



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:43 AM UTC

PDB ID : 3NL5 / pdb_00003nl5
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 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

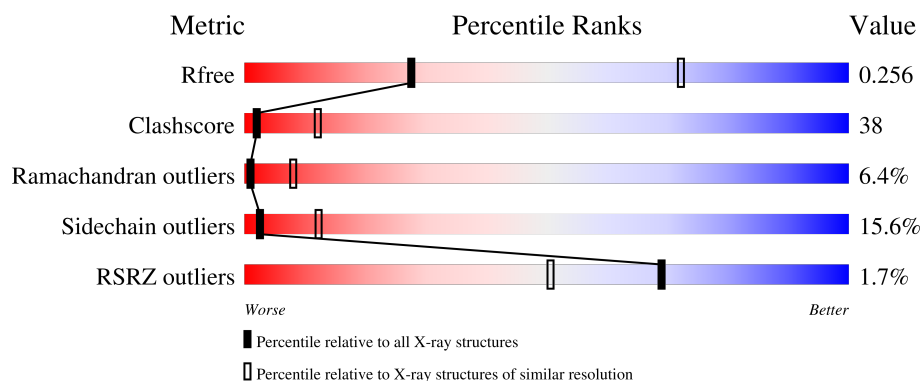
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	540	2% 39% 44% 12% 5%
1	B	540	2% 36% 46% 11% 6%
1	C	540	0% 38% 44% 12% 5%

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.

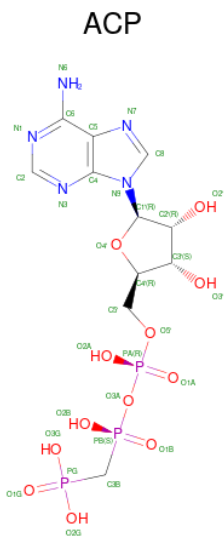
- Molecule 1 is a protein called Thiamine biosynthetic bifunctional enzyme.

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 (CCD ID: MG) (formula: Mg).

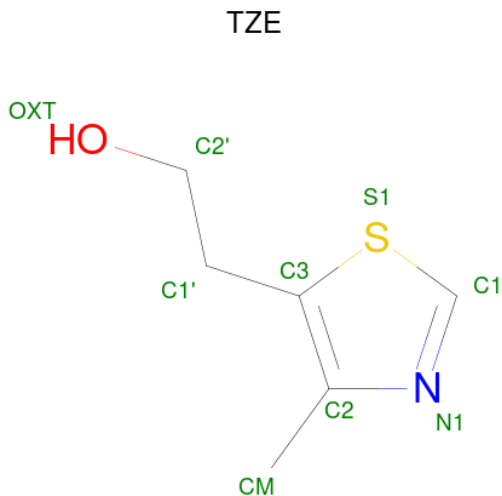
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: 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 (CCD ID: TZE) (formula: C_6H_9NOS).

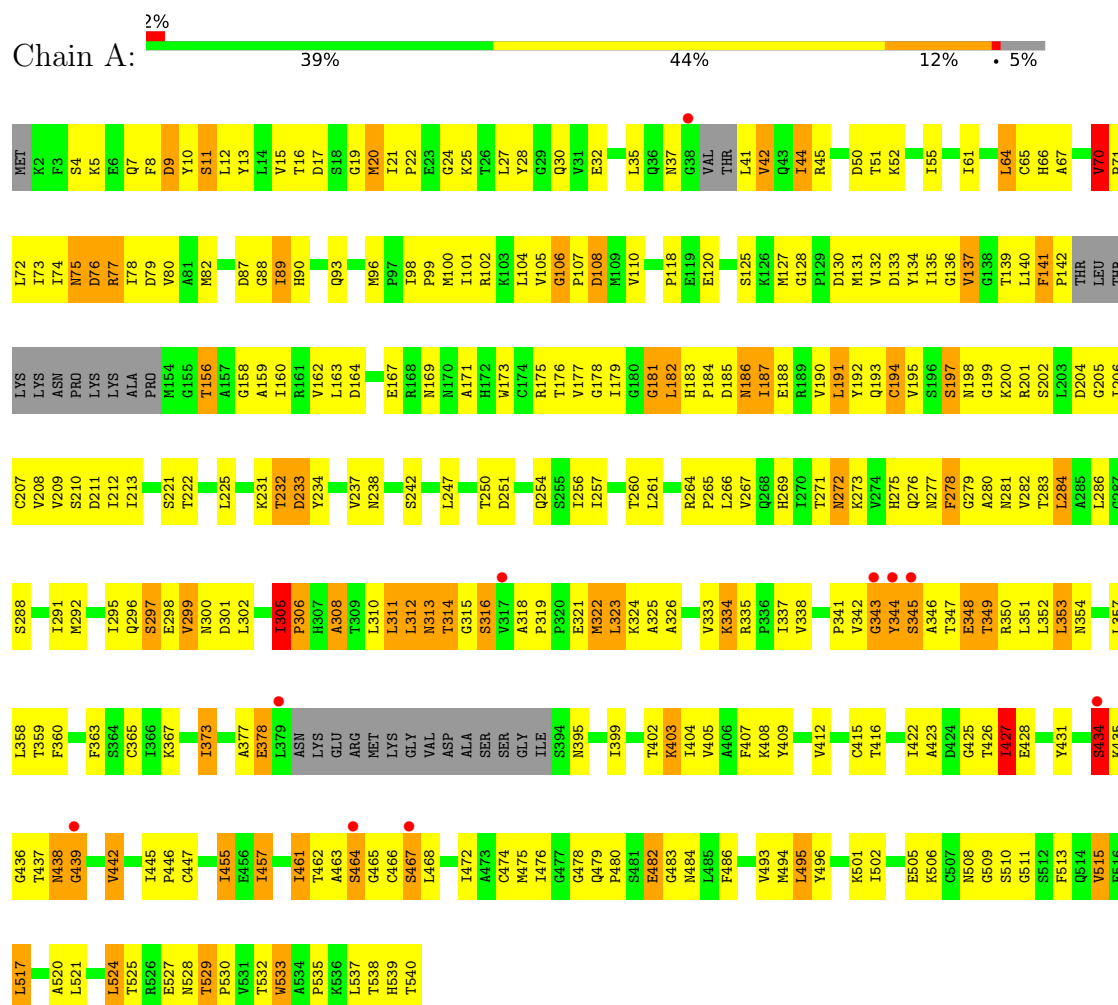


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			9	6	1	1	1		
4	B	1	Total	C	N	O	S	0	0
			9	6	1	1	1		
4	C	1	Total	C	N	O	S	0	0
			9	6	1	1	1		

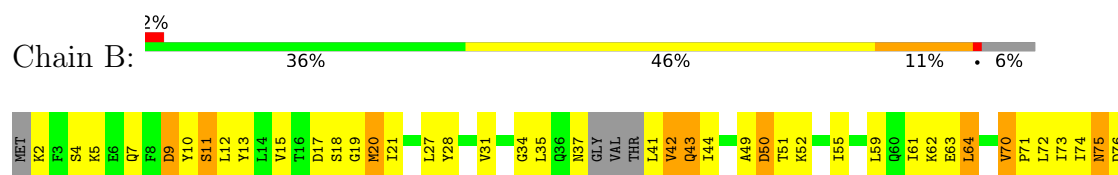
3 Residue-property plots

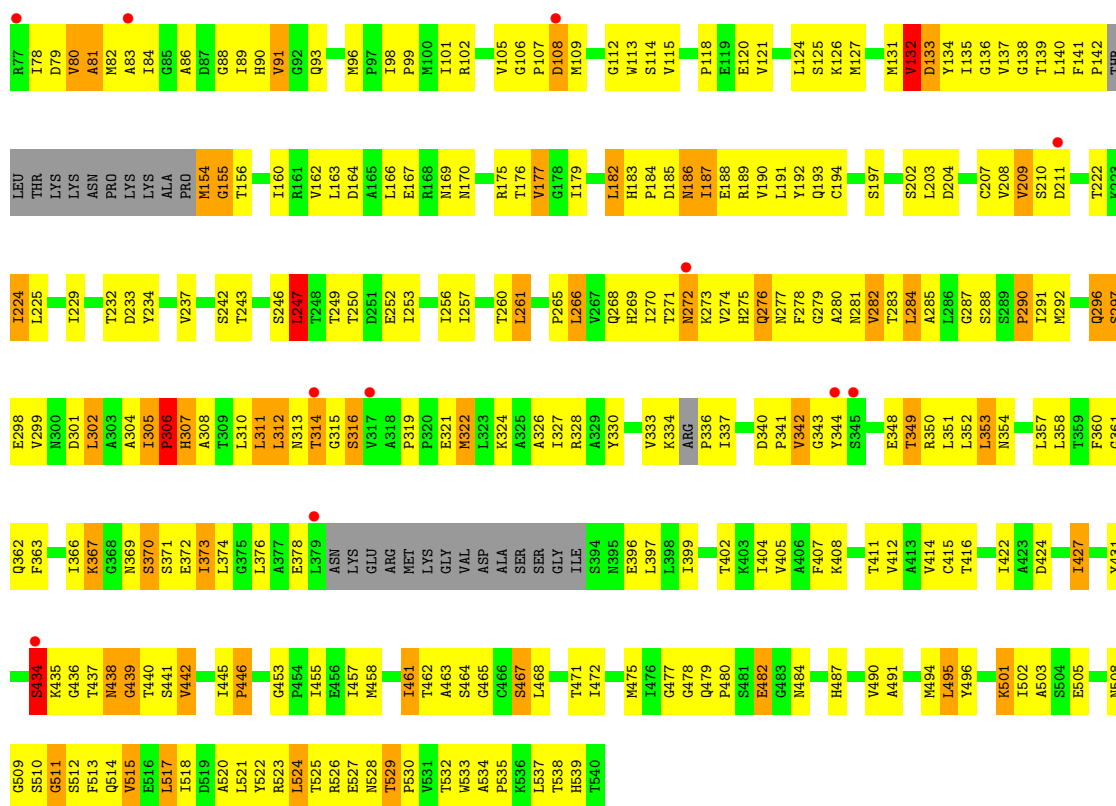
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

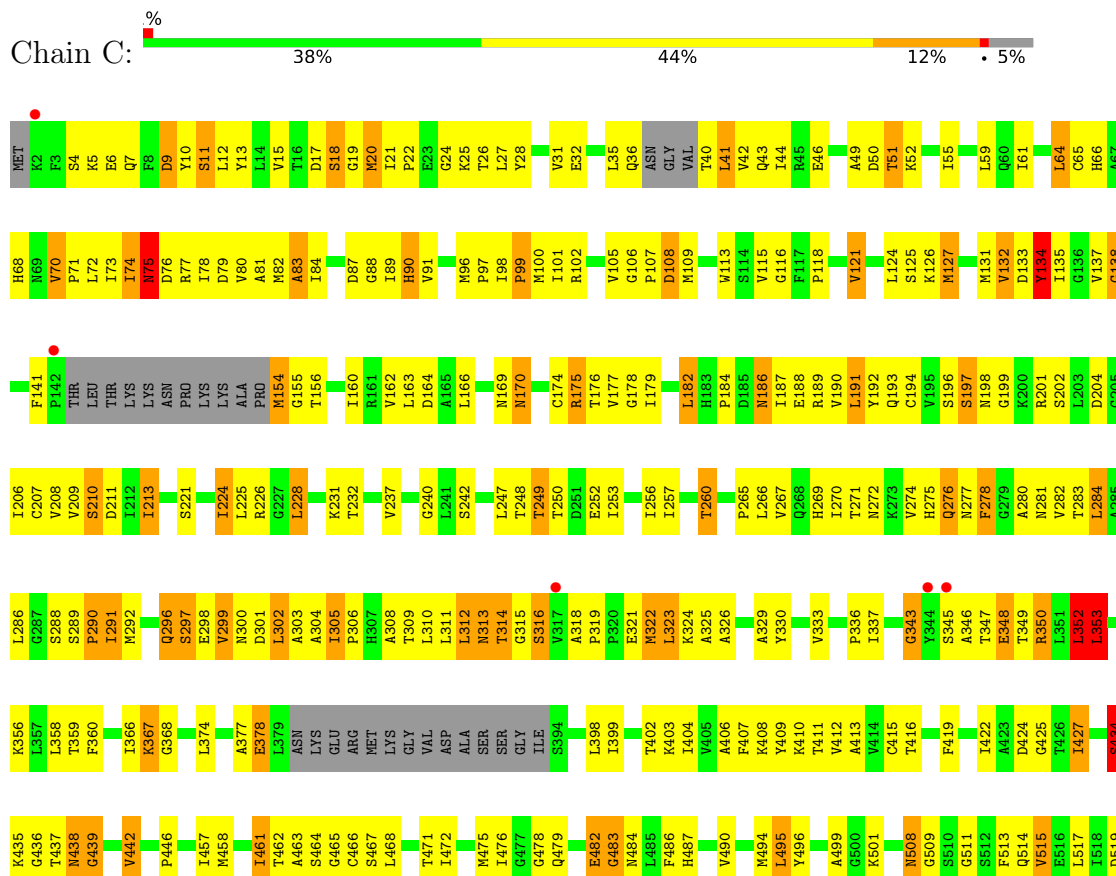


• Molecule 1: Thiamine biosynthetic bifunctional enzyme





• Molecule 1: Thiamine biosynthetic bifunctional enzyme



A520	L521	Y522	R523	L524	T525	R526	E527	N528	T529	P530	V531	T532	W533	A534	P535	R536	L537	T538	H539	T540
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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 36.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	91.3 (36.00-3.30) 91.6 (36.00-3.30)	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 0.202 , 0.256	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)	0.32 , 53.6	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	0.94	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: TZE, MG, ACP

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	0.59	0/3877	1.03	18/5259 (0.3%)
1	B	0.56	0/3858	1.01	16/5232 (0.3%)
1	C	0.54	0/3864	0.98	9/5242 (0.2%)
All	All	0.57	0/11599	1.01	43/15733 (0.3%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	LYS	N-CA-C	-16.56	91.10	114.12
1	C	435	LYS	N-CA-C	-12.31	98.24	113.38
1	B	435	LYS	N-CA-C	-12.19	97.18	114.12
1	B	434	SER	CB-CA-C	-11.09	93.85	111.48
1	B	305	ILE	CA-C-N	7.91	129.72	119.84
1	B	305	ILE	C-N-CA	7.91	129.72	119.84
1	A	434	SER	CB-CA-C	-7.84	94.83	110.42
1	B	396	GLU	N-CA-C	-7.59	103.02	111.82
1	A	305	ILE	CA-C-N	7.23	128.88	119.84
1	A	305	ILE	C-N-CA	7.23	128.88	119.84
1	B	434	SER	N-CA-C	7.10	121.28	112.47
1	C	533	TRP	N-CA-C	6.59	119.58	110.35
1	A	395	ASN	N-CA-C	6.54	121.88	113.18
1	A	179	ILE	N-CA-C	6.37	116.75	108.35
1	A	42	VAL	N-CA-C	6.24	116.82	108.27
1	A	70	VAL	CA-C-N	6.02	126.21	120.31
1	A	70	VAL	C-N-CA	6.02	126.21	120.31
1	B	42	VAL	N-CA-C	6.01	116.51	108.27
1	B	529	THR	CA-C-N	6.01	127.35	119.84
1	B	529	THR	C-N-CA	6.01	127.35	119.84
1	C	434	SER	CB-CA-C	-5.96	98.55	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	533	TRP	N-CA-C	5.89	119.36	110.64
1	C	479	GLN	CA-C-N	5.86	127.16	119.84
1	C	479	GLN	C-N-CA	5.86	127.16	119.84
1	B	179	ILE	N-CA-C	5.83	116.25	108.27
1	B	453	GLY	CA-C-N	5.74	127.01	119.84
1	B	453	GLY	C-N-CA	5.74	127.01	119.84
1	B	133	ASP	N-CA-C	-5.68	105.94	112.92
1	C	42	VAL	N-CA-C	5.68	116.65	108.48
1	B	532	THR	N-CA-C	5.57	117.16	111.14
1	C	532	THR	N-CA-C	5.46	116.92	111.07
1	A	529	THR	CA-C-N	5.24	126.39	119.84
1	A	529	THR	C-N-CA	5.24	126.39	119.84
1	A	212	ILE	N-CA-C	-5.22	106.71	111.67
1	A	532	THR	N-CA-C	5.20	116.64	110.97
1	B	435	LYS	N-CA-CB	5.20	118.05	110.88
1	C	127	MET	N-CA-C	-5.17	107.99	114.56
1	A	93	GLN	N-CA-C	-5.16	106.83	113.23
1	C	213	ILE	N-CA-C	5.11	115.23	110.42
1	A	435	LYS	N-CA-CB	5.09	117.91	110.88
1	A	159	ALA	N-CA-C	-5.06	105.85	112.23
1	A	181	GLY	N-CA-C	-5.05	108.47	114.48
1	B	370	SER	N-CA-C	5.04	118.20	111.75

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	291	0
1	B	3799	0	3785	315	0
1	C	3804	0	3795	287	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	875	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 38.

All (875) 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: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:342:VAL:C	1:A:344:TYR:H	1.86	0.81
1:C:79:ASP:HA	1:C:82:MET:HE2	1.59	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:482:GLU:CD	1:B:482:GLU:H	1.90	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: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:41:LEU:HD12	1:A:71:PRO:HG2	1.68	0.75
1:A:344:TYR:O	1:A:345:SER:CB	2.34	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:256:ILE:HG22	1:C:475:MET:HE3	1.73	0.70
1:B:190:VAL:O	1:B:194:CYS:HB2	1.91	0.70
1:A:256:ILE:HG22	1:A:475:MET:HE3	1.74	0.70
1:A:15:VAL:O	1:A:209:VAL:HG22	1.91	0.70
1:B:256:ILE:HG22	1:B:475:MET:HE3	1.72	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:4:SER:OG	1:B:7:GLN:HG3	1.92	0.69
1:B:463:ALA:O	1:B:467:SER:HB2	1.93	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:73:ILE:HG23	1:C:88:GLY:C	2.19	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:C:482:GLU:H	1:C:482:GLU:CD	2.02	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:59:LEU:HD21	1:C:84:ILE:HB	1.77	0.67
1:C:74:ILE:HG22	1:C:75:ASN:H	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:MET:N	4:B:543:TZE:N1	2.42	0.66
1:A:10:TYR:O	1:A:205:GLY:HA3	1.94	0.66
1:B:290:PRO:O	4:B:543:TZE:H3M	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:343:GLY:O	1:A:344:TYR:C	2.39	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:B:513:PHE:C	1:B:513:PHE:CD2	2.72	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:9:ASP:C	1:B:9:ASP:OD1	2.39	0.65
1:C:125:SER:C	1:C:127:MET:H	2.04	0.65
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: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:342:VAL:C	1:A:344:TYR:N	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:THR:HG23	1:B:446:PRO:HG3	1.81	0.62
1:B:265:PRO:HD2	1:B:288:SER:HB3	1.80	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
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:A:462:THR:C	1:A:464:SER:H	2.07	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: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:A:164:ASP:CG	1:A:197:SER:HB2	2.25	0.61
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:B:193:GLN:NE2	1:B:362:GLN:HE22	1.97	0.61
1:A:463:ALA:O	1:A:464:SER:C	2.44	0.61
1:B:528:ASN:C	1:B:530:PRO:HD3	2.26	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: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: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:9:ASP:OD1	1:A:9:ASP:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LEU:HD23	1:C:124:LEU:C	2.27	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:C:169:ASN:O	1:C:170:ASN:C	2.46	0.59
1:B:515:VAL:HG23	1:C:511:GLY:C	2.27	0.59
1:A:137:VAL:HG23	1:A:178:GLY:HA2	1.85	0.59
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:260:THR:HA	1:A:478:GLY:HA3	1.85	0.59
1:A:299:VAL:HG11	1:A:326:ALA:HB2	1.85	0.59
1:C:189:ARG:HH12	1:C:359:THR:C	2.10	0.59
1:A:513:PHE:C	1:A:513:PHE:CD2	2.81	0.58
1:C:267:VAL:HG12	1:C:269:HIS:CE1	2.38	0.58
1:B:17:ASP:HB3	1:B:20:MET:HE3	1.84	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:B:256:ILE:CG2	1:B:475:MET:HE3	2.34	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:B:81:ALA:O	1:B:82:MET:C	2.45	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:437:THR:O	1:A:438:ASN:C	2.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLN:HA	1:A:30:GLN:OE1	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:C:75:ASN:C	1:C:77:ARG:H	2.09	0.57
1:C:465:GLY:H	3:C:999:ACP:C3B	2.18	0.57
1:C:494:MET:O	1:C:495:LEU:C	2.48	0.57
1:A:269:HIS:CG	1:A:292:MET:HE3	2.39	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:C:513:PHE:C	1:C:513:PHE:CD2	2.83	0.56
1:A:5:LYS:HE3	1:A:133:ASP:CG	2.31	0.56
1:A:89:ILE:CG1	1:A:89:ILE:O	2.52	0.56
1:A:107:PRO:O	1:A:108:ASP:HB2	2.05	0.56
1:A:176:THR:O	1:A:204:ASP:HB2	2.05	0.56
1:B:81:ALA:HA	1:B:84:ILE:HG12	1.88	0.56
1:B:247:LEU:H	1:B:247:LEU:CD2	2.19	0.56
1:B:281:ASN:HA	1:B:284:LEU:CD2	2.34	0.56
1:C:65:CYS:HB3	1:C:70:VAL:O	2.04	0.56
1:C:78:ILE:HG12	1:C:89:ILE:HD12	1.87	0.56
1:C:347:THR:O	1:C:348:GLU:C	2.48	0.56
1:C:407:PHE:CB	1:C:442:VAL:HG23	2.33	0.56
1:B:272:ASN:OD1	1:B:315:GLY:C	2.46	0.56
1:C:457:ILE:O	1:C:457:ILE:HG13	2.05	0.56
1:B:209:VAL:C	1:B:211:ASP:H	2.14	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:A:482:GLU:H	1:A:482:GLU:CD	2.13	0.56
1:B:18:SER:O	1:B:21:ILE:HG13	2.06	0.56
1:A:528:ASN:C	1:A:530:PRO:HD3	2.31	0.56
1:B:305:ILE:HG23	1:B:306:PRO:HD2	1.88	0.56
1:B:247:LEU:H	1:B:247:LEU:HD22	1.71	0.55
4:B:543:TZE:H12'	1:C:274:VAL:HG22	1.88	0.55
1:C:406:ALA:O	1:C:425:GLY:HA3	2.06	0.55
1:C:407:PHE:HB3	1:C:442:VAL:CG2	2.31	0.55
1:A:125:SER:C	1:A:127:MET:H	2.13	0.55
1:A:322:MET:HG3	1:A:323:LEU:N	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ASN:C	1:B:283:THR:N	2.64	0.55
1:B:358:LEU:HD23	1:B:363:PHE:CE1	2.41	0.55
1:C:9:ASP:OD1	1:C:9:ASP:C	2.50	0.55
1:A:511:GLY:C	1:C:515:VAL:HG23	2.31	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:O	1:B:455:ILE:HG22	2.06	0.55
1:C:15:VAL:O	1:C:209:VAL:HG22	2.07	0.55
1:C:398:LEU:HD22	1:C:415:CYS:SG	2.47	0.55
1:B:98:ILE:HG21	1:B:127:MET:HE1	1.88	0.55
1:B:292:MET:N	1:B:292:MET:SD	2.80	0.55
1:C:281:ASN:HA	1:C:284:LEU:HD23	1.88	0.55
1:B:50:ASP:C	1:B:52:LYS:H	2.14	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:302:LEU:C	1:C:304:ALA:H	2.16	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:A:156:THR:HG21	1:A:193:GLN:HG3	1.90	0.54
1:B:281:ASN:O	1:B:283:THR:N	2.41	0.54
1:C:314:THR:CG2	1:C:315:GLY:N	2.70	0.54
1:A:509:GLY:HA2	1:C:522:TYR:HD2	1.72	0.54
1:B:465:GLY:N	3:B:899:ACP:H3B2	2.19	0.54
1:C:31:VAL:HG12	1:C:31:VAL:O	2.07	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:74:ILE:HG22	1:B:75:ASN:N	2.23	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:C:89:ILE:HD11	1:C:101:ILE:CG2	2.37	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:A:41:LEU:HG	1:A:42:VAL:N	2.23	0.53
1:A:163:LEU:HD22	1:A:201:ARG:HD3	1.90	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:A:102:ARG:HB3	1:A:131:MET:HE2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:515:VAL:HG23	1:B:511:GLY:C	2.33	0.53
1:C:179:ILE:HG13	1:C:207:CYS:HB2	1.90	0.53
1:C:298:GLU:O	1:C:299:VAL:C	2.52	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:B:28:TYR:HE1	1:B:64:LEU:HB2	1.73	0.53
1:B:121:VAL:CG1	1:B:166:LEU:HD23	2.39	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:HD23	1:A:495:LEU:O	2.08	0.53
1:B:34:GLY:HA2	1:B:222:THR:HG21	1.91	0.53
1:B:125:SER:C	1:B:127:MET:H	2.17	0.53
1:B:334:LYS:O	1:B:336:PRO:CD	2.57	0.53
1:C:18:SER:HB2	1:C:46:GLU:OE2	2.09	0.53
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:C:534:ALA:N	1:C:535:PRO:CD	2.71	0.52
1:B:118:PRO:C	1:B:120:GLU:N	2.65	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:44:ILE:HD11	1:A:61:ILE:HG21	1.92	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:C:266:LEU:HD22	1:C:305:ILE:HD13	1.91	0.52
1:B:522:TYR:CD2	1:C:509:GLY:HA2	2.45	0.52
1:C:202:SER:CB	1:C:436:GLY:HA2	2.36	0.52
1:A:198:ASN:OD1	1:A:200:LYS:HB2	2.09	0.52
1:C:4:SER:O	1:C:5:LYS:C	2.53	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:B:4:SER:O	1:B:5:LYS:C	2.53	0.52
1:C:75:ASN:C	1:C:77:ARG:N	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:MET:O	1:C:496:TYR:N	2.43	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:A:102:ARG:CB	1:A:131:MET:HE2	2.39	0.52
1:B:276:GLN:NE2	1:B:292:MET:HG2	2.24	0.52
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:A:533:TRP:C	1:A:535:PRO:HD2	2.34	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: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:32:GLU:O	1:C:36:GLN:HG3	2.10	0.51
1:C:107:PRO:O	1:C:108:ASP:CB	2.59	0.51
1:C:253:ILE:O	1:C:257:ILE:HG13	2.10	0.51
1:B:124:LEU:C	1:B:124:LEU:HD23	2.34	0.51
1:B:269:HIS:CG	1:B:292:MET:HE3	2.45	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:322:MET:O	1:B:322:MET:HE2	2.11	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: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:B:274:VAL:HG21	4:B:542:TZE:C1'	2.39	0.50
1:A:209:VAL:C	1:A:211:ASP:H	2.19	0.50
1:A:298:GLU:O	1:A:299:VAL:C	2.54	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:78:ILE:HD13	1:A:96:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:202:SER:OG	1:A:436:GLY:HA2	2.11	0.50
1:A:251:ASP:O	1:A:254:GLN:HB3	2.12	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:B:253:ILE:HD11	1:B:494:MET:HE2	1.94	0.50
1:B:282:VAL:HG21	1:B:467:SER:HG	1.75	0.50
1:C:28:TYR:CE1	1:C:64:LEU:HG	2.47	0.50
1:C:282:VAL:O	1:C:286:LEU:HG	2.12	0.50
1:C:353:LEU:C	1:C:353:LEU:HD12	2.36	0.50
1:B:10:TYR:O	1:B:11:SER:C	2.55	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
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:44:ILE:HD12	1:C:72:LEU:HD21	1.93	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: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:41:LEU:HG	1:B:42:VAL:N	2.27	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: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:72:LEU:HD12	1:C:73:ILE:H	1.78	0.49
1:C:407:PHE:CE2	1:C:427:ILE:HD11	2.46	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:C:345:SER:O	1:C:346:ALA:C	2.56	0.49
1:B:285:ALA:C	1:B:287:GLY:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:162:VAL:C	1:B:164:ASP:N	2.67	0.49
1:C:192:TYR:OH	1:C:410:LYS:HB3	2.13	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:28:TYR:CZ	1:B:64:LEU:HG	2.48	0.49
1:B:247:LEU:HD22	1:B:247:LEU:N	2.28	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:HD23	1:C:284:LEU:H	1.78	0.49
1:A:353:LEU:O	1:A:353:LEU:HD12	2.12	0.49
1:B:80:VAL:O	1:B:81:ALA:C	2.56	0.49
1:C:17:ASP:HB3	1:C:20:MET:HE3	1.95	0.48
1:C:275:HIS:CG	1:C:466:CYS:HB3	2.48	0.48
1:A:51:THR:O	1:A:55:ILE:HG13	2.12	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: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
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:98:ILE:N	1:C:99:PRO:CD	2.76	0.48
1:C:314:THR:C	1:C:316:SER:H	2.21	0.48
1:C:353:LEU:HD12	1:C:353:LEU:O	2.13	0.48
1:A:260:THR:HG22	1:A:478:GLY:HA3	1.95	0.48
1:A:357:LEU:C	1:A:359:THR:H	2.19	0.48
1:A:463:ALA:C	1:A:465:GLY:N	2.71	0.48
1:C:98:ILE:N	1:C:99:PRO:HD2	2.28	0.48
1:C:270:ILE:HD12	1:C:310:LEU:HD11	1.96	0.48
1:C:284:LEU:CD2	1:C:284:LEU:H	2.26	0.48
1:B:80:VAL:O	1:B:83:ALA:N	2.46	0.48
1:B:90:HIS:HE1	1:B:114:SER:OG	1.97	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:B:186:ASN:C	1:B:186:ASN:OD1	2.57	0.48
1:B:533:TRP:C	1:B:535:PRO:HD2	2.38	0.48
1:C:124:LEU:HD11	1:C:174:CYS:SG	2.54	0.48
1:A:278:PHE:CD2	1:A:463:ALA:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LYS:HA	1:A:360:PHE:CD1	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:B:73:ILE:HG23	1:B:88:GLY:C	2.39	0.48
1:B:113:TRP:HB2	1:B:132:VAL:HG13	1.96	0.48
1:A:4:SER:OG	1:A:7:GLN:HG3	2.14	0.48
1:A:494:MET:C	1:A:496:TYR:N	2.71	0.48
1:B:517:LEU:HD23	1:B:517:LEU:O	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:B:290:PRO:O	4:B:543:TZE:CM	2.60	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:5:LYS:HE3	1:B:133:ASP:CG	2.39	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:256:ILE:CG2	1:C:475:MET:HE3	2.43	0.47
1:C:495:LEU:HD22	1:C:521:LEU:CD2	2.45	0.47
1:A:37:ASN:HB2	1:A:222:THR:HG22	1.96	0.47
1:A:324:LYS:HB2	1:A:360:PHE:CD1	2.48	0.47
1:B:55:ILE:O	1:B:59:LEU:HG	2.15	0.47
1:B:107:PRO:O	1:B:108:ASP:HB2	2.14	0.47
1:B:156:THR:HG21	1:B:193:GLN:HG3	1.97	0.47
1:C:41:LEU:CD1	1:C:71:PRO:HG2	2.44	0.47
1:C:79:ASP:OD1	1:C:80:VAL:N	2.42	0.47
1:C:224:ILE:O	1:C:228:LEU:HD13	2.14	0.47
1:C:490:VAL:O	1:C:494:MET:HG2	2.15	0.47
1:A:10:TYR:O	1:A:11:SER:C	2.56	0.47
1:A:73:ILE:HG23	1:A:88:GLY:C	2.40	0.47
1:A:90:HIS:HD2	1:A:134:TYR:OH	1.98	0.47
1:A:277:ASN:O	1:A:280:ALA:N	2.47	0.47
1:B:247:LEU:CD2	1:B:539:HIS:NE2	2.78	0.47
1:B:269:HIS:CB	1:B:292:MET:HE3	2.45	0.47
1:B:343:GLY:O	1:B:372:GLU:HG2	2.15	0.47
1:B:517:LEU:C	1:B:517:LEU:CD2	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:ILE:HD11	1:C:514:GLN:HG3	1.97	0.47
1:A:50:ASP:C	1:A:52:LYS:H	2.22	0.47
1:A:242:SER:HA	1:A:428:GLU:HG2	1.97	0.47
1:B:140:LEU:HD23	1:B:154:MET:HE3	1.95	0.47
1:B:326:ALA:O	1:B:327:ILE:C	2.57	0.47
1:B:495:LEU:CD2	1:B:521:LEU:HD22	2.45	0.47
1:B:510:SER:O	1:B:511:GLY:C	2.58	0.47
1:C:134:TYR:CD1	1:C:134:TYR:C	2.93	0.47
1:A:455:ILE:HG22	1:A:455:ILE:O	2.14	0.47
1:B:162:VAL:C	1:B:164:ASP:H	2.22	0.47
1:C:98:ILE:HB	1:C:99:PRO:HD3	1.97	0.47
1:C:465:GLY:N	3:C:999:ACP:H3B2	2.30	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:45:ARG:HH11	1:A:45:ARG:HG2	1.79	0.46
1:A:75:ASN:O	1:A:76:ASP:C	2.58	0.46
1:A:271:THR:HA	1:A:313:ASN:HB2	1.96	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:A:462:THR:C	1:A:464:SER:N	2.73	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:C:257:ILE:HG12	1:C:475:MET:HE1	1.98	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:HD23	1:A:312:LEU:HA	1.60	0.46
1:B:81:ALA:O	1:B:84:ILE:N	2.48	0.46
1:B:312:LEU:HD23	1:B:312:LEU:HA	1.61	0.46
1:A:5:LYS:HE3	1:A:133:ASP:OD1	2.15	0.46
1:A:13:TYR:CD2	1:A:207:CYS:SG	3.09	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
1:C:35:LEU:HD22	1:C:70:VAL:CG1	2.44	0.46
1:C:125:SER:C	1:C:127:MET:N	2.69	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:C:533:TRP:C	1:C:535:PRO:HD2	2.41	0.46
1:A:323:LEU:HD23	1:A:323:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:186:ASN:OD1	1:A:186:ASN:C	2.58	0.46
1:C:256:ILE:O	1:C:260:THR:HG23	2.15	0.46
1:A:247:LEU:HD22	1:A:247:LEU:N	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:A:343:GLY:O	1:A:346:ALA:N	2.44	0.45
1:A:437:THR:O	1:A:437:THR:HG23	2.17	0.45
1:B:55:ILE:HG12	1:B:80:VAL:HG13	1.98	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:C:163:LEU:HD23	1:C:163:LEU:HA	1.79	0.45
1:C:302:LEU:C	1:C:304:ALA:N	2.73	0.45
1:A:247:LEU:H	1:A:247:LEU:CD2	2.28	0.45
1:A:533:TRP:CD1	1:A:533:TRP:H	2.35	0.45
1:B:118:PRO:C	1:B:120:GLU:H	2.23	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:B:471:THR:O	1:B:472:ILE:C	2.58	0.45
1:C:13:TYR:O	1:C:207:CYS:HA	2.16	0.45
1:C:292:MET:N	4:C:542:TZE:N1	2.50	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:A:265:PRO:O	1:A:288:SER:HB2	2.16	0.45
1:A:277:ASN:O	1:A:278:PHE:C	2.59	0.45
1:B:182:LEU:N	1:B:182:LEU:HD13	2.30	0.45
1:B:269:HIS:HB2	1:B:292:MET:SD	2.57	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:VAL:HG21	1:C:135:ILE:HG21	1.98	0.45
1:C:352:LEU:O	1:C:353:LEU:C	2.59	0.45
1:C:437:THR:O	1:C:438:ASN:C	2.58	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:O	1:A:264:ARG:HG2	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:274:VAL:CG2	4:B:542:TZE:C1'	2.94	0.45
1:B:495:LEU:HD23	1:B:495:LEU:O	2.16	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:B:512:SER:O	1:B:513:PHE:C	2.59	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:A:257:ILE:HG12	1:A:475:MET:HE1	1.99	0.45
1:C:276:GLN:NE2	1:C:292:MET:CG	2.80	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:A:517:LEU:C	1:A:517:LEU:CD2	2.89	0.44
1:B:281:ASN:C	1:B:283:THR:H	2.25	0.44
1:B:369:ASN:OD1	1:B:369:ASN:C	2.60	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:50:ASP:C	1:B:52:LYS:N	2.75	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:192:TYR:HB2	1:A:431:TYR:CD1	2.52	0.44
1:A:373:ILE:HD13	1:A:373:ILE:HA	1.71	0.44
1:B:43:GLN:HE22	1:B:90:HIS:CD2	2.35	0.44
1:B:253:ILE:O	1:B:257:ILE:HG13	2.18	0.44
1:C:66:HIS:HE1	1:C:87:ASP:OD1	2.00	0.44
1:A:79:ASP:HA	1:A:82:MET:CE	2.48	0.44
1:A:422:ILE:HG22	1:A:486:PHE:HE1	1.83	0.44
1:B:275:HIS:NE2	1:B:279:GLY:HA3	2.32	0.44
1:B:513:PHE:C	1:B:513:PHE:HD2	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:TYR:O	1:C:11:SER:C	2.60	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
1:A:50:ASP:C	1:A:52:LYS:N	2.76	0.44
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:102:ARG:HB3	1:B:131:MET:HE2	2.00	0.44
1:A:237:VAL:HA	1:A:334:LYS:O	2.17	0.44
1:B:88:GLY:HA2	1:B:109:MET:HG2	1.99	0.44
1:C:44:ILE:O	1:C:44:ILE:HG22	2.18	0.44
1:B:13:TYR:O	1:B:207:CYS:HA	2.18	0.44
1:B:204:ASP:CG	1:B:434:SER:HB3	2.42	0.44
1:B:502:ILE:O	1:B:503:ALA:C	2.60	0.44
1:C:78:ILE:HD13	1:C:96:MET:SD	2.57	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: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:A:13:TYR:O	1:A:207:CYS:HA	2.17	0.43
1:A:183:HIS:O	1:A:187:ILE:HG13	2.18	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:266:LEU:HD21	1:A:291:ILE:HD12	2.00	0.43
1:A:281:ASN:HA	1:A:284:LEU:HD21	1.99	0.43
1:B:342:VAL:O	1:B:342:VAL:HG22	2.17	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:277:ASN:O	1:B:278:PHE:C	2.61	0.43
1:B:343:GLY:H	1:B:350:ARG:NE	2.16	0.43
1:C:98:ILE:HG21	1:C:127:MET:HE1	1.99	0.43
1:A:79:ASP:OD1	1:A:80:VAL:N	2.44	0.43
1:A:137:VAL:CG2	1:A:178:GLY:HA2	2.48	0.43
1:A:286:LEU:HD21	1:A:521:LEU:HD22	2.00	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:B:266:LEU:C	1:B:266:LEU:HD12	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:LEU:C	1:B:304:ALA:N	2.76	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:B:402:THR:OG1	1:B:415:CYS:HB2	2.19	0.43
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:C:99:PRO:O	1:C:100:MET:C	2.61	0.43
1:C:247:LEU:H	1:C:247:LEU:HD22	1.84	0.43
1:C:281:ASN:C	1:C:283:THR:N	2.76	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:HD2	1:B:501:LYS:HA	1.73	0.43
1:A:125:SER:C	1:A:127:MET:N	2.73	0.43
1:B:43:GLN:HA	1:B:73:ILE:O	2.19	0.43
1:B:139:THR:O	1:B:140:LEU:C	2.62	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:A:35:LEU:C	1:A:37:ASN:H	2.27	0.43
1:B:302:LEU:C	1:B:304:ALA:H	2.26	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:281:ASN:C	1:A:283:THR:N	2.75	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:192:TYR:HA	1:B:431:TYR:HB3	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:C:74:ILE:CG2	1:C:75:ASN:N	2.76	0.42
1:A:275:HIS:CG	1:A:275:HIS:O	2.72	0.42
1:C:162:VAL:C	1:C:164:ASP:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:13:TYR:CE1	1:A:41:LEU:HD23	2.54	0.42
1:A:298:GLU:O	1:A:301:ASP:N	2.44	0.42
1:A:425:GLY:O	1:A:427:ILE:HG12	2.20	0.42
1:B:314:THR:CG2	1:B:315:GLY:N	2.83	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:513:PHE:C	1:A:513:PHE:HD2	2.25	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: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:397:LEU:HD12	1:B:397:LEU:HA	1.88	0.42
1:B:468:LEU:O	1:B:468:LEU:HD12	2.19	0.42
1:C:271:THR:CA	1:C:313:ASN:HB2	2.45	0.42
1:A:281:ASN:O	1:A:282:VAL:C	2.63	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:O	1:B:440:THR:HG22	2.20	0.42
1:C:41:LEU:HD12	1:C:71:PRO:HG2	2.02	0.42
1:C:275:HIS:CG	1:C:275:HIS:O	2.73	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:82:MET:O	1:C:83:ALA:C	2.63	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: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:322:MET:HG3	1:C:323:LEU:N	2.30	0.42
1:C:410:LYS:HA	1:C:410:LYS:HD3	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:44:ILE:N	1:B:73:ILE:O	2.41	0.42
1:B:187:ILE:HD12	1:B:225:LEU:HD22	2.02	0.42
1:C:527:GLU:O	1:C:529:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:315:GLY:HA3	1:A:350:ARG:NH2	2.35	0.41
1:A:501:LYS:HA	1:A:501:LYS:HD2	1.76	0.41
1:B:62:LYS:HA	1:B:72:LEU:HD22	2.02	0.41
1:B:125:SER:C	1:B:127:MET:N	2.78	0.41
1:C:22:PRO:HG2	1:C:25:LYS:HD3	2.01	0.41
1:C:73:ILE:HG23	1:C:89:ILE:N	2.35	0.41
1:C:484:ASN:HD21	1:C:486:PHE:HB3	1.84	0.41
1:A:278:PHE:C	1:A:278:PHE:CD1	2.99	0.41
1:A:427:ILE:O	1:A:427:ILE:HG22	2.21	0.41
1:A:462:THR:O	1:A:464:SER:N	2.53	0.41
1:B:281:ASN:O	1:B:282:VAL:C	2.63	0.41
1:B:373:ILE:HD13	1:B:373:ILE:HA	1.73	0.41
1:B:524:LEU:HD13	1:B:524:LEU:HA	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:98:ILE:N	1:A:99:PRO:CD	2.84	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:357:LEU:C	1:A:359:THR:N	2.78	0.41
1:B:98:ILE:N	1:B:99:PRO:CD	2.83	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:C:289:SER:HA	1:C:290:PRO:HD3	1.82	0.41
1:A:27:LEU:HD23	1:A:61:ILE:HD11	2.01	0.41
1:A:118:PRO:C	1:A:120:GLU:N	2.77	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:B:154:MET:HG3	1:B:155:GLY:N	2.34	0.41
1:B:437:THR:O	1:B:438:ASN:C	2.63	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:139:THR:O	1:A:140:LEU:C	2.63	0.41
1:A:403:LYS:HG2	1:A:447:CYS:HB2	2.01	0.41
1:A:494:MET:O	1:A:495:LEU:C	2.63	0.41
1:B:461:ILE:HG23	1:B:464:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LEU:HD22	1:B:521:LEU:HD22	2.02	0.41
1:C:131:MET:C	1:C:132:VAL:HG23	2.45	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:N	1:C:419:PHE:CD1	2.88	0.41
1:A:10:TYR:CD1	1:A:10:TYR:N	2.88	0.41
1:A:281:ASN:ND2	1:B:462:THR:H	2.18	0.41
1:B:15:VAL:O	1:B:209:VAL:HG22	2.21	0.41
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:B:495:LEU:HD23	1:B:521:LEU:CD2	2.51	0.41
1:C:50:ASP:C	1:C:52:LYS:N	2.79	0.41
1:C:416:THR:HB	3:C:999:ACP:H3'	2.02	0.41
1:A:17:ASP:HB3	1:A:20:MET:HE3	2.03	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:182:LEU:N	1:A:182:LEU:HD13	2.36	0.41
1:A:247:LEU:HD21	1:A:539:HIS:NE2	2.35	0.41
1:A:353:LEU:HD12	1:A:353:LEU:C	2.46	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:B:424:ASP:O	1:B:445:ILE:HB	2.21	0.41
1:C:31:VAL:O	1:C:31:VAL:CG1	2.69	0.41
1:C:105:VAL:HB	1:C:109:MET:SD	2.61	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:74:ILE:CG2	1:C:75:ASN:H	2.24	0.41
1:C:374:LEU:HD23	1:C:374:LEU:HA	1.95	0.41
1:A:8:PHE:CE1	1:A:110:VAL:HG21	2.56	0.40
1:A:135:ILE:CG1	1:A:176:THR:HG22	2.51	0.40
1:B:75:ASN:HB3	1:B:76:ASP:H	1.56	0.40
1:B:298:GLU:HG2	1:C:347:THR:OG1	2.21	0.40
1:B:341:PRO:O	1:B:343:GLY:O	2.39	0.40
1:C:176:THR:O	1:C:204:ASP:HB2	2.20	0.40
1:B:59:LEU:HD23	1:B:59:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:HG11	1:B:101:ILE:HD13	2.02	0.40
1:B:252:GLU:O	1:B:256:ILE:HG12	2.20	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:90:HIS:C	1:B:90:HIS:ND1	2.79	0.40
1:B:246:SER:O	1:B:247:LEU:C	2.65	0.40
1:C:74:ILE:HG13	1:C:81:ALA:HA	2.04	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
3:C:999:ACP:O5'	3:C:999:ACP:H8	2.21	0.40
1:A:89:ILE:O	1:A:89:ILE:HG12	2.21	0.40
1:A:341:PRO:HD2	1:A:367:LYS:O	2.22	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:B:533:TRP:CD1	1:B:533:TRP:H	2.39	0.40
1:C:4:SER:C	1:C:6:GLU:N	2.79	0.40
1:C:166:LEU:HD13	1:C:201:ARG:CZ	2.52	0.40
1:C:226:ARG:HA	1:C:226:ARG:HD3	1.61	0.40
1:B:353:LEU:HD12	1:B:353:LEU:C	2.46	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	8
1	B	500/540 (93%)	385 (77%)	85 (17%)	30 (6%)	1	9
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	8

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	MET
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	355 (86%)	59 (14%)	3	14
1	B	412/449 (92%)	344 (84%)	68 (16%)	2	11
1	C	412/449 (92%)	346 (84%)	66 (16%)	2	11
All	All	1238/1347 (92%)	1045 (84%)	193 (16%)	2	12

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP

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Mol	Chain	Res	Type
1	A	44	ILE
1	A	64	LEU
1	A	70	VAL
1	A	74	ILE
1	A	75	ASN
1	A	89	ILE
1	A	137	VAL
1	A	141	PHE
1	A	156	THR
1	A	167	GLU
1	A	169	ASN
1	A	175	ARG
1	A	182	LEU
1	A	187	ILE
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	250	THR
1	A	284	LEU
1	A	295	ILE
1	A	297	SER
1	A	302	LEU
1	A	305	ILE
1	A	306	PRO
1	A	311	LEU
1	A	312	LEU
1	A	313	ASN
1	A	314	THR
1	A	321	GLU
1	A	322	MET
1	A	323	LEU
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	373	ILE

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Mol	Chain	Res	Type
1	A	399	ILE
1	A	403	LYS
1	A	408	LYS
1	A	412	VAL
1	A	427	ILE
1	A	442	VAL
1	A	457	ILE
1	A	461	ILE
1	A	467	SER
1	A	482	GLU
1	A	484	ASN
1	A	508	ASN
1	A	515	VAL
1	A	517	LEU
1	A	524	LEU
1	A	538	THR
1	B	2	LYS
1	B	9	ASP
1	B	43	GLN
1	B	50	ASP
1	B	61	ILE
1	B	63	GLU
1	B	64	LEU
1	B	70	VAL
1	B	75	ASN
1	B	91	VAL
1	B	132	VAL
1	B	137	VAL
1	B	154	MET
1	B	167	GLU
1	B	169	ASN
1	B	175	ARG
1	B	177	VAL
1	B	182	LEU
1	B	187	ILE
1	B	188	GLU
1	B	191	LEU
1	B	197	SER
1	B	224	ILE
1	B	232	THR
1	B	233	ASP
1	B	242	SER

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Mol	Chain	Res	Type
1	B	247	LEU
1	B	261	LEU
1	B	266	LEU
1	B	276	GLN
1	B	284	LEU
1	B	296	GLN
1	B	297	SER
1	B	302	LEU
1	B	306	PRO
1	B	307	HIS
1	B	311	LEU
1	B	312	LEU
1	B	314	THR
1	B	321	GLU
1	B	322	MET
1	B	328	ARG
1	B	333	VAL
1	B	342	VAL
1	B	348	GLU
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	373	ILE
1	B	378	GLU
1	B	399	ILE
1	B	408	LYS
1	B	412	VAL
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	538	THR

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Mol	Chain	Res	Type
1	C	9	ASP
1	C	12	LEU
1	C	18	SER
1	C	26	THR
1	C	51	THR
1	C	64	LEU
1	C	70	VAL
1	C	75	ASN
1	C	90	HIS
1	C	91	VAL
1	C	121	VAL
1	C	134	TYR
1	C	141	PHE
1	C	154	MET
1	C	175	ARG
1	C	182	LEU
1	C	187	ILE
1	C	188	GLU
1	C	191	LEU
1	C	196	SER
1	C	197	SER
1	C	198	ASN
1	C	210	SER
1	C	221	SER
1	C	224	ILE
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	291	ILE
1	C	296	GLN
1	C	297	SER
1	C	302	LEU
1	C	305	ILE
1	C	311	LEU
1	C	312	LEU
1	C	313	ASN
1	C	314	THR
1	C	321	GLU

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Mol	Chain	Res	Type
1	C	322	MET
1	C	323	LEU
1	C	333	VAL
1	C	348	GLU
1	C	350	ARG
1	C	352	LEU
1	C	353	LEU
1	C	367	LYS
1	C	399	ILE
1	C	403	LYS
1	C	408	LYS
1	C	412	VAL
1	C	427	ILE
1	C	442	VAL
1	C	461	ILE
1	C	464	SER
1	C	467	SER
1	C	482	GLU
1	C	501	LYS
1	C	508	ASN
1	C	515	VAL
1	C	517	LEU
1	C	524	LEU
1	C	538	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	66	HIS
1	A	68	HIS
1	A	90	HIS
1	A	169	ASN
1	A	193	GLN
1	A	276	GLN
1	A	277	ASN
1	A	281	ASN
1	A	296	GLN
1	A	313	ASN
1	A	362	GLN
1	A	479	GLN
1	A	484	ASN

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Mol	Chain	Res	Type
1	A	514	GLN
1	B	66	HIS
1	B	68	HIS
1	B	75	ASN
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	313	ASN
1	B	355	ASN
1	B	362	GLN
1	B	395	ASN
1	B	484	ASN
1	B	528	ASN
1	C	43	GLN
1	C	66	HIS
1	C	68	HIS
1	C	93	GLN
1	C	169	ASN
1	C	183	HIS
1	C	193	GLN
1	C	269	HIS
1	C	272	ASN
1	C	276	GLN
1	C	281	ASN
1	C	354	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
4	TZE	C	542	-	8,9,9	3.04	4 (50%)	8,11,11	2.98	3 (37%)
3	ACP	C	999	2	31,33,33	3.51	14 (45%)	47,52,52	1.93	16 (34%)
4	TZE	B	542	-	8,9,9	3.08	4 (50%)	8,11,11	3.02	3 (37%)
3	ACP	B	899	2	31,33,33	3.69	15 (48%)	47,52,52	1.99	13 (27%)
3	ACP	A	799	2	31,33,33	3.54	15 (48%)	47,52,52	1.92	12 (25%)
4	TZE	B	543	-	8,9,9	3.07	4 (50%)	8,11,11	3.00	3 (37%)

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
4	TZE	C	542	-	-	1/3/3/3	0/1/1/1
3	ACP	C	999	2	-	7/19/38/38	0/3/3/3
4	TZE	B	542	-	-	1/3/3/3	0/1/1/1
3	ACP	B	899	2	-	7/19/38/38	0/3/3/3
3	ACP	A	799	2	-	11/19/38/38	0/3/3/3
4	TZE	B	543	-	-	1/3/3/3	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	899	ACP	PA-O3A	8.72	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	899	ACP	PB-O3A	8.47	1.67	1.58
3	A	799	ACP	PB-O3A	7.86	1.67	1.58
3	C	999	ACP	PB-O3A	7.86	1.67	1.58
3	C	999	ACP	PG-O1G	7.45	1.65	1.50
3	B	899	ACP	PG-O1G	7.45	1.65	1.50
3	A	799	ACP	PA-O3A	7.42	1.67	1.59
3	A	799	ACP	PG-O1G	7.39	1.65	1.50
4	B	542	TZE	C2-N1	7.15	1.47	1.38
4	B	543	TZE	C2-N1	7.01	1.47	1.38
4	C	542	TZE	C2-N1	6.98	1.47	1.38
3	C	999	ACP	PA-O3A	6.21	1.66	1.59
3	C	999	ACP	C8-N7	6.17	1.43	1.31
3	B	899	ACP	C8-N7	6.07	1.43	1.31
3	B	899	ACP	PB-O1B	5.93	1.65	1.51
3	A	799	ACP	C8-N7	5.90	1.43	1.31
3	C	999	ACP	PB-O1B	5.68	1.65	1.51
3	A	799	ACP	PB-O1B	5.59	1.64	1.51
3	C	999	ACP	C6-N6	5.03	1.47	1.34
3	A	799	ACP	C6-N6	4.93	1.46	1.34
3	B	899	ACP	C6-N6	4.86	1.46	1.34
3	C	999	ACP	PG-O2G	4.67	1.65	1.55
3	A	799	ACP	PG-O2G	4.57	1.65	1.55
3	C	999	ACP	C4-N9	4.51	1.47	1.37
3	B	899	ACP	PG-O2G	4.41	1.64	1.55
3	C	999	ACP	PA-O1A	4.40	1.66	1.50
3	B	899	ACP	PA-O1A	4.38	1.66	1.50
3	B	899	ACP	PB-O2B	-4.26	1.46	1.56
3	A	799	ACP	PA-O1A	4.20	1.65	1.50
3	A	799	ACP	PB-O2B	-4.17	1.46	1.56
3	A	799	ACP	C4-N9	3.99	1.46	1.37
3	B	899	ACP	C4-N9	3.93	1.45	1.37
3	C	999	ACP	PB-O2B	-3.81	1.47	1.56
3	A	799	ACP	PG-O3G	-3.76	1.46	1.55
3	C	999	ACP	C2-N3	3.67	1.40	1.33
4	B	543	TZE	C1-N1	3.42	1.39	1.30
3	B	899	ACP	C2-N3	3.39	1.40	1.33
3	A	799	ACP	C2-N3	3.36	1.39	1.33
4	B	542	TZE	C1-N1	3.31	1.38	1.30
4	C	542	TZE	C1-N1	3.26	1.38	1.30
3	B	899	ACP	PG-O3G	-3.21	1.47	1.55
3	C	999	ACP	PG-O3G	-3.10	1.48	1.55
4	C	542	TZE	C1-S1	2.90	1.77	1.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	542	TZE	C1-S1	2.86	1.77	1.72
4	B	543	TZE	C1-S1	2.84	1.77	1.72
3	C	999	ACP	O4'-C1'	2.45	1.47	1.42
3	C	999	ACP	C2-N1	2.44	1.38	1.33
3	B	899	ACP	C2-N1	2.25	1.37	1.33
3	A	799	ACP	O4'-C1'	2.20	1.47	1.42
4	B	543	TZE	CM-C2	2.19	1.54	1.49
3	A	799	ACP	C2-N1	2.17	1.37	1.33
4	B	542	TZE	CM-C2	2.13	1.54	1.49
3	B	899	ACP	PA-O5'	2.13	1.67	1.59
3	A	799	ACP	PA-O5'	2.06	1.67	1.59
3	B	899	ACP	O4'-C1'	2.04	1.46	1.42
4	C	542	TZE	CM-C2	2.02	1.53	1.49

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	542	TZE	S1-C1-N1	-6.60	110.41	116.08
4	B	543	TZE	S1-C1-N1	-6.48	110.52	116.08
4	C	542	TZE	S1-C1-N1	-6.46	110.53	116.08
3	B	899	ACP	N3-C2-N1	-5.81	119.79	128.58
3	A	799	ACP	N3-C2-N1	-5.62	120.08	128.58
3	C	999	ACP	N3-C2-N1	-5.41	120.39	128.58
3	C	999	ACP	C5-C4-N3	-5.34	119.37	126.72
3	B	899	ACP	C5-C4-N3	-4.89	119.98	126.72
3	A	799	ACP	C5-C4-N3	-4.85	120.04	126.72
3	A	799	ACP	N9-C8-N7	-4.17	108.02	113.94
3	B	899	ACP	N9-C8-N7	-3.95	108.34	113.94
3	A	799	ACP	PB-O3A-PA	-3.92	119.59	132.37
4	B	543	TZE	C1-N1-C2	3.63	114.79	110.71
4	C	542	TZE	C1-N1-C2	3.58	114.73	110.71
3	B	899	ACP	C2-N3-C4	3.55	120.50	111.83
4	B	542	TZE	C1-N1-C2	3.52	114.67	110.71
3	C	999	ACP	C2-N3-C4	3.44	120.22	111.83
3	C	999	ACP	N9-C8-N7	-3.43	109.06	113.94
4	B	543	TZE	C1'-C3-S1	-3.40	112.94	120.90
4	B	542	TZE	C1'-C3-S1	-3.37	113.01	120.90
3	A	799	ACP	C2-N3-C4	3.36	120.03	111.83
4	C	542	TZE	C1'-C3-S1	-3.31	113.16	120.90
3	B	899	ACP	C2'-C3'-C4'	3.23	108.84	102.61
3	B	899	ACP	PB-O3A-PA	-3.14	122.11	132.37
3	A	799	ACP	C5-N7-C8	2.89	107.99	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	999	ACP	PB-O3A-PA	-2.85	123.05	132.37
3	A	799	ACP	N3-C4-N9	2.83	131.99	127.17
3	C	999	ACP	C5-N7-C8	2.83	107.90	103.45
3	B	899	ACP	O5'-C5'-C4'	2.83	118.61	108.99
3	B	899	ACP	C5-N7-C8	2.80	107.86	103.45
3	C	999	ACP	N3-C4-N9	2.79	131.91	127.17
3	C	999	ACP	C5-C4-N9	2.67	108.72	105.81
3	C	999	ACP	C4-C5-N7	-2.58	107.63	110.58
3	B	899	ACP	N3-C4-N9	2.53	131.48	127.17
3	B	899	ACP	C5-C4-N9	2.51	108.55	105.81
3	A	799	ACP	O5'-C5'-C4'	2.50	117.51	108.99
3	B	899	ACP	C4-C5-N7	-2.49	107.74	110.58
3	C	999	ACP	O4'-C1'-N9	2.45	112.80	108.09
3	B	899	ACP	O4'-C4'-C5'	2.42	117.08	109.33
3	C	999	ACP	C6-C5-C4	2.32	120.35	117.18
3	A	799	ACP	O4'-C4'-C5'	2.28	116.65	109.33
3	C	999	ACP	O3'-C3'-C2'	2.28	119.12	111.82
3	A	799	ACP	C4-C5-N7	-2.25	108.01	110.58
3	B	899	ACP	O4'-C1'-N9	2.22	112.35	108.09
3	C	999	ACP	O2G-PG-O1G	-2.19	106.73	112.39
3	A	799	ACP	C4-N9-C8	2.16	108.01	105.74
3	C	999	ACP	C3'-C2'-C1'	2.11	105.45	101.46
3	C	999	ACP	O3'-C3'-C4'	2.05	116.97	111.08
3	A	799	ACP	C6-C5-C4	2.03	119.95	117.18
3	C	999	ACP	O2'-C2'-C1'	2.03	117.08	110.10

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C5'-O5'-PA-O3A
3	A	799	ACP	O4'-C4'-C5'-O5'
3	B	899	ACP	PB-C3B-PG-O1G
3	B	899	ACP	PB-C3B-PG-O2G

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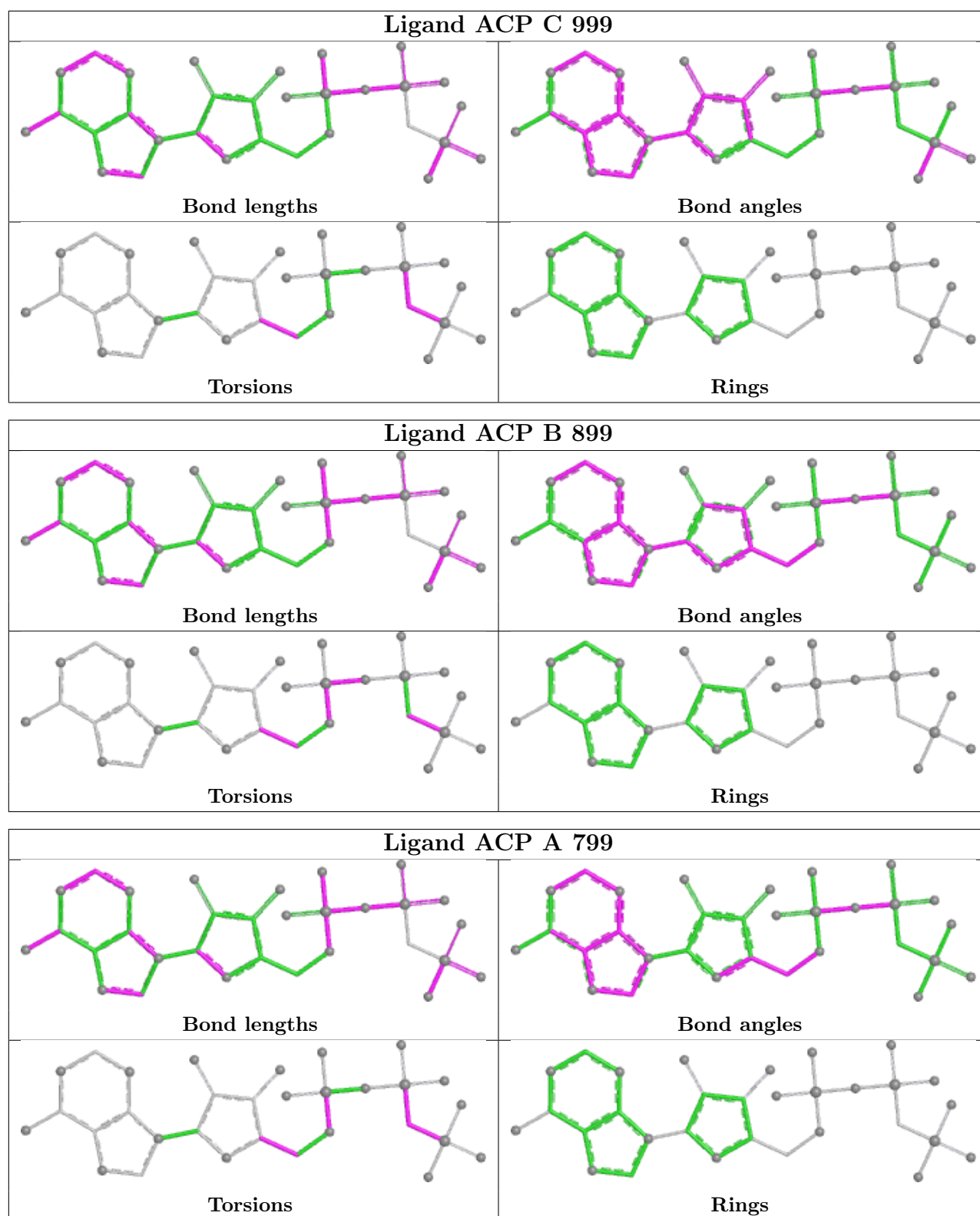
Mol	Chain	Res	Type	Atoms
3	B	899	ACP	PB-C3B-PG-O3G
3	B	899	ACP	C5'-O5'-PA-O1A
3	C	999	ACP	PB-C3B-PG-O1G
3	C	999	ACP	PG-C3B-PB-O3A
4	B	542	TZE	C3-C1'-C2'-OXT
4	B	543	TZE	C3-C1'-C2'-OXT
4	C	542	TZE	C3-C1'-C2'-OXT
3	A	799	ACP	C3'-C4'-C5'-O5'
3	B	899	ACP	O4'-C4'-C5'-O5'
3	C	999	ACP	O4'-C4'-C5'-O5'
3	B	899	ACP	C3'-C4'-C5'-O5'
3	B	899	ACP	PB-O3A-PA-O1A
3	C	999	ACP	C3'-C4'-C5'-O5'
3	C	999	ACP	PB-C3B-PG-O2G
3	C	999	ACP	PB-C3B-PG-O3G
3	C	999	ACP	PG-C3B-PB-O2B

There are no ring outliers.

6 monomers are involved in 36 short contacts:

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

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	512/540 (94%)	-0.01	10 (1%) 65 46	27, 70, 93, 122	0
1	B	510/540 (94%)	0.10	11 (2%) 62 43	30, 80, 100, 127	0
1	C	511/540 (94%)	0.07	5 (0%) 79 63	30, 77, 99, 125	0
All	All	1533/1620 (94%)	0.05	26 (1%) 69 50	27, 76, 98, 127	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	344	TYR	6.2
1	A	38	GLY	5.4
1	A	464	SER	3.8
1	B	434	SER	3.5
1	C	317	VAL	3.0
1	B	83	ALA	2.7
1	B	379	LEU	2.7
1	A	467	SER	2.7
1	B	317	VAL	2.7
1	B	108	ASP	2.7
1	A	317	VAL	2.6
1	B	77	ARG	2.6
1	B	345	SER	2.6
1	C	345	SER	2.6
1	B	344	TYR	2.6
1	A	439	GLY	2.5
1	A	434	SER	2.3
1	B	272	ASN	2.3
1	A	343	GLY	2.2
1	C	2	LYS	2.2
1	C	142	PRO	2.2
1	A	344	TYR	2.1
1	A	345	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	379	LEU	2.0
1	B	211	ASP	2.0
1	B	314	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

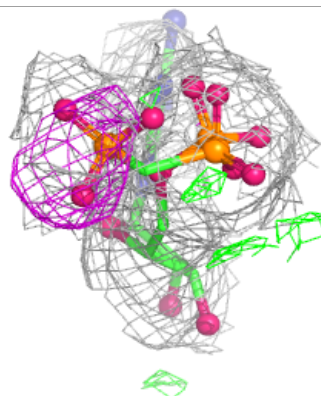
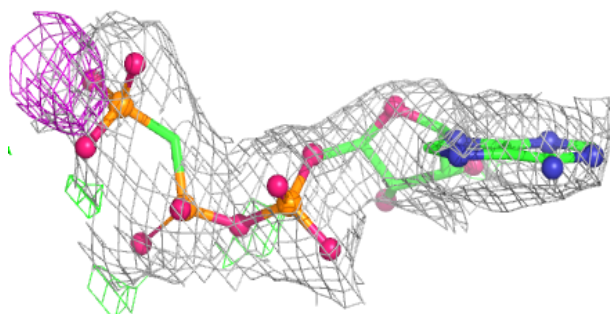
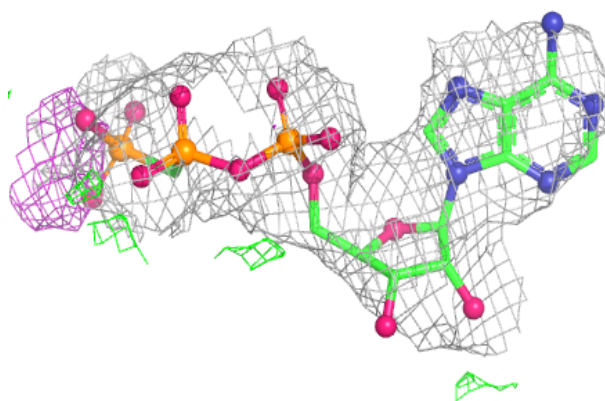
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	B	541	1/1	0.61	0.22	76,76,76,76	0
4	TZE	B	543	9/9	0.73	0.27	55,56,56,56	0
4	TZE	B	542	9/9	0.76	0.32	42,43,43,43	0
4	TZE	C	542	9/9	0.78	0.30	48,48,48,48	0
3	ACP	B	899	31/31	0.88	0.12	80,92,113,119	0
3	ACP	A	799	31/31	0.88	0.11	76,87,103,107	0
3	ACP	C	999	31/31	0.89	0.10	78,96,111,113	0
2	MG	C	541	1/1	0.89	0.14	76,76,76,76	0
2	MG	A	541	1/1	0.93	0.24	65,65,65,65	0

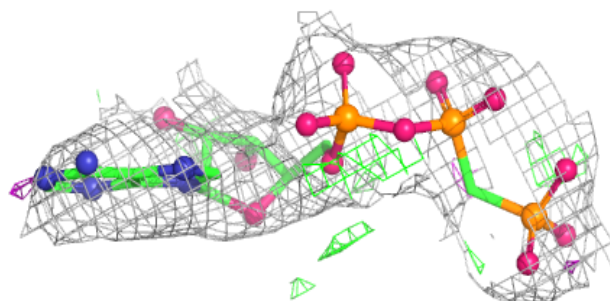
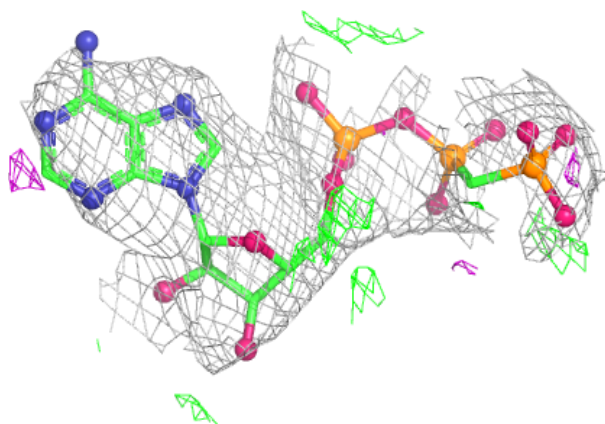
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

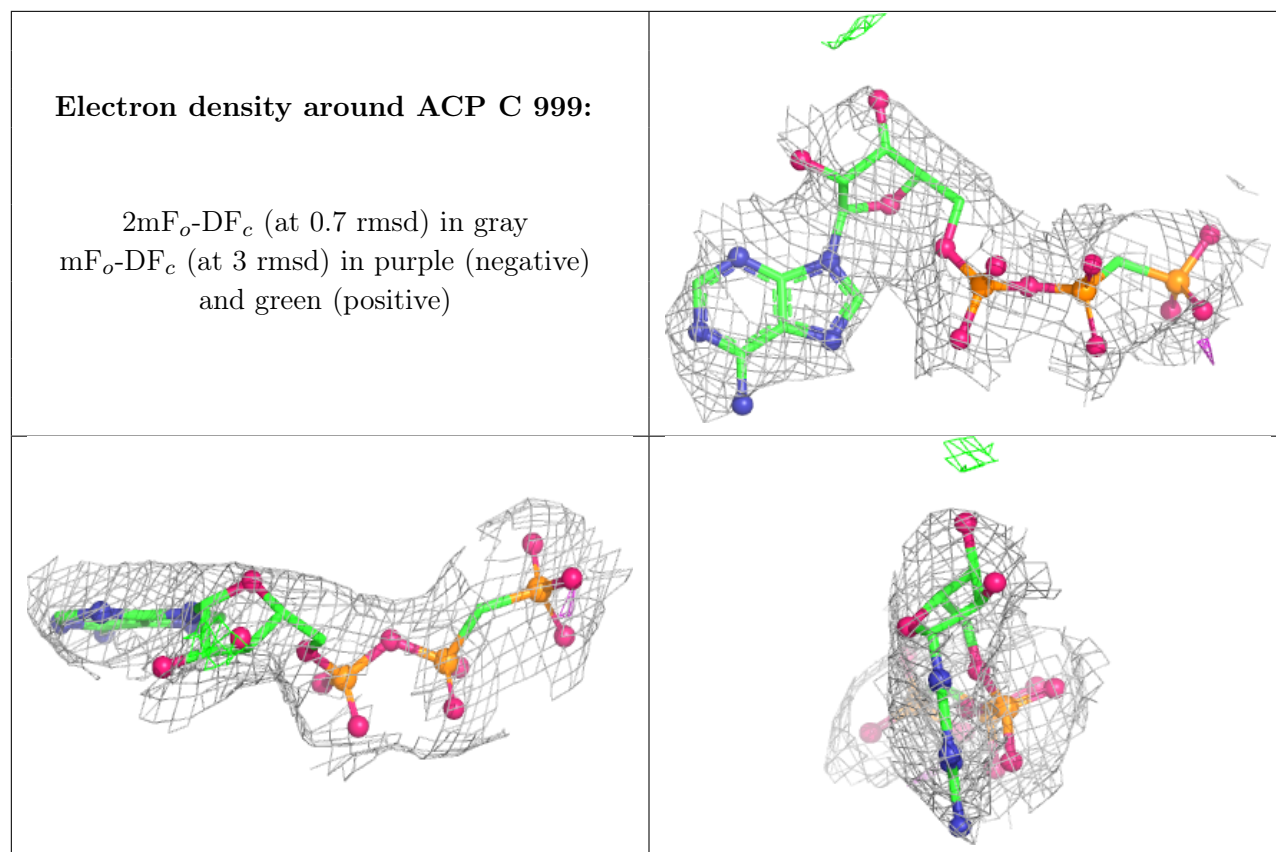
Electron density around ACP B 899:

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

**Electron density around ACP A 799:**

$2mF_o-DF_c$ (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.