



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 09:24 am BST

PDB ID : 1Z2B
Title : Tubulin-colchicine-vinblastine: stathmin-like domain complex
Authors : Gigant, B.; Wang, C.; Ravelli, R.B.G.; Roussi, F.; Steinmetz, M.O.; Curmi, P.A.; Sobel, A.; Knossow, M.
Deposited on : 2005-03-08
Resolution : 4.10 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

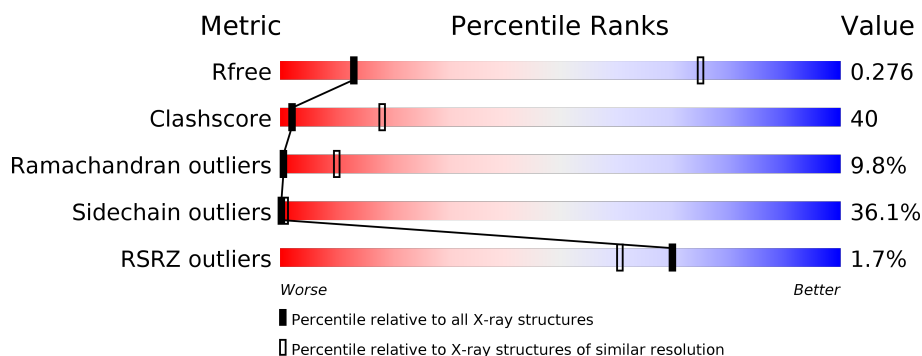
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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	448	<div> <div></div> <div> <div>32%</div> <div>43%</div> <div>18%</div> <div>• 5%</div> </div> </div>
1	C	448	<div> <div>2%</div> <div> <div>33%</div> <div>42%</div> <div>18%</div> <div>• 5%</div> </div> </div>
2	B	445	<div> <div>2%</div> <div> <div>30%</div> <div>38%</div> <div>24%</div> <div>• 6%</div> </div> </div>
2	D	445	<div> <div>2%</div> <div> <div>29%</div> <div>40%</div> <div>23%</div> <div>• 6%</div> </div> </div>
3	E	142	<div> <div>•</div> <div> <div>33%</div> <div>35%</div> <div>16%</div> <div>• 13%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	VLB	C	800	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14173 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3290	2091	556	622	21			
1	C	427	Total	C	N	O	S	38	0	0
			3248	2058	552	618	20			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ILE	VAL	SEE REMARK 999	GB 59858433
A	16	ILE	MET	SEE REMARK 999	GB 59858433
A	50	ASN	THR	SEE REMARK 999	GB 59858433
A	54	SER	CYS	SEE REMARK 999	GB 59858433
A	78	VAL	ILE	SEE REMARK 999	GB 59858433
A	80	THR	ASN	SEE REMARK 999	GB 59858433
A	82	THR	PRO	SEE REMARK 999	GB 59858433
A	117	LEU	PRO	SEE REMARK 999	GB 59858433
A	126	ALA	SER	SEE REMARK 999	GB 59858433
A	232	GLY	SER	SEE REMARK 999	GB 59858433
A	334	THR	ALA	SEE REMARK 999	GB 59858433
C	7	ILE	VAL	SEE REMARK 999	GB 59858433
C	16	ILE	MET	SEE REMARK 999	GB 59858433
C	50	ASN	THR	SEE REMARK 999	GB 59858433
C	54	SER	CYS	SEE REMARK 999	GB 59858433
C	78	VAL	ILE	SEE REMARK 999	GB 59858433
C	80	THR	ASN	SEE REMARK 999	GB 59858433
C	82	THR	PRO	SEE REMARK 999	GB 59858433
C	117	LEU	PRO	SEE REMARK 999	GB 59858433
C	126	ALA	SER	SEE REMARK 999	GB 59858433
C	232	GLY	SER	SEE REMARK 999	GB 59858433
C	334	THR	ALA	SEE REMARK 999	GB 59858433

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3240	2038	546	632	24			
2	D	419	Total	C	N	O	S	0	0	0
			3237	2037	544	632	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	172	VAL	MET	SEE REMARK 999	GB 50844501
B	318	VAL	ILE	SEE REMARK 999	GB 50844501
D	172	VAL	MET	SEE REMARK 999	GB 50844501
D	318	VAL	ILE	SEE REMARK 999	GB 50844501

- Molecule 3 is a protein called RB3 STATHMIN-LIKE DOMAIN 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			917	555	174	183	5			

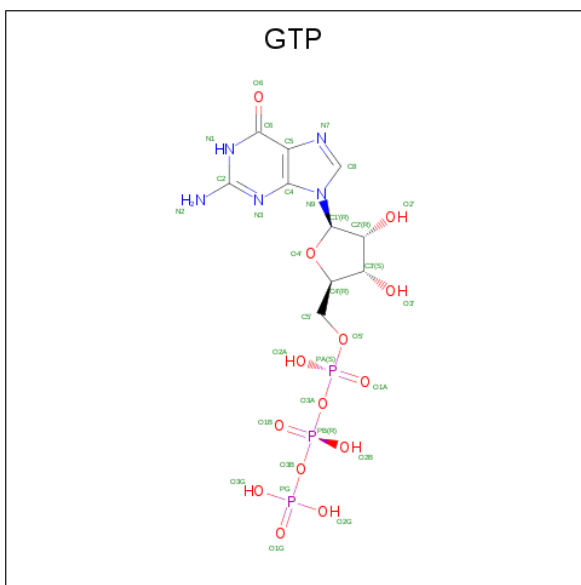
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	SEE REMARK 999	UNP P63043

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

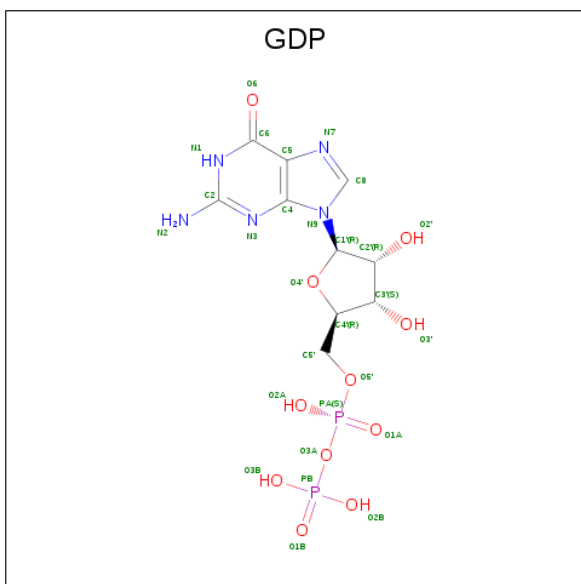
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



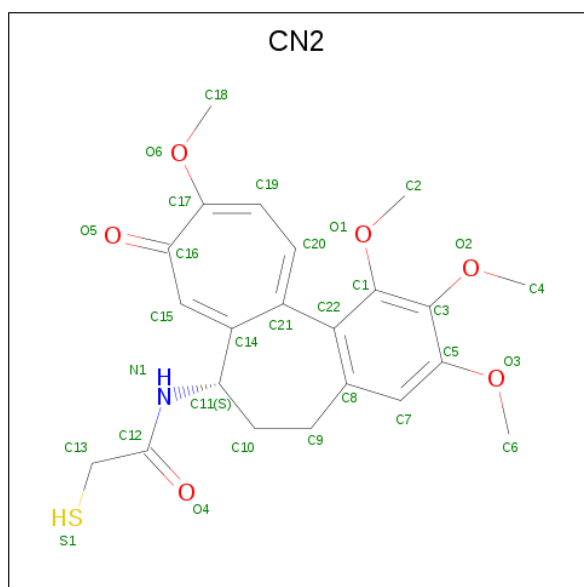
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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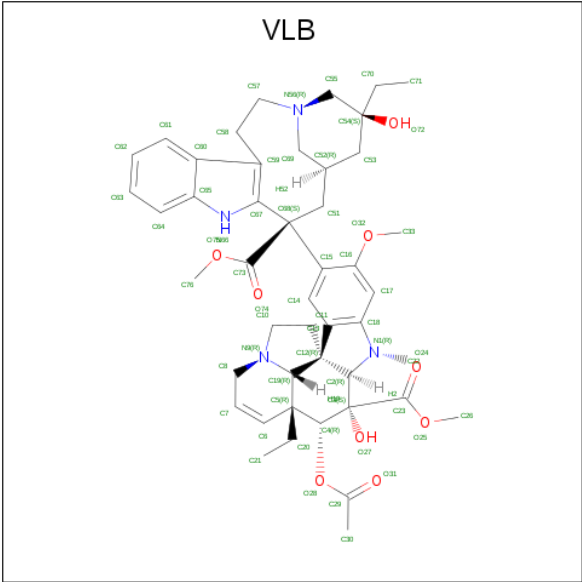
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 7 is 2-MERCAPTO-N-[1,2,3,10-TETRAMETHOXY-9-OXO-5,6,7,9-TETRAHYDRO-BENZO[A]HEPTALEN-7-YL]ACETAMIDE (three-letter code: CN2) (formula: $C_{22}H_{25}NO_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			30	22	1	6	1		
7	D	1	Total	C	N	O	S	0	0
			30	22	1	6	1		

- Molecule 8 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (three-letter code: VLB) (formula: $C_{46}H_{58}N_4O_9$).

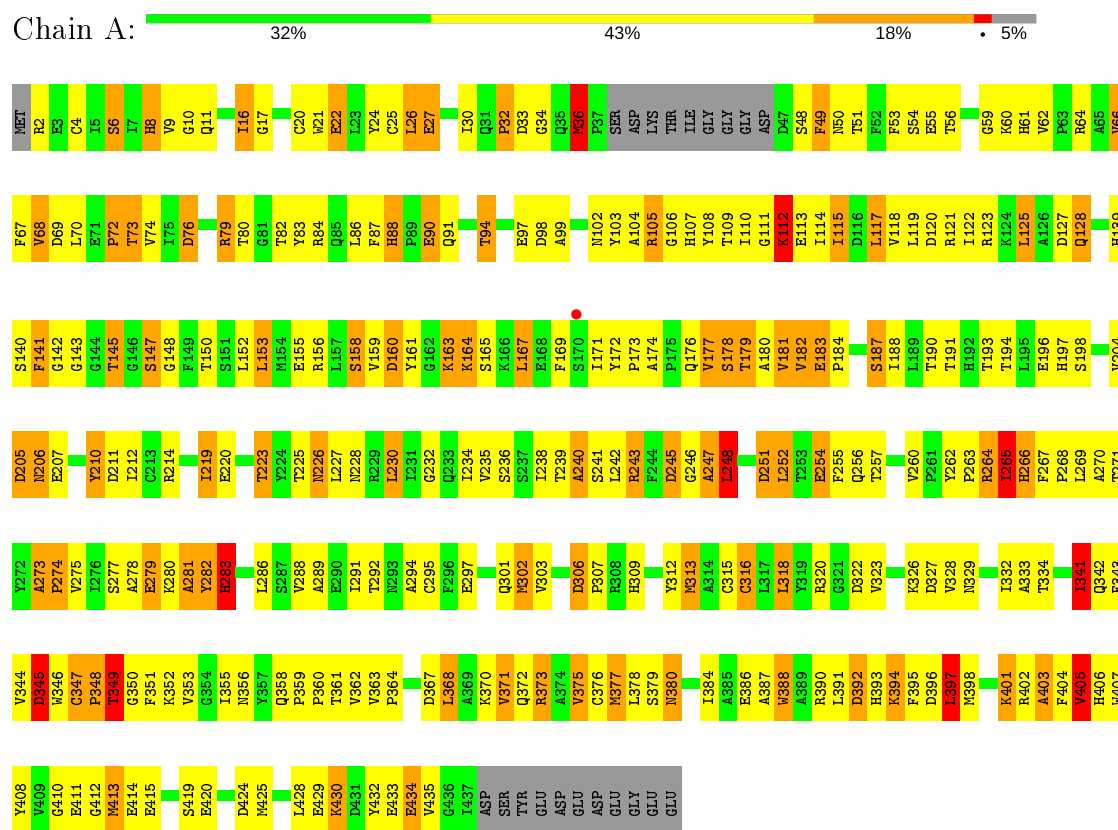


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			59	46	4	9		

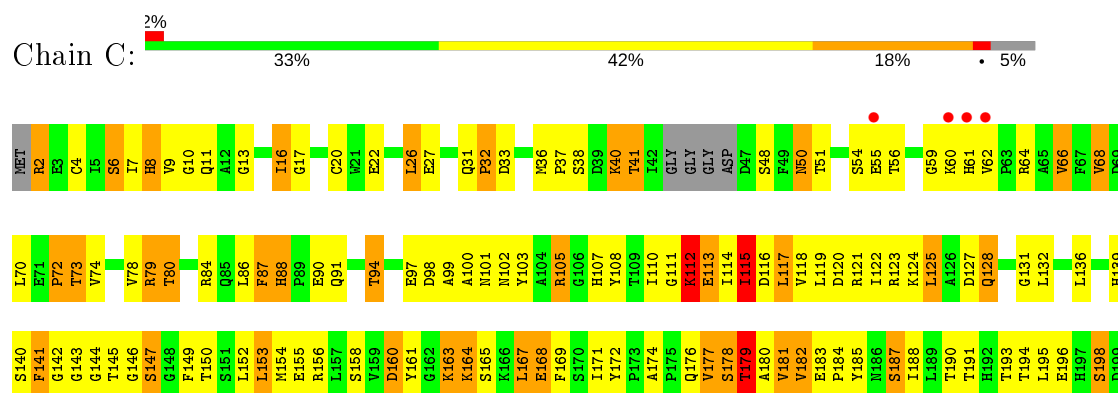
3 Residue-property plots

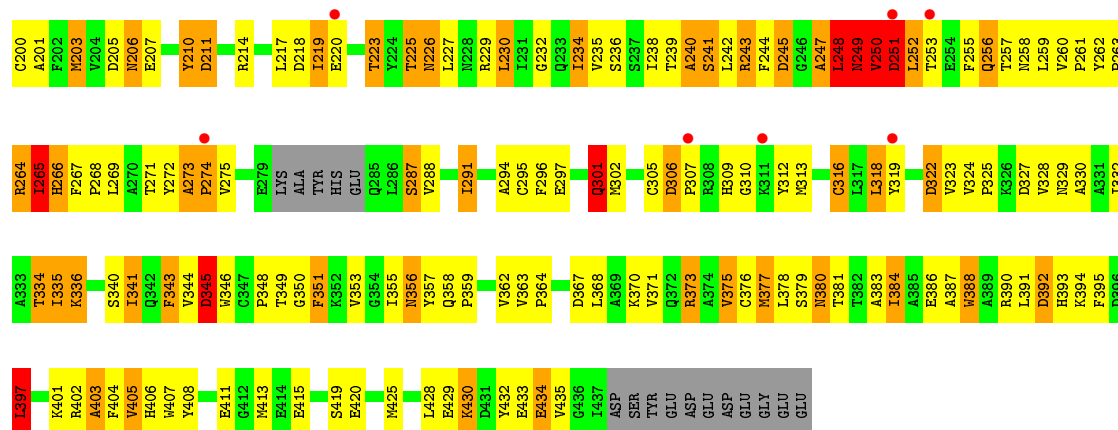
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

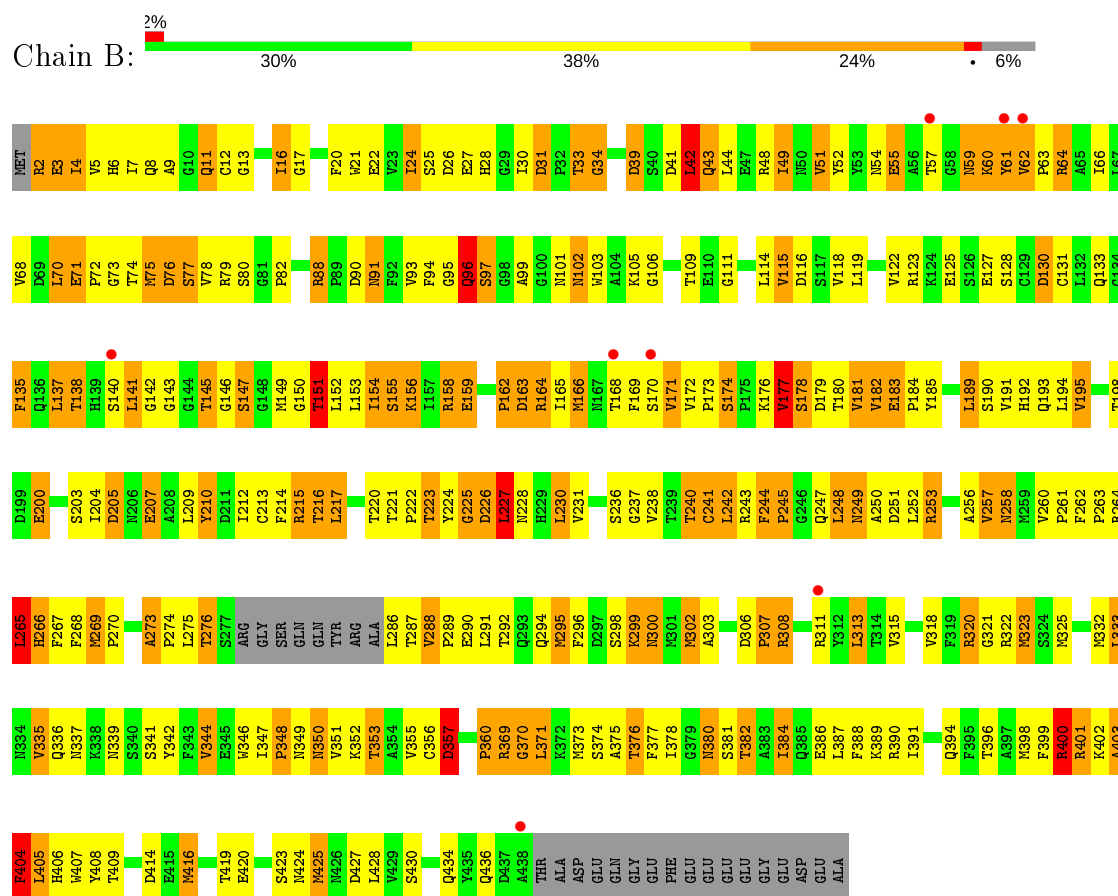


• Molecule 1: Tubulin alpha chain

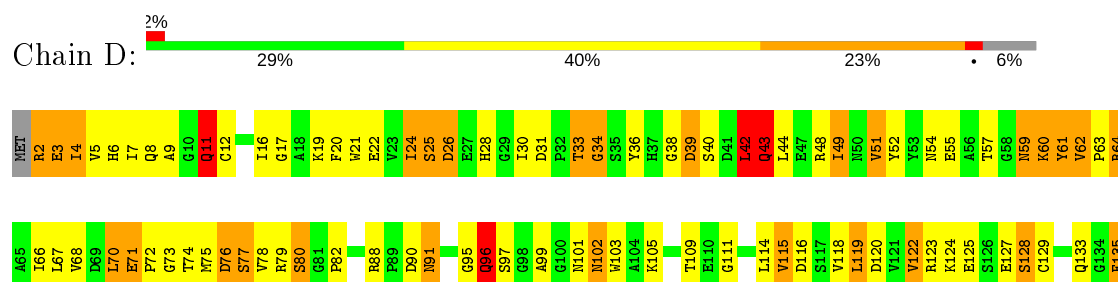


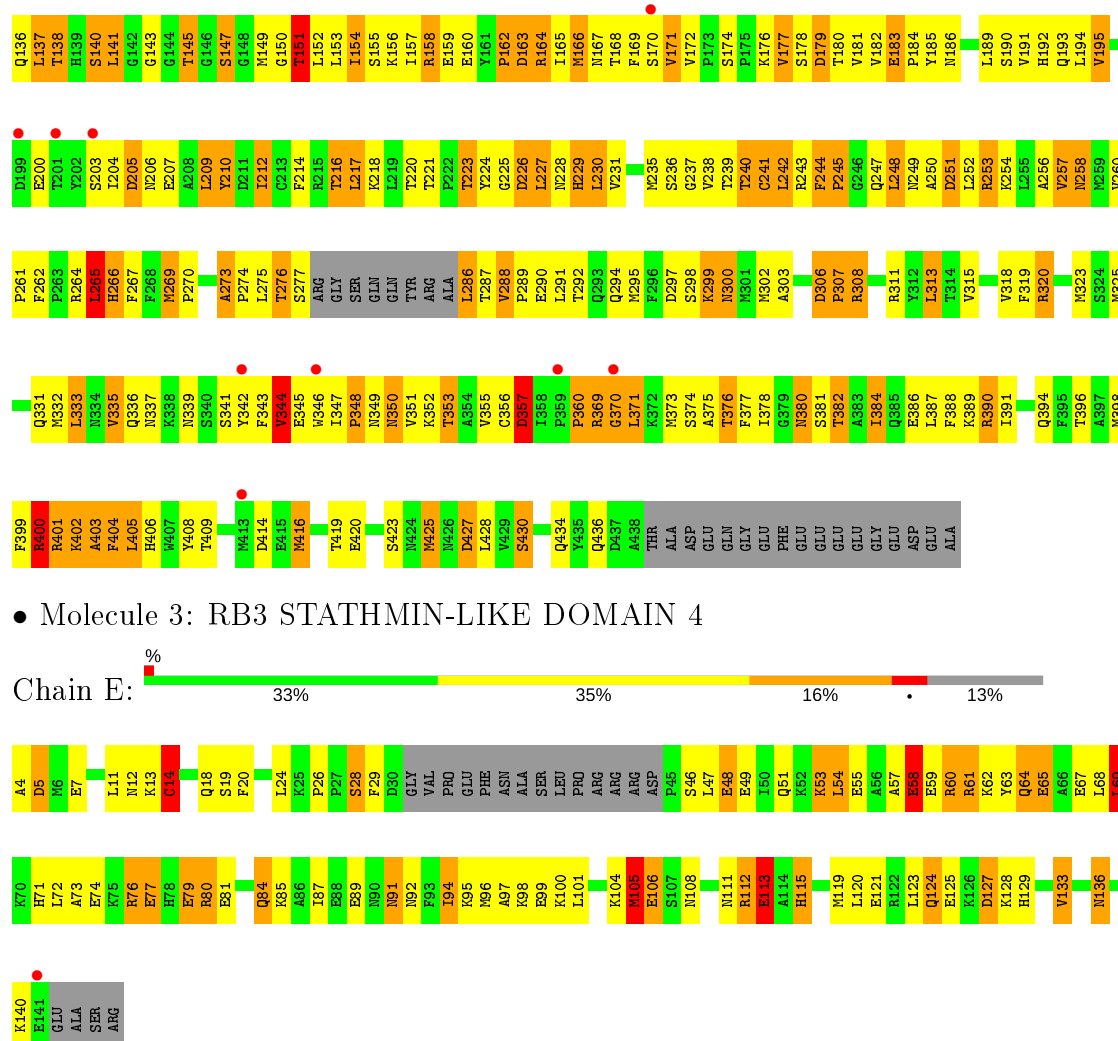


• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	324.85Å 324.85Å 54.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.10 38.31 – 4.09	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-4.10) 94.7 (38.31-4.09)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 4.13Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.209 , 0.269 0.211 , 0.276	Depositor DCC
R_{free} test set	1283 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	197.5	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 195.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14173	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: GDP, GTP, MG, VLB, CN2

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	0.80	1/3367 (0.0%)	0.97	12/4579 (0.3%)
1	C	0.79	3/3320 (0.1%)	1.02	16/4520 (0.4%)
2	B	0.75	0/3312	0.97	9/4498 (0.2%)
2	D	0.73	0/3309	1.00	13/4494 (0.3%)
3	E	0.73	1/925 (0.1%)	0.92	3/1241 (0.2%)
All	All	0.76	5/14233 (0.0%)	0.98	53/19332 (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	1
1	C	0	4
2	B	0	1
2	D	0	1
3	E	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	306	ASP	C-N	-6.13	1.22	1.34
3	E	105	MET	SD-CE	5.45	2.08	1.77
1	A	36	MET	SD-CE	5.41	2.08	1.77
1	C	203	MET	SD-CE	5.34	2.07	1.77
1	C	168	GLU	CD-OE1	5.03	1.31	1.25

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	301	GLN	O-C-N	-14.33	99.77	122.70
1	C	120	ASP	CB-CG-OD2	7.82	125.33	118.30
1	C	301	GLN	CA-C-N	7.40	133.48	117.20
1	C	160	ASP	CB-CG-OD2	7.29	124.86	118.30
1	A	205	ASP	CB-CG-OD2	7.25	124.83	118.30
2	D	357	ASP	CB-CG-OD2	7.15	124.74	118.30
2	B	26	ASP	CB-CG-OD2	7.00	124.60	118.30
1	C	211	ASP	CB-CG-OD2	6.97	124.58	118.30
1	A	120	ASP	CB-CG-OD2	6.97	124.58	118.30
1	C	250	VAL	N-CA-C	6.71	129.12	111.00
2	D	163	ASP	CB-CG-OD2	6.49	124.14	118.30
1	C	251	ASP	CB-CG-OD2	6.38	124.04	118.30
2	B	130	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	397	LEU	CA-CB-CG	6.27	129.72	115.30
2	B	242	LEU	CA-CB-CG	6.20	129.57	115.30
1	C	397	LEU	CA-CB-CG	6.20	129.57	115.30
1	C	322	ASP	CB-CG-OD2	6.18	123.87	118.30
1	A	322	ASP	CB-CG-OD2	6.08	123.78	118.30
1	C	345	ASP	CB-CG-OD2	5.98	123.69	118.30
2	D	205	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	69	ASP	CB-CG-OD2	5.84	123.55	118.30
2	D	120	ASP	CB-CG-OD2	5.82	123.54	118.30
2	D	306	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	349	THR	N-CA-C	-5.74	95.50	111.00
2	D	26	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	249	ASN	N-CA-C	5.72	126.44	111.00
3	E	106	GLU	N-CA-C	-5.61	95.84	111.00
1	A	345	ASP	CB-CG-OD2	5.58	123.33	118.30
2	B	205	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	160	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	248	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	76	ASP	CB-CG-OD2	5.52	123.27	118.30
2	D	226	ASP	CB-CG-OD2	5.51	123.26	118.30
2	D	39	ASP	CB-CG-OD2	5.49	123.24	118.30
2	D	31	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	245	ASP	CB-CG-OD2	5.43	123.18	118.30
3	E	69	LEU	CA-CB-CG	5.42	127.78	115.30
2	B	31	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	218	ASP	CB-CG-OD2	5.42	123.18	118.30
2	D	242	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	424	ASP	CB-CG-OD2	5.34	123.11	118.30
2	D	427	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	392	ASP	CB-CG-OD2	5.32	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	392	ASP	CB-CG-OD2	5.30	123.07	118.30
3	E	54	LEU	CA-CB-CG	5.25	127.39	115.30
1	C	205	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	163	ASP	CB-CG-OD2	5.18	122.97	118.30
2	B	39	ASP	CB-CG-OD2	5.15	122.93	118.30
2	D	297	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	306	ASP	CB-CG-OD2	5.14	122.92	118.30
2	B	357	ASP	CB-CG-OD2	5.12	122.91	118.30
2	D	179	ASP	CB-CG-OD2	5.10	122.89	118.30
2	B	226	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	VAL	Peptide
2	B	162	PRO	Peptide
1	C	177	VAL	Peptide
1	C	248	LEU	Peptide
1	C	249	ASN	Peptide
1	C	301	GLN	Mainchain
2	D	162	PRO	Peptide
3	E	5	ASP	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	3154	240	0
1	C	3248	0	3087	258	0
2	B	3240	0	3056	300	0
2	D	3237	0	3054	272	0
3	E	917	0	803	66	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	12	4	0
5	C	32	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	28	0	12	5	0
6	D	28	0	12	7	0
7	B	30	0	23	7	0
7	D	30	0	23	8	0
8	C	59	0	58	21	0
All	All	14173	0	13306	1096	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 40.

All (1096) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:MET:CE	1:C:203:MET:SD	2.07	1.42
1:A:36:MET:CE	1:A:36:MET:SD	2.08	1.40
3:E:105:MET:SD	3:E:105:MET:CE	2.08	1.39
2:B:241:CYS:HB3	2:B:247:GLN:NE2	1.55	1.20
1:A:346:TRP:O	1:A:346:TRP:HE3	1.27	1.17
1:C:329:ASN:HA	8:C:800:VLB:H211	1.19	1.15
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.29	1.14
1:A:273:ALA:CB	1:A:274:PRO:HD3	1.79	1.13
2:B:401:ARG:HG3	2:B:401:ARG:HH11	0.96	1.12
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.30	1.12
1:A:270:ALA:HB3	1:A:302:MET:HE2	1.30	1.12
2:D:241:CYS:HB3	2:D:247:GLN:NE2	1.63	1.12
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.30	1.11
1:A:79:ARG:HH22	1:A:94:THR:HG21	0.99	1.10
2:B:133:GLN:HE21	2:B:252:LEU:HB3	1.12	1.09
1:C:79:ARG:HH22	1:C:94:THR:HG21	0.97	1.08
2:D:223:THR:HB	2:D:225:GLY:H	1.14	1.07
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.19	1.07
1:A:8:HIS:CD2	1:A:17:GLY:HA3	1.90	1.07
1:A:278:ALA:O	1:A:279:GLU:HB3	1.52	1.06
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.09	1.05
2:D:401:ARG:HH11	2:D:401:ARG:HG3	0.94	1.05
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.37	1.04
1:C:8:HIS:CD2	1:C:17:GLY:HA3	1.93	1.04
1:C:8:HIS:HD2	1:C:17:GLY:HA3	1.21	1.03
2:D:133:GLN:HE21	2:D:252:LEU:HB3	1.22	1.02
1:C:79:ARG:HH22	1:C:94:THR:CG2	1.72	1.01
1:A:346:TRP:CE3	1:A:346:TRP:O	2.14	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:241:CYS:HB3	2:D:247:GLN:HE21	1.18	1.00
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.90	0.99
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.44	0.98
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.94	0.97
1:C:206:ASN:HD21	5:C:601:GTP:N2	1.62	0.97
1:C:79:ARG:NH2	1:C:94:THR:HG21	1.80	0.96
2:B:156:LYS:HG2	3:E:76:ARG:NH2	1.80	0.96
1:A:8:HIS:HD2	1:A:17:GLY:HA3	1.19	0.95
1:C:273:ALA:CB	1:C:274:PRO:HD3	1.94	0.95
1:A:273:ALA:HB3	1:A:274:PRO:CD	1.96	0.95
1:A:79:ARG:HH22	1:A:94:THR:CG2	1.78	0.95
1:C:206:ASN:HD21	5:C:601:GTP:HN22	0.97	0.95
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.28	0.95
2:B:241:CYS:CB	2:B:247:GLN:HE21	1.80	0.94
1:C:264:ARG:O	1:C:266:HIS:CD2	2.21	0.94
2:B:241:CYS:HB3	2:B:247:GLN:HE21	1.17	0.94
1:A:79:ARG:NH2	1:A:94:THR:HG21	1.83	0.93
2:B:352:LYS:HG3	7:B:700:CN2:O5	1.69	0.93
2:D:165:ILE:HD11	2:D:252:LEU:HG	1.52	0.91
2:B:247:GLN:HG3	2:B:248:LEU:HG	1.50	0.91
1:A:206:ASN:HD21	5:A:600:GTP:HN22	0.96	0.91
2:B:287:THR:HG22	2:B:290:GLU:HB2	1.53	0.91
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.52	0.91
2:D:247:GLN:HG3	2:D:248:LEU:HG	1.53	0.90
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.34	0.90
2:D:172:VAL:HG11	2:D:387:LEU:HD21	1.51	0.90
2:D:401:ARG:NH1	2:D:401:ARG:HG3	1.72	0.90
1:A:273:ALA:CB	1:A:375:VAL:H	1.84	0.90
8:C:800:VLB:H572	8:C:800:VLB:O72	1.70	0.90
2:B:401:ARG:HG3	2:B:401:ARG:NH1	1.75	0.89
1:C:99:ALA:HB2	1:C:145:THR:HG22	1.55	0.89
1:A:115:ILE:HG13	1:A:152:LEU:HD23	1.54	0.89
2:B:54:ASN:HB2	2:B:64:ARG:HD3	1.55	0.89
1:C:265:ILE:HG23	1:C:267:PHE:CZ	2.08	0.89
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.55	0.88
2:B:133:GLN:NE2	2:B:252:LEU:HB3	1.88	0.88
2:B:177:VAL:HA	8:C:800:VLB:H532	1.56	0.87
1:C:98:ASP:OD1	1:C:99:ALA:N	2.06	0.87
1:A:270:ALA:HB3	1:A:302:MET:CE	2.05	0.86
2:D:291:LEU:HD21	2:D:375:ALA:CB	2.03	0.86
1:A:99:ALA:HB2	1:A:145:THR:CG2	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:HD21	5:A:600:GTP:N2	1.73	0.86
1:C:178:SER:HB3	7:D:701:CN2:S1	2.16	0.86
2:D:287:THR:HG22	2:D:290:GLU:HB2	1.57	0.86
1:C:234:ILE:HD11	1:C:272:TYR:HB2	1.57	0.86
1:C:206:ASN:ND2	5:C:601:GTP:HN22	1.74	0.86
1:A:98:ASP:OD1	1:A:99:ALA:N	2.09	0.85
1:C:329:ASN:HA	8:C:800:VLB:C21	2.03	0.85
2:D:401:ARG:CG	2:D:401:ARG:HH11	1.85	0.85
1:A:270:ALA:O	1:A:302:MET:HB2	1.75	0.85
2:B:140:SER:HA	2:B:171:VAL:HG23	1.59	0.85
1:A:238:ILE:HG12	1:A:378:LEU:HD11	1.59	0.84
1:C:273:ALA:CB	1:C:375:VAL:H	1.91	0.84
2:D:350:ASN:H	2:D:350:ASN:HD22	1.22	0.84
2:D:241:CYS:CB	2:D:247:GLN:HE21	1.91	0.84
2:B:216:THR:CG2	2:B:299:LYS:HD3	2.09	0.83
2:D:164:ARG:HA	2:D:164:ARG:HE	1.42	0.83
1:C:115:ILE:HG13	1:C:152:LEU:HD23	1.58	0.83
2:B:180:THR:HB	2:B:183:GLU:OE2	1.76	0.83
8:C:800:VLB:H572	8:C:800:VLB:H511	1.60	0.83
3:E:4:ALA:HB3	3:E:24:LEU:HD11	1.60	0.82
2:B:241:CYS:CB	2:B:247:GLN:NE2	2.40	0.82
2:D:223:THR:HB	2:D:225:GLY:N	1.94	0.82
2:B:336:GLN:OE1	2:B:351:VAL:HG11	1.78	0.82
2:B:265:LEU:HD12	2:B:265:LEU:O	1.80	0.82
1:A:36:MET:HG2	1:A:61:HIS:NE2	1.94	0.82
1:C:41:THR:HG21	1:C:61:HIS:HE1	1.45	0.82
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.60	0.81
2:B:165:ILE:HD11	2:B:252:LEU:HG	1.61	0.81
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.05	0.81
2:B:401:ARG:HH11	2:B:401:ARG:CG	1.88	0.81
2:D:224:TYR:O	2:D:228:ASN:ND2	2.13	0.81
2:D:205:ASP:OD1	2:D:207:GLU:HB3	1.81	0.80
2:B:414:ASP:HB3	2:B:416:MET:HE3	1.63	0.80
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.10	0.80
2:B:177:VAL:HG22	8:C:800:VLB:H532	1.64	0.80
1:C:97:GLU:HG2	1:C:110:ILE:HD11	1.64	0.80
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.12	0.79
2:B:216:THR:HG23	2:B:299:LYS:HD3	1.63	0.79
2:B:88:ARG:O	2:B:91:ASN:HB2	1.82	0.79
1:C:99:ALA:HB2	1:C:145:THR:CG2	2.13	0.79
1:C:238:ILE:HG12	1:C:378:LEU:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.64	0.78
2:D:336:GLN:OE1	2:D:351:VAL:HG11	1.83	0.78
2:B:350:ASN:HD22	2:B:350:ASN:H	1.32	0.78
1:A:128:GLN:O	1:A:128:GLN:HG2	1.80	0.78
1:C:241:SER:HB2	1:C:250:VAL:O	1.83	0.78
2:D:250:ALA:CB	7:D:701:CN2:H7	2.14	0.78
2:D:70:LEU:HA	2:D:95:GLY:HA3	1.64	0.77
2:D:70:LEU:HD12	2:D:145:THR:HB	1.66	0.77
2:D:332:MET:HG3	2:D:353:THR:HG21	1.66	0.77
2:D:265:LEU:HD12	2:D:265:LEU:O	1.84	0.77
1:A:294:ALA:O	1:A:297:GLU:HB3	1.84	0.77
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.49	0.77
2:D:333:LEU:O	2:D:337:ASN:ND2	2.18	0.77
1:A:265:ILE:HG23	1:A:267:PHE:CZ	2.20	0.77
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.66	0.77
2:D:2:ARG:NH1	2:D:133:GLN:HA	2.01	0.76
2:D:133:GLN:NE2	2:D:252:LEU:HB3	2.01	0.76
1:A:388:TRP:HA	1:A:388:TRP:CE3	2.21	0.76
2:B:332:MET:HG3	2:B:353:THR:HG21	1.66	0.76
1:C:329:ASN:CA	8:C:800:VLB:H211	2.09	0.76
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.67	0.76
2:B:2:ARG:NH1	2:B:133:GLN:HA	2.01	0.76
1:A:178:SER:HB3	7:B:700:CN2:S1	2.25	0.76
2:B:264:ARG:O	2:B:266:HIS:CD2	2.40	0.75
2:D:245:PRO:HG2	2:D:247:GLN:HG2	1.68	0.75
2:D:264:ARG:O	2:D:266:HIS:CD2	2.40	0.75
1:A:260:VAL:HB	1:A:266:HIS:HB2	1.68	0.75
1:C:252:LEU:O	1:C:253:THR:HB	1.86	0.74
1:A:318:LEU:HB2	1:A:376:CYS:HB3	1.68	0.74
3:E:55:GLU:HA	3:E:58:GLU:HB2	1.69	0.74
2:B:291:LEU:HD21	2:B:375:ALA:CB	2.16	0.74
1:C:407:TRP:CD2	2:D:257:VAL:HG23	2.22	0.74
1:A:292:THR:O	1:A:295:CYS:HB2	1.88	0.74
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.70	0.74
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.23	0.73
2:D:180:THR:HG22	2:D:182:VAL:H	1.52	0.73
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.28	0.73
2:B:205:ASP:OD1	2:B:207:GLU:HB3	1.89	0.73
2:B:70:LEU:HA	2:B:95:GLY:HA3	1.70	0.73
2:D:48:ARG:NH1	2:D:245:PRO:HD2	2.03	0.73
1:A:206:ASN:ND2	5:A:600:GTP:HN22	1.80	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:ARG:O	2:D:91:ASN:HB2	1.89	0.73
1:C:330:ALA:O	1:C:334:THR:OG1	2.07	0.72
2:B:123:ARG:O	2:B:127:GLU:HB2	1.88	0.72
2:D:99:ALA:HB1	2:D:145:THR:HG21	1.70	0.72
2:D:140:SER:HA	2:D:171:VAL:HG23	1.70	0.72
2:D:48:ARG:HH12	2:D:245:PRO:HD2	1.55	0.72
2:B:99:ALA:HB1	2:B:145:THR:HG21	1.70	0.72
2:B:151:THR:HB	2:B:193:GLN:HG2	1.71	0.72
1:C:288:VAL:HG11	1:C:327:ASP:HB3	1.69	0.72
1:C:288:VAL:HG21	1:C:327:ASP:OD2	1.90	0.72
1:C:328:VAL:HG12	1:C:332:ILE:HD12	1.72	0.72
2:D:257:VAL:O	2:D:257:VAL:HG13	1.87	0.71
2:B:176:LYS:HB3	8:C:800:VLB:H222	1.72	0.71
2:B:273:ALA:CB	2:B:274:PRO:CD	2.66	0.71
1:C:90:GLU:HB3	1:C:121:ARG:HD3	1.73	0.71
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.19	0.71
2:B:156:LYS:HG2	3:E:76:ARG:HH21	1.56	0.71
1:A:273:ALA:HB2	1:A:375:VAL:H	1.53	0.71
2:D:315:VAL:HG12	2:D:351:VAL:HG23	1.71	0.71
1:C:6:SER:HB3	1:C:8:HIS:HE1	1.55	0.71
2:B:336:GLN:OE1	2:B:351:VAL:CG1	2.39	0.70
1:C:40:LYS:O	1:C:41:THR:HB	1.89	0.70
1:C:66:VAL:HG11	1:C:122:ILE:HG22	1.72	0.70
2:B:33:THR:O	2:B:34:GLY:O	2.09	0.70
2:D:2:ARG:O	2:D:3:GLU:HB2	1.91	0.70
2:D:5:VAL:HG22	2:D:135:PHE:CD2	2.27	0.70
3:E:123:LEU:C	3:E:125:GLU:H	1.95	0.70
1:C:128:GLN:O	1:C:128:GLN:HG2	1.92	0.70
1:A:99:ALA:CB	1:A:145:THR:HG22	2.16	0.69
2:B:403:ALA:O	2:B:405:LEU:N	2.25	0.69
1:C:288:VAL:HG13	1:C:323:VAL:HG13	1.73	0.69
2:B:221:THR:HA	8:C:800:VLB:H761	1.74	0.69
1:C:115:ILE:HG13	1:C:152:LEU:CD2	2.23	0.69
1:C:68:VAL:HG11	1:C:118:VAL:CG2	2.22	0.69
1:C:265:ILE:HG12	1:C:265:ILE:O	1.92	0.69
2:D:414:ASP:HB3	2:D:416:MET:HE3	1.75	0.69
2:D:5:VAL:HG12	2:D:64:ARG:HG2	1.74	0.69
2:B:220:THR:O	2:B:222:PRO:HD3	1.93	0.69
1:C:350:GLY:O	1:C:351:PHE:HB2	1.93	0.69
1:A:8:HIS:CD2	1:A:17:GLY:CA	2.74	0.69
1:C:328:VAL:HG12	1:C:332:ILE:CD1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:CB	1:A:274:PRO:CD	2.56	0.69
2:B:269:MET:HG2	2:B:384:ILE:HG12	1.75	0.69
1:A:323:VAL:HG12	1:A:355:ILE:HD13	1.75	0.68
1:A:291:ILE:HB	1:A:375:VAL:HG23	1.75	0.68
1:A:388:TRP:HA	1:A:388:TRP:HE3	1.58	0.68
1:C:68:VAL:HG11	1:C:118:VAL:HG22	1.76	0.68
2:B:212:ILE:HG22	2:B:230:LEU:HD21	1.75	0.68
2:D:111:GLY:HA2	2:D:149:MET:CE	2.23	0.68
2:D:237:GLY:CA	2:D:376:THR:HG21	2.24	0.68
3:E:127:ASP:C	3:E:129:HIS:H	1.95	0.68
1:C:88:HIS:HB2	1:C:91:GLN:NE2	2.04	0.68
1:A:68:VAL:HG11	1:A:118:VAL:HG22	1.75	0.68
1:A:341:ILE:HG12	1:A:342:GLN:H	1.59	0.68
2:B:133:GLN:HE21	2:B:252:LEU:CB	1.98	0.68
2:D:159:GLU:HB2	3:E:123:LEU:HD23	1.76	0.68
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.29	0.68
2:D:273:ALA:CB	2:D:274:PRO:CD	2.70	0.68
1:A:68:VAL:HG11	1:A:118:VAL:CG2	2.24	0.68
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.76	0.68
2:B:250:ALA:CB	7:B:700:CN2:H7	2.24	0.67
1:C:265:ILE:CG2	1:C:267:PHE:CZ	2.77	0.67
2:D:33:THR:O	2:D:34:GLY:O	2.12	0.67
1:A:115:ILE:HG13	1:A:152:LEU:CD2	2.23	0.67
1:A:6:SER:HB3	1:A:8:HIS:HE1	1.59	0.67
2:D:266:HIS:HB3	2:D:380:ASN:HD21	1.58	0.67
1:C:210:TYR:CE1	1:C:214:ARG:HD2	2.30	0.67
2:D:4:ILE:HG22	2:D:133:GLN:HB3	1.77	0.67
3:E:112:ARG:O	3:E:115:HIS:N	2.21	0.67
2:D:145:THR:HG23	6:D:603:GDP:O3B	1.95	0.67
2:B:114:LEU:O	2:B:116:ASP:N	2.28	0.67
2:B:135:PHE:HB2	2:B:166:MET:CE	2.25	0.67
1:A:407:TRP:CD2	2:B:257:VAL:HG23	2.30	0.67
1:C:316:CYS:O	1:C:377:MET:HA	1.95	0.66
1:C:41:THR:HG21	1:C:61:HIS:CE1	2.30	0.66
2:D:195:VAL:HA	2:D:265:LEU:HD23	1.76	0.66
2:B:154:ILE:HG12	2:B:155:SER:N	2.08	0.66
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.77	0.66
1:C:234:ILE:CD1	1:C:272:TYR:HB2	2.26	0.66
1:A:98:ASP:HB3	2:B:251:ASP:OD2	1.96	0.66
2:B:403:ALA:C	2:B:405:LEU:H	1.97	0.66
2:D:250:ALA:HB1	7:D:701:CN2:H7	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.78	0.66
2:B:12:CYS:SG	2:B:171:VAL:HG21	2.35	0.65
1:C:294:ALA:O	1:C:297:GLU:HB3	1.96	0.65
2:B:176:LYS:O	2:B:177:VAL:HB	1.96	0.65
2:B:111:GLY:HA2	2:B:149:MET:CE	2.25	0.65
2:D:164:ARG:HE	2:D:164:ARG:CA	2.03	0.65
2:B:308:ARG:HH11	2:B:308:ARG:CG	2.08	0.65
2:B:177:VAL:HG22	8:C:800:VLB:C53	2.25	0.65
1:C:181:VAL:HG23	2:D:258:ASN:HD22	1.62	0.65
2:B:224:TYR:OH	6:B:602:GDP:H2'	1.96	0.65
1:C:240:ALA:O	1:C:243:ARG:N	2.30	0.65
2:D:315:VAL:CG1	2:D:351:VAL:HG23	2.27	0.65
1:C:407:TRP:CG	2:D:257:VAL:HG23	2.32	0.65
2:B:250:ALA:HB1	7:B:700:CN2:H7	1.78	0.65
1:C:20:CYS:HB3	1:C:232:GLY:HA2	1.79	0.64
2:D:158:ARG:O	2:D:159:GLU:CB	2.46	0.64
2:D:5:VAL:CG2	2:D:135:PHE:HD2	2.10	0.64
1:A:8:HIS:HD2	1:A:17:GLY:CA	2.04	0.64
2:B:48:ARG:HH12	2:B:245:PRO:HD2	1.63	0.64
2:D:141:LEU:HD23	2:D:172:VAL:HG22	1.79	0.64
1:A:190:THR:CG2	1:A:191:THR:N	2.62	0.63
2:B:99:ALA:HB1	2:B:145:THR:CG2	2.29	0.63
2:D:42:LEU:O	2:D:44:LEU:N	2.31	0.63
1:A:407:TRP:HZ2	2:B:260:VAL:HG23	1.62	0.63
1:C:8:HIS:CD2	1:C:17:GLY:CA	2.77	0.63
2:B:333:LEU:O	2:B:337:ASN:ND2	2.31	0.63
2:D:114:LEU:O	2:D:116:ASP:N	2.31	0.63
1:A:265:ILE:HG12	1:A:265:ILE:O	1.99	0.63
1:A:273:ALA:HB2	1:A:375:VAL:N	2.14	0.63
1:C:253:THR:H	1:C:256:GLN:HB2	1.62	0.63
2:D:9:ALA:HA	2:D:68:VAL:O	1.99	0.63
2:D:336:GLN:OE1	2:D:351:VAL:CG1	2.46	0.63
2:D:95:GLY:O	2:D:96:GLN:HB2	1.97	0.63
2:B:147:SER:O	2:B:151:THR:OG1	2.15	0.63
2:B:414:ASP:HB3	2:B:416:MET:CE	2.28	0.63
2:D:251:ASP:C	2:D:253:ARG:H	2.01	0.63
2:D:347:ILE:O	2:D:348:PRO:O	2.17	0.63
2:B:95:GLY:O	2:B:96:GLN:HB2	1.98	0.62
2:D:54:ASN:HB2	2:D:64:ARG:HD3	1.80	0.62
2:B:159:GLU:HB2	3:E:72:LEU:HD23	1.81	0.62
2:B:212:ILE:CG2	2:B:230:LEU:HD21	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:VAL:HA	2:B:265:LEU:HD23	1.82	0.62
1:C:288:VAL:CG1	1:C:327:ASP:HB3	2.30	0.62
2:D:185:TYR:HE2	2:D:398:MET:HB3	1.65	0.62
1:A:262:TYR:O	1:A:266:HIS:HD2	1.82	0.62
1:A:266:HIS:O	1:A:268:PRO:HD3	1.99	0.62
2:B:251:ASP:C	2:B:253:ARG:H	2.01	0.62
2:B:4:ILE:HG22	2:B:133:GLN:HB3	1.81	0.62
1:C:181:VAL:CG2	2:D:258:ASN:HD22	2.11	0.62
1:A:66:VAL:HG11	1:A:122:ILE:HG22	1.82	0.62
2:B:156:LYS:HA	3:E:76:ARG:HH21	1.62	0.62
2:B:226:ASP:O	2:B:227:LEU:CB	2.47	0.62
2:B:135:PHE:HB2	2:B:166:MET:HE1	1.81	0.62
1:C:8:HIS:HD2	1:C:17:GLY:CA	2.06	0.62
2:B:141:LEU:HD23	2:B:172:VAL:HG22	1.82	0.62
3:E:84:GLN:HA	3:E:87:ILE:HG22	1.82	0.61
1:A:88:HIS:HB2	1:A:91:GLN:NE2	2.11	0.61
2:B:42:LEU:O	2:B:44:LEU:N	2.33	0.61
1:C:388:TRP:HA	1:C:388:TRP:HE3	1.64	0.61
2:B:320:ARG:HA	2:B:356:CYS:O	2.00	0.61
1:A:155:GLU:OE1	1:A:197:HIS:CE1	2.54	0.61
2:B:265:LEU:O	2:B:266:HIS:O	2.19	0.61
1:C:244:PHE:CZ	1:C:358:GLN:HG2	2.35	0.61
1:C:407:TRP:CG	2:D:257:VAL:CG2	2.83	0.61
1:A:177:VAL:HG22	1:A:210:TYR:CD2	2.35	0.61
1:C:260:VAL:HG12	1:C:266:HIS:HB2	1.82	0.61
2:B:236:SER:O	2:B:240:THR:HG23	2.01	0.61
2:B:315:VAL:HG12	2:B:351:VAL:HG23	1.82	0.61
2:B:70:LEU:HD12	2:B:145:THR:HB	1.82	0.61
2:B:20:PHE:O	2:B:24:ILE:HG23	2.01	0.61
1:C:48:SER:C	1:C:50:ASN:H	2.02	0.61
2:B:177:VAL:HG22	8:C:800:VLB:H712	1.81	0.61
1:C:312:TYR:HB3	1:C:343:PHE:CE2	2.36	0.61
8:C:800:VLB:H511	8:C:800:VLB:C57	2.31	0.61
2:D:70:LEU:CD1	2:D:145:THR:HB	2.30	0.61
2:B:210:TYR:C	2:B:210:TYR:HD1	2.04	0.60
2:D:404:PHE:HD1	2:D:404:PHE:N	1.99	0.60
1:C:6:SER:HB3	1:C:8:HIS:CE1	2.36	0.60
2:D:287:THR:HG22	2:D:290:GLU:H	1.66	0.60
3:E:94:ILE:CG2	3:E:95:LYS:N	2.63	0.60
2:B:48:ARG:NH1	2:B:245:PRO:HD2	2.16	0.60
3:E:115:HIS:C	3:E:115:HIS:HD1	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:CB	1:A:375:VAL:N	2.62	0.60
7:B:700:CN2:H15	7:B:700:CN2:C12	2.31	0.60
1:A:179:THR:O	7:B:700:CN2:H132	2.00	0.60
1:C:230:LEU:HD12	1:C:230:LEU:O	2.02	0.60
1:C:273:ALA:CB	1:C:375:VAL:N	2.63	0.60
2:D:99:ALA:HB1	2:D:145:THR:CG2	2.32	0.60
6:D:603:GDP:O2B	6:D:603:GDP:O1A	2.20	0.60
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.82	0.60
1:C:334:THR:C	1:C:336:LYS:H	2.04	0.60
2:B:151:THR:HG22	2:B:193:GLN:HB3	1.83	0.60
2:B:216:THR:HG21	2:B:299:LYS:HD3	1.84	0.60
2:B:266:HIS:HB3	2:B:380:ASN:HD21	1.65	0.59
1:C:142:GLY:HA3	1:C:183:GLU:HG3	1.84	0.59
1:A:246:GLY:O	1:A:247:ALA:O	2.20	0.59
2:B:185:TYR:HE2	2:B:398:MET:HB3	1.67	0.59
2:B:59:ASN:O	2:B:60:LYS:O	2.20	0.59
1:C:183:GLU:HB3	1:C:184:PRO:CD	2.32	0.59
2:B:306:ASP:O	2:B:308:ARG:N	2.35	0.59
1:C:111:GLY:O	1:C:113:GLU:N	2.35	0.59
2:D:123:ARG:O	2:D:127:GLU:HB2	2.03	0.59
2:D:352:LYS:HG3	7:D:701:CN2:O5	2.00	0.59
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.37	0.59
1:A:27:GLU:HG3	1:A:361:THR:OG1	2.02	0.59
2:B:237:GLY:CA	2:B:376:THR:HG21	2.32	0.59
2:B:287:THR:HG22	2:B:290:GLU:CB	2.31	0.59
2:B:4:ILE:HD11	2:B:52:TYR:CE2	2.38	0.59
1:C:125:LEU:HD23	1:C:128:GLN:HE22	1.67	0.59
1:A:163:LYS:H	1:A:163:LYS:HE3	1.67	0.59
1:C:36:MET:C	1:C:38:SER:H	2.05	0.59
2:B:158:ARG:O	2:B:159:GLU:CB	2.49	0.59
1:C:324:VAL:HG13	1:C:325:PRO:HD2	1.85	0.59
1:C:387:ALA:HA	1:C:390:ARG:NH1	2.18	0.59
2:D:154:ILE:HG12	2:D:155:SER:N	2.15	0.59
2:D:308:ARG:CG	2:D:308:ARG:HH11	2.16	0.59
2:B:262:PHE:O	2:B:266:HIS:CD2	2.56	0.59
2:D:151:THR:HA	2:D:154:ILE:HD13	1.85	0.59
1:C:143:GLY:O	1:C:147:SER:OG	2.20	0.59
1:C:177:VAL:HG22	1:C:210:TYR:CD2	2.37	0.59
1:C:346:TRP:HZ2	1:C:435:VAL:CG1	2.15	0.59
2:D:291:LEU:HD21	2:D:375:ALA:HB3	1.83	0.59
1:A:176:GLN:HG2	1:A:177:VAL:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:190:SER:O	2:D:193:GLN:N	2.36	0.58
2:D:306:ASP:O	2:D:308:ARG:N	2.36	0.58
1:A:411:GLU:O	3:E:61:ARG:HD3	2.03	0.58
2:B:407:TRP:CD1	1:C:257:THR:HG23	2.37	0.58
2:B:287:THR:HG22	2:B:290:GLU:H	1.68	0.58
2:B:347:ILE:CG2	2:B:350:ASN:HB3	2.26	0.58
1:C:51:THR:HG21	1:C:242:LEU:HD13	1.85	0.58
1:A:371:VAL:HG12	1:A:372:GLN:H	1.68	0.58
2:B:287:THR:O	2:B:288:VAL:HB	2.04	0.58
1:C:41:THR:O	1:C:41:THR:HG23	2.03	0.58
1:A:198:SER:O	1:A:265:ILE:HG13	2.03	0.58
2:D:404:PHE:N	2:D:404:PHE:CD1	2.70	0.58
2:B:156:LYS:HG2	3:E:76:ARG:CZ	2.32	0.58
1:C:223:THR:N	1:C:226:ASN:HB2	2.18	0.58
1:C:262:TYR:O	1:C:263:PRO:C	2.42	0.58
2:D:226:ASP:O	2:D:227:LEU:CB	2.51	0.58
2:D:209:LEU:HD21	2:D:231:VAL:HG22	1.84	0.58
1:A:167:LEU:HD13	1:A:252:LEU:HD13	1.85	0.58
1:A:315:CYS:HB3	1:A:351:PHE:CE2	2.38	0.58
3:E:87:ILE:O	3:E:91:ASN:ND2	2.37	0.58
1:A:271:THR:O	1:A:376:CYS:O	2.22	0.58
1:C:125:LEU:HD23	1:C:128:GLN:NE2	2.19	0.58
2:B:264:ARG:O	2:B:266:HIS:N	2.34	0.58
1:C:356:ASN:O	1:C:358:GLN:N	2.36	0.58
2:B:183:GLU:N	2:B:184:PRO:HD2	2.19	0.57
2:B:210:TYR:C	2:B:210:TYR:CD1	2.77	0.57
1:C:181:VAL:HG23	2:D:258:ASN:ND2	2.19	0.57
2:D:151:THR:HG22	2:D:193:GLN:HB3	1.86	0.57
1:C:182:VAL:CG2	1:C:408:TYR:OH	2.53	0.57
1:A:204:VAL:HG22	1:A:302:MET:HE1	1.86	0.57
1:C:291:ILE:HB	1:C:375:VAL:HG23	1.84	0.57
3:E:115:HIS:O	3:E:115:HIS:ND1	2.33	0.57
1:A:341:ILE:H	1:A:341:ILE:HD13	1.69	0.57
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.40	0.57
1:C:325:PRO:HB2	8:C:800:VLB:H763	1.86	0.57
1:A:190:THR:HG23	1:A:191:THR:N	2.18	0.57
2:B:262:PHE:O	2:B:266:HIS:HD2	1.87	0.57
1:C:288:VAL:HG11	1:C:327:ASP:CB	2.33	0.57
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.85	0.57
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.85	0.57
1:C:54:SER:HB3	1:C:64:ARG:HE	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:GLN:HA	2:D:167:ASN:O	2.05	0.57
1:C:266:HIS:O	1:C:268:PRO:HD3	2.03	0.57
2:B:6:HIS:CE1	2:B:8:GLN:HB2	2.40	0.57
8:C:800:VLB:O72	8:C:800:VLB:C57	2.50	0.57
2:D:133:GLN:HE21	2:D:252:LEU:CB	2.08	0.57
1:C:182:VAL:HG23	1:C:408:TYR:OH	2.05	0.56
1:C:191:THR:HG23	1:C:425:MET:CE	2.35	0.56
1:C:176:GLN:HG2	1:C:177:VAL:H	1.69	0.56
1:A:6:SER:HB3	1:A:8:HIS:CE1	2.41	0.56
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.39	0.56
2:D:265:LEU:O	2:D:266:HIS:O	2.23	0.56
2:B:2:ARG:O	2:B:3:GLU:HB2	2.04	0.56
2:B:145:THR:HG23	6:B:602:GDP:O3B	2.06	0.56
1:C:102:ASN:OD1	1:C:105:ARG:HB2	2.05	0.56
1:C:248:LEU:O	1:C:249:ASN:HB2	2.05	0.56
2:D:159:GLU:HB2	3:E:123:LEU:CD2	2.36	0.56
1:C:392:ASP:OD1	1:C:429:GLU:OE1	2.24	0.56
2:D:180:THR:HG22	2:D:181:VAL:N	2.20	0.56
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.87	0.56
3:E:94:ILE:HG22	3:E:95:LYS:H	1.69	0.56
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.87	0.56
2:B:262:PHE:O	2:B:264:ARG:N	2.38	0.56
2:B:4:ILE:HD11	2:B:52:TYR:CZ	2.40	0.56
3:E:76:ARG:O	3:E:79:GLU:HB2	2.05	0.56
1:A:265:ILE:CG2	1:A:267:PHE:CZ	2.89	0.56
2:D:224:TYR:CE2	6:D:603:GDP:C5	2.94	0.56
3:E:51:GLN:C	3:E:53:LYS:H	2.09	0.56
3:E:67:GLU:C	3:E:69:LEU:H	2.07	0.56
1:A:102:ASN:ND2	1:A:104:ALA:HB3	2.21	0.55
1:A:72:PRO:O	1:A:74:VAL:N	2.38	0.55
2:B:64:ARG:HG3	2:B:125:GLU:OE1	2.05	0.55
2:B:177:VAL:CG2	8:C:800:VLB:H532	2.33	0.55
2:D:298:SER:C	2:D:300:ASN:H	2.10	0.55
3:E:67:GLU:O	3:E:71:HIS:HB2	2.05	0.55
2:B:164:ARG:HE	2:B:164:ARG:HA	1.71	0.55
2:B:223:THR:HB	2:B:225:GLY:N	2.21	0.55
2:B:71:GLU:O	2:B:71:GLU:HG2	2.07	0.55
1:A:265:ILE:O	1:A:266:HIS:O	2.25	0.55
1:C:70:LEU:CD2	1:C:110:ILE:HG23	2.37	0.55
1:C:265:ILE:HG23	1:C:267:PHE:CE1	2.42	0.55
2:D:226:ASP:O	2:D:227:LEU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:264:ARG:O	2:D:266:HIS:N	2.32	0.55
1:A:412:GLY:O	3:E:60:ARG:NH1	2.40	0.55
2:B:158:ARG:HH11	2:B:158:ARG:CG	2.20	0.55
2:B:396:THR:O	2:B:400:ARG:HB2	2.07	0.55
2:D:147:SER:O	2:D:151:THR:OG1	2.15	0.55
2:B:213:CYS:HA	2:B:217:LEU:HD12	1.89	0.55
1:C:98:ASP:HB3	2:D:251:ASP:OD2	2.07	0.55
1:C:54:SER:O	1:C:56:THR:N	2.40	0.55
1:C:288:VAL:CG1	1:C:323:VAL:HG13	2.37	0.55
2:D:141:LEU:CD2	2:D:172:VAL:HG22	2.37	0.55
2:B:245:PRO:HG2	2:B:247:GLN:HG2	1.89	0.54
1:C:273:ALA:CB	1:C:274:PRO:CD	2.68	0.54
1:C:273:ALA:HB2	1:C:375:VAL:N	2.21	0.54
2:B:416:MET:O	2:B:420:GLU:HB2	2.07	0.54
2:B:70:LEU:CA	2:B:95:GLY:HA3	2.38	0.54
1:C:177:VAL:CG2	1:C:210:TYR:CD2	2.90	0.54
2:B:133:GLN:NE2	2:B:252:LEU:CB	2.65	0.54
1:C:318:LEU:HB2	1:C:376:CYS:HB3	1.89	0.54
1:A:313:MET:HG3	1:A:380:ASN:O	2.07	0.54
2:B:347:ILE:O	2:B:348:PRO:O	2.25	0.54
2:D:180:THR:HG21	2:D:182:VAL:HG22	1.89	0.54
2:D:5:VAL:CG2	2:D:135:PHE:CD2	2.87	0.54
2:B:228:ASN:HD21	6:B:602:GDP:HN1	1.55	0.54
2:D:124:LYS:O	2:D:128:SER:HB2	2.08	0.54
1:C:198:SER:O	1:C:265:ILE:HG13	2.08	0.54
2:D:183:GLU:O	2:D:184:PRO:C	2.44	0.54
2:D:241:CYS:CB	2:D:247:GLN:NE2	2.52	0.54
2:D:347:ILE:O	2:D:347:ILE:HG22	2.07	0.54
2:B:216:THR:O	2:B:217:LEU:HG	2.08	0.54
1:A:262:TYR:O	1:A:266:HIS:CD2	2.61	0.54
2:D:180:THR:HB	2:D:183:GLU:OE2	2.07	0.54
3:E:19:SER:O	3:E:20:PHE:HB3	2.07	0.54
1:A:205:ASP:CB	1:A:303:VAL:HA	2.38	0.54
1:A:230:LEU:O	1:A:230:LEU:HD12	2.07	0.54
1:C:344:VAL:O	1:C:346:TRP:N	2.35	0.54
2:D:59:ASN:O	2:D:60:LYS:O	2.25	0.54
1:A:387:ALA:HA	1:A:390:ARG:NH1	2.23	0.54
2:B:70:LEU:C	2:B:95:GLY:HA3	2.29	0.54
2:B:369:ARG:O	2:B:370:GLY:O	2.26	0.53
2:B:269:MET:HB3	2:B:303:ALA:HB3	1.89	0.53
2:D:7:ILE:HD13	2:D:153:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:VAL:HG23	1:A:408:TYR:OH	2.08	0.53
1:A:407:TRP:HZ2	2:B:260:VAL:CG2	2.20	0.53
2:D:51:VAL:HG12	2:D:52:TYR:CD1	2.43	0.53
3:E:125:GLU:C	3:E:127:ASP:H	2.12	0.53
1:C:287:SER:O	1:C:291:ILE:HG12	2.08	0.53
2:D:6:HIS:HD2	2:D:136:GLN:HG3	1.72	0.53
2:B:102:ASN:OD1	2:B:105:LYS:HB2	2.08	0.53
2:B:205:ASP:OD1	2:B:207:GLU:N	2.42	0.53
2:B:95:GLY:O	2:B:96:GLN:CB	2.57	0.53
1:C:108:TYR:O	1:C:112:LYS:HB2	2.08	0.53
1:C:187:SER:O	1:C:191:THR:HG22	2.09	0.53
1:C:79:ARG:NH2	1:C:94:THR:CG2	2.57	0.53
2:B:257:VAL:O	2:B:257:VAL:HG13	2.07	0.53
1:C:190:THR:CG2	1:C:191:THR:N	2.71	0.53
1:C:332:ILE:O	1:C:335:ILE:N	2.42	0.53
2:D:236:SER:O	2:D:240:THR:HG23	2.09	0.53
2:D:382:THR:HB	2:D:436:GLN:HE21	1.74	0.53
2:B:296:PHE:CE2	2:B:377:PHE:CE1	2.97	0.53
1:C:70:LEU:HD22	1:C:110:ILE:HG23	1.90	0.53
2:B:298:SER:C	2:B:300:ASN:H	2.13	0.53
1:C:111:GLY:C	1:C:113:GLU:N	2.62	0.53
2:D:224:TYR:CD2	6:D:603:GDP:C6	2.97	0.53
7:D:701:CN2:H62	7:D:701:CN2:H43	1.91	0.53
2:D:70:LEU:CA	2:D:95:GLY:HA3	2.37	0.53
1:A:177:VAL:CG2	1:A:210:TYR:CD2	2.93	0.52
2:D:11:GLN:CG	2:D:74:THR:HG21	2.34	0.52
2:B:295:MET:SD	2:B:377:PHE:HB2	2.49	0.52
1:C:190:THR:HG23	1:C:191:THR:N	2.23	0.52
1:C:88:HIS:H	1:C:91:GLN:NE2	2.07	0.52
2:D:153:LEU:O	2:D:157:ILE:HG12	2.09	0.52
2:D:183:GLU:O	2:D:186:ASN:N	2.42	0.52
2:D:185:TYR:CE2	2:D:398:MET:HB3	2.43	0.52
2:B:118:VAL:HG11	2:B:153:LEU:HD11	1.91	0.52
2:B:185:TYR:CE2	2:B:398:MET:HB3	2.45	0.52
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.44	0.52
1:C:48:SER:C	1:C:50:ASN:N	2.63	0.52
1:A:180:ALA:O	1:A:181:VAL:C	2.48	0.52
2:B:404:PHE:N	2:B:404:PHE:CD1	2.75	0.52
1:C:177:VAL:HG22	1:C:210:TYR:HD2	1.73	0.52
1:C:264:ARG:O	1:C:266:HIS:N	2.42	0.52
2:D:194:LEU:O	2:D:265:LEU:CD2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:273:ALA:CB	2:D:375:ALA:H	2.22	0.52
3:E:57:ALA:O	3:E:59:GLU:N	2.42	0.52
2:B:190:SER:O	2:B:191:VAL:C	2.48	0.52
2:B:7:ILE:O	2:B:137:LEU:HA	2.10	0.52
1:C:68:VAL:CG1	1:C:118:VAL:HG22	2.39	0.52
1:C:310:GLY:HA3	1:C:383:ALA:HB2	1.92	0.52
3:E:51:GLN:O	3:E:54:LEU:HB3	2.09	0.52
2:B:183:GLU:O	2:B:184:PRO:C	2.47	0.52
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.92	0.52
2:B:404:PHE:HD1	2:B:404:PHE:N	2.08	0.52
2:D:151:THR:HB	2:D:193:GLN:HG2	1.90	0.52
2:D:287:THR:HG22	2:D:290:GLU:CB	2.35	0.52
2:D:287:THR:O	2:D:288:VAL:HB	2.10	0.52
2:B:251:ASP:O	2:B:252:LEU:HB3	2.10	0.52
1:A:277:SER:O	1:A:280:LYS:HB2	2.10	0.52
2:B:238:VAL:HG13	2:B:378:ILE:HD11	1.91	0.52
1:A:49:PHE:HA	1:A:243:ARG:O	2.10	0.52
2:B:237:GLY:O	2:B:240:THR:OG1	2.27	0.52
2:D:205:ASP:OD2	2:D:390:ARG:NH1	2.42	0.52
1:A:87:PHE:N	1:A:87:PHE:CD2	2.78	0.51
1:C:36:MET:O	1:C:38:SER:N	2.43	0.51
1:C:7:ILE:HD13	1:C:153:LEU:HD11	1.92	0.51
2:D:135:PHE:HB2	2:D:166:MET:CE	2.40	0.51
2:D:416:MET:O	2:D:420:GLU:HB2	2.10	0.51
3:E:127:ASP:C	3:E:129:HIS:N	2.64	0.51
1:C:161:TYR:HB3	1:C:164:LYS:HG3	1.92	0.51
1:C:425:MET:O	1:C:429:GLU:HB2	2.09	0.51
1:A:281:ALA:O	1:A:283:HIS:N	2.42	0.51
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.25	0.51
2:B:347:ILE:O	2:B:347:ILE:HG22	2.10	0.51
1:C:264:ARG:C	1:C:266:HIS:CD2	2.84	0.51
1:C:435:VAL:O	1:C:435:VAL:HG12	2.10	0.51
2:D:182:VAL:O	2:D:185:TYR:HB2	2.11	0.51
1:A:90:GLU:O	1:A:121:ARG:CD	2.59	0.51
2:D:256:ALA:O	2:D:260:VAL:HG22	2.10	0.51
2:D:266:HIS:H	2:D:266:HIS:CD2	2.29	0.51
2:D:267:PHE:N	2:D:267:PHE:CD1	2.78	0.51
2:B:142:GLY:HA3	2:B:173:PRO:HG3	1.91	0.51
1:C:111:GLY:O	1:C:112:LYS:C	2.49	0.51
1:C:155:GLU:O	1:C:158:SER:HB2	2.11	0.51
1:C:313:MET:HG3	1:C:380:ASN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:THR:CB	2:D:225:GLY:H	2.05	0.51
1:C:68:VAL:HG11	1:C:118:VAL:HG21	1.93	0.51
1:C:273:ALA:HB2	1:C:375:VAL:H	1.70	0.51
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.92	0.51
2:B:31:ASP:HB2	2:B:34:GLY:CA	2.40	0.51
7:B:700:CN2:H62	7:B:700:CN2:H43	1.92	0.51
2:B:135:PHE:HB2	2:B:166:MET:HE2	1.93	0.51
2:B:158:ARG:NH1	2:B:158:ARG:HG3	2.26	0.51
1:C:100:ALA:HB1	2:D:253:ARG:HG2	1.93	0.51
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.41	0.51
2:D:76:ASP:N	2:D:76:ASP:OD1	2.44	0.51
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.46	0.50
1:A:177:VAL:HG22	1:A:210:TYR:HD2	1.76	0.50
1:A:392:ASP:OD1	1:A:429:GLU:OE1	2.29	0.50
2:B:176:LYS:HB3	8:C:800:VLB:C22	2.40	0.50
1:A:407:TRP:CZ2	2:B:260:VAL:HG23	2.45	0.50
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.24	0.50
1:C:201:ALA:O	1:C:268:PRO:HD2	2.11	0.50
1:C:405:VAL:CG1	1:C:406:HIS:N	2.73	0.50
7:D:701:CN2:C12	7:D:701:CN2:H15	2.39	0.50
1:A:262:TYR:O	1:A:264:ARG:N	2.45	0.50
2:D:165:ILE:HG23	2:D:253:ARG:NH1	2.26	0.50
3:E:13:LYS:HG3	3:E:18:GLN:HG3	1.92	0.50
2:B:7:ILE:HG22	2:B:137:LEU:CD1	2.42	0.50
2:B:342:TYR:CD2	2:B:342:TYR:N	2.80	0.50
2:B:11:GLN:CG	2:B:74:THR:HG21	2.36	0.50
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.47	0.50
2:D:115:VAL:HG21	2:D:152:LEU:CD2	2.41	0.50
2:D:270:PRO:HA	2:D:377:PHE:O	2.12	0.50
1:A:117:LEU:HD11	1:A:121:ARG:NH2	2.27	0.50
2:D:152:LEU:O	2:D:153:LEU:C	2.50	0.50
1:A:183:GLU:HB3	1:A:184:PRO:CD	2.42	0.50
1:A:247:ALA:O	1:A:248:LEU:O	2.29	0.50
2:B:172:VAL:HG11	2:B:387:LEU:HD21	1.92	0.50
1:C:325:PRO:HB3	8:C:800:VLB:C65	2.40	0.50
1:C:136:LEU:HD23	1:C:167:LEU:HB3	1.94	0.50
2:D:295:MET:SD	2:D:377:PHE:HB2	2.51	0.50
1:A:174:ALA:CB	1:A:207:GLU:HB2	2.41	0.50
1:A:288:VAL:HG13	1:A:323:VAL:HG22	1.92	0.50
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.60	0.50
1:C:328:VAL:O	1:C:332:ILE:HD12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:PHE:CD2	1:C:87:PHE:N	2.78	0.50
2:D:360:PRO:O	2:D:369:ARG:O	2.30	0.50
1:A:223:THR:N	1:A:226:ASN:HB2	2.27	0.49
1:A:316:CYS:O	1:A:377:MET:HA	2.12	0.49
1:A:344:VAL:O	1:A:346:TRP:N	2.45	0.49
1:A:291:ILE:HB	1:A:375:VAL:CG2	2.41	0.49
1:A:54:SER:O	1:A:56:THR:N	2.45	0.49
1:C:11:GLN:HB3	5:C:601:GTP:O2A	2.12	0.49
2:D:7:ILE:O	2:D:137:LEU:HA	2.13	0.49
2:D:4:ILE:HD11	2:D:52:TYR:CE2	2.47	0.49
1:A:155:GLU:OE1	1:A:197:HIS:HE1	1.95	0.49
1:A:176:GLN:HG2	1:A:177:VAL:N	2.27	0.49
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.92	0.49
2:B:401:ARG:O	1:C:262:TYR:OH	2.29	0.49
2:B:146:GLY:N	6:B:602:GDP:O1B	2.41	0.49
1:C:72:PRO:O	1:C:74:VAL:N	2.44	0.49
2:D:210:TYR:C	2:D:210:TYR:CD1	2.86	0.49
2:D:369:ARG:O	2:D:370:GLY:C	2.51	0.49
2:D:396:THR:O	2:D:400:ARG:HB2	2.12	0.49
1:A:184:PRO:O	1:A:188:ILE:HG12	2.12	0.49
1:A:435:VAL:O	1:A:435:VAL:HG12	2.12	0.49
2:D:250:ALA:O	2:D:252:LEU:N	2.44	0.49
2:D:224:TYR:CD2	6:D:603:GDP:C5	3.00	0.49
1:A:405:VAL:CG1	1:A:406:HIS:N	2.75	0.49
1:C:191:THR:O	1:C:195:LEU:HB2	2.12	0.49
2:D:414:ASP:HB3	2:D:416:MET:CE	2.41	0.49
3:E:123:LEU:C	3:E:125:GLU:N	2.64	0.49
2:B:181:VAL:O	2:B:398:MET:CE	2.61	0.49
2:B:291:LEU:HD21	2:B:375:ALA:HB3	1.94	0.49
2:B:357:ASP:N	2:B:357:ASP:OD2	2.46	0.49
3:E:105:MET:HB3	3:E:105:MET:CE	2.43	0.49
1:A:16:ILE:HG22	1:A:17:GLY:N	2.27	0.49
2:D:250:ALA:CB	7:D:701:CN2:C7	2.88	0.49
2:D:320:ARG:HA	2:D:356:CYS:O	2.12	0.49
2:D:224:TYR:HD2	6:D:603:GDP:C6	2.30	0.49
1:A:68:VAL:CG1	1:A:118:VAL:HG22	2.41	0.49
2:B:177:VAL:CG1	2:B:177:VAL:O	2.61	0.49
2:B:194:LEU:O	2:B:265:LEU:CD2	2.61	0.49
2:B:266:HIS:H	2:B:266:HIS:CD2	2.29	0.49
1:A:264:ARG:HB2	1:A:266:HIS:NE2	2.28	0.49
2:B:270:PRO:HA	2:B:377:PHE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ASN:HD21	8:C:800:VLB:H66	1.60	0.49
2:D:8:GLN:OE1	2:D:67:LEU:CD2	2.61	0.49
1:A:404:PHE:O	1:A:405:VAL:C	2.50	0.49
2:B:388:PHE:CD2	2:B:425:MET:HE2	2.48	0.49
1:A:90:GLU:O	1:A:121:ARG:HD3	2.12	0.48
2:B:152:LEU:O	2:B:153:LEU:C	2.47	0.48
1:C:261:PRO:HB2	1:C:262:TYR:CD1	2.48	0.48
1:C:404:PHE:O	1:C:405:VAL:C	2.51	0.48
2:D:114:LEU:O	2:D:115:VAL:C	2.51	0.48
1:A:239:THR:O	1:A:240:ALA:C	2.51	0.48
1:A:106:GLY:O	1:A:111:GLY:HA3	2.14	0.48
2:B:150:GLY:O	2:B:152:LEU:N	2.45	0.48
1:A:105:ARG:HH22	2:B:253:ARG:HH21	1.61	0.48
2:B:44:LEU:HA	2:B:49:ILE:HB	1.95	0.48
1:C:239:THR:O	1:C:240:ALA:C	2.52	0.48
3:E:4:ALA:HB3	3:E:24:LEU:CD1	2.37	0.48
2:B:226:ASP:O	2:B:227:LEU:HB2	2.12	0.48
2:B:267:PHE:CD1	2:B:267:PHE:N	2.81	0.48
1:C:309:HIS:ND1	1:C:386:GLU:OE1	2.47	0.48
2:D:2:ARG:HH12	2:D:133:GLN:HA	1.76	0.48
1:C:108:TYR:HB3	3:E:108:ASN:OD1	2.13	0.48
1:A:22:GLU:HB2	1:A:83:TYR:CE1	2.49	0.48
2:B:62:VAL:HA	2:B:63:PRO:HD2	1.72	0.48
1:A:159:VAL:HG11	3:E:48:GLU:HB2	1.94	0.48
3:E:73:ALA:HA	3:E:76:ARG:HB2	1.94	0.48
1:A:254:GLU:HA	1:A:257:THR:HB	1.95	0.48
1:A:145:THR:N	5:A:600:GTP:O2B	2.45	0.48
1:C:402:ARG:O	1:C:403:ALA:C	2.51	0.48
2:D:164:ARG:NH2	2:D:253:ARG:HH22	2.11	0.48
2:B:251:ASP:C	2:B:253:ARG:N	2.67	0.48
1:C:265:ILE:O	1:C:266:HIS:O	2.31	0.48
1:C:266:HIS:HB3	1:C:380:ASN:OD1	2.13	0.48
1:A:198:SER:HB3	1:A:265:ILE:CD1	2.43	0.48
1:A:182:VAL:CG2	1:A:408:TYR:OH	2.62	0.48
2:B:3:GLU:OE2	2:B:130:ASP:HB3	2.14	0.48
1:C:178:SER:OG	2:D:352:LYS:HD2	2.14	0.48
2:D:231:VAL:HG12	2:D:235:MET:CE	2.44	0.48
2:D:36:TYR:OH	2:D:40:SER:O	2.32	0.48
2:B:308:ARG:NH1	2:B:308:ARG:HG3	2.29	0.48
1:C:180:ALA:O	1:C:181:VAL:C	2.50	0.48
1:C:273:ALA:HB2	1:C:375:VAL:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:GLY:N	5:C:601:GTP:O1B	2.42	0.48
2:D:138:THR:HG22	2:D:169:PHE:HB2	1.95	0.48
1:C:296:PHE:HZ	1:C:351:PHE:HE2	1.62	0.48
1:A:105:ARG:NH2	2:B:253:ARG:HH21	2.11	0.47
1:A:66:VAL:C	1:A:67:PHE:HD1	2.18	0.47
2:B:16:ILE:HG22	2:B:17:GLY:N	2.29	0.47
2:D:250:ALA:C	2:D:252:LEU:H	2.17	0.47
1:A:139:HIS:CG	1:A:150:THR:HG21	2.49	0.47
1:A:402:ARG:O	1:A:403:ALA:C	2.51	0.47
2:B:155:SER:O	3:E:76:ARG:NH2	2.47	0.47
2:B:399:PHE:O	2:B:400:ARG:O	2.33	0.47
2:B:51:VAL:HG12	2:B:52:TYR:CD1	2.49	0.47
2:B:5:VAL:CG2	2:B:135:PHE:CD2	2.97	0.47
2:B:7:ILE:HG22	2:B:137:LEU:HD12	1.96	0.47
1:C:251:ASP:C	1:C:252:LEU:O	2.51	0.47
1:C:309:HIS:CE1	1:C:386:GLU:OE1	2.67	0.47
1:A:111:GLY:O	1:A:113:GLU:N	2.48	0.47
1:A:309:HIS:CE1	1:A:386:GLU:OE1	2.67	0.47
1:C:179:THR:HB	1:C:180:ALA:H	1.57	0.47
2:D:238:VAL:HG13	2:D:378:ILE:HD11	1.96	0.47
1:A:32:PRO:O	1:A:33:ASP:C	2.52	0.47
2:B:70:LEU:CD1	2:B:145:THR:HB	2.43	0.47
1:C:54:SER:HB3	1:C:64:ARG:NE	2.28	0.47
2:D:251:ASP:O	2:D:252:LEU:HB3	2.13	0.47
1:A:97:GLU:HG2	1:A:110:ILE:CD1	2.45	0.47
1:A:54:SER:HB3	1:A:64:ARG:HE	1.80	0.47
1:C:26:LEU:HD21	1:C:364:PRO:HD3	1.95	0.47
2:D:408:TYR:O	2:D:409:THR:C	2.53	0.47
2:D:103:TRP:CZ3	2:D:189:LEU:HD22	2.50	0.47
2:D:360:PRO:C	2:D:369:ARG:O	2.53	0.47
2:B:106:GLY:O	2:B:111:GLY:HA3	2.15	0.47
2:B:180:THR:O	2:B:182:VAL:N	2.47	0.47
2:B:256:ALA:O	2:B:260:VAL:HG22	2.15	0.47
2:B:407:TRP:NE1	1:C:257:THR:HG23	2.30	0.47
1:C:247:ALA:C	1:C:249:ASN:H	2.17	0.47
1:C:267:PHE:CD1	1:C:267:PHE:N	2.82	0.47
1:C:407:TRP:HZ2	2:D:260:VAL:HG23	1.78	0.47
2:D:273:ALA:HB3	2:D:375:ALA:H	1.79	0.47
1:A:393:HIS:O	1:A:394:LYS:C	2.51	0.47
2:B:381:SER:O	2:B:384:ILE:HB	2.14	0.47
1:C:152:LEU:O	1:C:153:LEU:C	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:TYR:CZ	1:C:328:VAL:HG13	2.50	0.47
3:E:115:HIS:C	3:E:115:HIS:ND1	2.67	0.47
1:A:251:ASP:OD1	1:A:251:ASP:C	2.53	0.47
1:A:88:HIS:H	1:A:91:GLN:NE2	2.13	0.47
2:B:190:SER:O	2:B:193:GLN:N	2.48	0.47
1:C:66:VAL:HG12	1:C:125:LEU:HD12	1.97	0.47
2:B:308:ARG:HG2	2:B:308:ARG:HH11	1.77	0.47
2:B:388:PHE:HD2	2:B:425:MET:CE	2.28	0.47
1:C:40:LYS:O	1:C:41:THR:CB	2.60	0.47
1:C:97:GLU:HG2	1:C:110:ILE:CD1	2.40	0.47
1:C:407:TRP:HZ2	2:D:260:VAL:CG2	2.28	0.47
3:E:112:ARG:HG2	3:E:113:GLU:N	2.28	0.47
3:E:69:LEU:C	3:E:71:HIS:H	2.17	0.47
2:B:360:PRO:O	2:B:369:ARG:O	2.32	0.47
2:B:75:MET:HE2	2:B:94:PHE:HA	1.96	0.47
3:E:85:LYS:O	3:E:89:GLU:HB2	2.15	0.47
1:A:347:CYS:O	1:A:348:PRO:C	2.54	0.46
2:B:102:ASN:OD1	2:B:105:LYS:N	2.36	0.46
2:B:263:PRO:O	2:B:265:LEU:N	2.48	0.46
2:D:308:ARG:HG2	2:D:308:ARG:HH11	1.80	0.46
3:E:63:TYR:O	3:E:64:GLN:C	2.53	0.46
1:A:51:THR:CB	1:A:243:ARG:HA	2.45	0.46
1:A:97:GLU:HG2	1:A:110:ILE:HD11	1.96	0.46
2:B:102:ASN:OD1	2:B:102:ASN:O	2.32	0.46
2:B:118:VAL:O	2:B:122:VAL:HG13	2.15	0.46
2:B:158:ARG:HH11	2:B:158:ARG:HG3	1.79	0.46
2:B:265:LEU:O	2:B:266:HIS:C	2.53	0.46
2:D:261:PRO:HG3	2:D:313:LEU:HG	1.97	0.46
2:D:381:SER:O	2:D:384:ILE:HB	2.15	0.46
2:D:95:GLY:O	2:D:96:GLN:CB	2.63	0.46
2:B:369:ARG:O	2:B:370:GLY:C	2.52	0.46
2:D:399:PHE:O	2:D:400:ARG:O	2.32	0.46
3:E:51:GLN:C	3:E:53:LYS:N	2.68	0.46
2:B:333:LEU:HA	2:B:336:GLN:HE21	1.81	0.46
2:B:315:VAL:CG1	2:B:351:VAL:HG23	2.44	0.46
1:C:249:ASN:HB3	1:C:250:VAL:HG22	1.96	0.46
2:D:209:LEU:HD12	2:D:209:LEU:HA	1.71	0.46
1:C:407:TRP:CD1	2:D:257:VAL:HG22	2.49	0.46
1:A:105:ARG:HH22	2:B:253:ARG:NH2	2.14	0.46
1:C:411:GLU:OE2	1:C:411:GLU:HA	2.15	0.46
2:D:212:ILE:HG22	2:D:230:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASN:OD1	1:A:105:ARG:HB2	2.15	0.46
1:A:368:LEU:H	1:A:368:LEU:HG	1.29	0.46
2:B:342:TYR:N	2:B:342:TYR:HD2	2.14	0.46
2:B:9:ALA:HA	2:B:68:VAL:O	2.16	0.46
2:D:6:HIS:CE1	2:D:8:GLN:HB2	2.51	0.46
1:A:99:ALA:CB	1:A:145:THR:CG2	2.87	0.46
1:A:393:HIS:CE1	1:A:397:LEU:HD13	2.51	0.46
2:D:177:VAL:O	2:D:177:VAL:HG12	2.16	0.46
3:E:13:LYS:O	3:E:14:CYS:O	2.33	0.46
3:E:67:GLU:O	3:E:69:LEU:N	2.49	0.46
1:A:210:TYR:CD1	1:A:210:TYR:C	2.89	0.46
1:A:251:ASP:OD1	1:A:252:LEU:N	2.48	0.46
1:A:36:MET:HG2	1:A:61:HIS:CD2	2.51	0.46
2:B:177:VAL:O	2:B:178:SER:HB3	2.16	0.46
1:A:20:CYS:HB3	1:A:232:GLY:HA2	1.98	0.46
1:A:315:CYS:HB3	1:A:351:PHE:HE2	1.81	0.46
2:B:209:LEU:HD21	2:B:231:VAL:HG22	1.97	0.46
2:B:308:ARG:NH1	2:B:308:ARG:CG	2.70	0.46
1:C:172:TYR:HE2	1:C:391:LEU:HD22	1.81	0.46
2:D:251:ASP:C	2:D:253:ARG:N	2.68	0.46
1:A:143:GLY:O	1:A:147:SER:OG	2.34	0.46
1:A:312:TYR:O	1:A:344:VAL:HG12	2.16	0.46
2:B:313:LEU:HD11	2:B:346:TRP:CH2	2.51	0.46
1:C:100:ALA:HB3	1:C:105:ARG:HE	1.81	0.46
2:D:262:PHE:O	2:D:266:HIS:CD2	2.69	0.46
2:D:342:TYR:N	2:D:342:TYR:CD2	2.84	0.46
1:A:181:VAL:HG23	2:B:258:ASN:HD22	1.81	0.45
2:D:195:VAL:HG21	2:D:428:LEU:HD13	1.97	0.45
1:A:30:ILE:HG23	1:A:34:GLY:O	2.16	0.45
2:B:228:ASN:ND2	6:B:602:GDP:HN1	2.14	0.45
2:B:5:VAL:HG12	2:B:64:ARG:HG2	1.98	0.45
1:C:184:PRO:O	1:C:188:ILE:HG12	2.15	0.45
1:A:190:THR:CG2	1:A:191:THR:H	2.30	0.45
1:A:82:THR:O	1:A:83:TYR:HB2	2.17	0.45
2:B:74:THR:HA	2:B:77:SER:HB2	1.99	0.45
2:D:269:MET:HE1	2:D:307:PRO:HG3	1.96	0.45
1:A:327:ASP:O	1:A:328:VAL:C	2.54	0.45
1:A:82:THR:O	1:A:83:TYR:CB	2.65	0.45
1:C:316:CYS:O	1:C:377:MET:HE3	2.17	0.45
2:D:115:VAL:HG12	2:D:116:ASP:N	2.30	0.45
2:D:269:MET:HG2	2:D:384:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:VAL:CG2	2:D:62:VAL:O	2.63	0.45
2:B:171:VAL:HA	2:B:204:ILE:O	2.16	0.45
2:D:427:ASP:O	2:D:430:SER:N	2.50	0.45
1:A:312:TYR:HE2	1:A:379:SER:HB2	1.82	0.45
2:B:135:PHE:CD1	2:B:135:PHE:N	2.83	0.45
2:B:150:GLY:C	2:B:152:LEU:N	2.69	0.45
2:B:382:THR:HB	2:B:436:GLN:HE21	1.81	0.45
1:C:141:PHE:HD1	1:C:172:TYR:HA	1.81	0.45
1:C:346:TRP:O	1:C:348:PRO:HD3	2.17	0.45
2:D:289:PRO:HA	2:D:331:GLN:NE2	2.32	0.45
1:A:332:ILE:O	1:A:333:ALA:C	2.54	0.45
1:C:183:GLU:CB	1:C:184:PRO:CD	2.94	0.45
2:D:118:VAL:O	2:D:122:VAL:HG13	2.16	0.45
2:D:8:GLN:NE2	2:D:17:GLY:HA3	2.32	0.45
2:D:260:VAL:HA	2:D:261:PRO:HD2	1.82	0.45
1:A:289:ALA:O	1:A:292:THR:HB	2.17	0.45
1:A:320:ARG:O	1:A:373:ARG:HA	2.17	0.45
1:A:348:PRO:HB2	1:A:349:THR:H	1.50	0.45
2:B:140:SER:HA	2:B:171:VAL:CG2	2.37	0.45
2:B:248:LEU:HB2	2:B:249:ASN:H	1.50	0.45
1:C:107:HIS:HD2	1:C:108:TYR:CE2	2.35	0.45
1:C:115:ILE:HD12	1:C:156:ARG:HD3	1.99	0.45
2:D:20:PHE:O	2:D:24:ILE:HG23	2.17	0.45
1:C:100:ALA:CB	2:D:253:ARG:HG2	2.47	0.45
2:D:191:VAL:HG11	2:D:425:MET:CE	2.47	0.45
3:E:79:GLU:C	3:E:81:GLU:H	2.21	0.45
1:A:111:GLY:O	1:A:112:LYS:C	2.55	0.45
1:A:68:VAL:HG11	1:A:118:VAL:HG21	1.98	0.45
2:B:212:ILE:HD12	2:B:215:ARG:NH2	2.32	0.45
2:B:388:PHE:CD2	2:B:425:MET:CE	2.99	0.45
1:C:358:GLN:HA	1:C:359:PRO:HD3	1.89	0.45
2:D:308:ARG:CG	2:D:308:ARG:NH1	2.76	0.45
2:B:141:LEU:CD2	2:B:172:VAL:HG22	2.46	0.45
2:B:408:TYR:O	2:B:409:THR:C	2.55	0.45
1:C:181:VAL:HG11	1:C:404:PHE:CZ	2.51	0.44
2:B:269:MET:HE1	2:B:307:PRO:HG3	2.00	0.44
1:C:149:PHE:O	1:C:150:THR:C	2.55	0.44
1:C:154:MET:HB3	1:C:154:MET:HE3	1.83	0.44
1:C:244:PHE:CE2	1:C:358:GLN:HG2	2.51	0.44
2:D:102:ASN:OD1	2:D:105:LYS:HB2	2.16	0.44
3:E:76:ARG:HA	3:E:76:ARG:HD3	1.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HD23	1:A:128:GLN:NE2	2.32	0.44
1:A:281:ALA:C	1:A:283:HIS:H	2.20	0.44
1:C:393:HIS:CE1	1:C:397:LEU:HD13	2.52	0.44
2:D:143:GLY:O	2:D:147:SER:HB3	2.17	0.44
1:A:112:LYS:HG3	3:E:54:LEU:HD11	1.99	0.44
1:A:26:LEU:HD21	1:A:364:PRO:HD3	1.99	0.44
1:A:108:TYR:CE1	1:A:413:MET:HG3	2.52	0.44
2:B:287:THR:O	2:B:288:VAL:CB	2.66	0.44
2:D:150:GLY:O	2:D:152:LEU:N	2.51	0.44
2:D:36:TYR:CZ	2:D:38:GLY:O	2.71	0.44
2:B:143:GLY:O	2:B:147:SER:HB3	2.16	0.44
1:C:247:ALA:C	1:C:249:ASN:N	2.71	0.44
2:D:210:TYR:HD1	2:D:210:TYR:C	2.21	0.44
1:C:180:ALA:O	1:C:183:GLU:HB2	2.18	0.44
1:C:223:THR:CG2	1:C:225:THR:HG23	2.48	0.44
1:A:410:GLY:HA2	3:E:64:GLN:NE2	2.32	0.44
2:B:332:MET:HG3	2:B:353:THR:CG2	2.43	0.44
1:C:223:THR:HB	1:C:226:ASN:H	1.83	0.44
1:C:36:MET:C	1:C:38:SER:N	2.71	0.44
1:C:381:THR:HG23	1:C:384:ILE:H	1.83	0.44
1:C:395:PHE:C	1:C:395:PHE:CD2	2.91	0.44
2:D:350:ASN:H	2:D:350:ASN:ND2	2.02	0.44
3:E:77:GLU:HG2	3:E:80:ARG:HB2	1.98	0.44
2:B:335:VAL:C	2:B:337:ASN:H	2.21	0.44
2:B:403:ALA:HB1	2:B:404:PHE:HD1	1.82	0.44
2:D:269:MET:HA	2:D:270:PRO:HD3	1.83	0.44
2:D:404:PHE:H	2:D:404:PHE:HD1	1.64	0.44
3:E:129:HIS:O	3:E:133:VAL:HG23	2.18	0.44
3:E:57:ALA:O	3:E:60:ARG:N	2.50	0.44
2:B:158:ARG:NH1	2:B:158:ARG:CG	2.81	0.44
1:C:70:LEU:HB2	1:C:145:THR:HG21	1.99	0.44
2:D:135:PHE:N	2:D:135:PHE:CD1	2.85	0.44
3:E:92:ASN:O	3:E:96:MET:HB2	2.18	0.44
1:A:407:TRP:CG	2:B:257:VAL:CG2	3.02	0.43
2:B:164:ARG:CA	2:B:164:ARG:HE	2.31	0.43
2:B:182:VAL:O	2:B:185:TYR:HB2	2.17	0.43
1:C:176:GLN:HG2	1:C:177:VAL:N	2.31	0.43
1:C:383:ALA:O	1:C:386:GLU:HB2	2.18	0.43
2:D:319:PHE:CD1	2:D:319:PHE:N	2.86	0.43
2:D:9:ALA:CB	2:D:68:VAL:HB	2.48	0.43
1:A:205:ASP:HB3	1:A:303:VAL:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:HZ3	1:A:53:PHE:CZ	2.36	0.43
1:A:359:PRO:HA	1:A:360:PRO:HD3	1.91	0.43
2:B:114:LEU:O	2:B:115:VAL:C	2.55	0.43
2:B:195:VAL:HG21	2:B:428:LEU:HD13	2.00	0.43
1:C:346:TRP:CZ2	1:C:435:VAL:HG13	2.40	0.43
1:C:8:HIS:ND1	1:C:8:HIS:N	2.66	0.43
2:D:269:MET:HB3	2:D:303:ALA:HB3	2.00	0.43
1:A:24:TYR:CE2	1:A:243:ARG:NH1	2.86	0.43
1:A:420:GLU:HG2	1:A:420:GLU:O	2.18	0.43
1:A:180:ALA:HB1	2:B:258:ASN:HD21	1.84	0.43
2:B:360:PRO:C	2:B:369:ARG:O	2.56	0.43
1:C:322:ASP:O	1:C:373:ARG:HD3	2.18	0.43
2:D:61:TYR:HD2	2:D:61:TYR:HA	1.72	0.43
1:A:158:SER:HB3	3:E:46:SER:CB	2.48	0.43
1:A:169:PHE:CE2	1:A:235:VAL:HG22	2.53	0.43
2:B:155:SER:C	3:E:76:ARG:HH22	2.21	0.43
2:B:61:TYR:HA	2:B:61:TYR:HD2	1.69	0.43
1:C:405:VAL:HG13	1:C:406:HIS:N	2.33	0.43
1:C:430:LYS:O	1:C:434:GLU:HB2	2.18	0.43
1:A:306:ASP:HA	1:A:307:PRO:HD3	1.83	0.43
1:A:401:LYS:C	1:A:403:ALA:H	2.21	0.43
2:B:321:GLY:O	2:B:323:MET:N	2.51	0.43
2:D:250:ALA:C	2:D:252:LEU:N	2.72	0.43
2:D:307:PRO:O	2:D:308:ARG:HD2	2.18	0.43
2:D:357:ASP:N	2:D:357:ASP:OD2	2.50	0.43
2:D:42:LEU:O	2:D:43:GLN:C	2.56	0.43
2:D:224:TYR:HE2	6:D:603:GDP:C4	2.36	0.43
2:B:111:GLY:HA2	2:B:149:MET:HE3	1.99	0.43
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.54	0.43
2:B:270:PRO:HG2	2:B:302:MET:CB	2.49	0.43
1:C:229:ARG:HG2	1:C:229:ARG:HH11	1.83	0.43
1:C:324:VAL:O	1:C:327:ASP:HB2	2.18	0.43
1:A:108:TYR:HE1	1:A:413:MET:HG3	1.83	0.43
2:B:273:ALA:CB	2:B:375:ALA:H	2.32	0.43
1:C:169:PHE:CE2	1:C:235:VAL:HG22	2.54	0.43
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.01	0.43
2:B:158:ARG:O	2:B:159:GLU:HB3	2.19	0.43
2:B:216:THR:HG21	2:B:299:LYS:CD	2.49	0.43
2:B:222:PRO:O	8:C:800:VLB:H713	2.19	0.43
8:C:800:VLB:N9	8:C:800:VLB:O27	2.52	0.43
3:E:97:ALA:HA	3:E:100:LYS:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ALA:CB	1:A:302:MET:CE	2.88	0.43
2:D:332:MET:HG3	2:D:353:THR:CG2	2.45	0.43
1:A:273:ALA:HB2	1:A:375:VAL:CA	2.49	0.43
1:A:425:MET:O	1:A:429:GLU:HB2	2.19	0.43
2:B:166:MET:HB3	2:B:198:THR:HA	2.01	0.43
2:B:76:ASP:OD1	2:B:76:ASP:N	2.52	0.43
3:E:123:LEU:O	3:E:125:GLU:N	2.52	0.43
1:A:118:VAL:O	1:A:121:ARG:N	2.51	0.42
1:A:280:LYS:HG2	1:A:283:HIS:CE1	2.54	0.42
1:A:320:ARG:HH21	1:A:358:GLN:HG3	1.84	0.42
2:B:55:GLU:H	2:B:55:GLU:HG3	1.71	0.42
2:D:135:PHE:HB2	2:D:166:MET:HE1	2.00	0.42
1:A:141:PHE:HD2	1:A:141:PHE:HA	1.74	0.42
2:B:115:VAL:HG12	2:B:116:ASP:N	2.32	0.42
1:C:249:ASN:HB2	1:C:355:ILE:H	1.83	0.42
2:D:251:ASP:HB2	2:D:254:LYS:H	1.85	0.42
2:B:12:CYS:O	2:B:13:GLY:C	2.57	0.42
3:E:77:GLU:OE2	3:E:80:ARG:HG3	2.19	0.42
1:A:107:HIS:HD2	1:A:108:TYR:CE2	2.37	0.42
1:A:152:LEU:O	1:A:153:LEU:C	2.58	0.42
2:B:241:CYS:SG	2:B:247:GLN:NE2	2.93	0.42
1:C:101:ASN:ND2	2:D:254:LYS:HE3	2.34	0.42
1:C:70:LEU:HD13	1:C:145:THR:HB	2.00	0.42
1:C:16:ILE:HG22	1:C:17:GLY:N	2.33	0.42
1:C:198:SER:HB3	1:C:265:ILE:CD1	2.50	0.42
1:C:78:VAL:C	1:C:80:THR:H	2.23	0.42
1:A:265:ILE:HG23	1:A:267:PHE:CE1	2.54	0.42
1:A:181:VAL:HG11	1:A:404:PHE:CZ	2.55	0.42
2:B:102:ASN:OD1	2:B:105:LYS:CB	2.67	0.42
2:B:41:ASP:O	2:B:42:LEU:C	2.56	0.42
1:C:111:GLY:C	1:C:113:GLU:H	2.22	0.42
2:D:216:THR:O	2:D:217:LEU:CB	2.68	0.42
7:D:701:CN2:C15	7:D:701:CN2:C12	2.97	0.42
2:D:74:THR:HA	2:D:77:SER:HB2	2.00	0.42
2:B:151:THR:CG2	2:B:193:GLN:HB3	2.48	0.42
1:A:398:MET:HG3	2:B:348:PRO:CD	2.50	0.42
2:B:416:MET:H	2:B:416:MET:HG3	1.68	0.42
2:D:64:ARG:HG3	2:D:125:GLU:OE1	2.19	0.42
2:B:403:ALA:C	2:B:405:LEU:N	2.61	0.42
1:C:163:LYS:O	1:C:164:LYS:C	2.58	0.42
1:C:255:PHE:O	1:C:259:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:231:VAL:HG12	2:D:235:MET:HE2	2.01	0.42
1:A:271:THR:HB	1:A:377:MET:HB3	2.00	0.42
1:A:309:HIS:ND1	1:A:386:GLU:OE1	2.53	0.42
2:B:2:ARG:HH12	2:B:133:GLN:HA	1.79	0.42
2:D:164:ARG:HH21	2:D:253:ARG:HH22	1.67	0.42
1:A:294:ALA:O	1:A:297:GLU:CB	2.63	0.42
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.79	0.42
1:A:109:THR:OG1	1:A:411:GLU:HB3	2.19	0.42
1:A:54:SER:HB3	1:A:64:ARG:NE	2.34	0.42
1:A:398:MET:HG3	2:B:348:PRO:HD3	2.00	0.42
1:C:2:ARG:HB2	1:C:131:GLY:O	2.20	0.42
1:C:177:VAL:CG2	1:C:210:TYR:HD2	2.31	0.42
1:C:223:THR:H	1:C:226:ASN:HB2	1.83	0.42
2:D:21:TRP:O	2:D:25:SER:HB2	2.19	0.42
2:D:70:LEU:C	2:D:95:GLY:HA3	2.40	0.42
1:A:187:SER:O	1:A:191:THR:HG22	2.20	0.42
1:A:191:THR:HG23	1:A:425:MET:CE	2.49	0.42
2:B:424:ASN:O	2:B:427:ASP:HB2	2.19	0.42
1:C:248:LEU:O	1:C:249:ASN:CB	2.67	0.42
1:C:350:GLY:O	1:C:351:PHE:CB	2.63	0.42
2:D:119:LEU:HD23	2:D:123:ARG:HH21	1.85	0.42
2:D:150:GLY:C	2:D:152:LEU:N	2.72	0.42
2:D:403:ALA:C	2:D:405:LEU:H	2.23	0.42
3:E:19:SER:O	3:E:20:PHE:CB	2.67	0.42
1:A:405:VAL:HG13	1:A:406:HIS:N	2.34	0.41
2:B:122:VAL:CG2	2:B:123:ARG:N	2.82	0.41
1:C:219:ILE:HD12	1:C:226:ASN:HD21	1.85	0.41
1:C:229:ARG:CG	1:C:229:ARG:HH11	2.33	0.41
2:D:239:THR:O	2:D:240:THR:C	2.58	0.41
2:D:274:PRO:HG3	2:D:286:LEU:HD22	2.00	0.41
2:D:216:THR:HG21	2:D:299:LYS:HD3	2.01	0.41
2:D:335:VAL:C	2:D:337:ASN:H	2.23	0.41
3:E:63:TYR:O	3:E:65:GLU:N	2.53	0.41
1:C:163:LYS:H	1:C:163:LYS:HE3	1.85	0.41
1:C:174:ALA:HB1	1:C:176:GLN:NE2	2.35	0.41
1:A:430:LYS:O	1:A:434:GLU:HB2	2.20	0.41
2:B:141:LEU:HA	2:B:147:SER:HB2	2.02	0.41
1:A:181:VAL:CG2	2:B:258:ASN:HD22	2.33	0.41
2:B:273:ALA:HB1	2:B:274:PRO:HD3	1.94	0.41
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.38	0.41
2:D:229:HIS:NE2	2:D:277:SER:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:HIS:CG	2:D:49:ILE:HD12	2.54	0.41
3:E:129:HIS:O	3:E:133:VAL:CG2	2.68	0.41
1:A:395:PHE:C	1:A:395:PHE:CD2	2.93	0.41
2:B:177:VAL:HG13	2:B:177:VAL:O	2.20	0.41
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.35	0.41
1:C:260:VAL:HA	1:C:261:PRO:HD3	1.73	0.41
1:C:271:THR:HG21	1:C:295:CYS:O	2.21	0.41
1:C:185:TYR:OH	1:C:403:ALA:HB3	2.21	0.41
2:D:261:PRO:HB2	2:D:262:PHE:CD1	2.56	0.41
1:A:16:ILE:CG2	1:A:17:GLY:N	2.82	0.41
1:A:323:VAL:HG12	1:A:355:ILE:CD1	2.47	0.41
1:C:182:VAL:O	1:C:182:VAL:CG2	2.68	0.41
2:D:135:PHE:HB2	2:D:166:MET:HE2	2.02	0.41
2:D:287:THR:CG2	2:D:290:GLU:H	2.32	0.41
3:E:121:GLU:HG3	3:E:121:GLU:O	2.21	0.41
2:B:2:ARG:HH11	2:B:133:GLN:HA	1.80	0.41
1:C:291:ILE:O	1:C:294:ALA:HB3	2.21	0.41
2:D:141:LEU:HA	2:D:141:LEU:HD12	1.67	0.41
2:D:190:SER:O	2:D:191:VAL:C	2.59	0.41
2:D:71:GLU:HG2	2:D:71:GLU:O	2.19	0.41
1:A:125:LEU:HD23	1:A:128:GLN:HE22	1.85	0.41
1:A:155:GLU:O	1:A:158:SER:HB2	2.21	0.41
1:A:171:ILE:N	1:A:171:ILE:HD12	2.36	0.41
1:A:219:ILE:HD12	1:A:226:ASN:HD21	1.86	0.41
1:A:73:THR:O	1:A:76:ASP:HB2	2.21	0.41
2:B:200:GLU:HB3	2:B:268:PHE:CE1	2.55	0.41
2:B:407:TRP:CD1	1:C:257:THR:CG2	3.03	0.41
2:D:333:LEU:HA	2:D:336:GLN:HE21	1.85	0.41
1:C:272:TYR:CE2	1:C:274:PRO:HD2	2.56	0.41
2:D:76:ASP:O	2:D:80:SER:HB2	2.21	0.41
1:A:395:PHE:O	1:A:396:ASP:C	2.59	0.41
1:A:98:ASP:CB	2:B:251:ASP:OD2	2.65	0.41
2:B:348:PRO:O	2:B:350:ASN:N	2.54	0.41
2:D:158:ARG:O	2:D:159:GLU:HB2	2.19	0.41
2:D:262:PHE:O	2:D:264:ARG:N	2.54	0.41
2:D:387:LEU:O	2:D:390:ARG:HG3	2.21	0.41
1:A:10:GLY:O	1:A:11:GLN:C	2.59	0.41
1:A:282:TYR:CD1	1:A:282:TYR:N	2.89	0.41
1:A:286:LEU:HD12	1:A:286:LEU:H	1.86	0.41
1:C:265:ILE:HD13	1:C:267:PHE:CE2	2.56	0.41
1:C:31:GLN:O	1:C:32:PRO:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ALA:O	2:D:261:PRO:O	2.39	0.41
1:C:420:GLU:O	1:C:420:GLU:HG2	2.19	0.41
2:D:205:ASP:OD1	2:D:207:GLU:N	2.54	0.41
2:D:343:PHE:O	2:D:344:VAL:C	2.59	0.41
3:E:94:ILE:CG2	3:E:95:LYS:H	2.28	0.41
2:B:28:HIS:CG	2:B:49:ILE:HD12	2.56	0.41
2:B:287:THR:CG2	2:B:290:GLU:H	2.32	0.41
1:C:171:ILE:HG22	1:C:171:ILE:O	2.21	0.41
1:C:168:GLU:HG2	1:C:201:ALA:HB2	2.03	0.41
2:D:178:SER:HB2	2:D:183:GLU:OE2	2.21	0.41
2:D:171:VAL:HA	2:D:204:ILE:O	2.20	0.41
2:D:262:PHE:O	2:D:266:HIS:HD2	2.03	0.41
2:D:237:GLY:HA2	2:D:376:THR:HG21	2.00	0.41
2:D:388:PHE:CD2	2:D:425:MET:HE2	2.56	0.41
1:A:115:ILE:HD12	1:A:156:ARG:HD3	2.02	0.40
1:A:141:PHE:CD1	1:A:172:TYR:HB2	2.55	0.40
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.86	0.40
1:A:346:TRP:HZ3	1:A:347:CYS:HG	1.64	0.40
2:B:177:VAL:HA	8:C:800:VLB:C53	2.38	0.40
2:B:103:TRP:CZ3	2:B:189:LEU:HD22	2.56	0.40
1:C:31:GLN:HG3	1:C:31:GLN:H	1.76	0.40
2:D:245:PRO:HG3	2:D:247:GLN:CD	2.41	0.40
2:D:401:ARG:O	2:D:402:LYS:C	2.59	0.40
1:A:404:PHE:O	1:A:406:HIS:N	2.54	0.40
2:B:269:MET:HG2	2:B:384:ILE:CG1	2.48	0.40
1:A:70:LEU:HB2	1:A:145:THR:HG21	2.02	0.40
1:A:228:ASN:O	1:A:232:GLY:N	2.45	0.40
1:A:318:LEU:CB	1:A:376:CYS:HB3	2.45	0.40
2:B:103:TRP:HD1	2:B:147:SER:OG	2.05	0.40
1:C:102:ASN:O	1:C:103:TYR:C	2.59	0.40
1:C:328:VAL:HG12	1:C:332:ILE:HD11	2.00	0.40
2:D:164:ARG:NE	2:D:164:ARG:CA	2.77	0.40
2:D:342:TYR:N	2:D:342:TYR:HD2	2.19	0.40
2:D:344:VAL:HG13	2:D:346:TRP:H	1.86	0.40
3:E:112:ARG:HA	3:E:115:HIS:HB3	2.02	0.40
2:B:62:VAL:CG2	2:B:62:VAL:O	2.69	0.40
1:C:10:GLY:O	1:C:13:GLY:N	2.55	0.40
2:D:111:GLY:HA2	2:D:149:MET:HE3	2.00	0.40
2:D:150:GLY:O	2:D:153:LEU:N	2.55	0.40
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.56	0.40
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:388:PHE:CE1	2:D:428:LEU:HD21	2.56	0.40
3:E:84:GLN:HE21	3:E:84:GLN:HB2	1.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	423/448 (94%)	317 (75%)	75 (18%)	31 (7%)	1	16
1	C	421/448 (94%)	315 (75%)	68 (16%)	38 (9%)	1	12
2	B	415/445 (93%)	298 (72%)	71 (17%)	46 (11%)	0	7
2	D	415/445 (93%)	297 (72%)	73 (18%)	45 (11%)	0	7
3	E	120/142 (84%)	68 (57%)	36 (30%)	16 (13%)	0	4
All	All	1794/1928 (93%)	1295 (72%)	323 (18%)	176 (10%)	0	10

All (176) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	62	VAL
1	A	72	PRO
1	A	112	LYS
1	A	240	ALA
1	A	247	ALA
1	A	248	LEU
1	A	345	ASP
1	A	348	PRO
1	A	403	ALA
2	B	3	GLU
2	B	34	GLY

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Mol	Chain	Res	Type
2	B	43	GLN
2	B	60	LYS
2	B	62	VAL
2	B	72	PRO
2	B	82	PRO
2	B	115	VAL
2	B	163	ASP
2	B	177	VAL
2	B	245	PRO
2	B	249	ASN
2	B	265	LEU
2	B	266	HIS
2	B	273	ALA
2	B	288	VAL
2	B	348	PRO
2	B	369	ARG
2	B	370	GLY
2	B	371	LEU
2	B	400	ARG
2	B	403	ALA
1	C	41	THR
1	C	62	VAL
1	C	72	PRO
1	C	73	THR
1	C	112	LYS
1	C	240	ALA
1	C	249	ASN
1	C	250	VAL
1	C	266	HIS
1	C	341	ILE
1	C	345	ASP
1	C	357	TYR
1	C	403	ALA
2	D	3	GLU
2	D	34	GLY
2	D	43	GLN
2	D	60	LYS
2	D	62	VAL
2	D	64	ARG
2	D	72	PRO
2	D	82	PRO
2	D	96	GLN

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Mol	Chain	Res	Type
2	D	115	VAL
2	D	163	ASP
2	D	217	LEU
2	D	227	LEU
2	D	245	PRO
2	D	249	ASN
2	D	265	LEU
2	D	266	HIS
2	D	273	ALA
2	D	288	VAL
2	D	348	PRO
2	D	369	ARG
2	D	370	GLY
2	D	400	ARG
2	D	403	ALA
3	E	14	CYS
3	E	28	SER
3	E	29	PHE
3	E	47	LEU
3	E	58	GLU
3	E	124	GLN
3	E	128	LYS
1	A	73	THR
1	A	164	LYS
1	A	241	SER
1	A	264	ARG
1	A	273	ALA
1	A	282	TYR
1	A	341	ILE
1	A	350	GLY
2	B	42	LEU
2	B	64	ARG
2	B	73	GLY
2	B	96	GLN
2	B	151	THR
2	B	178	SER
2	B	181	VAL
2	B	217	LEU
2	B	225	GLY
2	B	227	LEU
2	B	244	PHE
2	B	276	THR

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Mol	Chain	Res	Type
2	B	299	LYS
2	B	404	PHE
1	C	33	ASP
1	C	55	GLU
1	C	164	LYS
1	C	241	SER
1	C	252	LEU
1	C	265	ILE
1	C	335	ILE
1	C	351	PHE
1	C	377	MET
2	D	42	LEU
2	D	57	THR
2	D	73	GLY
2	D	151	THR
2	D	229	HIS
2	D	244	PHE
2	D	251	ASP
2	D	276	THR
2	D	299	LYS
2	D	371	LEU
3	E	7	GLU
3	E	12	ASN
3	E	64	GLN
3	E	68	LEU
3	E	113	GLU
3	E	140	LYS
1	A	59	GLY
1	A	181	VAL
1	A	263	PRO
1	A	266	HIS
1	A	274	PRO
1	A	281	ALA
1	A	283	HIS
2	B	57	THR
2	B	360	PRO
1	C	59	GLY
1	C	181	VAL
1	C	247	ALA
1	C	248	LEU
1	C	273	ALA
1	C	274	PRO

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Mol	Chain	Res	Type
1	C	305	CYS
2	D	344	VAL
2	D	360	PRO
3	E	136	ASN
1	A	245	ASP
1	A	349	THR
2	B	97	SER
2	B	159	GLU
2	B	322	ARG
1	C	179	THR
1	C	349	THR
2	D	59	ASN
2	D	129	CYS
2	D	218	LYS
2	D	402	LYS
1	A	32	PRO
2	B	59	ASN
2	B	307	PRO
2	B	402	LYS
1	C	37	PRO
1	C	40	LYS
1	C	307	PRO
2	D	11	GLN
2	D	220	THR
3	E	26	PRO
3	E	49	GLU
1	A	377	MET
1	C	32	PRO
2	D	307	PRO
1	A	405	VAL
1	C	115	ILE
2	D	177	VAL
2	B	162	PRO
1	C	405	VAL
1	A	265	ILE
2	B	344	VAL
1	C	144	GLY
2	D	162	PRO

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	345/377 (92%)	228 (66%)	117 (34%)	0	1
1	C	336/377 (89%)	224 (67%)	112 (33%)	0	2
2	B	348/383 (91%)	217 (62%)	131 (38%)	0	0
2	D	348/383 (91%)	218 (63%)	130 (37%)	0	0
3	E	80/126 (64%)	44 (55%)	36 (45%)	0	0
All	All	1457/1646 (88%)	931 (64%)	526 (36%)	0	1

All (526) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	4	CYS
1	A	6	SER
1	A	8	HIS
1	A	9	VAL
1	A	16	ILE
1	A	22	GLU
1	A	26	LEU
1	A	27	GLU
1	A	36	MET
1	A	48	SER
1	A	49	PHE
1	A	50	ASN
1	A	60	LYS
1	A	66	VAL
1	A	68	VAL
1	A	79	ARG
1	A	80	THR
1	A	84	ARG
1	A	88	HIS
1	A	90	GLU
1	A	94	THR
1	A	105	ARG

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Mol	Chain	Res	Type
1	A	112	LYS
1	A	114	ILE
1	A	115	ILE
1	A	117	LEU
1	A	119	LEU
1	A	123	ARG
1	A	125	LEU
1	A	127	ASP
1	A	128	GLN
1	A	140	SER
1	A	141	PHE
1	A	145	THR
1	A	147	SER
1	A	153	LEU
1	A	158	SER
1	A	160	ASP
1	A	163	LYS
1	A	165	SER
1	A	167	LEU
1	A	178	SER
1	A	179	THR
1	A	182	VAL
1	A	183	GLU
1	A	187	SER
1	A	193	THR
1	A	194	THR
1	A	196	GLU
1	A	206	ASN
1	A	210	TYR
1	A	211	ASP
1	A	212	ILE
1	A	219	ILE
1	A	220	GLU
1	A	223	THR
1	A	225	THR
1	A	226	ASN
1	A	227	LEU
1	A	230	LEU
1	A	234	ILE
1	A	236	SER
1	A	242	LEU
1	A	243	ARG

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Mol	Chain	Res	Type
1	A	245	ASP
1	A	248	LEU
1	A	251	ASP
1	A	252	LEU
1	A	254	GLU
1	A	255	PHE
1	A	256	GLN
1	A	265	ILE
1	A	269	LEU
1	A	275	VAL
1	A	279	GLU
1	A	283	HIS
1	A	301	GLN
1	A	302	MET
1	A	306	ASP
1	A	313	MET
1	A	316	CYS
1	A	318	LEU
1	A	326	LYS
1	A	329	ASN
1	A	334	THR
1	A	341	ILE
1	A	343	PHE
1	A	345	ASP
1	A	347	CYS
1	A	349	THR
1	A	352	LYS
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	373	ARG
1	A	375	VAL
1	A	380	ASN
1	A	384	ILE
1	A	388	TRP
1	A	394	LYS
1	A	397	LEU
1	A	401	LYS

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Mol	Chain	Res	Type
1	A	405	VAL
1	A	413	MET
1	A	414	GLU
1	A	415	GLU
1	A	419	SER
1	A	428	LEU
1	A	430	LYS
1	A	432	TYR
1	A	433	GLU
1	A	434	GLU
2	B	2	ARG
2	B	4	ILE
2	B	11	GLN
2	B	16	ILE
2	B	22	GLU
2	B	24	ILE
2	B	25	SER
2	B	27	GLU
2	B	30	ILE
2	B	33	THR
2	B	39	ASP
2	B	42	LEU
2	B	43	GLN
2	B	49	ILE
2	B	51	VAL
2	B	55	GLU
2	B	61	TYR
2	B	66	ILE
2	B	70	LEU
2	B	71	GLU
2	B	75	MET
2	B	76	ASP
2	B	77	SER
2	B	78	VAL
2	B	79	ARG
2	B	80	SER
2	B	88	ARG
2	B	90	ASP
2	B	91	ASN
2	B	93	VAL
2	B	96	GLN
2	B	97	SER

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Mol	Chain	Res	Type
2	B	101	ASN
2	B	102	ASN
2	B	109	THR
2	B	119	LEU
2	B	128	SER
2	B	131	CYS
2	B	135	PHE
2	B	137	LEU
2	B	138	THR
2	B	141	LEU
2	B	145	THR
2	B	147	SER
2	B	151	THR
2	B	154	ILE
2	B	155	SER
2	B	156	LYS
2	B	158	ARG
2	B	164	ARG
2	B	166	MET
2	B	168	THR
2	B	170	SER
2	B	171	VAL
2	B	174	SER
2	B	177	VAL
2	B	179	ASP
2	B	182	VAL
2	B	183	GLU
2	B	189	LEU
2	B	192	HIS
2	B	195	VAL
2	B	200	GLU
2	B	203	SER
2	B	207	GLU
2	B	210	TYR
2	B	214	PHE
2	B	215	ARG
2	B	216	THR
2	B	223	THR
2	B	227	LEU
2	B	230	LEU
2	B	240	THR
2	B	241	CYS

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Mol	Chain	Res	Type
2	B	242	LEU
2	B	243	ARG
2	B	244	PHE
2	B	248	LEU
2	B	253	ARG
2	B	257	VAL
2	B	258	ASN
2	B	265	LEU
2	B	269	MET
2	B	275	LEU
2	B	276	THR
2	B	286	LEU
2	B	292	THR
2	B	294	GLN
2	B	295	MET
2	B	300	ASN
2	B	302	MET
2	B	308	ARG
2	B	311	ARG
2	B	313	LEU
2	B	318	VAL
2	B	320	ARG
2	B	323	MET
2	B	325	MET
2	B	333	LEU
2	B	335	VAL
2	B	339	ASN
2	B	341	SER
2	B	344	VAL
2	B	349	ASN
2	B	350	ASN
2	B	353	THR
2	B	355	VAL
2	B	357	ASP
2	B	371	LEU
2	B	373	MET
2	B	374	SER
2	B	376	THR
2	B	380	ASN
2	B	382	THR
2	B	384	ILE
2	B	386	GLU

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Mol	Chain	Res	Type
2	B	389	LYS
2	B	390	ARG
2	B	391	ILE
2	B	394	GLN
2	B	400	ARG
2	B	401	ARG
2	B	404	PHE
2	B	405	LEU
2	B	406	HIS
2	B	416	MET
2	B	419	THR
2	B	423	SER
2	B	425	MET
2	B	430	SER
2	B	434	GLN
1	C	2	ARG
1	C	4	CYS
1	C	6	SER
1	C	8	HIS
1	C	9	VAL
1	C	16	ILE
1	C	22	GLU
1	C	26	LEU
1	C	27	GLU
1	C	50	ASN
1	C	60	LYS
1	C	66	VAL
1	C	68	VAL
1	C	73	THR
1	C	79	ARG
1	C	80	THR
1	C	84	ARG
1	C	86	LEU
1	C	87	PHE
1	C	88	HIS
1	C	94	THR
1	C	105	ARG
1	C	112	LYS
1	C	113	GLU
1	C	114	ILE
1	C	115	ILE
1	C	116	ASP

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Mol	Chain	Res	Type
1	C	117	LEU
1	C	119	LEU
1	C	123	ARG
1	C	124	LYS
1	C	125	LEU
1	C	127	ASP
1	C	128	GLN
1	C	132	LEU
1	C	140	SER
1	C	141	PHE
1	C	147	SER
1	C	153	LEU
1	C	160	ASP
1	C	163	LYS
1	C	165	SER
1	C	167	LEU
1	C	178	SER
1	C	179	THR
1	C	182	VAL
1	C	187	SER
1	C	193	THR
1	C	194	THR
1	C	196	GLU
1	C	198	SER
1	C	200	CYS
1	C	206	ASN
1	C	210	TYR
1	C	211	ASP
1	C	217	LEU
1	C	219	ILE
1	C	220	GLU
1	C	223	THR
1	C	225	THR
1	C	226	ASN
1	C	227	LEU
1	C	230	LEU
1	C	234	ILE
1	C	236	SER
1	C	243	ARG
1	C	245	ASP
1	C	251	ASP
1	C	256	GLN

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Mol	Chain	Res	Type
1	C	258	ASN
1	C	264	ARG
1	C	265	ILE
1	C	269	LEU
1	C	275	VAL
1	C	287	SER
1	C	291	ILE
1	C	301	GLN
1	C	302	MET
1	C	306	ASP
1	C	316	CYS
1	C	318	LEU
1	C	334	THR
1	C	336	LYS
1	C	340	SER
1	C	341	ILE
1	C	343	PHE
1	C	345	ASP
1	C	353	VAL
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	373	ARG
1	C	375	VAL
1	C	379	SER
1	C	380	ASN
1	C	384	ILE
1	C	388	TRP
1	C	394	LYS
1	C	397	LEU
1	C	401	LYS
1	C	413	MET
1	C	415	GLU
1	C	419	SER
1	C	428	LEU
1	C	430	LYS
1	C	432	TYR
1	C	433	GLU

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Mol	Chain	Res	Type
1	C	434	GLU
2	D	2	ARG
2	D	4	ILE
2	D	11	GLN
2	D	16	ILE
2	D	19	LYS
2	D	22	GLU
2	D	24	ILE
2	D	25	SER
2	D	26	ASP
2	D	30	ILE
2	D	33	THR
2	D	39	ASP
2	D	42	LEU
2	D	43	GLN
2	D	49	ILE
2	D	51	VAL
2	D	55	GLU
2	D	61	TYR
2	D	66	ILE
2	D	70	LEU
2	D	71	GLU
2	D	75	MET
2	D	76	ASP
2	D	77	SER
2	D	78	VAL
2	D	79	ARG
2	D	80	SER
2	D	90	ASP
2	D	91	ASN
2	D	96	GLN
2	D	97	SER
2	D	101	ASN
2	D	102	ASN
2	D	109	THR
2	D	119	LEU
2	D	122	VAL
2	D	128	SER
2	D	135	PHE
2	D	137	LEU
2	D	138	THR
2	D	140	SER

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Mol	Chain	Res	Type
2	D	141	LEU
2	D	145	THR
2	D	147	SER
2	D	151	THR
2	D	154	ILE
2	D	156	LYS
2	D	158	ARG
2	D	160	GLU
2	D	164	ARG
2	D	166	MET
2	D	168	THR
2	D	170	SER
2	D	171	VAL
2	D	174	SER
2	D	176	LYS
2	D	179	ASP
2	D	183	GLU
2	D	192	HIS
2	D	195	VAL
2	D	200	GLU
2	D	203	SER
2	D	206	ASN
2	D	209	LEU
2	D	210	TYR
2	D	212	ILE
2	D	214	PHE
2	D	216	THR
2	D	221	THR
2	D	223	THR
2	D	230	LEU
2	D	240	THR
2	D	241	CYS
2	D	242	LEU
2	D	243	ARG
2	D	244	PHE
2	D	248	LEU
2	D	253	ARG
2	D	257	VAL
2	D	258	ASN
2	D	265	LEU
2	D	269	MET
2	D	275	LEU

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Mol	Chain	Res	Type
2	D	276	THR
2	D	286	LEU
2	D	292	THR
2	D	294	GLN
2	D	300	ASN
2	D	302	MET
2	D	308	ARG
2	D	311	ARG
2	D	313	LEU
2	D	318	VAL
2	D	320	ARG
2	D	323	MET
2	D	325	MET
2	D	333	LEU
2	D	335	VAL
2	D	339	ASN
2	D	341	SER
2	D	344	VAL
2	D	345	GLU
2	D	349	ASN
2	D	350	ASN
2	D	353	THR
2	D	355	VAL
2	D	357	ASP
2	D	371	LEU
2	D	373	MET
2	D	374	SER
2	D	376	THR
2	D	380	ASN
2	D	382	THR
2	D	384	ILE
2	D	386	GLU
2	D	389	LYS
2	D	390	ARG
2	D	391	ILE
2	D	394	GLN
2	D	400	ARG
2	D	401	ARG
2	D	404	PHE
2	D	405	LEU
2	D	406	HIS
2	D	416	MET

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Mol	Chain	Res	Type
2	D	419	THR
2	D	423	SER
2	D	425	MET
2	D	430	SER
2	D	434	GLN
3	E	5	ASP
3	E	11	LEU
3	E	14	CYS
3	E	28	SER
3	E	48	GLU
3	E	53	LYS
3	E	58	GLU
3	E	60	ARG
3	E	61	ARG
3	E	62	LYS
3	E	65	GLU
3	E	69	LEU
3	E	74	GLU
3	E	76	ARG
3	E	77	GLU
3	E	79	GLU
3	E	80	ARG
3	E	84	GLN
3	E	91	ASN
3	E	94	ILE
3	E	98	LYS
3	E	99	GLU
3	E	101	LEU
3	E	104	LYS
3	E	105	MET
3	E	106	GLU
3	E	111	ASN
3	E	112	ARG
3	E	113	GLU
3	E	115	HIS
3	E	119	MET
3	E	120	LEU
3	E	124	GLN
3	E	127	ASP
3	E	133	VAL
3	E	136	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	91	GLN
1	A	101	ASN
1	A	107	HIS
1	A	139	HIS
1	A	176	GLN
1	A	197	HIS
1	A	206	ASN
1	A	216	ASN
1	A	249	ASN
1	A	258	ASN
1	A	266	HIS
1	A	329	ASN
1	A	393	HIS
2	B	6	HIS
2	B	8	GLN
2	B	133	GLN
2	B	136	GLN
2	B	139	HIS
2	B	228	ASN
2	B	258	ASN
2	B	266	HIS
2	B	294	GLN
2	B	300	ASN
2	B	331	GLN
2	B	334	ASN
2	B	337	ASN
2	B	339	ASN
2	B	350	ASN
2	B	380	ASN
2	B	436	GLN
1	C	8	HIS
1	C	61	HIS
1	C	91	GLN
1	C	101	ASN
1	C	107	HIS
1	C	128	GLN
1	C	139	HIS
1	C	176	GLN
1	C	197	HIS
1	C	206	ASN
1	C	266	HIS

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Mol	Chain	Res	Type
1	C	329	ASN
1	C	393	HIS
2	D	6	HIS
2	D	133	GLN
2	D	136	GLN
2	D	258	ASN
2	D	266	HIS
2	D	309	HIS
2	D	337	ASN
2	D	339	ASN
2	D	350	ASN
2	D	380	ASN
2	D	436	GLN
3	E	12	ASN
3	E	64	GLN
3	E	84	GLN
3	E	91	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
6	GDP	B	602	-	24,30,30	1.05	1 (4%)	31,47,47	2.20	9 (29%)
5	GTP	A	600	4	26,34,34	1.06	3 (11%)	33,54,54	1.91	8 (24%)
8	VLB	C	800	-	63,67,67	1.56	10 (15%)	79,108,108	2.52	26 (32%)
7	CN2	B	700	-	28,32,32	3.17	7 (25%)	27,45,45	2.56	13 (48%)
7	CN2	D	701	-	28,32,32	3.07	7 (25%)	27,45,45	2.60	11 (40%)
5	GTP	C	601	4	26,34,34	1.16	3 (11%)	33,54,54	2.36	10 (30%)
6	GDP	D	603	-	24,30,30	1.04	1 (4%)	31,47,47	2.18	7 (22%)

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
6	GDP	B	602	-	-	4/12/32/32	0/3/3/3
5	GTP	A	600	4	-	5/18/38/38	0/3/3/3
8	VLB	C	800	-	-	16/38/131/131	0/7/9/9
7	CN2	B	700	-	-	2/10/27/27	0/3/3/3
7	CN2	D	701	-	-	3/10/27/27	0/3/3/3
5	GTP	C	601	4	-	6/18/38/38	0/3/3/3
6	GDP	D	603	-	-	3/12/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	CN2	C19-C17	-8.37	1.24	1.39
7	D	701	CN2	C19-C17	-8.34	1.24	1.39
7	B	700	CN2	C15-C16	7.34	1.54	1.39
7	B	700	CN2	C19-C20	-7.13	1.19	1.40
7	D	701	CN2	C15-C16	7.07	1.53	1.39
7	B	700	CN2	C20-C21	-7.06	1.23	1.40
7	D	701	CN2	C19-C20	-6.60	1.21	1.40
7	D	701	CN2	C20-C21	-6.53	1.24	1.40
8	C	800	VLB	C5-C6	-5.90	1.39	1.51
7	B	700	CN2	O6-C17	5.21	1.45	1.37
7	D	701	CN2	O6-C17	4.78	1.44	1.37
7	D	701	CN2	C22-C8	4.56	1.47	1.40
8	C	800	VLB	C8-C7	-4.12	1.38	1.49
8	C	800	VLB	C6-C7	4.08	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	601	GTP	C6-N1	3.48	1.39	1.33
8	C	800	VLB	C18-N1	-3.39	1.33	1.39
6	B	602	GDP	C6-N1	3.29	1.38	1.33
6	D	603	GDP	C6-N1	3.07	1.38	1.33
8	C	800	VLB	C3-C23	2.83	1.59	1.52
8	C	800	VLB	C30-C29	-2.82	1.39	1.49
5	A	600	GTP	C6-C5	-2.73	1.36	1.41
8	C	800	VLB	O25-C23	2.73	1.38	1.33
7	B	700	CN2	C22-C8	2.57	1.44	1.40
8	C	800	VLB	O28-C4	-2.55	1.39	1.44
5	A	600	GTP	C6-N1	2.42	1.37	1.33
8	C	800	VLB	C64-C65	-2.25	1.38	1.41
5	C	601	GTP	O4'-C4'	-2.25	1.40	1.45
8	C	800	VLB	C65-N66	-2.22	1.31	1.38
7	B	700	CN2	O3-C5	2.19	1.40	1.37
5	A	600	GTP	O4'-C4'	-2.19	1.40	1.45
7	D	701	CN2	O2-C3	2.04	1.42	1.38
5	C	601	GTP	C6-C5	-2.01	1.37	1.41

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	800	VLB	C4-O28-C29	-9.58	102.87	117.65
8	C	800	VLB	C57-C58-C59	6.86	127.27	114.30
7	D	701	CN2	C20-C19-C17	6.72	145.96	129.69
7	B	700	CN2	C20-C19-C17	6.63	145.74	129.69
5	C	601	GTP	N3-C2-N1	-6.48	118.58	127.22
5	C	601	GTP	PB-O3B-PG	-6.38	110.92	132.83
6	D	603	GDP	N3-C2-N1	-6.33	118.78	127.22
8	C	800	VLB	O25-C23-C3	6.06	122.41	112.22
6	B	602	GDP	N3-C2-N1	-5.88	119.38	127.22
7	D	701	CN2	O3-C5-C7	-5.43	114.77	124.12
8	C	800	VLB	O75-C73-C68	5.41	119.45	111.32
6	B	602	GDP	C2-N3-C4	5.36	121.48	115.36
8	C	800	VLB	C22-N1-C18	-5.23	104.13	120.84
8	C	800	VLB	C22-N1-C2	-5.14	106.69	119.21
6	D	603	GDP	C2-N3-C4	5.06	121.14	115.36
5	A	600	GTP	N3-C2-N1	-4.89	120.71	127.22
6	D	603	GDP	PA-O3A-PB	-4.65	116.86	132.83
8	C	800	VLB	O28-C29-C30	4.63	119.61	111.09
8	C	800	VLB	O32-C16-C15	4.49	121.18	116.58
5	A	600	GTP	PB-O3B-PG	-4.47	117.47	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	701	CN2	C4-O2-C3	4.42	126.90	114.78
5	C	601	GTP	C2-N3-C4	4.24	120.20	115.36
7	D	701	CN2	O3-C5-C3	4.23	122.59	115.16
7	D	701	CN2	C10-C11-N1	-4.19	102.50	110.04
7	B	700	CN2	C9-C10-C11	4.19	117.86	112.29
8	C	800	VLB	O25-C23-O24	-4.18	116.60	123.93
5	A	600	GTP	C2-N3-C4	4.13	120.08	115.36
5	C	601	GTP	C1'-N9-C4	-4.12	119.40	126.64
7	B	700	CN2	O3-C5-C3	3.94	122.08	115.16
6	B	602	GDP	PA-O3A-PB	-3.85	119.61	132.83
8	C	800	VLB	C69-N56-C55	-3.74	106.55	111.01
7	B	700	CN2	C6-O3-C5	3.69	123.10	117.53
5	C	601	GTP	C6-C5-C4	-3.68	117.28	120.80
6	B	602	GDP	C5-C6-N1	-3.59	118.53	123.43
8	C	800	VLB	C76-O75-C73	-3.56	109.94	115.94
7	B	700	CN2	C9-C8-C22	-3.55	116.43	119.50
7	B	700	CN2	C10-C9-C8	-3.39	106.25	113.68
6	B	602	GDP	C6-N1-C2	3.37	121.28	115.93
8	C	800	VLB	C4-C3-C2	-3.36	102.31	109.23
6	D	603	GDP	C6-N1-C2	3.35	121.26	115.93
8	C	800	VLB	C58-C57-N56	3.33	120.86	113.44
7	D	701	CN2	O4-C12-N1	3.32	128.56	122.95
8	C	800	VLB	O32-C16-C17	-3.27	118.49	124.12
7	B	700	CN2	C10-C11-N1	-3.23	104.24	110.04
5	A	600	GTP	N2-C2-N1	3.19	122.21	117.25
5	A	600	GTP	C5-C6-N1	-3.18	119.09	123.43
8	C	800	VLB	C12-C19-C5	-3.07	115.92	118.20
6	D	603	GDP	C5-C6-N1	-3.06	119.24	123.43
7	B	700	CN2	O4-C12-N1	2.98	127.98	122.95
7	B	700	CN2	O3-C5-C7	-2.94	119.06	124.12
5	C	601	GTP	N2-C2-N1	2.94	121.82	117.25
8	C	800	VLB	C33-O32-C16	-2.91	113.13	117.53
7	B	700	CN2	O4-C12-C13	-2.86	116.66	121.59
5	C	601	GTP	C6-N1-C2	2.84	120.45	115.93
7	D	701	CN2	C6-O3-C5	2.75	121.67	117.53
8	C	800	VLB	C7-C8-N9	-2.73	104.54	111.03
5	A	600	GTP	PA-O3A-PB	-2.70	123.57	132.83
8	C	800	VLB	C13-C12-C19	-2.58	106.62	115.16
6	B	602	GDP	N2-C2-N3	-2.53	113.66	117.79
6	D	603	GDP	C2'-C3'-C4'	2.46	107.43	102.64
8	C	800	VLB	C17-C18-C13	-2.46	119.08	122.00
7	B	700	CN2	C21-C22-C8	-2.45	117.85	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	602	GDP	C3'-C2'-C1'	2.44	104.65	100.98
5	C	601	GTP	PA-O3A-PB	-2.44	124.47	132.83
6	B	602	GDP	C4-C5-N7	-2.40	106.89	109.40
6	B	602	GDP	O2B-PB-O3A	2.40	112.69	104.64
8	C	800	VLB	C21-C20-C5	-2.32	111.32	115.79
8	C	800	VLB	O74-C73-C68	-2.31	119.31	124.19
8	C	800	VLB	O28-C29-O31	-2.31	118.37	122.96
5	C	601	GTP	O4'-C1'-C2'	2.30	110.28	106.93
5	A	600	GTP	O3G-PG-O3B	2.29	112.31	104.64
7	B	700	CN2	C9-C8-C7	2.29	124.47	119.42
7	D	701	CN2	C21-C22-C8	-2.24	118.07	120.50
7	D	701	CN2	C9-C10-C11	2.22	115.23	112.29
8	C	800	VLB	C8-N9-C19	-2.21	106.72	112.50
8	C	800	VLB	C61-C60-C65	2.20	121.09	118.17
5	A	600	GTP	C6-N1-C2	2.17	119.38	115.93
7	D	701	CN2	O2-C3-C5	2.14	123.20	120.12
7	D	701	CN2	C7-C5-C3	2.13	122.63	120.22
6	D	603	GDP	O2B-PB-O3A	2.12	111.76	104.64
5	C	601	GTP	C5-C6-N1	-2.09	120.58	123.43
7	B	700	CN2	C4-O2-C3	2.08	120.48	114.78
8	C	800	VLB	C4-C3-C23	2.04	116.05	110.85
8	C	800	VLB	C17-C16-C15	-2.03	120.33	122.20

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	602	GDP	PA-O3A-PB-O2B
6	B	602	GDP	O4'-C4'-C5'-O5'
5	A	600	GTP	C5'-O5'-PA-O1A
8	C	800	VLB	C21-C20-C5-C19
8	C	800	VLB	C21-C20-C5-C6
8	C	800	VLB	C21-C20-C5-C4
8	C	800	VLB	O24-C23-C3-C4
8	C	800	VLB	O25-C23-C3-C4
8	C	800	VLB	O24-C23-C3-O27
8	C	800	VLB	O25-C23-C3-O27
8	C	800	VLB	O24-C23-C3-C2
8	C	800	VLB	O25-C23-C3-C2
5	C	601	GTP	C5'-O5'-PA-O1A
6	D	603	GDP	O4'-C4'-C5'-O5'
6	D	603	GDP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
8	C	800	VLB	C30-C29-O28-C4
6	B	602	GDP	C3'-C4'-C5'-O5'
7	B	700	CN2	C7-C5-O3-C6
7	D	701	CN2	C7-C5-O3-C6
7	B	700	CN2	C3-C5-O3-C6
8	C	800	VLB	O31-C29-O28-C4
7	D	701	CN2	C3-C5-O3-C6
5	C	601	GTP	PG-O3B-PB-O1B
7	D	701	CN2	C14-C11-N1-C12
5	A	600	GTP	C5'-O5'-PA-O3A
5	C	601	GTP	C5'-O5'-PA-O3A
5	A	600	GTP	C5'-O5'-PA-O2A
5	C	601	GTP	C5'-O5'-PA-O2A
6	D	603	GDP	PA-O3A-PB-O1B
8	C	800	VLB	C15-C68-C73-O75
8	C	800	VLB	C67-C68-C73-O75
5	A	600	GTP	PB-O3A-PA-O2A
8	C	800	VLB	C15-C68-C73-O74
8	C	800	VLB	C67-C68-C73-O74
6	B	602	GDP	PA-O3A-PB-O1B
5	A	600	GTP	PB-O3A-PA-O1A
5	C	601	GTP	PG-O3B-PB-O2B
5	C	601	GTP	PB-O3A-PA-O2A
8	C	800	VLB	C58-C57-N56-C55

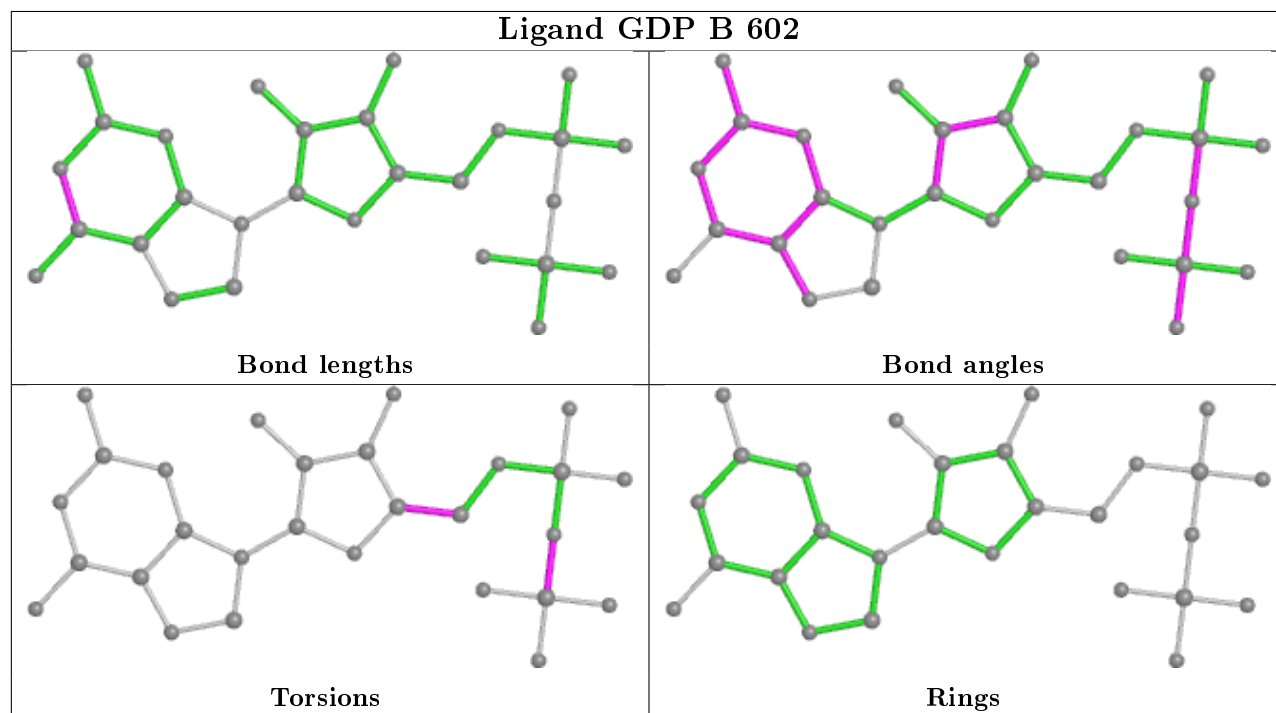
There are no ring outliers.

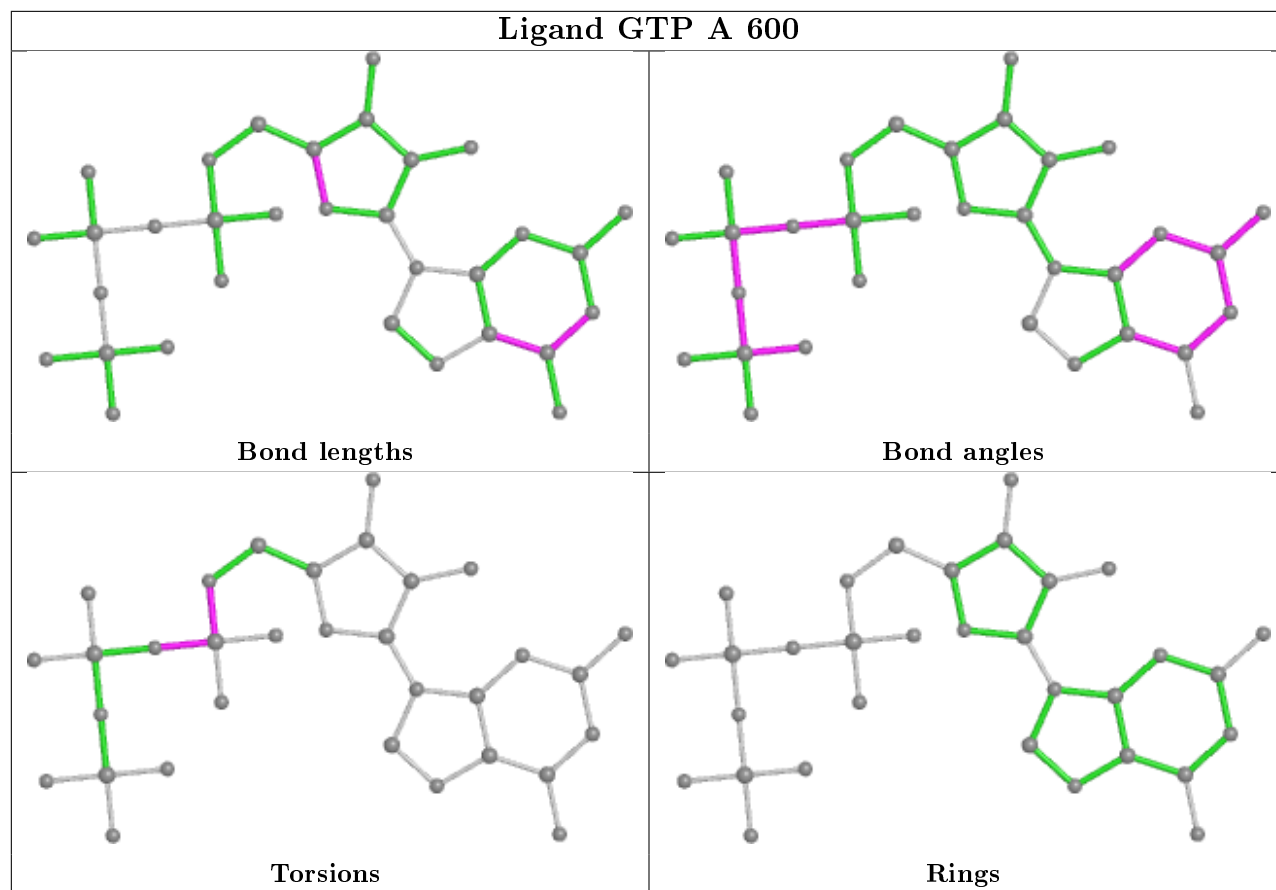
7 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	602	GDP	5	0
5	A	600	GTP	4	0
8	C	800	VLB	21	0
7	B	700	CN2	7	0
7	D	701	CN2	8	0
5	C	601	GTP	5	0
6	D	603	GDP	7	0

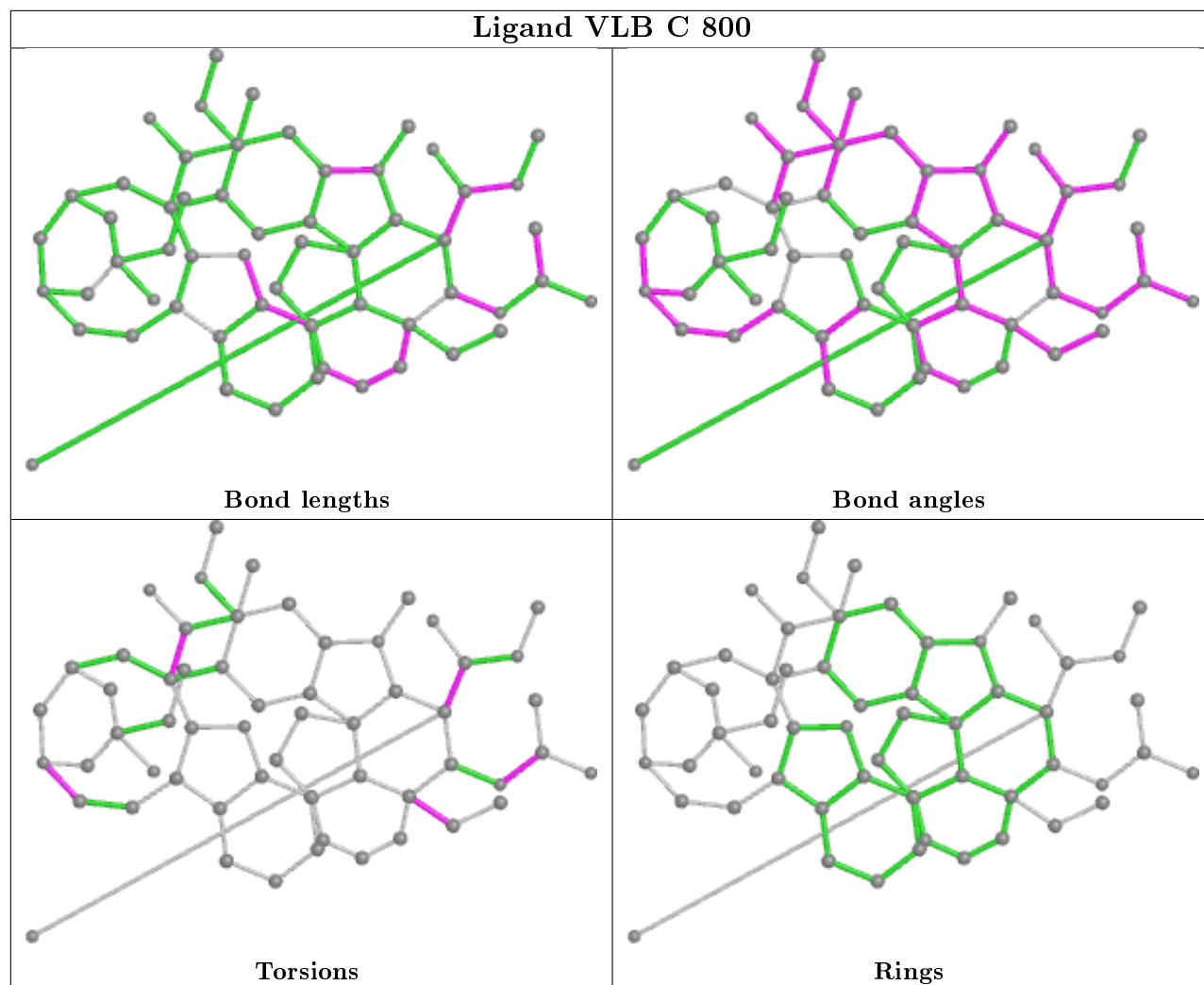
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

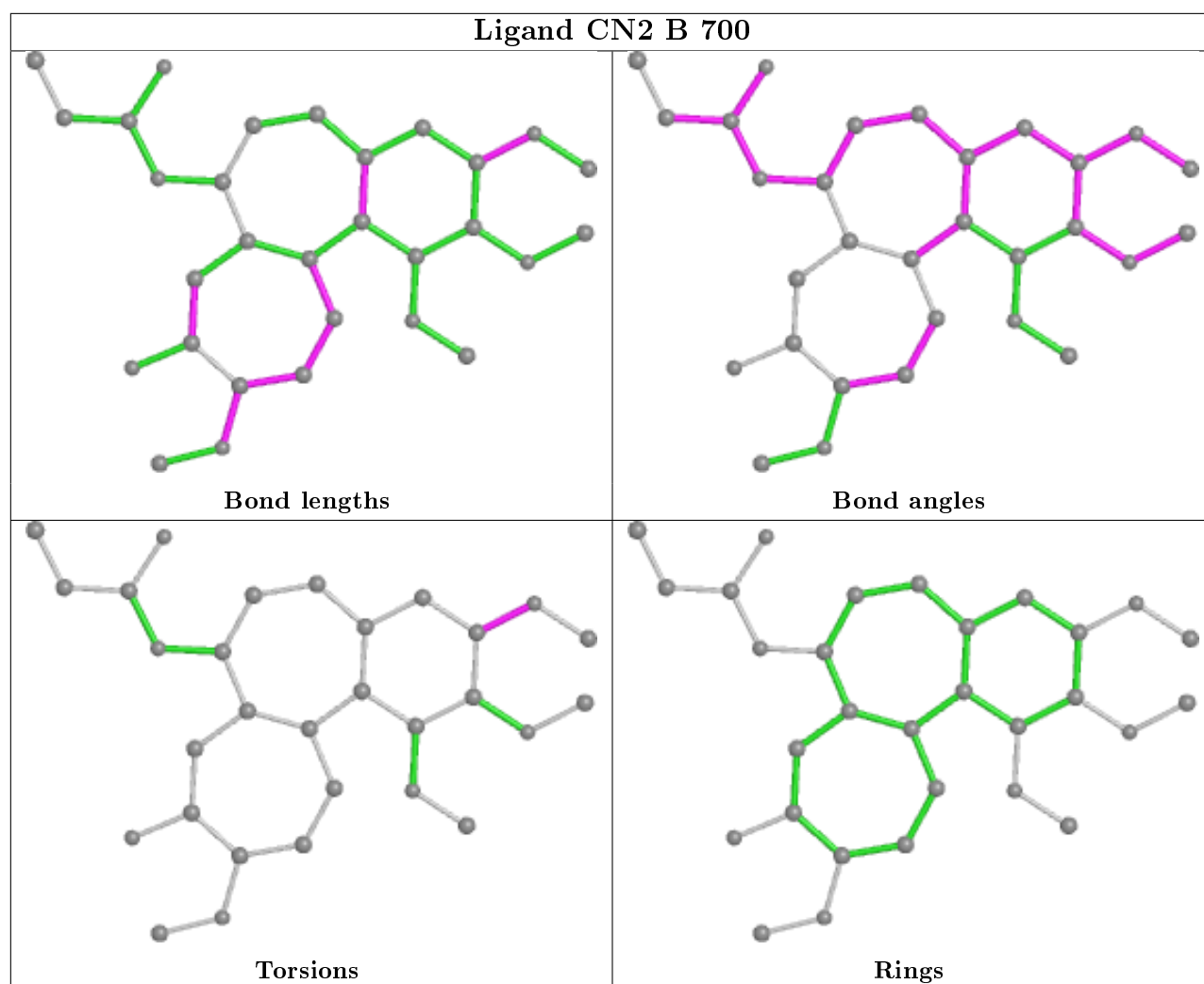
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

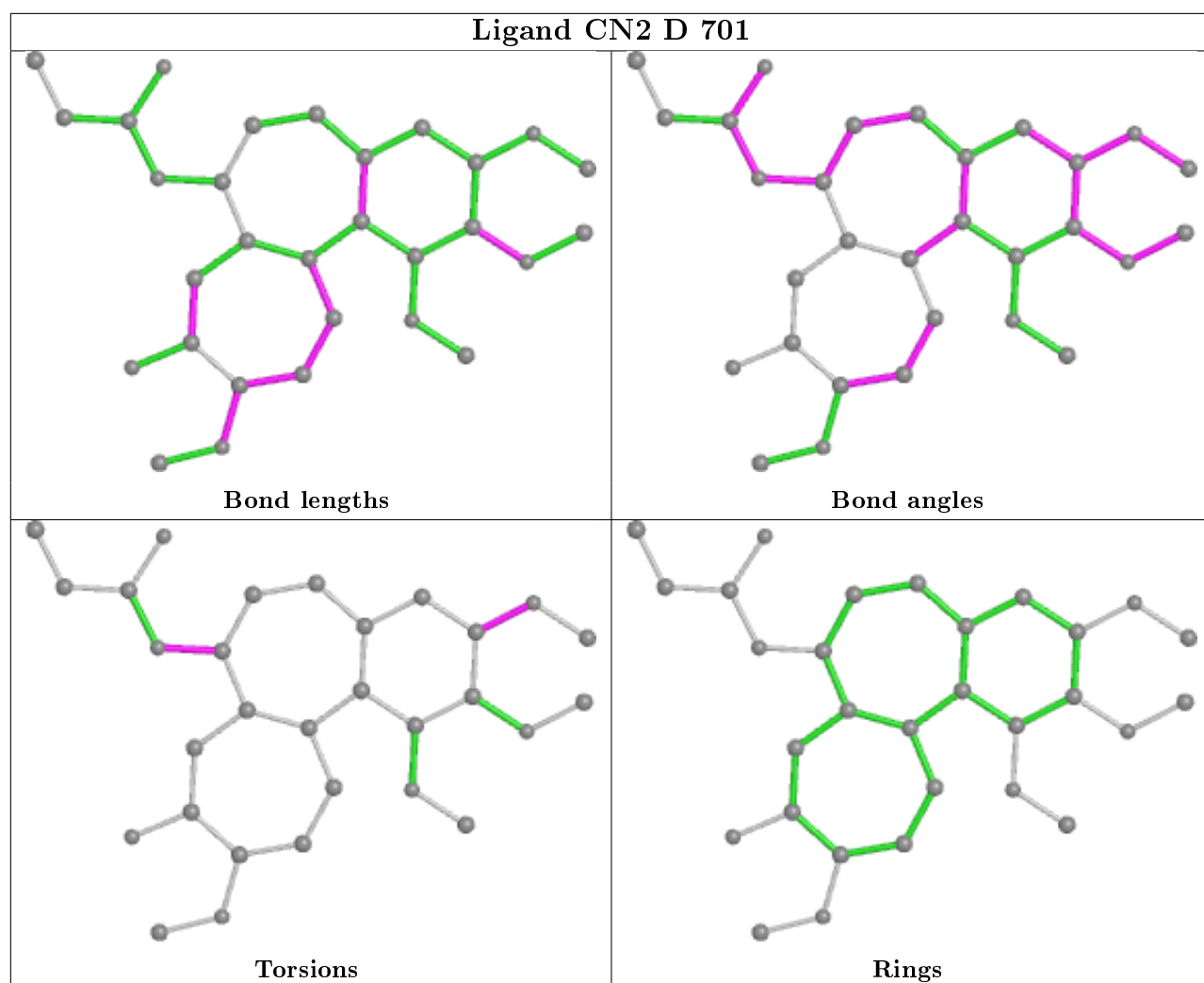


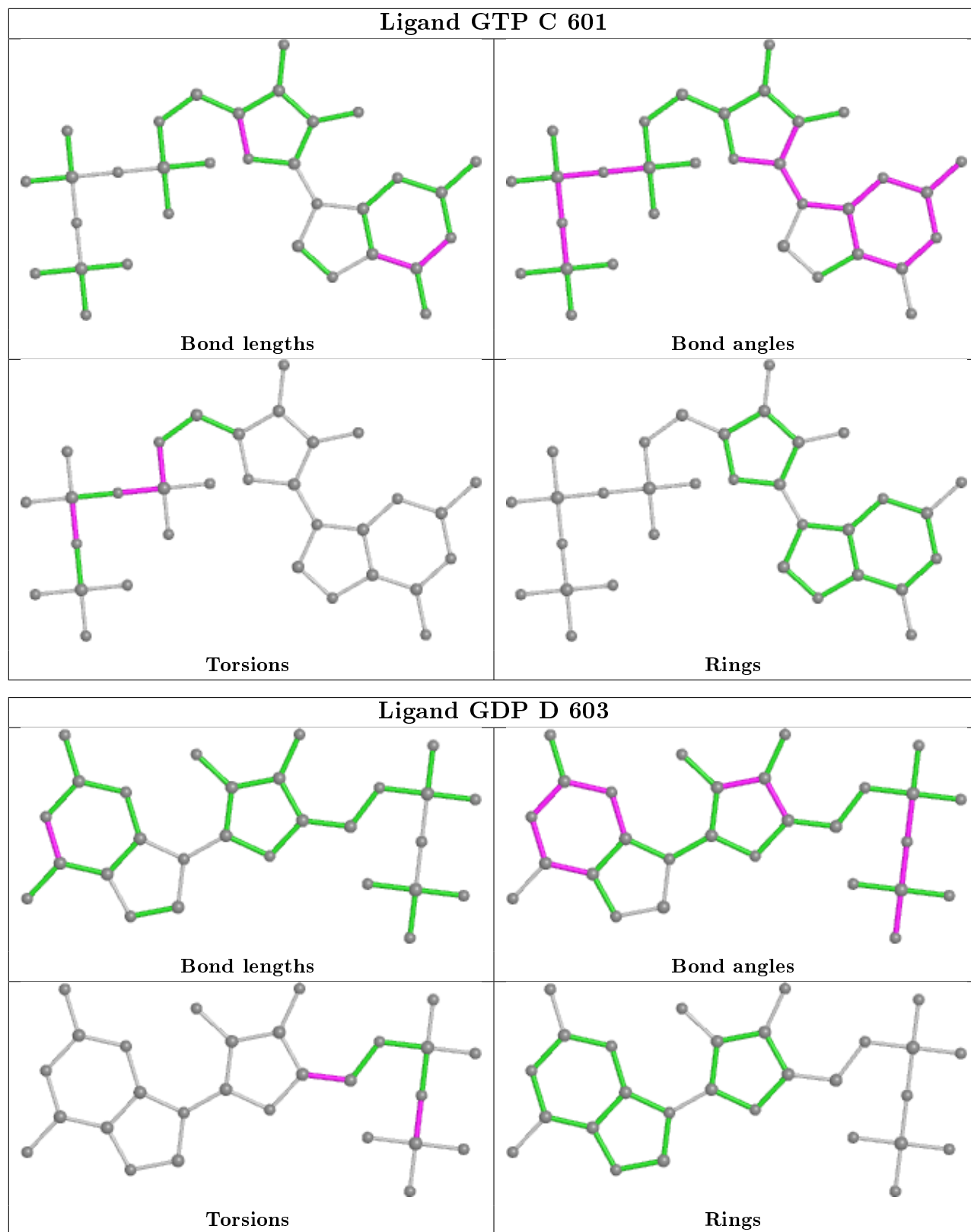


Ligand VLB C 800









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	427/448 (95%)	-0.31	1 (0%) 95 93	118, 118, 118, 118	1 (0%)
1	C	422/448 (94%)	-0.05	11 (2%) 56 45	118, 118, 118, 118	0
2	B	419/445 (94%)	-0.08	8 (1%) 66 58	118, 118, 118, 118	0
2	D	419/445 (94%)	-0.07	9 (2%) 63 54	118, 118, 118, 118	0
3	E	124/142 (87%)	-0.23	1 (0%) 86 79	118, 118, 118, 118	0
All	All	1811/1928 (93%)	-0.13	30 (1%) 70 60	118, 118, 118, 118	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	61	TYR	3.8
1	C	311	LYS	3.2
2	B	62	VAL	3.1
1	C	61	HIS	3.1
2	D	203	SER	2.9
2	B	311	ARG	2.9
1	C	253	THR	2.8
1	C	251	ASP	2.8
2	D	170	SER	2.6
3	E	141	GLU	2.5
2	D	199	ASP	2.5
2	B	140	SER	2.5
1	A	170	SER	2.4
2	D	370	GLY	2.4
1	C	307	PRO	2.3
1	C	319	TYR	2.2
1	C	274	PRO	2.2
2	D	201	THR	2.2
2	B	57	THR	2.2
2	D	413	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	220	GLU	2.1
2	B	170	SER	2.1
2	B	168	THR	2.1
2	D	346	TRP	2.1
1	C	60	LYS	2.1
1	C	62	VAL	2.1
2	D	359	PRO	2.0
2	D	342	TYR	2.0
2	B	438	ALA	2.0
1	C	55	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

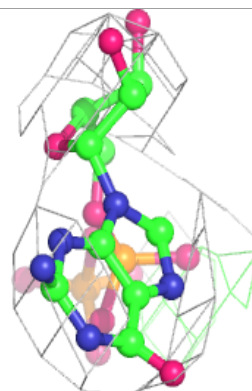
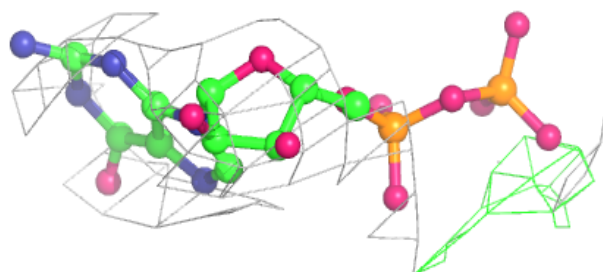
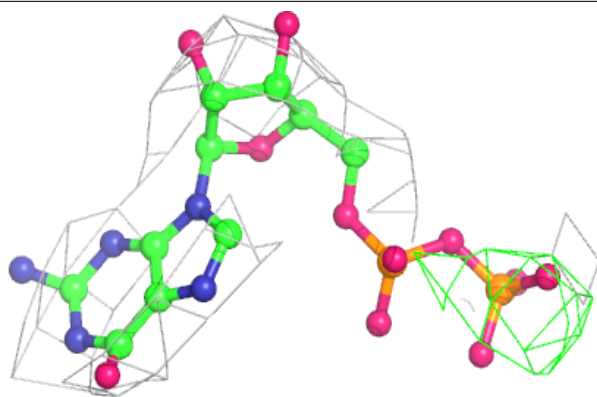
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GDP	B	602	28/28	0.85	0.44	117,117,117,117	0
8	VLB	C	800	59/59	0.88	0.28	117,117,117,117	0
7	CN2	B	700	30/30	0.89	0.28	117,117,117,117	0
7	CN2	D	701	30/30	0.94	0.22	117,117,117,117	0
5	GTP	A	600	32/32	0.94	0.29	117,117,117,117	0
5	GTP	C	601	32/32	0.95	0.25	117,117,117,117	0
6	GDP	D	603	28/28	0.97	0.23	117,117,117,117	0
4	MG	C	501	1/1	0.97	0.26	117,117,117,117	0
4	MG	A	500	1/1	0.98	0.34	117,117,117,117	0

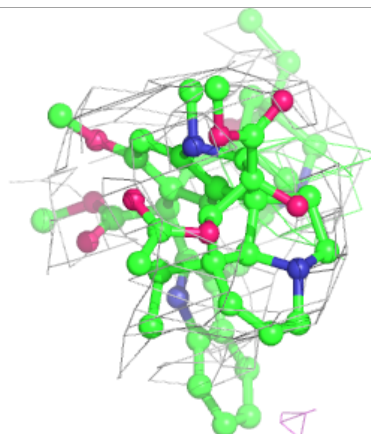
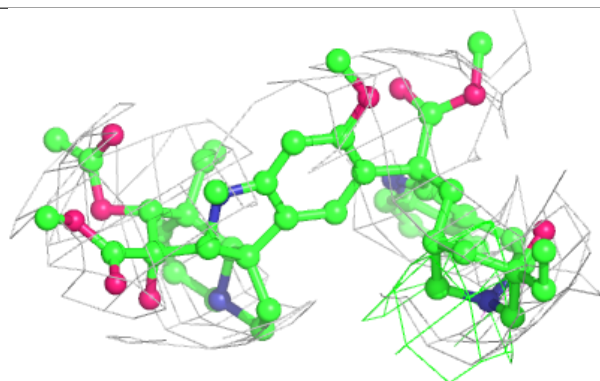
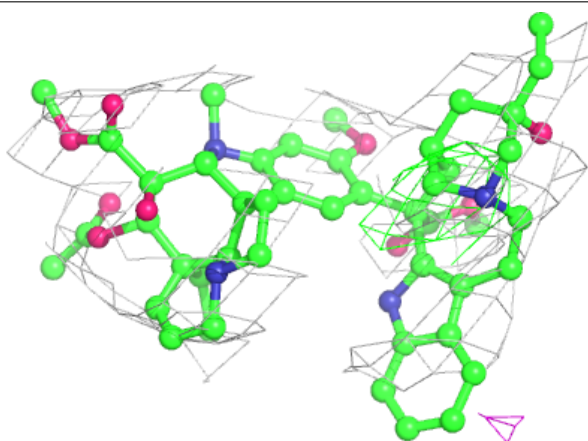
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP B 602:

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

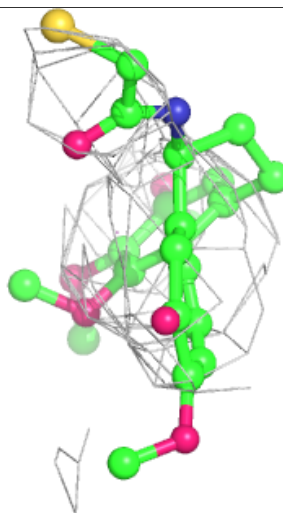
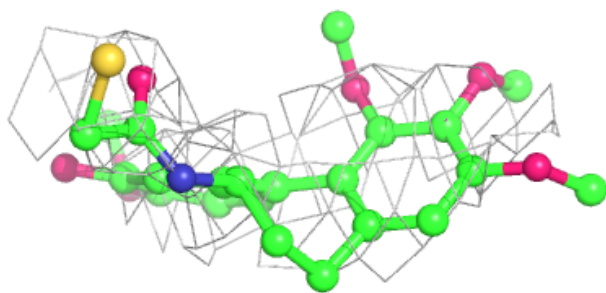
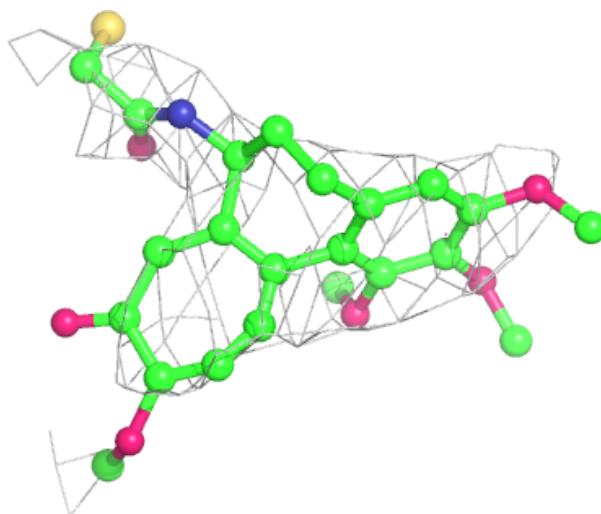
**Electron density around VLB C 800:**

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



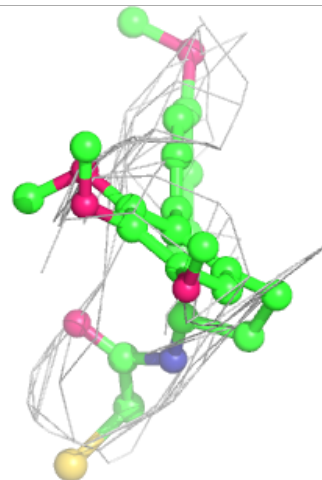
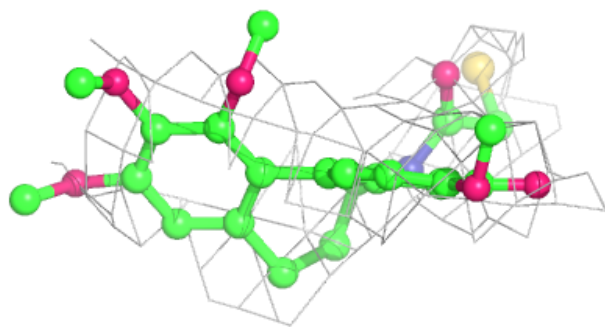
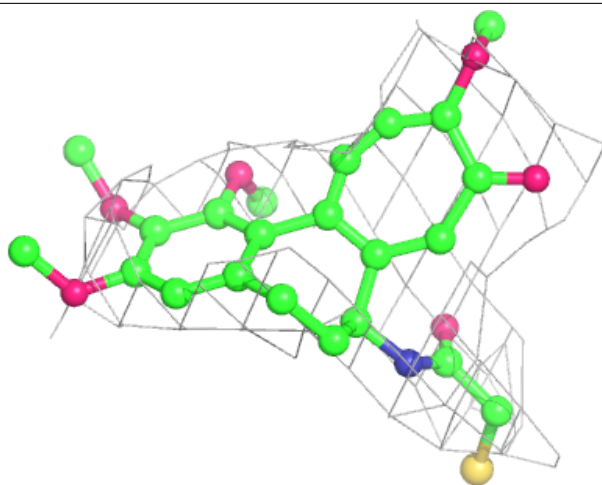
Electron density around CN2 B 700:

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



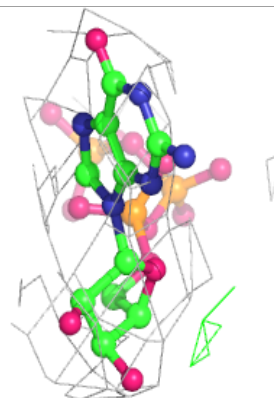
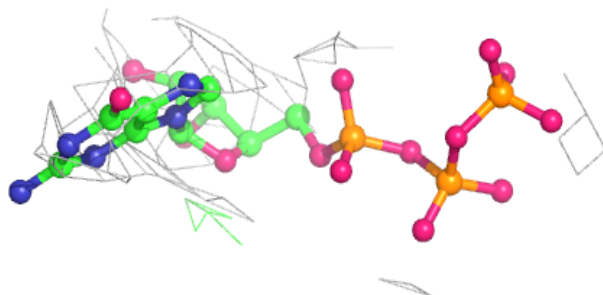
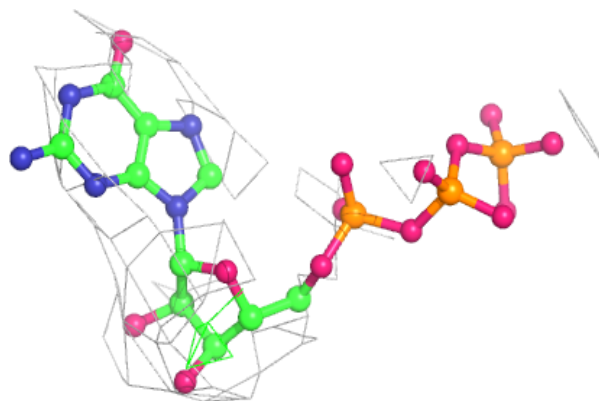
Electron density around CN2 D 701:

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

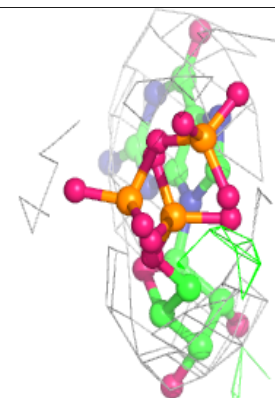
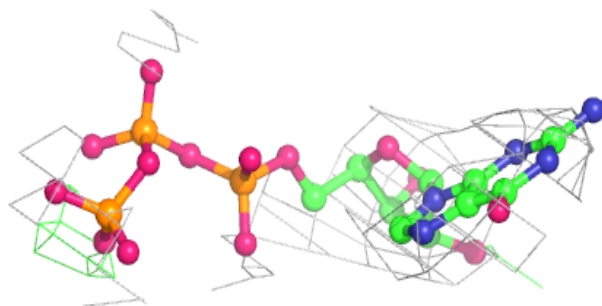
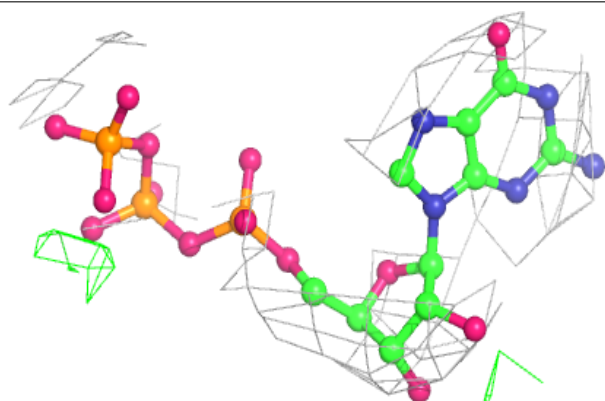


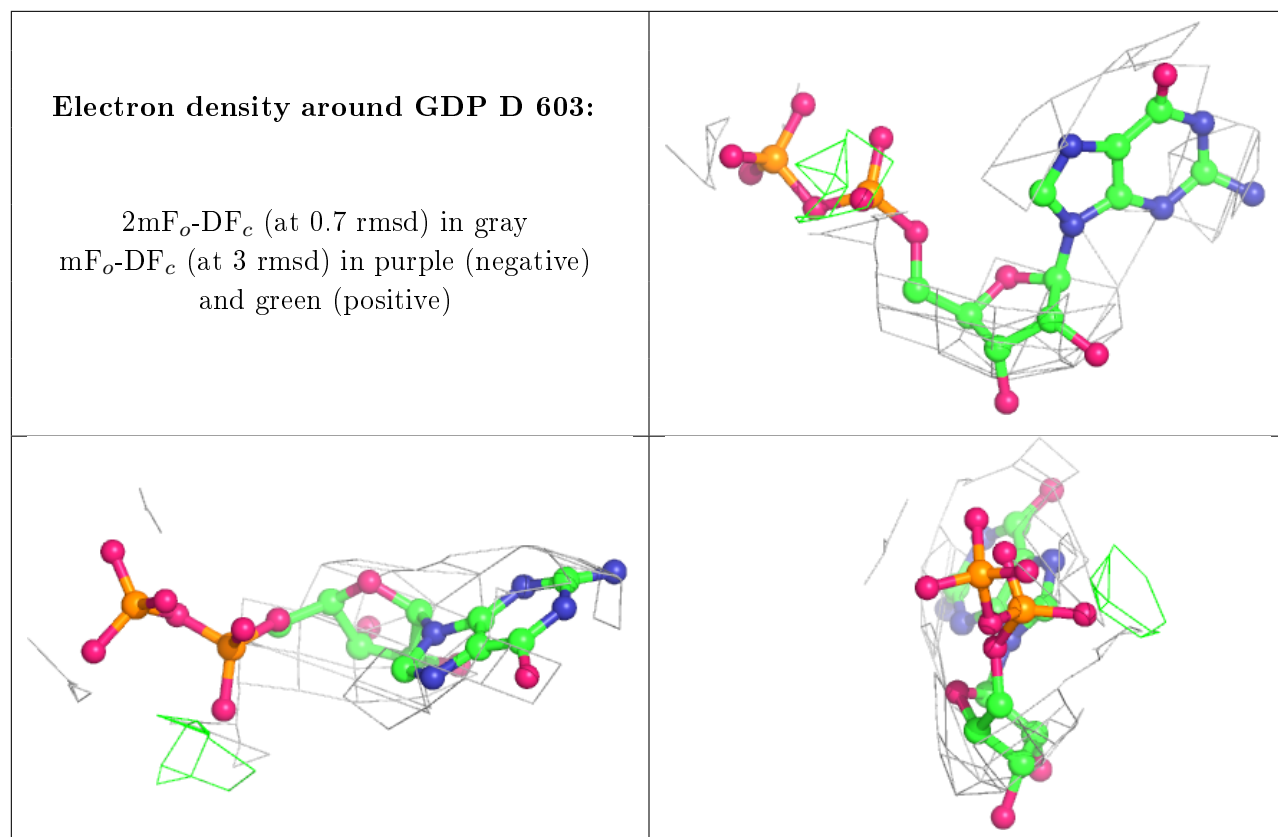
Electron density around GTP A 600:

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

**Electron density around GTP C 601:**

$2mF_o-DF_c$ (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.