1:C:284:LEU:HD23	1.88	0.55
1:B:515:VAL:HG23	1:C:511:GLY:C	2.27	0.54
1:C:296:GLN:HG3	1:C:322:MET:HB2	1.89	0.54
1:B:522:TYR:HD2	1:C:509:GLY:HA2	1.72	0.54
1:C:322:MET:O	1:C:325:ALA:HB3	2.07	0.54
1:A:28:TYR:CE1	1:A:64:LEU:HG	2.43	0.54
1:B:307:HIS:CD2	1:B:477:GLY:O	2.60	0.54
1:C:189:ARG:HH12	1:C:359:THR:C	2.10	0.54
1:A:156:THR:HG21	1:A:193:GLN:HG3	1.90	0.54
1:A:513:PHE:C	1:A:513:PHE:CD2	2.81	0.54
1:B:281:ASN:O	1:B:283:THR:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:THR:CG2	1:C:315:GLY:N	2.70	0.54
1:B:465:GLY:N	3:B:899:ACP:H3B2	2.19	0.54
1:C:31:VAL:O	1:C:31:VAL:HG12	2.07	0.54
1:A:509:GLY:HA2	1:C:522:TYR:HD2	1.72	0.54
1:C:124:LEU:HD23	1:C:124:LEU:C	2.27	0.54
1:A:107:PRO:O	1:A:108:ASP:CB	2.55	0.54
1:A:465:GLY:N	3:A:799:ACP:H3B2	2.22	0.54
1:A:527:GLU:O	1:A:529:THR:HG23	2.07	0.54
1:B:140:LEU:HD23	1:B:154:MET:CE	2.38	0.54
1:B:268:GLN:HA	1:B:291:ILE:O	2.08	0.54
1:B:74:ILE:HG22	1:B:75:ASN:N	2.23	0.54
1:C:267:VAL:CG1	1:C:269:HIS:CE1	2.91	0.54
1:C:314:THR:HG23	1:C:315:GLY:N	2.23	0.54
1:C:89:ILE:HD11	1:C:101:ILE:CG2	2.37	0.54
1:A:163:LEU:HD22	1:A:201:ARG:HD3	1.90	0.53
1:A:41:LEU:HG	1:A:42:VAL:N	2.23	0.53
1:A:501:LYS:HE3	1:A:505:GLU:OE2	2.07	0.53
1:A:28:TYR:O	1:A:32:GLU:HB2	2.08	0.53
1:B:414:VAL:HG22	1:B:422:ILE:HG23	1.89	0.53
1:A:358:LEU:HD23	1:A:363:PHE:HE1	1.73	0.53
1:A:422:ILE:HD11	1:A:493:VAL:HG21	1.89	0.53
1:C:280:ALA:O	1:C:284:LEU:HD22	2.08	0.53
1:A:299:VAL:HG23	1:A:300:ASN:N	2.24	0.53
1:B:81:ALA:O	1:B:82:MET:C	2.45	0.53
1:C:179:ILE:HG13	1:C:207:CYS:HB2	1.90	0.53
1:A:183:HIS:HB3	1:A:184:PRO:CD	2.39	0.53
1:B:370:SER:O	1:B:374:LEU:HG	2.09	0.53
1:A:16:THR:HG22	1:A:213:ILE:HD11	1.90	0.53
1:B:50:ASP:O	1:B:52:LYS:N	2.42	0.53
1:C:240:GLY:HA3	1:C:483:GLY:O	2.08	0.53
1:C:115:VAL:HG23	1:C:135:ILE:HB	1.89	0.53
1:C:135:ILE:CG1	1:C:176:THR:HG22	2.39	0.53
1:A:437:THR:O	1:A:438:ASN:C	2.47	0.53
1:B:121:VAL:CG1	1:B:166:LEU:HD23	2.39	0.53
1:B:28:TYR:HE1	1:B:64:LEU:HB2	1.73	0.53
1:B:296:GLN:O	1:B:299:VAL:HG22	2.08	0.53
1:B:283:THR:HG22	1:B:288:SER:O	2.08	0.53
1:A:495:LEU:O	1:A:495:LEU:HD23	2.08	0.53
1:B:334:LYS:O	1:B:336:PRO:CD	2.57	0.53
1:B:34:GLY:HA2	1:B:222:THR:HG21	1.91	0.53
1:C:18:SER:HB2	1:C:46:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD11	1:A:208:VAL:HG22	1.90	0.52
1:B:468:LEU:O	1:B:472:ILE:HG13	2.09	0.52
1:B:98:ILE:HG21	1:B:127:MET:HE1	1.90	0.52
1:C:534:ALA:N	1:C:535:PRO:CD	2.71	0.52
1:C:113:TRP:HB2	1:C:132:VAL:HG13	1.90	0.52
4:B:543:TZE:H12'	1:C:274:VAL:CG2	2.40	0.52
1:A:140:LEU:HD12	1:A:182:LEU:HD11	1.90	0.52
1:A:358:LEU:HD13	1:A:409:TYR:CE2	2.44	0.52
1:A:44:ILE:HD11	1:A:61:ILE:HG21	1.92	0.52
1:C:266:LEU:HD22	1:C:305:ILE:HD13	1.91	0.52
1:C:202:SER:CB	1:C:436:GLY:HA2	2.36	0.52
1:C:494:MET:O	1:C:495:LEU:C	2.48	0.52
1:B:522:TYR:CD2	1:C:509:GLY:HA2	2.45	0.52
1:A:198:ASN:OD1	1:A:200:LYS:HB2	2.09	0.52
1:B:140:LEU:HD23	1:B:154:MET:HE3	1.90	0.52
1:C:377:ALA:O	1:C:378:GLU:HB2	2.09	0.52
1:A:12:LEU:HD11	1:A:208:VAL:CG2	2.40	0.52
1:A:457:ILE:HG23	1:A:513:PHE:CE1	2.43	0.52
1:C:494:MET:O	1:C:496:TYR:N	2.43	0.52
1:C:513:PHE:C	1:C:513:PHE:CD2	2.83	0.52
1:A:130:ASP:O	1:A:131:MET:HG2	2.10	0.52
1:B:19:GLY:O	1:B:20:MET:HB3	2.10	0.52
1:B:28:TYR:CE1	1:B:64:LEU:HB2	2.45	0.52
1:C:347:THR:O	1:C:348:GLU:C	2.48	0.52
1:A:5:LYS:HE3	1:A:133:ASP:CG	2.31	0.52
1:B:276:GLN:NE2	1:B:292:MET:HG2	2.24	0.52
1:B:272:ASN:OD1	1:B:315:GLY:C	2.46	0.51
1:B:260:THR:HG22	1:B:478:GLY:HA3	1.92	0.51
1:C:442:VAL:O	1:C:442:VAL:HG13	2.09	0.51
1:B:43:GLN:HG3	1:B:44:ILE:N	2.25	0.51
1:B:292:MET:O	4:B:543:TZE:H1	2.10	0.51
1:A:208:VAL:HG11	1:A:225:LEU:CD1	2.38	0.51
1:A:257:ILE:HG22	1:A:261:LEU:HD12	1.90	0.51
1:A:347:THR:HG21	1:C:302:LEU:CD1	2.39	0.51
1:A:482:GLU:CD	1:A:482:GLU:H	2.13	0.51
1:B:121:VAL:HG11	1:B:166:LEU:HD23	1.92	0.51
1:C:208:VAL:HG11	1:C:225:LEU:HD13	1.92	0.51
1:C:260:THR:HG22	1:C:478:GLY:HA3	1.93	0.51
1:C:520:ALA:O	1:C:524:LEU:HB2	2.10	0.51
1:B:343:GLY:H	1:B:350:ARG:HE	1.59	0.51
1:C:107:PRO:O	1:C:108:ASP:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ILE:O	1:C:257:ILE:HG13	2.10	0.51
1:C:32:GLU:O	1:C:36:GLN:HG3	2.10	0.51
1:C:75:ASN:C	1:C:77:ARG:H	2.09	0.51
1:A:125:SER:C	1:A:127:MET:H	2.13	0.51
1:A:284:LEU:HA	1:A:288:SER:O	2.10	0.51
1:B:344:TYR:CA	1:B:354:ASN:ND2	2.71	0.51
1:B:455:ILE:HD11	1:B:501:LYS:HD3	1.92	0.51
1:C:22:PRO:O	1:C:25:LYS:HB2	2.10	0.51
1:B:281:ASN:C	1:B:283:THR:N	2.64	0.51
1:C:18:SER:O	1:C:21:ILE:HG13	2.10	0.51
1:A:495:LEU:HD22	1:A:521:LEU:CD2	2.41	0.51
1:B:209:VAL:C	1:B:211:ASP:H	2.14	0.51
1:A:308:ALA:O	1:A:335:ARG:HD3	2.11	0.50
1:B:266:LEU:O	1:B:308:ALA:HA	2.12	0.50
1:C:35:LEU:HD12	1:C:64:LEU:HD22	1.92	0.50
1:C:458:MET:O	1:C:461:ILE:HG22	2.12	0.50
1:C:9:ASP:C	1:C:9:ASP:OD1	2.50	0.50
1:B:274:VAL:HG21	4:B:542:TZE:C1'	2.39	0.50
1:B:50:ASP:C	1:B:52:LYS:H	2.14	0.50
4:B:543:TZE:C1'	1:C:274:VAL:CG2	2.89	0.50
1:C:416:THR:OG1	3:C:999:ACP:O2A	2.28	0.50
1:A:511:GLY:C	1:C:515:VAL:HG23	2.31	0.50
1:A:78:ILE:HD13	1:A:96:MET:SD	2.51	0.50
1:B:247:LEU:HD21	1:B:539:HIS:NE2	2.26	0.50
1:B:281:ASN:ND2	1:C:462:THR:H	2.09	0.50
1:C:55:ILE:O	1:C:59:LEU:HG	2.11	0.50
1:A:251:ASP:O	1:A:254:GLN:HB3	2.12	0.50
1:A:202:SER:OG	1:A:436:GLY:HA2	2.11	0.50
1:A:528:ASN:C	1:A:530:PRO:HD3	2.31	0.50
1:B:107:PRO:O	1:B:108:ASP:CB	2.59	0.50
1:B:247:LEU:HD12	1:B:537:LEU:HG	1.92	0.50
1:C:282:VAL:O	1:C:286:LEU:HG	2.12	0.50
1:C:28:TYR:CE1	1:C:64:LEU:HG	2.47	0.50
1:C:118:PRO:HA	1:C:121:VAL:HG23	1.92	0.50
1:C:299:VAL:HG23	1:C:300:ASN:N	2.26	0.50
1:A:19:GLY:O	1:A:20:MET:HB3	2.11	0.50
1:A:30:GLN:OE1	1:A:30:GLN:CA	2.59	0.50
1:B:93:GLN:NE2	1:B:114:SER:O	2.45	0.50
1:C:343:GLY:HA3	1:C:346:ALA:HB2	1.93	0.50
1:A:423:ALA:HB2	1:A:447:CYS:HB2	1.93	0.50
1:B:12:LEU:HD11	1:B:208:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:VAL:HA	1:B:334:LYS:HB3	1.93	0.50
1:B:407:PHE:HE2	1:B:427:ILE:HD11	1.76	0.50
1:C:107:PRO:O	1:C:108:ASP:HB2	2.11	0.50
1:C:204:ASP:OD1	1:C:434:SER:HB3	2.12	0.50
1:C:310:LEU:HD13	1:C:330:TYR:CE1	2.46	0.50
1:C:44:ILE:HD12	1:C:72:LEU:HD21	1.93	0.50
1:A:447:CYS:O	1:A:540:THR:CB	2.60	0.50
1:A:494:MET:O	1:A:496:TYR:N	2.44	0.49
1:B:118:PRO:C	1:B:120:GLU:N	2.65	0.49
1:B:183:HIS:HB3	1:B:184:PRO:CD	2.42	0.49
1:B:315:GLY:O	1:B:316:SER:O	2.30	0.49
1:B:41:LEU:HG	1:B:42:VAL:N	2.27	0.49
1:B:407:PHE:CB	1:B:442:VAL:HG23	2.42	0.49
1:C:366:ILE:HG13	1:C:411:THR:HG21	1.94	0.49
1:B:495:LEU:CD2	1:B:521:LEU:CD2	2.90	0.49
1:C:407:PHE:CE2	1:C:427:ILE:HD11	2.46	0.49
1:C:72:LEU:HD12	1:C:73:ILE:H	1.78	0.49
1:A:164:ASP:OD2	1:A:197:SER:HB2	2.12	0.49
1:B:224:ILE:HG22	1:B:225:LEU:N	2.27	0.49
1:A:265:PRO:HD2	1:A:288:SER:CB	2.39	0.49
1:A:276:GLN:HE22	1:A:292:MET:CG	2.24	0.49
1:C:192:TYR:OH	1:C:410:LYS:HB3	2.13	0.49
1:B:290:PRO:O	4:B:543:TZE:CM	2.60	0.49
1:C:231:LYS:HG2	1:C:232:THR:H	1.78	0.49
1:C:266:LEU:CD2	1:C:305:ILE:HD13	2.43	0.49
1:B:247:LEU:N	1:B:247:LEU:HD22	2.28	0.49
1:B:28:TYR:CZ	1:B:64:LEU:HG	2.48	0.49
1:C:175:ARG:NH1	1:C:204:ASP:OD1	2.41	0.49
1:B:265:PRO:HD2	1:B:288:SER:CB	2.43	0.49
1:B:324:LYS:HB2	1:B:360:PHE:CE1	2.47	0.49
1:B:366:ILE:HG13	1:B:411:THR:HG21	1.95	0.49
1:C:284:LEU:H	1:C:284:LEU:HD23	1.78	0.49
1:A:353:LEU:HD12	1:A:353:LEU:O	2.12	0.49
1:C:275:HIS:CG	1:C:466:CYS:HB3	2.48	0.48
1:C:302:LEU:C	1:C:304:ALA:H	2.16	0.48
1:A:105:VAL:O	1:A:106:GLY:O	2.31	0.48
1:A:305:ILE:HG23	1:A:306:PRO:HD2	1.95	0.48
1:A:515:VAL:HG23	1:B:511:GLY:C	2.33	0.48
1:A:51:THR:O	1:A:55:ILE:HG13	2.12	0.48
1:B:189:ARG:O	1:B:193:GLN:HG2	2.13	0.48
1:C:21:ILE:HD11	1:C:27:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:GLU:O	1:C:299:VAL:C	2.52	0.48
1:A:22:PRO:O	1:A:25:LYS:HB2	2.12	0.48
1:B:112:GLY:HA3	1:B:134:TYR:CZ	2.49	0.48
1:C:353:LEU:O	1:C:353:LEU:HD12	2.13	0.48
1:C:98:ILE:N	1:C:99:PRO:CD	2.76	0.48
1:A:260:THR:HG22	1:A:478:GLY:HA3	1.95	0.48
1:A:79:ASP:HA	1:A:82:MET:HE2	1.94	0.48
1:C:284:LEU:H	1:C:284:LEU:CD2	2.26	0.48
1:C:270:ILE:HD12	1:C:310:LEU:HD11	1.96	0.48
1:C:98:ILE:N	1:C:99:PRO:HD2	2.28	0.48
1:B:90:HIS:HE1	1:B:114:SER:OG	1.97	0.48
1:B:80:VAL:O	1:B:83:ALA:N	2.46	0.48
1:C:298:GLU:O	1:C:301:ASP:N	2.45	0.48
1:A:78:ILE:HG12	1:A:89:ILE:HD12	1.95	0.48
1:C:124:LEU:HD11	1:C:174:CYS:SG	2.54	0.48
1:A:324:LYS:HA	1:A:360:PHE:CD1	2.49	0.48
1:A:278:PHE:CD2	1:A:463:ALA:HB3	2.49	0.48
1:C:156:THR:HG22	1:C:194:CYS:SG	2.54	0.48
1:C:424:ASP:HB3	1:C:446:PRO:HG2	1.94	0.48
1:A:102:ARG:HB3	1:A:131:MET:HE2	1.96	0.48
1:B:125:SER:C	1:B:127:MET:H	2.17	0.48
1:B:113:TRP:HB2	1:B:132:VAL:HG13	1.96	0.48
1:B:162:VAL:C	1:B:164:ASP:N	2.67	0.48
1:A:4:SER:OG	1:A:7:GLN:HG3	2.14	0.48
1:B:517:LEU:O	1:B:517:LEU:HD23	2.14	0.48
1:B:334:LYS:O	1:B:336:PRO:N	2.47	0.47
1:B:416:THR:HB	3:B:899:ACP:C3'	2.33	0.47
1:C:484:ASN:ND2	1:C:487:HIS:H	2.12	0.47
1:A:66:HIS:HE1	1:A:87:ASP:OD1	1.98	0.47
1:C:137:VAL:HG23	1:C:178:GLY:HA2	1.97	0.47
1:C:274:VAL:HG23	1:C:275:HIS:N	2.29	0.47
1:A:21:ILE:HG23	1:A:22:PRO:HD2	1.95	0.47
1:B:276:GLN:HE22	1:B:292:MET:HG2	1.79	0.47
1:C:24:GLY:O	1:C:25:LYS:HG3	2.14	0.47
1:C:43:GLN:HE22	1:C:90:HIS:CD2	2.32	0.47
1:C:495:LEU:HD22	1:C:521:LEU:CD2	2.45	0.47
1:A:324:LYS:HB2	1:A:360:PHE:CD1	2.48	0.47
1:A:37:ASN:HB2	1:A:222:THR:HG22	1.96	0.47
1:B:107:PRO:O	1:B:108:ASP:HB2	2.14	0.47
1:B:55:ILE:O	1:B:59:LEU:HG	2.15	0.47
1:C:4:SER:O	1:C:5:LYS:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:THR:HG21	1:B:193:GLN:HG3	1.97	0.47
1:C:224:ILE:O	1:C:228:LEU:HD13	2.14	0.47
1:C:41:LEU:CD1	1:C:71:PRO:HG2	2.44	0.47
1:C:75:ASN:C	1:C:77:ARG:N	2.67	0.47
1:C:79:ASP:OD1	1:C:80:VAL:N	2.42	0.47
1:B:124:LEU:C	1:B:124:LEU:HD23	2.34	0.47
1:B:4:SER:O	1:B:5:LYS:C	2.53	0.47
1:C:490:VAL:O	1:C:494:MET:HG2	2.15	0.47
1:A:277:ASN:O	1:A:280:ALA:N	2.47	0.47
1:A:90:HIS:HD2	1:A:134:TYR:OH	1.98	0.47
1:B:247:LEU:CD2	1:B:539:HIS:NE2	2.78	0.47
1:B:343:GLY:O	1:B:372:GLU:HG2	2.15	0.47
1:C:21:ILE:HG23	1:C:22:PRO:HD2	1.97	0.47
1:C:312:LEU:HD23	1:C:312:LEU:HA	1.63	0.47
1:C:461:ILE:HD11	1:C:514:GLN:HG3	1.97	0.47
1:A:242:SER:HA	1:A:428:GLU:HG2	1.97	0.47
1:B:495:LEU:CD2	1:B:521:LEU:HD22	2.45	0.47
1:C:322:MET:HG3	1:C:323:LEU:N	2.30	0.47
1:A:455:ILE:HG22	1:A:455:ILE:O	2.14	0.47
1:C:465:GLY:N	3:C:999:ACP:H3B2	2.30	0.47
1:C:98:ILE:HB	1:C:99:PRO:HD3	1.97	0.47
1:A:533:TRP:C	1:A:535:PRO:HD2	2.34	0.47
1:B:455:ILE:HG22	1:B:458:MET:HG3	1.97	0.47
1:B:458:MET:HG2	1:B:513:PHE:CZ	2.49	0.47
1:B:533:TRP:N	1:B:533:TRP:CD1	2.80	0.47
1:A:271:THR:HA	1:A:313:ASN:HB2	1.96	0.46
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.79	0.46
1:A:186:ASN:O	1:A:190:VAL:HG23	2.15	0.46
1:A:348:GLU:O	1:A:351:LEU:HB3	2.15	0.46
1:B:510:SER:O	1:B:513:PHE:N	2.48	0.46
1:C:21:ILE:HD11	1:C:27:LEU:CD1	2.45	0.46
1:A:231:LYS:HG2	1:A:232:THR:N	2.28	0.46
1:A:247:LEU:H	1:A:247:LEU:HD22	1.80	0.46
1:A:312:LEU:HA	1:A:312:LEU:HD23	1.60	0.46
1:B:312:LEU:HA	1:B:312:LEU:HD23	1.61	0.46
1:B:81:ALA:O	1:B:84:ILE:N	2.48	0.46
1:A:13:TYR:CD2	1:A:207:CYS:SG	3.09	0.46
1:A:5:LYS:HE3	1:A:133:ASP:OD1	2.15	0.46
1:B:141:PHE:HA	1:B:142:PRO:HD3	1.68	0.46
1:B:319:PRO:HD2	1:B:322:MET:HG2	1.97	0.46
1:B:343:GLY:N	1:B:350:ARG:HE	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:HD22	1:C:70:VAL:CG1	2.44	0.46
1:C:522:TYR:O	1:C:526:ARG:HD3	2.16	0.46
1:B:513:PHE:HE2	1:B:517:LEU:HD12	1.79	0.46
1:C:102:ARG:NH1	1:C:107:PRO:HA	2.28	0.46
1:A:323:LEU:N	1:A:323:LEU:HD23	2.30	0.46
1:B:28:TYR:CE1	1:B:64:LEU:HG	2.50	0.46
1:B:523:ARG:NH1	1:C:508:ASN:HB2	2.30	0.46
1:B:484:ASN:ND2	1:B:487:HIS:H	2.13	0.46
1:A:275:HIS:CG	1:A:466:CYS:HB3	2.50	0.46
1:B:271:THR:CA	1:B:313:ASN:HB2	2.42	0.46
1:B:324:LYS:HG3	1:B:360:PHE:CG	2.51	0.46
1:B:494:MET:O	1:B:496:TYR:N	2.49	0.46
1:C:11:SER:HB3	1:C:226:ARG:HH12	1.80	0.46
1:A:209:VAL:C	1:A:211:ASP:H	2.19	0.46
1:A:298:GLU:O	1:A:299:VAL:C	2.54	0.46
1:C:98:ILE:HG21	1:C:127:MET:HE1	1.97	0.46
1:C:256:ILE:O	1:C:260:THR:HG23	2.15	0.46
1:A:247:LEU:N	1:A:247:LEU:HD22	2.32	0.45
1:B:280:ALA:O	1:B:284:LEU:HD22	2.16	0.45
1:C:179:ILE:HG13	1:C:207:CYS:CB	2.46	0.45
1:C:353:LEU:C	1:C:353:LEU:HD12	2.36	0.45
1:A:343:GLY:O	1:A:346:ALA:N	2.44	0.45
1:A:437:THR:HG23	1:A:437:THR:O	2.17	0.45
1:B:257:ILE:HD11	1:B:533:TRP:CH2	2.41	0.45
1:B:270:ILE:HB	1:B:312:LEU:HD23	1.98	0.45
1:B:55:ILE:HG12	1:B:80:VAL:HG13	1.98	0.45
1:C:163:LEU:HD23	1:C:163:LEU:HA	1.79	0.45
1:A:247:LEU:H	1:A:247:LEU:CD2	2.28	0.45
1:B:10:TYR:O	1:B:11:SER:C	2.55	0.45
1:B:407:PHE:CD1	1:B:442:VAL:HG23	2.51	0.45
1:B:487:HIS:O	1:B:491:ALA:N	2.41	0.45
1:C:276:GLN:NE2	1:C:292:MET:HG2	2.32	0.45
1:C:465:GLY:HA3	3:C:999:ACP:H3B2	1.97	0.45
1:A:404:ILE:HA	1:A:442:VAL:HG21	1.99	0.45
1:C:13:TYR:O	1:C:207:CYS:HA	2.16	0.45
1:C:299:VAL:HG23	1:C:300:ASN:H	1.81	0.45
1:C:367:LYS:HE2	1:C:465:GLY:O	2.17	0.45
1:C:292:MET:N	4:C:542:TZE:N1	2.50	0.45
1:A:265:PRO:O	1:A:288:SER:HB2	2.16	0.45
1:B:182:LEU:HD13	1:B:182:LEU:N	2.30	0.45
1:B:269:HIS:HB2	1:B:292:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:GLU:O	1:B:301:ASP:N	2.50	0.45
1:C:199:GLY:O	1:C:437:THR:O	2.34	0.45
1:A:462:THR:HG22	1:C:281:ASN:HD21	1.81	0.45
1:A:533:TRP:CD1	1:A:533:TRP:N	2.82	0.45
1:C:115:VAL:HG21	1:C:135:ILE:HG21	1.98	0.45
1:C:495:LEU:HD11	1:C:525:THR:CG2	2.46	0.45
1:A:156:THR:HG21	1:A:193:GLN:CG	2.46	0.45
1:A:264:ARG:HG2	1:A:264:ARG:O	2.17	0.45
1:A:296:GLN:CG	1:A:322:MET:HB2	2.47	0.45
1:A:426:THR:O	1:A:428:GLU:N	2.49	0.45
1:B:162:VAL:O	1:B:164:ASP:N	2.50	0.45
1:B:495:LEU:O	1:B:495:LEU:HD23	2.16	0.45
1:B:274:VAL:CG2	4:B:542:TZE:C1'	2.94	0.45
1:C:358:LEU:HD22	1:C:409:TYR:CE2	2.52	0.45
1:A:403:LYS:O	1:A:445:ILE:HD11	2.16	0.45
1:C:125:SER:C	1:C:127:MET:N	2.69	0.45
1:B:202:SER:OG	1:B:434:SER:N	2.50	0.45
1:B:340:ASP:OD1	1:B:367:LYS:HE2	2.17	0.45
1:B:367:LYS:HE3	1:B:367:LYS:O	2.17	0.45
1:C:266:LEU:O	1:C:309:THR:N	2.50	0.45
1:C:406:ALA:HB2	1:C:413:ALA:CB	2.42	0.45
1:C:276:GLN:NE2	1:C:292:MET:CG	2.80	0.45
1:C:345:SER:O	1:C:346:ALA:C	2.56	0.45
1:A:277:ASN:O	1:A:280:ALA:HB3	2.17	0.44
1:A:283:THR:HG23	1:A:474:CYS:SG	2.58	0.44
1:B:285:ALA:C	1:B:287:GLY:H	2.19	0.44
1:C:247:LEU:HD21	1:C:539:HIS:CD2	2.52	0.44
1:A:423:ALA:HA	1:A:446:PRO:O	2.16	0.44
1:A:525:THR:O	1:A:528:ASN:HB2	2.17	0.44
1:B:458:MET:HG2	1:B:513:PHE:HZ	1.82	0.44
1:C:305:ILE:HG23	1:C:306:PRO:HD2	1.98	0.44
1:A:373:ILE:HA	1:A:373:ILE:HD13	1.71	0.44
1:A:192:TYR:HB2	1:A:431:TYR:CD1	2.52	0.44
1:B:253:ILE:O	1:B:257:ILE:HG13	2.18	0.44
1:B:43:GLN:HE22	1:B:90:HIS:CD2	2.35	0.44
1:C:66:HIS:HE1	1:C:87:ASP:OD1	2.00	0.44
1:A:422:ILE:HG22	1:A:486:PHE:HE1	1.83	0.44
1:A:79:ASP:HA	1:A:82:MET:CE	2.48	0.44
1:B:275:HIS:NE2	1:B:279:GLY:HA3	2.32	0.44
1:C:164:ASP:OD1	1:C:197:SER:HB2	2.17	0.44
1:A:37:ASN:HB2	1:A:222:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LYS:NZ	1:A:431:TYR:OH	2.41	0.44
1:B:21:ILE:HD11	1:B:27:LEU:CD1	2.48	0.44
1:A:171:ALA:HA	1:A:173:TRP:CZ3	2.52	0.44
1:A:315:GLY:O	1:A:316:SER:O	2.35	0.44
1:B:80:VAL:O	1:B:81:ALA:C	2.56	0.44
1:A:237:VAL:HA	1:A:334:LYS:O	2.17	0.44
1:A:357:LEU:C	1:A:359:THR:H	2.19	0.44
1:B:88:GLY:HA2	1:B:109:MET:HG2	1.99	0.44
1:C:44:ILE:HG22	1:C:44:ILE:O	2.18	0.44
1:B:13:TYR:O	1:B:207:CYS:HA	2.18	0.44
1:C:280:ALA:O	1:C:284:LEU:CD2	2.65	0.44
1:C:461:ILE:HD11	1:C:514:GLN:CG	2.48	0.44
1:C:78:ILE:HD13	1:C:96:MET:SD	2.57	0.44
1:A:271:THR:HA	1:A:313:ASN:CB	2.48	0.44
1:A:272:ASN:O	1:A:276:GLN:HG2	2.17	0.44
1:A:511:GLY:N	1:C:519:ASP:OD1	2.50	0.44
1:B:115:VAL:HG23	1:B:135:ILE:HB	2.00	0.44
1:B:269:HIS:CD2	1:B:311:LEU:HD12	2.53	0.44
1:B:342:VAL:O	1:B:342:VAL:HG22	2.17	0.44
1:C:314:THR:C	1:C:316:SER:H	2.21	0.44
1:A:183:HIS:O	1:A:187:ILE:HG13	2.18	0.43
1:A:13:TYR:O	1:A:207:CYS:HA	2.17	0.43
1:A:463:ALA:C	1:A:465:GLY:N	2.71	0.43
1:A:495:LEU:HD22	1:A:521:LEU:HD23	1.99	0.43
1:A:136:GLY:HA2	1:A:177:VAL:O	2.18	0.43
1:A:281:ASN:HA	1:A:284:LEU:HD21	1.99	0.43
1:A:266:LEU:HD21	1:A:291:ILE:HD12	2.00	0.43
1:B:462:THR:O	1:B:463:ALA:HB3	2.18	0.43
1:B:274:VAL:HG23	1:B:275:HIS:N	2.33	0.43
1:B:343:GLY:H	1:B:350:ARG:NE	2.16	0.43
1:A:137:VAL:CG2	1:A:178:GLY:HA2	2.48	0.43
1:A:322:MET:O	1:A:325:ALA:HB3	2.19	0.43
1:A:479:GLN:HA	1:A:480:PRO:HD3	1.86	0.43
1:A:286:LEU:HD21	1:A:521:LEU:HD22	2.00	0.43
1:A:79:ASP:OD1	1:A:80:VAL:N	2.44	0.43
1:B:186:ASN:OD1	1:B:186:ASN:C	2.57	0.43
1:B:533:TRP:C	1:B:535:PRO:HD2	2.38	0.43
1:A:181:GLY:O	1:A:183:HIS:CD2	2.72	0.43
1:A:275:HIS:NE2	1:A:279:GLY:HA3	2.33	0.43
1:A:494:MET:C	1:A:496:TYR:N	2.71	0.43
1:B:402:THR:OG1	1:B:415:CYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:LYS:HG2	1:C:232:THR:N	2.34	0.43
1:C:277:ASN:O	1:C:280:ALA:HB3	2.19	0.43
1:B:79:ASP:O	1:B:82:MET:HB2	2.18	0.43
1:B:73:ILE:HG23	1:B:88:GLY:C	2.39	0.43
1:C:247:LEU:H	1:C:247:LEU:HD22	1.84	0.43
1:C:495:LEU:CD2	1:C:521:LEU:HD23	2.49	0.43
1:A:198:ASN:O	1:A:200:LYS:N	2.51	0.43
1:A:350:ARG:O	1:A:354:ASN:ND2	2.52	0.43
1:B:17:ASP:O	1:B:20:MET:HG2	2.19	0.43
1:B:225:LEU:O	1:B:229:ILE:HG13	2.19	0.43
1:C:499:ALA:HB1	1:C:520:ALA:HB3	1.98	0.43
1:A:280:ALA:O	1:A:284:LEU:HD22	2.19	0.43
1:B:501:LYS:HA	1:B:501:LYS:HD2	1.73	0.43
1:A:50:ASP:C	1:A:52:LYS:H	2.22	0.43
1:B:43:GLN:HA	1:B:73:ILE:O	2.19	0.43
1:C:318:ALA:HB1	1:C:322:MET:HG2	2.01	0.43
1:C:356:LYS:HG2	1:C:360:PHE:CZ	2.54	0.43
1:C:248:THR:HG21	1:C:253:ILE:HG12	2.01	0.43
1:C:522:TYR:CE1	1:C:526:ARG:CZ	3.01	0.43
1:A:141:PHE:HA	1:A:142:PRO:HD3	1.91	0.42
1:A:269:HIS:HB3	1:A:271:THR:HG22	2.01	0.42
1:A:282:VAL:HG21	1:A:467:SER:HG	1.81	0.42
1:A:297:SER:HB2	1:B:349:THR:HG21	2.01	0.42
1:B:376:LEU:HB2	1:B:405:VAL:HG21	2.00	0.42
1:B:407:PHE:CE2	1:B:427:ILE:HD11	2.53	0.42
1:B:192:TYR:HA	1:B:431:TYR:HB3	2.01	0.42
1:B:5:LYS:HE3	1:B:133:ASP:CG	2.39	0.42
1:C:74:ILE:CG2	1:C:75:ASN:N	2.76	0.42
1:A:275:HIS:O	1:A:275:HIS:CG	2.72	0.42
1:A:185:ASP:O	1:A:185:ASP:OD2	2.38	0.42
1:A:324:LYS:CA	1:A:360:PHE:CD1	3.02	0.42
1:A:402:THR:OG1	1:A:415:CYS:HB2	2.19	0.42
1:B:13:TYR:CD1	1:B:41:LEU:HD23	2.54	0.42
1:B:247:LEU:HD21	1:B:539:HIS:HD2	1.79	0.42
1:C:35:LEU:O	1:C:68:HIS:CD2	2.72	0.42
1:A:10:TYR:O	1:A:11:SER:C	2.56	0.42
1:A:298:GLU:O	1:A:301:ASP:N	2.44	0.42
1:A:13:TYR:CE1	1:A:41:LEU:HD23	2.54	0.42
1:A:425:GLY:O	1:A:427:ILE:HG12	2.20	0.42
1:A:73:ILE:HG23	1:A:88:GLY:C	2.40	0.42
1:B:154:MET:HG3	1:B:155:GLY:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:THR:CG2	1:B:315:GLY:N	2.83	0.42
1:B:517:LEU:C	1:B:517:LEU:CD2	2.88	0.42
1:C:269:HIS:HB2	1:C:292:MET:SD	2.59	0.42
1:C:323:LEU:HD23	1:C:323:LEU:N	2.35	0.42
1:A:125:SER:C	1:A:127:MET:N	2.73	0.42
1:A:231:LYS:CG	1:A:232:THR:H	2.28	0.42
1:B:115:VAL:HB	1:B:135:ILE:HD12	2.01	0.42
1:B:162:VAL:C	1:B:164:ASP:H	2.22	0.42
1:B:136:GLY:HA2	1:B:177:VAL:O	2.19	0.42
1:B:203:LEU:HA	1:B:203:LEU:HD23	1.81	0.42
1:B:326:ALA:O	1:B:327:ILE:C	2.57	0.42
1:B:397:LEU:HA	1:B:397:LEU:HD12	1.88	0.42
1:B:468:LEU:HD12	1:B:468:LEU:O	2.19	0.42
1:B:510:SER:O	1:B:511:GLY:C	2.58	0.42
1:C:271:THR:CA	1:C:313:ASN:HB2	2.45	0.42
1:A:324:LYS:CB	1:A:360:PHE:CD1	3.03	0.42
1:A:423:ALA:HA	1:A:447:CYS:HA	2.00	0.42
1:B:20:MET:O	1:B:20:MET:HG3	2.19	0.42
1:B:202:SER:CB	1:B:436:GLY:HA2	2.41	0.42
1:B:440:THR:HG22	1:B:440:THR:O	2.20	0.42
1:C:134:TYR:C	1:C:134:TYR:CD1	2.93	0.42
1:C:275:HIS:CG	1:C:275:HIS:O	2.73	0.42
1:C:41:LEU:HD12	1:C:71:PRO:HG2	2.02	0.42
1:A:186:ASN:C	1:A:186:ASN:OD1	2.58	0.42
1:A:21:ILE:HD11	1:A:27:LEU:HD12	2.02	0.42
1:B:154:MET:CG	1:B:155:GLY:N	2.82	0.42
1:C:184:PRO:HD3	1:C:211:ASP:OD2	2.20	0.42
1:C:471:THR:O	1:C:475:MET:HG2	2.20	0.42
1:A:247:LEU:CD2	1:A:539:HIS:NE2	2.83	0.42
1:A:373:ILE:O	1:A:373:ILE:CG2	2.66	0.42
1:A:75:ASN:O	1:A:76:ASP:C	2.58	0.42
1:B:297:SER:OG	1:C:349:THR:HG21	2.20	0.42
1:C:318:ALA:HA	1:C:319:PRO:HD3	1.86	0.42
1:C:410:LYS:HD3	1:C:410:LYS:HA	1.82	0.42
1:A:266:LEU:HD12	1:A:267:VAL:N	2.35	0.42
1:A:318:ALA:HB3	1:A:323:LEU:HD21	2.02	0.42
1:B:187:ILE:HD12	1:B:225:LEU:HD22	2.02	0.42
1:B:44:ILE:N	1:B:73:ILE:O	2.41	0.42
1:C:527:GLU:O	1:C:529:THR:HG23	2.20	0.42
1:A:64:LEU:O	1:A:67:ALA:HB3	2.20	0.41
1:C:18:SER:O	1:C:20:MET:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:GLY:HA3	1:A:350:ARG:NH2	2.35	0.41
1:A:501:LYS:HD2	1:A:501:LYS:HA	1.76	0.41
1:A:65:CYS:HB3	1:A:70:VAL:O	2.20	0.41
1:A:89:ILE:O	1:A:89:ILE:HG13	2.20	0.41
1:B:62:LYS:HA	1:B:72:LEU:HD22	2.02	0.41
1:C:22:PRO:HG2	1:C:25:LYS:HD3	2.01	0.41
1:C:484:ASN:HD21	1:C:486:PHE:HB3	1.84	0.41
1:C:73:ILE:HG23	1:C:89:ILE:N	2.35	0.41
1:C:79:ASP:HA	1:C:82:MET:CE	2.42	0.41
1:A:427:ILE:HG22	1:A:427:ILE:O	2.21	0.41
1:A:462:THR:O	1:A:464:SER:N	2.53	0.41
1:B:373:ILE:HA	1:B:373:ILE:HD13	1.73	0.41
1:B:524:LEU:HA	1:B:524:LEU:HD13	1.64	0.41
1:C:191:LEU:HD12	1:C:191:LEU:HA	1.70	0.41
1:C:326:ALA:O	1:C:329:ALA:HB3	2.20	0.41
1:C:404:ILE:HA	1:C:442:VAL:HG21	2.00	0.41
1:C:422:ILE:HG22	1:C:486:PHE:HE1	1.85	0.41
1:A:277:ASN:O	1:A:278:PHE:C	2.59	0.41
1:A:311:LEU:HD23	1:A:338:VAL:HB	2.02	0.41
1:A:319:PRO:HD2	1:A:322:MET:HG2	2.02	0.41
1:A:98:ILE:N	1:A:99:PRO:CD	2.84	0.41
1:B:342:VAL:HA	1:B:343:GLY:HA2	1.76	0.41
1:B:501:LYS:HE3	1:B:505:GLU:OE2	2.20	0.41
1:B:98:ILE:N	1:B:99:PRO:CD	2.83	0.41
1:C:289:SER:HA	1:C:290:PRO:HD3	1.82	0.41
1:C:533:TRP:C	1:C:535:PRO:HD2	2.41	0.41
1:A:27:LEU:HD23	1:A:61:ILE:HD11	2.01	0.41
1:A:468:LEU:O	1:A:472:ILE:HG13	2.20	0.41
1:B:12:LEU:HD11	1:B:208:VAL:CG2	2.50	0.41
1:C:13:TYR:CD2	1:C:207:CYS:SG	3.13	0.41
1:A:128:GLY:O	1:A:173:TRP:CZ2	2.73	0.41
1:A:403:LYS:HG2	1:A:447:CYS:HB2	2.01	0.41
1:B:461:ILE:HG23	1:B:464:SER:HB2	2.02	0.41
1:B:495:LEU:HD22	1:B:521:LEU:HD22	2.02	0.41
1:C:135:ILE:HG13	1:C:176:THR:HG22	2.01	0.41
1:C:154:MET:CG	1:C:155:GLY:N	2.83	0.41
1:C:213:ILE:HD13	1:C:213:ILE:HA	1.85	0.41
1:C:402:THR:OG1	1:C:415:CYS:HB2	2.21	0.41
1:C:419:PHE:CD1	1:C:419:PHE:N	2.88	0.41
1:A:10:TYR:CD1	1:A:10:TYR:N	2.88	0.41
1:B:15:VAL:O	1:B:209:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASN:ND2	1:B:314:THR:O	2.54	0.41
1:B:442:VAL:O	1:B:442:VAL:HG13	2.19	0.41
1:A:281:ASN:ND2	1:B:462:THR:H	2.18	0.41
1:B:495:LEU:HD23	1:B:521:LEU:CD2	2.51	0.41
1:C:416:THR:HB	3:C:999:ACP:H3'	2.02	0.41
1:A:273:LYS:HA	1:A:276:GLN:CG	2.51	0.41
1:A:510:SER:O	1:A:513:PHE:HB3	2.20	0.41
1:B:138:GLY:HA3	1:B:154:MET:CE	2.50	0.41
1:B:176:THR:O	1:B:204:ASP:HB2	2.20	0.41
1:B:357:LEU:HD23	1:B:360:PHE:CE1	2.55	0.41
1:A:247:LEU:HD21	1:A:539:HIS:NE2	2.35	0.41
1:A:506:LYS:HE2	1:A:506:LYS:HB3	1.98	0.41
1:B:273:LYS:HA	1:B:276:GLN:HG3	2.03	0.41
1:A:182:LEU:HD13	1:A:182:LEU:N	2.36	0.41
1:B:118:PRO:C	1:B:120:GLU:H	2.23	0.41
1:B:424:ASP:O	1:B:445:ILE:HB	2.21	0.41
1:C:105:VAL:HB	1:C:109:MET:SD	2.61	0.41
1:C:31:VAL:O	1:C:31:VAL:CG1	2.69	0.41
1:C:257:ILE:CD1	1:C:533:TRP:HH2	2.27	0.41
1:A:314:THR:CG2	1:A:315:GLY:N	2.84	0.41
1:B:327:ILE:HG22	1:B:361:GLY:HA3	2.03	0.41
1:C:374:LEU:HA	1:C:374:LEU:HD23	1.95	0.41
1:C:74:ILE:CG2	1:C:75:ASN:H	2.24	0.41
1:A:135:ILE:CG1	1:A:176:THR:HG22	2.51	0.40
1:A:8:PHE:CE1	1:A:110:VAL:HG21	2.56	0.40
1:B:341:PRO:O	1:B:343:GLY:O	2.39	0.40
1:B:471:THR:O	1:B:472:ILE:C	2.58	0.40
1:B:75:ASN:HB3	1:B:76:ASP:H	1.56	0.40
1:C:176:THR:O	1:C:204:ASP:HB2	2.20	0.40
1:C:302:LEU:C	1:C:304:ALA:N	2.73	0.40
1:B:298:GLU:HG2	1:C:347:THR:OG1	2.21	0.40
1:B:252:GLU:O	1:B:256:ILE:HG12	2.20	0.40
1:B:59:LEU:HD23	1:B:59:LEU:HA	1.87	0.40
1:B:91:VAL:HG11	1:B:101:ILE:HD13	2.02	0.40
1:C:121:VAL:O	1:C:124:LEU:HB3	2.22	0.40
1:A:416:THR:HB	3:A:799:ACP:H3'	2.04	0.40
1:A:457:ILE:HD12	1:C:522:TYR:CZ	2.56	0.40
1:B:512:SER:O	1:B:513:PHE:C	2.59	0.40
1:C:237:VAL:HG21	1:C:336:PRO:HB3	2.03	0.40
1:C:368:GLY:O	1:C:415:CYS:HA	2.22	0.40
1:C:437:THR:O	1:C:438:ASN:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ILE:HG13	1:C:81:ALA:HA	2.04	0.40
3:C:999:ACP:O5'	3:C:999:ACP:H8	2.21	0.40
1:A:341:PRO:HD2	1:A:367:LYS:O	2.22	0.40
1:A:462:THR:C	1:A:464:SER:N	2.73	0.40
1:A:89:ILE:HG12	1:A:89:ILE:O	2.21	0.40
1:B:31:VAL:O	1:B:35:LEU:HG	2.21	0.40
1:B:479:GLN:HA	1:B:480:PRO:HD3	1.89	0.40
1:B:509:GLY:O	1:B:513:PHE:HB2	2.21	0.40
1:C:166:LEU:HD13	1:C:201:ARG:CZ	2.52	0.40
1:C:226:ARG:HD3	1:C:226:ARG:HA	1.61	0.40
1:C:352:LEU:O	1:C:353:LEU:C	2.59	0.40
1:B:465:GLY:CA	3:B:899:ACP:H3B2	2.52	0.40
1:B:522:TYR:CE1	1:B:526:ARG:CZ	3.05	0.40
1:B:527:GLU:O	1:B:529:THR:HG23	2.21	0.40
1:C:282:VAL:O	1:C:282:VAL:HG12	2.21	0.40
1:C:465:GLY:CA	3:C:999:ACP:H3B2	2.52	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	504/540 (93%)	399 (79%)	73 (14%)	32 (6%)	1	9
1	B	500/540 (93%)	385 (77%)	85 (17%)	30 (6%)	1	10
1	C	503/540 (93%)	407 (81%)	61 (12%)	35 (7%)	1	7
All	All	1507/1620 (93%)	1191 (79%)	219 (14%)	97 (6%)	1	9

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	MET

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Mol	Chain	Res	Type
1	A	76	ASP
1	A	186	ASN
1	A	272	ASN
1	A	316	SER
1	A	343	GLY
1	A	344	TYR
1	A	345	SER
1	A	438	ASN
1	B	20	MET
1	B	80	VAL
1	B	186	ASN
1	B	272	ASN
1	B	316	SER
1	B	438	ASN
1	C	20	MET
1	C	41	LEU
1	C	49	ALA
1	C	74	ILE
1	C	126	LYS
1	C	170	ASN
1	C	308	ALA
1	C	316	SER
1	C	438	ASN
1	A	106	GLY
1	A	378	GLU
1	A	434	SER
1	A	439	GLY
1	A	464	SER
1	A	483	GLY
1	A	495	LEU
1	B	11	SER
1	B	49	ALA
1	B	51	THR
1	B	106	GLY
1	B	163	LEU
1	B	282	VAL
1	B	495	LEU
1	C	11	SER
1	C	75	ASN
1	C	134	TYR
1	C	303	ALA
1	C	343	GLY

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Mol	Chain	Res	Type
1	C	434	SER
1	C	495	LEU
1	A	77	ARG
1	A	238	ASN
1	B	108	ASP
1	B	306	PRO
1	B	441	SER
1	C	76	ASP
1	C	186	ASN
1	C	272	ASN
1	C	378	GLU
1	C	483	GLY
1	A	11	SER
1	A	199	GLY
1	A	232	THR
1	A	308	ALA
1	A	405	VAL
1	B	210	SER
1	B	247	LEU
1	B	434	SER
1	B	511	GLY
1	C	83	ALA
1	C	278	PHE
1	C	299	VAL
1	C	352	LEU
1	C	353	LEU
1	A	108	ASP
1	A	233	ASP
1	B	126	LYS
1	B	132	VAL
1	B	170	ASN
1	B	209	VAL
1	C	108	ASP
1	C	290	PRO
1	A	132	VAL
1	A	210	SER
1	A	278	PHE
1	A	427	ILE
1	B	81	ALA
1	B	155	GLY
1	B	290	PRO
1	B	439	GLY

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Mol	Chain	Res	Type
1	C	132	VAL
1	B	446	PRO
1	C	99	PRO
1	C	116	GLY
1	C	138	GLY
1	A	455	ILE
1	A	502	ILE
1	B	534	ALA
1	C	19	GLY
1	C	439	GLY
1	A	299	VAL
1	C	106	GLY

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	414/449 (92%)	358 (86%)	56 (14%)	4	16
1	B	412/449 (92%)	353 (86%)	59 (14%)	3	15
1	C	412/449 (92%)	356 (86%)	56 (14%)	3	16
All	All	1238/1347 (92%)	1067 (86%)	171 (14%)	3	16

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	43	GLN
1	A	54	PHE
1	A	64	LEU
1	A	66	HIS
1	A	70	VAL
1	A	74	ILE
1	A	75	ASN
1	A	89	ILE
1	A	134	TYR

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Mol	Chain	Res	Type
1	A	137	VAL
1	A	141	PHE
1	A	167	GLU
1	A	175	ARG
1	A	182	LEU
1	A	188	GLU
1	A	191	LEU
1	A	194	CYS
1	A	197	SER
1	A	221	SER
1	A	233	ASP
1	A	245	ASN
1	A	250	THR
1	A	284	LEU
1	A	292	MET
1	A	297	SER
1	A	302	LEU
1	A	305	ILE
1	A	312	LEU
1	A	313	ASN
1	A	321	GLU
1	A	322	MET
1	A	323	LEU
1	A	328	ARG
1	A	333	VAL
1	A	334	LYS
1	A	348	GLU
1	A	349	THR
1	A	352	LEU
1	A	353	LEU
1	A	365	CYS
1	A	367	LYS
1	A	399	ILE
1	A	408	LYS
1	A	412	VAL
1	A	427	ILE
1	A	442	VAL
1	A	451	GLU
1	A	457	ILE
1	A	467	SER
1	A	482	GLU
1	A	484	ASN

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Mol	Chain	Res	Type
1	A	508	ASN
1	A	517	LEU
1	A	524	LEU
1	A	538	THR
1	B	2	LYS
1	B	43	GLN
1	B	50	ASP
1	B	54	PHE
1	B	61	ILE
1	B	64	LEU
1	B	70	VAL
1	B	75	ASN
1	B	93	GLN
1	B	113	TRP
1	B	137	VAL
1	B	154	MET
1	B	167	GLU
1	B	175	ARG
1	B	177	VAL
1	B	182	LEU
1	B	188	GLU
1	B	191	LEU
1	B	197	SER
1	B	232	THR
1	B	233	ASP
1	B	242	SER
1	B	247	LEU
1	B	261	LEU
1	B	266	LEU
1	B	276	GLN
1	B	284	LEU
1	B	292	MET
1	B	296	GLN
1	B	297	SER
1	B	302	LEU
1	B	306	PRO
1	B	311	LEU
1	B	312	LEU
1	B	322	MET
1	B	328	ARG
1	B	333	VAL
1	B	342	VAL

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Mol	Chain	Res	Type
1	B	349	THR
1	B	351	LEU
1	B	352	LEU
1	B	353	LEU
1	B	367	LYS
1	B	371	SER
1	B	399	ILE
1	B	408	LYS
1	B	427	ILE
1	B	434	SER
1	B	442	VAL
1	B	461	ILE
1	B	467	SER
1	B	482	GLU
1	B	501	LYS
1	B	508	ASN
1	B	515	VAL
1	B	517	LEU
1	B	524	LEU
1	B	526	ARG
1	B	538	THR
1	C	9	ASP
1	C	12	LEU
1	C	18	SER
1	C	26	THR
1	C	51	THR
1	C	54	PHE
1	C	64	LEU
1	C	70	VAL
1	C	75	ASN
1	C	90	HIS
1	C	91	VAL
1	C	134	TYR
1	C	141	PHE
1	C	154	MET
1	C	175	ARG
1	C	182	LEU
1	C	188	GLU
1	C	191	LEU
1	C	196	SER
1	C	197	SER
1	C	198	ASN

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Mol	Chain	Res	Type
1	C	210	SER
1	C	221	SER
1	C	228	LEU
1	C	242	SER
1	C	249	THR
1	C	250	THR
1	C	260	THR
1	C	276	GLN
1	C	284	LEU
1	C	292	MET
1	C	297	SER
1	C	302	LEU
1	C	305	ILE
1	C	312	LEU
1	C	314	THR
1	C	321	GLU
1	C	322	MET
1	C	323	LEU
1	C	333	VAL
1	C	350	ARG
1	C	352	LEU
1	C	353	LEU
1	C	367	LYS
1	C	408	LYS
1	C	419	PHE
1	C	427	ILE
1	C	442	VAL
1	C	464	SER
1	C	467	SER
1	C	501	LYS
1	C	508	ASN
1	C	515	VAL
1	C	517	LEU
1	C	524	LEU
1	C	538	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	90	HIS
1	A	93	GLN

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	193	GLN
1	A	276	GLN
1	A	277	ASN
1	A	281	ASN
1	A	313	ASN
1	A	362	GLN
1	A	479	GLN
1	A	484	ASN
1	B	43	GLN
1	B	66	HIS
1	B	90	HIS
1	B	93	GLN
1	B	193	GLN
1	B	276	GLN
1	B	281	ASN
1	B	307	HIS
1	B	355	ASN
1	B	484	ASN
1	C	43	GLN
1	C	66	HIS
1	C	68	HIS
1	C	93	GLN
1	C	183	HIS
1	C	193	GLN
1	C	272	ASN
1	C	276	GLN
1	C	281	ASN
1	C	362	GLN
1	C	484	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACP	A	799	2	27,33,33	3.39	13 (48%)	32,52,52	1.61	4 (12%)
4	TZE	B	543	-	5,9,9	2.03	3 (60%)	3,11,11	3.01	1 (33%)
4	TZE	B	542	-	5,9,9	1.96	3 (60%)	3,11,11	2.99	1 (33%)
3	ACP	B	899	2	27,33,33	3.45	13 (48%)	32,52,52	1.73	5 (15%)
3	ACP	C	999	2	27,33,33	3.42	12 (44%)	32,52,52	1.63	6 (18%)
4	TZE	C	542	-	5,9,9	2.18	3 (60%)	3,11,11	2.98	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACP	A	799	2	-	11/15/38/38	0/3/3/3
4	TZE	B	543	-	-	0/2/3/3	0/1/1/1
4	TZE	B	542	-	-	1/2/3/3	0/1/1/1
3	ACP	B	899	2	-	8/15/38/38	0/3/3/3
3	ACP	C	999	2	-	6/15/38/38	0/3/3/3
4	TZE	C	542	-	-	1/2/3/3	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	899	ACP	PB-O3A	8.48	1.67	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	799	ACP	PB-O3A	7.87	1.67	1.58
3	C	999	ACP	PB-O3A	7.87	1.67	1.58
3	C	999	ACP	PG-O1G	7.20	1.65	1.50
3	B	899	ACP	PG-O1G	7.20	1.65	1.50
3	A	799	ACP	PG-O1G	7.15	1.65	1.50
3	B	899	ACP	PB-O1B	5.81	1.65	1.51
3	C	999	ACP	PB-O1B	5.57	1.65	1.51
3	A	799	ACP	PB-O1B	5.48	1.64	1.51
3	C	999	ACP	C2-N3	5.18	1.40	1.32
3	C	999	ACP	C8-N7	4.96	1.43	1.34
3	B	899	ACP	C2-N3	4.88	1.40	1.32
3	B	899	ACP	C8-N7	4.86	1.43	1.34
3	A	799	ACP	C2-N3	4.84	1.39	1.32
3	C	999	ACP	O4'-C1'	4.73	1.47	1.41
3	A	799	ACP	C8-N7	4.67	1.43	1.34
3	C	999	ACP	PG-O2G	4.58	1.65	1.54
3	A	799	ACP	PG-O2G	4.49	1.65	1.54
3	B	899	ACP	PB-O2B	-4.43	1.46	1.56
3	A	799	ACP	PB-O2B	-4.34	1.46	1.56
3	B	899	ACP	PG-O2G	4.32	1.64	1.54
3	A	799	ACP	O4'-C1'	4.30	1.47	1.41
3	C	999	ACP	PA-O1A	4.28	1.66	1.50
3	B	899	ACP	PA-O1A	4.25	1.66	1.50
3	A	799	ACP	PA-O1A	4.08	1.65	1.50
3	B	899	ACP	O4'-C1'	4.04	1.46	1.41
3	C	999	ACP	PB-O2B	-3.96	1.47	1.56
3	A	799	ACP	PG-O3G	-3.65	1.46	1.54
3	C	999	ACP	C6-N6	3.57	1.47	1.34
3	A	799	ACP	C6-N6	3.50	1.46	1.34
3	B	899	ACP	C6-N6	3.44	1.46	1.34
4	C	542	TZE	C1'-C3	3.36	1.52	1.50
3	B	899	ACP	PG-O3G	-3.11	1.47	1.54
3	C	999	ACP	PG-O3G	-3.00	1.48	1.54
4	B	543	TZE	C1'-C3	2.99	1.52	1.50
4	C	542	TZE	C3-C2	-2.75	1.37	1.42
4	B	542	TZE	C3-C2	-2.67	1.37	1.42
4	B	542	TZE	C1'-C3	2.58	1.52	1.50
4	B	543	TZE	C3-C2	-2.42	1.37	1.42
3	C	999	ACP	C2-N1	2.35	1.38	1.33
4	B	543	TZE	CM-C2	2.22	1.54	1.50
3	B	899	ACP	C2-N1	2.17	1.37	1.33
4	B	542	TZE	CM-C2	2.15	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	799	ACP	C2-N1	2.09	1.37	1.33
3	B	899	ACP	PA-O5'	2.08	1.67	1.59
4	C	542	TZE	CM-C2	2.02	1.53	1.50
3	A	799	ACP	PA-O5'	2.01	1.67	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	899	ACP	N3-C2-N1	-5.68	119.79	128.68
3	A	799	ACP	N3-C2-N1	-5.50	120.08	128.68
3	C	999	ACP	N3-C2-N1	-5.31	120.39	128.68
4	B	543	TZE	C1'-C3-C2	5.05	131.49	127.43
4	B	542	TZE	C1'-C3-C2	5.02	131.46	127.43
4	C	542	TZE	C1'-C3-C2	4.94	131.40	127.43
3	A	799	ACP	PA-O3A-PB	-4.09	119.59	132.56
3	B	899	ACP	PA-O3A-PB	-3.29	122.11	132.56
3	B	899	ACP	C2'-C3'-C4'	3.19	108.84	102.64
3	C	999	ACP	PA-O3A-PB	-3.00	123.05	132.56
3	C	999	ACP	C3'-C2'-C1'	2.97	105.45	100.98
3	B	899	ACP	O5'-C5'-C4'	2.80	118.61	108.99
3	A	799	ACP	O5'-C5'-C4'	2.47	117.51	108.99
3	B	899	ACP	O4'-C4'-C5'	2.34	117.08	109.37
3	C	999	ACP	O3'-C3'-C2'	2.26	119.12	111.82
3	A	799	ACP	O4'-C4'-C5'	2.21	116.65	109.37
3	C	999	ACP	O2G-PG-O1G	-2.14	106.73	112.39
3	C	999	ACP	O3'-C3'-C4'	2.05	116.97	111.05

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	542	TZE	C3-C1'-C2'-OXT
3	A	799	ACP	PB-C3B-PG-O1G
3	A	799	ACP	PB-C3B-PG-O2G
3	A	799	ACP	PB-C3B-PG-O3G
3	A	799	ACP	PG-C3B-PB-O1B
3	A	799	ACP	PG-C3B-PB-O2B
3	A	799	ACP	PG-C3B-PB-O3A
3	A	799	ACP	C5'-O5'-PA-O1A
3	A	799	ACP	C5'-O5'-PA-O2A
3	A	799	ACP	O4'-C4'-C5'-O5'
3	A	799	ACP	C3'-C4'-C5'-O5'

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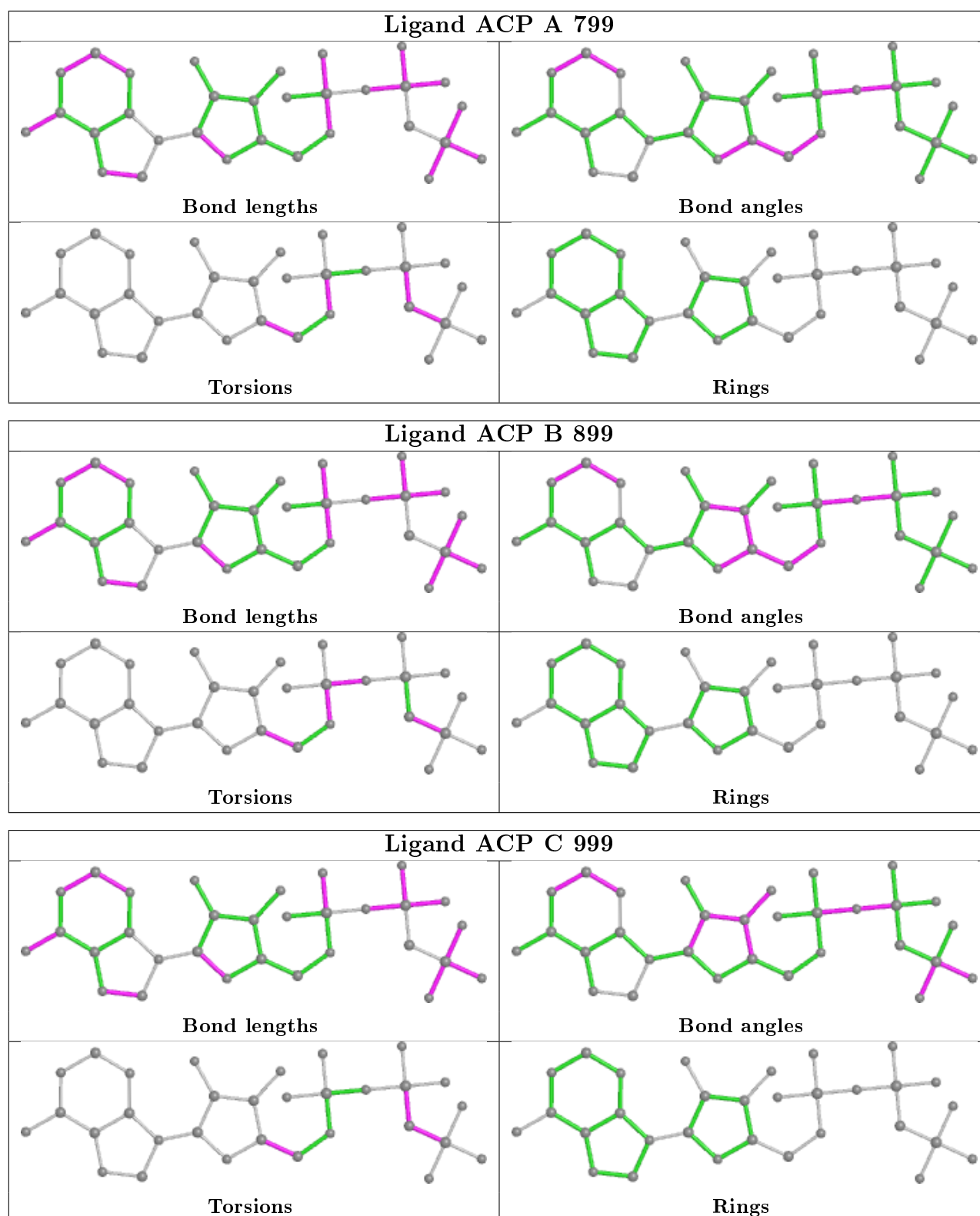
Mol	Chain	Res	Type	Atoms
3	B	899	ACP	PB-C3B-PG-O1G
3	B	899	ACP	PB-C3B-PG-O2G
3	B	899	ACP	PB-C3B-PG-O3G
3	B	899	ACP	C5'-O5'-PA-O1A
3	C	999	ACP	PB-C3B-PG-O1G
3	C	999	ACP	PG-C3B-PB-O3A
4	C	542	TZE	C3-C1'-C2'-OXT
3	B	899	ACP	O4'-C4'-C5'-O5'
3	B	899	ACP	C3'-C4'-C5'-O5'
3	C	999	ACP	O4'-C4'-C5'-O5'
3	C	999	ACP	C3'-C4'-C5'-O5'
3	B	899	ACP	PB-O3A-PA-O1A
3	C	999	ACP	PB-C3B-PG-O2G
3	C	999	ACP	PB-C3B-PG-O3G
3	A	799	ACP	C5'-O5'-PA-O3A
3	B	899	ACP	C5'-O5'-PA-O3A

There are no ring outliers.

6 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	799	ACP	4	0
4	B	543	TZE	10	0
4	B	542	TZE	7	0
3	B	899	ACP	8	0
3	C	999	ACP	8	0
4	C	542	TZE	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	512/540 (94%)	-0.24	2 (0%) 92 93	27, 70, 93, 122	0
1	B	510/540 (94%)	-0.10	1 (0%) 95 96	30, 80, 100, 127	0
1	C	511/540 (94%)	-0.09	2 (0%) 92 93	30, 77, 99, 125	0
All	All	1533/1620 (94%)	-0.14	5 (0%) 94 94	27, 76, 98, 127	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108	ASP	2.7
1	A	24	GLY	2.3
1	C	248	THR	2.2
1	C	535	PRO	2.1
1	A	25	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

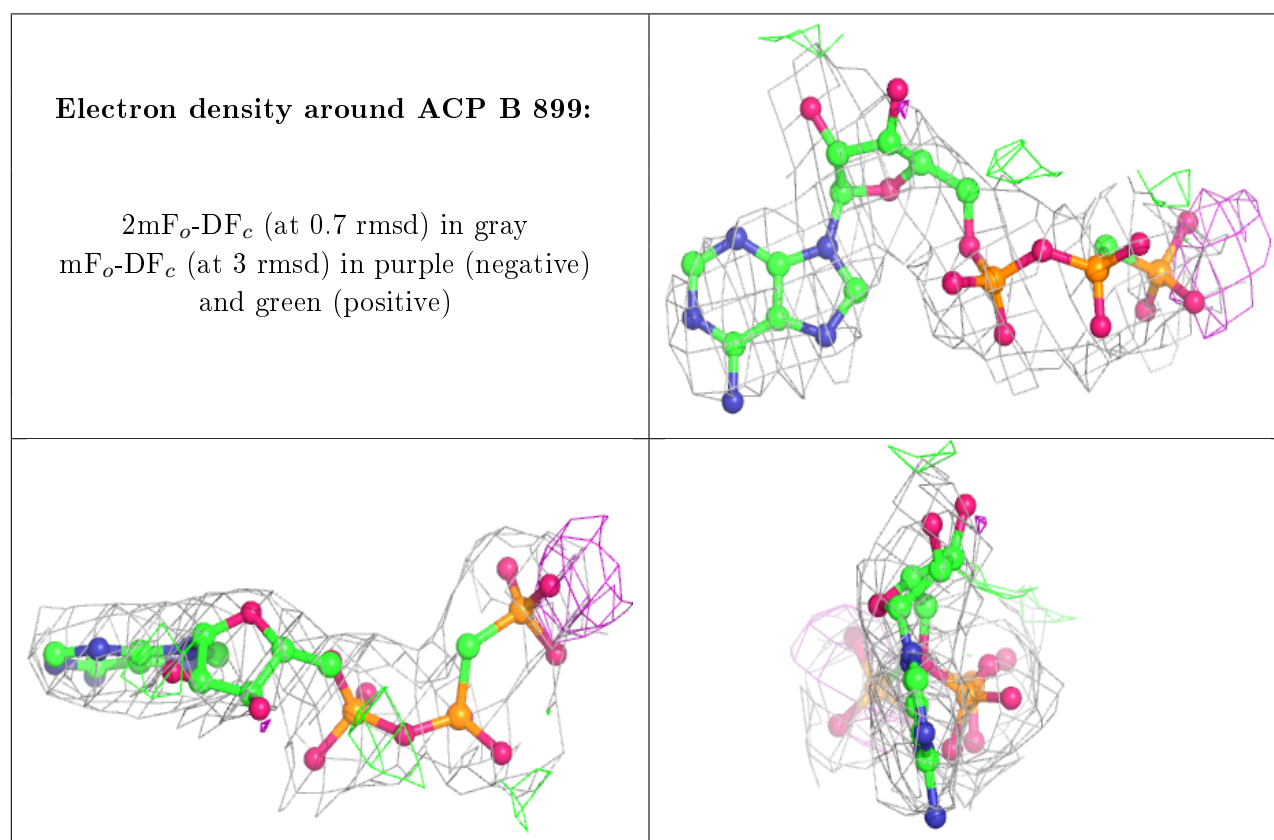
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

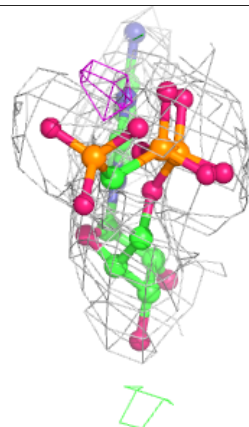
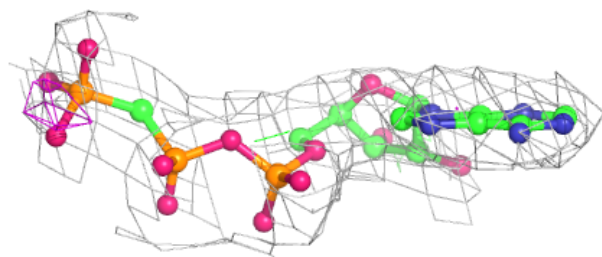
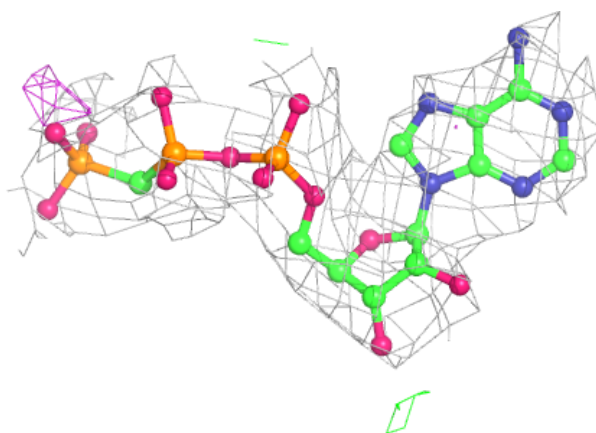
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	TZE	B	543	9/9	0.83	0.34	55,56,56,56	0
4	TZE	C	542	9/9	0.84	0.40	48,48,48,48	0
3	ACP	B	899	31/31	0.87	0.26	80,92,113,119	0
4	TZE	B	542	9/9	0.87	0.40	42,43,43,43	0
3	ACP	C	999	31/31	0.88	0.21	78,96,111,113	0
3	ACP	A	799	31/31	0.89	0.21	76,87,103,107	0
2	MG	B	541	1/1	0.91	0.29	76,76,76,76	0
2	MG	A	541	1/1	0.95	0.28	65,65,65,65	0
2	MG	C	541	1/1	0.97	0.24	76,76,76,76	0

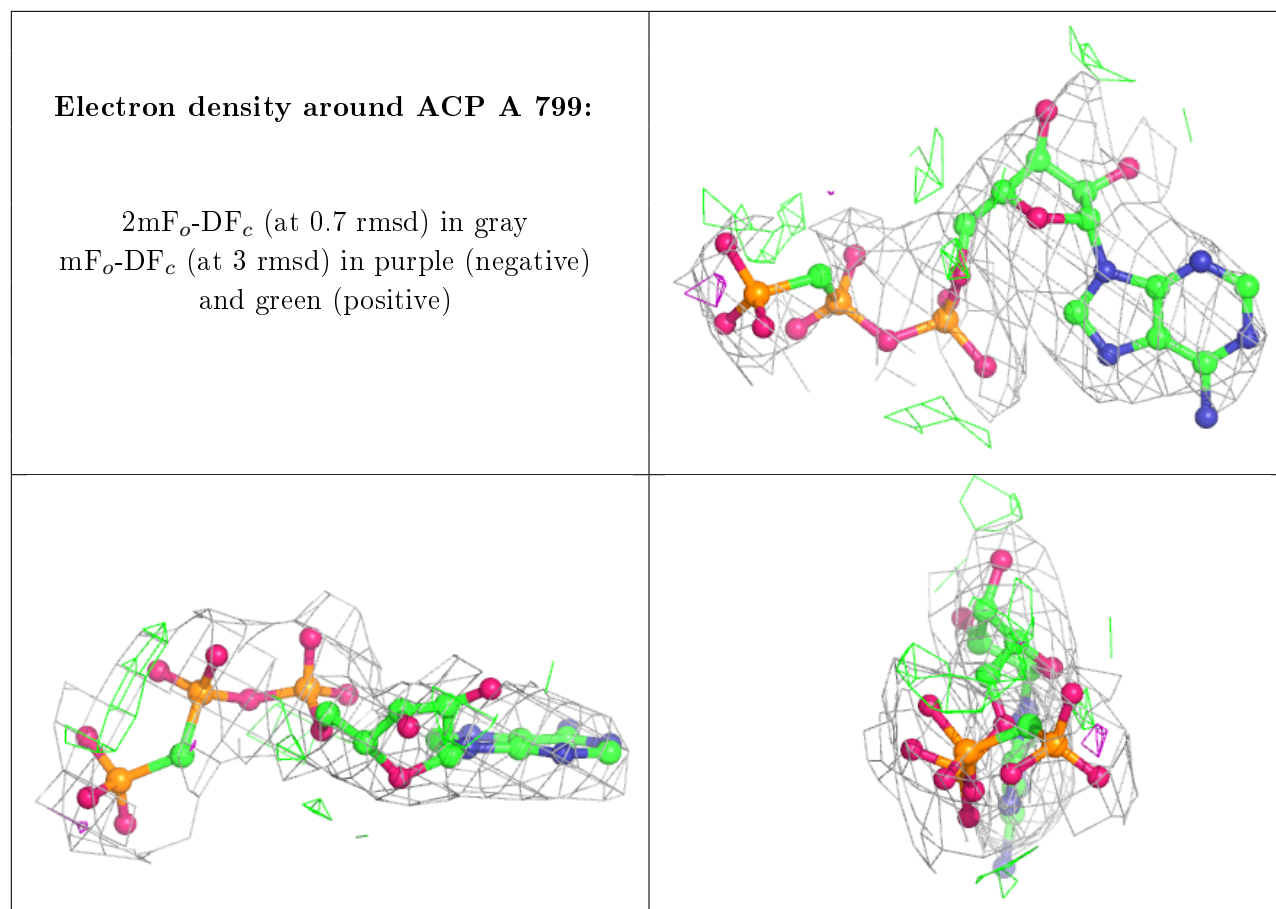
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around ACP C 999:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.