



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:45 pm BST

PDB ID : 3E22
Title : Tubulin-colchicine-soblidotin: Stathmin-like domain complex
Authors : Cormier, A.; Marchand, M.; Ravelli, R.B.; Knossow, M.; Gigant, B.
Deposited on : 2008-08-05
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

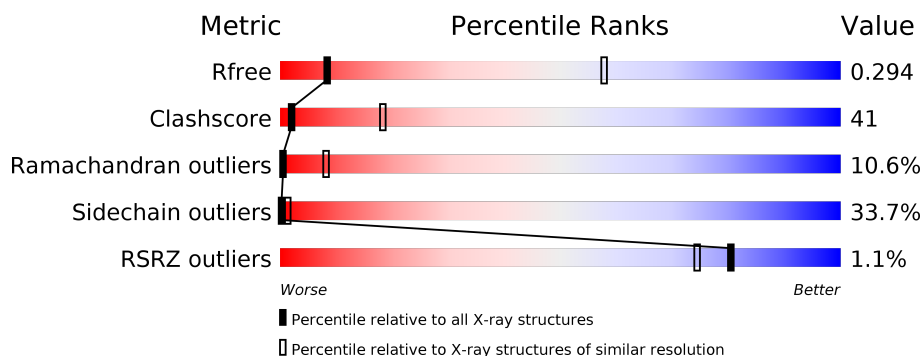
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	449	<div> <div>31%</div> <div>42%</div> <div>19%</div> <div>• 5%</div> </div>
1	C	449	<div>2%</div> <div>33%</div> <div>41%</div> <div>18%</div> <div>• 6%</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
8	TZT	B	800	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14154 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 Tubulin alpha-1C chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3290	2089	556	624	21			
1	C	421	Total	C	N	O	S	0	0	0
			3234	2055	547	611	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	TYR	ALA	SEE REMARK 999	UNP Q3ZCJ7
A	442	ASP	GLY	SEE REMARK 999	UNP Q3ZCJ7
A	443	GLU	ASP	SEE REMARK 999	UNP Q3ZCJ7
A	447	GLU	ASP	SEE REMARK 999	UNP Q3ZCJ7
C	440	TYR	ALA	SEE REMARK 999	UNP Q3ZCJ7
C	442	ASP	GLY	SEE REMARK 999	UNP Q3ZCJ7
C	443	GLU	ASP	SEE REMARK 999	UNP Q3ZCJ7
C	447	GLU	ASP	SEE REMARK 999	UNP Q3ZCJ7

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3238	2036	546	632	24			
2	D	419	Total	C	N	O	S	0	0	0
			3246	2041	549	632	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	SER	CYS	SEE REMARK 999	UNP Q6B856
B	318	VAL	ILE	SEE REMARK 999	UNP Q6B856
D	203	SER	CYS	SEE REMARK 999	UNP Q6B856
D	318	VAL	ILE	SEE REMARK 999	UNP Q6B856

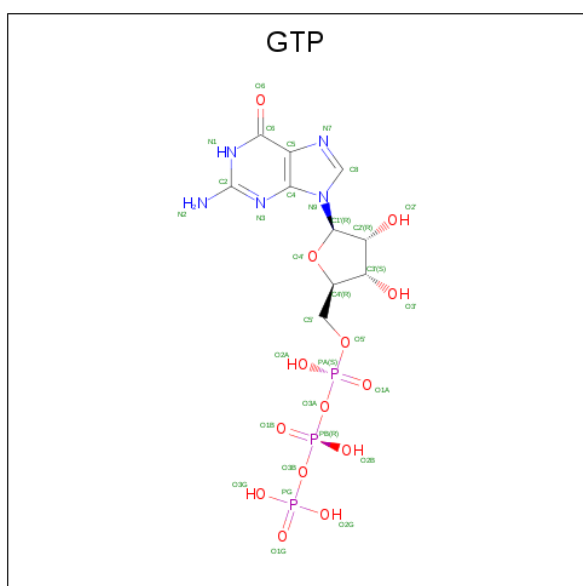
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			916	555	173	183	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	EXPRESSION TAG	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

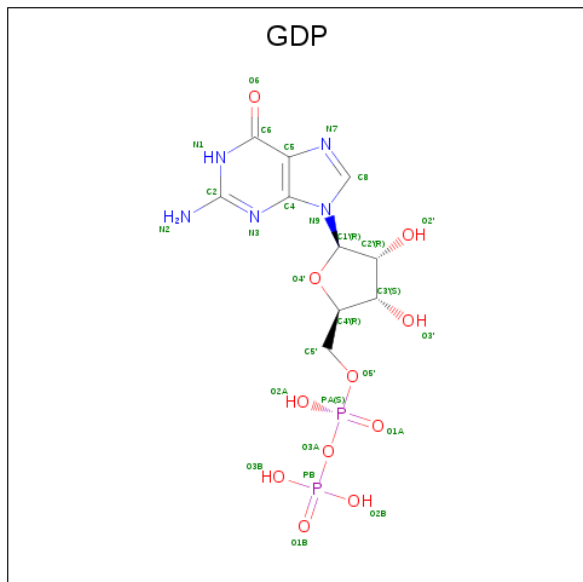


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

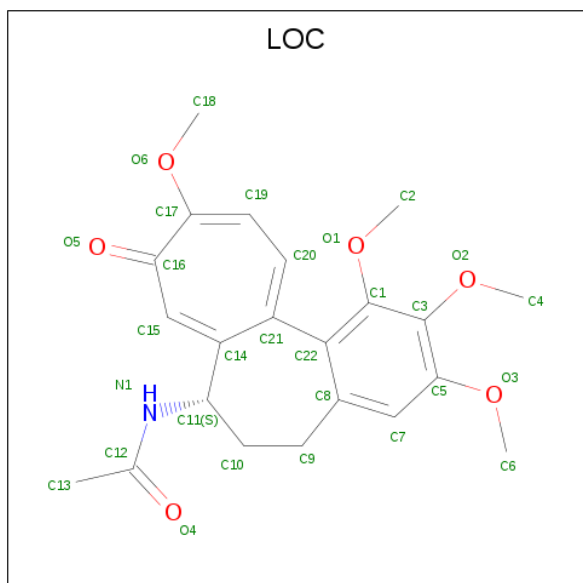
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



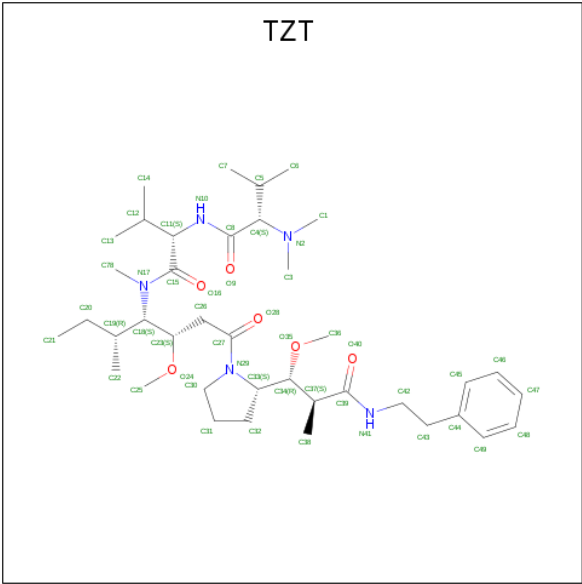
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 7 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]ethanamide (three-letter code: LOC) (formula: $C_{22}H_{25}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			29	22	1	6		
7	D	1	Total	C	N	O	0	0
			29	22	1	6		

- Molecule 8 is SOBLIDOTIN (three-letter code: TZT) (formula: C₃₉H₆₇N₅O₆).

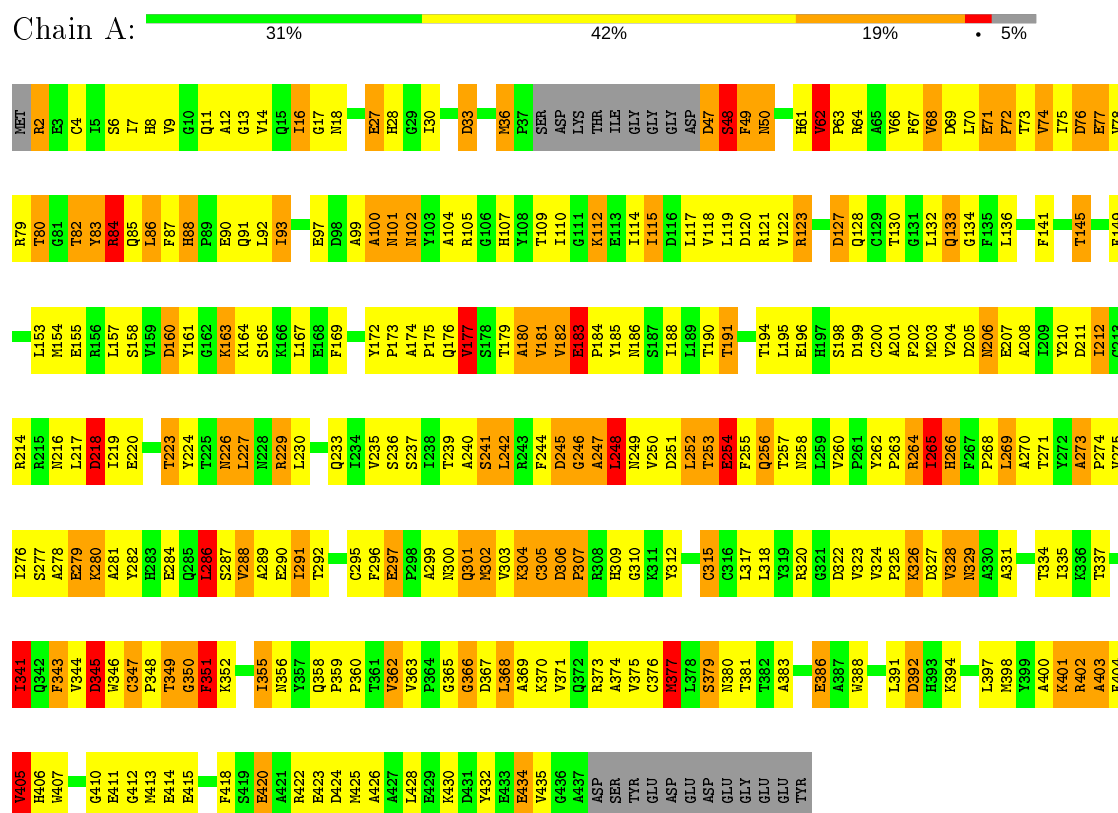


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			50	39	5	6		

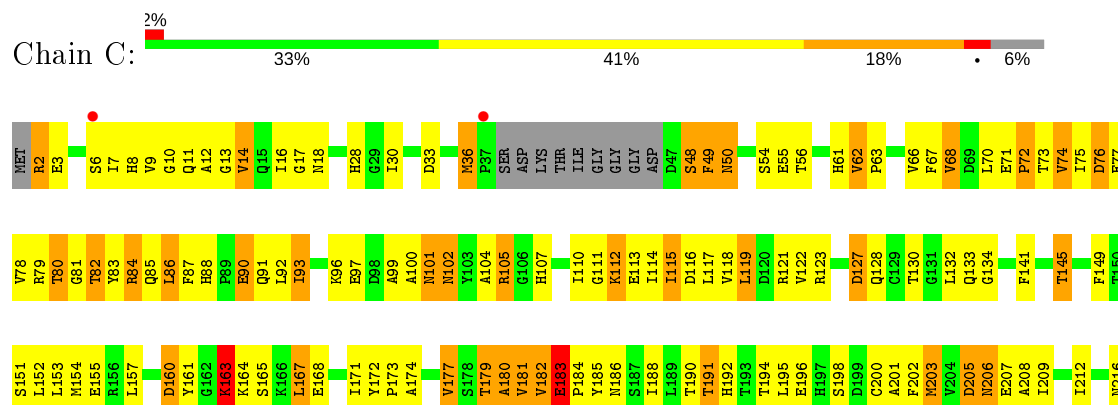
3 Residue-property plots

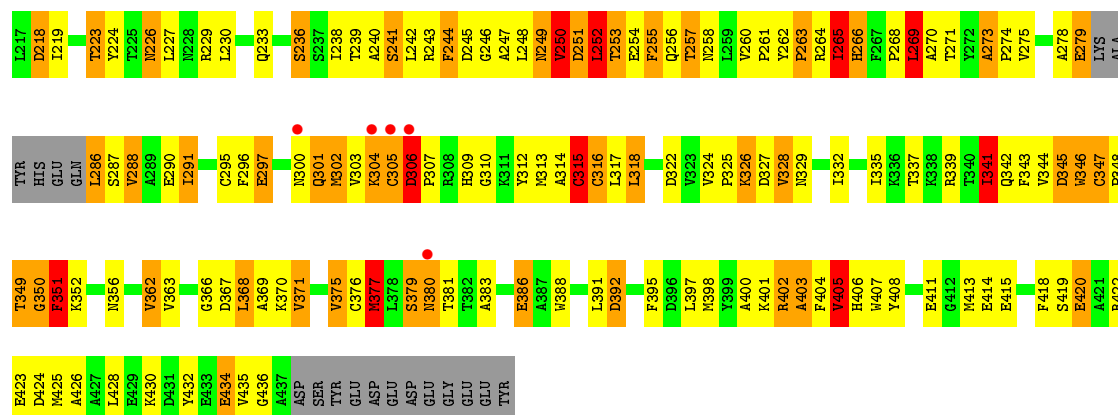
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Tubulin alpha-1C chain



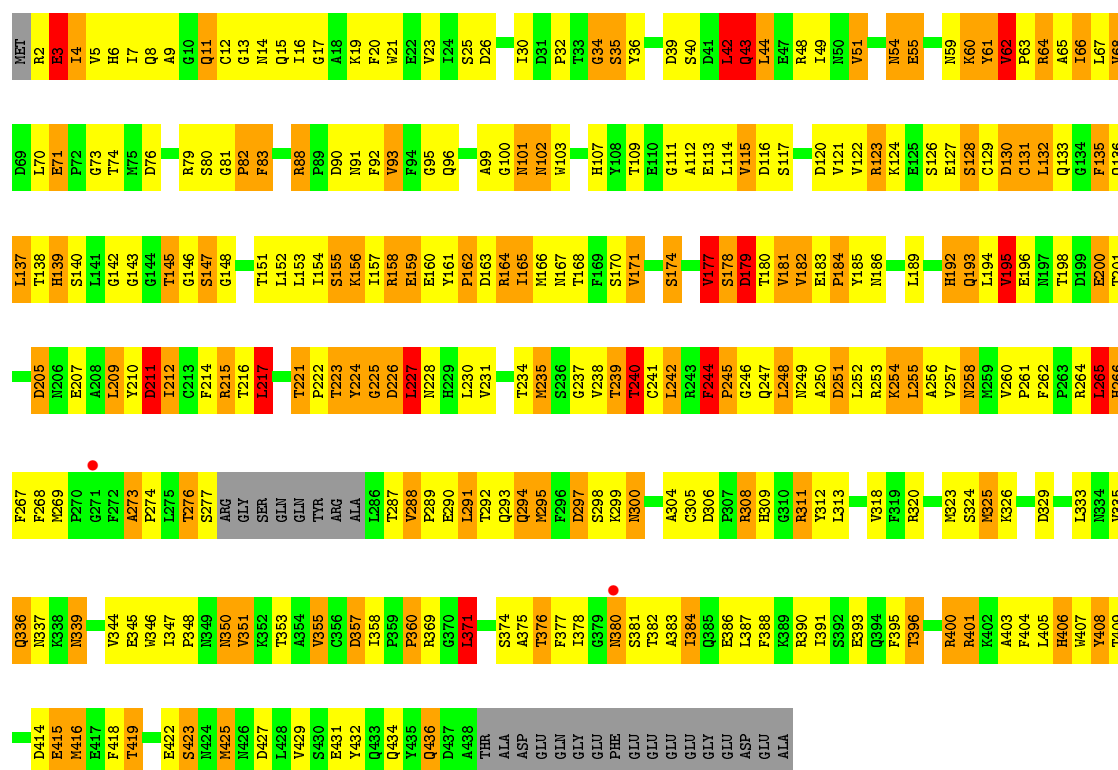
- Molecule 1: Tubulin alpha-1C chain





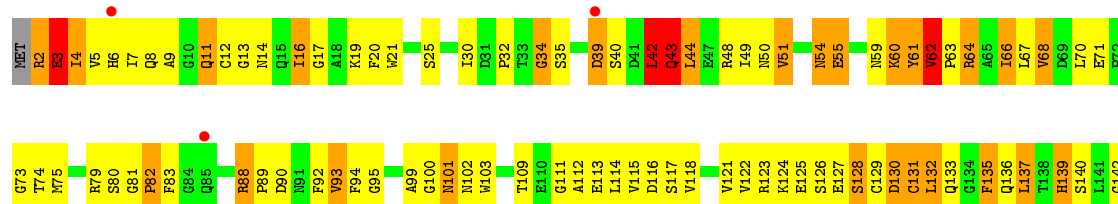
• Molecule 2: Tubulin beta-2B chain

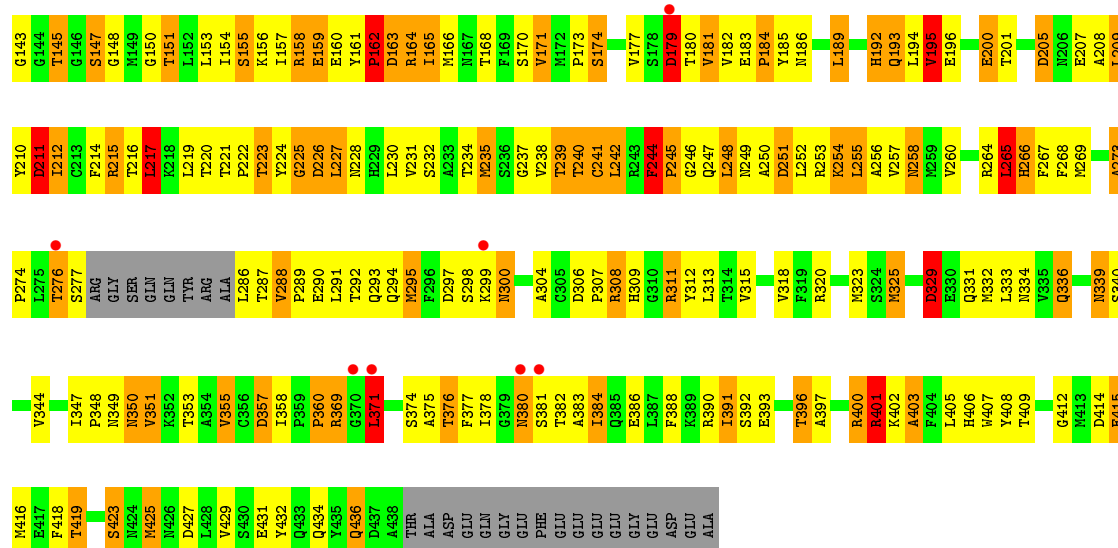
Chain B: 30% 39% 22% 6%



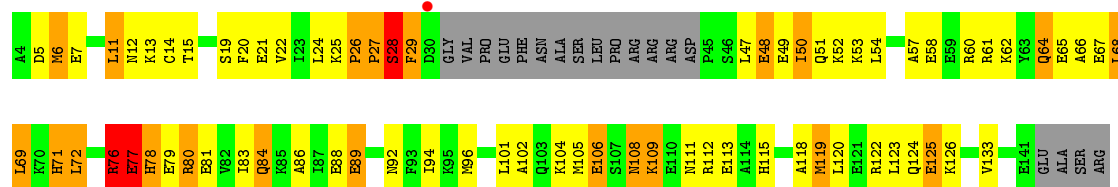
• Molecule 2: Tubulin beta-2B chain

Chain D: 2% 31% 40% 20% 6%





• Molecule 3: Stathmin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	324.09 Å 324.09 Å 53.28 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.80 19.91 – 3.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-3.80) 97.6 (19.91-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 3.82 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.229 , 0.295 0.240 , 0.294	Depositor DCC
R_{free} test set	1598 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	140.1	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 108.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14154	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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: GTP, LOC, MG, GDP, TZT

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	0.95	1/3367 (0.0%)	1.09	19/4579 (0.4%)
1	C	0.67	1/3308 (0.0%)	0.96	15/4498 (0.3%)
2	B	0.76	0/3310	0.99	11/4495 (0.2%)
2	D	0.61	0/3318	0.92	13/4505 (0.3%)
3	E	0.72	0/924	0.90	0/1239
All	All	0.76	2/14227 (0.0%)	0.99	58/19316 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	3
2	B	0	3
2	D	0	2
3	E	0	3
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	GLU	CD-OE1	5.64	1.31	1.25
1	C	436	GLY	C-O	-5.23	1.15	1.23

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	LEU	CA-CB-CG	7.48	132.51	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	ASP	CB-CG-OD2	7.28	124.86	118.30
1	A	33	ASP	CB-CG-OD2	6.95	124.55	118.30
1	A	76	ASP	CB-CG-OD2	6.82	124.43	118.30
1	A	47	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	160	ASP	CB-CG-OD2	6.59	124.23	118.30
2	D	427	ASP	CB-CG-OD2	6.56	124.21	118.30
2	B	226	ASP	CB-CG-OD2	6.38	124.04	118.30
2	B	120	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	127	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	345	ASP	CB-CG-OD2	6.14	123.83	118.30
2	D	357	ASP	CB-CG-OD2	5.98	123.69	118.30
2	D	179	ASP	CB-CG-OD2	5.97	123.67	118.30
2	D	211	ASP	CB-CG-OD2	5.96	123.66	118.30
2	D	116	ASP	CB-CG-OD2	5.91	123.62	118.30
1	C	345	ASP	CB-CG-OD2	5.87	123.58	118.30
1	C	160	ASP	CB-CG-OD2	5.80	123.53	118.30
1	C	116	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	424	ASP	CB-CG-OD2	5.77	123.50	118.30
1	C	76	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	69	ASP	CB-CG-OD2	5.74	123.47	118.30
2	B	179	ASP	CB-CG-OD2	5.73	123.45	118.30
1	C	205	ASP	CB-CG-OD2	5.72	123.45	118.30
2	B	211	ASP	CB-CG-OD2	5.72	123.44	118.30
1	C	424	ASP	CB-CG-OD2	5.71	123.44	118.30
2	D	414	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	218	ASP	CB-CG-OD2	5.68	123.41	118.30
1	C	250	VAL	CB-CA-C	5.68	122.19	111.40
1	A	245	ASP	CB-CG-OD2	5.62	123.36	118.30
2	D	205	ASP	CB-CG-OD2	5.62	123.36	118.30
2	B	205	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	199	ASP	CB-CG-OD2	5.51	123.26	118.30
2	D	306	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	120	ASP	CB-CG-OD2	5.46	123.21	118.30
1	C	306	ASP	CB-CG-OD2	5.46	123.21	118.30
2	D	39	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	315	CYS	CA-CB-SG	-5.45	104.20	114.00
1	C	269	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	84	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	C	134	GLY	N-CA-C	5.38	126.54	113.10
2	B	306	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	127	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	134	GLY	N-CA-C	5.32	126.40	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	GLY	N-CA-C	-5.32	99.81	113.10
2	B	297	ASP	CB-CG-OD2	5.27	123.04	118.30
2	D	226	ASP	CB-CG-OD2	5.26	123.03	118.30
2	D	371	LEU	CA-CB-CG	5.25	127.37	115.30
2	D	130	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	123	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	252	LEU	CA-CB-CG	5.17	127.19	115.30
2	B	76	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	218	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	119	LEU	CA-CB-CG	-5.12	103.52	115.30
1	A	286	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	A	229	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	D	329	ASP	CB-CG-OD2	5.04	122.83	118.30
2	B	26	ASP	CB-CG-OD2	5.01	122.81	118.30
2	B	291	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	VAL	Peptide
1	A	265	ILE	Peptide
2	B	162	PRO	Peptide
2	B	244	PHE	Peptide
2	B	265	LEU	Peptide
1	C	177	VAL	Peptide
1	C	265	ILE	Peptide
1	C	315	CYS	Peptide
2	D	162	PRO	Peptide
2	D	244	PHE	Peptide
3	E	5	ASP	Peptide
3	E	50	ILE	Peptide
3	E	77	GLU	Peptide

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	3290	0	3149	276	0
1	C	3234	0	3102	267	0
2	B	3238	0	3049	290	0
2	D	3246	0	3067	253	0
3	E	916	0	799	62	0
4	A	32	0	12	4	0
4	C	32	0	12	6	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	4	0
6	D	28	0	12	1	0
7	B	29	0	23	3	0
7	D	29	0	23	3	0
8	B	50	0	67	30	0
All	All	14154	0	13327	1115	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 41.

All (1115) 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)
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.77	1.14
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.81	1.10
1:C:273:ALA:HB1	1:C:274:PRO:HD3	1.23	1.10
1:A:273:ALA:HB1	1:A:274:PRO:HD3	1.20	1.09
2:B:336:GLN:OE1	2:B:351:VAL:HG11	1.53	1.07
1:A:286:LEU:HD12	1:A:286:LEU:H	1.17	1.07
1:C:183:GLU:HB3	1:C:184:PRO:CD	1.85	1.06
1:C:271:THR:HG21	1:C:295:CYS:HA	1.34	1.06
1:C:273:ALA:CB	1:C:274:PRO:HD3	1.84	1.06
2:B:223:THR:HA	8:B:800:TZT:H25	1.35	1.06
1:A:350:GLY:O	1:A:351:PHE:HB2	1.54	1.05
1:A:273:ALA:CB	1:A:274:PRO:HD3	1.87	1.04
1:C:249:ASN:O	1:C:250:VAL:HB	1.55	1.04
1:A:183:GLU:HB3	1:A:184:PRO:CD	1.89	1.03
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.40	1.03
2:B:401:ARG:HG3	2:B:401:ARG:HH11	1.22	1.03
3:E:76:ARG:O	3:E:78:HIS:N	1.92	1.03
2:D:276:THR:HG23	2:D:277:SER:H	1.20	1.02
1:C:206:ASN:HD21	4:C:600:GTP:HN22	1.05	1.02
1:A:247:ALA:HB2	3:E:12:ASN:HB3	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:350:ASN:H	2:D:350:ASN:HD22	1.02	1.01
2:B:287:THR:HG22	2:B:290:GLU:HB2	1.39	1.00
1:A:346:TRP:O	1:A:346:TRP:HE3	1.44	1.00
1:A:167:LEU:HD13	1:A:252:LEU:HD13	1.41	0.99
2:D:180:THR:HG22	2:D:182:VAL:H	1.27	0.99
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.40	0.99
2:B:276:THR:HG23	2:B:277:SER:H	1.26	0.98
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.45	0.97
1:A:273:ALA:HB2	1:A:375:VAL:N	1.79	0.97
8:B:800:TZT:O16	8:B:800:TZT:H19	1.64	0.97
1:C:265:ILE:HG12	1:C:265:ILE:O	1.63	0.97
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.42	0.96
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.47	0.96
2:D:99:ALA:HB1	2:D:145:THR:HG22	1.46	0.96
1:C:273:ALA:CB	1:C:274:PRO:CD	2.44	0.95
2:B:350:ASN:HD22	2:B:350:ASN:H	1.02	0.94
1:A:273:ALA:CB	1:A:274:PRO:CD	2.42	0.94
2:D:396:THR:O	2:D:400:ARG:HB3	1.67	0.94
2:D:158:ARG:O	2:D:159:GLU:HB3	1.65	0.94
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.50	0.94
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.50	0.94
2:B:396:THR:O	2:B:400:ARG:HB2	1.69	0.93
1:C:48:SER:O	1:C:50:ASN:N	2.03	0.92
2:D:400:ARG:HG2	2:D:400:ARG:O	1.66	0.92
1:C:273:ALA:HB2	1:C:375:VAL:N	1.84	0.91
2:B:158:ARG:O	2:B:159:GLU:HB3	1.70	0.91
1:A:70:LEU:HD13	1:A:145:THR:HB	1.52	0.91
1:A:273:ALA:HB2	1:A:375:VAL:H	1.31	0.91
8:B:800:TZT:H13A	8:B:800:TZT:O9	1.71	0.90
1:A:102:ASN:HD21	1:A:104:ALA:HB3	1.34	0.90
2:B:273:ALA:CB	2:B:274:PRO:CD	2.49	0.90
1:C:8:HIS:CD2	1:C:17:GLY:HA3	2.06	0.90
1:A:265:ILE:HG12	1:A:265:ILE:O	1.71	0.90
2:D:287:THR:HG22	2:D:290:GLU:HB2	1.54	0.89
2:B:226:ASP:O	2:B:227:LEU:HB3	1.70	0.89
2:B:245:PRO:HB2	2:B:247:GLN:HG2	1.54	0.89
1:C:70:LEU:HD13	1:C:145:THR:HB	1.52	0.89
2:B:224:TYR:CE1	8:B:800:TZT:H20	2.08	0.89
1:C:101:ASN:ND2	2:D:254:LYS:HG2	1.86	0.89
2:B:273:ALA:HB1	2:B:274:PRO:HD3	1.52	0.89
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LEU:HD12	1:A:286:LEU:N	1.89	0.87
1:C:273:ALA:HB1	1:C:274:PRO:CD	2.05	0.87
1:A:368:LEU:HD12	1:A:368:LEU:H	1.38	0.87
2:B:99:ALA:HB1	2:B:145:THR:HG22	1.57	0.87
2:D:140:SER:HA	2:D:171:VAL:HG23	1.57	0.86
2:D:273:ALA:CB	2:D:274:PRO:CD	2.52	0.86
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.06	0.86
1:C:205:ASP:HB2	1:C:303:VAL:HA	1.56	0.85
2:B:224:TYR:O	2:B:228:ASN:HB2	1.77	0.85
2:B:273:ALA:HB2	2:B:375:ALA:H	1.41	0.85
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.11	0.85
2:D:245:PRO:HB2	2:D:247:GLN:HG2	1.58	0.85
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.05	0.85
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.58	0.85
1:A:271:THR:HG21	1:A:295:CYS:HA	1.58	0.85
1:C:241:SER:HA	1:C:250:VAL:HG22	1.59	0.85
1:C:368:LEU:H	1:C:368:LEU:HD12	1.41	0.85
2:B:140:SER:HA	2:B:171:VAL:HG23	1.56	0.85
1:A:247:ALA:CB	3:E:12:ASN:HB3	2.06	0.84
1:A:346:TRP:CE3	1:A:346:TRP:O	2.29	0.83
2:B:265:LEU:HD12	2:B:265:LEU:O	1.76	0.83
2:B:350:ASN:ND2	2:B:350:ASN:H	1.73	0.83
2:D:7:ILE:HB	2:D:137:LEU:HB2	1.61	0.83
2:D:153:LEU:O	2:D:157:ILE:HG12	1.78	0.83
1:C:350:GLY:O	1:C:351:PHE:HB2	1.77	0.83
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.19	0.83
2:D:350:ASN:H	2:D:350:ASN:ND2	1.76	0.82
2:D:131:CYS:O	2:D:131:CYS:SG	2.36	0.82
3:E:27:PRO:O	3:E:28:SER:HB2	1.79	0.82
2:B:70:LEU:HA	2:B:95:GLY:HA3	1.62	0.82
2:D:273:ALA:HB1	2:D:274:PRO:HD3	1.59	0.82
2:B:7:ILE:HB	2:B:137:LEU:HB2	1.62	0.82
2:B:131:CYS:O	2:B:131:CYS:SG	2.37	0.81
2:B:350:ASN:HD22	2:B:350:ASN:N	1.74	0.81
1:A:273:ALA:HB1	1:A:274:PRO:CD	1.99	0.81
2:B:273:ALA:CB	2:B:375:ALA:H	1.92	0.81
1:C:420:GLU:HA	1:C:423:GLU:HG3	1.61	0.81
1:A:206:ASN:HD21	4:A:600:GTP:HN22	1.27	0.80
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.60	0.80
2:D:350:ASN:HD22	2:D:350:ASN:N	1.76	0.80
2:B:8:GLN:OE1	2:B:67:LEU:HD21	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:265:LEU:HD12	2:D:265:LEU:O	1.81	0.80
1:A:247:ALA:HB1	3:E:19:SER:CB	2.12	0.79
1:A:6:SER:HB3	1:A:8:HIS:HE1	1.46	0.79
2:D:223:THR:HB	2:D:225:GLY:H	1.46	0.79
1:C:101:ASN:HD22	2:D:254:LYS:HG2	1.46	0.79
2:B:223:THR:HA	8:B:800:TZT:C25	2.14	0.78
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.65	0.78
1:A:273:ALA:CB	1:A:375:VAL:H	1.96	0.78
1:C:271:THR:CG2	1:C:295:CYS:HA	2.11	0.78
1:C:105:ARG:HH22	2:D:253:ARG:HH21	1.31	0.78
1:C:271:THR:HG21	1:C:295:CYS:CA	2.11	0.77
2:D:159:GLU:HB2	3:E:123:LEU:HD13	1.66	0.77
1:C:102:ASN:HD21	1:C:104:ALA:HB3	1.48	0.77
1:A:174:ALA:CB	1:A:207:GLU:HB2	2.15	0.77
2:D:276:THR:CG2	2:D:277:SER:H	1.98	0.77
2:B:192:HIS:O	2:B:195:VAL:HG12	1.84	0.77
1:C:273:ALA:HB2	1:C:375:VAL:H	1.50	0.76
8:B:800:TZT:HN10	8:B:800:TZT:H6	1.50	0.76
1:A:6:SER:HB3	1:A:8:HIS:CE1	2.21	0.76
1:A:109:THR:HA	3:E:61:ARG:NH2	2.01	0.75
2:B:401:ARG:HG3	2:B:401:ARG:NH1	1.91	0.75
2:D:226:ASP:O	2:D:227:LEU:HB3	1.86	0.75
1:A:278:ALA:O	1:A:279:GLU:HB3	1.86	0.75
2:D:8:GLN:NE2	2:D:17:GLY:HA3	2.02	0.75
2:B:164:ARG:HH12	2:B:253:ARG:HH22	1.35	0.75
1:A:115:ILE:HD13	1:A:115:ILE:O	1.87	0.74
2:B:336:GLN:OE1	2:B:351:VAL:CG1	2.34	0.74
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.18	0.74
1:A:262:TYR:O	1:A:266:HIS:HD2	1.68	0.74
1:C:206:ASN:ND2	4:C:600:GTP:HN22	1.82	0.74
1:C:205:ASP:CB	1:C:303:VAL:HA	2.18	0.74
1:A:350:GLY:O	1:A:351:PHE:CB	2.32	0.73
1:A:247:ALA:HB2	3:E:12:ASN:CB	2.16	0.73
3:E:102:ALA:O	3:E:106:GLU:HB2	1.89	0.73
2:D:223:THR:HB	2:D:225:GLY:N	2.04	0.73
2:D:336:GLN:OE1	2:D:351:VAL:HG11	1.89	0.73
1:A:412:GLY:O	3:E:60:ARG:NH1	2.21	0.72
2:D:276:THR:HG23	2:D:277:SER:N	2.02	0.72
2:D:419:THR:O	2:D:423:SER:HB2	1.89	0.72
1:C:99:ALA:CB	1:C:145:THR:HG22	2.18	0.72
1:C:185:TYR:OH	1:C:403:ALA:HB3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:TYR:O	1:A:266:HIS:CD2	2.42	0.72
1:A:258:ASN:HD21	1:A:352:LYS:CE	2.02	0.72
2:B:325:MET:HG2	2:B:355:VAL:HG21	1.71	0.72
1:A:183:GLU:CB	1:A:184:PRO:CD	2.66	0.72
2:D:70:LEU:HA	2:D:95:GLY:HA3	1.72	0.71
2:B:12:CYS:SG	2:B:171:VAL:HG21	2.31	0.71
2:D:241:CYS:HB3	2:D:247:GLN:HE21	1.54	0.71
2:B:151:THR:HB	2:B:193:GLN:HG2	1.73	0.71
1:A:273:ALA:HB3	1:A:274:PRO:CD	2.20	0.71
2:B:247:GLN:HG3	2:B:248:LEU:H	1.56	0.71
2:B:269:MET:HB3	2:B:384:ILE:HD11	1.72	0.71
2:B:276:THR:CG2	2:B:277:SER:H	2.03	0.71
1:C:183:GLU:CB	1:C:184:PRO:CD	2.64	0.71
2:D:8:GLN:OE1	2:D:67:LEU:HD21	1.91	0.71
3:E:109:LYS:O	3:E:113:GLU:HB2	1.91	0.71
1:C:6:SER:HB3	1:C:8:HIS:HE1	1.56	0.70
3:E:112:ARG:HA	3:E:115:HIS:HB3	1.72	0.70
1:A:296:PHE:CE2	1:A:377:MET:SD	2.85	0.70
1:A:309:HIS:ND1	1:A:386:GLU:OE1	2.25	0.70
1:A:323:VAL:HG12	1:A:355:ILE:HD11	1.73	0.70
2:B:273:ALA:HB2	2:B:375:ALA:N	2.06	0.70
1:A:258:ASN:HD21	1:A:352:LYS:HE3	1.56	0.70
2:D:151:THR:HB	2:D:193:GLN:HG2	1.74	0.70
1:A:392:ASP:OD1	1:A:422:ARG:CZ	2.40	0.70
2:B:419:THR:O	2:B:423:SER:HB2	1.92	0.70
2:B:287:THR:CG2	2:B:290:GLU:H	2.05	0.69
2:B:404:PHE:CD2	1:C:261:PRO:HA	2.27	0.69
1:C:291:ILE:HB	1:C:375:VAL:CG2	2.22	0.69
1:C:270:ALA:O	1:C:302:MET:HB2	1.92	0.69
1:A:48:SER:O	1:A:50:ASN:N	2.25	0.69
1:A:287:SER:OG	1:A:290:GLU:HG3	1.92	0.69
1:C:392:ASP:OD1	1:C:422:ARG:CZ	2.40	0.69
1:A:99:ALA:CB	1:A:145:THR:HG22	2.22	0.69
2:B:153:LEU:O	2:B:157:ILE:HG12	1.92	0.69
2:D:273:ALA:HB2	2:D:375:ALA:H	1.57	0.69
1:A:102:ASN:ND2	1:A:104:ALA:HB3	2.08	0.69
1:A:8:HIS:HD2	1:A:17:GLY:HA3	1.57	0.69
2:B:287:THR:O	2:B:288:VAL:HB	1.92	0.69
1:A:420:GLU:HA	1:A:423:GLU:HG3	1.74	0.69
1:A:205:ASP:CB	1:A:303:VAL:HA	2.21	0.69
1:C:201:ALA:O	1:C:268:PRO:HD2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:ASP:OD1	8:B:800:TZT:H3	1.92	0.68
1:C:180:ALA:O	1:C:182:VAL:N	2.26	0.68
8:B:800:TZT:C19	8:B:800:TZT:O16	2.38	0.68
2:B:177:VAL:HG12	2:B:177:VAL:O	1.93	0.68
2:B:276:THR:HG23	2:B:277:SER:N	2.07	0.68
1:A:376:CYS:SG	1:A:376:CYS:O	2.52	0.68
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.76	0.68
1:C:264:ARG:O	1:C:266:HIS:CD2	2.47	0.68
2:D:247:GLN:HG3	2:D:248:LEU:H	1.58	0.68
1:C:105:ARG:NH2	2:D:253:ARG:HE	1.92	0.68
2:D:273:ALA:CB	2:D:375:ALA:H	2.07	0.68
2:D:396:THR:O	2:D:400:ARG:CB	2.40	0.67
1:C:270:ALA:O	1:C:302:MET:CB	2.41	0.67
2:B:265:LEU:O	2:B:266:HIS:O	2.12	0.67
2:D:168:THR:HG1	2:D:201:THR:HG1	1.40	0.67
1:C:291:ILE:HB	1:C:375:VAL:HG23	1.77	0.67
2:D:180:THR:HG22	2:D:181:VAL:N	2.09	0.67
2:B:137:LEU:HD23	2:B:168:THR:HG22	1.77	0.67
1:C:273:ALA:CB	1:C:375:VAL:H	2.07	0.67
1:A:185:TYR:OH	1:A:403:ALA:HB3	1.95	0.67
1:C:315:CYS:HB3	1:C:351:PHE:CD2	2.30	0.66
1:C:8:HIS:HD2	1:C:17:GLY:HA3	1.58	0.66
1:A:277:SER:O	1:A:280:LYS:HB2	1.95	0.66
1:A:64:ARG:HH11	1:A:64:ARG:HG3	1.59	0.66
1:C:255:PHE:CE2	1:C:318:LEU:HD11	2.30	0.66
1:C:278:ALA:O	1:C:279:GLU:HB3	1.95	0.66
2:B:180:THR:O	2:B:182:VAL:N	2.28	0.66
2:B:6:HIS:CE1	2:B:8:GLN:HG3	2.30	0.66
1:C:145:THR:HG23	4:C:600:GTP:O2B	1.95	0.66
1:C:288:VAL:HG11	1:C:327:ASP:HB3	1.77	0.66
2:B:200:GLU:OE2	2:B:255:LEU:HD12	1.95	0.66
2:B:262:PHE:O	2:B:264:ARG:N	2.29	0.66
1:C:6:SER:HB3	1:C:8:HIS:CE1	2.31	0.66
2:D:54:ASN:ND2	2:D:64:ARG:HD2	2.10	0.66
1:C:287:SER:OG	1:C:290:GLU:HG3	1.96	0.66
2:D:133:GLN:NE2	2:D:252:LEU:HD22	2.10	0.66
2:D:224:TYR:O	2:D:228:ASN:HB2	1.94	0.66
1:C:420:GLU:HA	1:C:423:GLU:CG	2.25	0.66
2:D:133:GLN:HE21	2:D:252:LEU:HD22	1.59	0.66
1:A:286:LEU:H	1:A:286:LEU:CD1	2.01	0.66
2:D:194:LEU:O	2:D:196:GLU:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:THR:O	2:B:217:LEU:HB2	1.94	0.65
2:B:251:ASP:H	2:B:254:LYS:HD3	1.60	0.65
1:C:262:TYR:O	1:C:264:ARG:N	2.29	0.65
1:A:260:VAL:HG12	1:A:266:HIS:HB2	1.78	0.65
2:B:406:HIS:CD2	1:C:263:PRO:HG3	2.31	0.65
1:C:49:PHE:HA	1:C:243:ARG:O	1.96	0.65
2:D:325:MET:HG2	2:D:355:VAL:HG21	1.78	0.65
2:D:5:VAL:HG12	2:D:64:ARG:HG2	1.78	0.65
2:D:251:ASP:H	2:D:254:LYS:HD3	1.62	0.65
2:B:224:TYR:CD1	8:B:800:TZT:H20	2.32	0.65
2:B:401:ARG:HH11	2:B:401:ARG:CG	2.02	0.65
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.24	0.65
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.27	0.64
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.61	0.64
1:A:410:GLY:HA2	3:E:64:GLN:NE2	2.11	0.64
1:A:145:THR:HG23	4:A:600:GTP:O2B	1.96	0.64
1:A:203:MET:O	1:A:302:MET:CE	2.45	0.64
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.62	0.64
2:B:139:HIS:HE1	2:B:170:SER:OG	1.80	0.64
2:B:297:ASP:OD2	2:B:299:LYS:HB2	1.97	0.64
1:C:70:LEU:HD13	1:C:145:THR:CB	2.27	0.64
1:A:305:CYS:O	1:A:306:ASP:HB3	1.97	0.64
1:C:315:CYS:SG	1:C:377:MET:HE2	2.37	0.64
1:C:249:ASN:ND2	1:C:250:VAL:O	2.30	0.64
1:A:183:GLU:HB3	1:A:184:PRO:HD2	1.78	0.64
1:C:63:PRO:HD3	1:C:86:LEU:HD12	1.79	0.64
2:B:241:CYS:HB3	2:B:247:GLN:HE21	1.63	0.64
1:C:115:ILE:HD13	1:C:115:ILE:O	1.98	0.64
1:C:249:ASN:ND2	1:C:250:VAL:H	1.96	0.64
1:A:128:GLN:O	1:A:128:GLN:HG3	1.98	0.63
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.80	0.63
1:A:179:THR:O	1:A:180:ALA:CB	2.46	0.63
1:A:262:TYR:O	1:A:264:ARG:N	2.31	0.63
8:B:800:TZT:H12	1:C:325:PRO:HB3	1.80	0.63
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.79	0.63
1:C:425:MET:CE	1:C:425:MET:HA	2.29	0.63
2:B:406:HIS:CG	1:C:263:PRO:HG3	2.34	0.63
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.79	0.63
1:C:99:ALA:HB2	1:C:145:THR:HG22	1.80	0.63
1:C:262:TYR:O	1:C:266:HIS:CD2	2.52	0.62
1:C:273:ALA:CB	1:C:375:VAL:N	2.59	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:CB	1:A:375:VAL:N	2.57	0.62
1:A:323:VAL:CG1	1:A:355:ILE:HD11	2.29	0.62
1:A:398:MET:HG3	2:B:348:PRO:HD3	1.81	0.62
8:B:800:TZT:O9	8:B:800:TZT:C13	2.45	0.62
3:E:68:LEU:O	3:E:72:LEU:HB2	1.99	0.62
1:A:203:MET:O	1:A:302:MET:HE1	2.00	0.62
1:A:72:PRO:O	1:A:74:VAL:N	2.32	0.62
2:B:414:ASP:HB3	2:B:416:MET:HE2	1.80	0.62
1:A:70:LEU:HD13	1:A:145:THR:CB	2.28	0.62
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.14	0.62
2:B:194:LEU:O	2:B:196:GLU:N	2.33	0.62
2:D:164:ARG:HH12	2:D:253:ARG:HH22	1.46	0.62
1:A:291:ILE:HB	1:A:375:VAL:CG2	2.30	0.62
1:C:77:GLU:HA	1:C:80:THR:HB	1.82	0.62
1:A:287:SER:O	1:A:289:ALA:N	2.33	0.62
1:A:348:PRO:O	3:E:25:LYS:O	2.17	0.62
2:B:210:TYR:CD1	2:B:222:PRO:HG2	2.35	0.62
1:C:79:ARG:HD3	1:C:92:LEU:HD12	1.81	0.62
2:D:54:ASN:HD22	2:D:64:ARG:HD2	1.62	0.62
1:A:36:MET:HG2	1:A:61:HIS:CD2	2.34	0.62
2:D:382:THR:HG22	2:D:432:TYR:HD2	1.65	0.62
2:B:192:HIS:C	2:B:192:HIS:HD1	2.03	0.62
2:D:223:THR:CB	2:D:225:GLY:H	2.13	0.62
2:B:185:TYR:CD1	2:B:418:PHE:HE2	2.18	0.62
1:A:266:HIS:O	1:A:268:PRO:HD3	2.00	0.62
2:B:168:THR:HG1	2:B:201:THR:HG1	1.40	0.62
1:C:208:ALA:O	1:C:212:ILE:HD12	2.00	0.61
1:A:208:ALA:O	1:A:212:ILE:HD12	2.01	0.61
1:C:305:CYS:O	1:C:306:ASP:HB3	1.99	0.61
2:D:137:LEU:HD23	2:D:168:THR:HG22	1.82	0.61
2:D:241:CYS:HB3	2:D:247:GLN:NE2	2.14	0.61
1:A:88:HIS:HB2	1:A:91:GLN:NE2	2.15	0.61
2:D:192:HIS:HD1	2:D:192:HIS:C	2.03	0.61
2:B:287:THR:HG22	2:B:290:GLU:H	1.66	0.61
1:C:105:ARG:HH22	2:D:253:ARG:NH2	1.99	0.61
1:A:343:PHE:CD1	1:A:349:THR:HA	2.35	0.61
2:B:42:LEU:O	2:B:44:LEU:N	2.33	0.61
1:C:288:VAL:HG21	1:C:327:ASP:OD2	2.01	0.61
2:B:135:PHE:CD1	2:B:135:PHE:N	2.68	0.60
2:D:216:THR:O	2:D:217:LEU:HB2	2.00	0.60
3:E:84:GLN:O	3:E:88:GLU:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ILE:HB	1:A:375:VAL:HG23	1.83	0.60
2:D:66:ILE:HD11	2:D:121:VAL:HG12	1.82	0.60
1:A:179:THR:O	1:A:180:ALA:HB2	1.99	0.60
2:B:54:ASN:ND2	2:B:64:ARG:HD2	2.16	0.60
1:C:99:ALA:HB3	1:C:145:THR:HG22	1.81	0.60
1:A:64:ARG:NH1	1:A:64:ARG:HG3	2.16	0.60
1:C:246:GLY:O	1:C:248:LEU:N	2.34	0.60
2:D:164:ARG:HA	2:D:164:ARG:HH11	1.65	0.60
1:A:317:LEU:CD2	1:A:377:MET:HE3	2.31	0.60
2:B:5:VAL:HG12	2:B:64:ARG:HG2	1.83	0.60
2:D:9:ALA:HA	2:D:68:VAL:O	2.02	0.60
2:D:4:ILE:HG23	2:D:51:VAL:HG22	1.84	0.60
1:C:203:MET:O	1:C:302:MET:CE	2.50	0.60
2:D:180:THR:HG22	2:D:182:VAL:N	2.07	0.60
1:A:2:ARG:HG2	1:A:2:ARG:O	2.02	0.60
2:B:312:TYR:CD2	2:B:381:SER:HB2	2.37	0.60
8:B:800:TZT:C30	8:B:800:TZT:H25B	2.32	0.60
1:A:180:ALA:O	1:A:182:VAL:N	2.34	0.59
1:A:183:GLU:CB	1:A:184:PRO:HD2	2.32	0.59
2:B:347:ILE:CG2	2:B:350:ASN:HB3	2.26	0.59
1:C:383:ALA:O	1:C:386:GLU:HB2	2.01	0.59
1:C:75:ILE:O	1:C:78:VAL:HB	2.01	0.59
2:B:168:THR:OG1	2:B:201:THR:OG1	2.15	0.59
1:C:171:ILE:CG2	1:C:206:ASN:ND2	2.65	0.59
2:D:143:GLY:H	2:D:186:ASN:HD22	1.51	0.59
2:D:165:ILE:HG23	2:D:253:ARG:NH1	2.17	0.59
1:A:407:TRP:CD2	2:B:257:VAL:HG23	2.37	0.59
1:C:315:CYS:SG	1:C:377:MET:CE	2.90	0.59
2:D:331:GLN:O	2:D:334:ASN:HB3	2.02	0.59
1:A:63:PRO:HD3	1:A:86:LEU:HD12	1.84	0.59
1:A:80:THR:O	1:A:84:ARG:HD2	2.02	0.59
2:B:179:ASP:OD2	8:B:800:TZT:H1	2.02	0.59
1:C:36:MET:HG2	1:C:61:HIS:CD2	2.37	0.59
8:B:800:TZT:H30A	8:B:800:TZT:H25B	1.85	0.59
1:C:266:HIS:O	1:C:268:PRO:HD3	2.03	0.59
1:C:88:HIS:HB2	1:C:91:GLN:NE2	2.17	0.59
1:A:296:PHE:HE2	1:A:377:MET:SD	2.26	0.59
1:A:7:ILE:HG12	1:A:66:VAL:CG2	2.33	0.59
1:C:260:VAL:HG12	1:C:266:HIS:HB2	1.84	0.59
1:A:315:CYS:SG	1:A:377:MET:CE	2.91	0.58
1:C:128:GLN:HG3	1:C:128:GLN:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:VAL:HG13	1:C:251:ASP:H	1.68	0.58
1:C:2:ARG:O	1:C:2:ARG:HG2	2.03	0.58
2:D:192:HIS:O	2:D:195:VAL:HG12	2.03	0.58
1:A:271:THR:CG2	1:A:295:CYS:HA	2.31	0.58
2:D:288:VAL:HA	2:D:291:LEU:HB3	1.86	0.58
2:D:287:THR:O	2:D:288:VAL:HB	2.04	0.58
1:C:173:PRO:HB3	4:C:600:GTP:O3'	2.03	0.58
3:E:84:GLN:C	3:E:86:ALA:H	2.06	0.58
1:A:247:ALA:CB	3:E:19:SER:CB	2.82	0.58
3:E:78:HIS:O	3:E:81:GLU:HB3	2.02	0.58
1:A:256:GLN:HA	1:A:260:VAL:HG22	1.84	0.58
1:C:117:LEU:HD21	1:C:121:ARG:HH21	1.69	0.58
1:C:269:LEU:HD21	1:C:301:GLN:HG2	1.84	0.58
2:D:225:GLY:O	2:D:228:ASN:HB2	2.04	0.58
1:A:288:VAL:HA	1:A:291:ILE:HD11	1.86	0.58
1:A:383:ALA:O	1:A:386:GLU:HB2	2.04	0.58
1:A:341:ILE:H	1:A:341:ILE:HD13	1.69	0.58
2:D:4:ILE:HG12	2:D:4:ILE:O	2.04	0.58
3:E:65:GLU:C	3:E:67:GLU:H	2.07	0.58
1:C:425:MET:HE2	1:C:425:MET:HA	1.85	0.57
3:E:22:VAL:O	3:E:22:VAL:HG13	2.03	0.57
1:A:212:ILE:HG23	1:A:216:ASN:HD22	1.68	0.57
8:B:800:TZT:C8	8:B:800:TZT:H13A	2.34	0.57
2:D:139:HIS:HE1	2:D:170:SER:OG	1.87	0.57
2:D:165:ILE:HG23	2:D:253:ARG:HH11	1.69	0.57
1:A:315:CYS:SG	1:A:377:MET:HE2	2.44	0.57
2:B:210:TYR:CE1	2:B:222:PRO:HG2	2.40	0.57
2:D:180:THR:HG21	2:D:182:VAL:HG22	1.84	0.57
2:B:133:GLN:HE21	2:B:252:LEU:HD22	1.70	0.57
2:B:262:PHE:C	2:B:264:ARG:H	2.07	0.57
2:B:207:GLU:O	2:B:211:ASP:HB2	2.04	0.57
2:D:132:LEU:HD23	2:D:164:ARG:HD2	1.86	0.57
2:D:185:TYR:CD1	2:D:418:PHE:HE2	2.23	0.57
2:B:177:VAL:CG1	2:B:177:VAL:O	2.53	0.57
2:D:11:GLN:CG	2:D:74:THR:HG21	2.34	0.57
2:D:266:HIS:HB3	2:D:380:ASN:HD21	1.68	0.57
2:D:30:ILE:HD11	2:D:49:ILE:HD11	1.86	0.57
2:D:383:ALA:O	2:D:386:GLU:HB2	2.05	0.57
3:E:104:LYS:O	3:E:108:ASN:HB2	2.05	0.57
1:C:344:VAL:O	1:C:346:TRP:N	2.37	0.57
3:E:67:GLU:O	3:E:71:HIS:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:78:HIS:CD2	3:E:78:HIS:C	2.77	0.57
1:C:420:GLU:O	1:C:420:GLU:HG2	2.03	0.57
2:D:273:ALA:HB2	2:D:375:ALA:N	2.20	0.57
1:A:278:ALA:O	1:A:279:GLU:CB	2.52	0.56
2:B:7:ILE:HA	2:B:66:ILE:HG22	1.87	0.56
3:E:67:GLU:O	3:E:69:LEU:N	2.38	0.56
1:A:167:LEU:HD23	1:A:202:PHE:HE1	1.68	0.56
1:C:183:GLU:HB3	1:C:184:PRO:HD2	1.83	0.56
2:B:287:THR:HG22	2:B:290:GLU:CB	2.25	0.56
1:C:101:ASN:HD22	2:D:254:LYS:CG	2.14	0.56
2:D:194:LEU:C	2:D:196:GLU:H	2.08	0.56
2:B:266:HIS:HB3	2:B:380:ASN:HD21	1.70	0.56
1:C:229:ARG:HG2	1:C:229:ARG:HH11	1.70	0.56
1:A:101:ASN:ND2	2:B:254:LYS:HG2	2.20	0.56
1:A:430:LYS:O	1:A:434:GLU:N	2.39	0.56
2:D:145:THR:HG23	6:D:600:GDP:PB	2.46	0.56
1:A:270:ALA:O	1:A:302:MET:CB	2.54	0.56
1:A:420:GLU:HG2	1:A:420:GLU:O	2.05	0.56
2:B:238:VAL:HG13	2:B:378:ILE:HD11	1.88	0.56
8:B:800:TZT:H21A	8:B:800:TZT:O16	2.06	0.56
1:C:262:TYR:O	1:C:266:HIS:HD2	1.89	0.56
2:D:42:LEU:O	2:D:44:LEU:N	2.38	0.56
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.54	0.56
2:D:30:ILE:HG23	2:D:34:GLY:O	2.05	0.56
2:B:13:GLY:O	2:B:16:ILE:HG22	2.06	0.56
1:C:118:VAL:HG21	1:C:149:PHE:CZ	2.41	0.56
1:C:203:MET:HE1	1:C:303:VAL:HG11	1.87	0.56
1:A:420:GLU:HA	1:A:423:GLU:CG	2.36	0.56
2:B:6:HIS:HE1	2:B:8:GLN:HG3	1.71	0.55
1:C:181:VAL:HG11	1:C:404:PHE:CZ	2.41	0.55
1:A:278:ALA:C	1:A:280:LYS:H	2.09	0.55
2:B:55:GLU:HB3	2:B:61:TYR:CD2	2.41	0.55
2:D:3:GLU:O	2:D:133:GLN:HB3	2.06	0.55
2:D:48:ARG:NH1	2:D:245:PRO:HD2	2.21	0.55
1:A:115:ILE:C	1:A:115:ILE:HD13	2.26	0.55
2:B:100:GLY:O	2:B:101:ASN:HB2	2.05	0.55
2:B:9:ALA:HA	2:B:68:VAL:O	2.07	0.55
1:C:310:GLY:HA3	1:C:383:ALA:HB2	1.88	0.55
1:C:309:HIS:ND1	1:C:386:GLU:OE1	2.37	0.55
2:D:135:PHE:CD1	2:D:135:PHE:N	2.74	0.55
1:A:273:ALA:HB3	1:A:374:ALA:HB1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LYS:HG3	2:B:348:PRO:HB3	1.89	0.55
2:B:20:PHE:CD2	2:B:235:MET:HG2	2.42	0.55
1:C:88:HIS:O	1:C:91:GLN:HG2	2.06	0.55
2:D:59:ASN:O	2:D:60:LYS:O	2.24	0.55
1:A:229:ARG:HH11	1:A:229:ARG:HG2	1.72	0.55
1:A:256:GLN:HA	1:A:260:VAL:CG2	2.37	0.55
1:A:265:ILE:O	1:A:266:HIS:O	2.25	0.55
2:B:273:ALA:CB	2:B:375:ALA:N	2.66	0.55
1:A:328:VAL:HG11	3:E:20:PHE:HZ	1.71	0.55
1:A:435:VAL:HG12	1:A:435:VAL:O	2.06	0.55
2:B:59:ASN:O	2:B:60:LYS:O	2.25	0.54
2:B:6:HIS:HD2	2:B:136:GLN:HG3	1.73	0.54
1:A:297:GLU:HB3	1:A:300:ASN:HB2	1.89	0.54
2:B:386:GLU:O	2:B:390:ARG:HG2	2.07	0.54
1:C:288:VAL:HA	1:C:291:ILE:HD11	1.89	0.54
1:C:270:ALA:O	1:C:302:MET:HB3	2.08	0.54
2:D:19:LYS:O	2:D:232:SER:HB2	2.07	0.54
1:A:99:ALA:HB3	1:A:145:THR:HG22	1.90	0.54
1:A:180:ALA:O	1:A:181:VAL:C	2.45	0.54
1:A:271:THR:HG21	1:A:295:CYS:CA	2.34	0.54
2:B:133:GLN:NE2	2:B:252:LEU:HD22	2.22	0.54
2:B:3:GLU:O	2:B:133:GLN:HB3	2.08	0.54
2:B:19:LYS:O	2:B:23:VAL:HG23	2.08	0.54
1:A:270:ALA:O	1:A:302:MET:HB3	2.07	0.54
2:D:264:ARG:O	2:D:266:HIS:CD2	2.61	0.54
3:E:50:ILE:HA	3:E:52:LYS:H	1.73	0.54
1:A:177:VAL:HG11	1:A:227:LEU:HD21	1.89	0.54
1:A:173:PRO:HB2	1:A:179:THR:HG22	1.89	0.54
1:A:86:LEU:HB3	1:A:87:PHE:CD2	2.43	0.54
1:A:323:VAL:CG1	1:A:324:VAL:N	2.71	0.54
2:D:118:VAL:O	2:D:122:VAL:HG13	2.07	0.54
2:D:66:ILE:HD11	2:D:121:VAL:CG1	2.38	0.54
2:B:155:SER:O	3:E:76:ARG:NH2	2.37	0.53
1:C:185:TYR:CD2	1:C:418:PHE:HE2	2.26	0.53
2:B:241:CYS:HB3	2:B:247:GLN:NE2	2.23	0.53
1:C:271:THR:HB	1:C:377:MET:HG2	1.89	0.53
1:A:181:VAL:HG23	2:B:258:ASN:ND2	2.23	0.53
1:A:233:GLN:HE22	1:A:362:VAL:HG12	1.73	0.53
1:C:168:GLU:HG2	1:C:201:ALA:HB2	1.89	0.53
1:A:287:SER:O	1:A:290:GLU:N	2.40	0.53
2:B:132:LEU:HG	2:B:133:GLN:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:THR:O	1:C:180:ALA:HB2	2.08	0.53
1:C:252:LEU:HA	1:C:255:PHE:HB2	1.90	0.53
1:C:407:TRP:CD2	2:D:257:VAL:HG23	2.44	0.53
1:C:239:THR:O	1:C:240:ALA:C	2.47	0.53
2:D:401:ARG:O	2:D:402:LYS:C	2.44	0.53
1:A:328:VAL:HG12	1:A:329:ASN:N	2.22	0.53
1:A:407:TRP:CG	2:B:257:VAL:HG23	2.44	0.53
2:B:148:GLY:O	2:B:151:THR:OG1	2.26	0.53
2:B:8:GLN:OE1	2:B:67:LEU:CD2	2.52	0.53
1:C:403:ALA:HB1	1:C:404:PHE:HD1	1.74	0.53
1:A:312:TYR:HE2	1:A:379:SER:CB	2.22	0.53
2:B:225:GLY:O	2:B:228:ASN:N	2.42	0.53
2:B:30:ILE:HD11	2:B:49:ILE:HD11	1.90	0.53
2:D:132:LEU:HG	2:D:133:GLN:N	2.17	0.53
1:A:253:THR:O	1:A:256:GLN:HG2	2.09	0.53
1:A:327:ASP:C	1:A:329:ASN:N	2.59	0.53
1:A:401:LYS:C	1:A:403:ALA:H	2.13	0.53
1:C:315:CYS:HB3	1:C:351:PHE:HD2	1.73	0.53
1:C:7:ILE:HG12	1:C:66:VAL:CG2	2.38	0.53
2:D:148:GLY:O	2:D:151:THR:OG1	2.27	0.53
2:D:174:SER:HB2	2:D:207:GLU:HB2	1.91	0.53
2:B:185:TYR:CD1	2:B:418:PHE:CE2	2.97	0.52
2:B:146:GLY:N	6:B:600:GDP:O1B	2.37	0.52
2:D:3:GLU:HG2	2:D:64:ARG:NH2	2.24	0.52
2:B:4:ILE:H	2:B:64:ARG:HH21	1.57	0.52
2:B:179:ASP:CG	8:B:800:TZT:H1	2.29	0.52
2:D:269:MET:HB3	2:D:384:ILE:HD11	1.90	0.52
3:E:60:ARG:HH11	3:E:60:ARG:HB2	1.74	0.52
1:A:327:ASP:O	1:A:328:VAL:C	2.46	0.52
8:B:800:TZT:N10	8:B:800:TZT:H6	2.19	0.52
2:D:17:GLY:HA2	2:D:20:PHE:HB3	1.90	0.52
2:D:180:THR:HG22	2:D:181:VAL:H	1.73	0.52
2:D:287:THR:CG2	2:D:290:GLU:H	2.22	0.52
2:B:251:ASP:H	2:B:254:LYS:HB2	1.73	0.52
2:B:264:ARG:HB2	2:B:266:HIS:NE2	2.24	0.52
1:C:312:TYR:HE2	1:C:379:SER:CB	2.22	0.52
1:A:269:LEU:HD21	1:A:301:GLN:HG2	1.89	0.52
1:A:70:LEU:HD22	1:A:110:ILE:HG23	1.90	0.52
2:B:209:LEU:HD21	2:B:231:VAL:HG22	1.91	0.52
2:B:40:SER:HB2	2:B:43:GLN:NE2	2.25	0.52
2:B:158:ARG:HA	2:B:161:TYR:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:179:ASP:N	2:D:179:ASP:OD1	2.42	0.52
1:A:241:SER:HB2	1:A:249:ASN:O	2.10	0.52
2:B:145:THR:HG23	6:B:600:GDP:PB	2.49	0.52
1:C:407:TRP:CG	2:D:257:VAL:HG23	2.44	0.52
1:C:90:GLU:O	1:C:121:ARG:CD	2.58	0.52
2:D:391:ILE:C	2:D:393:GLU:H	2.13	0.52
2:D:397:ALA:HA	2:D:400:ARG:HE	1.75	0.52
2:B:165:ILE:HD11	2:B:252:LEU:HG	1.92	0.52
2:B:200:GLU:HB3	2:B:268:PHE:CE1	2.44	0.52
2:B:414:ASP:HB3	2:B:416:MET:CE	2.40	0.52
2:B:55:GLU:HB3	2:B:61:TYR:HD2	1.74	0.52
1:C:188:ILE:HG23	1:C:425:MET:HG3	1.91	0.52
1:A:410:GLY:HA2	3:E:64:GLN:HE22	1.75	0.51
2:B:245:PRO:HB2	2:B:247:GLN:CG	2.34	0.51
1:C:238:ILE:CG2	1:C:252:LEU:HD21	2.40	0.51
1:A:310:GLY:HA3	1:A:383:ALA:HB2	1.92	0.51
1:A:402:ARG:O	1:A:403:ALA:C	2.48	0.51
1:A:47:ASP:O	1:A:49:PHE:N	2.43	0.51
1:A:79:ARG:HD3	1:A:92:LEU:HD12	1.92	0.51
2:B:253:ARG:O	2:B:257:VAL:HG12	2.10	0.51
1:C:182:VAL:HG23	1:C:408:TYR:OH	2.11	0.51
1:C:296:PHE:CE2	1:C:377:MET:SD	3.04	0.51
1:C:86:LEU:HB3	1:C:87:PHE:CD2	2.45	0.51
1:A:61:HIS:O	1:A:62:VAL:O	2.28	0.51
1:C:430:LYS:O	1:C:434:GLU:N	2.43	0.51
2:D:100:GLY:O	2:D:101:ASN:HB2	2.11	0.51
2:B:350:ASN:N	2:B:350:ASN:ND2	2.45	0.51
1:C:115:ILE:HD13	1:C:115:ILE:C	2.30	0.51
1:C:54:SER:O	1:C:56:THR:N	2.36	0.51
2:D:238:VAL:HG13	2:D:378:ILE:HD11	1.92	0.51
1:A:223:THR:N	1:A:226:ASN:HB2	2.26	0.51
1:C:171:ILE:HG23	1:C:206:ASN:ND2	2.25	0.51
2:D:292:THR:HA	2:D:295:MET:HE3	1.93	0.51
2:B:401:ARG:O	1:C:262:TYR:OH	2.28	0.51
2:B:111:GLY:O	2:B:112:ALA:C	2.48	0.51
1:A:78:VAL:C	1:A:80:THR:H	2.14	0.51
1:C:70:LEU:N	1:C:70:LEU:HD12	2.26	0.51
2:D:192:HIS:C	2:D:192:HIS:ND1	2.64	0.51
1:A:205:ASP:OD2	1:A:304:LYS:HB2	2.11	0.51
2:B:181:VAL:H	1:C:258:ASN:ND2	2.08	0.51
2:B:194:LEU:C	2:B:196:GLU:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:ILE:C	2:B:393:GLU:H	2.15	0.51
1:C:78:VAL:C	1:C:80:THR:H	2.15	0.51
2:D:207:GLU:O	2:D:211:ASP:HB2	2.09	0.51
1:C:2:ARG:O	1:C:2:ARG:CG	2.59	0.50
2:B:133:GLN:HE21	2:B:252:LEU:CD2	2.23	0.50
2:B:142:GLY:HA2	2:B:186:ASN:HB2	1.93	0.50
2:B:30:ILE:HG23	2:B:34:GLY:O	2.11	0.50
2:D:210:TYR:CD1	2:D:222:PRO:HG2	2.46	0.50
2:B:192:HIS:ND1	2:B:192:HIS:C	2.64	0.50
2:D:211:ASP:HB3	2:D:215:ARG:NH1	2.27	0.50
1:C:100:ALA:CB	2:D:253:ARG:HG2	2.41	0.50
3:E:65:GLU:O	3:E:69:LEU:HB2	2.11	0.50
2:B:70:LEU:HD12	2:B:145:THR:HB	1.93	0.50
2:B:267:PHE:CD1	2:B:267:PHE:N	2.79	0.50
2:D:247:GLN:HG3	2:D:248:LEU:HG	1.92	0.50
1:A:83:TYR:C	1:A:85:GLN:N	2.64	0.50
2:B:212:ILE:HD12	2:B:215:ARG:NH2	2.26	0.50
2:B:66:ILE:HD11	2:B:121:VAL:HG12	1.92	0.50
2:B:262:PHE:C	2:B:264:ARG:N	2.65	0.50
2:B:273:ALA:HB1	2:B:274:PRO:CD	2.30	0.50
8:B:800:TZT:H78A	8:B:800:TZT:H12	1.93	0.50
1:C:203:MET:O	1:C:302:MET:HE1	2.10	0.50
1:A:239:THR:O	1:A:240:ALA:C	2.50	0.50
2:B:99:ALA:CB	2:B:145:THR:HG22	2.35	0.50
2:B:54:ASN:N	2:B:64:ARG:HH11	2.10	0.50
7:B:700:LOC:C6	7:B:700:LOC:H4B	2.41	0.50
1:C:223:THR:N	1:C:226:ASN:HB2	2.27	0.50
2:D:133:GLN:HE21	2:D:252:LEU:CD2	2.23	0.50
1:A:68:VAL:HG11	1:A:118:VAL:CG2	2.42	0.50
1:C:111:GLY:O	1:C:113:GLU:N	2.44	0.50
1:C:72:PRO:O	1:C:74:VAL:N	2.44	0.50
3:E:119:MET:HG3	3:E:119:MET:O	2.12	0.50
1:A:133:GLN:NE2	1:A:252:LEU:HG	2.27	0.50
1:C:180:ALA:HB1	2:D:258:ASN:HD21	1.77	0.50
1:C:205:ASP:OD2	1:C:304:LYS:HB2	2.12	0.50
1:C:325:PRO:HA	1:C:328:VAL:HB	1.93	0.50
1:C:377:MET:HG3	1:C:377:MET:O	2.11	0.50
2:D:124:LYS:O	2:D:128:SER:HB2	2.12	0.50
1:A:70:LEU:CD1	1:A:145:THR:HB	2.35	0.49
1:C:241:SER:CA	1:C:250:VAL:HG22	2.37	0.49
1:A:33:ASP:HA	1:A:85:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TRP:HD1	2:B:147:SER:OG	1.95	0.49
2:B:193:GLN:HA	2:B:193:GLN:HE21	1.77	0.49
2:B:288:VAL:HA	2:B:291:LEU:HB3	1.93	0.49
2:B:383:ALA:O	2:B:386:GLU:HB2	2.12	0.49
1:C:183:GLU:CB	1:C:184:PRO:HD2	2.38	0.49
2:B:179:ASP:OD2	2:B:179:ASP:N	2.44	0.49
1:C:102:ASN:ND2	1:C:104:ALA:HB3	2.23	0.49
2:D:180:THR:CG2	2:D:181:VAL:N	2.74	0.49
1:A:323:VAL:HG12	1:A:324:VAL:N	2.27	0.49
1:A:75:ILE:O	1:A:78:VAL:HB	2.12	0.49
2:B:227:LEU:HD23	2:B:228:ASN:N	2.27	0.49
1:C:422:ARG:HH12	1:C:426:ALA:HB2	1.77	0.49
2:D:267:PHE:N	2:D:267:PHE:CD1	2.80	0.49
2:B:152:LEU:O	2:B:156:LYS:N	2.45	0.49
2:B:132:LEU:HD23	2:B:164:ARG:HD2	1.94	0.49
2:D:242:LEU:HD21	2:D:252:LEU:HB2	1.94	0.49
2:D:264:ARG:O	2:D:266:HIS:N	2.46	0.49
2:D:265:LEU:O	2:D:266:HIS:O	2.30	0.49
1:A:68:VAL:HG11	1:A:118:VAL:HG22	1.93	0.49
2:B:54:ASN:HD22	2:B:64:ARG:HD2	1.76	0.49
1:C:315:CYS:HB3	1:C:351:PHE:CE2	2.47	0.49
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.77	0.49
1:C:68:VAL:HG11	1:C:118:VAL:HG22	1.94	0.49
1:A:67:PHE:HB3	1:A:75:ILE:CD1	2.43	0.49
2:D:226:ASP:N	2:D:226:ASP:OD1	2.46	0.49
4:C:600:GTP:O3G	2:D:254:LYS:NZ	2.46	0.49
2:D:350:ASN:ND2	2:D:350:ASN:N	2.46	0.49
2:B:70:LEU:CA	2:B:95:GLY:HA3	2.39	0.49
1:C:154:MET:HA	1:C:157:LEU:HD12	1.95	0.49
1:C:179:THR:O	1:C:180:ALA:CB	2.61	0.49
2:D:8:GLN:HB3	2:D:14:ASN:OD1	2.12	0.49
2:D:242:LEU:HD11	2:D:252:LEU:HD13	1.93	0.49
3:E:76:ARG:O	3:E:79:GLU:N	2.41	0.49
2:B:251:ASP:O	2:B:252:LEU:HB3	2.13	0.49
1:C:195:LEU:HD12	1:C:265:ILE:CG2	2.43	0.49
1:C:167:LEU:HD23	1:C:202:PHE:HE1	1.78	0.49
1:C:49:PHE:N	1:C:243:ARG:O	2.45	0.49
1:A:101:ASN:HD22	2:B:254:LYS:HG2	1.78	0.49
2:D:273:ALA:HB2	2:D:375:ALA:O	2.13	0.49
1:A:181:VAL:HG11	1:A:404:PHE:CZ	2.48	0.48
1:A:403:ALA:HB1	1:A:404:PHE:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:PHE:HB3	2:B:425:MET:HE1	1.95	0.48
1:C:233:GLN:HE22	1:C:362:VAL:HG12	1.78	0.48
1:C:376:CYS:SG	1:C:376:CYS:O	2.71	0.48
1:C:33:ASP:HA	1:C:85:GLN:HB2	1.94	0.48
2:D:251:ASP:O	2:D:252:LEU:HB3	2.13	0.48
1:A:182:VAL:O	1:A:185:TYR:HB2	2.13	0.48
1:A:280:LYS:O	1:A:281:ALA:C	2.51	0.48
2:B:180:THR:C	2:B:182:VAL:H	2.16	0.48
1:C:270:ALA:HB3	1:C:302:MET:SD	2.53	0.48
2:D:142:GLY:HA3	2:D:173:PRO:HG3	1.96	0.48
2:D:200:GLU:HB3	2:D:268:PHE:CE1	2.48	0.48
2:D:336:GLN:OE1	2:D:351:VAL:CG1	2.59	0.48
1:C:10:GLY:O	1:C:12:ALA:N	2.46	0.48
1:C:191:THR:O	1:C:195:LEU:HB2	2.13	0.48
1:C:368:LEU:N	1:C:368:LEU:HD12	2.21	0.48
2:B:165:ILE:HG23	2:B:253:ARG:NH1	2.28	0.48
2:B:205:ASP:OD2	2:B:304:ALA:HB3	2.13	0.48
2:B:96:GLN:HE21	1:C:2:ARG:HH12	1.59	0.48
1:C:190:THR:HG23	1:C:191:THR:N	2.27	0.48
1:C:255:PHE:HE1	1:C:352:LYS:HB3	1.77	0.48
2:B:404:PHE:CE2	1:C:261:PRO:HA	2.47	0.48
3:E:27:PRO:O	3:E:28:SER:CB	2.56	0.48
1:A:174:ALA:HB1	1:A:207:GLU:HB2	1.94	0.48
1:A:264:ARG:O	1:A:266:HIS:CD2	2.66	0.48
2:B:255:LEU:O	2:B:256:ALA:C	2.49	0.48
2:B:136:GLN:HA	2:B:167:ASN:O	2.13	0.48
1:C:180:ALA:HB1	2:D:258:ASN:ND2	2.29	0.48
1:C:343:PHE:CD1	1:C:349:THR:HG22	2.48	0.48
2:D:251:ASP:C	2:D:253:ARG:H	2.16	0.48
1:C:168:GLU:HG2	1:C:201:ALA:CB	2.43	0.48
1:C:212:ILE:HG23	1:C:216:ASN:HD22	1.77	0.48
2:D:48:ARG:O	2:D:51:VAL:N	2.40	0.48
2:D:6:HIS:CE1	2:D:8:GLN:HG3	2.49	0.48
1:A:248:LEU:HD22	1:A:249:ASN:N	2.29	0.48
1:A:203:MET:O	1:A:302:MET:HE3	2.14	0.48
1:A:276:ILE:HD11	1:A:280:LYS:NZ	2.28	0.48
2:B:126:SER:C	2:B:128:SER:H	2.17	0.48
2:B:251:ASP:HB3	2:B:254:LYS:H	1.79	0.48
2:B:251:ASP:C	2:B:253:ARG:H	2.18	0.48
1:C:249:ASN:ND2	1:C:250:VAL:N	2.62	0.48
1:C:278:ALA:O	1:C:279:GLU:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:28:SER:O	3:E:29:PHE:CB	2.62	0.48
1:A:2:ARG:CG	1:A:2:ARG:O	2.62	0.48
2:B:66:ILE:HD11	2:B:121:VAL:CG1	2.44	0.48
8:B:800:TZT:C12	1:C:325:PRO:HB3	2.44	0.48
1:C:61:HIS:O	1:C:62:VAL:O	2.31	0.48
2:B:15:GLN:NE2	8:B:800:TZT:H43	2.29	0.47
2:B:177:VAL:HG22	8:B:800:TZT:H21B	1.96	0.47
1:C:203:MET:O	1:C:302:MET:HE3	2.12	0.47
2:D:111:GLY:O	2:D:112:ALA:C	2.51	0.47
2:D:2:ARG:HD2	2:D:131:CYS:SG	2.54	0.47
2:D:8:GLN:OE1	2:D:67:LEU:CD2	2.60	0.47
2:B:7:ILE:O	2:B:137:LEU:HA	2.15	0.47
1:C:100:ALA:O	1:C:102:ASN:N	2.46	0.47
1:C:111:GLY:O	1:C:112:LYS:C	2.52	0.47
3:E:67:GLU:C	3:E:69:LEU:H	2.17	0.47
1:A:368:LEU:H	1:A:368:LEU:CD1	2.14	0.47
1:A:317:LEU:HD21	1:A:377:MET:HE3	1.95	0.47
2:D:4:ILE:HD11	2:D:136:GLN:HG2	1.97	0.47
2:D:339:ASN:HD22	2:D:339:ASN:HA	1.58	0.47
2:D:99:ALA:CB	2:D:145:THR:HG22	2.30	0.47
1:A:425:MET:HE2	1:A:425:MET:HA	1.96	0.47
2:D:185:TYR:CD1	2:D:418:PHE:CE2	3.02	0.47
1:A:317:LEU:HD23	1:A:377:MET:HE3	1.97	0.47
2:B:292:THR:HA	2:B:295:MET:HE3	1.97	0.47
2:D:81:GLY:O	2:D:82:PRO:O	2.33	0.47
1:A:325:PRO:HD3	1:A:355:ILE:HD12	1.97	0.47
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.95	0.47
2:B:287:THR:CG2	2:B:290:GLU:HB2	2.27	0.47
2:B:67:LEU:HD13	2:B:92:PHE:HE2	1.80	0.47
1:C:317:LEU:CD2	1:C:377:MET:HE3	2.45	0.47
2:D:158:ARG:O	2:D:159:GLU:CB	2.45	0.47
1:A:246:GLY:HA2	3:E:14:CYS:SG	2.54	0.47
1:A:270:ALA:H	1:A:302:MET:HE2	1.78	0.47
2:B:17:GLY:HA2	2:B:20:PHE:HB3	1.97	0.47
2:B:244:PHE:H	2:B:245:PRO:CD	2.28	0.47
1:C:70:LEU:CD2	1:C:110:ILE:HG23	2.45	0.47
1:C:14:VAL:HG21	1:C:75:ILE:HD11	1.96	0.47
1:C:270:ALA:H	1:C:302:MET:HE2	1.79	0.47
1:C:30:ILE:HA	1:C:36:MET:HB3	1.96	0.47
1:A:217:LEU:O	1:A:218:ASP:CB	2.63	0.47
1:A:77:GLU:HA	1:A:80:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:O	2:B:159:GLU:CB	2.50	0.47
2:B:294:GLN:CD	2:B:300:ASN:HD21	2.17	0.47
2:B:42:LEU:O	2:B:43:GLN:C	2.53	0.47
7:B:700:LOC:H6A	7:B:700:LOC:C4	2.45	0.47
1:C:312:TYR:HE2	1:C:379:SER:HB2	1.78	0.47
2:D:264:ARG:HB2	2:D:266:HIS:NE2	2.29	0.47
2:D:287:THR:HG22	2:D:290:GLU:H	1.79	0.47
2:B:54:ASN:HB2	2:B:64:ARG:HD3	1.96	0.47
1:C:118:VAL:HG21	1:C:149:PHE:HZ	1.79	0.47
1:C:286:LEU:HD12	1:C:286:LEU:N	2.30	0.47
2:D:13:GLY:O	2:D:16:ILE:HG22	2.15	0.47
2:D:200:GLU:OE2	2:D:255:LEU:HD12	2.15	0.47
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.63	0.47
1:C:250:VAL:CG1	1:C:251:ASP:H	2.26	0.47
1:C:67:PHE:HB3	1:C:75:ILE:HD12	1.96	0.47
2:D:6:HIS:HD2	2:D:136:GLN:HG3	1.80	0.47
1:A:112:LYS:HE3	3:E:58:GLU:HG3	1.97	0.46
1:A:315:CYS:SG	1:A:377:MET:HE1	2.55	0.46
2:B:217:LEU:HD23	2:B:217:LEU:O	2.15	0.46
1:A:368:LEU:N	1:A:368:LEU:HD12	2.19	0.46
1:C:402:ARG:O	1:C:405:VAL:N	2.48	0.46
2:D:4:ILE:CG2	2:D:51:VAL:HG22	2.44	0.46
1:A:190:THR:HG23	1:A:191:THR:N	2.30	0.46
1:C:180:ALA:O	1:C:181:VAL:C	2.53	0.46
2:D:16:ILE:HD11	2:D:231:VAL:HG11	1.97	0.46
2:B:179:ASP:HB2	2:B:180:THR:H	1.55	0.46
2:B:215:ARG:HH21	2:B:299:LYS:HA	1.81	0.46
1:C:404:PHE:O	1:C:406:HIS:N	2.48	0.46
2:D:194:LEU:C	2:D:196:GLU:N	2.68	0.46
2:D:212:ILE:HD12	2:D:215:ARG:NH2	2.30	0.46
2:D:386:GLU:O	2:D:390:ARG:HG2	2.15	0.46
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.51	0.46
1:C:236:SER:HA	1:C:243:ARG:HH12	1.79	0.46
1:C:419:SER:O	1:C:423:GLU:HG2	2.16	0.46
2:D:297:ASP:OD2	2:D:299:LYS:HB2	2.15	0.46
1:A:411:GLU:O	3:E:61:ARG:NH1	2.47	0.46
1:A:292:THR:O	1:A:295:CYS:HB2	2.15	0.46
2:B:276:THR:CG2	2:B:277:SER:N	2.75	0.46
2:B:240:THR:O	2:B:244:PHE:HB2	2.15	0.46
2:B:260:VAL:HA	2:B:261:PRO:HD2	1.68	0.46
2:B:62:VAL:HA	2:B:63:PRO:HD2	1.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:PRO:HA	2:B:83:PHE:CD2	2.50	0.46
2:D:255:LEU:O	2:D:256:ALA:C	2.54	0.46
2:D:67:LEU:HD13	2:D:92:PHE:HE2	1.80	0.46
1:A:112:LYS:NZ	3:E:58:GLU:OE1	2.48	0.46
1:A:185:TYR:CD2	1:A:418:PHE:HE2	2.34	0.46
2:D:142:GLY:N	2:D:173:PRO:HG3	2.30	0.46
2:D:244:PHE:H	2:D:245:PRO:HD3	1.81	0.46
2:D:347:ILE:HA	2:D:348:PRO:HD3	1.82	0.46
2:D:99:ALA:HB1	2:D:145:THR:CG2	2.33	0.46
1:A:16:ILE:HG22	1:A:17:GLY:N	2.30	0.46
2:B:183:GLU:O	2:B:184:PRO:C	2.55	0.46
1:C:102:ASN:HA	1:C:186:ASN:HD21	1.81	0.46
2:D:251:ASP:C	2:D:253:ARG:N	2.70	0.46
2:D:75:MET:HE3	2:D:94:PHE:CD2	2.51	0.46
1:A:242:LEU:HD23	1:A:249:ASN:O	2.16	0.46
2:B:256:ALA:O	2:B:260:VAL:HG22	2.16	0.46
3:E:19:SER:O	3:E:20:PHE:HB3	2.16	0.46
2:B:357:ASP:OD2	2:B:357:ASP:N	2.49	0.45
2:B:35:SER:OG	2:B:36:TYR:N	2.48	0.45
2:B:11:GLN:CG	2:B:74:THR:HG21	2.46	0.45
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.98	0.45
3:E:112:ARG:CA	3:E:115:HIS:HB3	2.41	0.45
1:A:100:ALA:O	1:A:102:ASN:N	2.49	0.45
1:A:248:LEU:HA	1:A:254:GLU:OE1	2.16	0.45
1:A:309:HIS:CE1	1:A:386:GLU:OE1	2.68	0.45
1:A:375:VAL:HG12	1:A:376:CYS:H	1.82	0.45
2:B:382:THR:HG22	2:B:432:TYR:HD2	1.81	0.45
2:D:400:ARG:O	2:D:400:ARG:CG	2.51	0.45
1:A:169:PHE:CE2	1:A:235:VAL:HG22	2.52	0.45
2:B:122:VAL:HG23	2:B:123:ARG:N	2.30	0.45
2:B:142:GLY:HA3	2:B:183:GLU:HB3	1.99	0.45
2:D:21:TRP:O	2:D:25:SER:HB2	2.16	0.45
1:A:349:THR:O	1:A:350:GLY:O	2.35	0.45
1:A:30:ILE:HA	1:A:36:MET:HB3	1.99	0.45
2:B:223:THR:OG1	2:B:226:ASP:OD1	2.23	0.45
2:B:71:GLU:O	2:B:71:GLU:HG2	2.14	0.45
1:C:249:ASN:CG	1:C:250:VAL:N	2.68	0.45
1:C:255:PHE:CD1	1:C:316:CYS:SG	3.10	0.45
1:A:181:VAL:HG23	2:B:258:ASN:HD22	1.80	0.45
2:B:227:LEU:HD23	2:B:228:ASN:H	1.81	0.45
2:D:158:ARG:HA	2:D:161:TYR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:TYR:HE2	1:A:379:SER:HB2	1.81	0.45
2:B:114:LEU:O	2:B:116:ASP:N	2.50	0.45
1:C:398:MET:HG3	2:D:348:PRO:HD3	1.99	0.45
1:A:117:LEU:HD21	1:A:121:ARG:HH21	1.81	0.45
1:A:201:ALA:O	1:A:268:PRO:HD2	2.17	0.45
1:A:82:THR:O	1:A:83:TYR:CG	2.70	0.45
2:B:164:ARG:HA	2:B:164:ARG:HH11	1.81	0.45
2:B:212:ILE:CD1	2:B:215:ARG:NH2	2.79	0.45
2:B:21:TRP:O	2:B:25:SER:HB2	2.16	0.45
2:B:265:LEU:O	2:B:265:LEU:CD1	2.58	0.45
1:C:107:HIS:CE1	1:C:155:GLU:OE2	2.70	0.45
1:C:240:ALA:O	1:C:241:SER:C	2.54	0.45
1:C:265:ILE:O	1:C:266:HIS:O	2.35	0.45
1:C:68:VAL:HG11	1:C:118:VAL:CG2	2.46	0.45
2:D:251:ASP:H	2:D:254:LYS:HB2	1.81	0.45
1:A:422:ARG:HH12	1:A:426:ALA:HB2	1.81	0.45
1:A:88:HIS:O	1:A:91:GLN:HG2	2.15	0.45
2:B:93:VAL:HG12	2:B:114:LEU:HD11	1.99	0.45
3:E:83:ILE:O	3:E:86:ALA:HB3	2.16	0.45
1:A:320:ARG:O	1:A:373:ARG:HA	2.17	0.45
2:B:143:GLY:H	2:B:186:ASN:HD22	1.65	0.45
2:B:242:LEU:HD21	2:B:252:LEU:HB2	1.99	0.45
2:B:339:ASN:HD22	2:B:339:ASN:HA	1.59	0.45
2:D:32:PRO:HA	2:D:83:PHE:CD2	2.52	0.45
1:A:270:ALA:O	1:A:302:MET:HB2	2.16	0.45
2:B:124:LYS:O	2:B:128:SER:HB2	2.17	0.45
2:B:8:GLN:HB3	2:B:14:ASN:OD1	2.16	0.45
2:B:179:ASP:O	2:B:180:THR:CB	2.64	0.45
1:C:173:PRO:HB2	1:C:179:THR:HG22	1.97	0.45
1:C:209:ILE:HG22	1:C:227:LEU:HG	1.99	0.45
1:C:198:SER:HB3	1:C:265:ILE:HD12	1.99	0.45
1:C:67:PHE:HB3	1:C:75:ILE:CD1	2.47	0.45
1:C:80:THR:O	1:C:84:ARG:HD2	2.16	0.45
2:B:244:PHE:H	2:B:245:PRO:HD3	1.81	0.44
2:B:224:TYR:OH	6:B:600:GDP:H2'	2.16	0.44
8:B:800:TZT:HN10	8:B:800:TZT:C6	2.26	0.44
2:B:82:PRO:HB2	2:B:83:PHE:H	1.60	0.44
1:C:241:SER:O	1:C:250:VAL:HG22	2.17	0.44
1:A:188:ILE:HG23	1:A:425:MET:HG3	2.00	0.44
1:C:198:SER:O	1:C:265:ILE:HB	2.16	0.44
2:D:225:GLY:O	2:D:228:ASN:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:388:PHE:HB3	2:D:425:MET:HE1	1.99	0.44
3:E:25:LYS:HA	3:E:26:PRO:HD2	1.82	0.44
3:E:76:ARG:HA	3:E:76:ARG:HD3	1.74	0.44
1:A:154:MET:HA	1:A:157:LEU:HD12	1.99	0.44
1:A:306:ASP:O	1:A:309:HIS:HB3	2.18	0.44
1:A:68:VAL:HA	1:A:93:ILE:O	2.16	0.44
2:B:147:SER:O	2:B:151:THR:HG23	2.17	0.44
2:B:223:THR:HB	2:B:225:GLY:N	2.31	0.44
2:D:40:SER:HB2	2:D:43:GLN:NE2	2.32	0.44
2:B:16:ILE:HG21	2:B:138:THR:HB	1.98	0.44
8:B:800:TZT:N10	8:B:800:TZT:C6	2.79	0.44
2:D:183:GLU:O	2:D:184:PRO:C	2.55	0.44
2:D:265:LEU:O	2:D:266:HIS:C	2.56	0.44
2:D:274:PRO:HB3	2:D:286:LEU:HD21	1.99	0.44
3:E:67:GLU:C	3:E:69:LEU:N	2.71	0.44
1:A:278:ALA:C	1:A:280:LYS:N	2.71	0.44
1:A:405:VAL:CG1	1:A:406:HIS:N	2.81	0.44
1:C:105:ARG:NH2	2:D:253:ARG:NE	2.62	0.44
2:D:48:ARG:CZ	2:D:245:PRO:HD2	2.47	0.44
1:A:70:LEU:CD2	1:A:110:ILE:HG23	2.48	0.44
1:A:190:THR:O	1:A:191:THR:C	2.56	0.44
1:A:83:TYR:O	1:A:84:ARG:C	2.55	0.44
2:B:337:ASN:C	2:B:339:ASN:H	2.20	0.44
2:B:48:ARG:O	2:B:51:VAL:N	2.47	0.44
3:E:57:ALA:O	3:E:58:GLU:C	2.54	0.44
2:B:287:THR:O	2:B:288:VAL:CB	2.62	0.44
1:C:255:PHE:CE1	1:C:352:LYS:HB3	2.52	0.44
1:C:104:ALA:HB1	1:C:411:GLU:HB2	1.99	0.44
2:D:7:ILE:O	2:D:137:LEU:HA	2.18	0.44
2:D:70:LEU:HD12	2:D:145:THR:HB	2.00	0.44
2:D:150:GLY:O	2:D:151:THR:C	2.54	0.44
2:D:180:THR:CG2	2:D:181:VAL:H	2.30	0.44
2:D:336:GLN:H	2:D:336:GLN:HG2	1.47	0.44
1:A:329:ASN:O	1:A:331:ALA:N	2.51	0.44
1:A:48:SER:C	1:A:50:ASN:H	2.20	0.44
2:D:332:MET:C	2:D:334:ASN:H	2.20	0.44
1:A:287:SER:C	1:A:289:ALA:N	2.70	0.44
2:B:298:SER:C	2:B:300:ASN:H	2.21	0.44
1:C:115:ILE:HG13	1:C:152:LEU:HG	1.99	0.43
2:D:250:ALA:CB	7:D:700:LOC:H7	2.48	0.43
3:E:48:GLU:C	3:E:48:GLU:CD	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:92:ASN:O	3:E:96:MET:HB3	2.18	0.43
1:A:79:ARG:HG2	1:A:79:ARG:H	1.51	0.43
8:B:800:TZT:H1A	8:B:800:TZT:H5	1.72	0.43
1:C:172:TYR:HA	1:C:173:PRO:HD3	1.91	0.43
1:A:287:SER:O	1:A:288:VAL:C	2.57	0.43
1:C:123:ARG:NH1	1:C:161:TYR:HE2	2.17	0.43
1:C:254:GLU:OE1	1:C:352:LYS:NZ	2.51	0.43
2:D:360:PRO:HB2	2:D:369:ARG:H	1.63	0.43
3:E:104:LYS:C	3:E:106:GLU:H	2.20	0.43
1:A:123:ARG:NH1	1:A:161:TYR:HE2	2.16	0.43
1:A:325:PRO:O	1:A:326:LYS:C	2.54	0.43
1:A:83:TYR:O	1:A:85:GLN:N	2.52	0.43
2:B:225:GLY:O	2:B:228:ASN:HB2	2.18	0.43
2:B:249:ASN:OD1	2:B:254:LYS:HE2	2.19	0.43
2:B:336:GLN:H	2:B:336:GLN:HG2	1.51	0.43
3:E:115:HIS:O	3:E:118:ALA:HB3	2.18	0.43
3:E:123:LEU:C	3:E:125:GLU:H	2.22	0.43
1:A:306:ASP:HA	1:A:307:PRO:HD3	1.80	0.43
1:A:365:GLY:O	1:A:366:GLY:O	2.37	0.43
1:A:425:MET:CE	1:A:425:MET:HA	2.49	0.43
1:A:67:PHE:O	1:A:93:ILE:N	2.41	0.43
2:B:241:CYS:CB	2:B:247:GLN:NE2	2.81	0.43
2:B:177:VAL:HG22	8:B:800:TZT:C21	2.49	0.43
1:C:96:LYS:HG2	2:D:131:CYS:HB2	1.99	0.43
1:A:12:ALA:O	1:A:13:GLY:C	2.57	0.43
1:C:123:ARG:HD2	1:C:161:TYR:OH	2.17	0.43
1:C:28:HIS:CE1	1:C:244:PHE:CE2	3.07	0.43
1:A:191:THR:O	1:A:195:LEU:HB2	2.17	0.43
1:C:49:PHE:CA	1:C:243:ARG:O	2.65	0.43
2:D:162:PRO:HD2	2:D:163:ASP:HB2	2.01	0.43
3:E:76:ARG:HB3	3:E:77:GLU:H	1.59	0.43
1:A:154:MET:HE1	1:A:198:SER:HB2	2.01	0.43
1:A:430:LYS:O	1:A:434:GLU:HB2	2.18	0.43
1:C:117:LEU:HD21	1:C:121:ARG:NH2	2.34	0.43
1:C:395:PHE:C	1:C:395:PHE:CD2	2.91	0.43
1:C:435:VAL:O	1:C:435:VAL:HG12	2.18	0.43
2:D:208:ALA:HB2	2:D:304:ALA:N	2.33	0.43
3:E:86:ALA:HA	3:E:89:GLU:HG2	2.00	0.43
3:E:92:ASN:O	3:E:96:MET:CB	2.66	0.43
2:B:100:GLY:O	2:B:101:ASN:CB	2.66	0.43
2:B:165:ILE:HG23	2:B:253:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:245:PRO:CB	2:D:247:GLN:HG2	2.41	0.43
2:D:42:LEU:O	2:D:43:GLN:C	2.57	0.43
1:A:407:TRP:CE2	2:B:257:VAL:HA	2.54	0.43
2:B:344:VAL:HG13	2:B:346:TRP:H	1.84	0.43
1:C:297:GLU:HB3	1:C:300:ASN:HB2	2.01	0.43
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.54	0.43
2:D:253:ARG:O	2:D:257:VAL:HG12	2.18	0.43
3:E:65:GLU:C	3:E:67:GLU:N	2.71	0.43
1:A:223:THR:H	1:A:226:ASN:HB2	1.84	0.42
1:A:66:VAL:O	1:A:67:PHE:HD1	2.02	0.42
1:C:313:MET:HG2	1:C:380:ASN:O	2.19	0.42
1:C:402:ARG:O	1:C:403:ALA:C	2.56	0.42
1:C:81:GLY:O	1:C:82:THR:C	2.56	0.42
2:D:312:TYR:CD2	2:D:381:SER:HB2	2.54	0.42
2:B:66:ILE:HD11	2:B:121:VAL:HB	2.01	0.42
2:B:360:PRO:HG2	2:B:371:LEU:HD23	2.01	0.42
8:B:800:TZT:C30	8:B:800:TZT:C25	2.97	0.42
1:C:171:ILE:HG21	1:C:206:ASN:ND2	2.32	0.42
1:C:48:SER:C	1:C:50:ASN:H	2.15	0.42
2:D:50:ASN:O	2:D:64:ARG:NH1	2.51	0.42
2:B:3:GLU:CD	2:B:130:ASP:H	2.23	0.42
1:C:339:ARG:O	1:C:341:ILE:HD13	2.19	0.42
1:C:70:LEU:HD22	1:C:110:ILE:HG23	2.01	0.42
1:C:14:VAL:HG21	1:C:75:ILE:CD1	2.49	0.42
2:D:142:GLY:HA3	2:D:183:GLU:HB3	2.01	0.42
1:C:105:ARG:NH2	2:D:253:ARG:HH21	2.09	0.42
2:D:88:ARG:HA	2:D:89:PRO:HD3	1.84	0.42
1:A:28:HIS:CE1	1:A:244:PHE:CE2	3.07	0.42
1:A:27:GLU:OE2	1:A:320:ARG:NH1	2.44	0.42
1:A:323:VAL:HG12	1:A:355:ILE:CD1	2.47	0.42
1:C:112:LYS:O	1:C:115:ILE:HG22	2.19	0.42
1:C:12:ALA:O	1:C:13:GLY:C	2.57	0.42
1:C:274:PRO:HG2	1:C:371:VAL:HG11	2.02	0.42
1:C:346:TRP:CZ2	1:C:435:VAL:HG13	2.54	0.42
2:D:401:ARG:C	2:D:403:ALA:N	2.73	0.42
2:D:82:PRO:HB2	2:D:83:PHE:H	1.57	0.42
2:B:156:LYS:HE3	3:E:76:ARG:HD2	2.01	0.42
1:A:358:GLN:HA	1:A:359:PRO:HD3	1.79	0.42
1:A:173:PRO:HB3	4:A:600:GTP:O3'	2.19	0.42
2:B:2:ARG:HD2	2:B:131:CYS:SG	2.60	0.42
2:B:7:ILE:HG12	2:B:66:ILE:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:800:TZT:H78	8:B:800:TZT:H23	1.77	0.42
1:C:206:ASN:HD21	4:C:600:GTP:N2	1.90	0.42
2:B:221:THR:HG21	1:C:326:LYS:N	2.35	0.42
2:D:55:GLU:HB3	2:D:61:TYR:CD2	2.54	0.42
1:A:359:PRO:HA	1:A:360:PRO:HD3	1.86	0.42
1:C:258:ASN:O	1:C:314:ALA:HB2	2.20	0.42
1:C:347:CYS:SG	1:C:348:PRO:HD2	2.59	0.42
1:C:67:PHE:O	1:C:93:ILE:N	2.46	0.42
2:D:273:ALA:CB	2:D:375:ALA:N	2.78	0.42
2:B:291:LEU:HD21	2:B:375:ALA:HB2	2.00	0.42
2:B:6:HIS:HB3	2:B:64:ARG:O	2.20	0.42
8:B:800:TZT:H25A	8:B:800:TZT:H18	1.76	0.42
1:C:223:THR:H	1:C:226:ASN:HB2	1.85	0.42
2:D:11:GLN:HG3	2:D:74:THR:CG2	2.46	0.42
2:D:257:VAL:O	2:D:257:VAL:HG22	2.19	0.42
2:D:276:THR:CG2	2:D:277:SER:N	2.71	0.42
1:A:102:ASN:HA	1:A:186:ASN:HD21	1.84	0.42
2:B:114:LEU:O	2:B:115:VAL:C	2.57	0.42
8:B:800:TZT:H30	8:B:800:TZT:H25B	2.01	0.42
3:E:60:ARG:NH1	3:E:60:ARG:HB2	2.34	0.42
1:A:280:LYS:O	1:A:282:TYR:N	2.53	0.42
1:A:83:TYR:C	1:A:85:GLN:H	2.23	0.42
2:B:194:LEU:C	2:B:196:GLU:N	2.72	0.42
2:D:215:ARG:HH21	2:D:299:LYS:HA	1.84	0.42
2:D:332:MET:C	2:D:334:ASN:N	2.72	0.42
1:A:71:GLU:OE2	4:A:600:GTP:O1G	2.37	0.42
2:B:242:LEU:HD11	2:B:252:LEU:HD13	2.02	0.42
2:B:250:ALA:CB	7:B:700:LOC:H7	2.50	0.42
2:B:181:VAL:H	1:C:258:ASN:HD21	1.66	0.42
2:D:142:GLY:CA	2:D:173:PRO:HG3	2.50	0.42
1:A:329:ASN:C	1:A:331:ALA:N	2.72	0.41
2:B:265:LEU:O	2:B:266:HIS:C	2.57	0.41
2:B:55:GLU:H	2:B:55:GLU:HG3	1.54	0.41
2:D:212:ILE:CD1	2:D:215:ARG:NH2	2.83	0.41
3:E:80:ARG:HE	3:E:84:GLN:HE22	1.66	0.41
1:A:167:LEU:CD1	1:A:252:LEU:HD13	2.30	0.41
1:A:394:LYS:HG3	2:B:348:PRO:CB	2.49	0.41
2:B:180:THR:C	2:B:182:VAL:N	2.72	0.41
2:B:209:LEU:HD12	2:B:209:LEU:HA	1.89	0.41
2:B:211:ASP:HB3	2:B:215:ARG:NH1	2.34	0.41
2:B:88:ARG:HB3	2:B:91:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:PHE:O	1:C:405:VAL:C	2.58	0.41
2:D:231:VAL:HG12	2:D:235:MET:HE1	2.02	0.41
2:D:349:ASN:HD22	2:D:349:ASN:HA	1.70	0.41
1:A:198:SER:O	1:A:265:ILE:HB	2.21	0.41
1:A:273:ALA:HB3	1:A:274:PRO:HD2	2.00	0.41
1:A:289:ALA:O	1:A:292:THR:HB	2.21	0.41
2:B:107:HIS:O	2:B:152:LEU:HD22	2.21	0.41
2:B:182:VAL:O	2:B:183:GLU:C	2.59	0.41
2:B:251:ASP:C	2:B:253:ARG:N	2.72	0.41
1:A:180:ALA:HB1	2:B:258:ASN:HD21	1.86	0.41
2:B:294:GLN:HE21	2:B:294:GLN:HB2	1.66	0.41
2:B:273:ALA:HB2	2:B:375:ALA:O	2.20	0.41
2:D:256:ALA:O	2:D:260:VAL:HG22	2.21	0.41
2:D:269:MET:HE1	2:D:307:PRO:HD3	2.01	0.41
7:D:700:LOC:C6	7:D:700:LOC:H4B	2.51	0.41
2:D:93:VAL:HG12	2:D:114:LEU:HD11	2.03	0.41
1:C:163:LYS:H	1:C:163:LYS:HE3	1.86	0.41
2:D:165:ILE:HD11	2:D:252:LEU:HG	2.01	0.41
2:D:205:ASP:OD2	2:D:304:ALA:HB3	2.20	0.41
2:D:247:GLN:HG3	2:D:248:LEU:N	2.31	0.41
1:A:179:THR:HA	1:A:183:GLU:OE2	2.20	0.41
1:A:210:TYR:CZ	1:A:214:ARG:HD2	2.55	0.41
1:A:404:PHE:CD1	1:A:404:PHE:N	2.87	0.41
2:B:136:GLN:HG3	2:B:136:GLN:O	2.20	0.41
1:C:377:MET:O	1:C:377:MET:CG	2.68	0.41
2:D:62:VAL:HA	2:D:63:PRO:HD2	1.75	0.41
1:A:70:LEU:HD12	1:A:70:LEU:N	2.35	0.41
2:B:102:ASN:OD1	2:B:102:ASN:O	2.38	0.41
2:B:225:GLY:O	2:B:228:ASN:CB	2.69	0.41
2:B:388:PHE:HB3	2:B:425:MET:CE	2.49	0.41
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.54	0.41
2:D:103:TRP:CZ3	2:D:189:LEU:HD22	2.55	0.41
1:A:17:GLY:O	1:A:18:ASN:C	2.59	0.41
1:C:246:GLY:C	1:C:248:LEU:H	2.23	0.41
1:C:88:HIS:H	1:C:91:GLN:NE2	2.18	0.41
2:D:64:ARG:HG3	2:D:125:GLU:OE1	2.21	0.41
2:D:142:GLY:H	2:D:173:PRO:HG3	1.85	0.41
2:D:48:ARG:C	2:D:50:ASN:N	2.73	0.41
1:A:185:TYR:HH	1:A:403:ALA:HB3	1.82	0.41
2:B:103:TRP:CZ3	2:B:189:LEU:HD22	2.56	0.41
2:B:387:LEU:O	2:B:390:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:GLY:O	1:C:18:ASN:C	2.59	0.41
1:C:190:THR:CG2	1:C:191:THR:N	2.84	0.41
1:C:236:SER:O	1:C:240:ALA:N	2.37	0.41
1:C:271:THR:HG21	1:C:295:CYS:O	2.21	0.41
1:C:79:ARG:H	1:C:79:ARG:HG2	1.57	0.41
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.55	0.41
2:D:325:MET:O	2:D:329:ASP:HB2	2.21	0.41
2:D:311:ARG:HD3	2:D:436:GLN:HG3	2.02	0.41
7:D:700:LOC:C4	7:D:700:LOC:H6A	2.50	0.41
1:A:204:VAL:HG22	1:A:302:MET:SD	2.60	0.41
2:B:311:ARG:HD3	2:B:436:GLN:HG3	2.03	0.41
1:C:278:ALA:CA	1:C:369:ALA:HB2	2.44	0.41
2:D:103:TRP:HD1	2:D:147:SER:OG	2.03	0.41
2:D:55:GLU:HB3	2:D:61:TYR:HD2	1.86	0.41
2:D:75:MET:CE	2:D:94:PHE:CD2	3.04	0.41
2:B:164:ARG:NH1	2:B:253:ARG:HH22	2.11	0.41
2:B:81:GLY:O	2:B:82:PRO:O	2.39	0.41
1:C:302:MET:HE2	1:C:302:MET:HB3	1.66	0.41
2:D:126:SER:C	2:D:128:SER:H	2.24	0.41
2:D:209:LEU:HD12	2:D:209:LEU:HA	1.94	0.41
1:A:288:VAL:HG11	1:A:327:ASP:HB2	2.03	0.41
1:A:104:ALA:HB1	1:A:411:GLU:HB2	2.02	0.41
2:B:11:GLN:HB3	6:B:600:GDP:O1A	2.21	0.41
2:B:133:GLN:NE2	2:B:252:LEU:CD2	2.84	0.41
2:B:324:SER:C	2:B:326:LYS:H	2.25	0.41
2:B:305:CYS:SG	2:B:384:ILE:HA	2.61	0.41
2:B:395:PHE:CE2	2:B:422:GLU:HB2	2.56	0.41
2:B:408:TYR:CD1	2:B:408:TYR:N	2.89	0.41
1:C:262:TYR:HA	1:C:263:PRO:HD3	1.90	0.41
1:C:315:CYS:SG	1:C:377:MET:HE1	2.60	0.41
2:D:245:PRO:HB2	2:D:246:GLY:H	1.56	0.41
2:D:4:ILE:H	2:D:64:ARG:HH21	1.69	0.41
1:A:253:THR:O	1:A:255:PHE:N	2.54	0.40
1:A:271:THR:HB	1:A:377:MET:HG2	2.02	0.40
1:A:305:CYS:SG	1:A:306:ASP:N	2.94	0.40
1:A:62:VAL:HA	1:A:63:PRO:HD3	1.98	0.40
1:C:191:THR:HG22	1:C:192:HIS:N	2.37	0.40
2:D:388:PHE:HB3	2:D:425:MET:CE	2.51	0.40
1:A:207:GLU:HG2	1:A:304:LYS:HD3	2.03	0.40
1:A:279:GLU:HG2	1:A:279:GLU:O	2.21	0.40
1:C:151:SER:O	1:C:155:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:THR:O	1:C:191:THR:C	2.59	0.40
1:C:324:VAL:HA	1:C:325:PRO:HD2	1.90	0.40
2:D:133:GLN:NE2	2:D:252:LEU:CD2	2.81	0.40
2:D:16:ILE:HD11	2:D:231:VAL:CB	2.51	0.40
1:A:107:HIS:CE1	1:A:155:GLU:OE2	2.75	0.40
1:A:136:LEU:HD23	1:A:167:LEU:HB2	2.03	0.40
1:A:344:VAL:HG13	1:A:347:CYS:HB2	2.04	0.40
2:B:247:GLN:HG3	2:B:248:LEU:HG	2.03	0.40
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.56	0.40
2:B:67:LEU:HD13	2:B:92:PHE:CE2	2.57	0.40
1:C:107:HIS:HE1	1:C:155:GLU:OE2	2.04	0.40
2:D:142:GLY:HA2	2:D:186:ASN:HB2	2.02	0.40
2:D:298:SER:C	2:D:300:ASN:H	2.23	0.40
2:D:412:GLY:O	3:E:133:VAL:HB	2.21	0.40
1:A:190:THR:CG2	1:A:191:THR:N	2.84	0.40
2:B:54:ASN:H	2:B:64:ARG:HD3	1.85	0.40
2:B:65:ALA:O	2:B:91:ASN:HB3	2.21	0.40
1:C:256:GLN:O	1:C:257:THR:C	2.60	0.40
2:D:155:SER:O	3:E:123:LEU:HD21	2.22	0.40
2:D:7:ILE:HA	2:D:66:ILE:HG22	2.02	0.40
1:A:118:VAL:HG21	1:A:149:PHE:CZ	2.56	0.40
1:A:176:GLN:H	1:A:176:GLN:NE2	2.19	0.40
1:A:388:TRP:HA	1:A:388:TRP:CE3	2.57	0.40
1:A:401:LYS:C	1:A:403:ALA:N	2.74	0.40
2:B:198:THR:OG1	2:B:265:LEU:HD22	2.21	0.40
2:B:245:PRO:HB2	2:B:246:GLY:H	1.49	0.40
1:C:179:THR:HB	1:C:180:ALA:H	1.61	0.40
2:D:2:ARG:CZ	2:D:133:GLN:HB2	2.51	0.40
3:E:6:MET:HE2	3:E:24:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	423/449 (94%)	295 (70%)	85 (20%)	43 (10%)	0	9
1	C	415/449 (92%)	300 (72%)	73 (18%)	42 (10%)	0	9
2	B	415/445 (93%)	289 (70%)	81 (20%)	45 (11%)	0	8
2	D	415/445 (93%)	297 (72%)	73 (18%)	45 (11%)	0	8
3	E	120/142 (84%)	71 (59%)	35 (29%)	14 (12%)	0	6
All	All	1788/1930 (93%)	1252 (70%)	347 (19%)	189 (11%)	0	8

All (189) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	48	SER
1	A	49	PHE
1	A	62	VAL
1	A	72	PRO
1	A	73	THR
1	A	82	THR
1	A	101	ASN
1	A	180	ALA
1	A	181	VAL
1	A	245	ASP
1	A	247	ALA
1	A	257	THR
1	A	273	ALA
1	A	288	VAL
1	A	341	ILE
1	A	345	ASP
1	A	349	THR
1	A	350	GLY
1	A	351	PHE
1	A	377	MET
2	B	43	GLN
2	B	60	LYS
2	B	82	PRO
2	B	113	GLU
2	B	115	VAL
2	B	162	PRO
2	B	163	ASP
2	B	181	VAL
2	B	195	VAL
2	B	217	LEU

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Mol	Chain	Res	Type
2	B	227	LEU
2	B	265	LEU
2	B	273	ALA
2	B	276	THR
2	B	288	VAL
2	B	369	ARG
2	B	400	ARG
2	B	403	ALA
1	C	11	GLN
1	C	49	PHE
1	C	62	VAL
1	C	72	PRO
1	C	73	THR
1	C	82	THR
1	C	180	ALA
1	C	181	VAL
1	C	241	SER
1	C	247	ALA
1	C	250	VAL
1	C	253	THR
1	C	266	HIS
1	C	273	ALA
1	C	305	CYS
1	C	345	ASP
1	C	350	GLY
1	C	351	PHE
1	C	377	MET
2	D	43	GLN
2	D	60	LYS
2	D	62	VAL
2	D	82	PRO
2	D	115	VAL
2	D	162	PRO
2	D	163	ASP
2	D	195	VAL
2	D	217	LEU
2	D	220	THR
2	D	240	THR
2	D	265	LEU
2	D	273	ALA
2	D	276	THR
2	D	288	VAL

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Mol	Chain	Res	Type
2	D	369	ARG
2	D	403	ALA
3	E	7	GLU
3	E	27	PRO
3	E	28	SER
3	E	29	PHE
3	E	68	LEU
3	E	77	GLU
1	A	83	TYR
1	A	84	ARG
1	A	100	ALA
1	A	112	LYS
1	A	183	GLU
1	A	263	PRO
1	A	266	HIS
1	A	305	CYS
1	A	366	GLY
1	A	403	ALA
1	A	405	VAL
2	B	3	GLU
2	B	11	GLN
2	B	62	VAL
2	B	73	GLY
2	B	159	GLU
2	B	225	GLY
2	B	240	THR
2	B	244	PHE
2	B	308	ARG
2	B	360	PRO
2	B	415	GLU
1	C	83	TYR
1	C	101	ASN
1	C	112	LYS
1	C	249	ASN
1	C	251	ASP
1	C	257	THR
1	C	265	ILE
1	C	288	VAL
1	C	341	ILE
1	C	342	GLN
1	C	366	GLY
1	C	403	ALA

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Mol	Chain	Res	Type
1	C	405	VAL
2	D	11	GLN
2	D	73	GLY
2	D	113	GLU
2	D	159	GLU
2	D	225	GLY
2	D	244	PHE
2	D	360	PRO
2	D	401	ARG
2	D	415	GLU
3	E	49	GLU
3	E	108	ASN
1	A	254	GLU
1	A	265	ILE
1	A	299	ALA
1	A	400	ALA
2	B	35	SER
2	B	42	LEU
2	B	123	ARG
2	B	129	CYS
2	B	179	ASP
2	B	239	THR
2	B	245	PRO
2	B	266	HIS
1	C	55	GLU
1	C	84	ARG
1	C	183	GLU
1	C	400	ALA
2	D	42	LEU
2	D	219	LEU
2	D	245	PRO
2	D	308	ARG
2	D	371	LEU
3	E	11	LEU
3	E	64	GLN
1	A	164	LYS
2	B	34	GLY
2	B	178	SER
2	B	371	LEU
2	B	405	LEU
1	C	163	LYS
1	C	164	LYS

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Mol	Chain	Res	Type
1	C	263	PRO
2	D	3	GLU
2	D	34	GLY
2	D	35	SER
2	D	123	ARG
2	D	129	CYS
2	D	239	THR
2	D	255	LEU
2	D	266	HIS
2	D	392	SER
2	D	405	LEU
3	E	47	LEU
3	E	66	ALA
1	A	77	GLU
1	A	163	LYS
1	A	248	LEU
1	A	307	PRO
2	B	184	PRO
2	B	255	LEU
1	C	179	THR
1	C	307	PRO
2	D	177	VAL
2	D	184	PRO
3	E	26	PRO
2	B	177	VAL
2	D	151	THR
3	E	76	ARG
2	B	335	VAL
2	D	344	VAL
1	A	175	PRO
1	A	14	VAL
1	C	14	VAL

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	346/378 (92%)	230 (66%)	116 (34%)	0	1
1	C	340/378 (90%)	234 (69%)	106 (31%)	0	2
2	B	347/383 (91%)	229 (66%)	118 (34%)	0	1
2	D	349/383 (91%)	227 (65%)	122 (35%)	0	1
3	E	80/126 (64%)	49 (61%)	31 (39%)	0	0
All	All	1462/1648 (89%)	969 (66%)	493 (34%)	0	1

All (493) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	4	CYS
1	A	9	VAL
1	A	16	ILE
1	A	27	GLU
1	A	36	MET
1	A	48	SER
1	A	50	ASN
1	A	62	VAL
1	A	68	VAL
1	A	71	GLU
1	A	74	VAL
1	A	76	ASP
1	A	80	THR
1	A	86	LEU
1	A	88	HIS
1	A	90	GLU
1	A	93	ILE
1	A	97	GLU
1	A	102	ASN
1	A	105	ARG
1	A	114	ILE
1	A	115	ILE
1	A	119	LEU
1	A	122	VAL
1	A	127	ASP
1	A	130	THR
1	A	132	LEU
1	A	133	GLN
1	A	141	PHE
1	A	145	THR

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Mol	Chain	Res	Type
1	A	153	LEU
1	A	158	SER
1	A	160	ASP
1	A	163	LYS
1	A	165	SER
1	A	177	VAL
1	A	182	VAL
1	A	183	GLU
1	A	191	THR
1	A	194	THR
1	A	196	GLU
1	A	200	CYS
1	A	206	ASN
1	A	211	ASP
1	A	212	ILE
1	A	218	ASP
1	A	219	ILE
1	A	223	THR
1	A	224	TYR
1	A	226	ASN
1	A	230	LEU
1	A	236	SER
1	A	237	SER
1	A	241	SER
1	A	242	LEU
1	A	248	LEU
1	A	250	VAL
1	A	251	ASP
1	A	252	LEU
1	A	253	THR
1	A	254	GLU
1	A	256	GLN
1	A	264	ARG
1	A	265	ILE
1	A	269	LEU
1	A	275	VAL
1	A	279	GLU
1	A	280	LYS
1	A	284	GLU
1	A	286	LEU
1	A	291	ILE
1	A	297	GLU

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Mol	Chain	Res	Type
1	A	301	GLN
1	A	302	MET
1	A	304	LYS
1	A	306	ASP
1	A	315	CYS
1	A	318	LEU
1	A	322	ASP
1	A	326	LYS
1	A	328	VAL
1	A	329	ASN
1	A	334	THR
1	A	335	ILE
1	A	337	THR
1	A	341	ILE
1	A	343	PHE
1	A	345	ASP
1	A	347	CYS
1	A	351	PHE
1	A	355	ILE
1	A	356	ASN
1	A	362	VAL
1	A	363	VAL
1	A	367	ASP
1	A	368	LEU
1	A	370	LYS
1	A	371	VAL
1	A	377	MET
1	A	379	SER
1	A	380	ASN
1	A	381	THR
1	A	386	GLU
1	A	392	ASP
1	A	397	LEU
1	A	401	LYS
1	A	402	ARG
1	A	405	VAL
1	A	413	MET
1	A	414	GLU
1	A	415	GLU
1	A	420	GLU
1	A	428	LEU
1	A	432	TYR

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Mol	Chain	Res	Type
1	A	434	GLU
2	B	3	GLU
2	B	4	ILE
2	B	39	ASP
2	B	42	LEU
2	B	43	GLN
2	B	44	LEU
2	B	51	VAL
2	B	54	ASN
2	B	55	GLU
2	B	61	TYR
2	B	62	VAL
2	B	64	ARG
2	B	66	ILE
2	B	68	VAL
2	B	71	GLU
2	B	79	ARG
2	B	80	SER
2	B	83	PHE
2	B	88	ARG
2	B	90	ASP
2	B	93	VAL
2	B	101	ASN
2	B	102	ASN
2	B	109	THR
2	B	117	SER
2	B	127	GLU
2	B	128	SER
2	B	130	ASP
2	B	131	CYS
2	B	132	LEU
2	B	135	PHE
2	B	137	LEU
2	B	139	HIS
2	B	145	THR
2	B	147	SER
2	B	154	ILE
2	B	155	SER
2	B	156	LYS
2	B	158	ARG
2	B	160	GLU
2	B	164	ARG

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Mol	Chain	Res	Type
2	B	165	ILE
2	B	166	MET
2	B	171	VAL
2	B	174	SER
2	B	177	VAL
2	B	178	SER
2	B	179	ASP
2	B	182	VAL
2	B	192	HIS
2	B	193	GLN
2	B	195	VAL
2	B	200	GLU
2	B	209	LEU
2	B	211	ASP
2	B	212	ILE
2	B	214	PHE
2	B	215	ARG
2	B	217	LEU
2	B	221	THR
2	B	223	THR
2	B	224	TYR
2	B	227	LEU
2	B	230	LEU
2	B	234	THR
2	B	235	MET
2	B	239	THR
2	B	240	THR
2	B	242	LEU
2	B	248	LEU
2	B	251	ASP
2	B	254	LYS
2	B	258	ASN
2	B	265	LEU
2	B	293	GLN
2	B	294	GLN
2	B	295	MET
2	B	300	ASN
2	B	308	ARG
2	B	309	HIS
2	B	311	ARG
2	B	313	LEU
2	B	318	VAL

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Mol	Chain	Res	Type
2	B	320	ARG
2	B	323	MET
2	B	325	MET
2	B	329	ASP
2	B	333	LEU
2	B	336	GLN
2	B	339	ASN
2	B	345	GLU
2	B	350	ASN
2	B	351	VAL
2	B	353	THR
2	B	355	VAL
2	B	357	ASP
2	B	358	ILE
2	B	371	LEU
2	B	374	SER
2	B	376	THR
2	B	377	PHE
2	B	380	ASN
2	B	384	ILE
2	B	396	THR
2	B	401	ARG
2	B	406	HIS
2	B	407	TRP
2	B	408	TYR
2	B	409	THR
2	B	415	GLU
2	B	416	MET
2	B	419	THR
2	B	423	SER
2	B	425	MET
2	B	429	VAL
2	B	431	GLU
2	B	434	GLN
2	B	436	GLN
1	C	2	ARG
1	C	3	GLU
1	C	9	VAL
1	C	16	ILE
1	C	36	MET
1	C	48	SER
1	C	50	ASN

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Mol	Chain	Res	Type
1	C	68	VAL
1	C	71	GLU
1	C	74	VAL
1	C	76	ASP
1	C	80	THR
1	C	86	LEU
1	C	90	GLU
1	C	93	ILE
1	C	97	GLU
1	C	102	ASN
1	C	105	ARG
1	C	114	ILE
1	C	115	ILE
1	C	119	LEU
1	C	122	VAL
1	C	127	ASP
1	C	130	THR
1	C	132	LEU
1	C	133	GLN
1	C	141	PHE
1	C	145	THR
1	C	153	LEU
1	C	160	ASP
1	C	163	LYS
1	C	165	SER
1	C	167	LEU
1	C	177	VAL
1	C	182	VAL
1	C	183	GLU
1	C	191	THR
1	C	194	THR
1	C	196	GLU
1	C	200	CYS
1	C	203	MET
1	C	206	ASN
1	C	218	ASP
1	C	219	ILE
1	C	223	THR
1	C	224	TYR
1	C	226	ASN
1	C	230	LEU
1	C	236	SER

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Mol	Chain	Res	Type
1	C	242	LEU
1	C	244	PHE
1	C	245	ASP
1	C	252	LEU
1	C	253	THR
1	C	255	PHE
1	C	265	ILE
1	C	269	LEU
1	C	275	VAL
1	C	279	GLU
1	C	286	LEU
1	C	291	ILE
1	C	297	GLU
1	C	301	GLN
1	C	302	MET
1	C	304	LYS
1	C	306	ASP
1	C	315	CYS
1	C	316	CYS
1	C	318	LEU
1	C	322	ASP
1	C	326	LYS
1	C	328	VAL
1	C	329	ASN
1	C	332	ILE
1	C	335	ILE
1	C	337	THR
1	C	341	ILE
1	C	346	TRP
1	C	347	CYS
1	C	349	THR
1	C	351	PHE
1	C	356	ASN
1	C	362	VAL
1	C	363	VAL
1	C	367	ASP
1	C	368	LEU
1	C	370	LYS
1	C	371	VAL
1	C	375	VAL
1	C	377	MET
1	C	379	SER

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Mol	Chain	Res	Type
1	C	380	ASN
1	C	381	THR
1	C	386	GLU
1	C	392	ASP
1	C	397	LEU
1	C	401	LYS
1	C	402	ARG
1	C	405	VAL
1	C	413	MET
1	C	414	GLU
1	C	415	GLU
1	C	420	GLU
1	C	428	LEU
1	C	432	TYR
1	C	434	GLU
2	D	2	ARG
2	D	3	GLU
2	D	4	ILE
2	D	16	ILE
2	D	39	ASP
2	D	42	LEU
2	D	43	GLN
2	D	44	LEU
2	D	51	VAL
2	D	54	ASN
2	D	55	GLU
2	D	61	TYR
2	D	62	VAL
2	D	64	ARG
2	D	66	ILE
2	D	68	VAL
2	D	71	GLU
2	D	79	ARG
2	D	80	SER
2	D	88	ARG
2	D	90	ASP
2	D	93	VAL
2	D	101	ASN
2	D	102	ASN
2	D	109	THR
2	D	117	SER
2	D	127	GLU

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Mol	Chain	Res	Type
2	D	128	SER
2	D	130	ASP
2	D	131	CYS
2	D	132	LEU
2	D	135	PHE
2	D	137	LEU
2	D	139	HIS
2	D	145	THR
2	D	147	SER
2	D	154	ILE
2	D	155	SER
2	D	156	LYS
2	D	158	ARG
2	D	160	GLU
2	D	164	ARG
2	D	165	ILE
2	D	166	MET
2	D	171	VAL
2	D	174	SER
2	D	179	ASP
2	D	181	VAL
2	D	189	LEU
2	D	192	HIS
2	D	193	GLN
2	D	195	VAL
2	D	200	GLU
2	D	209	LEU
2	D	211	ASP
2	D	212	ILE
2	D	214	PHE
2	D	215	ARG
2	D	217	LEU
2	D	221	THR
2	D	223	THR
2	D	227	LEU
2	D	230	LEU
2	D	234	THR
2	D	235	MET
2	D	239	THR
2	D	240	THR
2	D	241	CYS
2	D	242	LEU

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Mol	Chain	Res	Type
2	D	248	LEU
2	D	249	ASN
2	D	251	ASP
2	D	254	LYS
2	D	258	ASN
2	D	265	LEU
2	D	293	GLN
2	D	294	GLN
2	D	295	MET
2	D	300	ASN
2	D	308	ARG
2	D	309	HIS
2	D	311	ARG
2	D	313	LEU
2	D	315	VAL
2	D	318	VAL
2	D	320	ARG
2	D	323	MET
2	D	325	MET
2	D	329	ASP
2	D	333	LEU
2	D	336	GLN
2	D	339	ASN
2	D	340	SER
2	D	350	ASN
2	D	351	VAL
2	D	353	THR
2	D	355	VAL
2	D	357	ASP
2	D	358	ILE
2	D	371	LEU
2	D	374	SER
2	D	376	THR
2	D	377	PHE
2	D	380	ASN
2	D	384	ILE
2	D	391	ILE
2	D	396	THR
2	D	400	ARG
2	D	401	ARG
2	D	406	HIS
2	D	407	TRP

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Mol	Chain	Res	Type
2	D	408	TYR
2	D	409	THR
2	D	415	GLU
2	D	416	MET
2	D	419	THR
2	D	423	SER
2	D	425	MET
2	D	429	VAL
2	D	431	GLU
2	D	434	GLN
2	D	436	GLN
3	E	6	MET
3	E	11	LEU
3	E	13	LYS
3	E	15	THR
3	E	21	GLU
3	E	28	SER
3	E	48	GLU
3	E	51	GLN
3	E	53	LYS
3	E	54	LEU
3	E	62	LYS
3	E	69	LEU
3	E	71	HIS
3	E	72	LEU
3	E	76	ARG
3	E	78	HIS
3	E	80	ARG
3	E	84	GLN
3	E	89	GLU
3	E	94	ILE
3	E	101	LEU
3	E	105	MET
3	E	106	GLU
3	E	109	LYS
3	E	111	ASN
3	E	119	MET
3	E	120	LEU
3	E	122	ARG
3	E	124	GLN
3	E	125	GLU
3	E	126	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	50	ASN
1	A	85	GLN
1	A	91	GLN
1	A	101	ASN
1	A	102	ASN
1	A	107	HIS
1	A	133	GLN
1	A	139	HIS
1	A	176	GLN
1	A	206	ASN
1	A	216	ASN
1	A	233	GLN
1	A	256	GLN
1	A	258	ASN
1	A	266	HIS
1	A	301	GLN
1	A	329	ASN
1	A	356	ASN
1	A	380	ASN
2	B	6	HIS
2	B	15	GLN
2	B	54	ASN
2	B	96	GLN
2	B	133	GLN
2	B	136	GLN
2	B	139	HIS
2	B	186	ASN
2	B	193	GLN
2	B	197	ASN
2	B	247	GLN
2	B	258	ASN
2	B	294	GLN
2	B	300	ASN
2	B	331	GLN
2	B	339	ASN
2	B	349	ASN
2	B	350	ASN
2	B	380	ASN
2	B	385	GLN
2	B	434	GLN

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Mol	Chain	Res	Type
1	C	8	HIS
1	C	28	HIS
1	C	50	ASN
1	C	85	GLN
1	C	91	GLN
1	C	101	ASN
1	C	102	ASN
1	C	107	HIS
1	C	139	HIS
1	C	176	GLN
1	C	206	ASN
1	C	216	ASN
1	C	233	GLN
1	C	249	ASN
1	C	258	ASN
1	C	266	HIS
1	C	380	ASN
2	D	6	HIS
2	D	8	GLN
2	D	15	GLN
2	D	43	GLN
2	D	54	ASN
2	D	133	GLN
2	D	136	GLN
2	D	139	HIS
2	D	193	GLN
2	D	197	ASN
2	D	247	GLN
2	D	258	ASN
2	D	294	GLN
2	D	300	ASN
2	D	331	GLN
2	D	339	ASN
2	D	349	ASN
2	D	350	ASN
2	D	380	ASN
2	D	434	GLN
3	E	51	GLN
3	E	64	GLN
3	E	78	HIS
3	E	84	GLN
3	E	111	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, 2 are monoatomic - leaving 7 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	GTP	C	600	-	26,34,34	1.15	2 (7%)	33,54,54	2.07	11 (33%)
8	TZT	B	800	-	51,51,51	1.82	12 (23%)	54,70,70	2.19	14 (25%)
6	GDP	B	600	-	24,30,30	0.98	1 (4%)	31,47,47	2.24	12 (38%)
6	GDP	D	600	-	24,30,30	1.05	1 (4%)	31,47,47	2.06	8 (25%)
7	LOC	B	700	-	28,31,31	3.46	7 (25%)	28,44,44	3.16	10 (35%)
7	LOC	D	700	-	28,31,31	3.24	6 (21%)	28,44,44	3.18	11 (39%)
4	GTP	A	600	-	26,34,34	0.98	2 (7%)	33,54,54	1.71	6 (18%)

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	GTP	C	600	-	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	TZT	B	800	-	-	30/72/82/82	0/2/2/2
6	GDP	B	600	-	-	3/12/32/32	0/3/3/3
6	GDP	D	600	-	-	2/12/32/32	0/3/3/3
7	LOC	B	700	-	-	2/10/25/25	0/3/3/3
7	LOC	D	700	-	-	2/10/25/25	0/3/3/3
4	GTP	A	600	-	-	5/18/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	LOC	C19-C17	-9.91	1.21	1.39
7	D	700	LOC	C19-C17	-9.64	1.22	1.39
7	B	700	LOC	C19-C20	-9.35	1.13	1.40
7	D	700	LOC	C19-C20	-8.60	1.15	1.40
7	B	700	LOC	C20-C21	-8.23	1.20	1.40
7	D	700	LOC	C20-C21	-7.13	1.22	1.40
8	B	800	TZT	C34-C33	7.04	1.61	1.52
7	D	700	LOC	C15-C16	6.55	1.52	1.39
7	B	700	LOC	C15-C16	5.63	1.50	1.39
7	B	700	LOC	O6-C17	5.30	1.45	1.37
7	D	700	LOC	O6-C17	4.00	1.43	1.37
8	B	800	TZT	C33-N29	3.97	1.52	1.47
8	B	800	TZT	C43-C44	3.95	1.63	1.51
4	C	600	GTP	C6-N1	3.53	1.39	1.33
8	B	800	TZT	C23-C18	3.31	1.59	1.52
6	D	600	GDP	C6-N1	3.25	1.38	1.33
8	B	800	TZT	O35-C34	3.22	1.50	1.42
8	B	800	TZT	C26-C27	3.21	1.57	1.51
7	B	700	LOC	C22-C8	3.06	1.45	1.40
4	A	600	GTP	C6-N1	3.05	1.38	1.33
6	B	600	GDP	C6-N1	3.00	1.38	1.33
7	D	700	LOC	C22-C8	2.92	1.45	1.40
4	A	600	GTP	O4'-C1'	2.54	1.44	1.41
8	B	800	TZT	C49-C44	2.42	1.44	1.38
8	B	800	TZT	C37-C39	2.32	1.56	1.52
4	C	600	GTP	O4'-C4'	-2.24	1.40	1.45
8	B	800	TZT	C45-C44	2.19	1.43	1.38
8	B	800	TZT	C42-C43	2.16	1.59	1.51
8	B	800	TZT	C46-C45	2.05	1.43	1.38
7	B	700	LOC	O1-C1	-2.03	1.34	1.38
8	B	800	TZT	C37-C34	2.00	1.59	1.55

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	LOC	C20-C19-C17	8.36	149.93	129.69
7	D	700	LOC	C20-C19-C17	7.80	148.58	129.69
7	D	700	LOC	C6-O3-C5	7.64	129.07	117.53
7	B	700	LOC	C6-O3-C5	7.47	128.80	117.53
6	D	600	GDP	N3-C2-N1	-6.19	118.97	127.22
8	B	800	TZT	C5-C4-C8	5.71	119.53	111.85
7	D	700	LOC	C21-C22-C8	-5.67	114.36	120.50
4	C	600	GTP	N3-C2-N1	-5.63	119.72	127.22
6	B	600	GDP	N3-C2-N1	-5.61	119.73	127.22
6	D	600	GDP	C2-N3-C4	5.55	121.69	115.36
6	B	600	GDP	C2-N3-C4	5.35	121.47	115.36
8	B	800	TZT	O28-C27-C26	-5.34	112.56	122.20
8	B	800	TZT	C42-C43-C44	5.08	124.63	112.87
7	B	700	LOC	O3-C5-C3	4.88	123.74	115.16
7	D	700	LOC	O3-C5-C3	4.66	123.36	115.16
7	B	700	LOC	C21-C22-C8	-4.63	115.48	120.50
7	D	700	LOC	C21-C22-C1	4.54	127.27	121.07
8	B	800	TZT	C12-C11-C15	-4.49	101.64	110.73
4	A	600	GTP	N3-C2-N1	-4.44	121.31	127.22
7	D	700	LOC	C11-N1-C12	4.43	127.31	122.44
4	C	600	GTP	C2-N3-C4	4.43	120.42	115.36
8	B	800	TZT	C25-O24-C23	-4.43	102.11	114.03
7	B	700	LOC	C11-N1-C12	4.42	127.30	122.44
4	C	600	GTP	PA-O3A-PB	-4.23	118.32	132.83
4	A	600	GTP	C2-N3-C4	4.21	120.17	115.36
6	B	600	GDP	PA-O3A-PB	-4.14	118.63	132.83
8	B	800	TZT	C42-N41-C39	4.12	129.93	122.59
7	D	700	LOC	O3-C5-C7	-4.02	117.21	124.12
7	B	700	LOC	C21-C22-C1	3.99	126.52	121.07
7	B	700	LOC	C10-C11-N1	-3.77	103.27	110.04
7	B	700	LOC	O3-C5-C7	-3.74	117.68	124.12
8	B	800	TZT	C30-N29-C33	-3.66	105.98	111.74
4	A	600	GTP	PB-O3B-PG	-3.62	120.42	132.83
7	B	700	LOC	O4-C12-N1	3.59	128.55	121.95
8	B	800	TZT	C3-N2-C4	-3.37	106.17	114.09
6	B	600	GDP	C6-C5-C4	-3.37	117.58	120.80
4	C	600	GTP	PB-O3B-PG	-3.35	121.32	132.83
8	B	800	TZT	C23-C26-C27	3.29	117.50	112.42
6	D	600	GDP	PA-O3A-PB	-3.22	121.76	132.83
7	B	700	LOC	O4-C12-C13	-3.19	116.13	122.06
7	D	700	LOC	O4-C12-N1	3.17	127.78	121.95
4	C	600	GTP	C5-C6-N1	-3.02	119.30	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	800	TZT	O9-C8-C4	-3.01	116.21	121.09
4	C	600	GTP	C6-N1-C2	2.97	120.66	115.93
6	B	600	GDP	C4-C5-N7	-2.96	106.32	109.40
8	B	800	TZT	O28-C27-N29	-2.94	115.17	121.54
6	B	600	GDP	C1'-N9-C4	-2.88	121.59	126.64
4	A	600	GTP	PA-O3A-PB	-2.84	123.07	132.83
8	B	800	TZT	C78-N17-C18	2.82	125.01	119.46
6	B	600	GDP	C6-N1-C2	2.78	120.35	115.93
7	D	700	LOC	C10-C11-N1	-2.78	105.05	110.04
7	D	700	LOC	C4-O2-C3	2.72	122.23	114.78
6	D	600	GDP	O3B-PB-O3A	2.68	113.63	104.64
6	D	600	GDP	C6-N1-C2	2.67	120.16	115.93
4	C	600	GTP	N2-C2-N1	2.66	121.39	117.25
8	B	800	TZT	C6-C5-C4	2.61	117.67	110.82
4	A	600	GTP	C5-C6-N1	-2.56	119.93	123.43
4	C	600	GTP	C1'-N9-C4	-2.53	122.19	126.64
6	D	600	GDP	C5-C6-N1	-2.42	120.13	123.43
6	B	600	GDP	O3B-PB-O3A	2.42	112.74	104.64
7	D	700	LOC	C9-C10-C11	2.30	115.34	112.29
6	B	600	GDP	O2B-PB-O3A	2.29	112.32	104.64
6	B	600	GDP	N2-C2-N1	2.26	120.76	117.25
6	D	600	GDP	C2'-C3'-C4'	2.26	107.03	102.64
6	B	600	GDP	C5-C6-N1	-2.23	120.38	123.43
4	C	600	GTP	C6-C5-C4	-2.19	118.71	120.80
4	C	600	GTP	C4-C5-N7	-2.10	107.21	109.40
6	D	600	GDP	C4-C5-N7	-2.07	107.24	109.40
4	A	600	GTP	C6-N1-C2	2.06	119.20	115.93
4	C	600	GTP	O2G-PG-O3B	2.05	111.52	104.64
6	B	600	GDP	C3'-C2'-C1'	2.01	104.01	100.98
8	B	800	TZT	C49-C44-C45	-2.01	115.00	118.17

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	600	GTP	C5'-O5'-PA-O1A
8	B	800	TZT	C8-C4-C5-C7
8	B	800	TZT	C5-C4-N2-C3
8	B	800	TZT	C5-C4-N2-C1
8	B	800	TZT	C8-C4-N2-C3
8	B	800	TZT	C8-C4-N2-C1
8	B	800	TZT	C5-C4-C8-O9

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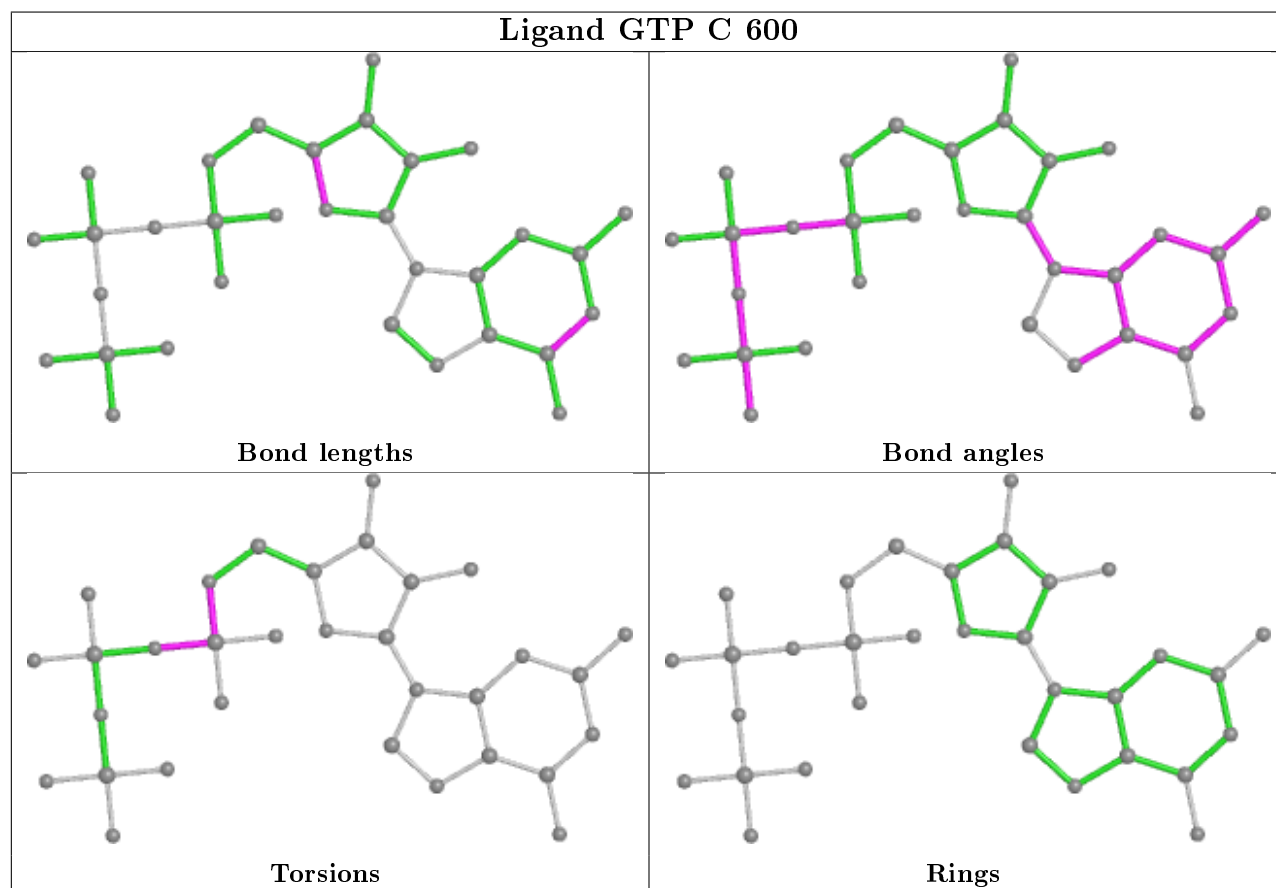
Mol	Chain	Res	Type	Atoms
8	B	800	TZT	C19-C18-N17-C15
8	B	800	TZT	C23-C18-N17-C15
8	B	800	TZT	C19-C18-N17-C78
8	B	800	TZT	C23-C18-N17-C78
8	B	800	TZT	C23-C26-C27-O28
8	B	800	TZT	C23-C26-C27-N29
8	B	800	TZT	C37-C34-O35-C36
8	B	800	TZT	O35-C34-C37-C38
6	B	600	GDP	O4'-C4'-C5'-O5'
6	B	600	GDP	C3'-C4'-C5'-O5'
6	D	600	GDP	O4'-C4'-C5'-O5'
6	D	600	GDP	C3'-C4'-C5'-O5'
4	A	600	GTP	C5'-O5'-PA-O1A
7	B	700	LOC	C7-C5-O3-C6
7	D	700	LOC	C7-C5-O3-C6
7	B	700	LOC	C3-C5-O3-C6
7	D	700	LOC	C3-C5-O3-C6
8	B	800	TZT	N41-C42-C43-C44
8	B	800	TZT	N2-C4-C5-C6
8	B	800	TZT	C8-C4-C5-C6
8	B	800	TZT	C12-C11-N10-C8
8	B	800	TZT	C15-C11-N10-C8
8	B	800	TZT	C18-C19-C20-C21
8	B	800	TZT	N2-C4-C5-C7
8	B	800	TZT	C5-C4-C8-N10
4	C	600	GTP	C5'-O5'-PA-O3A
8	B	800	TZT	O24-C23-C26-C27
4	A	600	GTP	C5'-O5'-PA-O3A
8	B	800	TZT	C22-C19-C20-C21
4	C	600	GTP	C5'-O5'-PA-O2A
4	A	600	GTP	C5'-O5'-PA-O2A
8	B	800	TZT	C32-C33-C34-C37
8	B	800	TZT	N29-C33-C34-C37
8	B	800	TZT	C33-C34-C37-C38
8	B	800	TZT	C33-C34-O35-C36
8	B	800	TZT	C38-C37-C39-O40
8	B	800	TZT	C38-C37-C39-N41
4	C	600	GTP	PB-O3A-PA-O2A
4	A	600	GTP	PB-O3A-PA-O1A
4	A	600	GTP	PB-O3A-PA-O2A
6	B	600	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

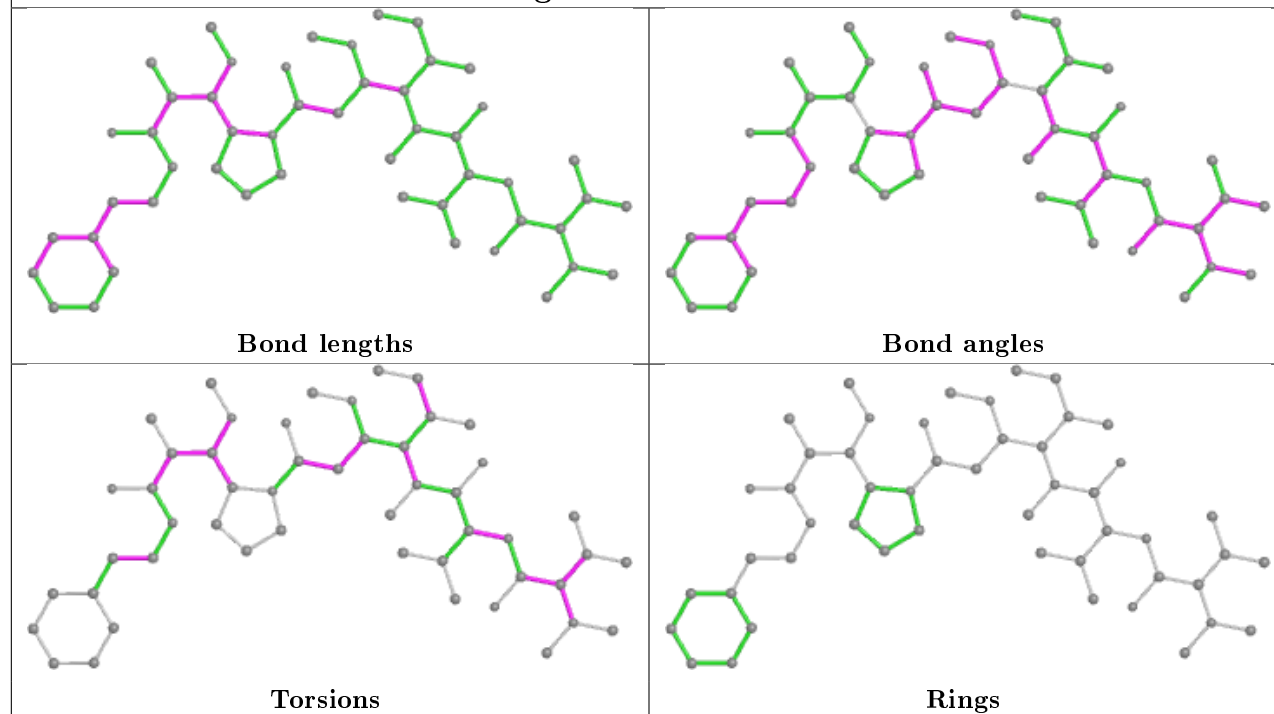
7 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	600	GTP	6	0
8	B	800	TZT	30	0
6	B	600	GDP	4	0
6	D	600	GDP	1	0
7	B	700	LOC	3	0
7	D	700	LOC	3	0
4	A	600	GTP	4	0

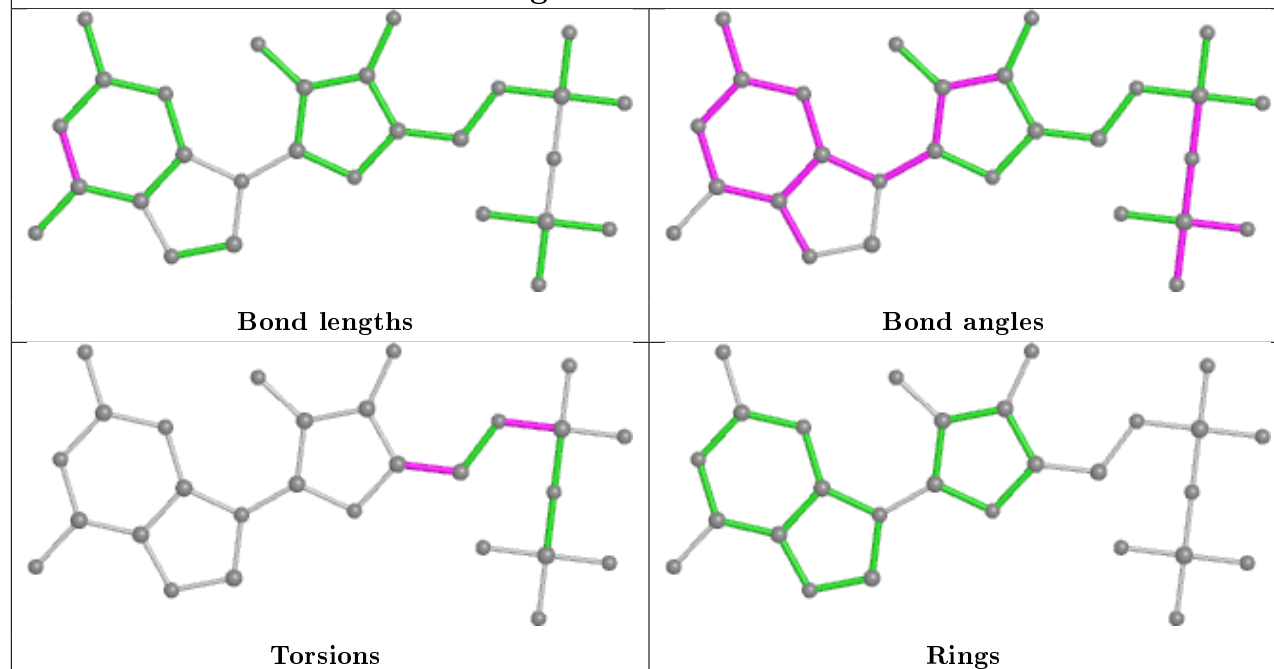
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

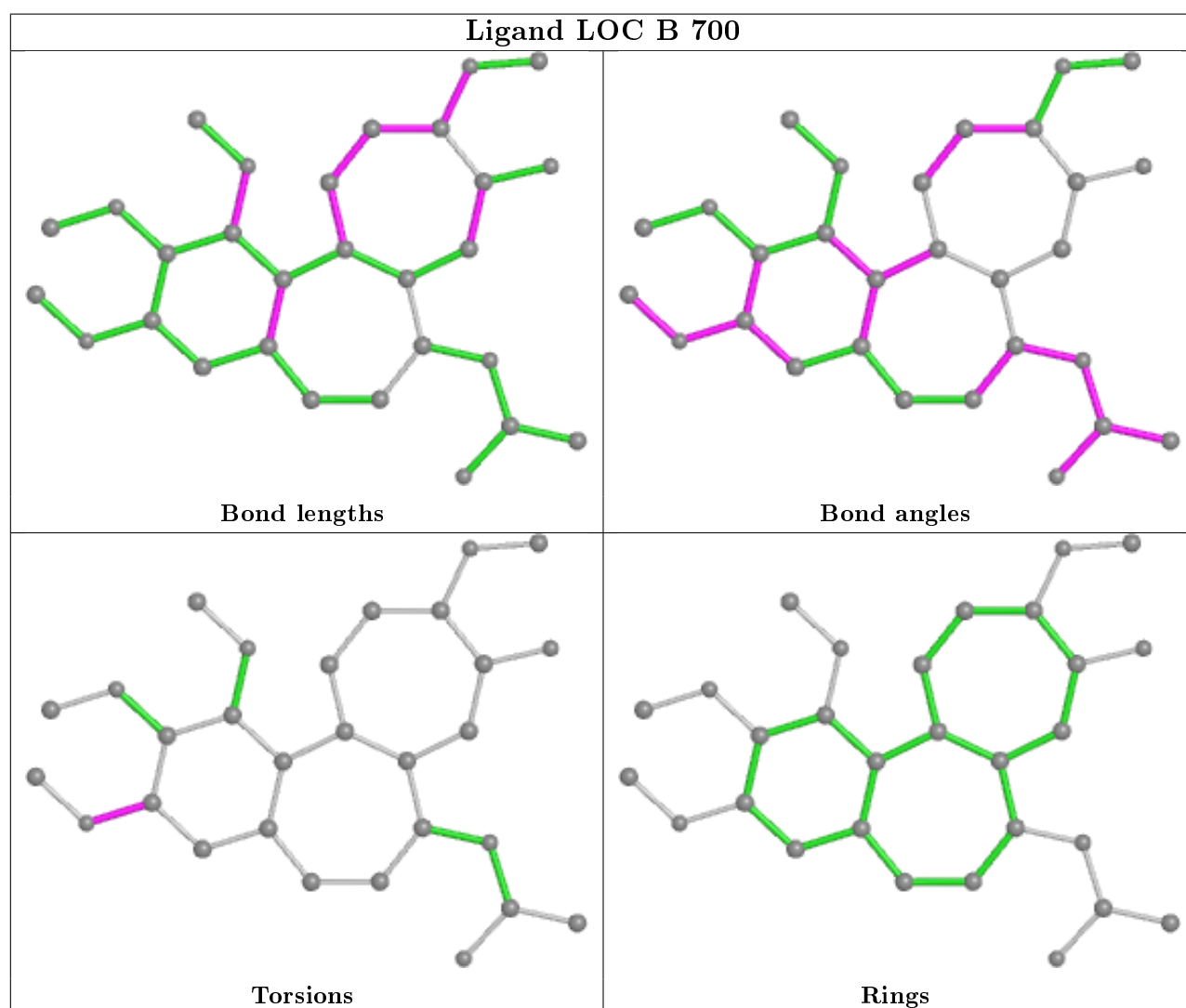
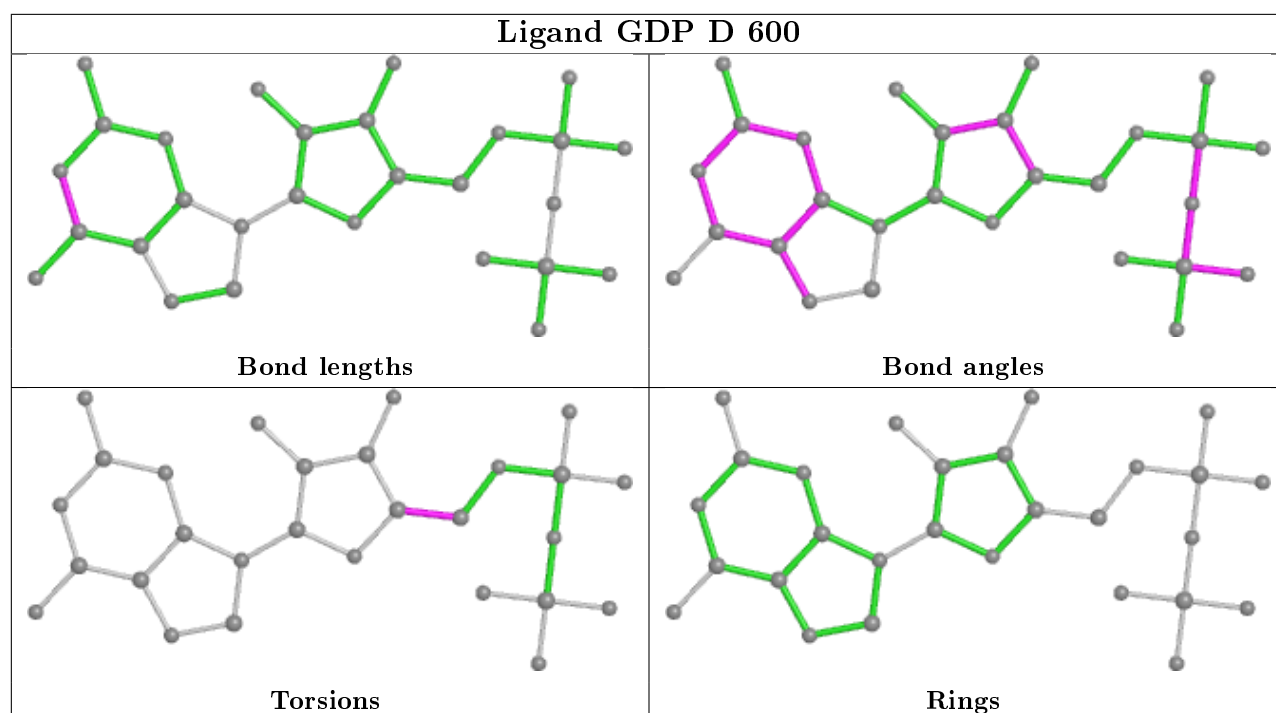


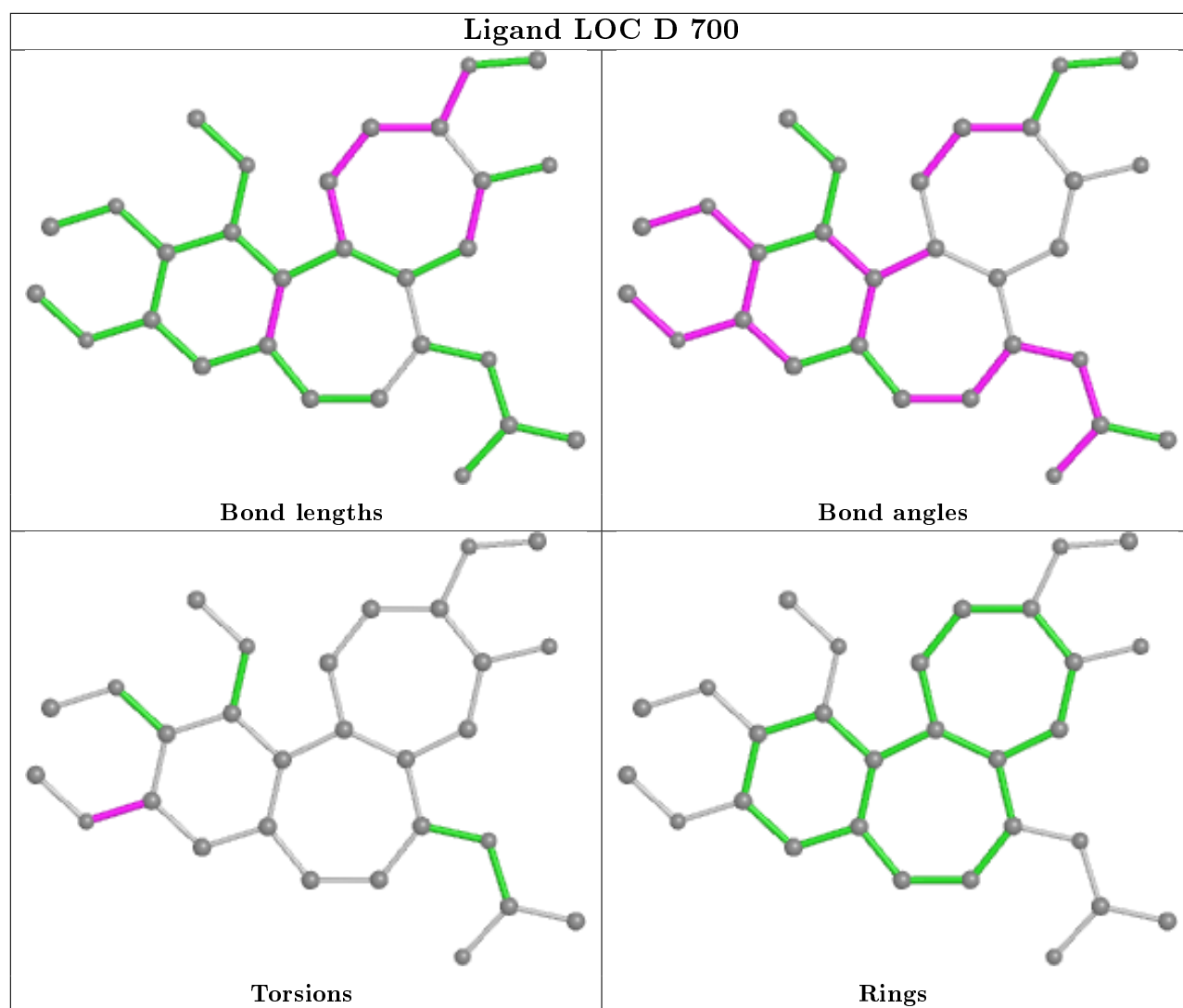
Ligand TZT B 800

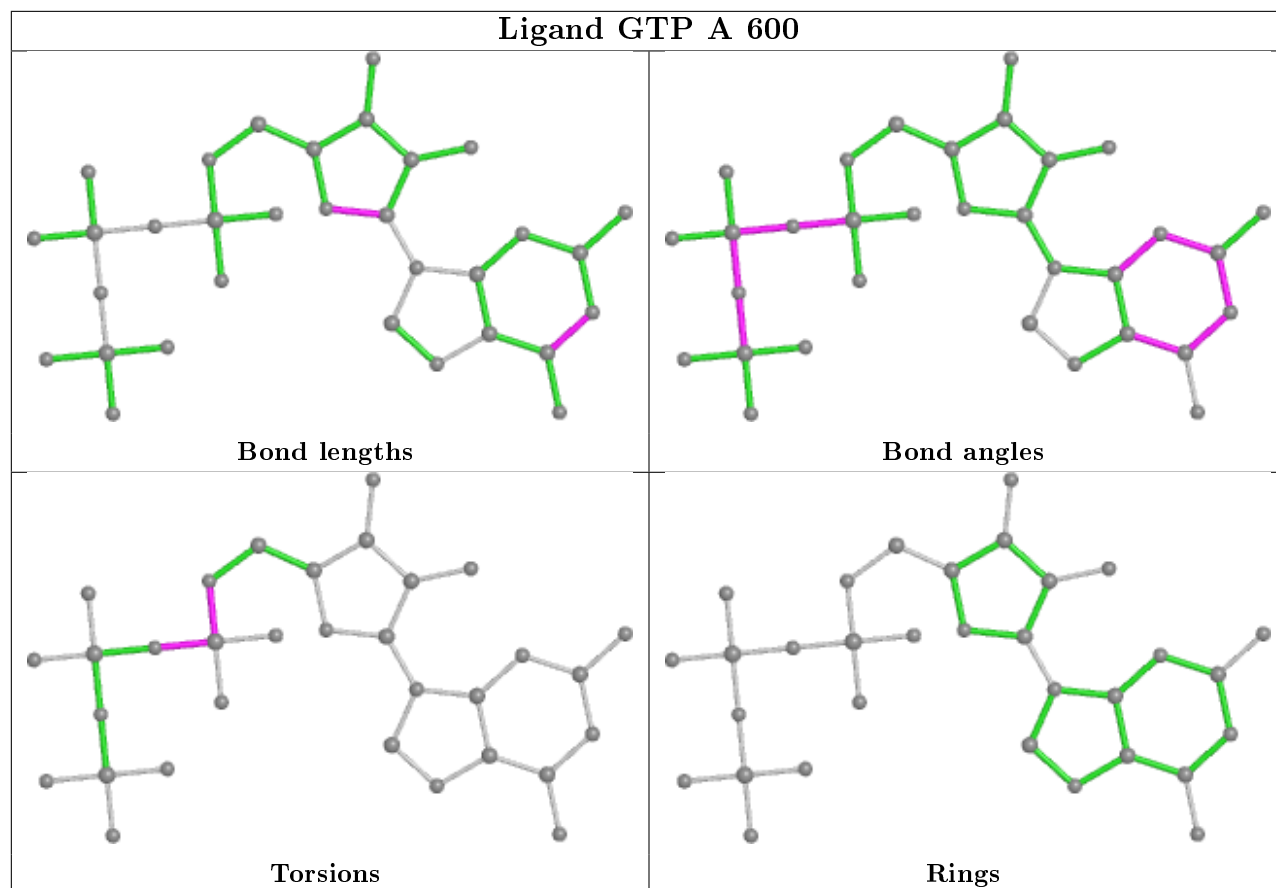


Ligand GDP B 600









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	427/449 (95%)	-0.62	0 100 100	91, 95, 97, 103	0
1	C	421/449 (93%)	-0.34	7 (1%) 70 62	94, 95, 96, 98	1 (0%)
2	B	419/445 (94%)	-0.49	2 (0%) 91 87	94, 95, 96, 97	0
2	D	419/445 (94%)	-0.29	10 (2%) 59 50	94, 95, 96, 96	0
3	E	124/142 (87%)	-0.38	1 (0%) 86 81	91, 95, 97, 99	0
All	All	1810/1930 (93%)	-0.43	20 (1%) 80 74	91, 95, 96, 103	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	304	LYS	3.5
1	C	305	CYS	3.4
1	C	306	ASP	3.3
2	D	299	LYS	3.3
1	C	6	SER	3.2
2	D	6	HIS	3.2
3	E	30	ASP	3.0
2	D	381	SER	2.8
1	C	300	ASN	2.8
2	D	39	ASP	2.8
2	D	371	LEU	2.8
2	B	271	GLY	2.7
2	D	85	GLN	2.5
1	C	380	ASN	2.4
2	D	276	THR	2.4
2	D	380	ASN	2.3
1	C	37	PRO	2.2
2	D	370	GLY	2.1
2	D	179	ASP	2.1
2	B	380	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

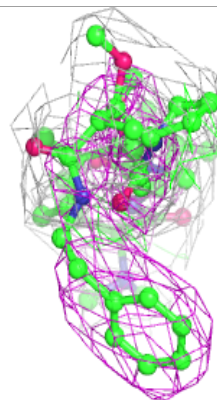
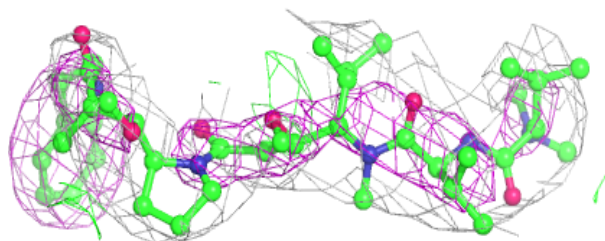
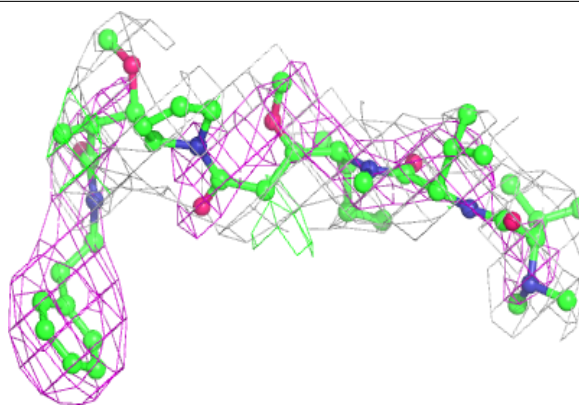
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	TZT	B	800	50/50	0.82	0.33	92,94,102,102	0
6	GDP	D	600	28/28	0.91	0.23	95,95,95,95	0
6	GDP	B	600	28/28	0.92	0.23	94,95,95,96	0
4	GTP	C	600	32/32	0.92	0.20	94,95,95,95	0
7	LOC	B	700	29/29	0.94	0.28	95,95,95,95	0
7	LOC	D	700	29/29	0.94	0.33	94,95,95,95	0
4	GTP	A	600	32/32	0.94	0.15	94,95,95,96	0
5	MG	C	601	1/1	0.96	0.20	96,96,96,96	0
5	MG	A	601	1/1	0.98	0.24	93,93,93,93	0

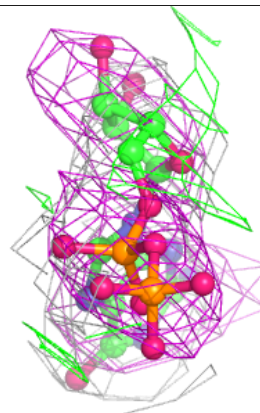
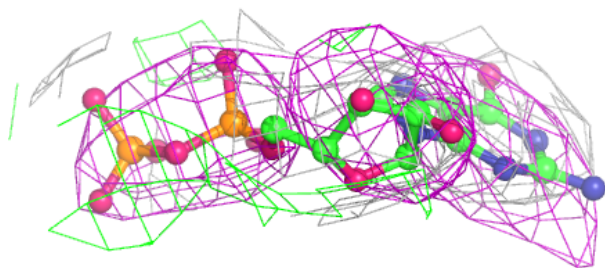
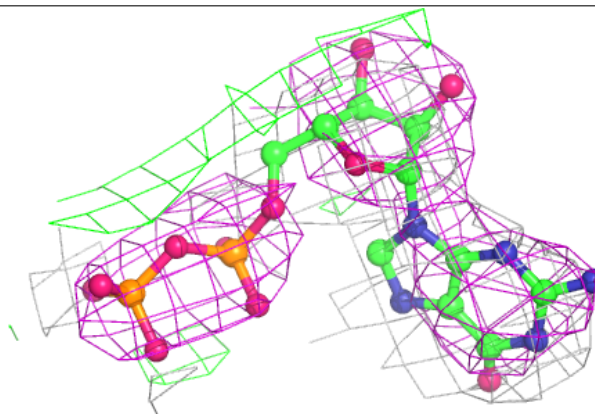
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TZT B 800:

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

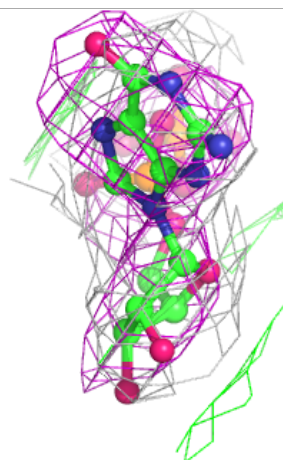
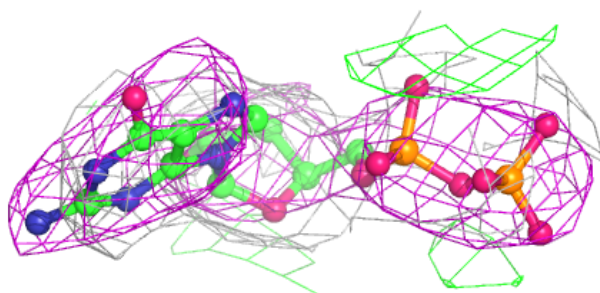
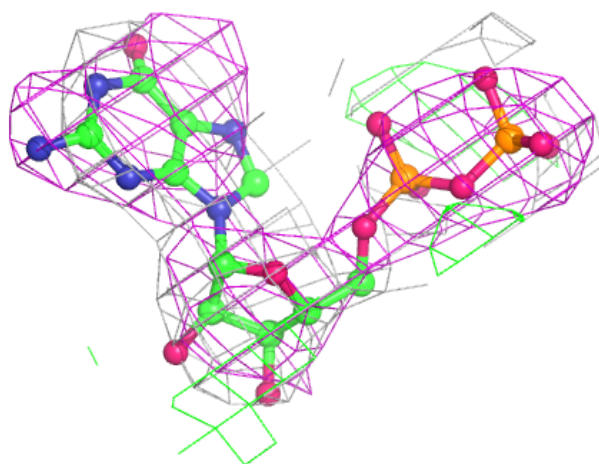
**Electron density around GDP D 600:**

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



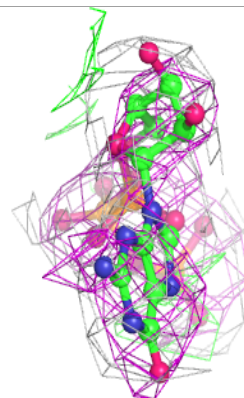
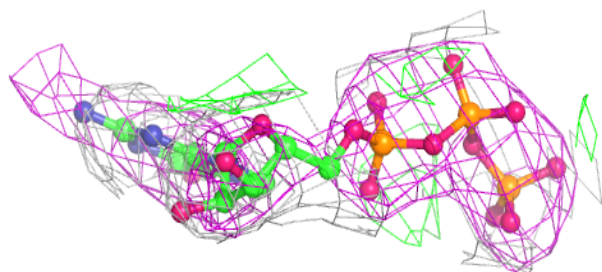
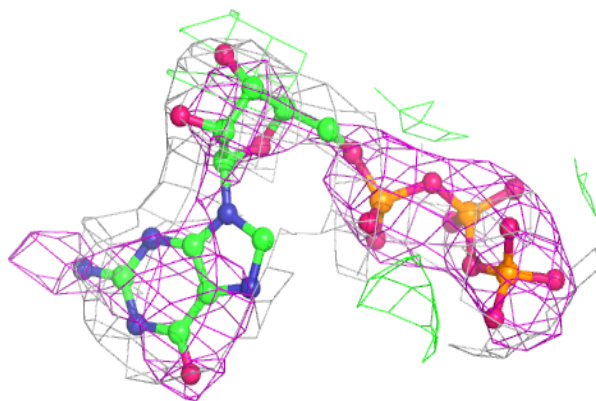
Electron density around GDP B 600:

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

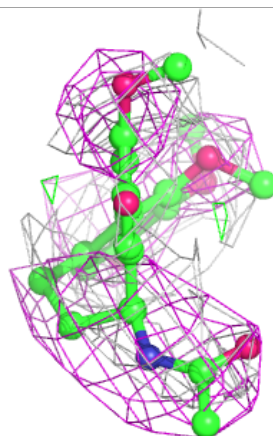
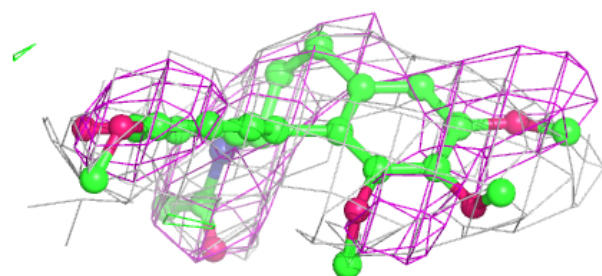
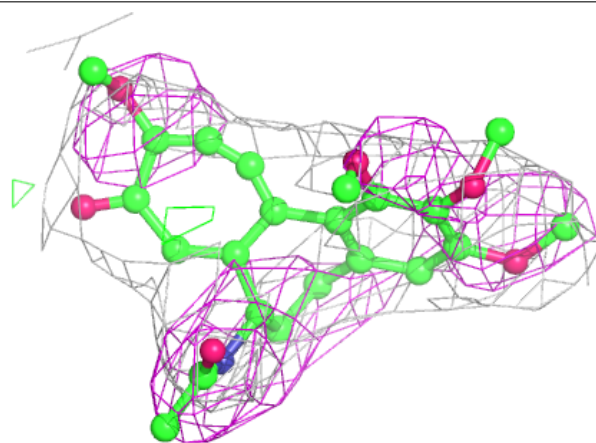


Electron density around GTP C 600:

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

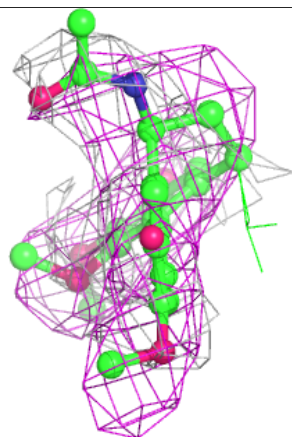
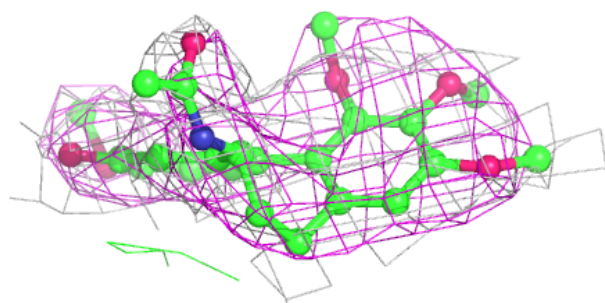
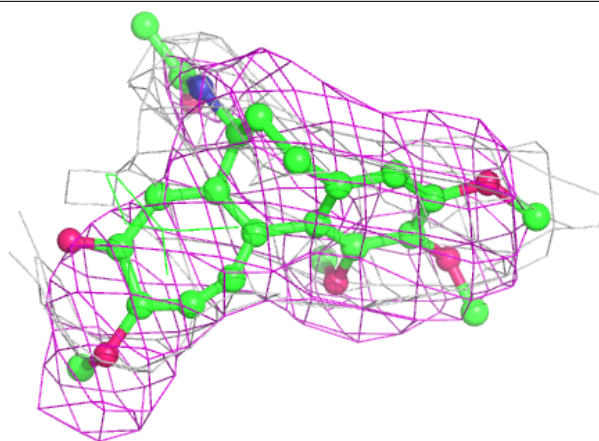
**Electron density around LOC B 700:**

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

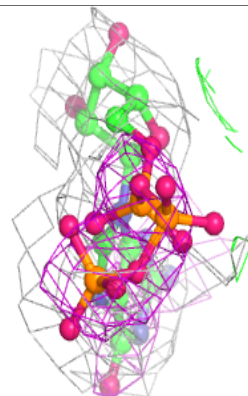
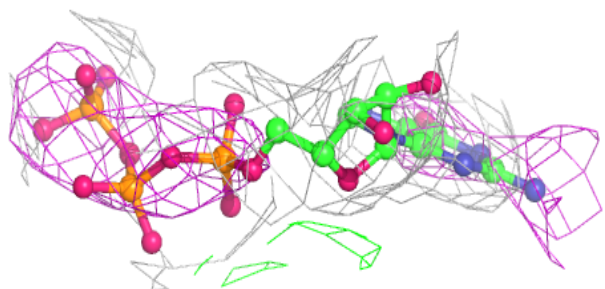
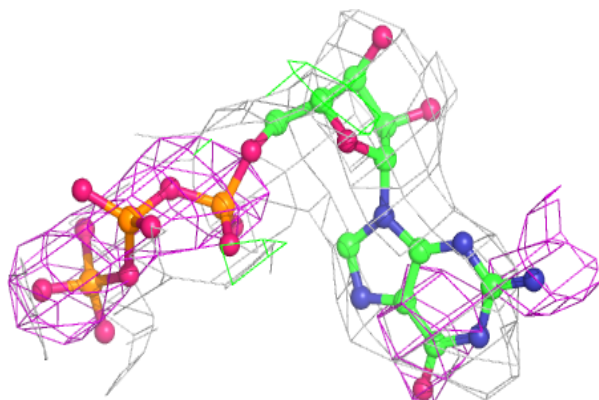


Electron density around LOC D 700:

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

**Electron density around GTP A 600:**

$2mF_o-DF_c$ (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.