



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:23 pm BST

PDB ID : 3DU7  
Title : Tubulin-colchicine-phomopsin A: Stathmin-like domain complex  
Authors : Cormier, A.; Marchand, M.; Ravelli, R.B.; Knossow, M.; Gigant, B.  
Deposited on : 2008-07-17  
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](mailto: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.

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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

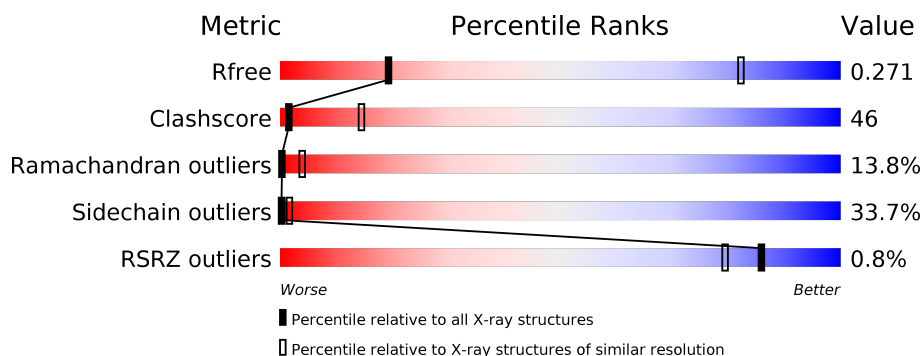
# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	449	
1	C	449	
2	B	445	
2	D	445	
3	E	142	

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
5	CN2	B	700	-	-	X	-
5	CN2	D	701	-	-	X	-
6	HOS	B	800	-	-	X	-
6	HOS	D	801	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14258 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1C chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3265	2070	554	620	21			
1	C	438	Total	C	N	O	S	0	0	0
			3317	2098	564	634	21			

There are 8 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	0	0
			3282	2061	556	641	24			
2	D	426	Total	C	N	O	S	0	0	0
			3272	2056	551	641	24			

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			830	504	158	163	5			

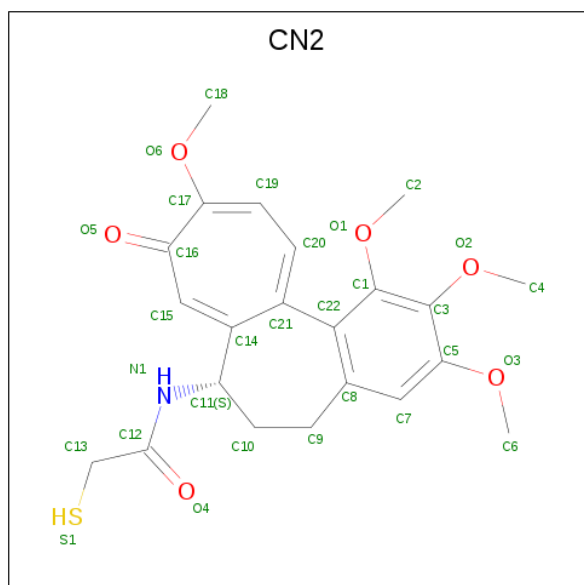
There is a discrepancy between the modelled and reference sequences:

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

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

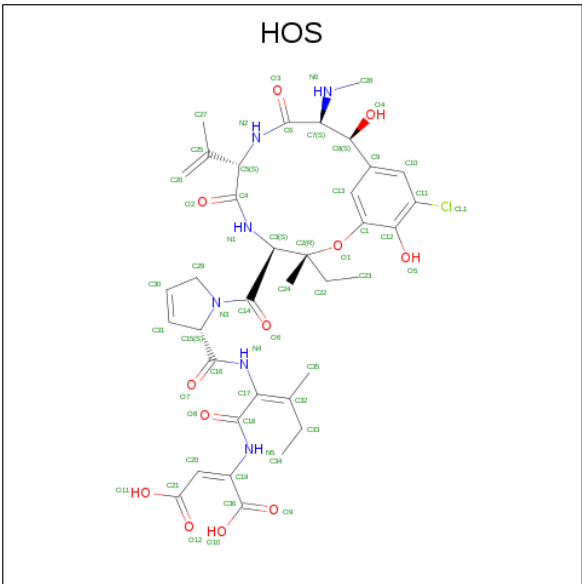
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 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<sub>22</sub>H<sub>25</sub>NO<sub>6</sub>S).



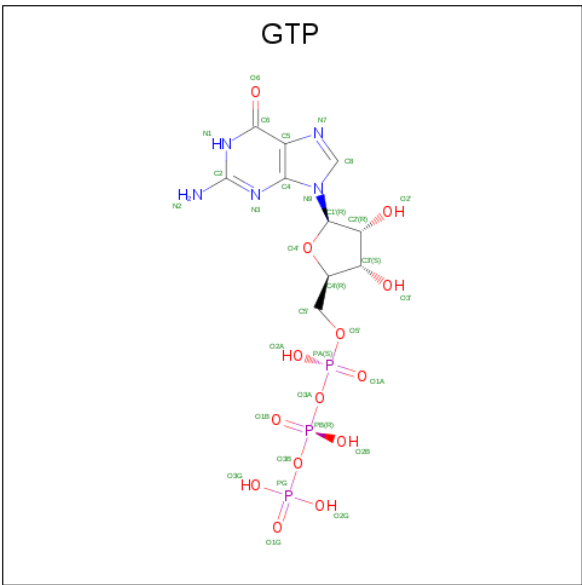
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			30	22	1	6	1		
5	D	1	Total	C	N	O	S	0	0
			30	22	1	6	1		

- Molecule 6 is Phomopsin A (three-letter code: HOS) (formula: C<sub>36</sub>H<sub>45</sub>ClN<sub>6</sub>O<sub>12</sub>).



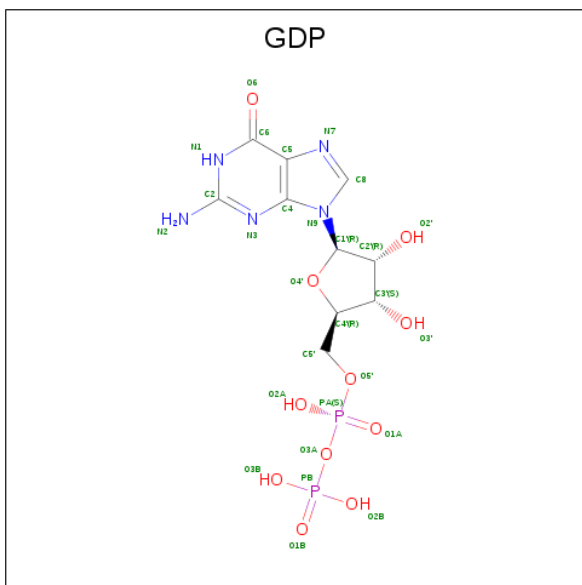
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Cl	N	O	0	0
			55	36	1	6	12		
6	D	1	Total	C	Cl	N	O	0	0
			55	36	1	6	12		

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).

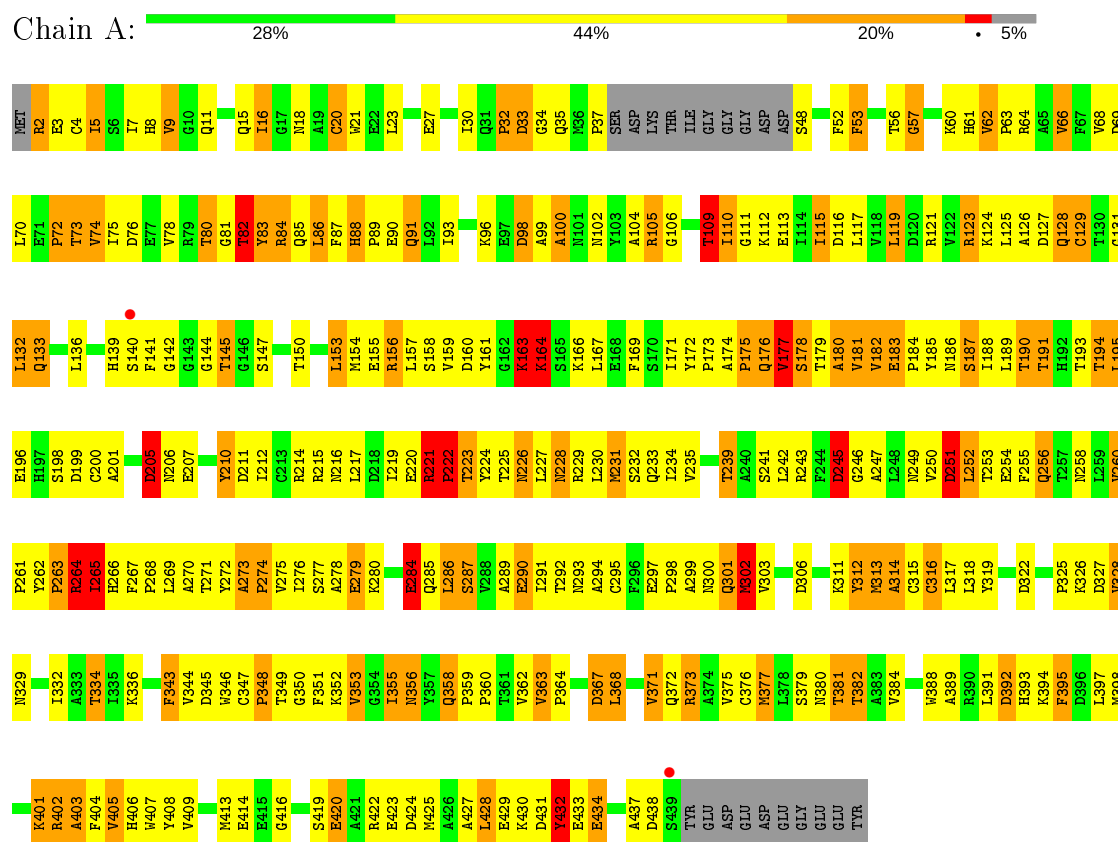


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

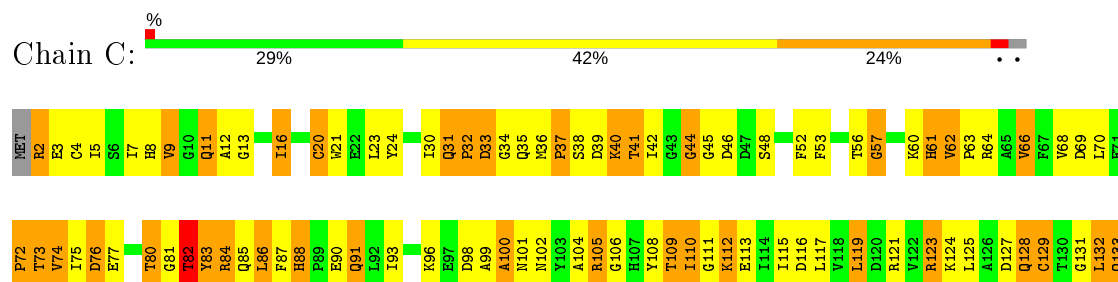
### 3 Residue-property plots

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

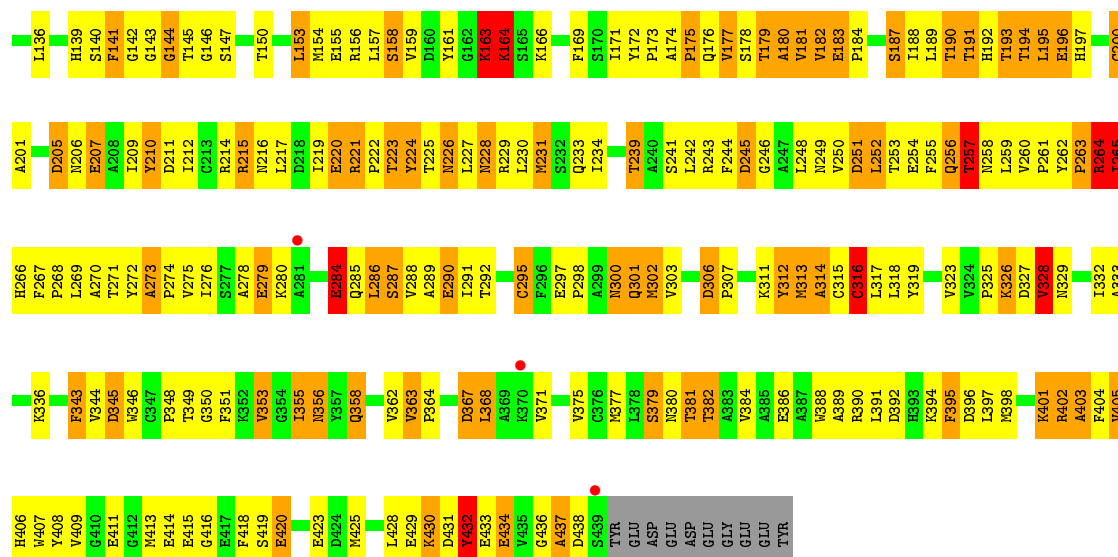
- Molecule 1: Tubulin alpha-1C chain



- Molecule 1: Tubulin alpha-1C chain

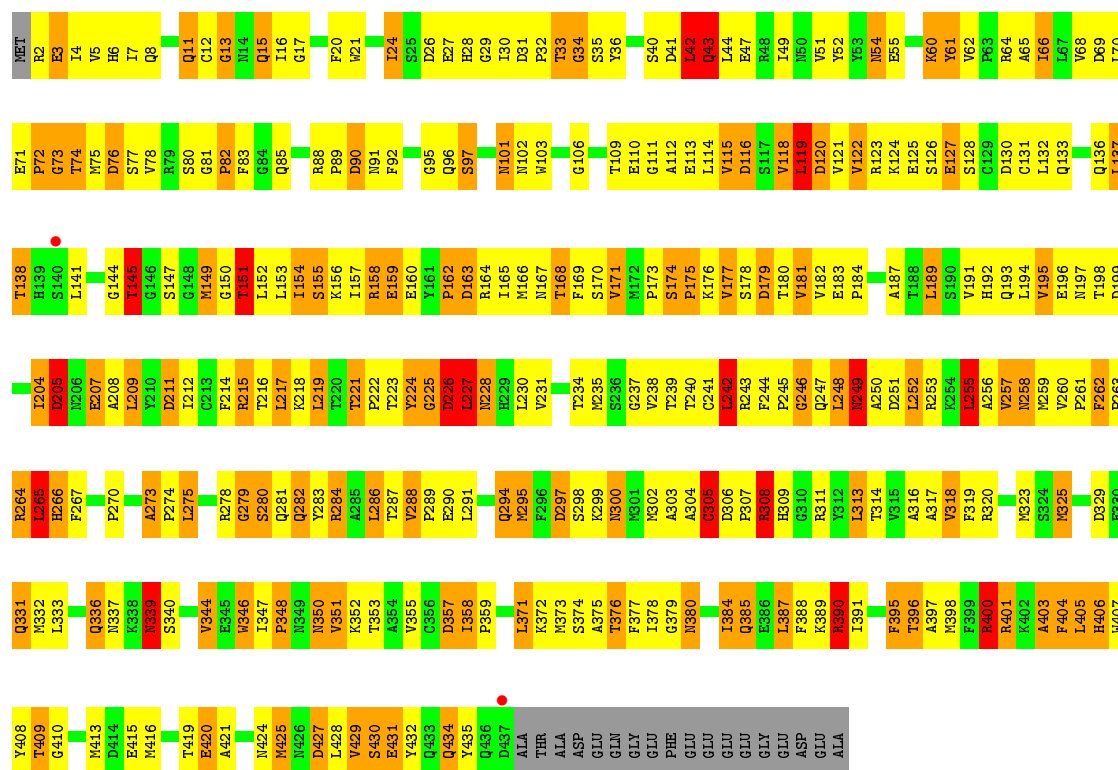






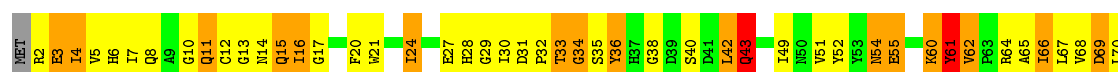
• Molecule 2: Tubulin beta-2B chain

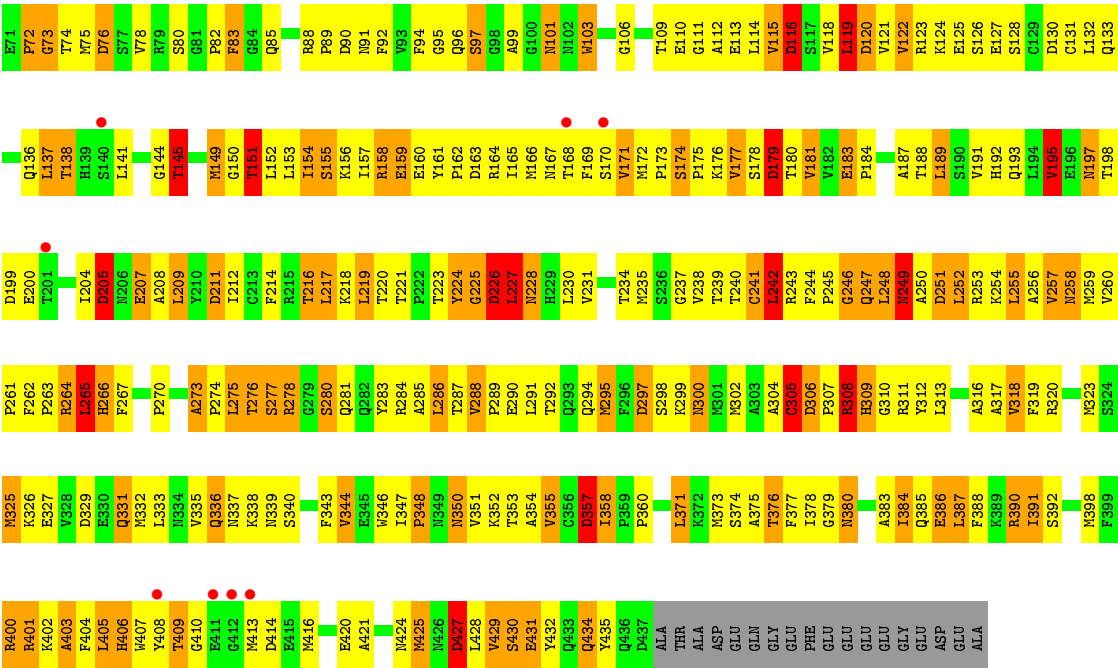
Chain B: 26% 42% 24%



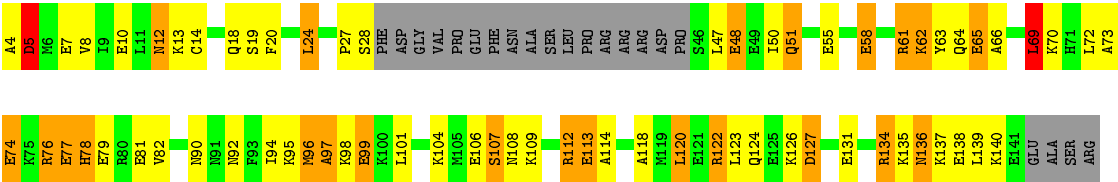
• Molecule 2: Tubulin beta-2B chain

Chain D: 2% 25% 44% 23%





● Molecule 3: Stathmin-4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	327.13 Å   327.13 Å   53.67 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	20.00 – 4.10 38.97 – 4.09	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-4.10) 95.9 (38.97-4.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 4.13 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.215 , 0.265 0.216 , 0.271	Depositor DCC
$R_{free}$ test set	1286 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	181.9	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 162.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14258	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, CN2, HOS

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	0.82	0/3340	1.02	17/4547 (0.4%)
1	C	0.79	1/3393 (0.0%)	0.99	10/4622 (0.2%)
2	B	0.77	0/3356	1.05	17/4561 (0.4%)
2	D	0.77	0/3346	1.02	15/4548 (0.3%)
3	E	0.74	0/836	0.91	4/1127 (0.4%)
All	All	0.78	1/14271 (0.0%)	1.02	63/19405 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
2	B	0	5
2	D	0	6
3	E	0	1
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	231	MET	SD-CE	5.35	2.07	1.77

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	242	LEU	CA-CB-CG	9.96	138.20	115.30
2	D	242	LEU	CA-CB-CG	8.73	135.38	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	ASP	CB-CG-OD2	8.14	125.63	118.30
1	A	160	ASP	CB-CG-OD2	7.68	125.21	118.30
2	B	26	ASP	CB-CG-OD2	7.12	124.71	118.30
1	C	211	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	245	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	127	ASP	CB-CG-OD2	6.98	124.58	118.30
2	B	390	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	306	ASP	CB-CG-OD2	6.86	124.47	118.30
2	D	69	ASP	CB-CG-OD2	6.77	124.39	118.30
2	D	297	ASP	CB-CG-OD2	6.74	124.36	118.30
2	B	130	ASP	CB-CG-OD2	6.59	124.23	118.30
2	D	226	ASP	CB-CG-OD2	6.41	124.07	118.30
1	C	367	ASP	CB-CG-OD2	6.38	124.05	118.30
3	E	5	ASP	CB-CG-OD2	6.38	124.04	118.30
2	B	61	TYR	N-CA-C	6.33	128.09	111.00
2	D	61	TYR	N-CA-C	6.25	127.88	111.00
2	D	205	ASP	CB-CG-OD2	6.25	123.92	118.30
3	E	127	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	116	ASP	CB-CG-OD2	6.08	123.77	118.30
1	C	245	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	69	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	211	ASP	CB-CG-OD2	6.01	123.71	118.30
2	B	211	ASP	CB-CG-OD2	5.99	123.69	118.30
2	D	357	ASP	CB-CG-OD2	5.98	123.68	118.30
2	D	211	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	424	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	231	MET	CB-CG-SD	-5.79	95.03	112.40
1	A	251	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	199	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	306	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	127	ASP	CB-CG-OD2	5.68	123.41	118.30
2	D	427	ASP	CB-CG-OD2	5.66	123.39	118.30
1	C	76	ASP	CB-CG-OD2	5.64	123.37	118.30
2	B	297	ASP	CB-CG-OD2	5.63	123.36	118.30
2	D	414	ASP	CB-CG-OD2	5.62	123.36	118.30
2	B	163	ASP	CB-CG-OD2	5.60	123.34	118.30
2	B	255	LEU	CA-CB-CG	5.58	128.14	115.30
3	E	24	LEU	CA-CB-CG	5.58	128.14	115.30
1	C	431	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	76	ASP	CB-CG-OD2	5.55	123.30	118.30
2	B	226	ASP	CB-CG-OD2	5.44	123.20	118.30
1	C	345	ASP	CB-CG-OD2	5.44	123.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	251	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	69	ASP	CB-CG-OD2	5.41	123.17	118.30
2	B	41	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	322	ASP	CB-CG-OD2	5.37	123.13	118.30
2	B	390	ARG	NE-CZ-NH2	-5.37	117.62	120.30
2	D	116	ASP	CB-CG-OD2	5.35	123.12	118.30
2	B	90	ASP	CB-CG-OD2	5.33	123.09	118.30
2	B	308	ARG	CG-CD-NE	5.32	122.97	111.80
2	D	277	SER	N-CA-C	5.29	125.27	111.00
2	B	306	ASP	CB-CG-OD2	5.25	123.02	118.30
3	E	69	LEU	CA-CB-CG	5.24	127.36	115.30
1	C	116	ASP	CB-CG-OD2	5.24	123.02	118.30
2	D	179	ASP	CB-CG-OD2	5.19	122.97	118.30
2	D	306	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	222	PRO	N-CD-CG	-5.09	95.56	103.20
2	B	205	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	392	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	98	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	205	ASP	CB-CG-OD2	5.06	122.85	118.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	ARG	Peptide
1	A	284	GLU	Peptide
2	B	165	ILE	Peptide
2	B	246	GLY	Peptide
2	B	247	GLN	Peptide
2	B	262	PHE	Peptide
2	B	286	LEU	Peptide
1	C	256	GLN	Peptide
1	C	284	GLU	Peptide
2	D	197	ASN	Peptide
2	D	246	GLY	Peptide
2	D	247	GLN	Peptide
2	D	276	THR	Peptide
2	D	286	LEU	Peptide
2	D	304	ALA	Peptide
3	E	48	GLU	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3265	0	3102	280	0
1	C	3317	0	3128	299	0
2	B	3282	0	3072	318	0
2	D	3272	0	3054	327	0
3	E	830	0	672	56	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	B	30	0	23	12	0
5	D	30	0	23	12	0
6	B	55	0	43	26	0
6	D	55	0	43	24	0
7	D	64	0	24	6	0
8	D	56	0	24	8	0
All	All	14258	0	13208	1258	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 46.

All (1258) 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:231:MET:CE	1:C:231:MET:SD	2.07	1.41
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.23	1.14
1:C:99:ALA:HB2	1:C:145:THR:HG22	1.20	1.12
1:A:99:ALA:CB	1:A:145:THR:HG22	1.78	1.12
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.11	1.10
1:C:252:LEU:HA	1:C:255:PHE:HB2	1.30	1.10
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.15	1.09
1:C:273:ALA:CB	1:C:274:PRO:HD3	1.82	1.08
2:B:316:ALA:HB1	5:B:700:CN2:H21	1.33	1.08
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.19	1.08
2:B:251:ASP:O	2:B:253:ARG:N	1.88	1.06
1:A:273:ALA:CB	1:A:274:PRO:HD3	1.85	1.06
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.83	1.06
1:C:105:ARG:CZ	2:D:253:ARG:HH12	1.66	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:307:PRO:O	2:D:308:ARG:HB2	1.52	1.05
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.10	1.05
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.36	1.05
2:D:262:PHE:CE1	2:D:435:TYR:HE2	1.74	1.05
1:C:36:MET:O	1:C:38:SER:N	1.90	1.04
6:D:801:HOS:O8	6:D:801:HOS:H20	1.53	1.04
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.88	1.02
1:C:99:ALA:CB	1:C:145:THR:HG22	1.90	1.02
2:B:224:TYR:CD1	6:B:800:HOS:H22	1.94	1.02
2:D:331:GLN:HA	2:D:331:GLN:NE2	1.75	1.02
1:A:133:GLN:HE21	1:A:252:LEU:HG	1.21	1.02
2:B:4:ILE:HG22	2:B:133:GLN:HB3	1.39	1.01
2:B:318:VAL:HG23	2:B:376:THR:HG23	1.42	1.01
2:D:158:ARG:O	2:D:159:GLU:HB3	1.60	1.01
1:A:133:GLN:NE2	1:A:252:LEU:HG	1.76	1.00
2:B:273:ALA:HB3	2:B:274:PRO:CD	1.92	0.99
2:D:251:ASP:O	2:D:253:ARG:N	1.96	0.98
2:D:151:THR:HB	2:D:193:GLN:HG2	1.45	0.98
2:B:401:ARG:O	1:C:262:TYR:OH	1.82	0.98
1:C:171:ILE:CG2	1:C:206:ASN:HD21	1.78	0.97
1:C:430:LYS:O	1:C:434:GLU:HB2	1.65	0.96
1:C:101:ASN:HD22	2:D:254:LYS:HG2	1.28	0.95
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.43	0.95
1:C:273:ALA:HB3	1:C:274:PRO:CD	1.97	0.95
2:D:4:ILE:HG22	2:D:133:GLN:HB3	1.47	0.95
2:B:307:PRO:O	2:B:308:ARG:HG2	1.65	0.94
2:D:223:THR:HA	6:D:801:HOS:H29	1.47	0.94
2:B:158:ARG:O	2:B:159:GLU:HB3	1.65	0.93
1:A:355:ILE:HD11	3:E:18:GLN:HB3	1.50	0.93
1:A:109:THR:HG23	3:E:61:ARG:CZ	1.99	0.93
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.47	0.93
1:A:430:LYS:O	1:A:434:GLU:HB2	1.69	0.91
2:B:390:ARG:HG3	2:B:390:ARG:HH11	1.36	0.91
2:B:234:THR:O	2:B:238:VAL:HG23	1.70	0.91
1:C:171:ILE:HG23	1:C:206:ASN:HD21	1.34	0.91
1:A:171:ILE:CG2	1:A:206:ASN:HD21	1.84	0.90
2:B:284:ARG:HD2	2:B:372:LYS:CB	2.01	0.90
2:B:401:ARG:HG3	2:B:401:ARG:HH11	1.35	0.90
1:C:233:GLN:HE22	1:C:362:VAL:HG12	1.38	0.90
1:C:231:MET:HB2	1:C:231:MET:CE	2.01	0.89
2:D:318:VAL:HG23	2:D:376:THR:HG23	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.02	0.89
2:B:305:CYS:SG	2:B:384:ILE:HA	2.14	0.88
1:A:273:ALA:HB3	1:A:274:PRO:CD	2.02	0.87
1:A:70:LEU:HD23	1:A:110:ILE:HG23	1.56	0.87
1:C:101:ASN:ND2	2:D:254:LYS:HG2	1.88	0.87
2:B:54:ASN:HD22	2:B:64:ARG:HD3	1.37	0.87
2:B:431:GLU:HA	2:B:434:GLN:HB2	1.56	0.87
3:E:4:ALA:O	3:E:5:ASP:HB2	1.75	0.86
2:B:151:THR:HB	2:B:193:GLN:HG2	1.57	0.86
6:B:800:HOS:O7	6:B:800:HOS:C35	2.24	0.86
1:C:205:ASP:HB3	1:C:303:VAL:HA	1.57	0.86
1:C:30:ILE:HG23	1:C:34:GLY:O	1.75	0.86
1:C:317:LEU:HB2	1:C:353:VAL:HG12	1.55	0.86
2:B:401:ARG:HH11	2:B:401:ARG:CG	1.88	0.86
2:B:403:ALA:O	2:B:405:LEU:N	2.07	0.86
1:A:273:ALA:CB	1:A:375:VAL:H	1.87	0.86
2:B:262:PHE:CE1	2:B:435:TYR:HE2	1.93	0.85
3:E:112:ARG:HG3	3:E:113:GLU:N	1.90	0.85
3:E:76:ARG:O	3:E:78:HIS:N	2.09	0.85
6:B:800:HOS:C29	6:B:800:HOS:H22A	2.07	0.84
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.58	0.84
2:B:404:PHE:CE2	1:C:261:PRO:HB3	2.11	0.84
2:D:138:THR:HG22	2:D:169:PHE:HB2	1.59	0.84
2:B:207:GLU:HB2	2:B:390:ARG:HH22	1.41	0.84
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.13	0.84
2:D:54:ASN:HD22	2:D:64:ARG:HD3	1.42	0.84
1:C:287:SER:HB2	1:C:290:GLU:HB2	1.61	0.83
5:B:700:CN2:H62	5:B:700:CN2:H43	1.60	0.83
2:B:3:GLU:HB3	2:B:64:ARG:NH2	1.92	0.83
2:D:234:THR:O	2:D:238:VAL:HG23	1.79	0.82
1:C:16:ILE:O	1:C:20:CYS:HB3	1.79	0.82
2:B:54:ASN:HD22	2:B:64:ARG:CD	1.92	0.82
2:D:331:GLN:HA	2:D:331:GLN:HE21	1.39	0.82
2:D:305:CYS:SG	2:D:384:ILE:HA	2.19	0.82
1:C:231:MET:CE	1:C:231:MET:CB	2.57	0.82
2:B:251:ASP:C	2:B:253:ARG:H	1.82	0.81
3:E:106:GLU:C	3:E:108:ASN:H	1.84	0.81
6:B:800:HOS:O8	6:B:800:HOS:H33A	1.78	0.81
1:A:105:ARG:CZ	2:B:253:ARG:HH12	1.94	0.81
1:A:171:ILE:HG23	1:A:206:ASN:HD21	1.44	0.80
1:A:98:ASP:OD1	1:A:99:ALA:N	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:MET:HB2	1:C:231:MET:HE2	1.61	0.80
2:B:331:GLN:HA	2:B:331:GLN:NE2	1.95	0.80
2:B:256:ALA:O	2:B:258:ASN:N	2.13	0.80
2:D:223:THR:HA	6:D:801:HOS:C29	2.11	0.80
2:D:431:GLU:HA	2:D:434:GLN:HB2	1.62	0.80
2:D:401:ARG:CG	2:D:401:ARG:HH11	1.95	0.79
6:B:800:HOS:O8	6:B:800:HOS:H20	1.82	0.79
1:C:264:ARG:O	1:C:266:HIS:CD2	2.36	0.79
2:B:205:ASP:HB2	2:B:387:LEU:HD11	1.63	0.79
1:A:398:MET:CE	2:B:348:PRO:HD2	2.12	0.79
2:B:88:ARG:HB3	2:B:91:ASN:OD1	1.81	0.79
2:B:177:VAL:HA	6:B:800:HOS:C13	2.12	0.79
1:C:171:ILE:CG2	1:C:206:ASN:ND2	2.46	0.79
2:D:401:ARG:HH11	2:D:401:ARG:HG3	1.47	0.78
1:A:348:PRO:HA	3:E:27:PRO:HA	1.66	0.78
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.63	0.78
1:A:88:HIS:O	1:A:91:GLN:HG3	1.84	0.78
2:D:262:PHE:CE1	2:D:435:TYR:CE2	2.67	0.78
2:B:401:ARG:HG3	2:B:401:ARG:NH1	1.98	0.77
6:B:800:HOS:H29	6:B:800:HOS:H22A	1.66	0.77
2:D:158:ARG:O	2:D:159:GLU:CB	2.31	0.77
1:C:105:ARG:NH2	2:D:253:ARG:HH12	1.82	0.77
2:D:287:THR:HG22	2:D:290:GLU:HB2	1.65	0.77
6:B:800:HOS:H23B	6:B:800:HOS:O5	1.85	0.77
2:B:5:VAL:HG12	2:B:64:ARG:HG2	1.67	0.77
1:C:105:ARG:CZ	2:D:253:ARG:NH1	2.45	0.76
2:D:3:GLU:HB3	2:D:64:ARG:HH22	1.48	0.76
1:C:171:ILE:HG23	1:C:206:ASN:ND2	1.99	0.76
1:C:273:ALA:CB	1:C:375:VAL:H	1.98	0.76
3:E:131:GLU:HA	3:E:134:ARG:HE	1.50	0.76
1:A:30:ILE:HG23	1:A:34:GLY:O	1.84	0.76
2:D:3:GLU:HB3	2:D:64:ARG:NH2	2.00	0.76
2:D:237:GLY:HA2	2:D:240:THR:HG23	1.66	0.76
1:C:389:ALA:HA	1:C:392:ASP:HB2	1.68	0.76
3:E:10:GLU:OE2	3:E:18:GLN:NE2	2.19	0.76
2:D:66:ILE:HD11	2:D:121:VAL:HB	1.65	0.75
1:C:190:THR:O	1:C:194:THR:HB	1.86	0.75
1:C:98:ASP:OD1	1:C:99:ALA:N	2.18	0.75
2:D:224:TYR:O	2:D:228:ASN:HB2	1.85	0.75
1:A:109:THR:HG23	3:E:61:ARG:NH1	2.01	0.75
2:D:54:ASN:HD22	2:D:64:ARG:CD	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.68	0.75
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.67	0.75
2:B:24:ILE:HD12	2:B:243:ARG:HD3	1.66	0.75
2:D:205:ASP:HB2	2:D:387:LEU:HD11	1.69	0.75
1:C:363:VAL:HG12	1:C:364:PRO:HD2	1.69	0.75
1:A:205:ASP:HB3	1:A:303:VAL:HA	1.69	0.74
1:A:398:MET:HE2	2:B:348:PRO:HD2	1.69	0.74
1:C:88:HIS:O	1:C:91:GLN:HG3	1.86	0.74
2:B:149:MET:O	2:B:152:LEU:HB3	1.87	0.74
2:B:316:ALA:CB	5:B:700:CN2:H21	2.15	0.74
2:D:205:ASP:OD2	2:D:390:ARG:NH2	2.19	0.74
6:D:801:HOS:C35	6:D:801:HOS:O7	2.35	0.74
2:B:316:ALA:HB1	5:B:700:CN2:C2	2.14	0.74
1:C:210:TYR:CE1	1:C:214:ARG:HD2	2.22	0.74
1:A:405:VAL:HG13	1:A:406:HIS:N	2.01	0.74
1:A:289:ALA:O	1:A:292:THR:HB	1.87	0.74
1:A:221:ARG:HH21	2:B:325:MET:CE	1.99	0.73
2:B:337:ASN:C	2:B:339:ASN:H	1.91	0.73
1:C:233:GLN:NE2	1:C:362:VAL:HG12	2.03	0.73
1:A:363:VAL:HG12	1:A:364:PRO:HD2	1.69	0.73
1:C:171:ILE:HD12	1:C:171:ILE:N	2.04	0.73
2:D:5:VAL:HG12	2:D:64:ARG:HG2	1.69	0.73
1:A:2:ARG:HB2	1:A:131:GLY:O	1.88	0.73
2:B:221:THR:HG22	6:B:800:HOS:CL1	2.26	0.73
1:A:3:GLU:HB2	1:A:129:CYS:SG	2.29	0.73
1:A:182:VAL:HG23	1:A:408:TYR:OH	1.88	0.73
1:A:221:ARG:HH21	2:B:325:MET:HE3	1.51	0.73
2:B:403:ALA:C	2:B:405:LEU:H	1.91	0.73
1:C:270:ALA:O	1:C:302:MET:HB2	1.89	0.72
2:B:266:HIS:HB3	2:B:380:ASN:HD21	1.53	0.72
1:C:106:GLY:O	1:C:111:GLY:HA3	1.88	0.72
1:C:123:ARG:HD2	1:C:161:TYR:OH	1.89	0.72
2:B:191:VAL:HG21	2:B:425:MET:HE3	1.69	0.72
2:B:262:PHE:O	2:B:264:ARG:N	2.22	0.72
1:C:3:GLU:HB2	1:C:129:CYS:SG	2.30	0.72
1:A:344:VAL:O	1:A:346:TRP:N	2.22	0.72
1:A:123:ARG:HD2	1:A:161:TYR:OH	1.90	0.72
1:C:289:ALA:O	1:C:292:THR:HB	1.90	0.72
2:B:3:GLU:HB3	2:B:64:ARG:HH22	1.52	0.71
2:B:237:GLY:HA2	2:B:240:THR:HG23	1.72	0.71
1:C:344:VAL:O	1:C:346:TRP:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:ARG:HG3	2:B:125:GLU:OE2	1.90	0.71
2:D:33:THR:O	2:D:34:GLY:O	2.08	0.71
2:D:111:GLY:C	2:D:113:GLU:H	1.92	0.71
2:B:7:ILE:O	2:B:137:LEU:HA	1.90	0.71
1:C:70:LEU:HD23	1:C:110:ILE:HG23	1.73	0.71
2:B:273:ALA:CB	2:B:274:PRO:CD	2.57	0.71
2:B:406:HIS:CE1	2:B:407:TRP:CD1	2.79	0.71
1:C:262:TYR:O	1:C:264:ARG:N	2.23	0.71
1:A:273:ALA:HB2	1:A:375:VAL:H	1.52	0.70
2:D:124:LYS:O	2:D:128:SER:HB2	1.90	0.70
1:A:246:GLY:HA2	3:E:14:CYS:SG	2.30	0.70
2:B:224:TYR:CE1	6:B:800:HOS:H24A	2.26	0.70
2:B:336:GLN:HE22	2:B:351:VAL:HG11	1.55	0.70
1:C:406:HIS:HE1	2:D:261:PRO:O	1.74	0.70
2:D:278:ARG:N	2:D:278:ARG:HE	1.88	0.70
2:B:224:TYR:O	2:B:228:ASN:HB2	1.92	0.70
1:A:287:SER:HB2	1:A:290:GLU:HB2	1.72	0.70
5:D:701:CN2:H43	5:D:701:CN2:H63	1.73	0.70
6:B:800:HOS:O7	6:B:800:HOS:H35B	1.92	0.70
1:A:102:ASN:ND2	1:A:104:ALA:HB3	2.06	0.69
1:C:273:ALA:CB	1:C:274:PRO:CD	2.57	0.69
1:A:233:GLN:HE22	1:A:362:VAL:HG12	1.57	0.69
1:A:106:GLY:O	1:A:111:GLY:HA3	1.93	0.69
1:A:403:ALA:HB1	1:A:404:PHE:HD1	1.56	0.69
2:D:207:GLU:HB2	2:D:390:ARG:HH22	1.56	0.69
1:A:133:GLN:HE21	1:A:252:LEU:CG	2.01	0.69
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.27	0.69
1:C:255:PHE:O	1:C:259:LEU:HG	1.93	0.69
2:D:336:GLN:HE22	2:D:351:VAL:HG11	1.57	0.69
1:A:163:LYS:H	1:A:163:LYS:HE3	1.56	0.69
2:B:66:ILE:HD11	2:B:121:VAL:HB	1.74	0.69
2:B:207:GLU:HB2	2:B:390:ARG:NH2	2.06	0.68
2:D:256:ALA:O	2:D:258:ASN:N	2.24	0.68
1:A:317:LEU:HB2	1:A:353:VAL:HG12	1.74	0.68
6:B:800:HOS:H35A	6:B:800:HOS:O7	1.93	0.68
1:A:102:ASN:HB2	1:A:408:TYR:CE2	2.28	0.68
1:C:405:VAL:HG13	1:C:406:HIS:N	2.08	0.68
2:D:291:LEU:HD21	2:D:375:ALA:CB	2.24	0.68
2:D:424:ASN:O	2:D:427:ASP:HB2	1.93	0.68
2:B:307:PRO:O	2:B:308:ARG:CG	2.39	0.68
1:C:2:ARG:HB2	1:C:131:GLY:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:237:GLY:CA	2:D:376:THR:HG21	2.18	0.68
6:D:801:HOS:O8	6:D:801:HOS:H33	1.94	0.68
1:A:171:ILE:CG2	1:A:206:ASN:ND2	2.56	0.68
2:B:205:ASP:OD2	2:B:390:ARG:NH2	2.27	0.68
2:B:275:LEU:HD12	2:B:281:GLN:OE1	1.92	0.68
1:C:403:ALA:HB1	1:C:404:PHE:HD1	1.58	0.68
1:A:278:ALA:O	1:A:279:GLU:CB	2.40	0.68
1:A:223:THR:HB	1:A:226:ASN:HB2	1.76	0.68
1:A:273:ALA:CB	1:A:274:PRO:CD	2.60	0.68
1:C:99:ALA:HB2	1:C:145:THR:CG2	2.12	0.68
1:C:105:ARG:NH1	2:D:253:ARG:HH12	1.92	0.68
1:A:375:VAL:HG12	1:A:376:CYS:H	1.59	0.67
2:B:217:LEU:O	2:B:219:LEU:N	2.26	0.67
2:B:223:THR:HA	6:B:800:HOS:C30	2.25	0.67
2:D:237:GLY:HA2	2:D:240:THR:CG2	2.24	0.67
2:B:424:ASN:O	2:B:427:ASP:HB2	1.94	0.67
1:C:398:MET:CE	2:D:348:PRO:HD2	2.24	0.67
2:D:257:VAL:O	2:D:257:VAL:HG22	1.94	0.67
2:B:178:SER:H	6:B:800:HOS:H13	1.60	0.67
1:C:48:SER:O	1:C:243:ARG:O	2.13	0.67
2:D:217:LEU:O	2:D:219:LEU:N	2.26	0.67
1:A:233:GLN:NE2	1:A:362:VAL:HG12	2.10	0.67
1:C:241:SER:HB2	1:C:249:ASN:ND2	2.09	0.67
2:B:33:THR:O	2:B:34:GLY:O	2.13	0.67
1:C:99:ALA:CB	1:C:145:THR:CG2	2.70	0.67
1:A:171:ILE:HG23	1:A:206:ASN:ND2	2.10	0.67
2:B:96:GLN:HG3	2:B:97:SER:H	1.59	0.67
1:C:302:MET:HE2	1:C:302:MET:HA	1.74	0.67
2:D:278:ARG:H	2:D:278:ARG:HE	1.40	0.67
1:A:99:ALA:HB3	1:A:145:THR:HG22	1.75	0.66
1:A:181:VAL:O	1:A:398:MET:HE1	1.95	0.66
1:C:266:HIS:O	1:C:268:PRO:HD3	1.95	0.66
2:B:331:GLN:HA	2:B:331:GLN:HE21	1.58	0.66
1:A:32:PRO:O	1:A:33:ASP:C	2.32	0.66
1:A:265:ILE:HG23	1:A:267:PHE:CZ	2.31	0.66
2:B:89:PRO:O	2:B:92:PHE:HB2	1.96	0.66
1:C:273:ALA:HB2	1:C:375:VAL:H	1.61	0.66
2:B:158:ARG:O	2:B:159:GLU:CB	2.39	0.66
2:B:257:VAL:O	2:B:257:VAL:HG22	1.96	0.66
3:E:134:ARG:C	3:E:136:ASN:H	1.97	0.66
2:B:114:LEU:O	2:B:116:ASP:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:700:CN2:H15	5:B:700:CN2:O4	1.96	0.66
2:B:174:SER:HB2	2:B:207:GLU:CG	2.26	0.66
1:A:205:ASP:OD1	1:A:205:ASP:C	2.34	0.65
1:A:406:HIS:HE1	2:B:261:PRO:O	1.80	0.65
2:D:273:ALA:CB	2:D:375:ALA:H	2.10	0.65
2:D:273:ALA:HB3	2:D:375:ALA:H	1.60	0.65
1:A:70:LEU:HD23	1:A:110:ILE:CG2	2.25	0.65
1:C:209:ILE:HG22	1:C:227:LEU:HD12	1.78	0.65
1:A:167:LEU:HD13	1:A:252:LEU:HD13	1.78	0.65
2:D:28:HIS:HA	2:D:43:GLN:HB3	1.78	0.65
2:B:251:ASP:C	2:B:253:ARG:N	2.41	0.65
1:C:182:VAL:HG23	1:C:408:TYR:OH	1.97	0.65
2:D:401:ARG:NH1	2:D:401:ARG:HG3	2.07	0.65
2:D:251:ASP:C	2:D:253:ARG:N	2.49	0.65
2:D:406:HIS:CE1	2:D:407:TRP:CD1	2.85	0.65
2:B:167:ASN:HD22	2:B:252:LEU:HD11	1.63	0.64
2:B:31:ASP:HB3	2:B:32:PRO:HD2	1.79	0.64
2:D:287:THR:HG22	2:D:290:GLU:H	1.63	0.64
1:A:228:ASN:HD21	7:D:600:GTP:HN1	1.45	0.64
2:D:212:ILE:HG21	2:D:230:LEU:HD21	1.79	0.64
2:D:344:VAL:HG11	2:D:347:ILE:HD12	1.79	0.64
2:B:287:THR:HG22	2:B:290:GLU:HB2	1.79	0.64
2:B:396:THR:HG22	2:B:400:ARG:HH21	1.62	0.64
2:D:64:ARG:HG3	2:D:125:GLU:OE2	1.98	0.64
1:A:353:VAL:HG21	3:E:20:PHE:CZ	2.33	0.64
1:A:180:ALA:HB1	2:B:258:ASN:HD21	1.62	0.64
1:A:223:THR:CB	1:A:226:ASN:HB2	2.28	0.64
2:B:111:GLY:C	2:B:113:GLU:H	2.00	0.64
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.38	0.63
1:A:402:ARG:O	1:A:403:ALA:C	2.35	0.63
5:B:700:CN2:C6	5:B:700:CN2:H43	2.28	0.63
1:A:389:ALA:HB2	1:A:429:GLU:OE2	1.97	0.63
2:B:132:LEU:HG	2:B:133:GLN:N	2.14	0.63
2:D:287:THR:HG22	2:D:290:GLU:CB	2.27	0.63
1:A:265:ILE:HG12	1:A:265:ILE:O	1.98	0.63
2:B:4:ILE:HG22	2:B:133:GLN:CB	2.23	0.63
1:C:108:TYR:CE1	1:C:413:MET:HG3	2.33	0.63
2:D:174:SER:HB2	2:D:207:GLU:CG	2.29	0.63
1:A:190:THR:O	1:A:194:THR:HB	1.99	0.62
2:D:114:LEU:O	2:D:116:ASP:N	2.32	0.62
1:A:372:GLN:O	1:A:373:ARG:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:224:TYR:CE1	6:D:801:HOS:H24A	2.34	0.62
2:B:36:TYR:OH	2:B:40:SER:O	2.17	0.62
1:C:157:LEU:C	1:C:159:VAL:H	2.00	0.62
1:C:239:THR:OG1	1:C:243:ARG:NH1	2.33	0.62
1:C:251:ASP:O	1:C:255:PHE:HD1	1.82	0.62
2:D:223:THR:HA	6:D:801:HOS:C30	2.29	0.62
2:B:237:GLY:CA	2:B:376:THR:HG21	2.23	0.62
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.35	0.62
1:C:317:LEU:HB3	1:C:319:TYR:HE1	1.64	0.62
2:D:225:GLY:O	2:D:227:LEU:N	2.32	0.62
2:D:31:ASP:HB3	2:D:32:PRO:HD2	1.80	0.62
2:B:224:TYR:HE1	6:B:800:HOS:H24A	1.65	0.62
1:C:11:GLN:NE2	2:D:248:LEU:HD22	2.15	0.62
1:A:302:MET:HA	1:A:302:MET:HE2	1.82	0.62
1:C:228:ASN:HD22	1:C:228:ASN:N	1.97	0.62
2:D:111:GLY:C	2:D:113:GLU:N	2.53	0.62
2:D:224:TYR:CD1	6:D:801:HOS:H22	2.35	0.62
2:D:403:ALA:C	2:D:405:LEU:H	2.03	0.61
1:A:258:ASN:ND2	1:A:352:LYS:HG3	2.14	0.61
1:A:344:VAL:O	1:A:344:VAL:HG13	2.00	0.61
1:C:111:GLY:O	1:C:113:GLU:N	2.32	0.61
1:C:128:GLN:O	1:C:129:CYS:HB2	1.99	0.61
3:E:4:ALA:O	3:E:5:ASP:CB	2.48	0.61
1:A:171:ILE:N	1:A:171:ILE:HD12	2.16	0.61
1:C:100:ALA:HB1	2:D:253:ARG:HG2	1.82	0.61
1:C:40:LYS:O	1:C:41:THR:HG22	2.01	0.61
1:C:163:LYS:H	1:C:163:LYS:HE3	1.65	0.61
1:C:173:PRO:HB3	7:D:601:GTP:O3'	2.01	0.61
2:D:262:PHE:CD1	2:D:435:TYR:HE2	2.19	0.61
1:A:7:ILE:HG12	1:A:66:VAL:CG2	2.30	0.61
2:D:132:LEU:HD23	2:D:164:ARG:HG3	1.81	0.61
1:C:136:LEU:HD22	1:C:169:PHE:HE1	1.65	0.61
2:D:106:GLY:O	2:D:149:MET:HA	2.00	0.61
2:D:177:VAL:HG22	6:D:801:HOS:C12	2.30	0.61
2:B:173:PRO:HB3	8:D:602:GDP:O3'	2.01	0.61
1:A:401:LYS:O	2:B:262:PHE:HZ	1.84	0.61
1:A:398:MET:HE3	2:B:348:PRO:HD2	1.83	0.61
1:C:234:ILE:HG13	1:C:272:TYR:HB2	1.82	0.61
1:A:219:ILE:HG22	1:A:221:ARG:H	1.65	0.61
1:A:99:ALA:CB	1:A:145:THR:CG2	2.69	0.61
2:B:124:LYS:O	2:B:128:SER:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:801:HOS:H35B	6:D:801:HOS:O7	2.00	0.61
2:D:17:GLY:HA2	2:D:20:PHE:HB3	1.82	0.61
2:D:241:CYS:HB3	5:D:701:CN2:H62	1.83	0.61
2:B:388:PHE:CE1	2:B:428:LEU:HD21	2.36	0.60
2:D:227:LEU:HG	2:D:228:ASN:N	2.15	0.60
1:A:206:ASN:O	1:A:207:GLU:C	2.38	0.60
2:B:132:LEU:HD23	2:B:164:ARG:HG3	1.83	0.60
2:B:223:THR:HA	6:B:800:HOS:C29	2.30	0.60
2:D:7:ILE:O	2:D:137:LEU:HA	2.01	0.60
1:A:195:LEU:HB2	1:A:265:ILE:HG21	1.84	0.60
2:D:96:GLN:HG3	2:D:97:SER:H	1.67	0.60
1:A:16:ILE:O	1:A:20:CYS:HB3	2.01	0.60
2:D:4:ILE:HG22	2:D:133:GLN:CB	2.28	0.60
1:C:180:ALA:HB1	2:D:258:ASN:HD21	1.67	0.60
2:D:132:LEU:HG	2:D:133:GLN:N	2.16	0.60
1:C:105:ARG:NH2	2:D:253:ARG:NH1	2.50	0.60
3:E:124:GLN:HA	3:E:127:ASP:OD1	2.00	0.60
1:A:273:ALA:HB3	1:A:375:VAL:H	1.67	0.60
1:C:403:ALA:HB1	1:C:404:PHE:CD1	2.36	0.60
2:D:237:GLY:CA	2:D:240:THR:HG23	2.32	0.60
1:C:252:LEU:CA	1:C:255:PHE:HB2	2.20	0.59
2:B:174:SER:HB2	2:B:207:GLU:HG3	1.84	0.59
1:C:256:GLN:C	1:C:258:ASN:N	2.55	0.59
2:D:191:VAL:HG21	2:D:425:MET:HE3	1.83	0.59
2:B:279:GLY:H	2:B:282:GLN:HB3	1.66	0.59
2:B:287:THR:HG22	2:B:290:GLU:H	1.64	0.59
2:B:287:THR:HG23	2:B:288:VAL:N	2.17	0.59
2:B:28:HIS:HA	2:B:43:GLN:HB3	1.83	0.59
1:C:262:TYR:O	1:C:263:PRO:C	2.40	0.59
2:D:111:GLY:O	2:D:113:GLU:N	2.35	0.59
1:A:128:GLN:O	1:A:129:CYS:HB2	2.02	0.59
1:A:273:ALA:HB2	1:A:375:VAL:CB	2.32	0.59
2:D:287:THR:CG2	2:D:290:GLU:H	2.15	0.59
2:B:163:ASP:OD1	2:B:164:ARG:HG2	2.03	0.59
2:B:223:THR:HA	6:B:800:HOS:H29	1.84	0.59
1:A:388:TRP:HA	1:A:388:TRP:CE3	2.37	0.59
2:D:403:ALA:O	2:D:405:LEU:N	2.31	0.59
1:C:8:HIS:HE1	1:C:21:TRP:HE1	1.51	0.59
1:A:405:VAL:CG1	1:A:406:HIS:N	2.65	0.58
3:E:48:GLU:C	3:E:50:ILE:H	2.06	0.58
1:A:7:ILE:HG12	1:A:66:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:THR:HG23	1:C:61:HIS:CE1	2.38	0.58
2:D:207:GLU:HB2	2:D:390:ARG:NH2	2.18	0.58
1:A:105:ARG:NH2	2:B:253:ARG:HH12	2.01	0.58
1:A:125:LEU:HA	1:A:128:GLN:HE21	1.67	0.58
1:A:273:ALA:CB	1:A:375:VAL:HG23	2.34	0.58
1:C:85:GLN:HA	1:C:85:GLN:HE21	1.68	0.58
2:D:332:MET:CE	2:D:353:THR:CG2	2.81	0.58
2:B:167:ASN:ND2	2:B:252:LEU:HD11	2.18	0.58
1:C:80:THR:CG2	1:C:81:GLY:N	2.66	0.58
2:D:254:LYS:O	2:D:258:ASN:HB2	2.02	0.58
1:A:256:GLN:HB2	1:A:260:VAL:HG13	1.85	0.58
1:A:389:ALA:HA	1:A:392:ASP:HB2	1.86	0.58
2:D:120:ASP:HB2	2:D:123:ARG:NH1	2.17	0.58
2:D:149:MET:O	2:D:152:LEU:HB3	2.04	0.58
2:D:316:ALA:HB1	5:D:701:CN2:H21	1.85	0.58
1:A:258:ASN:HD21	1:A:352:LYS:CD	2.16	0.58
1:A:266:HIS:O	1:A:268:PRO:HD3	2.03	0.58
1:A:276:ILE:HD11	1:A:280:LYS:HD3	1.86	0.58
1:A:175:PRO:HD3	1:A:394:LYS:NZ	2.19	0.58
1:C:271:THR:HG21	1:C:295:CYS:O	2.04	0.58
2:D:336:GLN:HE22	2:D:351:VAL:CG1	2.16	0.58
2:D:76:ASP:N	2:D:76:ASP:OD1	2.37	0.58
2:B:212:ILE:HG21	2:B:230:LEU:HD21	1.84	0.57
2:D:36:TYR:OH	2:D:38:GLY:O	2.14	0.57
2:D:145:THR:HG23	8:D:603:GDP:O3B	2.04	0.57
2:D:209:LEU:HD21	2:D:231:VAL:CG2	2.33	0.57
1:C:278:ALA:O	1:C:279:GLU:CB	2.52	0.57
1:A:262:TYR:O	1:A:263:PRO:C	2.42	0.57
2:B:115:VAL:HG12	2:B:116:ASP:N	2.19	0.57
2:D:111:GLY:HA2	2:D:149:MET:HE3	1.86	0.57
1:C:146:GLY:N	7:D:601:GTP:O1B	2.30	0.57
1:A:100:ALA:HB1	2:B:253:ARG:HG2	1.85	0.57
1:C:265:ILE:HG23	1:C:267:PHE:CZ	2.39	0.57
2:D:297:ASP:HB3	2:D:300:ASN:HB2	1.86	0.57
2:B:66:ILE:HD11	2:B:121:VAL:CB	2.34	0.57
2:D:184:PRO:HG2	2:D:398:MET:CE	2.34	0.57
2:D:383:ALA:O	2:D:386:GLU:HB2	2.05	0.57
2:D:241:CYS:HB3	5:D:701:CN2:C6	2.35	0.57
6:D:801:HOS:H35A	6:D:801:HOS:O7	2.03	0.57
1:A:403:ALA:HB1	1:A:404:PHE:CD1	2.37	0.57
1:C:32:PRO:O	1:C:33:ASP:C	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:701:CN2:H63	5:D:701:CN2:C4	2.34	0.57
2:B:207:GLU:CB	2:B:390:ARG:HH22	2.16	0.57
2:B:406:HIS:HE1	2:B:407:TRP:CD1	2.23	0.57
1:C:436:GLY:O	1:C:437:ALA:O	2.23	0.57
1:C:100:ALA:CB	2:D:253:ARG:HG2	2.34	0.57
1:A:228:ASN:N	1:A:228:ASN:HD22	2.03	0.57
1:A:3:GLU:CB	1:A:129:CYS:SG	2.93	0.57
2:B:166:MET:HB3	2:B:198:THR:HG22	1.86	0.57
1:A:111:GLY:O	1:A:113:GLU:N	2.38	0.57
1:A:273:ALA:HB2	1:A:375:VAL:N	2.20	0.57
2:B:33:THR:HB	2:B:60:LYS:HD2	1.87	0.57
2:D:388:PHE:CE1	2:D:428:LEU:HD21	2.39	0.57
6:D:801:HOS:H29	6:D:801:HOS:H22A	1.87	0.56
2:B:111:GLY:O	2:B:113:GLU:N	2.38	0.56
1:C:156:ARG:O	1:C:159:VAL:HB	2.05	0.56
2:D:265:LEU:O	2:D:266:HIS:C	2.42	0.56
2:B:406:HIS:HA	2:B:409:THR:HB	1.86	0.56
6:D:801:HOS:C6	6:D:801:HOS:C13	2.84	0.56
2:B:227:LEU:HG	2:B:228:ASN:N	2.20	0.56
2:B:54:ASN:ND2	2:B:64:ARG:HD3	2.15	0.56
1:C:241:SER:HB2	1:C:249:ASN:HD21	1.70	0.56
1:C:201:ALA:O	1:C:268:PRO:HD2	2.06	0.56
3:E:122:ARG:C	3:E:124:GLN:H	2.09	0.56
1:A:264:ARG:O	1:A:266:HIS:CD2	2.59	0.56
1:A:83:TYR:C	1:A:85:GLN:N	2.57	0.56
1:C:270:ALA:HB3	1:C:302:MET:SD	2.45	0.56
1:C:85:GLN:HA	1:C:85:GLN:NE2	2.21	0.56
2:D:89:PRO:O	2:D:92:PHE:HB2	2.05	0.56
3:E:92:ASN:HA	3:E:95:LYS:CB	2.36	0.56
2:B:332:MET:CE	2:B:353:THR:CG2	2.83	0.56
1:C:291:ILE:HB	1:C:375:VAL:CG2	2.36	0.56
1:A:157:LEU:C	1:A:159:VAL:H	2.06	0.56
1:A:267:PHE:CD1	1:A:267:PHE:N	2.73	0.56
2:B:66:ILE:HD11	2:B:121:VAL:CG1	2.36	0.56
1:A:234:ILE:HG13	1:A:272:TYR:HB2	1.88	0.56
2:B:169:PHE:CE2	2:B:235:MET:HG2	2.41	0.56
1:C:291:ILE:HG13	1:C:292:THR:H	1.71	0.56
2:D:88:ARG:HB3	2:D:91:ASN:OD1	2.06	0.56
1:C:7:ILE:HD12	1:C:153:LEU:HD11	1.87	0.56
2:B:111:GLY:C	2:B:113:GLU:N	2.60	0.55
2:B:181:VAL:HG21	2:B:404:PHE:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:212:ILE:CG2	2:D:230:LEU:HD21	2.37	0.55
1:C:195:LEU:HD11	1:C:264:ARG:HH11	1.71	0.55
1:A:217:LEU:HB3	1:A:219:ILE:HD12	1.87	0.55
1:C:228:ASN:HD21	7:D:601:GTP:HN1	1.54	0.55
2:B:12:CYS:SG	2:B:171:VAL:HG21	2.47	0.55
1:C:180:ALA:O	1:C:181:VAL:C	2.44	0.55
2:D:174:SER:HB2	2:D:207:GLU:HG3	1.88	0.55
2:D:51:VAL:O	2:D:64:ARG:NH2	2.39	0.55
1:A:7:ILE:HA	1:A:66:VAL:HG23	1.87	0.55
2:D:101:ASN:HA	2:D:144:GLY:N	2.21	0.55
1:C:398:MET:HE2	2:D:348:PRO:HD2	1.87	0.55
1:A:86:LEU:C	1:A:87:PHE:HD2	2.10	0.55
2:B:304:ALA:O	2:B:305:CYS:HB2	2.06	0.55
1:C:143:GLY:O	1:C:147:SER:OG	2.21	0.55
1:C:56:THR:O	1:C:57:GLY:C	2.44	0.55
1:C:74:VAL:O	1:C:77:GLU:HB3	2.07	0.55
1:C:205:ASP:C	1:C:205:ASP:OD1	2.45	0.55
1:C:219:ILE:HG22	1:C:221:ARG:H	1.72	0.55
2:D:332:MET:HE1	2:D:353:THR:CG2	2.37	0.55
1:A:355:ILE:HD11	3:E:18:GLN:CB	2.32	0.55
1:A:52:PHE:O	1:A:64:ARG:HB2	2.07	0.55
2:B:209:LEU:HD21	2:B:231:VAL:HG23	1.89	0.55
2:B:408:TYR:O	2:B:409:THR:C	2.44	0.55
1:C:108:TYR:HE1	1:C:413:MET:HG3	1.71	0.55
1:C:402:ARG:O	1:C:403:ALA:C	2.45	0.55
2:D:408:TYR:O	2:D:409:THR:C	2.45	0.54
2:D:4:ILE:HD11	2:D:52:TYR:CZ	2.41	0.54
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.90	0.54
1:C:416:GLY:O	1:C:420:GLU:HB3	2.06	0.54
1:C:398:MET:HE3	2:D:348:PRO:HD2	1.89	0.54
2:D:192:HIS:HD2	2:D:421:ALA:HA	1.72	0.54
2:D:406:HIS:HA	2:D:409:THR:HB	1.90	0.54
1:A:60:LYS:HE2	1:A:85:GLN:O	2.08	0.54
2:B:30:ILE:HG23	2:B:34:GLY:O	2.07	0.54
2:B:287:THR:HG23	2:B:289:PRO:CD	2.30	0.54
1:C:132:LEU:HG	1:C:133:GLN:N	2.19	0.54
1:A:375:VAL:HG12	1:A:376:CYS:N	2.23	0.54
1:C:195:LEU:HB2	1:C:265:ILE:HG21	1.90	0.54
1:C:406:HIS:CE1	2:D:263:PRO:HD3	2.43	0.54
3:E:69:LEU:O	3:E:73:ALA:HB2	2.07	0.54
2:B:297:ASP:HB3	2:B:300:ASN:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:MET:HG3	2:B:353:THR:HG21	1.89	0.54
1:C:407:TRP:CG	2:D:257:VAL:HG23	2.43	0.54
2:D:266:HIS:HB3	2:D:380:ASN:HD21	1.72	0.54
2:D:255:LEU:HD23	5:D:701:CN2:C22	2.38	0.54
1:A:432:TYR:O	1:A:434:GLU:N	2.41	0.54
2:D:119:LEU:HD23	2:D:123:ARG:NH2	2.23	0.54
1:A:265:ILE:HG23	1:A:267:PHE:CE1	2.43	0.54
2:B:238:VAL:HG13	2:B:378:ILE:HD11	1.89	0.54
2:D:249:ASN:N	2:D:249:ASN:OD1	2.41	0.54
2:B:265:LEU:O	2:B:266:HIS:C	2.45	0.54
1:C:31:GLN:O	1:C:33:ASP:HB3	2.07	0.54
2:D:24:ILE:HD12	2:D:243:ARG:HD3	1.90	0.54
2:D:316:ALA:HA	2:D:352:LYS:O	2.08	0.54
2:D:2:ARG:C	2:D:3:GLU:HG3	2.29	0.54
1:A:86:LEU:HB3	1:A:87:PHE:CD2	2.43	0.53
2:B:274:PRO:C	2:B:275:LEU:HG	2.27	0.53
1:C:181:VAL:O	1:C:184:PRO:HD2	2.08	0.53
1:C:317:LEU:HB3	1:C:319:TYR:CE1	2.42	0.53
3:E:106:GLU:C	3:E:108:ASN:N	2.54	0.53
2:D:180:THR:O	2:D:181:VAL:C	2.46	0.53
2:D:241:CYS:CB	5:D:701:CN2:H62	2.39	0.53
2:B:287:THR:CG2	2:B:290:GLU:H	2.21	0.53
2:D:101:ASN:HA	2:D:144:GLY:H	1.73	0.53
2:D:247:GLN:HE22	2:D:354:ALA:HB1	1.72	0.53
1:C:171:ILE:N	1:C:171:ILE:CD1	2.72	0.53
1:C:404:PHE:N	1:C:404:PHE:CD1	2.76	0.53
1:A:9:VAL:HA	1:A:68:VAL:O	2.09	0.53
2:B:144:GLY:O	2:B:145:THR:C	2.46	0.53
2:D:126:SER:C	2:D:128:SER:H	2.12	0.53
2:D:4:ILE:HD11	2:D:52:TYR:OH	2.09	0.53
3:E:114:ALA:O	3:E:118:ALA:HB3	2.09	0.53
1:A:109:THR:HG23	3:E:61:ARG:NH2	2.23	0.53
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.55	0.53
2:B:287:THR:CG2	2:B:288:VAL:N	2.71	0.53
1:C:287:SER:CB	1:C:290:GLU:HB2	2.36	0.53
1:C:102:ASN:HB2	1:C:408:TYR:CE2	2.44	0.53
1:A:182:VAL:CG2	1:A:408:TYR:OH	2.56	0.53
2:B:168:THR:OG1	2:B:170:SER:OG	2.27	0.53
2:B:404:PHE:CD2	1:C:261:PRO:HB3	2.43	0.53
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.91	0.53
1:C:271:THR:HG23	1:C:301:GLN:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:ASN:HD22	2:D:252:LEU:HD11	1.74	0.53
1:A:83:TYR:O	1:A:85:GLN:N	2.42	0.53
1:C:255:PHE:HA	1:C:258:ASN:HB2	1.91	0.53
1:C:432:TYR:O	1:C:434:GLU:N	2.42	0.53
2:D:115:VAL:O	2:D:118:VAL:HG23	2.09	0.53
2:D:332:MET:CE	2:D:353:THR:HG21	2.38	0.53
3:E:106:GLU:O	3:E:108:ASN:N	2.40	0.53
2:B:8:GLN:HG2	2:B:13:GLY:O	2.08	0.53
6:B:800:HOS:O12	6:B:800:HOS:O10	2.26	0.53
1:C:83:TYR:C	1:C:85:GLN:N	2.61	0.53
2:D:262:PHE:O	2:D:264:ARG:N	2.41	0.53
1:C:157:LEU:C	1:C:159:VAL:N	2.63	0.52
1:C:189:LEU:HD11	1:C:413:MET:HE1	1.91	0.52
1:A:271:THR:HG23	1:A:301:GLN:HA	1.90	0.52
1:C:175:PRO:HD3	1:C:394:LYS:NZ	2.25	0.52
2:D:126:SER:O	2:D:128:SER:N	2.42	0.52
2:D:209:LEU:HD21	2:D:231:VAL:HG23	1.91	0.52
2:B:428:LEU:O	2:B:429:VAL:C	2.47	0.52
2:B:431:GLU:HA	2:B:434:GLN:CB	2.35	0.52
2:D:308:ARG:HB3	2:D:309:HIS:CD2	2.44	0.52
2:D:250:ALA:CB	5:D:701:CN2:H7	2.39	0.52
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.75	0.52
2:B:223:THR:CG2	2:B:226:ASP:HB3	2.39	0.52
1:C:125:LEU:HA	1:C:128:GLN:HE21	1.75	0.52
1:C:291:ILE:HB	1:C:375:VAL:HG23	1.92	0.52
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.43	0.52
1:A:83:TYR:C	1:A:85:GLN:H	2.12	0.52
1:C:264:ARG:O	1:C:266:HIS:N	2.42	0.52
1:A:290:GLU:O	1:A:293:ASN:N	2.43	0.52
1:A:189:LEU:HD11	1:A:413:MET:HE1	1.92	0.52
1:C:100:ALA:O	1:C:101:ASN:HB2	2.10	0.52
1:C:254:GLU:HA	1:C:257:THR:HB	1.90	0.52
1:C:325:PRO:O	1:C:327:ASP:N	2.43	0.52
2:B:224:TYR:CE1	6:B:800:HOS:H22	2.44	0.52
1:C:223:THR:CB	1:C:226:ASN:HB2	2.40	0.52
1:A:273:ALA:HB2	1:A:375:VAL:HB	1.92	0.52
2:D:66:ILE:HD11	2:D:121:VAL:CB	2.37	0.52
2:D:28:HIS:HD1	2:D:49:ILE:HD12	1.75	0.52
2:B:204:ILE:H	2:B:204:ILE:HD12	1.75	0.52
2:B:291:LEU:HD21	2:B:375:ALA:CB	2.39	0.52
2:D:176:LYS:O	2:D:177:VAL:HB	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:O	1:A:243:ARG:O	2.28	0.52
1:C:7:ILE:HG12	1:C:66:VAL:CG2	2.40	0.52
2:D:15:GLN:O	2:D:17:GLY:N	2.43	0.52
2:D:264:ARG:O	2:D:266:HIS:N	2.43	0.52
2:D:193:GLN:OE1	3:E:126:LYS:HE3	2.09	0.52
2:B:17:GLY:HA2	2:B:20:PHE:HB3	1.90	0.51
1:C:362:VAL:HB	1:C:368:LEU:HD12	1.92	0.51
1:C:52:PHE:O	1:C:64:ARG:HB2	2.10	0.51
1:C:7:ILE:HG12	1:C:66:VAL:HG23	1.91	0.51
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.92	0.51
2:B:332:MET:HE2	2:B:353:THR:CG2	2.39	0.51
1:C:136:LEU:HD22	1:C:169:PHE:CE1	2.44	0.51
1:C:389:ALA:HB2	1:C:429:GLU:OE2	2.10	0.51
2:D:332:MET:HG3	2:D:353:THR:HG21	1.91	0.51
2:D:96:GLN:HA	2:D:96:GLN:OE1	2.10	0.51
2:B:216:THR:O	2:B:217:LEU:CB	2.59	0.51
2:B:259:MET:HE3	2:B:314:THR:O	2.10	0.51
6:B:800:HOS:C33	6:B:800:HOS:O8	2.53	0.51
2:D:195:VAL:HA	2:D:265:LEU:HD23	1.91	0.51
2:B:407:TRP:CZ2	1:C:257:THR:N	2.79	0.51
2:D:216:THR:O	2:D:217:LEU:CB	2.58	0.51
2:D:224:TYR:HB3	6:D:801:HOS:H34A	1.92	0.51
1:A:262:TYR:O	1:A:264:ARG:N	2.44	0.51
1:C:265:ILE:HG12	1:C:265:ILE:O	2.10	0.51
2:D:256:ALA:C	2:D:258:ASN:H	2.12	0.51
3:E:134:ARG:C	3:E:136:ASN:N	2.63	0.51
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.44	0.51
1:A:251:ASP:O	1:A:254:GLU:HB2	2.10	0.51
2:B:208:ALA:O	2:B:211:ASP:N	2.43	0.51
1:C:90:GLU:HB3	1:C:121:ARG:CD	2.40	0.51
2:B:211:ASP:HB3	2:B:215:ARG:HH12	1.75	0.51
6:B:800:HOS:H3	6:B:800:HOS:C12	2.41	0.51
1:C:223:THR:HB	1:C:226:ASN:HB2	1.92	0.51
1:C:405:VAL:CG1	1:C:406:HIS:N	2.73	0.51
1:C:81:GLY:O	1:C:82:THR:C	2.48	0.51
2:D:119:LEU:HD23	2:D:123:ARG:HH22	1.76	0.51
2:B:262:PHE:O	2:B:266:HIS:CD2	2.63	0.51
1:C:381:THR:O	1:C:384:VAL:HG23	2.11	0.51
1:C:86:LEU:C	1:C:87:PHE:HD2	2.13	0.51
3:E:72:LEU:C	3:E:74:GLU:H	2.12	0.51
1:A:252:LEU:O	1:A:255:PHE:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:TYR:O	1:A:86:LEU:N	2.25	0.51
2:B:227:LEU:O	2:B:228:ASN:C	2.48	0.51
2:B:237:GLY:HA2	2:B:240:THR:CG2	2.39	0.51
2:B:337:ASN:C	2:B:339:ASN:N	2.63	0.51
1:C:123:ARG:O	1:C:125:LEU:N	2.44	0.51
3:E:136:ASN:C	3:E:138:GLU:H	2.14	0.51
3:E:48:GLU:C	3:E:50:ILE:N	2.63	0.51
1:A:154:MET:O	1:A:155:GLU:C	2.49	0.51
5:B:700:CN2:H15	5:B:700:CN2:C12	2.40	0.51
1:C:141:PHE:HD1	1:C:172:TYR:HB2	1.76	0.51
2:D:174:SER:CB	2:D:175:PRO:CD	2.89	0.51
2:D:262:PHE:CD1	2:D:435:TYR:CE2	2.98	0.51
2:B:351:VAL:HG12	2:B:351:VAL:O	2.12	0.50
2:B:54:ASN:HD22	2:B:64:ARG:HD2	1.74	0.50
2:D:332:MET:HE1	2:D:353:THR:HG22	1.93	0.50
2:B:223:THR:HG21	2:B:226:ASP:HB3	1.92	0.50
2:B:332:MET:CE	2:B:353:THR:HG21	2.41	0.50
2:D:103:TRP:HZ2	2:D:193:GLN:HE21	1.59	0.50
6:D:801:HOS:H22A	6:D:801:HOS:C29	2.42	0.50
1:A:427:ALA:O	1:A:431:ASP:N	2.36	0.50
2:B:390:ARG:HG3	2:B:390:ARG:NH1	2.13	0.50
1:C:264:ARG:O	1:C:266:HIS:CG	2.64	0.50
1:A:416:GLY:O	1:A:420:GLU:HB3	2.11	0.50
2:B:403:ALA:C	2:B:405:LEU:N	2.57	0.50
1:C:315:CYS:HB3	1:C:351:PHE:CD2	2.46	0.50
2:B:114:LEU:O	2:B:115:VAL:C	2.49	0.50
2:D:191:VAL:HG11	2:D:425:MET:CG	2.41	0.50
2:D:208:ALA:O	2:D:211:ASP:N	2.45	0.50
2:D:227:LEU:CG	2:D:228:ASN:N	2.74	0.50
2:D:238:VAL:HG13	2:D:378:ILE:HD11	1.93	0.50
2:D:431:GLU:HA	2:D:434:GLN:CB	2.38	0.50
2:B:224:TYR:CE1	6:B:800:HOS:C24	2.94	0.50
2:D:120:ASP:HB2	2:D:123:ARG:HH12	1.77	0.50
6:D:801:HOS:C33	6:D:801:HOS:O8	2.59	0.50
1:A:297:GLU:HG3	1:A:299:ALA:H	1.75	0.50
2:B:151:THR:CB	2:B:193:GLN:HG2	2.37	0.50
1:C:313:MET:O	1:C:314:ALA:HB2	2.12	0.50
1:C:273:ALA:HB2	1:C:375:VAL:N	2.26	0.50
1:C:70:LEU:HD23	1:C:110:ILE:CG2	2.40	0.50
2:D:16:ILE:HG21	2:D:138:THR:HB	1.94	0.50
3:E:51:GLN:HG2	3:E:51:GLN:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:LEU:O	2:B:390:ARG:HB3	2.12	0.50
6:B:800:HOS:H3	6:B:800:HOS:O5	2.12	0.50
1:C:217:LEU:HB3	1:C:219:ILE:HD12	1.93	0.50
2:D:168:THR:CG2	2:D:198:THR:HG21	2.42	0.50
1:A:406:HIS:HA	1:A:409:VAL:HG23	1.94	0.49
2:B:249:ASN:N	2:B:249:ASN:OD1	2.44	0.49
2:B:242:LEU:HG	5:B:700:CN2:H61	1.94	0.49
2:D:126:SER:C	2:D:128:SER:N	2.65	0.49
2:D:31:ASP:HB2	2:D:34:GLY:HA3	1.94	0.49
2:B:110:GLU:O	2:B:113:GLU:HB3	2.12	0.49
1:A:327:ASP:O	1:A:328:VAL:C	2.51	0.49
1:A:393:HIS:O	1:A:394:LYS:C	2.50	0.49
1:C:311:LYS:O	1:C:382:THR:HG22	2.13	0.49
1:C:405:VAL:HG13	1:C:406:HIS:H	1.77	0.49
2:D:277:SER:HB3	2:D:281:GLN:N	2.28	0.49
1:A:250:VAL:HG12	1:A:254:GLU:OE1	2.13	0.49
1:A:313:MET:O	1:A:314:ALA:HB2	2.12	0.49
2:B:316:ALA:HA	2:B:352:LYS:O	2.13	0.49
2:D:30:ILE:HG22	2:D:31:ASP:O	2.12	0.49
1:A:187:SER:HB2	1:A:391:LEU:HD21	1.95	0.49
1:A:401:LYS:C	1:A:403:ALA:H	2.15	0.49
2:B:225:GLY:O	2:B:227:LEU:N	2.46	0.49
1:C:180:ALA:O	1:C:182:VAL:N	2.45	0.49
2:B:406:HIS:HE1	2:B:407:TRP:NE1	2.10	0.49
1:C:99:ALA:HA	1:C:105:ARG:HG2	1.95	0.49
1:C:35:GLN:O	1:C:37:PRO:HD3	2.13	0.49
3:E:61:ARG:O	3:E:63:TYR:N	2.46	0.49
1:A:99:ALA:HB3	1:A:145:THR:CG2	2.40	0.49
2:B:69:ASP:O	2:B:95:GLY:N	2.45	0.49
2:D:377:PHE:CE2	2:D:379:GLY:HA3	2.48	0.49
2:B:282:GLN:O	2:B:282:GLN:NE2	2.45	0.49
1:C:233:GLN:HE22	1:C:362:VAL:CG1	2.17	0.49
1:A:298:PRO:O	1:A:301:GLN:HG3	2.12	0.49
2:B:28:HIS:HD1	2:B:49:ILE:HD12	1.78	0.49
1:C:157:LEU:O	1:C:159:VAL:N	2.45	0.49
1:C:273:ALA:HB2	1:C:375:VAL:CB	2.42	0.49
1:C:356:ASN:C	1:C:358:GLN:H	2.16	0.49
2:D:118:VAL:O	2:D:122:VAL:HG13	2.13	0.49
2:D:153:LEU:O	2:D:157:ILE:HG12	2.11	0.49
2:D:224:TYR:HB3	6:D:801:HOS:C34	2.43	0.49
2:D:69:ASP:O	2:D:95:GLY:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLN:O	1:A:373:ARG:CB	2.61	0.49
2:D:165:ILE:HD11	2:D:252:LEU:HD23	1.94	0.49
2:B:101:ASN:HA	2:B:144:GLY:N	2.28	0.48
2:B:184:PRO:HG2	2:B:398:MET:CE	2.43	0.48
2:B:171:VAL:HA	2:B:204:ILE:O	2.13	0.48
2:B:273:ALA:HB3	2:B:375:ALA:H	1.78	0.48
1:C:62:VAL:CG2	1:C:91:GLN:HE22	2.26	0.48
2:B:224:TYR:CE2	8:D:602:GDP:C5	3.01	0.48
5:D:701:CN2:C6	5:D:701:CN2:O2	2.60	0.48
2:B:103:TRP:HZ2	2:B:193:GLN:HE21	1.62	0.48
2:D:237:GLY:O	2:D:240:THR:HG23	2.13	0.48
1:A:353:VAL:CG2	3:E:20:PHE:CZ	2.97	0.48
2:B:120:ASP:HB2	2:B:123:ARG:NH1	2.28	0.48
2:B:211:ASP:HB3	2:B:215:ARG:NH1	2.29	0.48
2:B:212:ILE:CG2	2:B:230:LEU:HD21	2.42	0.48
1:A:325:PRO:O	1:A:327:ASP:N	2.47	0.48
1:C:111:GLY:C	1:C:113:GLU:H	2.16	0.48
2:D:273:ALA:CB	2:D:274:PRO:CD	2.65	0.48
2:D:387:LEU:O	2:D:390:ARG:HG3	2.13	0.48
2:B:145:THR:HG23	8:D:602:GDP:O3B	2.14	0.48
1:A:228:ASN:O	1:A:231:MET:N	2.46	0.48
1:A:88:HIS:HB2	1:A:91:GLN:NE2	2.28	0.48
2:B:192:HIS:HD2	2:B:421:ALA:HA	1.79	0.48
2:B:96:GLN:HG3	2:B:97:SER:N	2.27	0.48
1:C:343:PHE:CD1	1:C:349:THR:HA	2.48	0.48
2:D:166:MET:HB3	2:D:198:THR:HG22	1.95	0.48
2:D:242:LEU:HA	2:D:250:ALA:HB3	1.95	0.48
2:D:428:LEU:O	2:D:429:VAL:C	2.52	0.48
1:A:102:ASN:HD22	1:A:104:ALA:HB3	1.74	0.48
1:A:291:ILE:HB	1:A:375:VAL:CG2	2.43	0.48
2:B:280:SER:HA	2:B:283:TYR:HB2	1.96	0.48
2:B:398:MET:C	2:B:400:ARG:N	2.65	0.48
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.49	0.48
2:B:76:ASP:OD1	2:B:76:ASP:N	2.47	0.48
1:C:21:TRP:O	1:C:24:TYR:HB2	2.13	0.48
1:C:269:LEU:O	1:C:269:LEU:HD12	2.13	0.48
3:E:136:ASN:C	3:E:138:GLU:N	2.67	0.48
1:A:210:TYR:C	1:A:210:TYR:CD1	2.87	0.48
2:B:396:THR:HG22	2:B:400:ARG:NH2	2.29	0.48
1:C:255:PHE:CD2	1:C:316:CYS:SG	3.07	0.48
1:C:265:ILE:HG23	1:C:267:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:ARG:O	2:B:266:HIS:N	2.46	0.48
2:D:274:PRO:C	2:D:275:LEU:HG	2.34	0.48
1:A:105:ARG:CZ	2:B:253:ARG:NH1	2.73	0.48
1:A:100:ALA:CB	2:B:253:ARG:HG2	2.44	0.48
2:B:287:THR:HG22	2:B:290:GLU:CB	2.44	0.48
2:D:154:ILE:HG12	2:D:155:SER:N	2.29	0.48
2:D:151:THR:CB	2:D:193:GLN:HG2	2.30	0.48
3:E:79:GLU:C	3:E:81:GLU:H	2.17	0.48
1:A:404:PHE:CD1	1:A:404:PHE:N	2.80	0.47
5:B:700:CN2:C4	5:B:700:CN2:H62	2.39	0.47
1:C:11:GLN:HA	1:C:74:VAL:HG11	1.96	0.47
1:C:221:ARG:HH21	2:D:325:MET:HE3	1.79	0.47
2:D:336:GLN:NE2	2:D:351:VAL:HG11	2.27	0.47
2:B:316:ALA:CB	5:B:700:CN2:C2	2.86	0.47
1:C:123:ARG:HD2	1:C:161:TYR:CZ	2.48	0.47
1:C:139:HIS:CG	1:C:150:THR:HG21	2.49	0.47
1:C:267:PHE:CD1	1:C:267:PHE:N	2.83	0.47
2:D:174:SER:HB2	2:D:207:GLU:HG2	1.95	0.47
1:C:406:HIS:CE1	2:D:261:PRO:O	2.62	0.47
1:A:291:ILE:HG13	1:A:292:THR:H	1.79	0.47
2:D:21:TRP:CZ2	2:D:65:ALA:HB2	2.49	0.47
3:E:96:MET:O	3:E:98:LYS:N	2.47	0.47
2:B:31:ASP:HB2	2:B:34:GLY:HA3	1.96	0.47
2:B:66:ILE:HD11	2:B:121:VAL:HG12	1.97	0.47
1:C:36:MET:C	1:C:38:SER:N	2.60	0.47
1:A:123:ARG:O	1:A:125:LEU:N	2.48	0.47
1:A:7:ILE:HD12	1:A:153:LEU:HD11	1.95	0.47
1:C:44:GLY:O	1:C:46:ASP:N	2.48	0.47
1:A:80:THR:CG2	1:A:81:GLY:N	2.77	0.47
2:B:395:PHE:O	2:B:397:ALA:N	2.47	0.47
2:D:352:LYS:HG3	5:D:701:CN2:O5	2.14	0.47
1:A:85:GLN:HA	1:A:85:GLN:HE21	1.79	0.47
1:A:87:PHE:N	1:A:87:PHE:CD2	2.83	0.47
1:A:62:VAL:CG2	1:A:91:GLN:HE22	2.28	0.47
2:B:102:ASN:OD1	2:B:102:ASN:O	2.33	0.47
2:B:176:LYS:O	2:B:176:LYS:HG3	2.15	0.47
2:B:273:ALA:CB	2:B:375:ALA:H	2.27	0.47
1:C:179:THR:HB	1:C:183:GLU:OE1	2.14	0.47
1:C:344:VAL:HG13	1:C:344:VAL:O	2.14	0.47
1:A:328:VAL:HG12	1:A:332:ILE:HD11	1.96	0.47
2:B:317:ALA:HB3	2:B:353:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:GLN:HE22	2:B:351:VAL:CG1	2.24	0.47
3:E:112:ARG:C	3:E:114:ALA:N	2.67	0.47
1:A:104:ALA:HB2	1:A:408:TYR:HD2	1.79	0.47
1:A:184:PRO:O	1:A:188:ILE:HG12	2.14	0.47
1:A:35:GLN:O	1:A:37:PRO:HD3	2.14	0.47
2:B:191:VAL:HG11	2:B:425:MET:CE	2.45	0.47
2:B:385:GLN:HG2	2:B:385:GLN:O	2.14	0.47
1:C:133:GLN:HG2	1:C:133:GLN:O	2.14	0.47
2:D:292:THR:HA	2:D:295:MET:HE3	1.95	0.47
1:A:270:ALA:HA	1:A:377:MET:O	2.14	0.47
1:C:142:GLY:HA3	1:C:183:GLU:HG3	1.97	0.47
1:C:190:THR:CG2	1:C:191:THR:N	2.78	0.47
2:D:36:TYR:OH	2:D:40:SER:O	2.33	0.47
1:C:111:GLY:C	1:C:113:GLU:N	2.69	0.46
1:C:209:ILE:CG2	1:C:227:LEU:HD12	2.45	0.46
1:C:34:GLY:HA3	1:C:60:LYS:HA	1.96	0.46
2:D:406:HIS:HE1	2:D:407:TRP:NE1	2.13	0.46
3:E:63:TYR:O	3:E:65:GLU:N	2.49	0.46
1:A:136:LEU:HD22	1:A:169:PHE:HE1	1.79	0.46
1:A:219:ILE:O	1:A:222:PRO:HD3	2.14	0.46
2:B:406:HIS:HA	2:B:409:THR:CB	2.45	0.46
2:B:6:HIS:HE1	2:B:8:GLN:HG3	1.79	0.46
1:C:187:SER:HB2	1:C:391:LEU:HD21	1.97	0.46
1:C:82:THR:O	1:C:83:TYR:HB2	2.15	0.46
1:A:256:GLN:HB2	1:A:260:VAL:CG1	2.46	0.46
1:A:56:THR:O	1:A:57:GLY:C	2.54	0.46
2:D:231:VAL:HG12	2:D:235:MET:CE	2.45	0.46
2:D:277:SER:HB3	2:D:281:GLN:H	1.79	0.46
2:D:7:ILE:HG12	2:D:66:ILE:CG2	2.45	0.46
1:A:195:LEU:HD11	1:A:264:ARG:HH11	1.80	0.46
2:B:262:PHE:O	2:B:266:HIS:HD2	1.99	0.46
2:B:405:LEU:C	2:B:407:TRP:H	2.19	0.46
1:C:297:GLU:HA	1:C:298:PRO:HD2	1.82	0.46
1:C:80:THR:HG22	1:C:81:GLY:H	1.80	0.46
2:D:184:PRO:HG2	2:D:398:MET:HE1	1.95	0.46
1:A:315:CYS:HB3	1:A:351:PHE:CD2	2.51	0.46
1:C:317:LEU:HB2	1:C:353:VAL:CG1	2.36	0.46
1:C:333:ALA:O	1:C:336:LYS:HB3	2.16	0.46
2:B:255:LEU:HD23	5:B:700:CN2:C22	2.44	0.46
3:E:62:LYS:O	3:E:66:ALA:HB3	2.14	0.46
1:A:273:ALA:HB2	1:A:375:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:CD1	1:A:126:ALA:HB2	2.46	0.46
2:B:209:LEU:HD21	2:B:231:VAL:CG2	2.45	0.46
2:B:332:MET:HE1	2:B:353:THR:CG2	2.46	0.46
2:B:71:GLU:O	2:B:71:GLU:HG2	2.16	0.46
1:C:119:LEU:HD11	1:C:156:ARG:HG2	1.97	0.46
1:C:395:PHE:O	1:C:396:ASP:C	2.54	0.46
2:D:150:GLY:C	2:D:152:LEU:N	2.67	0.46
2:D:15:GLN:O	2:D:16:ILE:C	2.51	0.46
2:D:204:ILE:H	2:D:204:ILE:HD12	1.81	0.46
1:A:174:ALA:HB2	1:A:207:GLU:H	1.81	0.46
2:B:28:HIS:N	2:B:28:HIS:CD2	2.84	0.46
1:C:83:TYR:C	1:C:85:GLN:H	2.19	0.46
2:D:317:ALA:HB3	2:D:353:THR:HG22	1.97	0.46
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.98	0.46
1:A:284:GLU:HG2	1:A:286:LEU:HD12	1.97	0.46
1:A:381:THR:O	1:A:384:VAL:HG23	2.15	0.46
2:B:205:ASP:OD1	2:B:208:ALA:N	2.46	0.46
2:B:237:GLY:CA	2:B:240:THR:HG23	2.42	0.46
1:C:196:GLU:HG3	1:C:196:GLU:H	1.61	0.46
1:A:334:THR:C	1:A:336:LYS:H	2.19	0.46
1:A:407:TRP:CG	2:B:257:VAL:HG23	2.50	0.46
2:D:223:THR:HG23	2:D:226:ASP:OD2	2.16	0.46
1:A:311:LYS:O	1:A:382:THR:HG22	2.15	0.45
1:A:347:CYS:O	1:A:348:PRO:C	2.55	0.45
1:A:349:THR:CG2	3:E:24:LEU:HB3	2.47	0.45
2:B:89:PRO:HA	2:B:92:PHE:HD1	1.81	0.45
1:C:132:LEU:HD23	1:C:164:LYS:HD2	1.99	0.45
1:C:206:ASN:O	1:C:207:GLU:C	2.54	0.45
1:C:298:PRO:O	1:C:301:GLN:HG3	2.17	0.45
1:C:273:ALA:CB	1:C:375:VAL:HG23	2.46	0.45
2:D:28:HIS:CD2	2:D:28:HIS:N	2.83	0.45
2:D:406:HIS:HE1	2:D:407:TRP:CD1	2.34	0.45
2:D:427:ASP:O	2:D:430:SER:N	2.47	0.45
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.97	0.45
3:E:72:LEU:C	3:E:74:GLU:N	2.69	0.45
1:A:223:THR:CA	1:A:226:ASN:HB2	2.46	0.45
1:A:356:ASN:C	1:A:358:GLN:H	2.20	0.45
2:B:5:VAL:HG12	2:B:64:ARG:CG	2.42	0.45
2:D:33:THR:HB	2:D:60:LYS:HD2	1.97	0.45
2:D:55:GLU:HB3	2:D:61:TYR:CE2	2.51	0.45
6:D:801:HOS:O3	6:D:801:HOS:C13	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLU:O	1:A:291:ILE:C	2.54	0.45
1:A:297:GLU:HA	1:A:298:PRO:HD2	1.79	0.45
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.31	0.45
2:B:72:PRO:O	2:B:73:GLY:C	2.54	0.45
1:C:112:LYS:O	1:C:112:LYS:HG2	2.16	0.45
1:C:174:ALA:HB2	1:C:207:GLU:H	1.81	0.45
1:C:200:CYS:HB3	1:C:256:GLN:HE21	1.80	0.45
2:D:99:ALA:HB1	2:D:145:THR:HG21	1.99	0.45
2:D:70:LEU:HA	2:D:95:GLY:HA3	1.97	0.45
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.73	0.45
2:B:174:SER:CB	2:B:175:PRO:CD	2.93	0.45
2:B:357:ASP:OD2	2:B:357:ASP:N	2.47	0.45
2:B:377:PHE:CE2	2:B:379:GLY:HA3	2.52	0.45
1:C:250:VAL:HG12	1:C:251:ASP:H	1.80	0.45
2:D:103:TRP:CH2	2:D:189:LEU:HD22	2.51	0.45
2:D:223:THR:CG2	2:D:226:ASP:HB3	2.47	0.45
1:A:173:PRO:HB3	7:D:600:GTP:O3'	2.16	0.45
2:B:207:GLU:O	2:B:211:ASP:HB2	2.16	0.45
1:C:317:LEU:CB	1:C:319:TYR:HE1	2.27	0.45
1:C:356:ASN:O	1:C:358:GLN:N	2.46	0.45
2:D:132:LEU:CG	2:D:133:GLN:N	2.79	0.45
2:D:358:ILE:O	2:D:358:ILE:CG2	2.63	0.45
1:C:144:GLY:HA3	7:D:601:GTP:O2B	2.17	0.45
1:A:313:MET:HG3	1:A:380:ASN:O	2.16	0.45
1:A:82:THR:O	1:A:83:TYR:HB2	2.16	0.45
1:A:99:ALA:HA	1:A:105:ARG:HG2	1.99	0.45
2:B:106:GLY:O	2:B:149:MET:HA	2.15	0.45
2:B:332:MET:HE1	2:B:353:THR:HG22	1.99	0.45
1:C:7:ILE:CD1	1:C:153:LEU:HD11	2.47	0.45
2:D:191:VAL:HG11	2:D:425:MET:HG2	1.96	0.45
2:D:198:THR:O	2:D:265:LEU:HD22	2.16	0.45
1:A:269:LEU:O	1:A:269:LEU:HD12	2.15	0.45
2:B:122:VAL:CG2	2:B:123:ARG:N	2.79	0.45
2:B:126:SER:C	2:B:128:SER:H	2.18	0.45
1:C:287:SER:O	1:C:291:ILE:HG12	2.17	0.45
1:C:87:PHE:CD2	1:C:87:PHE:N	2.84	0.45
2:D:332:MET:HE2	2:D:353:THR:CG2	2.47	0.45
1:A:395:PHE:CD2	1:A:422:ARG:HD3	2.52	0.45
2:B:150:GLY:O	2:B:153:LEU:N	2.50	0.45
2:B:174:SER:HB2	2:B:207:GLU:HG2	1.96	0.45
2:B:194:LEU:O	2:B:196:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:PRO:HB2	1:C:73:THR:H	1.66	0.45
2:D:184:PRO:HG2	2:D:398:MET:HE3	1.98	0.45
2:D:287:THR:HG23	2:D:289:PRO:CD	2.42	0.45
2:D:309:HIS:H	2:D:309:HIS:CD2	2.33	0.45
2:B:16:ILE:HG21	2:B:138:THR:HB	1.98	0.45
2:B:262:PHE:CE1	2:B:435:TYR:CE2	2.86	0.45
2:B:51:VAL:O	2:B:64:ARG:NH2	2.50	0.45
1:C:312:TYR:HD2	1:C:381:THR:HB	1.82	0.45
1:C:432:TYR:C	1:C:434:GLU:N	2.70	0.45
1:C:80:THR:HG22	1:C:81:GLY:N	2.31	0.45
2:D:172:MET:HA	2:D:173:PRO:HD3	1.73	0.45
2:D:253:ARG:O	2:D:254:LYS:C	2.55	0.45
1:A:349:THR:HB	3:E:24:LEU:H	1.82	0.45
1:A:123:ARG:HD2	1:A:161:TYR:CZ	2.52	0.45
2:B:224:TYR:HE2	8:D:602:GDP:C5	2.35	0.45
2:B:16:ILE:HD12	2:B:228:ASN:OD1	2.17	0.45
2:B:29:GLY:O	2:B:36:TYR:HA	2.17	0.45
1:C:183:GLU:HB3	1:C:184:PRO:CD	2.46	0.45
1:C:306:ASP:HA	1:C:307:PRO:HD3	1.78	0.45
2:D:150:GLY:O	2:D:153:LEU:N	2.50	0.45
2:D:180:THR:HB	2:D:183:GLU:OE2	2.16	0.45
2:D:325:MET:HG2	2:D:355:VAL:HG21	1.98	0.45
2:D:36:TYR:CZ	2:D:38:GLY:O	2.69	0.45
1:A:190:THR:CG2	1:A:191:THR:N	2.80	0.44
1:A:104:ALA:HB2	1:A:408:TYR:CD2	2.52	0.44
1:C:3:GLU:CB	1:C:129:CYS:SG	3.02	0.44
1:C:408:TYR:O	1:C:411:GLU:N	2.50	0.44
1:C:70:LEU:N	1:C:70:LEU:HD12	2.32	0.44
2:D:114:LEU:O	2:D:115:VAL:C	2.54	0.44
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.64	0.44
3:E:19:SER:O	3:E:20:PHE:HB3	2.17	0.44
1:A:157:LEU:C	1:A:159:VAL:N	2.71	0.44
1:A:85:GLN:HA	1:A:85:GLN:NE2	2.33	0.44
2:B:81:GLY:HA3	2:B:82:PRO:HD3	1.83	0.44
3:E:120:LEU:O	3:E:124:GLN:HB2	2.18	0.44
1:A:174:ALA:CB	1:A:207:GLU:H	2.31	0.44
1:A:72:PRO:O	1:A:74:VAL:N	2.51	0.44
6:B:800:HOS:N3	6:B:800:HOS:H22A	2.24	0.44
1:C:288:VAL:HG11	1:C:327:ASP:HB3	1.99	0.44
1:C:406:HIS:HA	1:C:409:VAL:HG23	2.00	0.44
1:C:74:VAL:O	1:C:77:GLU:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:LEU:O	2:B:187:ALA:HA	2.17	0.44
2:B:198:THR:OG1	2:B:265:LEU:HD22	2.18	0.44
2:B:336:GLN:NE2	2:B:351:VAL:HG11	2.27	0.44
2:D:224:TYR:CE2	8:D:603:GDP:C5	3.05	0.44
2:D:350:ASN:H	2:D:350:ASN:HD22	1.65	0.44
1:A:359:PRO:HA	1:A:360:PRO:HD3	1.66	0.44
2:B:358:ILE:HA	2:B:359:PRO:HD3	1.91	0.44
1:C:163:LYS:HB2	1:C:164:LYS:H	1.71	0.44
2:D:270:PRO:HG2	2:D:302:MET:HB2	2.00	0.44
6:D:801:HOS:H23B	6:D:801:HOS:O5	2.17	0.44
6:D:801:HOS:O8	6:D:801:HOS:C20	2.37	0.44
2:D:115:VAL:HG12	2:D:116:ASP:N	2.32	0.44
2:D:166:MET:O	2:D:200:GLU:HG2	2.17	0.44
2:D:306:ASP:C	2:D:307:PRO:O	2.55	0.44
2:B:119:LEU:HD23	2:B:123:ARG:NH2	2.33	0.44
2:B:248:LEU:HG	2:B:248:LEU:H	1.70	0.44
2:D:12:CYS:O	2:D:14:ASN:N	2.50	0.44
2:D:308:ARG:C	2:D:310:GLY:H	2.21	0.44
1:A:20:CYS:HA	1:A:232:SER:HB2	2.00	0.44
1:A:273:ALA:HB1	1:A:375:VAL:HG23	1.98	0.44
1:A:420:GLU:HA	1:A:423:GLU:HB2	2.00	0.44
2:B:127:GLU:O	2:B:127:GLU:HG2	2.16	0.44
2:B:262:PHE:O	2:B:263:PRO:C	2.55	0.44
2:B:337:ASN:HA	2:B:340:SER:HB3	1.99	0.44
1:C:432:TYR:C	1:C:434:GLU:H	2.21	0.44
2:D:207:GLU:O	2:D:211:ASP:HB2	2.17	0.44
2:D:403:ALA:C	2:D:405:LEU:N	2.71	0.44
1:A:205:ASP:OD1	1:A:206:ASN:N	2.51	0.44
1:A:263:PRO:O	1:A:265:ILE:N	2.50	0.44
1:A:348:PRO:HA	3:E:27:PRO:CA	2.44	0.44
1:C:266:HIS:HB3	1:C:380:ASN:OD1	2.18	0.44
2:D:250:ALA:HB1	5:D:701:CN2:H7	2.00	0.44
2:B:224:TYR:HE1	6:B:800:HOS:C24	2.30	0.43
1:C:256:GLN:O	1:C:257:THR:C	2.56	0.43
2:D:110:GLU:O	2:D:113:GLU:HB3	2.17	0.43
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.53	0.43
1:A:109:THR:CG2	3:E:61:ARG:CZ	2.85	0.43
1:A:258:ASN:HD21	1:A:352:LYS:HD2	1.82	0.43
2:B:115:VAL:O	2:B:118:VAL:HG23	2.18	0.43
2:B:205:ASP:HB3	2:B:303:ALA:HA	2.00	0.43
2:B:308:ARG:HB2	2:B:309:HIS:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:VAL:O	2:B:351:VAL:CG1	2.66	0.43
2:B:191:VAL:HG11	2:B:425:MET:HE2	2.00	0.43
2:D:111:GLY:O	2:D:114:LEU:N	2.51	0.43
2:D:171:VAL:HA	2:D:204:ILE:O	2.18	0.43
2:D:83:PHE:HD2	2:D:83:PHE:HA	1.73	0.43
3:E:112:ARG:HG3	3:E:113:GLU:H	1.79	0.43
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.99	0.43
1:A:88:HIS:CD2	1:A:89:PRO:HD2	2.54	0.43
2:D:167:ASN:ND2	2:D:252:LEU:HD11	2.32	0.43
2:D:257:VAL:O	2:D:257:VAL:HG13	2.16	0.43
2:D:265:LEU:O	2:D:266:HIS:O	2.36	0.43
1:C:193:THR:HG21	3:E:104:LYS:NZ	2.32	0.43
3:E:122:ARG:HB2	3:E:122:ARG:HE	1.54	0.43
1:A:252:LEU:C	1:A:254:GLU:H	2.22	0.43
1:A:358:GLN:HA	1:A:359:PRO:HD2	1.90	0.43
2:B:227:LEU:CG	2:B:228:ASN:N	2.78	0.43
2:B:427:ASP:O	2:B:430:SER:N	2.44	0.43
1:C:273:ALA:HB2	1:C:375:VAL:HB	2.00	0.43
2:D:239:THR:O	2:D:240:THR:C	2.56	0.43
2:D:7:ILE:HG12	2:D:66:ILE:HG22	2.01	0.43
1:A:182:VAL:CG2	1:A:182:VAL:O	2.66	0.43
2:B:101:ASN:HA	2:B:144:GLY:H	1.83	0.43
2:B:181:VAL:CG2	2:B:404:PHE:CE1	3.01	0.43
1:A:294:ALA:O	1:A:297:GLU:HB3	2.18	0.43
1:A:62:VAL:HG21	1:A:91:GLN:HE22	1.82	0.43
2:B:332:MET:HE2	2:B:353:THR:HG21	1.98	0.43
1:A:156:ARG:O	1:A:159:VAL:HB	2.19	0.43
1:A:239:THR:O	1:A:241:SER:N	2.46	0.43
2:B:295:MET:HE1	2:B:319:PHE:CZ	2.54	0.43
2:B:388:PHE:C	2:B:390:ARG:N	2.72	0.43
1:C:171:ILE:HG22	1:C:206:ASN:ND2	2.31	0.43
1:C:284:GLU:HG2	1:C:286:LEU:HD12	1.99	0.43
2:D:307:PRO:O	2:D:308:ARG:CB	2.38	0.43
2:D:357:ASP:N	2:D:357:ASP:OD2	2.47	0.43
1:A:132:LEU:HG	1:A:133:GLN:N	2.27	0.43
1:A:201:ALA:O	1:A:268:PRO:HD2	2.19	0.43
2:B:132:LEU:CG	2:B:133:GLN:N	2.81	0.43
2:B:262:PHE:CD1	2:B:435:TYR:HE2	2.34	0.43
1:C:154:MET:O	1:C:155:GLU:C	2.56	0.43
1:C:184:PRO:O	1:C:188:ILE:HG12	2.17	0.43
1:C:41:THR:HG23	1:C:61:HIS:HE1	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:ILE:HD13	2:D:153:LEU:HD13	2.01	0.43
1:A:115:ILE:O	1:A:119:LEU:HB2	2.18	0.43
1:A:147:SER:O	1:A:190:THR:OG1	2.31	0.43
2:B:239:THR:O	2:B:240:THR:C	2.58	0.43
2:B:7:ILE:HG12	2:B:66:ILE:CG2	2.49	0.43
1:C:123:ARG:C	1:C:125:LEU:H	2.22	0.43
1:C:158:SER:OG	1:C:197:HIS:HB3	2.19	0.43
2:D:332:MET:O	2:D:335:VAL:N	2.49	0.43
2:D:337:ASN:HA	2:D:340:SER:HB3	2.01	0.43
1:A:176:GLN:HG2	1:A:177:VAL:H	1.83	0.43
2:B:122:VAL:HG22	2:B:123:ARG:N	2.34	0.43
1:C:255:PHE:CE2	1:C:316:CYS:SG	3.07	0.43
1:C:312:TYR:CD2	1:C:381:THR:HB	2.54	0.43
6:D:801:HOS:H24B	6:D:801:HOS:O6	2.18	0.43
3:E:96:MET:HE3	3:E:97:ALA:HB2	2.01	0.43
1:A:287:SER:O	1:A:290:GLU:N	2.52	0.42
1:A:358:GLN:O	1:A:359:PRO:C	2.57	0.42
1:A:82:THR:O	1:A:83:TYR:CB	2.67	0.42
1:A:88:HIS:C	1:A:90:GLU:N	2.72	0.42
2:B:180:THR:O	2:B:182:VAL:N	2.52	0.42
1:C:183:GLU:O	1:C:184:PRO:C	2.55	0.42
1:C:68:VAL:HG22	1:C:93:ILE:HB	2.01	0.42
2:D:2:ARG:CB	2:D:133:GLN:OE1	2.67	0.42
3:E:99:GLU:C	3:E:101:LEU:N	2.69	0.42
1:A:182:VAL:O	1:A:185:TYR:HB2	2.19	0.42
1:A:290:GLU:O	1:A:294:ALA:N	2.43	0.42
2:B:4:ILE:HD11	2:B:52:TYR:CZ	2.55	0.42
1:C:402:ARG:HD3	1:C:402:ARG:HA	1.84	0.42
2:D:288:VAL:O	2:D:292:THR:HG23	2.19	0.42
1:A:72:PRO:HB2	1:A:73:THR:H	1.71	0.42
2:B:231:VAL:HG12	2:B:235:MET:CE	2.49	0.42
1:C:314:ALA:O	1:C:379:SER:HA	2.19	0.42
1:C:386:GLU:O	1:C:390:ARG:HG3	2.19	0.42
1:C:7:ILE:HA	1:C:66:VAL:HG23	2.02	0.42
2:D:141:LEU:O	2:D:187:ALA:HA	2.18	0.42
2:D:255:LEU:HD22	2:D:259:MET:HG2	2.01	0.42
2:D:29:GLY:O	2:D:36:TYR:HA	2.19	0.42
1:A:157:LEU:O	1:A:159:VAL:N	2.53	0.42
1:A:223:THR:O	1:A:226:ASN:CB	2.68	0.42
2:B:198:THR:OG1	2:B:265:LEU:CD2	2.68	0.42
2:B:221:THR:HA	2:B:222:PRO:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:ILE:HG22	2:B:31:ASP:O	2.19	0.42
1:C:102:ASN:O	1:C:105:ARG:N	2.50	0.42
2:D:145:THR:HG23	8:D:603:GDP:PB	2.59	0.42
2:D:174:SER:OG	2:D:175:PRO:N	2.52	0.42
1:A:325:PRO:HA	1:A:328:VAL:HG23	2.01	0.42
2:B:141:LEU:HD13	2:B:170:SER:HB3	2.00	0.42
1:C:104:ALA:HB2	1:C:408:TYR:HD2	1.84	0.42
1:C:327:ASP:O	1:C:328:VAL:C	2.57	0.42
2:D:262:PHE:O	2:D:266:HIS:CD2	2.72	0.42
2:D:350:ASN:HD22	2:D:350:ASN:N	2.17	0.42
2:B:154:ILE:HG12	2:B:155:SER:N	2.35	0.42
2:D:54:ASN:ND2	2:D:64:ARG:HD3	2.22	0.42
1:A:271:THR:O	1:A:272:TYR:C	2.58	0.42
1:A:312:TYR:CD2	1:A:381:THR:HB	2.54	0.42
1:C:154:MET:HE3	1:C:154:MET:HA	2.01	0.42
1:C:328:VAL:HG12	1:C:332:ILE:CD1	2.49	0.42
1:C:404:PHE:HD1	1:C:404:PHE:N	2.16	0.42
2:D:103:TRP:CD2	2:D:189:LEU:HD13	2.55	0.42
2:D:163:ASP:OD1	2:D:164:ARG:HG2	2.20	0.42
2:D:2:ARG:O	2:D:3:GLU:HG3	2.20	0.42
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.38	0.42
2:D:72:PRO:O	2:D:73:GLY:C	2.58	0.42
1:A:362:VAL:HB	1:A:368:LEU:HD12	2.01	0.42
1:A:422:ARG:NH1	1:A:425:MET:HB2	2.35	0.42
2:B:294:GLN:HG3	2:B:300:ASN:ND2	2.35	0.42
1:C:179:THR:O	1:C:180:ALA:HB2	2.20	0.42
2:D:277:SER:HB3	2:D:280:SER:H	1.85	0.42
2:D:312:TYR:CD1	2:D:343:PHE:CE2	3.08	0.42
1:A:277:SER:HA	1:A:367:ASP:O	2.20	0.42
1:A:53:PHE:CD1	1:A:53:PHE:N	2.87	0.42
2:B:126:SER:C	2:B:128:SER:N	2.72	0.42
2:B:141:LEU:HD12	2:B:141:LEU:HA	1.86	0.42
2:B:153:LEU:O	2:B:157:ILE:HG12	2.19	0.42
2:B:221:THR:HG21	1:C:326:LYS:HA	2.01	0.42
2:B:250:ALA:HB1	5:B:700:CN2:H7	2.01	0.42
1:C:181:VAL:HG11	1:C:404:PHE:CZ	2.55	0.42
1:C:220:GLU:OE2	2:D:326:LYS:CB	2.68	0.42
2:D:248:LEU:H	2:D:248:LEU:HG	1.64	0.42
3:E:112:ARG:O	3:E:114:ALA:N	2.53	0.42
1:A:175:PRO:HD3	1:A:394:LYS:HZ1	1.83	0.42
1:C:174:ALA:HA	1:C:175:PRO:HD2	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:PRO:O	1:C:74:VAL:N	2.53	0.42
2:D:10:GLY:O	2:D:14:ASN:N	2.52	0.42
2:D:20:PHE:O	2:D:21:TRP:C	2.57	0.42
1:A:432:TYR:C	1:A:434:GLU:N	2.73	0.41
1:A:88:HIS:C	1:A:90:GLU:H	2.22	0.41
2:B:103:TRP:CD2	2:B:189:LEU:HD13	2.55	0.41
2:B:136:GLN:HG3	2:B:136:GLN:O	2.20	0.41
1:C:249:ASN:CG	1:C:250:VAL:N	2.73	0.41
1:C:276:ILE:HD11	1:C:280:LYS:HD3	2.02	0.41
1:A:181:VAL:O	1:A:184:PRO:HD2	2.20	0.41
1:A:312:TYR:HD2	1:A:381:THR:HB	1.83	0.41
1:A:428:LEU:HA	1:A:431:ASP:HB2	2.02	0.41
1:C:163:LYS:O	1:C:164:LYS:C	2.58	0.41
2:D:132:LEU:HD23	2:D:164:ARG:CG	2.46	0.41
1:A:210:TYR:CZ	1:A:214:ARG:HD2	2.55	0.41
2:B:6:HIS:HD2	2:B:136:GLN:OE1	2.03	0.41
2:B:150:GLY:C	2:B:152:LEU:N	2.73	0.41
2:B:169:PHE:CD2	2:B:235:MET:HG2	2.56	0.41
6:B:800:HOS:C3	6:B:800:HOS:C12	2.97	0.41
1:C:256:GLN:O	1:C:259:LEU:N	2.53	0.41
1:C:287:SER:HB2	1:C:290:GLU:H	1.84	0.41
2:D:295:MET:HE1	2:D:319:PHE:CZ	2.55	0.41
1:C:179:THR:H	2:D:352:LYS:HZ1	1.68	0.41
2:D:223:THR:CA	6:D:801:HOS:H29	2.35	0.41
3:E:58:GLU:HA	3:E:61:ARG:HB3	2.01	0.41
1:A:273:ALA:HB2	1:A:375:VAL:CA	2.51	0.41
1:A:328:VAL:HG12	1:A:332:ILE:CD1	2.50	0.41
1:A:388:TRP:HA	1:A:388:TRP:HE3	1.82	0.41
2:B:270:PRO:HG2	2:B:302:MET:HB2	2.02	0.41
2:B:36:TYR:CE1	2:B:43:GLN:OE1	2.73	0.41
1:C:172:TYR:HA	1:C:173:PRO:HD3	1.72	0.41
1:C:401:LYS:O	2:D:262:PHE:HZ	2.03	0.41
2:D:75:MET:HG3	2:D:94:PHE:HB3	2.01	0.41
3:E:63:TYR:C	3:E:65:GLU:H	2.24	0.41
1:A:343:PHE:CD1	1:A:349:THR:HA	2.55	0.41
2:B:337:ASN:O	2:B:339:ASN:N	2.53	0.41
2:B:419:THR:C	2:B:421:ALA:H	2.23	0.41
1:C:405:VAL:CG1	1:C:406:HIS:H	2.33	0.41
1:C:420:GLU:HA	1:C:423:GLU:HB2	2.02	0.41
1:C:72:PRO:O	1:C:74:VAL:HG23	2.20	0.41
2:D:66:ILE:HD11	2:D:121:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:GLY:O	2:D:152:LEU:N	2.52	0.41
2:D:54:ASN:O	2:D:62:VAL:HG13	2.20	0.41
1:A:260:VAL:HA	1:A:261:PRO:HD3	1.79	0.41
2:B:15:GLN:O	2:B:16:ILE:C	2.59	0.41
2:D:231:VAL:HG12	2:D:235:MET:HE2	2.02	0.41
2:D:8:GLN:HB3	2:D:67:LEU:CD2	2.50	0.41
1:A:139:HIS:CG	1:A:150:THR:HG21	2.56	0.41
1:A:190:THR:HG22	1:A:191:THR:N	2.36	0.41
1:A:219:ILE:HG22	1:A:221:ARG:N	2.34	0.41
2:B:16:ILE:HA	2:B:16:ILE:HD12	1.70	0.41
2:B:431:GLU:CA	2:B:434:GLN:HB2	2.40	0.41
2:B:42:LEU:O	2:B:44:LEU:N	2.53	0.41
1:C:212:ILE:HD11	1:C:300:ASN:HA	2.03	0.41
1:C:245:ASP:HB3	1:C:246:GLY:H	1.67	0.41
2:D:223:THR:HG21	2:D:226:ASP:HB3	2.02	0.41
2:D:227:LEU:O	2:D:228:ASN:C	2.59	0.41
2:D:331:GLN:NE2	2:D:331:GLN:CA	2.62	0.41
2:D:425:MET:C	2:D:427:ASP:H	2.23	0.41
1:A:401:LYS:C	1:A:403:ALA:N	2.74	0.41
1:A:68:VAL:HG22	1:A:93:ILE:HB	2.02	0.41
2:B:119:LEU:O	2:B:122:VAL:HG22	2.20	0.41
2:B:195:VAL:HA	2:B:265:LEU:HD23	2.03	0.41
1:C:224:TYR:O	1:C:228:ASN:ND2	2.54	0.41
1:C:273:ALA:HB3	1:C:375:VAL:H	1.80	0.41
1:C:9:VAL:HA	1:C:68:VAL:O	2.20	0.41
1:A:405:VAL:HG13	1:A:406:HIS:H	1.83	0.41
2:B:307:PRO:O	2:B:308:ARG:CB	2.69	0.41
1:C:123:ARG:C	1:C:125:LEU:N	2.74	0.41
1:C:183:GLU:CB	1:C:184:PRO:CD	2.98	0.41
2:D:122:VAL:CG2	2:D:123:ARG:N	2.83	0.41
2:D:157:ILE:O	2:D:161:TYR:N	2.49	0.41
2:D:264:ARG:C	2:D:266:HIS:H	2.23	0.41
2:D:278:ARG:N	2:D:278:ARG:NE	2.65	0.41
2:D:207:GLU:CB	2:D:390:ARG:HH22	2.30	0.41
2:D:391:ILE:HG13	2:D:392:SER:N	2.36	0.41
2:B:2:ARG:C	2:B:3:GLU:HG3	2.40	0.41
1:C:323:VAL:O	1:C:355:ILE:HG21	2.20	0.41
1:C:86:LEU:HB3	1:C:87:PHE:CD2	2.56	0.41
2:D:406:HIS:HA	2:D:409:THR:CB	2.51	0.41
1:A:182:VAL:HG23	1:A:182:VAL:O	2.21	0.41
1:A:360:PRO:HD2	1:A:371:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:LEU:HB2	2:B:380:ASN:O	2.20	0.41
1:C:415:GLU:O	1:C:418:PHE:HB2	2.21	0.41
2:D:153:LEU:HD23	2:D:153:LEU:HA	1.91	0.41
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.55	0.41
2:D:205:ASP:OD1	2:D:208:ALA:N	2.46	0.41
2:D:287:THR:HG22	2:D:290:GLU:N	2.33	0.41
2:D:61:TYR:HD2	2:D:61:TYR:HA	1.63	0.41
3:E:78:HIS:O	3:E:82:VAL:N	2.45	0.41
1:A:187:SER:O	1:A:191:THR:HB	2.21	0.40
2:B:347:ILE:O	2:B:350:ASN:HB3	2.21	0.40
2:B:4:ILE:HD11	2:B:52:TYR:OH	2.20	0.40
1:C:221:ARG:HH21	2:D:325:MET:CE	2.35	0.40
2:D:3:GLU:OE2	2:D:130:ASP:HB3	2.21	0.40
2:D:99:ALA:HB1	2:D:145:THR:CG2	2.51	0.40
2:D:177:VAL:HA	6:D:801:HOS:C13	2.51	0.40
2:D:224:TYR:HE2	8:D:603:GDP:C5	2.39	0.40
1:A:297:GLU:HG3	1:A:299:ALA:N	2.36	0.40
2:B:144:GLY:O	2:B:147:SER:N	2.53	0.40
2:B:181:VAL:HG21	2:B:404:PHE:HE1	1.85	0.40
2:B:227:LEU:O	2:B:230:LEU:N	2.51	0.40
2:B:75:MET:C	2:B:77:SER:H	2.24	0.40
1:C:82:THR:O	1:C:83:TYR:CB	2.68	0.40
1:C:83:TYR:O	1:C:85:GLN:N	2.54	0.40
6:D:801:HOS:C16	6:D:801:HOS:C35	2.99	0.40
1:A:102:ASN:HA	1:A:186:ASN:HD21	1.86	0.40
1:A:404:PHE:N	1:A:404:PHE:HD1	2.19	0.40
2:B:168:THR:CG2	2:B:198:THR:HG21	2.51	0.40
2:B:242:LEU:HA	2:B:250:ALA:HB3	2.04	0.40
1:C:99:ALA:HB3	1:C:145:THR:CG2	2.49	0.40
1:C:191:THR:HG23	1:C:425:MET:CE	2.51	0.40
2:D:153:LEU:O	2:D:157:ILE:N	2.48	0.40
2:D:262:PHE:O	2:D:266:HIS:HD2	2.03	0.40
3:E:61:ARG:HG2	3:E:62:LYS:HE2	2.03	0.40
1:A:317:LEU:HB3	1:A:319:TYR:HE1	1.86	0.40
2:B:344:VAL:HG13	2:B:346:TRP:CD1	2.57	0.40
2:B:70:LEU:HA	2:B:95:GLY:HA3	2.04	0.40
1:C:12:ALA:O	1:C:13:GLY:C	2.60	0.40
1:C:190:THR:HG22	1:C:191:THR:N	2.37	0.40
1:C:325:PRO:C	1:C:327:ASP:N	2.75	0.40
2:D:259:MET:SD	5:D:701:CN2:H182	2.61	0.40
3:E:12:ASN:O	3:E:13:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:CD1	1:A:172:TYR:C	2.95	0.40
1:A:221:ARG:N	1:A:222:PRO:CD	2.85	0.40
1:A:169:PHE:CE2	1:A:235:VAL:HG22	2.56	0.40
1:A:291:ILE:HB	1:A:375:VAL:HG23	2.03	0.40
1:A:8:HIS:HE1	1:A:21:TRP:NE1	2.18	0.40
2:B:168:THR:HG1	2:B:170:SER:HG	1.55	0.40
1:A:406:HIS:CE1	2:B:261:PRO:O	2.68	0.40
2:B:184:PRO:HG2	2:B:398:MET:HE1	2.04	0.40
2:B:405:LEU:C	2:B:407:TRP:N	2.74	0.40
2:B:409:THR:HG22	2:B:410:GLY:N	2.36	0.40
1:C:355:ILE:H	1:C:355:ILE:HG13	1.55	0.40
2:D:30:ILE:O	2:D:83:PHE:CZ	2.74	0.40
2:D:409:THR:HG22	2:D:410:GLY:N	2.36	0.40
2:D:425:MET:C	2:D:427:ASP:N	2.74	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	424/449 (94%)	297 (70%)	72 (17%)	55 (13%)	0	4
1	C	436/449 (97%)	303 (70%)	72 (16%)	61 (14%)	0	4
2	B	424/445 (95%)	276 (65%)	90 (21%)	58 (14%)	0	4
2	D	424/445 (95%)	274 (65%)	90 (21%)	60 (14%)	0	4
3	E	117/142 (82%)	72 (62%)	28 (24%)	17 (14%)	0	3
All	All	1825/1930 (95%)	1222 (67%)	352 (19%)	251 (14%)	0	4

All (251) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	62	VAL
1	A	72	PRO
1	A	112	LYS
1	A	124	LYS
1	A	129	CYS
1	A	163	LYS
1	A	180	ALA
1	A	181	VAL
1	A	222	PRO
1	A	239	THR
1	A	247	ALA
1	A	273	ALA
1	A	284	GLU
1	A	314	ALA
1	A	316	CYS
1	A	345	ASP
1	A	348	PRO
1	A	350	GLY
1	A	403	ALA
1	A	405	VAL
1	A	433	GLU
1	A	437	ALA
2	B	34	GLY
2	B	35	SER
2	B	43	GLN
2	B	62	VAL
2	B	73	GLY
2	B	82	PRO
2	B	97	SER
2	B	115	VAL
2	B	145	THR
2	B	217	LEU
2	B	218	LYS
2	B	226	ASP
2	B	227	LEU
2	B	228	ASN
2	B	244	PHE
2	B	245	PRO
2	B	249	ASN
2	B	257	VAL
2	B	265	LEU
2	B	288	VAL

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Mol	Chain	Res	Type
2	B	305	CYS
2	B	308	ARG
2	B	348	PRO
2	B	404	PHE
1	C	32	PRO
1	C	33	ASP
1	C	45	GLY
1	C	62	VAL
1	C	72	PRO
1	C	112	LYS
1	C	124	LYS
1	C	129	CYS
1	C	163	LYS
1	C	178	SER
1	C	181	VAL
1	C	222	PRO
1	C	239	THR
1	C	257	THR
1	C	265	ILE
1	C	273	ALA
1	C	284	GLU
1	C	314	ALA
1	C	345	ASP
1	C	348	PRO
1	C	350	GLY
1	C	403	ALA
1	C	405	VAL
1	C	437	ALA
2	D	34	GLY
2	D	35	SER
2	D	43	GLN
2	D	62	VAL
2	D	73	GLY
2	D	82	PRO
2	D	97	SER
2	D	115	VAL
2	D	145	THR
2	D	181	VAL
2	D	217	LEU
2	D	218	LYS
2	D	226	ASP
2	D	227	LEU

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Mol	Chain	Res	Type
2	D	244	PHE
2	D	245	PRO
2	D	249	ASN
2	D	257	VAL
2	D	265	LEU
2	D	288	VAL
2	D	298	SER
2	D	305	CYS
2	D	308	ARG
2	D	348	PRO
2	D	400	ARG
2	D	403	ALA
2	D	404	PHE
3	E	5	ASP
3	E	8	VAL
3	E	76	ARG
3	E	77	GLU
3	E	97	ALA
3	E	140	LYS
1	A	57	GLY
1	A	73	THR
1	A	83	TYR
1	A	84	ARG
1	A	109	THR
1	A	144	GLY
1	A	158	SER
1	A	164	LYS
1	A	178	SER
1	A	264	ARG
1	A	279	GLU
1	A	373	ARG
1	A	377	MET
1	A	432	TYR
2	B	42	LEU
2	B	112	ALA
2	B	118	VAL
2	B	119	LEU
2	B	159	GLU
2	B	177	VAL
2	B	179	ASP
2	B	181	VAL
2	B	215	ARG

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Mol	Chain	Res	Type
2	B	339	ASN
2	B	400	ARG
2	B	403	ALA
1	C	41	THR
1	C	42	ILE
1	C	44	GLY
1	C	57	GLY
1	C	73	THR
1	C	84	ARG
1	C	109	THR
1	C	144	GLY
1	C	158	SER
1	C	164	LYS
1	C	180	ALA
1	C	248	LEU
1	C	264	ARG
1	C	279	GLU
1	C	326	LYS
1	C	377	MET
1	C	432	TYR
1	C	433	GLU
2	D	42	LEU
2	D	112	ALA
2	D	151	THR
2	D	159	GLU
2	D	219	LEU
2	D	228	ASN
2	D	266	HIS
2	D	276	THR
2	D	285	ALA
2	D	371	LEU
3	E	64	GLN
3	E	96	MET
3	E	107	SER
3	E	139	LEU
1	A	82	THR
1	A	179	THR
1	A	245	ASP
1	A	265	ILE
1	A	285	GLN
1	A	301	GLN
1	A	326	LYS

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Mol	Chain	Res	Type
2	B	13	GLY
2	B	72	PRO
2	B	151	THR
2	B	162	PRO
2	B	219	LEU
2	B	252	LEU
2	B	266	HIS
2	B	273	ALA
2	B	371	LEU
2	B	389	LYS
2	B	395	PHE
2	B	396	THR
2	B	429	VAL
1	C	82	THR
1	C	83	TYR
1	C	215	ARG
1	C	301	GLN
2	D	13	GLY
2	D	72	PRO
2	D	119	LEU
2	D	162	PRO
2	D	177	VAL
2	D	284	ARG
2	D	409	THR
2	D	429	VAL
3	E	12	ASN
3	E	123	LEU
3	E	135	LYS
3	E	137	LYS
1	A	32	PRO
1	A	253	THR
1	A	302	MET
2	B	11	GLN
2	B	127	GLU
2	B	298	SER
1	C	37	PRO
1	C	39	ASP
1	C	40	LYS
1	C	100	ALA
1	C	179	THR
1	C	285	GLN
1	C	395	PHE

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Mol	Chain	Res	Type
2	D	11	GLN
2	D	103	TRP
2	D	127	GLU
2	D	178	SER
2	D	220	THR
2	D	273	ALA
2	D	309	HIS
3	E	7	GLU
3	E	61	ARG
1	A	100	ALA
1	A	395	PHE
2	B	47	GLU
2	B	420	GLU
1	C	207	GLU
1	C	316	CYS
2	D	179	ASP
2	D	252	LEU
3	E	47	LEU
1	A	175	PRO
1	A	249	ASN
1	C	175	PRO
1	C	177	VAL
1	C	251	ASP
1	C	263	PRO
2	D	299	LYS
2	D	402	LYS
1	A	263	PRO
2	B	246	GLY
2	B	279	GLY
1	C	328	VAL
2	D	246	GLY
2	D	195	VAL
1	A	177	VAL
2	B	175	PRO
2	B	225	GLY
1	C	221	ARG
1	A	221	ARG
1	A	274	PRO
2	D	16	ILE
2	D	225	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/378 (89%)	224 (66%)	114 (34%)	0	2
1	C	340/378 (90%)	232 (68%)	108 (32%)	0	2
2	B	349/383 (91%)	231 (66%)	118 (34%)	0	1
2	D	347/383 (91%)	226 (65%)	121 (35%)	0	1
3	E	60/126 (48%)	38 (63%)	22 (37%)	0	1
All	All	1434/1648 (87%)	951 (66%)	483 (34%)	0	2

All (483) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	4	CYS
1	A	5	ILE
1	A	9	VAL
1	A	11	GLN
1	A	15	GLN
1	A	16	ILE
1	A	20	CYS
1	A	23	LEU
1	A	27	GLU
1	A	53	PHE
1	A	61	HIS
1	A	66	VAL
1	A	74	VAL
1	A	75	ILE
1	A	80	THR
1	A	82	THR
1	A	84	ARG
1	A	86	LEU
1	A	88	HIS
1	A	91	GLN
1	A	96	LYS
1	A	105	ARG

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Mol	Chain	Res	Type
1	A	109	THR
1	A	110	ILE
1	A	115	ILE
1	A	117	LEU
1	A	119	LEU
1	A	121	ARG
1	A	123	ARG
1	A	128	GLN
1	A	132	LEU
1	A	133	GLN
1	A	140	SER
1	A	141	PHE
1	A	145	THR
1	A	153	LEU
1	A	156	ARG
1	A	163	LYS
1	A	164	LYS
1	A	166	LYS
1	A	176	GLN
1	A	177	VAL
1	A	178	SER
1	A	182	VAL
1	A	183	GLU
1	A	187	SER
1	A	190	THR
1	A	191	THR
1	A	193	THR
1	A	194	THR
1	A	195	LEU
1	A	196	GLU
1	A	198	SER
1	A	200	CYS
1	A	205	ASP
1	A	210	TYR
1	A	212	ILE
1	A	215	ARG
1	A	216	ASN
1	A	220	GLU
1	A	223	THR
1	A	224	TYR
1	A	225	THR
1	A	226	ASN

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Mol	Chain	Res	Type
1	A	227	LEU
1	A	228	ASN
1	A	229	ARG
1	A	230	LEU
1	A	242	LEU
1	A	245	ASP
1	A	251	ASP
1	A	252	LEU
1	A	256	GLN
1	A	260	VAL
1	A	264	ARG
1	A	265	ILE
1	A	275	VAL
1	A	284	GLU
1	A	286	LEU
1	A	287	SER
1	A	290	GLU
1	A	295	CYS
1	A	300	ASN
1	A	302	MET
1	A	312	TYR
1	A	313	MET
1	A	316	CYS
1	A	318	LEU
1	A	328	VAL
1	A	329	ASN
1	A	334	THR
1	A	343	PHE
1	A	353	VAL
1	A	355	ILE
1	A	356	ASN
1	A	358	GLN
1	A	363	VAL
1	A	367	ASP
1	A	368	LEU
1	A	371	VAL
1	A	379	SER
1	A	381	THR
1	A	382	THR
1	A	397	LEU
1	A	401	LYS
1	A	402	ARG

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Mol	Chain	Res	Type
1	A	414	GLU
1	A	419	SER
1	A	420	GLU
1	A	428	LEU
1	A	432	TYR
1	A	434	GLU
1	A	438	ASP
2	B	3	GLU
2	B	15	GLN
2	B	24	ILE
2	B	27	GLU
2	B	33	THR
2	B	42	LEU
2	B	43	GLN
2	B	54	ASN
2	B	55	GLU
2	B	60	LYS
2	B	61	TYR
2	B	66	ILE
2	B	68	VAL
2	B	74	THR
2	B	76	ASP
2	B	78	VAL
2	B	80	SER
2	B	83	PHE
2	B	85	GLN
2	B	90	ASP
2	B	101	ASN
2	B	109	THR
2	B	116	ASP
2	B	119	LEU
2	B	120	ASP
2	B	122	VAL
2	B	131	CYS
2	B	137	LEU
2	B	138	THR
2	B	145	THR
2	B	149	MET
2	B	151	THR
2	B	154	ILE
2	B	155	SER
2	B	156	LYS

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Mol	Chain	Res	Type
2	B	158	ARG
2	B	160	GLU
2	B	162	PRO
2	B	168	THR
2	B	171	VAL
2	B	174	SER
2	B	179	ASP
2	B	183	GLU
2	B	189	LEU
2	B	195	VAL
2	B	197	ASN
2	B	199	ASP
2	B	204	ILE
2	B	205	ASP
2	B	207	GLU
2	B	209	LEU
2	B	214	PHE
2	B	221	THR
2	B	224	TYR
2	B	227	LEU
2	B	241	CYS
2	B	242	LEU
2	B	248	LEU
2	B	249	ASN
2	B	255	LEU
2	B	258	ASN
2	B	260	VAL
2	B	264	ARG
2	B	265	LEU
2	B	267	PHE
2	B	275	LEU
2	B	278	ARG
2	B	280	SER
2	B	282	GLN
2	B	284	ARG
2	B	286	LEU
2	B	294	GLN
2	B	295	MET
2	B	299	LYS
2	B	300	ASN
2	B	305	CYS
2	B	311	ARG

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Mol	Chain	Res	Type
2	B	313	LEU
2	B	318	VAL
2	B	320	ARG
2	B	323	MET
2	B	325	MET
2	B	329	ASP
2	B	331	GLN
2	B	333	LEU
2	B	336	GLN
2	B	339	ASN
2	B	344	VAL
2	B	346	TRP
2	B	350	ASN
2	B	351	VAL
2	B	355	VAL
2	B	357	ASP
2	B	358	ILE
2	B	371	LEU
2	B	373	MET
2	B	374	SER
2	B	376	THR
2	B	380	ASN
2	B	384	ILE
2	B	385	GLN
2	B	387	LEU
2	B	390	ARG
2	B	391	ILE
2	B	400	ARG
2	B	401	ARG
2	B	405	LEU
2	B	406	HIS
2	B	409	THR
2	B	413	MET
2	B	415	GLU
2	B	416	MET
2	B	420	GLU
2	B	425	MET
2	B	430	SER
2	B	431	GLU
2	B	432	TYR
2	B	434	GLN
1	C	2	ARG

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Mol	Chain	Res	Type
1	C	4	CYS
1	C	5	ILE
1	C	9	VAL
1	C	11	GLN
1	C	16	ILE
1	C	20	CYS
1	C	23	LEU
1	C	31	GLN
1	C	53	PHE
1	C	61	HIS
1	C	66	VAL
1	C	74	VAL
1	C	75	ILE
1	C	76	ASP
1	C	80	THR
1	C	82	THR
1	C	84	ARG
1	C	86	LEU
1	C	88	HIS
1	C	91	GLN
1	C	96	LYS
1	C	105	ARG
1	C	109	THR
1	C	110	ILE
1	C	115	ILE
1	C	117	LEU
1	C	119	LEU
1	C	123	ARG
1	C	128	GLN
1	C	132	LEU
1	C	133	GLN
1	C	140	SER
1	C	141	PHE
1	C	153	LEU
1	C	163	LYS
1	C	164	LYS
1	C	166	LYS
1	C	176	GLN
1	C	177	VAL
1	C	182	VAL
1	C	183	GLU
1	C	187	SER

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Mol	Chain	Res	Type
1	C	190	THR
1	C	191	THR
1	C	192	HIS
1	C	193	THR
1	C	194	THR
1	C	195	LEU
1	C	196	GLU
1	C	200	CYS
1	C	205	ASP
1	C	210	TYR
1	C	215	ARG
1	C	216	ASN
1	C	220	GLU
1	C	223	THR
1	C	224	TYR
1	C	225	THR
1	C	226	ASN
1	C	228	ASN
1	C	229	ARG
1	C	230	LEU
1	C	242	LEU
1	C	244	PHE
1	C	252	LEU
1	C	253	THR
1	C	257	THR
1	C	260	VAL
1	C	264	ARG
1	C	265	ILE
1	C	275	VAL
1	C	284	GLU
1	C	286	LEU
1	C	287	SER
1	C	290	GLU
1	C	295	CYS
1	C	300	ASN
1	C	302	MET
1	C	312	TYR
1	C	313	MET
1	C	316	CYS
1	C	318	LEU
1	C	328	VAL
1	C	329	ASN

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Mol	Chain	Res	Type
1	C	343	PHE
1	C	353	VAL
1	C	355	ILE
1	C	356	ASN
1	C	358	GLN
1	C	363	VAL
1	C	367	ASP
1	C	368	LEU
1	C	371	VAL
1	C	379	SER
1	C	381	THR
1	C	382	THR
1	C	397	LEU
1	C	401	LYS
1	C	402	ARG
1	C	414	GLU
1	C	419	SER
1	C	420	GLU
1	C	428	LEU
1	C	430	LYS
1	C	432	TYR
1	C	434	GLU
1	C	438	ASP
2	D	3	GLU
2	D	4	ILE
2	D	15	GLN
2	D	24	ILE
2	D	27	GLU
2	D	33	THR
2	D	36	TYR
2	D	42	LEU
2	D	43	GLN
2	D	54	ASN
2	D	55	GLU
2	D	60	LYS
2	D	61	TYR
2	D	66	ILE
2	D	68	VAL
2	D	76	ASP
2	D	78	VAL
2	D	80	SER
2	D	83	PHE

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Mol	Chain	Res	Type
2	D	85	GLN
2	D	90	ASP
2	D	101	ASN
2	D	109	THR
2	D	116	ASP
2	D	119	LEU
2	D	120	ASP
2	D	122	VAL
2	D	131	CYS
2	D	136	GLN
2	D	137	LEU
2	D	138	THR
2	D	145	THR
2	D	149	MET
2	D	151	THR
2	D	154	ILE
2	D	155	SER
2	D	156	LYS
2	D	158	ARG
2	D	160	GLU
2	D	170	SER
2	D	171	VAL
2	D	174	SER
2	D	179	ASP
2	D	183	GLU
2	D	188	THR
2	D	189	LEU
2	D	195	VAL
2	D	197	ASN
2	D	199	ASP
2	D	205	ASP
2	D	207	GLU
2	D	209	LEU
2	D	214	PHE
2	D	216	THR
2	D	221	THR
2	D	224	TYR
2	D	227	LEU
2	D	241	CYS
2	D	242	LEU
2	D	248	LEU
2	D	249	ASN

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Mol	Chain	Res	Type
2	D	255	LEU
2	D	258	ASN
2	D	260	VAL
2	D	264	ARG
2	D	265	LEU
2	D	267	PHE
2	D	275	LEU
2	D	278	ARG
2	D	280	SER
2	D	283	TYR
2	D	286	LEU
2	D	294	GLN
2	D	295	MET
2	D	300	ASN
2	D	305	CYS
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	327	GLU
2	D	329	ASP
2	D	331	GLN
2	D	333	LEU
2	D	336	GLN
2	D	338	LYS
2	D	339	ASN
2	D	344	VAL
2	D	346	TRP
2	D	350	ASN
2	D	355	VAL
2	D	357	ASP
2	D	358	ILE
2	D	360	PRO
2	D	371	LEU
2	D	373	MET
2	D	374	SER
2	D	376	THR
2	D	380	ASN
2	D	384	ILE

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Mol	Chain	Res	Type
2	D	385	GLN
2	D	386	GLU
2	D	387	LEU
2	D	390	ARG
2	D	391	ILE
2	D	400	ARG
2	D	401	ARG
2	D	405	LEU
2	D	406	HIS
2	D	413	MET
2	D	416	MET
2	D	420	GLU
2	D	425	MET
2	D	427	ASP
2	D	430	SER
2	D	431	GLU
2	D	432	TYR
2	D	434	GLN
3	E	28	SER
3	E	51	GLN
3	E	55	GLU
3	E	58	GLU
3	E	62	LYS
3	E	65	GLU
3	E	69	LEU
3	E	70	LYS
3	E	74	GLU
3	E	77	GLU
3	E	78	HIS
3	E	90	ASN
3	E	94	ILE
3	E	99	GLU
3	E	107	SER
3	E	109	LYS
3	E	112	ARG
3	E	113	GLU
3	E	120	LEU
3	E	122	ARG
3	E	134	ARG
3	E	136	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	8	HIS
1	A	85	GLN
1	A	88	HIS
1	A	91	GLN
1	A	128	GLN
1	A	133	GLN
1	A	139	HIS
1	A	176	GLN
1	A	206	ASN
1	A	228	ASN
1	A	258	ASN
1	A	266	HIS
1	A	283	HIS
1	A	301	GLN
1	A	406	HIS
2	B	6	HIS
2	B	43	GLN
2	B	54	ASN
2	B	136	GLN
2	B	167	ASN
2	B	192	HIS
2	B	193	GLN
2	B	206	ASN
2	B	247	GLN
2	B	294	GLN
2	B	300	ASN
2	B	309	HIS
2	B	339	ASN
2	B	350	ASN
2	B	380	ASN
2	B	406	HIS
1	C	8	HIS
1	C	50	ASN
1	C	85	GLN
1	C	88	HIS
1	C	91	GLN
1	C	101	ASN
1	C	128	GLN
1	C	139	HIS
1	C	206	ASN
1	C	228	ASN
1	C	233	GLN
1	C	249	ASN

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Mol	Chain	Res	Type
1	C	256	GLN
1	C	258	ASN
1	C	266	HIS
1	C	406	HIS
2	D	6	HIS
2	D	8	GLN
2	D	54	ASN
2	D	136	GLN
2	D	192	HIS
2	D	247	GLN
2	D	294	GLN
2	D	300	ASN
2	D	309	HIS
2	D	350	ASN
2	D	380	ASN
2	D	394	GLN
2	D	406	HIS
3	E	90	ASN
3	E	108	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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$
7	GTP	D	601	-	26,34,34	1.14	2 (7%)	33,54,54	2.63	12 (36%)
5	CN2	B	700	-	28,32,32	3.30	7 (25%)	27,45,45	2.46	8 (29%)
5	CN2	D	701	-	28,32,32	3.15	6 (21%)	27,45,45	2.72	11 (40%)
7	GTP	D	600	-	26,34,34	0.99	2 (7%)	33,54,54	1.91	7 (21%)
8	GDP	D	602	-	24,30,30	1.01	2 (8%)	31,47,47	2.34	10 (32%)
6	HOS	B	800	-	45,57,57	1.55	6 (13%)	43,83,83	1.75	14 (32%)
8	GDP	D	603	-	24,30,30	1.14	2 (8%)	31,47,47	2.13	7 (22%)
6	HOS	D	801	-	45,57,57	1.57	9 (20%)	43,83,83	1.58	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GTP	D	601	-	-	5/18/38/38	0/3/3/3
5	CN2	B	700	-	-	3/10/27/27	0/3/3/3
5	CN2	D	701	-	-	3/10/27/27	0/3/3/3
7	GTP	D	600	-	-	5/18/38/38	0/3/3/3
8	GDP	D	602	-	-	4/12/32/32	0/3/3/3
6	HOS	B	800	-	-	16/76/92/92	0/2/3/3
8	GDP	D	603	-	-	6/12/32/32	0/3/3/3
6	HOS	D	801	-	-	23/76/92/92	0/2/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	700	CN2	C19-C17	-9.12	1.23	1.39
5	B	700	CN2	C19-C20	-7.98	1.17	1.40
5	D	701	CN2	C19-C17	-7.63	1.25	1.39
5	B	700	CN2	C20-C21	-7.57	1.21	1.40
5	D	701	CN2	C15-C16	7.39	1.54	1.39
5	D	701	CN2	C19-C20	-6.82	1.20	1.40
5	D	701	CN2	C20-C21	-6.73	1.23	1.40
5	B	700	CN2	C15-C16	6.58	1.52	1.39
5	D	701	CN2	O6-C17	5.94	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	700	CN2	O6-C17	5.17	1.45	1.37
6	B	800	HOS	C9-C8	4.96	1.59	1.51
5	D	701	CN2	C22-C8	4.65	1.48	1.40
6	D	801	HOS	C36-C19	4.35	1.58	1.52
6	B	800	HOS	C36-C19	4.34	1.58	1.52
6	D	801	HOS	C3-N1	4.32	1.52	1.45
6	B	800	HOS	C17-C18	4.12	1.54	1.47
5	B	700	CN2	C22-C8	4.01	1.47	1.40
8	D	603	GDP	C6-N1	3.46	1.39	1.33
6	D	801	HOS	C17-C18	3.27	1.53	1.47
7	D	601	GTP	C6-N1	3.14	1.38	1.33
6	D	801	HOS	C5-N2	2.97	1.49	1.45
6	D	801	HOS	C17-N4	-2.74	1.35	1.41
8	D	602	GDP	C6-N1	2.59	1.37	1.33
7	D	600	GTP	C6-N1	2.58	1.37	1.33
6	D	801	HOS	C29-C30	2.45	1.53	1.49
6	D	801	HOS	C19-N5	-2.40	1.35	1.40
7	D	601	GTP	O4'-C4'	-2.38	1.39	1.45
8	D	603	GDP	C6-C5	-2.27	1.37	1.41
7	D	600	GTP	O4'-C1'	2.20	1.44	1.41
6	B	800	HOS	C13-C1	2.16	1.42	1.38
6	D	801	HOS	C9-C8	2.11	1.55	1.51
5	B	700	CN2	O1-C1	-2.10	1.34	1.38
8	D	602	GDP	O4'-C1'	2.06	1.43	1.41
6	B	800	HOS	C1-C12	-2.05	1.37	1.40
6	B	800	HOS	C19-N5	-2.05	1.35	1.40
6	D	801	HOS	C3-C14	2.04	1.56	1.53

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	701	CN2	C20-C19-C17	7.50	147.84	129.69
8	D	602	GDP	N3-C2-N1	-7.12	117.72	127.22
5	B	700	CN2	C20-C19-C17	7.05	146.76	129.69
8	D	603	GDP	N3-C2-N1	-6.91	118.01	127.22
7	D	601	GTP	PB-O3B-PG	-6.86	109.30	132.83
7	D	601	GTP	C2-N3-C4	6.10	122.33	115.36
5	D	701	CN2	C11-N1-C12	6.08	133.01	123.33
7	D	601	GTP	N3-C2-N1	-5.97	119.26	127.22
8	D	602	GDP	C2-N3-C4	5.72	121.89	115.36
7	D	600	GTP	PB-O3B-PG	-5.28	114.69	132.83
5	B	700	CN2	C10-C11-N1	5.27	119.52	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	600	GTP	N3-C2-N1	-4.70	120.95	127.22
7	D	600	GTP	C2-N3-C4	4.68	120.70	115.36
6	D	801	HOS	C20-C19-N5	-4.45	114.09	121.30
5	B	700	CN2	C4-O2-C3	4.33	126.64	114.78
8	D	603	GDP	C1'-N9-C4	-4.23	119.20	126.64
7	D	601	GTP	C1'-N9-C4	-4.21	119.25	126.64
5	D	701	CN2	C6-O3-C5	4.17	123.82	117.53
6	D	801	HOS	C3-C14-N3	4.15	123.51	118.52
8	D	602	GDP	N2-C2-N3	-4.11	111.09	117.79
7	D	601	GTP	PA-O3A-PB	-3.91	119.40	132.83
7	D	601	GTP	C6-C5-C4	-3.91	117.06	120.80
6	B	800	HOS	C3-C14-N3	3.91	123.21	118.52
8	D	603	GDP	C2-N3-C4	3.89	119.80	115.36
5	D	701	CN2	O4-C12-N1	3.87	129.48	122.95
8	D	603	GDP	C6-C5-C4	-3.66	117.30	120.80
8	D	603	GDP	C6-N1-C2	3.63	121.70	115.93
5	D	701	CN2	O3-C5-C3	3.61	121.51	115.16
5	D	701	CN2	O3-C5-C7	-3.57	117.98	124.12
8	D	602	GDP	C6-N1-C2	3.56	121.58	115.93
5	B	700	CN2	C21-C22-C8	-3.55	116.65	120.50
6	B	800	HOS	C13-C9-C8	3.53	125.57	119.55
7	D	601	GTP	C4-C5-N7	-3.53	105.72	109.40
5	B	700	CN2	C9-C8-C22	-3.42	116.55	119.50
7	D	601	GTP	N2-C2-N1	3.15	122.15	117.25
8	D	602	GDP	PA-O3A-PB	-3.13	122.08	132.83
8	D	602	GDP	C5-C6-N1	-2.99	119.34	123.43
5	D	701	CN2	C21-C22-C1	2.96	125.12	121.07
8	D	603	GDP	C5-C6-N1	-2.93	119.42	123.43
5	D	701	CN2	C9-C10-C11	-2.87	108.47	112.29
6	B	800	HOS	O1-C2-C3	2.85	117.59	104.54
8	D	603	GDP	O2B-PB-O3A	2.84	114.17	104.64
6	D	801	HOS	O6-C14-N3	-2.76	116.45	121.38
6	B	800	HOS	O3-C6-N2	2.69	127.92	122.93
8	D	602	GDP	C6-C5-C4	-2.69	118.23	120.80
5	B	700	CN2	C9-C8-C7	2.64	125.25	119.42
6	B	800	HOS	C5-N2-C6	2.62	126.57	121.13
5	B	700	CN2	C21-C22-C1	2.61	124.63	121.07
7	D	601	GTP	O4'-C1'-C2'	2.59	110.72	106.93
5	B	700	CN2	C10-C9-C8	-2.57	108.07	113.68
7	D	600	GTP	N2-C2-N1	2.55	121.22	117.25
6	D	801	HOS	C10-C11-CL1	2.52	122.56	118.49
5	D	701	CN2	C21-C22-C8	-2.52	117.77	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	601	GTP	O2G-PG-O3B	2.50	113.03	104.64
6	B	800	HOS	C7-C6-N2	-2.47	111.16	116.48
6	D	801	HOS	O1-C2-C3	2.44	115.68	104.54
6	B	800	HOS	C8-C7-C6	-2.43	105.13	112.92
7	D	600	GTP	C6-C5-C4	-2.40	118.51	120.80
8	D	602	GDP	C1'-N9-C4	-2.39	122.43	126.64
6	D	801	HOS	O7-C16-N4	2.39	126.33	122.57
7	D	601	GTP	O5'-C5'-C4'	2.39	117.21	108.99
6	B	800	HOS	O7-C16-C15	-2.38	117.62	120.98
7	D	600	GTP	C5-C6-N1	-2.37	120.19	123.43
6	D	801	HOS	C13-C9-C8	2.37	123.59	119.55
7	D	601	GTP	C2'-C3'-C4'	2.33	107.18	102.64
6	B	800	HOS	C12-C11-CL1	-2.30	115.89	118.78
5	D	701	CN2	C4-O2-C3	2.30	121.08	114.78
8	D	602	GDP	O4'-C1'-C2'	2.30	110.28	106.93
6	B	800	HOS	C31-C15-C16	2.28	113.69	110.11
6	B	800	HOS	C20-C19-N5	-2.24	117.68	121.30
5	D	701	CN2	C10-C11-N1	2.22	114.02	110.04
6	D	801	HOS	C2-O1-C1	2.20	129.60	123.41
6	B	800	HOS	C10-C9-C13	-2.19	114.96	118.08
6	B	800	HOS	C10-C11-CL1	2.17	121.98	118.49
7	D	600	GTP	C1'-N9-C4	-2.08	122.98	126.64
6	B	800	HOS	C14-C3-N1	2.06	109.58	107.34
8	D	602	GDP	N2-C2-N1	-2.02	114.11	117.25

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	701	CN2	C10-C11-N1-C12
7	D	600	GTP	C5'-O5'-PA-O1A
8	D	602	GDP	C5'-O5'-PA-O1A
8	D	602	GDP	C5'-O5'-PA-O2A
6	B	800	HOS	C24-C2-C22-C23
6	B	800	HOS	O1-C2-C22-C23
6	B	800	HOS	C3-C2-C22-C23
6	B	800	HOS	C3-C2-O1-C1
6	B	800	HOS	C13-C1-O1-C2
6	B	800	HOS	C12-C1-O1-C2
6	B	800	HOS	C6-C7-N6-C28
6	B	800	HOS	C32-C17-N4-C16
6	B	800	HOS	C18-C17-N4-C16

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Mol	Chain	Res	Type	Atoms
8	D	603	GDP	C5'-O5'-PA-O2A
6	D	801	HOS	O1-C2-C22-C23
6	D	801	HOS	C3-C2-C22-C23
6	D	801	HOS	C22-C2-O1-C1
6	D	801	HOS	C3-C2-O1-C1
6	D	801	HOS	C13-C1-O1-C2
6	D	801	HOS	C12-C1-O1-C2
6	D	801	HOS	N6-C7-C8-C9
6	D	801	HOS	C6-C7-C8-C9
6	D	801	HOS	N6-C7-C8-O4
6	D	801	HOS	C6-C7-C8-O4
6	D	801	HOS	N1-C4-C5-C25
6	D	801	HOS	C32-C17-N4-C16
6	D	801	HOS	C18-C17-N4-C16
5	D	701	CN2	C3-C5-O3-C6
5	D	701	CN2	C7-C5-O3-C6
6	B	800	HOS	C31-C15-C16-O7
6	D	801	HOS	C31-C15-C16-O7
6	B	800	HOS	C31-C15-C16-N4
6	D	801	HOS	C31-C15-C16-N4
5	B	700	CN2	C7-C5-O3-C6
5	B	700	CN2	C3-C5-O3-C6
5	B	700	CN2	C10-C11-N1-C12
6	D	801	HOS	C24-C2-C22-C23
7	D	601	GTP	C5'-O5'-PA-O3A
7	D	600	GTP	C5'-O5'-PA-O3A
8	D	603	GDP	C5'-O5'-PA-O3A
6	D	801	HOS	O2-C4-C5-C25
6	B	800	HOS	C24-C2-O1-C1
6	D	801	HOS	O2-C4-C5-N2
7	D	601	GTP	C5'-O5'-PA-O2A
7	D	600	GTP	C5'-O5'-PA-O2A
8	D	603	GDP	C5'-O5'-PA-O1A
6	B	800	HOS	C8-C7-N6-C28
6	B	800	HOS	C22-C2-O1-C1
6	B	800	HOS	C20-C19-N5-C18
6	D	801	HOS	C20-C19-N5-C18
8	D	603	GDP	C3'-C4'-C5'-O5'
6	D	801	HOS	C24-C2-O1-C1
7	D	601	GTP	PB-O3A-PA-O2A
7	D	600	GTP	PG-O3B-PB-O2B
7	D	601	GTP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
8	D	603	GDP	O4'-C4'-C5'-O5'
8	D	602	GDP	C5'-O5'-PA-O3A
6	D	801	HOS	N1-C4-C5-N2
7	D	600	GTP	PG-O3B-PB-O1B
8	D	602	GDP	PB-O3A-PA-O2A
8	D	603	GDP	PB-O3A-PA-O1A
6	B	800	HOS	C36-C19-N5-C18
6	D	801	HOS	C36-C19-N5-C18
7	D	601	GTP	PB-O3B-PG-O1G
6	D	801	HOS	O1-C2-C3-C14

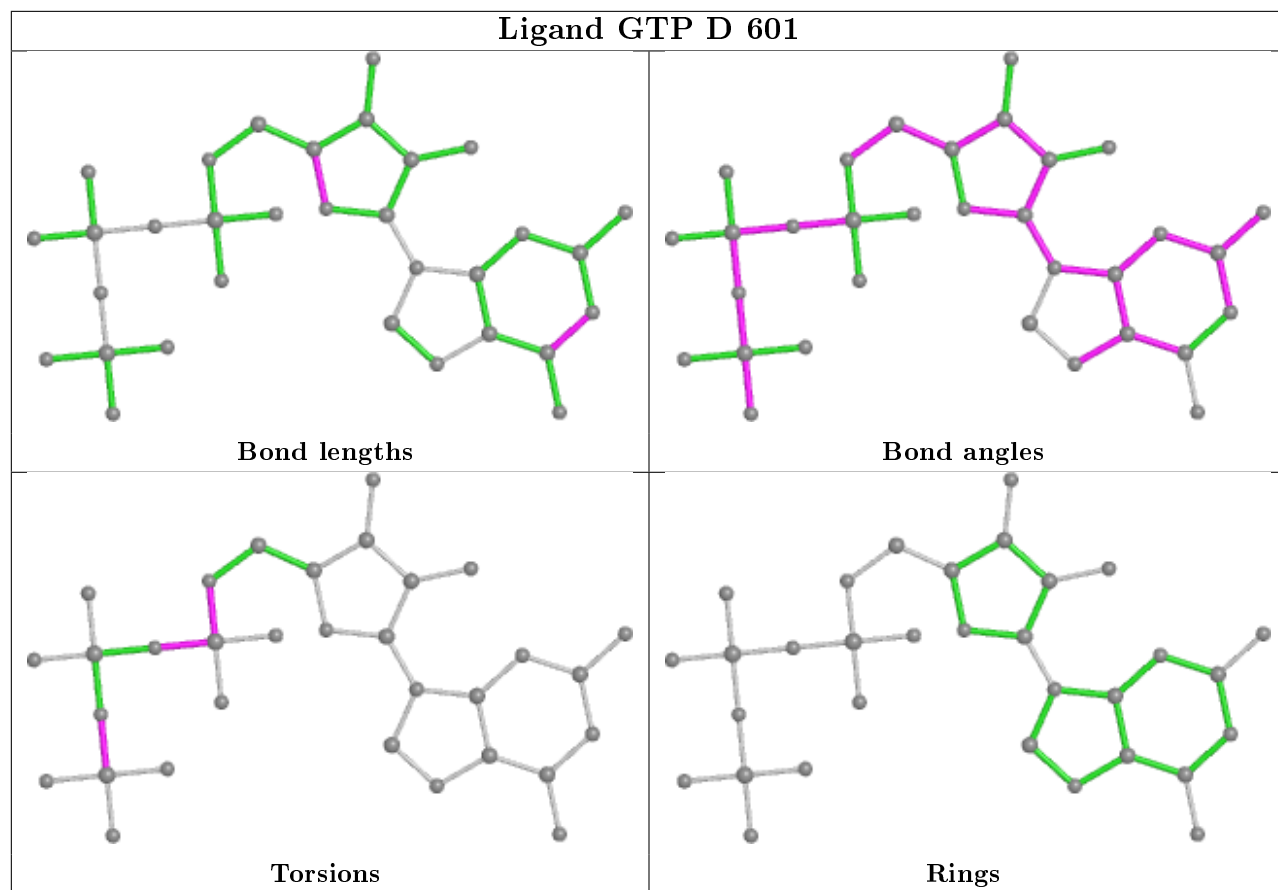
There are no ring outliers.

8 monomers are involved in 88 short contacts:

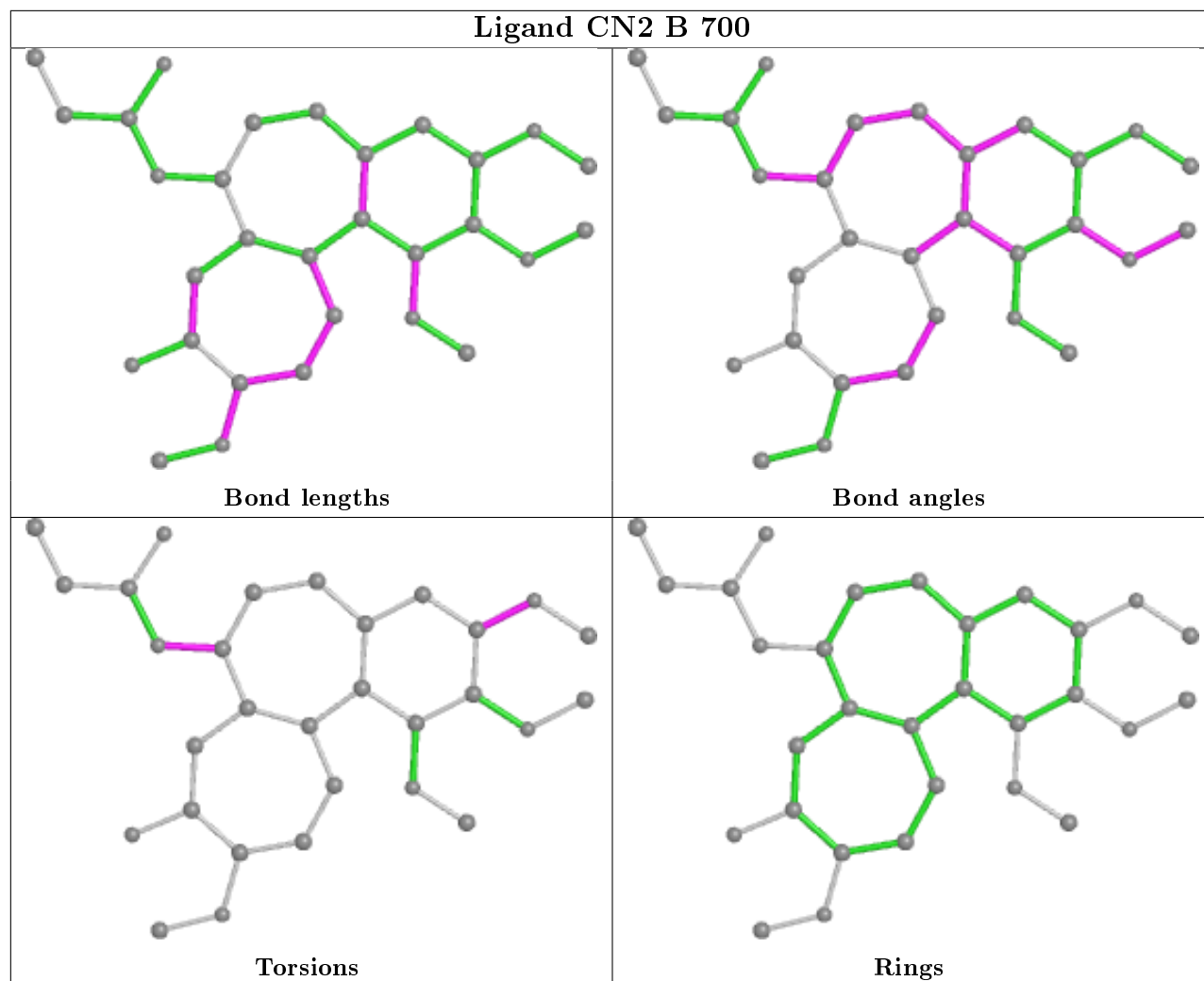
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	601	GTP	4	0
5	B	700	CN2	12	0
5	D	701	CN2	12	0
7	D	600	GTP	2	0
8	D	602	GDP	4	0
6	B	800	HOS	26	0
8	D	603	GDP	4	0
6	D	801	HOS	24	0

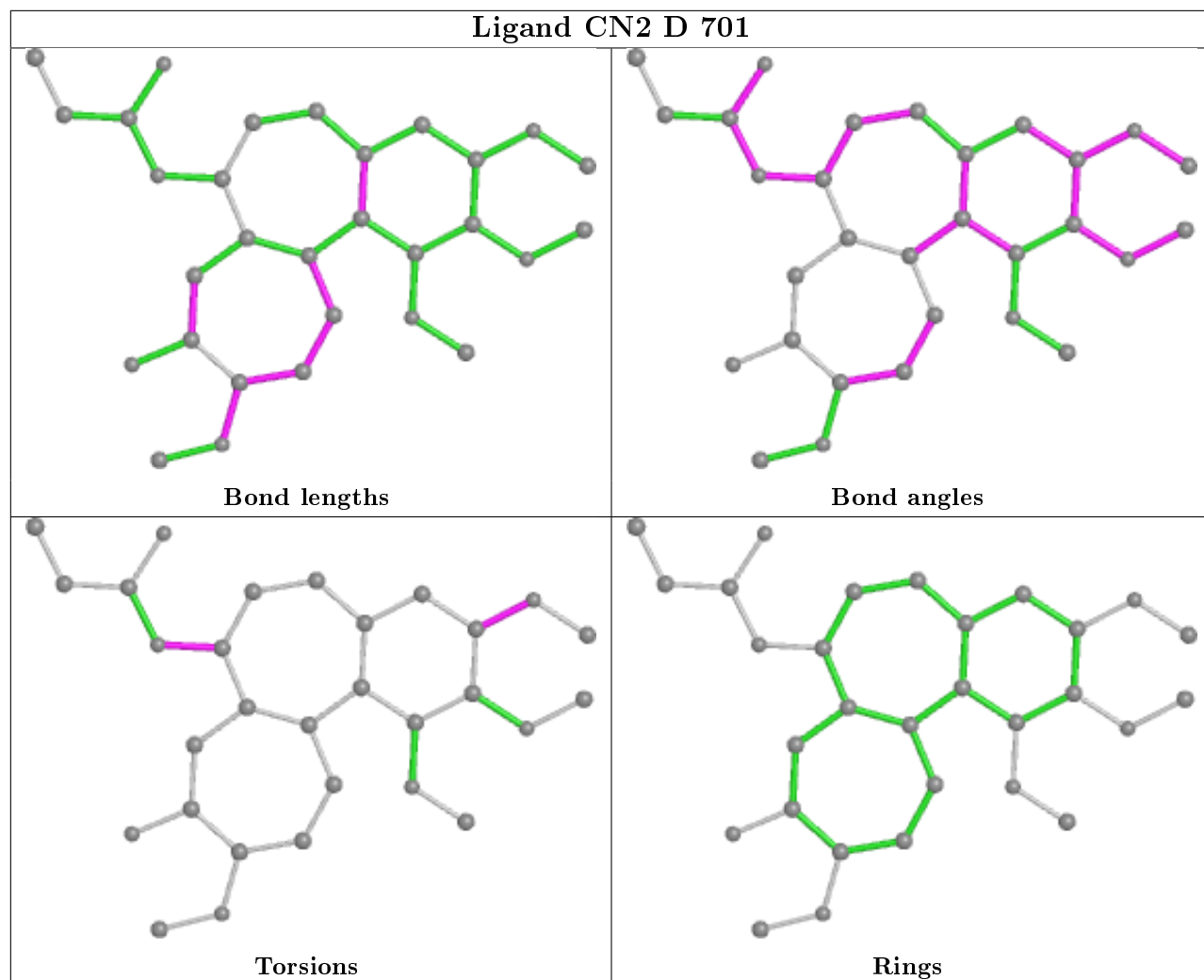
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

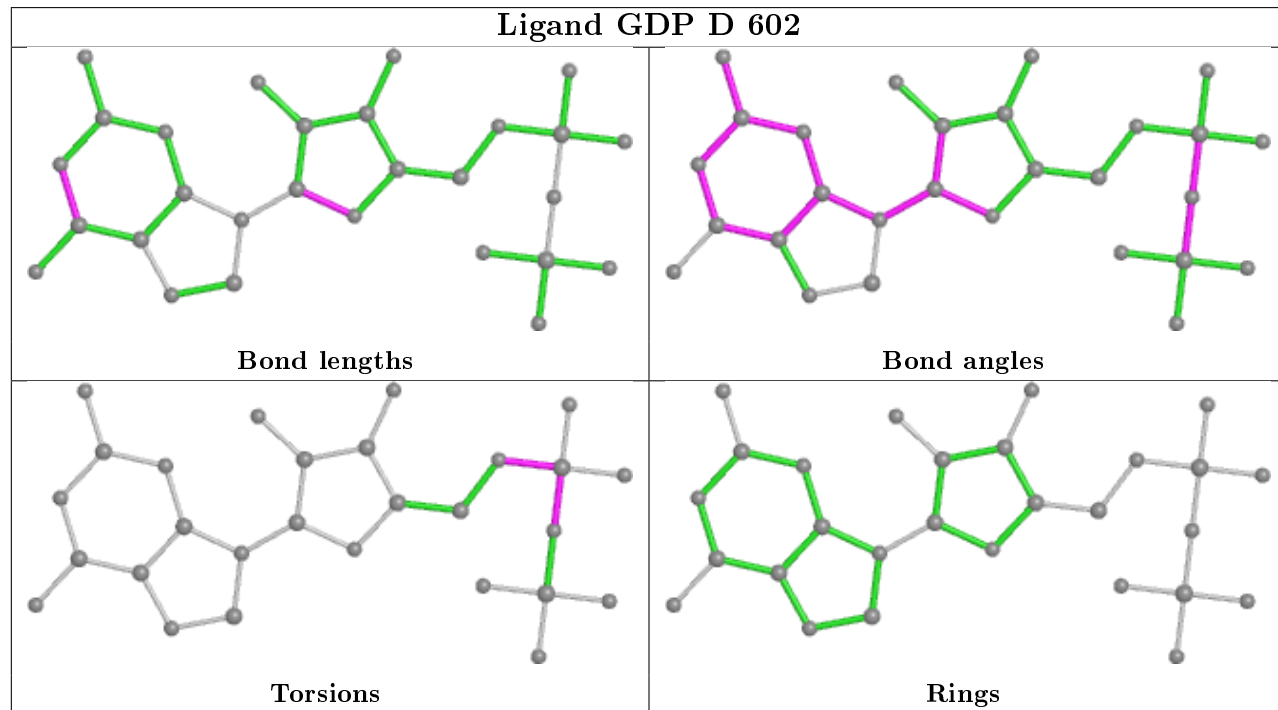
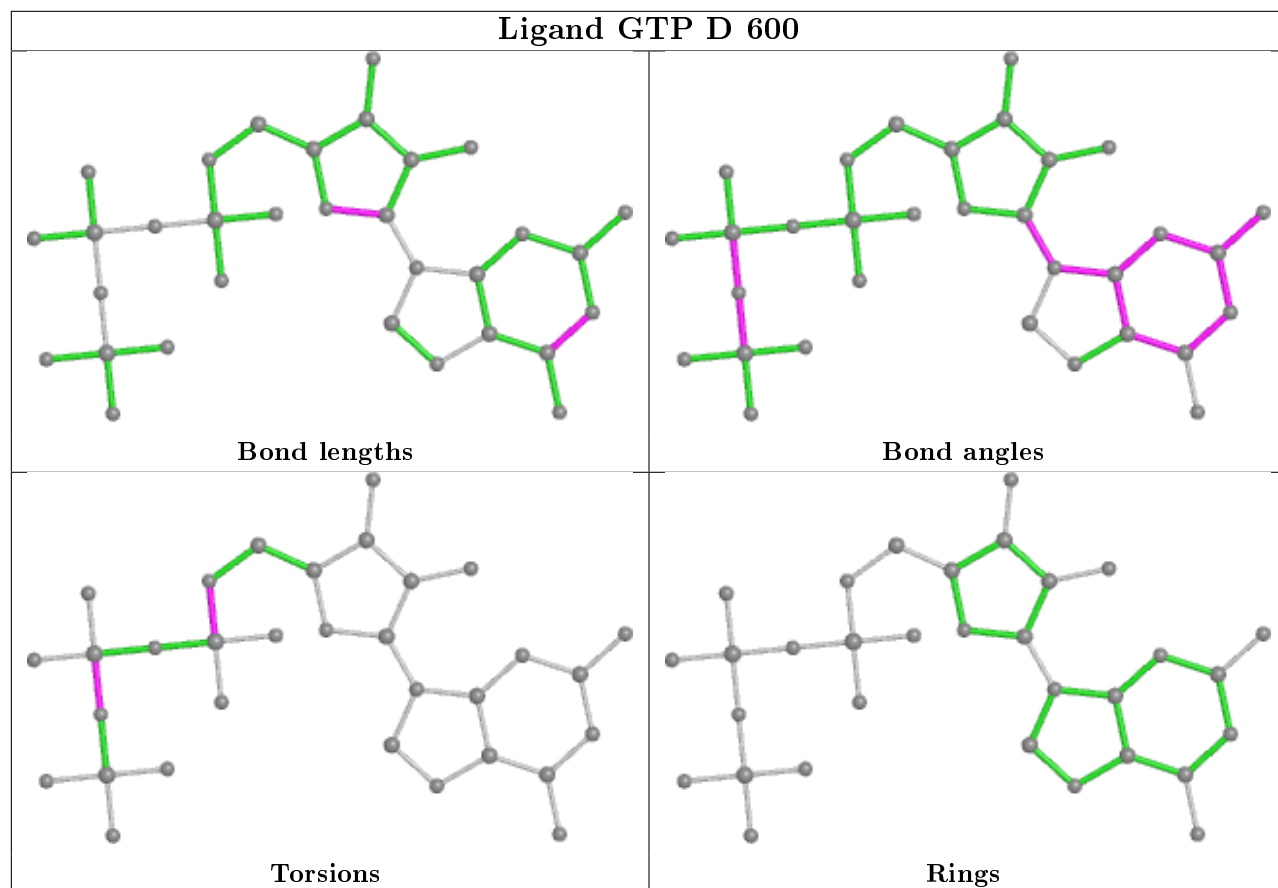




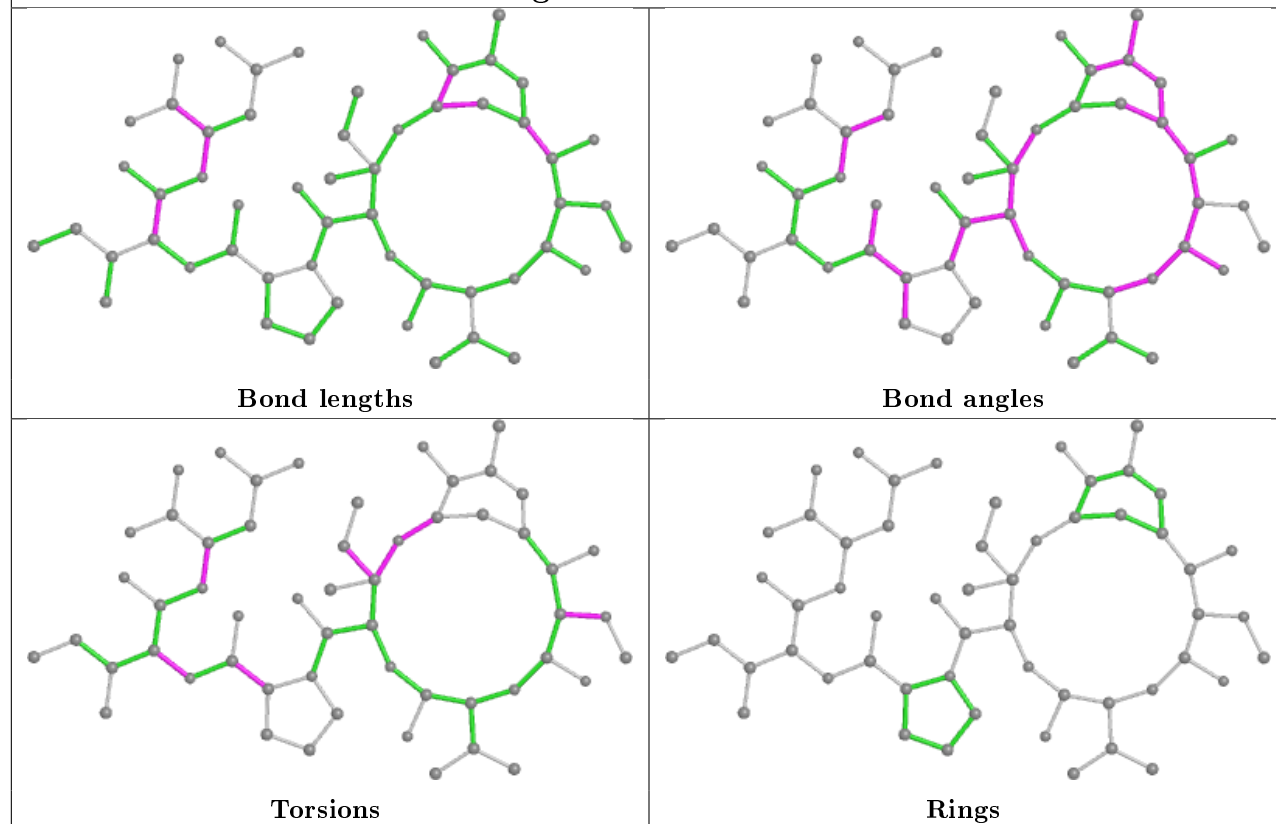
## Ligand CN2 B 700



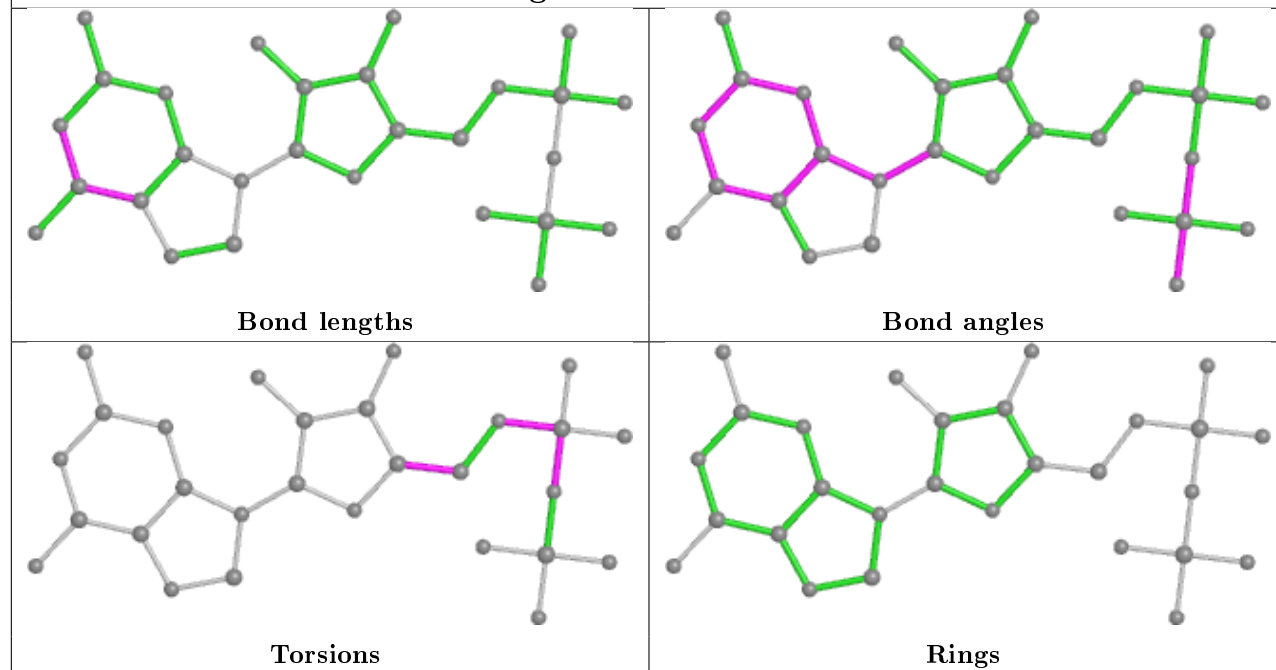


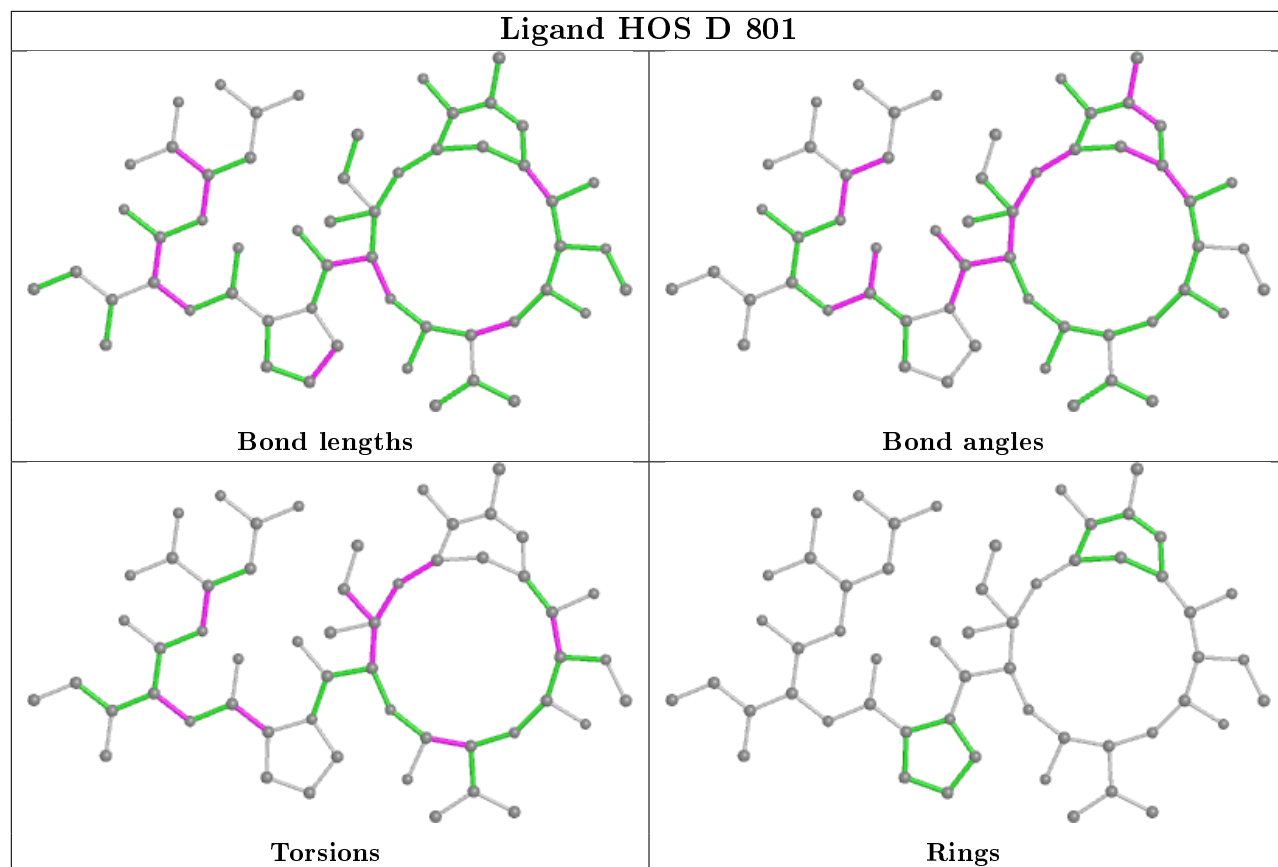


## Ligand HOS B 800



## Ligand GDP D 603





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	428/449 (95%)	-0.42	2 (0%) 91 85	96, 96, 96, 96	0
1	C	438/449 (97%)	-0.26	3 (0%) 87 82	96, 96, 96, 96	0
2	B	426/445 (95%)	-0.35	2 (0%) 91 85	96, 96, 96, 96	0
2	D	426/445 (95%)	-0.22	8 (1%) 66 58	96, 96, 96, 96	0
3	E	121/142 (85%)	-0.27	0 100 100	96, 96, 96, 96	0
All	All	1839/1930 (95%)	-0.31	15 (0%) 86 79	96, 96, 96, 96	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	281	ALA	4.0
1	C	370	LYS	3.5
2	D	412	GLY	3.0
2	D	201	THR	3.0
2	D	413	MET	2.8
2	D	168	THR	2.5
2	B	437	ASP	2.4
2	D	140	SER	2.3
2	D	408	TYR	2.3
1	A	439	SER	2.2
2	D	411	GLU	2.2
1	C	439	SER	2.1
1	A	140	SER	2.1
2	D	170	SER	2.1
2	B	140	SER	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, 95<sup>th</sup> 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.

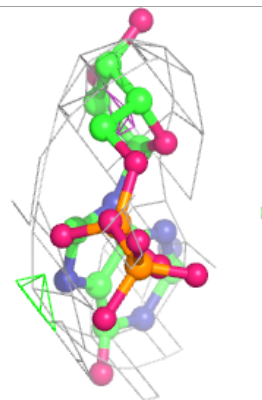
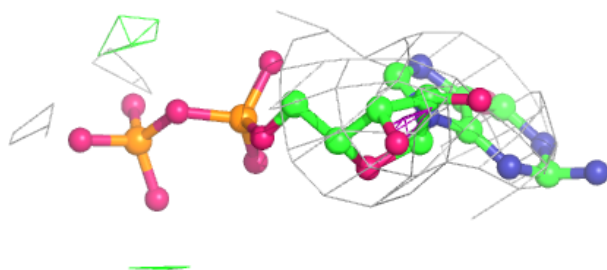
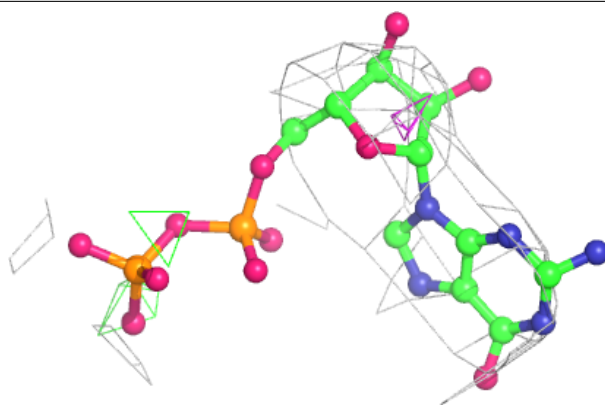
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	GDP	D	602	28/28	0.87	0.37	98,98,98,98	0
6	HOS	B	800	55/55	0.89	0.21	98,98,98,98	0
8	GDP	D	603	28/28	0.90	0.33	98,98,98,98	0
5	CN2	B	700	30/30	0.92	0.24	98,98,98,98	0
6	HOS	D	801	55/55	0.93	0.21	98,98,98,98	0
7	GTP	D	600	32/32	0.94	0.36	98,98,98,98	0
5	CN2	D	701	30/30	0.94	0.25	98,98,98,98	0
4	MG	A	500	1/1	0.96	0.55	98,98,98,98	0
7	GTP	D	601	32/32	0.96	0.33	98,98,98,98	0
4	MG	C	501	1/1	0.98	0.32	98,98,98,98	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.

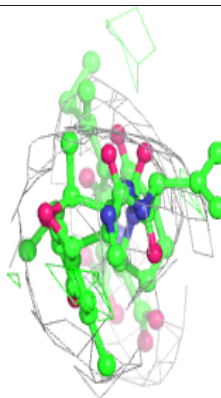
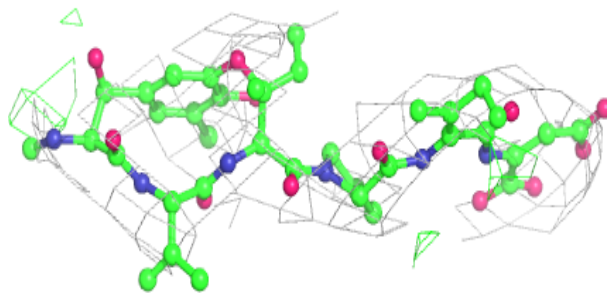
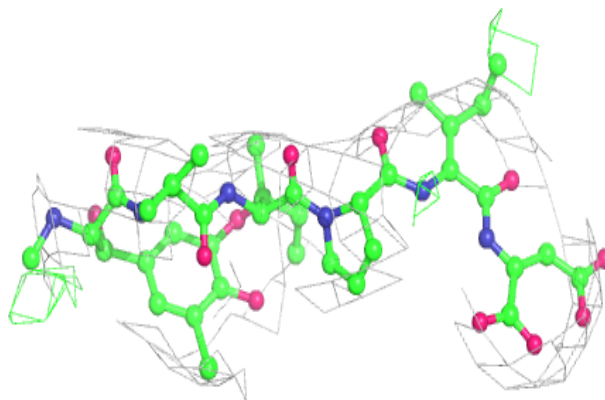


**Electron density around GDP D 602:**

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

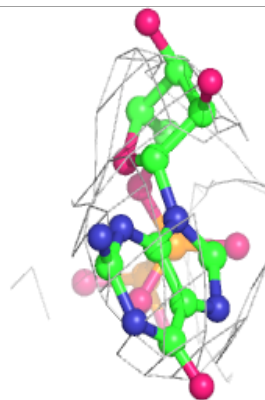
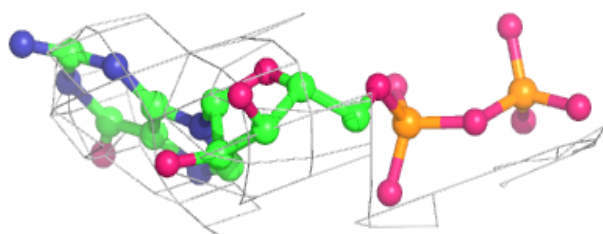
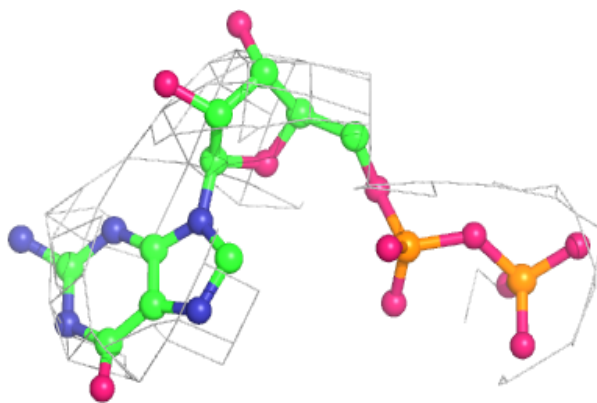
**Electron density around HOS B 800:**

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



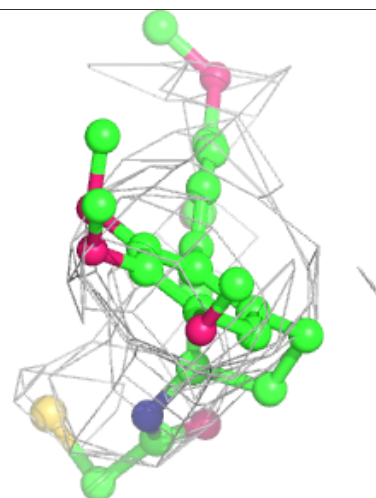
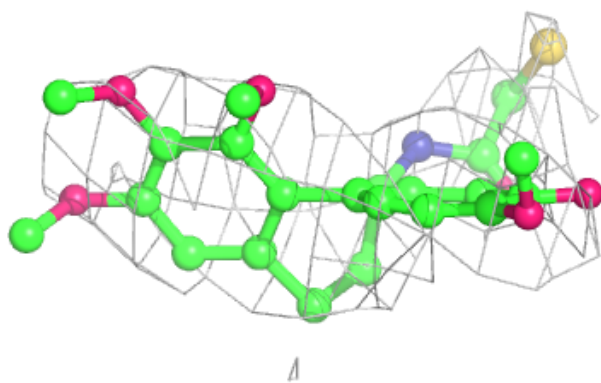
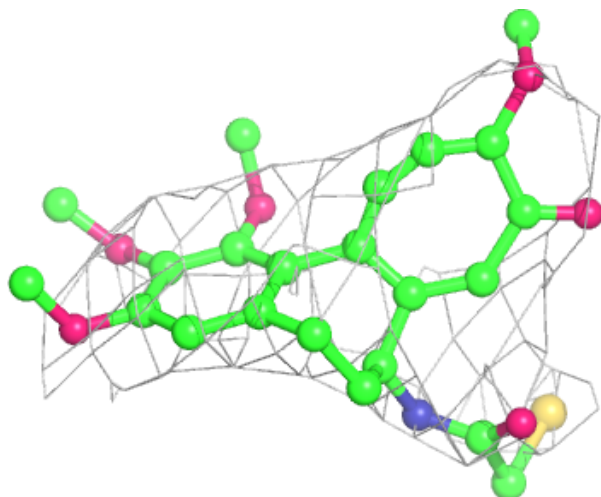
**Electron density around GDP D 603:**

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



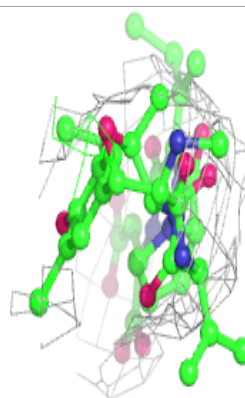
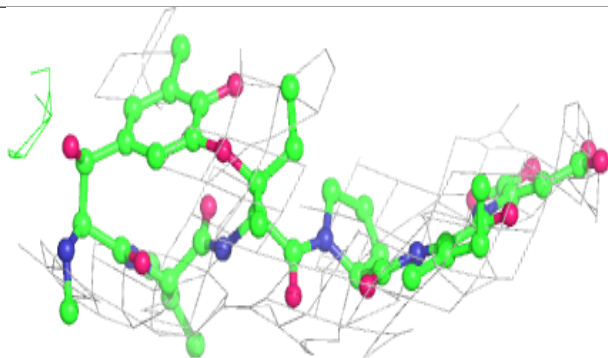
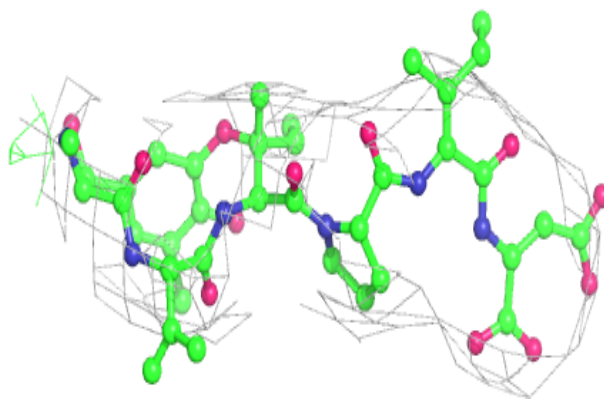
**Electron density around CN2 B 700:**

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

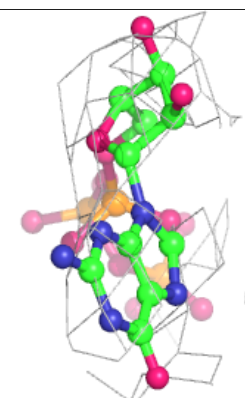
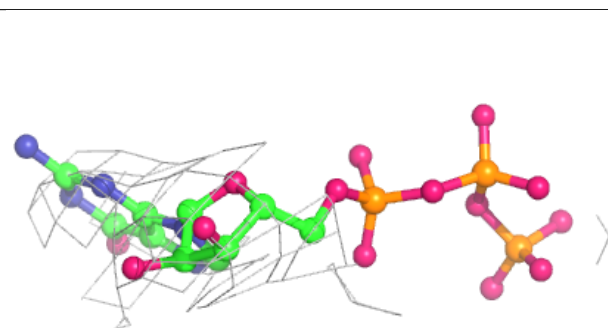
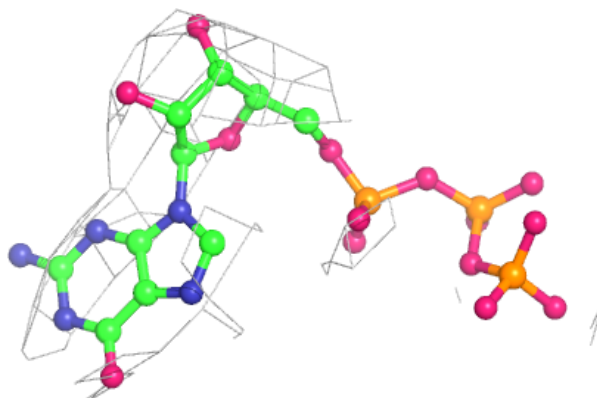


**Electron density around HOS D 801:**

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

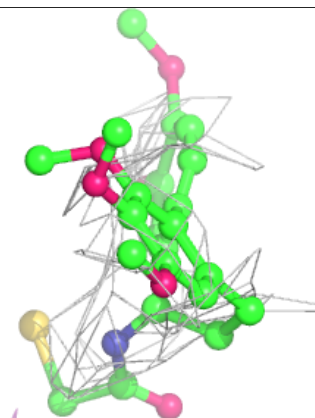
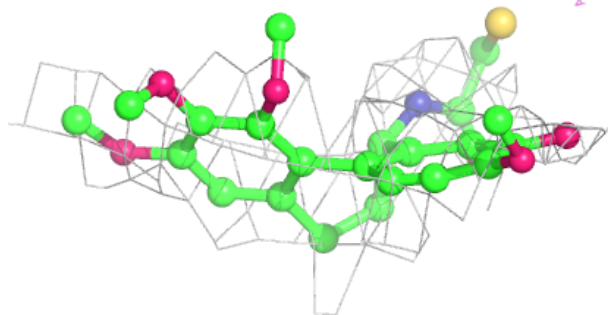
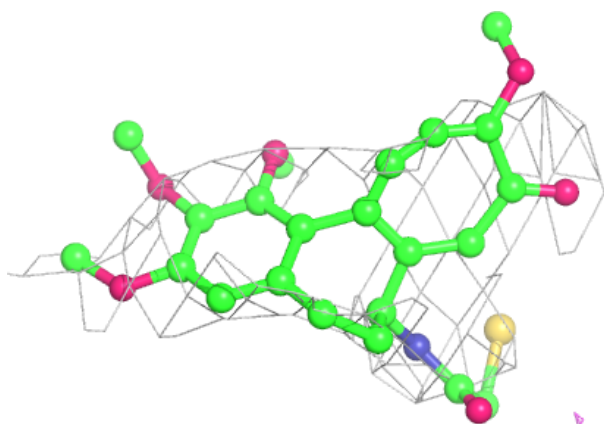
**Electron density around GTP D 600:**

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

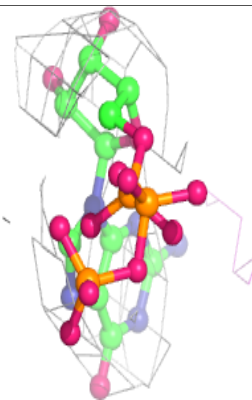
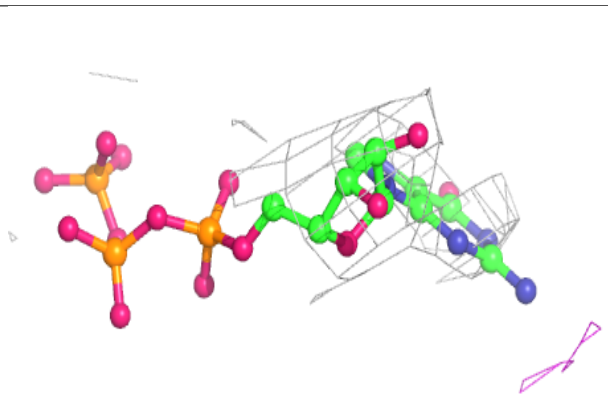
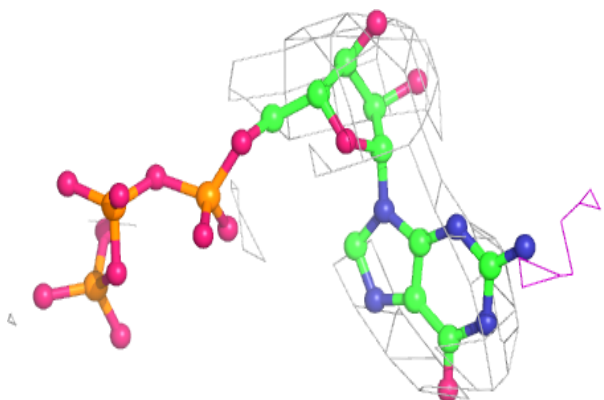


**Electron density around CN2 D 701:**

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

**Electron density around GTP D 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

There are no such residues in this entry.