



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:29 am BST

PDB ID : 3N2G
Title : TUBULIN-NSC 613863: RB3 Stathmin-like domain complex
Authors : Barbier, P.; Dorleans, A.; Devred, F.; Sanz, L.; Allegro, D.; Alfonso, C.; Knossow, M.; Peyrot, V.; Andreu, J.M.
Deposited on : 2010-05-18
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

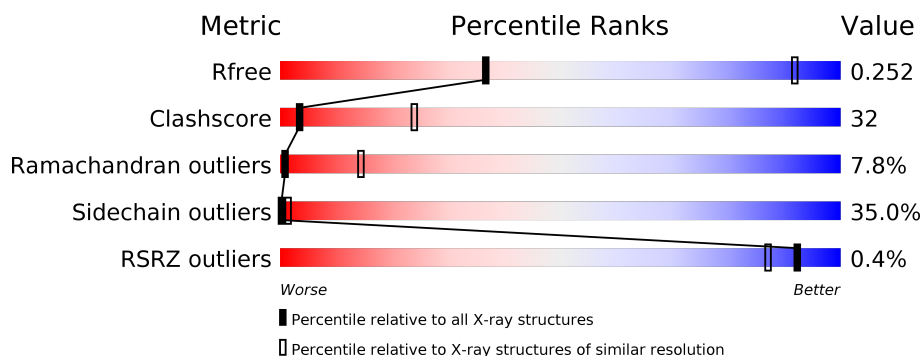
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div></div> <div>41% 37% 14% • 5%</div> </div>
1	C	451	<div> <div></div> <div>45% 33% 14% • 5%</div> </div>
2	B	445	<div> <div></div> <div>29% 43% 18% • 6%</div> </div>
2	D	445	<div> <div>%</div> <div>27% 43% 22% • •</div> </div>
3	E	142	<div> <div>%</div> <div>36% 32% 17% • 13%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GDP	D	600	-	-	X	-
7	G2N	D	700	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14220 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3300	2097	557	625	21			
1	C	429	Total	C	N	O	S	0	0	0
			3286	2084	554	627	21			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3246	2043	546	632	25			
2	D	427	Total	C	N	O	S	0	0	0
			3297	2071	559	643	24			

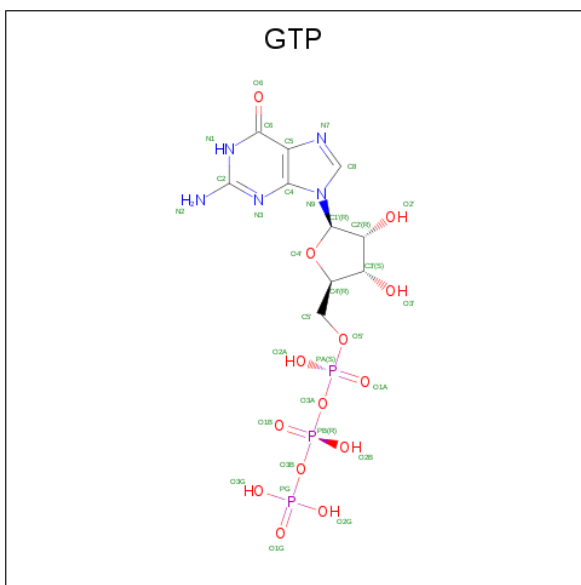
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			920	557	174	184	5			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

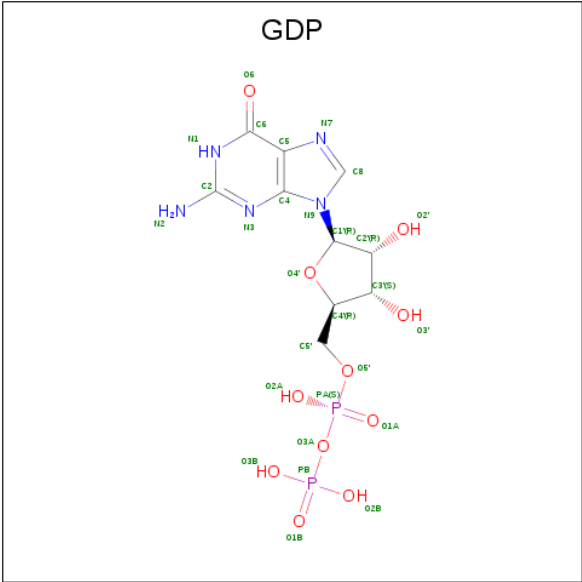


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

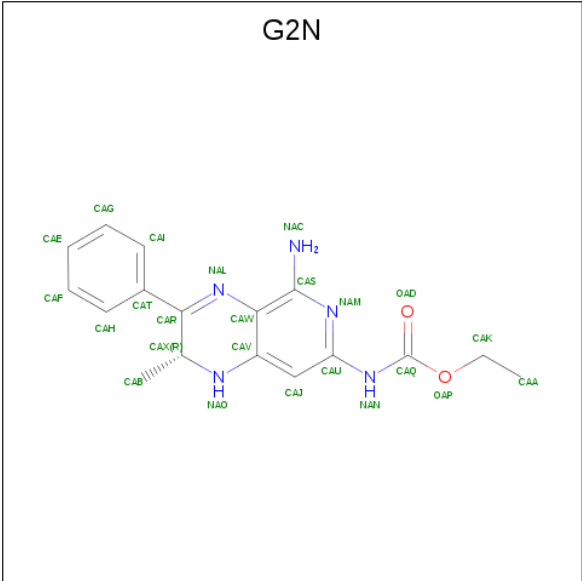
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 7 is ethyl [(2R)-5-amino-2-methyl-3-phenyl-1,2-dihydropyrido[3,4-b]pyrazin-7-yl]carbamate (three-letter code: G2N) (formula: C₁₇H₁₉N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			24	17	5	2		

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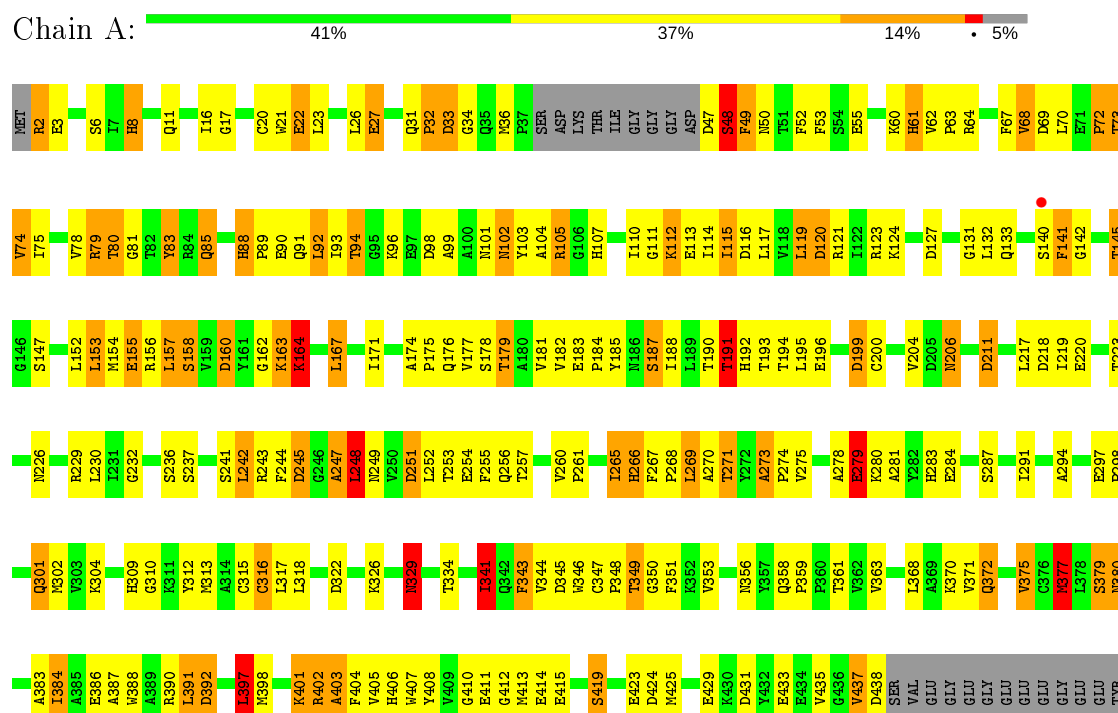
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			24	17	5	2		

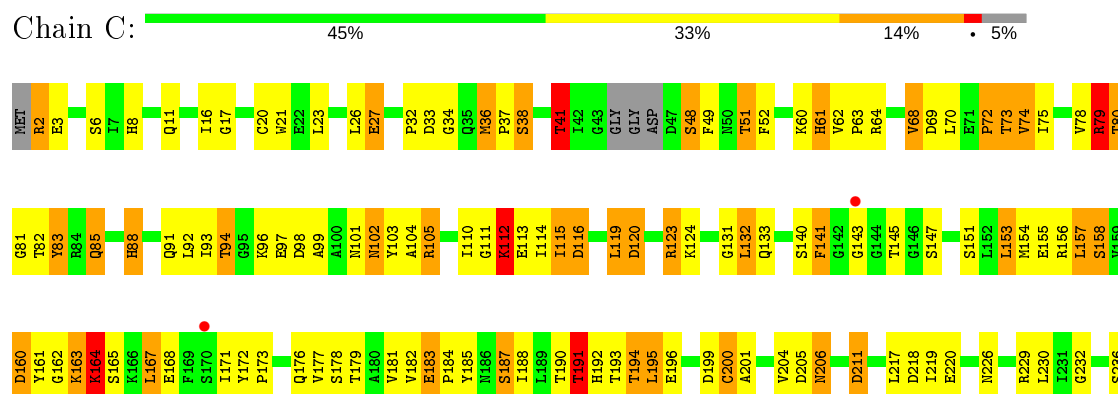
3 Residue-property plots

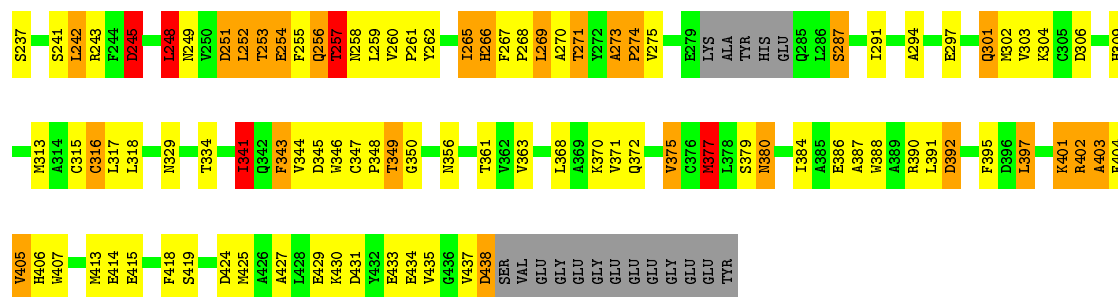
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



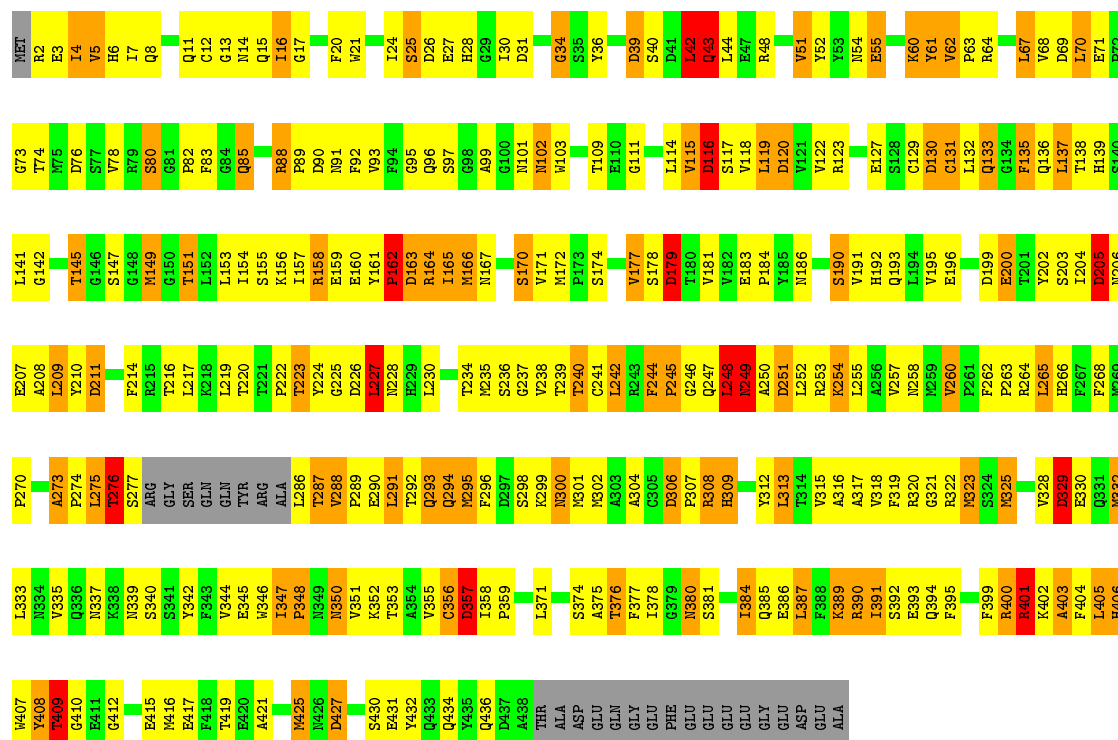
• Molecule 1: Tubulin alpha chain





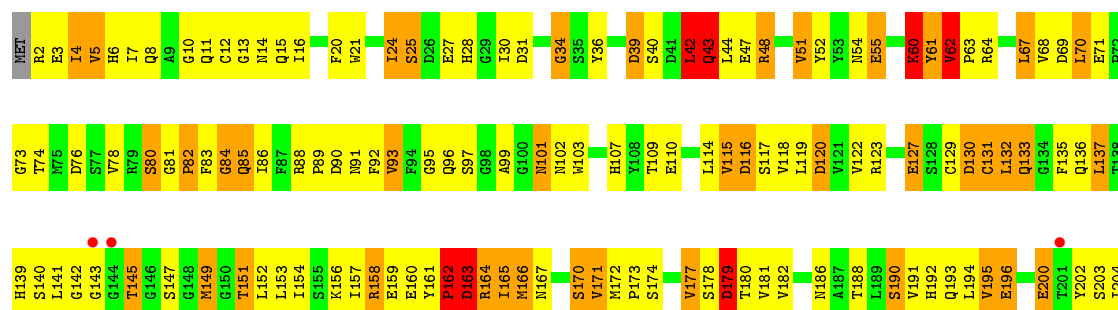
• Molecule 2: Tubulin beta chain

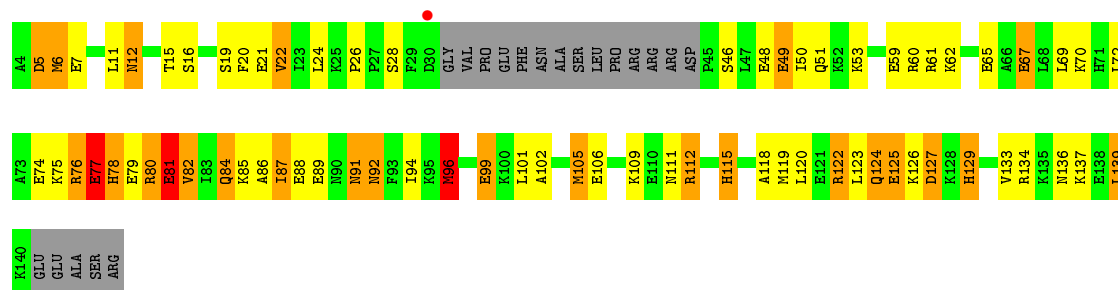
Chain B: 29% 43% 18% 6%



• Molecule 2: Tubulin beta chain

Chain D: 27% 43% 22%





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	328.55Å 328.55Å 54.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.00 29.83 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-4.00) 98.3 (29.83-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.98Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.209 , 0.241 0.238 , 0.252	Depositor DCC
R_{free} test set	1472 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	168.5	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 173.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14220	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, MG, G2N

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	0.79	0/3377	0.98	18/4593 (0.4%)
1	C	0.69	0/3360	0.94	15/4572 (0.3%)
2	B	0.78	0/3318	0.98	16/4505 (0.4%)
2	D	0.73	1/3370 (0.0%)	0.96	14/4574 (0.3%)
3	E	0.79	1/928 (0.1%)	0.90	2/1243 (0.2%)
All	All	0.75	2/14353 (0.0%)	0.96	65/19487 (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	C	0	2
2	B	0	3
2	D	0	4
3	E	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	127	GLU	CD-OE2	5.89	1.32	1.25
3	E	96	MET	SD-CE	5.26	2.07	1.77

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	ASP	CB-CG-OD2	8.53	125.98	118.30
1	A	397	LEU	CA-CB-CG	8.00	133.71	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ASP	CB-CG-OD2	7.82	125.34	118.30
1	C	397	LEU	CA-CB-CG	7.41	132.34	115.30
1	C	160	ASP	CB-CG-OD2	7.33	124.89	118.30
1	A	269	LEU	CA-CB-CG	7.32	132.14	115.30
2	D	242	LEU	CA-CB-CG	7.12	131.66	115.30
2	D	179	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	248	LEU	CA-CB-CG	6.98	131.36	115.30
1	C	269	LEU	CA-CB-CG	6.97	131.33	115.30
1	C	211	ASP	CB-CG-OD2	6.87	124.48	118.30
1	C	424	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	160	ASP	CB-CG-OD2	6.61	124.25	118.30
2	B	306	ASP	CB-CG-OD2	6.61	124.25	118.30
2	D	211	ASP	CB-CG-OD2	6.55	124.20	118.30
1	A	424	ASP	CB-CG-OD2	6.47	124.12	118.30
2	B	130	ASP	CB-CG-OD2	6.42	124.08	118.30
2	B	116	ASP	CB-CG-OD2	6.39	124.05	118.30
2	B	179	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	211	ASP	CB-CG-OD2	6.33	124.00	118.30
1	C	33	ASP	CB-CG-OD2	6.24	123.91	118.30
1	C	120	ASP	CB-CG-OD2	6.23	123.91	118.30
2	D	427	ASP	CB-CG-OD2	6.21	123.89	118.30
2	D	297	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	116	ASP	CB-CG-OD2	6.09	123.78	118.30
2	D	357	ASP	CB-CG-OD2	6.05	123.75	118.30
2	B	39	ASP	CB-CG-OD2	6.04	123.73	118.30
1	C	345	ASP	CB-CG-OD2	6.00	123.70	118.30
2	B	199	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	120	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	322	ASP	CB-CG-OD2	5.92	123.63	118.30
2	B	120	ASP	CB-CG-OD2	5.85	123.56	118.30
2	B	211	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	33	ASP	CB-CG-OD2	5.73	123.46	118.30
2	B	242	LEU	CA-CB-CG	5.70	128.41	115.30
2	D	120	ASP	CB-CG-OD2	5.70	123.43	118.30
2	B	357	ASP	CB-CG-OD2	5.67	123.40	118.30
2	D	39	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	218	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	127	ASP	CB-CG-OD2	5.63	123.37	118.30
1	C	248	LEU	CA-CB-CG	5.59	128.16	115.30
1	C	306	ASP	CB-CG-OD2	5.54	123.28	118.30
3	E	127	ASP	CB-CG-OD2	5.52	123.27	118.30
2	D	379	GLY	N-CA-C	5.51	126.89	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	130	ASP	CB-CG-OD2	5.50	123.25	118.30
2	B	329	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	251	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	266	HIS	CB-CA-C	-5.39	99.62	110.40
1	A	345	ASP	CB-CG-OD2	5.39	123.15	118.30
2	B	205	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	69	ASP	CB-CG-OD2	5.34	123.11	118.30
2	D	329	ASP	CB-CG-OD2	5.32	123.08	118.30
2	D	116	ASP	CB-CG-OD2	5.28	123.06	118.30
2	D	226	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	248	LEU	CB-CG-CD2	5.25	119.92	111.00
1	C	218	ASP	CB-CG-OD2	5.24	123.02	118.30
2	B	26	ASP	CB-CG-OD2	5.22	123.00	118.30
2	B	69	ASP	CB-CG-OD2	5.17	122.96	118.30
1	C	438	ASP	CB-CG-OD2	5.15	122.94	118.30
3	E	6	MET	N-CA-C	5.11	124.80	111.00
1	A	392	ASP	CB-CG-OD2	5.11	122.90	118.30
2	B	249	ASN	CB-CA-C	5.11	120.61	110.40
1	A	199	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	245	ASP	CB-CG-OD2	5.03	122.82	118.30
2	D	69	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	162	PRO	Peptide
2	B	248	LEU	Peptide
2	B	249	ASN	Peptide
1	C	266	HIS	Peptide
1	C	41	THR	Peptide
2	D	162	PRO	Peptide
2	D	248	LEU	Peptide
2	D	249	ASN	Peptide
2	D	262	PHE	Peptide
3	E	5	ASP	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3300	0	3162	166	0
1	C	3286	0	3133	164	0
2	B	3246	0	3072	255	0
2	D	3297	0	3116	285	0
3	E	920	0	816	56	0
4	A	32	0	12	3	0
4	C	32	0	12	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	8	0
6	D	28	0	12	15	0
7	B	24	0	19	7	0
7	D	24	0	19	11	0
All	All	14220	0	13385	890	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 32.

All (890) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:MET:SD	2:B:325:MET:CE	2.04	1.45
3:E:105:MET:SD	3:E:105:MET:CE	2.04	1.43
3:E:96:MET:CE	3:E:96:MET:SD	2.07	1.42
2:B:308:ARG:HH11	2:B:308:ARG:HG3	1.09	1.17
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.16	1.14
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.18	1.12
2:D:223:THR:HB	2:D:225:GLY:H	1.06	1.11
2:B:223:THR:HB	2:B:225:GLY:H	1.11	1.09
2:D:319:PHE:HB2	2:D:355:VAL:HG12	1.29	1.09
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.82	1.08
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.29	1.07
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.83	1.07
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.12	1.05
2:D:387:LEU:O	2:D:390:ARG:HG2	1.54	1.05
1:C:105:ARG:NH2	2:D:253:ARG:HH21	1.53	1.04
2:D:140:SER:HB2	6:D:600:GDP:H5'	1.37	1.03
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:261:PRO:HG3	2:D:313:LEU:HD12	1.37	1.02
2:D:140:SER:CB	6:D:600:GDP:H5'	1.95	0.97
1:C:79:ARG:NH2	1:C:94:THR:HG21	1.80	0.97
1:A:273:ALA:CB	1:A:274:PRO:HD3	1.94	0.97
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.48	0.95
2:D:123:ARG:O	2:D:127:GLU:HB2	1.66	0.95
2:D:5:VAL:HG22	2:D:135:PHE:HD2	1.30	0.95
1:C:105:ARG:HH22	2:D:253:ARG:NH2	1.66	0.94
1:A:79:ARG:NH2	1:A:94:THR:HG21	1.83	0.94
2:D:261:PRO:HG3	2:D:313:LEU:CD1	1.98	0.94
2:B:133:GLN:HE21	2:B:252:LEU:HD22	1.33	0.94
2:B:273:ALA:HB3	2:B:274:PRO:CD	1.98	0.93
1:C:206:ASN:HD21	4:C:600:GTP:N2	1.66	0.93
3:E:60:ARG:HH11	3:E:60:ARG:HB2	1.30	0.93
2:D:273:ALA:HB3	2:D:274:PRO:CD	1.99	0.92
2:D:135:PHE:HB2	2:D:166:MET:CE	1.99	0.91
2:D:223:THR:HB	2:D:225:GLY:N	1.86	0.91
2:B:5:VAL:HG22	2:B:135:PHE:HD2	1.35	0.91
1:A:70:LEU:HD12	1:A:145:THR:HB	1.52	0.91
2:D:133:GLN:HE21	2:D:252:LEU:HD22	1.36	0.91
1:C:70:LEU:HD12	1:C:145:THR:HB	1.54	0.90
1:A:278:ALA:O	1:A:279:GLU:HB3	1.72	0.89
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.51	0.89
2:B:223:THR:HB	2:B:225:GLY:N	1.88	0.89
1:C:206:ASN:HD21	4:C:600:GTP:HN22	0.90	0.89
1:A:105:ARG:HH22	2:B:253:ARG:HH21	1.20	0.87
2:B:142:GLY:O	6:B:600:GDP:H5'	1.75	0.86
2:D:312:TYR:HE2	2:D:377:PHE:HZ	1.24	0.86
2:D:99:ALA:HB1	2:D:145:THR:CG2	2.05	0.85
1:C:273:ALA:CB	1:C:274:PRO:HD3	2.07	0.85
2:B:270:PRO:HD2	2:B:302:MET:HB2	1.58	0.85
3:E:118:ALA:O	3:E:122:ARG:NH1	2.09	0.85
2:D:384:ILE:HG22	2:D:432:TYR:CE1	2.12	0.84
1:C:99:ALA:HB2	1:C:145:THR:HG22	1.60	0.83
2:D:171:VAL:HG12	2:D:206:ASN:HD21	1.43	0.83
1:C:183:GLU:HB3	1:C:184:PRO:CD	2.07	0.83
2:B:145:THR:HG23	6:B:600:GDP:O3B	1.78	0.82
2:B:387:LEU:O	2:B:390:ARG:HG2	1.78	0.82
2:D:295:MET:HG3	2:D:377:PHE:HB2	1.62	0.82
2:B:403:ALA:O	2:B:405:LEU:N	2.13	0.81
2:D:223:THR:CB	2:D:225:GLY:H	1.90	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.62	0.81
2:D:151:THR:HB	2:D:193:GLN:HG2	1.61	0.81
2:D:250:ALA:HA	2:D:255:LEU:HD13	1.63	0.81
2:B:192:HIS:HD2	2:B:421:ALA:HA	1.46	0.80
1:A:85:GLN:HA	1:A:85:GLN:HE21	1.47	0.79
2:B:308:ARG:NH1	2:B:308:ARG:HG3	1.90	0.79
2:D:162:PRO:HD2	2:D:163:ASP:HB2	1.64	0.79
2:D:159:GLU:HB2	3:E:123:LEU:HD13	1.63	0.79
2:D:224:TYR:O	2:D:228:ASN:ND2	2.16	0.79
2:B:308:ARG:HH11	2:B:308:ARG:CG	1.93	0.79
1:C:206:ASN:ND2	4:C:600:GTP:HN22	1.75	0.79
1:A:206:ASN:HD21	4:A:600:GTP:HN22	1.29	0.79
1:A:273:ALA:HB3	1:A:274:PRO:CD	2.07	0.78
1:A:278:ALA:HA	1:A:281:ALA:HB2	1.64	0.78
2:B:292:THR:HA	2:B:295:MET:CE	2.13	0.78
1:C:271:THR:HG23	1:C:301:GLN:HA	1.66	0.78
2:D:135:PHE:HB2	2:D:166:MET:HE1	1.65	0.78
2:B:135:PHE:HB2	2:B:166:MET:CE	2.13	0.78
2:B:123:ARG:O	2:B:127:GLU:HB2	1.84	0.78
2:D:265:LEU:HB2	2:D:432:TYR:CE2	2.19	0.77
2:D:265:LEU:HB2	2:D:432:TYR:HE2	1.49	0.77
1:C:105:ARG:HH22	2:D:253:ARG:HH21	0.81	0.77
2:B:99:ALA:HB1	2:B:145:THR:CG2	2.14	0.77
1:C:256:GLN:C	1:C:258:ASN:N	2.37	0.77
2:D:200:GLU:HB3	2:D:268:PHE:CE1	2.20	0.77
1:C:273:ALA:HB3	1:C:375:VAL:H	1.50	0.77
1:C:99:ALA:CB	1:C:145:THR:HG22	2.13	0.77
2:D:287:THR:HG23	2:D:290:GLU:HB2	1.67	0.77
3:E:60:ARG:NH1	3:E:60:ARG:HB2	2.00	0.77
2:B:151:THR:HB	2:B:193:GLN:HG2	1.67	0.77
2:D:273:ALA:HB2	2:D:375:ALA:H	1.50	0.77
2:B:273:ALA:CB	2:B:274:PRO:CD	2.59	0.76
2:D:273:ALA:CB	2:D:375:ALA:H	1.97	0.76
2:B:391:ILE:HG13	2:B:392:SER:N	1.99	0.76
2:D:220:THR:O	2:D:222:PRO:HD3	1.86	0.76
2:B:292:THR:HA	2:B:295:MET:HE3	1.68	0.76
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.02	0.76
2:D:265:LEU:CB	2:D:432:TYR:CE2	2.69	0.76
2:B:145:THR:O	2:B:149:MET:HB2	1.85	0.76
2:B:217:LEU:HB3	2:B:219:LEU:HG	1.67	0.76
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:350:ASN:H	2:D:350:ASN:HD22	1.32	0.76
1:A:79:ARG:NH2	1:A:94:THR:CG2	2.48	0.75
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.66	0.75
2:D:171:VAL:HG12	2:D:206:ASN:ND2	2.01	0.75
1:C:256:GLN:C	1:C:258:ASN:H	1.87	0.75
1:C:85:GLN:HA	1:C:85:GLN:HE21	1.52	0.75
2:D:403:ALA:O	2:D:405:LEU:N	2.20	0.75
1:A:99:ALA:CB	1:A:145:THR:HG22	2.17	0.75
2:B:312:TYR:HE2	2:B:377:PHE:HZ	1.35	0.75
2:D:289:PRO:HA	2:D:331:GLN:NE2	2.01	0.75
1:C:343:PHE:CD1	1:C:349:THR:HG22	2.22	0.75
2:B:223:THR:CB	2:B:225:GLY:H	1.94	0.75
2:B:42:LEU:O	2:B:44:LEU:N	2.20	0.74
2:D:399:PHE:O	2:D:400:ARG:O	2.06	0.74
1:C:79:ARG:NH2	1:C:94:THR:CG2	2.50	0.74
1:C:265:ILE:HD12	1:C:265:ILE:H	1.53	0.74
2:D:345:GLU:N	2:D:345:GLU:OE1	2.20	0.74
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.23	0.74
2:D:312:TYR:HE2	2:D:377:PHE:CZ	2.06	0.73
2:B:200:GLU:HB3	2:B:268:PHE:CE1	2.23	0.73
1:A:270:ALA:O	1:A:302:MET:HB2	1.89	0.73
2:B:36:TYR:OH	2:B:40:SER:O	2.04	0.73
2:D:427:ASP:O	2:D:431:GLU:HG3	1.88	0.73
2:B:159:GLU:HB2	3:E:72:LEU:HD23	1.71	0.73
1:A:101:ASN:HD22	2:B:254:LYS:HG2	1.54	0.72
2:D:42:LEU:O	2:D:44:LEU:N	2.22	0.72
2:D:145:THR:O	2:D:149:MET:HB2	1.89	0.72
2:D:179:ASP:N	2:D:179:ASP:OD1	2.21	0.72
2:D:234:THR:HG21	2:D:302:MET:HG3	1.71	0.72
2:D:99:ALA:HB1	2:D:145:THR:HG22	1.70	0.72
2:B:241:CYS:HB2	7:B:700:G2N:CAB	2.20	0.72
2:B:399:PHE:O	2:B:400:ARG:O	2.06	0.72
1:A:271:THR:HG23	1:A:301:GLN:HA	1.70	0.72
2:B:70:LEU:HD11	2:B:149:MET:HG3	1.72	0.72
1:A:183:GLU:HB3	1:A:184:PRO:CD	2.20	0.71
1:A:68:VAL:HG12	1:A:93:ILE:HB	1.71	0.71
1:A:105:ARG:HH22	2:B:253:ARG:NH2	1.88	0.71
6:D:600:GDP:H3'	6:D:600:GDP:H8	1.55	0.71
2:B:306:ASP:O	2:B:308:ARG:N	2.23	0.71
2:D:384:ILE:CG2	2:D:432:TYR:HE1	2.02	0.71
2:B:220:THR:O	2:B:222:PRO:HD3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:LEU:HD11	2:D:149:MET:HG3	1.71	0.71
2:B:276:THR:HG23	2:B:277:SER:N	2.06	0.70
2:D:262:PHE:HB2	2:D:265:LEU:HD11	1.73	0.70
1:C:153:LEU:HD13	1:C:157:LEU:HD11	1.71	0.70
2:B:171:VAL:HG12	2:B:206:ASN:ND2	2.07	0.70
2:B:191:VAL:HG11	2:B:425:MET:CE	2.20	0.70
1:A:273:ALA:CB	1:A:274:PRO:CD	2.68	0.70
1:C:229:ARG:HG2	1:C:229:ARG:HH11	1.57	0.70
1:A:265:ILE:H	1:A:265:ILE:HD12	1.56	0.70
2:B:2:ARG:N	2:B:133:GLN:OE1	2.25	0.70
2:B:224:TYR:O	2:B:228:ASN:ND2	2.23	0.70
1:C:273:ALA:CB	1:C:375:VAL:H	2.04	0.70
2:D:89:PRO:O	2:D:92:PHE:HD1	1.75	0.70
2:B:133:GLN:HE21	2:B:252:LEU:CD2	2.05	0.69
2:B:250:ALA:HA	2:B:255:LEU:HD13	1.74	0.69
2:D:292:THR:HA	2:D:295:MET:CE	2.22	0.69
2:B:99:ALA:HB1	2:B:145:THR:HG22	1.73	0.69
2:D:384:ILE:CG2	2:D:432:TYR:CE1	2.75	0.69
2:D:308:ARG:HH11	2:D:308:ARG:HG3	1.57	0.69
2:D:4:ILE:HG23	2:D:51:VAL:HG22	1.73	0.69
1:A:229:ARG:HH11	1:A:229:ARG:HG2	1.58	0.69
1:C:270:ALA:O	1:C:302:MET:HB2	1.92	0.69
1:A:317:LEU:CD2	1:A:377:MET:HE3	2.22	0.69
2:B:329:ASP:HA	2:B:332:MET:HB2	1.74	0.69
2:D:36:TYR:OH	2:D:40:SER:O	2.09	0.69
2:B:276:THR:HG23	2:B:277:SER:H	1.57	0.69
7:B:700:G2N:CAA	7:B:700:G2N:OAD	2.39	0.68
2:B:136:GLN:HE21	7:B:700:G2N:HAA	1.58	0.68
2:D:242:LEU:HD11	7:D:700:G2N:H16	1.75	0.68
3:E:84:GLN:C	3:E:86:ALA:H	1.97	0.68
1:A:105:ARG:HD3	1:A:411:GLU:OE1	1.93	0.68
2:B:51:VAL:HG13	2:B:52:TYR:CD1	2.28	0.68
2:D:171:VAL:CG1	2:D:206:ASN:HD21	2.06	0.68
2:D:265:LEU:CB	2:D:432:TYR:HE2	2.06	0.68
6:D:600:GDP:C8	6:D:600:GDP:H3'	2.28	0.68
2:B:114:LEU:O	2:B:116:ASP:N	2.27	0.68
3:E:70:LYS:O	3:E:70:LYS:HD2	1.94	0.67
1:A:343:PHE:CD1	1:A:349:THR:HG22	2.29	0.67
2:D:136:GLN:HE21	7:D:700:G2N:HAA	1.59	0.67
2:D:133:GLN:HE21	2:D:252:LEU:CD2	2.06	0.67
2:D:270:PRO:HD2	2:D:302:MET:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:SER:HA	2:B:301:MET:HG2	1.77	0.67
1:C:8:HIS:CD2	1:C:17:GLY:HA3	2.29	0.67
2:B:309:HIS:CD2	2:B:309:HIS:H	2.10	0.67
2:D:312:TYR:CD2	2:D:315:VAL:HG21	2.29	0.67
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.17	0.67
2:D:312:TYR:CD2	2:D:315:VAL:CG2	2.78	0.67
2:B:89:PRO:O	2:B:92:PHE:HD1	1.77	0.66
1:A:273:ALA:HB3	1:A:375:VAL:H	1.60	0.66
1:A:79:ARG:HH21	1:A:94:THR:HG21	1.60	0.66
2:B:298:SER:C	2:B:300:ASN:H	1.97	0.66
2:B:306:ASP:C	2:B:308:ARG:H	1.98	0.66
2:B:141:LEU:HA	2:B:147:SER:HB3	1.75	0.66
2:B:4:ILE:HG23	2:B:51:VAL:HG22	1.77	0.66
1:A:190:THR:HG23	1:A:191:THR:H	1.58	0.66
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.29	0.66
2:B:403:ALA:C	2:B:405:LEU:H	1.99	0.66
1:C:183:GLU:CB	1:C:184:PRO:HD3	2.20	0.66
2:B:192:HIS:O	2:B:195:VAL:HG12	1.96	0.66
3:E:22:VAL:O	3:E:22:VAL:HG13	1.95	0.66
1:A:145:THR:HG23	4:A:600:GTP:O2B	1.97	0.65
7:B:700:G2N:OAD	7:B:700:G2N:HAAA	1.96	0.65
1:C:27:GLU:OE2	1:C:243:ARG:NH2	2.28	0.65
2:D:54:ASN:HB2	2:D:64:ARG:HD3	1.79	0.65
2:B:265:LEU:HB2	2:B:432:TYR:CE2	2.31	0.65
2:D:5:VAL:CG2	2:D:135:PHE:HD2	2.08	0.65
2:B:147:SER:O	2:B:151:THR:OG1	2.09	0.65
2:D:298:SER:HA	2:D:301:MET:HG2	1.76	0.65
1:A:204:VAL:HG22	1:A:302:MET:CE	2.27	0.65
2:B:319:PHE:HB2	2:B:355:VAL:HG12	1.79	0.65
2:D:265:LEU:HB3	2:D:432:TYR:CE2	2.32	0.65
2:D:5:VAL:HG22	2:D:135:PHE:CD2	2.21	0.65
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.25	0.65
1:A:266:HIS:O	1:A:268:PRO:HD3	1.96	0.65
1:A:133:GLN:NE2	1:A:252:LEU:HG	2.12	0.65
2:D:248:LEU:HD11	7:D:700:G2N:CAH	2.27	0.65
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.32	0.64
1:A:70:LEU:CD1	1:A:145:THR:HB	2.25	0.64
2:D:114:LEU:O	2:D:116:ASP:N	2.30	0.64
1:C:101:ASN:HD22	2:D:254:LYS:HG2	1.62	0.64
2:D:309:HIS:H	2:D:309:HIS:CD2	2.16	0.64
2:B:115:VAL:HG12	2:B:116:ASP:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ALA:HB3	1:A:302:MET:HE2	1.78	0.64
2:D:383:ALA:O	2:D:386:GLU:HB2	1.98	0.64
2:D:2:ARG:N	2:D:133:GLN:OE1	2.31	0.64
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.33	0.63
1:C:105:ARG:NH2	2:D:253:ARG:NH2	2.36	0.63
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.80	0.63
2:B:337:ASN:HA	2:B:340:SER:HB3	1.79	0.63
3:E:112:ARG:O	3:E:115:HIS:N	2.28	0.63
1:A:273:ALA:CB	1:A:375:VAL:H	2.12	0.63
2:D:320:ARG:HA	2:D:356:CYS:O	1.99	0.62
2:B:141:LEU:HD13	2:B:170:SER:HB3	1.81	0.62
2:B:54:ASN:HB2	2:B:64:ARG:HD3	1.80	0.62
2:B:51:VAL:HG13	2:B:52:TYR:HD1	1.63	0.62
2:D:51:VAL:HG13	2:D:52:TYR:CD1	2.34	0.62
3:E:72:LEU:C	3:E:74:GLU:H	2.00	0.62
1:C:256:GLN:O	1:C:258:ASN:N	2.32	0.62
1:A:153:LEU:HD13	1:A:157:LEU:HD11	1.81	0.62
1:C:190:THR:HG23	1:C:191:THR:H	1.64	0.62
1:A:317:LEU:HD21	1:A:377:MET:HE3	1.81	0.62
1:C:315:CYS:SG	1:C:377:MET:CE	2.88	0.62
1:C:68:VAL:HG12	1:C:93:ILE:HB	1.80	0.62
2:D:248:LEU:HD11	7:D:700:G2N:CAF	2.30	0.62
1:A:204:VAL:HG22	1:A:302:MET:HE1	1.81	0.62
2:B:114:LEU:HB3	2:B:149:MET:HE1	1.82	0.62
2:B:262:PHE:HB2	2:B:265:LEU:HD11	1.80	0.62
2:D:200:GLU:HB3	2:D:268:PHE:HE1	1.65	0.62
2:D:385:GLN:HE21	2:D:389:LYS:HD2	1.65	0.62
2:D:250:ALA:HA	2:D:255:LEU:CD1	2.29	0.62
1:A:388:TRP:HA	1:A:388:TRP:CE3	2.35	0.61
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.09	0.61
2:B:317:ALA:HB3	2:B:353:THR:HG22	1.82	0.61
2:B:248:LEU:O	2:B:249:ASN:HB3	1.99	0.61
1:A:182:VAL:HG22	1:A:182:VAL:O	2.00	0.61
1:A:229:ARG:HH11	1:A:229:ARG:CG	2.12	0.61
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.81	0.61
2:B:241:CYS:HB2	7:B:700:G2N:HABA	1.81	0.61
2:D:208:ALA:O	2:D:211:ASP:N	2.32	0.61
1:A:190:THR:HG23	1:A:191:THR:N	2.16	0.61
1:C:315:CYS:SG	1:C:377:MET:HE2	2.41	0.61
1:C:79:ARG:HH21	1:C:94:THR:HG21	1.63	0.61
3:E:48:GLU:O	3:E:50:ILE:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ASN:OD1	2:B:200:GLU:HG3	2.00	0.61
2:B:21:TRP:O	2:B:25:SER:HB2	2.00	0.61
1:C:88:HIS:HB2	1:C:91:GLN:NE2	2.15	0.61
1:A:412:GLY:O	3:E:60:ARG:NH1	2.34	0.60
2:D:316:ALA:HB1	7:D:700:G2N:HAI	1.83	0.60
1:A:351:PHE:HB2	3:E:22:VAL:HG12	1.83	0.60
2:B:131:CYS:O	2:B:131:CYS:SG	2.59	0.60
2:B:135:PHE:HB2	2:B:166:MET:HE1	1.81	0.60
2:B:191:VAL:HG11	2:B:425:MET:HE3	1.84	0.60
2:D:385:GLN:HE21	2:D:389:LYS:CD	2.13	0.60
1:C:36:MET:CE	1:C:38:SER:O	2.49	0.60
2:D:140:SER:CB	6:D:600:GDP:C5'	2.75	0.60
2:D:312:TYR:HD2	2:D:315:VAL:CG2	2.14	0.60
2:D:55:GLU:HB3	2:D:61:TYR:HD2	1.66	0.60
1:C:253:THR:O	1:C:256:GLN:N	2.31	0.60
2:B:133:GLN:NE2	2:B:252:LEU:HB2	2.16	0.59
1:C:190:THR:HG23	1:C:191:THR:N	2.17	0.59
1:C:167:LEU:HD13	1:C:252:LEU:CD1	2.32	0.59
2:D:282:GLN:HE21	2:D:286:LEU:HD11	1.66	0.59
2:D:358:ILE:HG23	2:D:358:ILE:O	2.02	0.59
1:A:167:LEU:HD13	1:A:252:LEU:HD13	1.84	0.59
2:B:251:ASP:HB2	2:B:254:LYS:HB2	1.84	0.59
2:B:70:LEU:C	2:B:95:GLY:HA3	2.23	0.59
2:B:400:ARG:C	2:B:402:LYS:H	2.05	0.59
2:D:312:TYR:CE2	2:D:377:PHE:HZ	2.15	0.59
2:D:296:PHE:HE1	2:D:332:MET:CE	2.16	0.59
1:A:85:GLN:HA	1:A:85:GLN:NE2	2.16	0.59
2:B:179:ASP:N	2:B:179:ASP:OD1	2.35	0.59
1:C:204:VAL:HG22	1:C:302:MET:HE1	1.85	0.59
1:A:101:ASN:ND2	2:B:254:LYS:HG2	2.18	0.58
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.84	0.58
2:D:114:LEU:HB3	2:D:149:MET:HE1	1.85	0.58
3:E:74:GLU:C	3:E:76:ARG:H	2.05	0.58
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.86	0.58
1:A:280:LYS:HG2	1:A:283:HIS:HE1	1.69	0.58
3:E:77:GLU:HG2	3:E:80:ARG:HB2	1.86	0.58
1:A:280:LYS:HG2	1:A:283:HIS:CE1	2.39	0.58
2:D:162:PRO:CD	2:D:163:ASP:HB2	2.32	0.58
1:C:387:ALA:HB2	1:C:390:ARG:HH12	1.68	0.58
1:C:154:MET:O	1:C:158:SER:HB2	2.04	0.58
2:B:55:GLU:HB3	2:B:61:TYR:HD2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:GLU:OE2	2:D:268:PHE:HE1	1.86	0.57
2:D:34:GLY:HA2	2:D:60:LYS:HE2	1.86	0.57
1:C:70:LEU:CD1	1:C:145:THR:HB	2.32	0.57
2:D:164:ARG:HA	2:D:164:ARG:HE	1.68	0.57
2:D:292:THR:HA	2:D:295:MET:HE3	1.86	0.57
1:A:52:PHE:O	1:A:64:ARG:HB2	2.05	0.57
2:B:172:MET:CE	2:B:203:SER:HB3	2.34	0.57
1:C:111:GLY:O	1:C:113:GLU:N	2.37	0.57
2:D:282:GLN:HG2	2:D:282:GLN:O	2.04	0.57
1:C:229:ARG:CG	1:C:229:ARG:HH11	2.18	0.57
6:D:600:GDP:C8	6:D:600:GDP:C3'	2.87	0.57
2:D:14:ASN:HD21	2:D:67:LEU:HB3	1.70	0.57
1:A:275:VAL:HG23	1:A:275:VAL:O	2.05	0.57
2:B:200:GLU:HB3	2:B:268:PHE:HE1	1.67	0.57
2:D:141:LEU:HA	2:D:147:SER:HB3	1.87	0.57
3:E:81:GLU:O	3:E:82:VAL:C	2.43	0.57
1:A:177:VAL:O	1:A:177:VAL:HG13	2.04	0.56
1:A:387:ALA:HB2	1:A:390:ARG:HH12	1.70	0.56
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.87	0.56
1:A:154:MET:O	1:A:158:SER:HB2	2.04	0.56
2:D:273:ALA:CB	2:D:274:PRO:CD	2.61	0.56
2:D:298:SER:C	2:D:300:ASN:H	2.07	0.56
2:D:412:GLY:O	3:E:133:VAL:HB	2.05	0.56
2:B:384:ILE:HG22	2:B:432:TYR:CE1	2.40	0.56
2:B:407:TRP:CE2	1:C:257:THR:HA	2.40	0.56
2:D:306:ASP:O	2:D:308:ARG:N	2.35	0.56
2:D:55:GLU:HB3	2:D:61:TYR:CD2	2.39	0.56
2:B:265:LEU:HB2	2:B:432:TYR:HE2	1.69	0.56
2:D:292:THR:C	2:D:294:GLN:H	2.08	0.56
3:E:88:GLU:O	3:E:92:ASN:ND2	2.27	0.56
2:B:164:ARG:NH2	2:B:253:ARG:HH22	2.04	0.56
1:A:133:GLN:CD	1:A:252:LEU:H	2.09	0.56
1:C:256:GLN:O	1:C:259:LEU:N	2.28	0.56
2:D:115:VAL:HG12	2:D:116:ASP:N	2.20	0.56
2:D:203:SER:O	2:D:204:ILE:HG13	2.06	0.56
2:D:306:ASP:C	2:D:308:ARG:H	2.09	0.56
2:B:205:ASP:OD2	2:B:387:LEU:HD12	2.06	0.56
1:A:407:TRP:CD2	2:B:257:VAL:HG22	2.41	0.56
2:B:312:TYR:CE2	2:B:377:PHE:CZ	2.90	0.56
2:B:51:VAL:CG1	2:B:52:TYR:HD1	2.17	0.56
2:B:412:GLY:HA3	3:E:86:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LEU:HA	2:B:95:GLY:HA3	1.89	0.55
2:B:151:THR:HG21	2:B:190:SER:HB3	1.89	0.55
2:B:171:VAL:HG12	2:B:206:ASN:HD21	1.72	0.55
2:D:260:VAL:HG11	2:D:266:HIS:HB3	1.88	0.55
2:B:203:SER:O	2:B:204:ILE:HG13	2.06	0.55
2:D:202:TYR:OH	7:D:700:G2N:NAN	2.38	0.55
2:B:14:ASN:HD21	2:B:67:LEU:HB3	1.71	0.55
2:B:162:PRO:HD2	2:B:163:ASP:HB2	1.88	0.55
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.87	0.55
3:E:60:ARG:HH11	3:E:60:ARG:CB	2.12	0.55
1:A:111:GLY:O	1:A:113:GLU:N	2.39	0.55
2:B:171:VAL:CG1	2:B:206:ASN:HD21	2.19	0.55
2:B:210:TYR:CE2	2:B:222:PRO:HG2	2.42	0.55
3:E:67:GLU:C	3:E:69:LEU:H	2.08	0.55
2:B:2:ARG:HD2	2:B:131:CYS:SG	2.46	0.55
1:C:75:ILE:HG21	1:C:94:THR:HG22	1.89	0.55
1:A:8:HIS:CD2	1:A:17:GLY:CA	2.88	0.55
1:A:183:GLU:CB	1:A:184:PRO:HD3	2.30	0.55
2:D:416:MET:O	2:D:420:GLU:HB2	2.06	0.55
2:D:316:ALA:HB1	7:D:700:G2N:CAI	2.37	0.55
1:C:404:PHE:HE1	2:D:347:ILE:HG21	1.72	0.55
2:B:427:ASP:O	2:B:431:GLU:HG3	2.07	0.54
1:C:179:THR:O	2:D:352:LYS:HG3	2.07	0.54
1:C:78:VAL:C	1:C:80:THR:H	2.11	0.54
2:B:313:LEU:HB2	2:B:380:ASN:O	2.06	0.54
1:C:260:VAL:O	1:C:260:VAL:HG23	2.07	0.54
1:C:344:VAL:HG13	1:C:346:TRP:H	1.72	0.54
1:A:260:VAL:O	1:A:260:VAL:HG23	2.06	0.54
2:B:274:PRO:C	2:B:275:LEU:HG	2.26	0.54
2:D:391:ILE:HG13	2:D:392:SER:N	2.21	0.54
1:A:70:LEU:HD12	1:A:145:THR:CB	2.32	0.54
2:B:191:VAL:HG11	2:B:425:MET:HE2	1.88	0.54
2:D:285:ALA:O	2:D:287:THR:HG22	2.07	0.54
2:B:7:ILE:O	2:B:137:LEU:HA	2.07	0.54
3:E:84:GLN:C	3:E:86:ALA:N	2.61	0.54
2:B:158:ARG:O	2:B:159:GLU:HB3	2.07	0.54
1:A:181:VAL:H	2:B:258:ASN:ND2	2.05	0.54
2:B:312:TYR:HE2	2:B:377:PHE:CZ	2.23	0.54
1:C:101:ASN:ND2	2:D:254:LYS:HG2	2.23	0.54
1:C:102:ASN:C	1:C:102:ASN:ND2	2.61	0.54
2:D:191:VAL:HG11	2:D:425:MET:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:NH2	2:B:253:ARG:HH21	1.98	0.54
1:A:408:TYR:C	1:A:410:GLY:N	2.60	0.54
1:A:34:GLY:O	1:A:61:HIS:HB2	2.07	0.54
2:B:265:LEU:CB	2:B:432:TYR:CE2	2.91	0.54
1:C:72:PRO:O	1:C:74:VAL:N	2.41	0.54
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.42	0.54
2:D:321:GLY:O	2:D:323:MET:N	2.40	0.54
2:D:296:PHE:HE1	2:D:332:MET:HE3	1.73	0.53
2:B:55:GLU:HB3	2:B:61:TYR:CD2	2.42	0.53
1:C:266:HIS:O	1:C:268:PRO:HD3	2.08	0.53
3:E:74:GLU:C	3:E:76:ARG:N	2.62	0.53
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.43	0.53
2:D:10:GLY:O	2:D:14:ASN:N	2.37	0.53
1:C:102:ASN:HD21	1:C:104:ALA:HB3	1.73	0.53
1:C:431:ASP:O	1:C:435:VAL:HG23	2.08	0.53
2:D:163:ASP:HB3	2:D:164:ARG:HG2	1.91	0.53
1:A:401:LYS:C	1:A:403:ALA:H	2.12	0.53
1:A:88:HIS:HB2	1:A:91:GLN:NE2	2.24	0.53
2:B:8:GLN:OE1	2:B:67:LEU:HD23	2.09	0.53
1:C:190:THR:CG2	1:C:191:THR:H	2.22	0.53
1:A:316:CYS:O	1:A:377:MET:HA	2.08	0.53
2:B:345:GLU:OE1	2:B:345:GLU:N	2.42	0.53
1:C:143:GLY:HA3	4:C:600:GTP:H5'	1.89	0.53
1:C:200:CYS:HA	1:C:266:HIS:HB3	1.89	0.53
1:A:68:VAL:CG1	1:A:93:ILE:HB	2.37	0.53
2:D:191:VAL:HG11	2:D:425:MET:CE	2.39	0.53
1:C:313:MET:HG2	1:C:380:ASN:O	2.08	0.53
1:C:6:SER:HB3	1:C:8:HIS:HE1	1.74	0.53
2:D:88:ARG:HB3	2:D:91:ASN:OD1	2.09	0.53
2:D:210:TYR:CE2	2:D:222:PRO:HG2	2.43	0.53
1:C:406:HIS:CG	2:D:263:PRO:HG3	2.43	0.53
2:B:202:TYR:N	2:B:202:TYR:CD1	2.76	0.52
2:B:21:TRP:CH2	2:B:63:PRO:HB3	2.45	0.52
1:A:185:TYR:OH	1:A:403:ALA:HB3	2.10	0.52
2:B:208:ALA:O	2:B:211:ASP:N	2.42	0.52
1:C:36:MET:HE1	1:C:38:SER:O	2.09	0.52
2:D:242:LEU:HD11	7:D:700:G2N:CAK	2.40	0.52
2:D:276:THR:CG2	2:D:277:SER:N	2.72	0.52
1:A:22:GLU:HB2	1:A:83:TYR:HE1	1.75	0.52
1:C:52:PHE:O	1:C:64:ARG:HB2	2.09	0.52
2:D:251:ASP:HB3	2:D:254:LYS:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:76:ARG:O	3:E:79:GLU:HB2	2.10	0.52
1:A:315:CYS:SG	1:A:377:MET:HE1	2.50	0.52
1:C:177:VAL:O	1:C:177:VAL:HG13	2.09	0.52
2:D:139:HIS:O	2:D:171:VAL:HG23	2.08	0.52
2:D:408:TYR:N	2:D:408:TYR:CD1	2.78	0.52
2:B:164:ARG:HE	2:B:164:ARG:HA	1.75	0.52
2:B:200:GLU:OE2	2:B:268:PHE:HE1	1.92	0.52
1:C:187:SER:O	1:C:191:THR:HB	2.10	0.52
1:C:407:TRP:CG	2:D:257:VAL:HG22	2.45	0.52
2:D:15:GLN:HG3	2:D:15:GLN:O	2.10	0.52
1:C:183:GLU:CB	1:C:184:PRO:CD	2.78	0.52
1:C:251:ASP:O	1:C:255:PHE:CB	2.58	0.52
2:D:318:VAL:HA	2:D:354:ALA:O	2.09	0.52
2:D:255:LEU:HD21	7:D:700:G2N:HABB	1.92	0.52
2:B:313:LEU:HD12	2:B:347:ILE:HD11	1.92	0.52
2:B:313:LEU:CD1	2:B:347:ILE:HD11	2.39	0.52
1:C:167:LEU:HD13	1:C:252:LEU:HD11	1.91	0.52
3:E:19:SER:O	3:E:20:PHE:HB3	2.09	0.52
2:B:237:GLY:CA	2:B:376:THR:HG21	2.40	0.52
1:C:20:CYS:HB3	1:C:232:GLY:HA2	1.91	0.52
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.10	0.51
2:D:273:ALA:HB2	2:D:375:ALA:N	2.22	0.51
2:D:51:VAL:CG1	2:D:52:TYR:HD1	2.23	0.51
1:C:204:VAL:HG22	1:C:302:MET:CE	2.40	0.51
1:C:182:VAL:HG12	2:D:258:ASN:HD21	1.75	0.51
2:D:271:GLY:HA2	2:D:302:MET:HG2	1.92	0.51
2:D:282:GLN:HG3	2:D:286:LEU:HD21	1.92	0.51
1:A:249:ASN:HD22	1:A:254:GLU:HG2	1.75	0.51
1:A:72:PRO:O	1:A:74:VAL:N	2.44	0.51
2:B:260:VAL:HG11	2:B:266:HIS:HB3	1.91	0.51
1:C:427:ALA:O	1:C:430:LYS:HB3	2.11	0.51
2:D:224:TYR:CE2	6:D:600:GDP:C5	2.97	0.51
2:D:13:GLY:CA	2:D:139:HIS:HA	2.40	0.51
1:A:419:SER:O	1:A:423:GLU:HG2	2.11	0.51
1:A:404:PHE:HE1	2:B:347:ILE:HG21	1.76	0.51
1:C:407:TRP:CD2	2:D:257:VAL:HG22	2.45	0.51
2:D:224:TYR:OH	6:D:600:GDP:H2'	2.11	0.51
1:C:267:PHE:CD1	1:C:267:PHE:N	2.79	0.51
2:D:276:THR:HG21	2:D:280:SER:HB3	1.93	0.51
1:A:190:THR:CG2	1:A:191:THR:H	2.24	0.51
2:D:154:ILE:HA	2:D:157:ILE:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HD11	1:A:121:ARG:HD2	1.92	0.51
2:B:70:LEU:HD12	2:B:145:THR:HB	1.93	0.51
1:A:398:MET:HG3	2:B:348:PRO:HD3	1.91	0.51
2:B:381:SER:O	2:B:384:ILE:HB	2.10	0.51
1:C:291:ILE:HD12	1:C:375:VAL:CG2	2.41	0.51
2:D:255:LEU:O	7:D:700:G2N:NAC	2.44	0.51
2:D:350:ASN:H	2:D:350:ASN:ND2	2.06	0.51
2:D:21:TRP:CH2	2:D:63:PRO:HB3	2.46	0.51
1:C:190:THR:O	1:C:194:THR:HB	2.10	0.51
2:D:165:ILE:HD11	2:D:252:LEU:HG	1.93	0.51
2:D:287:THR:CG2	2:D:290:GLU:HB2	2.38	0.51
3:E:123:LEU:C	3:E:125:GLU:H	2.13	0.51
1:A:99:ALA:HB3	1:A:145:THR:HG22	1.93	0.50
1:A:8:HIS:HD2	1:A:17:GLY:HA3	1.75	0.50
2:B:76:ASP:O	2:B:80:SER:HB2	2.11	0.50
3:E:129:HIS:O	3:E:133:VAL:HG22	2.11	0.50
1:A:102:ASN:ND2	1:A:102:ASN:C	2.64	0.50
1:C:315:CYS:SG	1:C:377:MET:HE1	2.51	0.50
1:C:405:VAL:CG1	1:C:406:HIS:N	2.75	0.50
1:C:80:THR:HG22	1:C:81:GLY:N	2.26	0.50
2:D:2:ARG:HD2	2:D:131:CYS:SG	2.52	0.50
1:A:406:HIS:CG	2:B:263:PRO:HG3	2.46	0.50
2:B:306:ASP:C	2:B:308:ARG:N	2.63	0.50
2:B:88:ARG:HB3	2:B:91:ASN:OD1	2.11	0.50
1:C:401:LYS:C	1:C:403:ALA:H	2.14	0.50
1:C:34:GLY:O	1:C:61:HIS:HB2	2.11	0.50
2:D:224:TYR:CD2	6:D:600:GDP:C5	2.99	0.50
2:D:275:LEU:O	2:D:276:THR:HB	2.11	0.50
1:A:315:CYS:SG	1:A:377:MET:CE	3.00	0.50
2:B:155:SER:HB3	3:E:76:ARG:HH22	1.76	0.50
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.93	0.50
2:B:114:LEU:HD12	2:B:117:SER:HB2	1.92	0.50
2:B:15:GLN:O	2:B:15:GLN:HG3	2.12	0.50
2:B:54:ASN:HD22	2:B:64:ARG:HD2	1.77	0.50
2:B:34:GLY:HA2	2:B:60:LYS:HE2	1.93	0.50
1:C:165:SER:OG	1:C:252:LEU:HD12	2.12	0.50
2:D:251:ASP:HB2	2:D:254:LYS:HB2	1.93	0.50
2:B:205:ASP:OD1	2:B:207:GLU:HB3	2.11	0.49
1:C:85:GLN:HA	1:C:85:GLN:NE2	2.23	0.49
2:D:135:PHE:HZ	2:D:161:TYR:CD1	2.30	0.49
2:D:21:TRP:O	2:D:25:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:VAL:O	1:A:438:ASP:CB	2.60	0.49
2:B:135:PHE:HZ	2:B:161:TYR:CD1	2.30	0.49
2:B:224:TYR:CE2	6:B:600:GDP:C4	2.99	0.49
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.47	0.49
2:D:20:PHE:O	2:D:24:ILE:HG23	2.12	0.49
2:B:316:ALA:HB1	7:B:700:G2N:CAI	2.42	0.49
1:C:6:SER:HB3	1:C:8:HIS:CE1	2.47	0.49
1:C:341:ILE:HD13	1:C:341:ILE:H	1.77	0.49
2:D:118:VAL:O	2:D:122:VAL:HG13	2.12	0.49
3:E:118:ALA:O	3:E:122:ARG:CZ	2.59	0.49
1:A:78:VAL:C	1:A:80:THR:H	2.14	0.49
2:B:192:HIS:HD2	2:B:421:ALA:CA	2.21	0.49
2:B:236:SER:O	2:B:240:THR:HG23	2.12	0.49
1:C:273:ALA:CB	1:C:274:PRO:CD	2.78	0.49
2:D:151:THR:HG21	2:D:190:SER:HB3	1.94	0.49
2:D:84:GLY:O	2:D:86:ILE:N	2.44	0.49
7:B:700:G2N:OAP	7:B:700:G2N:HAJ	2.13	0.49
1:C:99:ALA:HB3	1:C:145:THR:HG22	1.94	0.49
1:C:387:ALA:HB2	1:C:390:ARG:NH1	2.27	0.49
2:D:135:PHE:CZ	2:D:161:TYR:CD1	3.00	0.49
2:D:224:TYR:CE2	6:D:600:GDP:C4	3.01	0.49
3:E:11:LEU:O	3:E:12:ASN:CB	2.61	0.49
3:E:137:LYS:C	3:E:139:LEU:H	2.16	0.49
1:A:133:GLN:HE21	1:A:252:LEU:HG	1.78	0.49
2:B:205:ASP:HB2	2:B:304:ALA:H	1.78	0.49
2:B:321:GLY:O	2:B:323:MET:N	2.45	0.49
2:B:12:CYS:SG	6:B:600:GDP:C4	3.06	0.49
2:D:402:LYS:HB3	2:D:405:LEU:HD22	1.94	0.49
2:B:234:THR:HG21	2:B:302:MET:HG3	1.95	0.48
2:B:320:ARG:HA	2:B:356:CYS:O	2.13	0.48
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.61	0.48
1:C:185:TYR:OH	1:C:403:ALA:HB3	2.13	0.48
2:D:224:TYR:CD2	6:D:600:GDP:C6	3.01	0.48
3:E:120:LEU:HA	3:E:123:LEU:HD12	1.95	0.48
2:B:357:ASP:O	2:B:359:PRO:HD3	2.13	0.48
1:C:181:VAL:H	2:D:258:ASN:ND2	2.10	0.48
1:C:188:ILE:HG23	1:C:425:MET:HG3	1.95	0.48
2:D:114:LEU:HD12	2:D:117:SER:HB2	1.95	0.48
2:B:276:THR:CG2	2:B:277:SER:N	2.74	0.48
2:B:391:ILE:HG13	2:B:392:SER:H	1.78	0.48
1:C:402:ARG:O	1:C:403:ALA:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:LEU:HD13	2:D:170:SER:HB3	1.95	0.48
2:D:51:VAL:HG13	2:D:52:TYR:HD1	1.78	0.48
2:B:406:HIS:HA	2:B:409:THR:HB	1.94	0.48
2:B:54:ASN:ND2	2:B:64:ARG:HD2	2.28	0.48
1:C:70:LEU:HD12	1:C:145:THR:CB	2.36	0.48
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.76	0.48
1:A:267:PHE:CD1	1:A:267:PHE:N	2.81	0.48
1:A:75:ILE:HG21	1:A:94:THR:HG22	1.96	0.48
1:A:80:THR:HG22	1:A:81:GLY:N	2.28	0.48
1:C:343:PHE:HD1	1:C:349:THR:HG22	1.71	0.48
2:D:202:TYR:CD1	2:D:202:TYR:N	2.81	0.48
2:D:245:PRO:HG2	2:D:246:GLY:H	1.78	0.48
3:E:123:LEU:O	3:E:127:ASP:HB2	2.14	0.48
3:E:81:GLU:O	3:E:84:GLN:N	2.43	0.48
2:B:298:SER:C	2:B:300:ASN:N	2.67	0.48
2:B:308:ARG:NH1	2:B:308:ARG:CG	2.62	0.48
1:C:115:ILE:HD11	1:C:156:ARG:HG3	1.96	0.48
1:C:167:LEU:HD13	1:C:252:LEU:HD13	1.96	0.48
1:C:98:ASP:OD1	1:C:99:ALA:N	2.47	0.48
1:A:171:ILE:O	1:A:171:ILE:HG22	2.14	0.48
1:A:397:LEU:HG	2:B:346:TRP:HA	1.94	0.48
2:D:99:ALA:CB	2:D:145:THR:CG2	2.85	0.48
2:D:381:SER:O	2:D:384:ILE:HB	2.14	0.48
2:B:209:LEU:HB3	2:B:227:LEU:CD1	2.43	0.47
2:D:229:HIS:CE1	2:D:277:SER:HB3	2.49	0.47
2:D:2:ARG:CZ	2:D:133:GLN:HB2	2.44	0.47
2:B:251:ASP:HB3	2:B:254:LYS:H	1.78	0.47
2:B:287:THR:HG23	2:B:290:GLU:HB2	1.95	0.47
2:B:403:ALA:C	2:B:405:LEU:N	2.62	0.47
2:D:93:VAL:HG21	2:D:118:VAL:HG13	1.96	0.47
2:D:7:ILE:O	2:D:137:LEU:HA	2.14	0.47
2:D:101:ASN:HD22	2:D:143:GLY:HA2	1.78	0.47
2:B:12:CYS:SG	6:B:600:GDP:N3	2.87	0.47
2:D:8:GLN:OE1	2:D:67:LEU:HD23	2.14	0.47
1:A:353:VAL:HG11	3:E:20:PHE:CZ	2.49	0.47
1:A:407:TRP:CG	2:B:257:VAL:HG22	2.49	0.47
2:D:103:TRP:HB2	2:D:186:ASN:OD1	2.13	0.47
2:D:226:ASP:O	2:D:227:LEU:HB2	2.15	0.47
3:E:72:LEU:C	3:E:74:GLU:N	2.67	0.47
1:C:405:VAL:HG13	1:C:406:HIS:N	2.30	0.47
2:D:132:LEU:HG	2:D:133:GLN:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:THR:HG23	6:D:600:GDP:O3B	2.14	0.47
2:D:180:THR:CG2	2:D:182:VAL:HG22	2.44	0.47
1:C:404:PHE:CE1	2:D:347:ILE:HG21	2.49	0.47
2:D:251:ASP:HB2	2:D:254:LYS:HD3	1.96	0.47
3:E:78:HIS:CD2	3:E:78:HIS:C	2.87	0.47
1:A:431:ASP:O	1:A:435:VAL:HG23	2.15	0.47
2:B:167:ASN:ND2	2:B:252:LEU:HD11	2.30	0.47
2:B:203:SER:C	2:B:204:ILE:HG13	2.35	0.47
1:C:275:VAL:HG23	1:C:275:VAL:O	2.15	0.47
1:C:317:LEU:CD2	1:C:377:MET:HE3	2.44	0.47
2:D:158:ARG:O	2:D:159:GLU:HB3	2.13	0.47
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.97	0.47
1:A:117:LEU:HD11	1:A:121:ARG:NH2	2.30	0.47
1:A:310:GLY:HA3	1:A:383:ALA:HB2	1.97	0.47
2:B:350:ASN:ND2	2:B:350:ASN:C	2.67	0.47
1:C:191:THR:HG23	1:C:425:MET:CE	2.45	0.47
2:D:276:THR:HG21	2:D:280:SER:CB	2.44	0.47
3:E:118:ALA:O	3:E:122:ARG:NH2	2.47	0.47
2:B:171:VAL:CG1	2:B:206:ASN:ND2	2.77	0.47
2:D:164:ARG:HE	2:D:164:ARG:CA	2.27	0.47
1:A:182:VAL:CG2	1:A:182:VAL:O	2.62	0.47
1:A:294:ALA:O	1:A:297:GLU:HB3	2.15	0.47
2:B:312:TYR:CD2	2:B:315:VAL:CG2	2.98	0.47
1:C:8:HIS:CD2	1:C:17:GLY:CA	2.97	0.47
2:D:177:VAL:O	2:D:177:VAL:HG12	2.15	0.47
2:D:307:PRO:HB2	2:D:312:TYR:CZ	2.50	0.47
3:E:78:HIS:O	3:E:81:GLU:HB2	2.14	0.47
2:B:163:ASP:HB3	2:B:164:ARG:HG2	1.96	0.47
2:D:202:TYR:OH	7:D:700:G2N:CAU	2.63	0.47
2:B:20:PHE:HD2	2:B:235:MET:HB3	1.80	0.46
2:D:5:VAL:HG13	2:D:132:LEU:CD1	2.44	0.46
1:A:313:MET:HG2	1:A:380:ASN:O	2.16	0.46
2:B:296:PHE:HE1	2:B:332:MET:CE	2.28	0.46
2:B:325:MET:HG2	2:B:355:VAL:HG21	1.97	0.46
1:C:48:SER:O	1:C:243:ARG:O	2.31	0.46
2:D:245:PRO:HB2	2:D:247:GLN:HG3	1.98	0.46
2:D:358:ILE:O	2:D:358:ILE:CG2	2.62	0.46
2:D:12:CYS:SG	6:D:600:GDP:C4	3.08	0.46
1:A:372:GLN:HG2	1:A:372:GLN:H	1.44	0.46
2:D:229:HIS:CE1	2:D:277:SER:CB	2.99	0.46
3:E:59:GLU:OE1	3:E:59:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:OH	1:A:107:HIS:ND1	2.45	0.46
2:D:200:GLU:HA	2:D:266:HIS:HB2	1.96	0.46
2:D:70:LEU:HA	2:D:95:GLY:HA3	1.97	0.46
3:E:22:VAL:CG1	3:E:22:VAL:O	2.61	0.46
2:B:103:TRP:HB2	2:B:186:ASN:OD1	2.15	0.46
2:B:400:ARG:O	2:B:402:LYS:N	2.48	0.46
2:B:13:GLY:CA	2:B:139:HIS:HA	2.45	0.46
2:B:154:ILE:HA	2:B:157:ILE:HB	1.97	0.46
2:B:70:LEU:CA	2:B:95:GLY:HA3	2.46	0.46
1:C:316:CYS:O	1:C:377:MET:HA	2.14	0.46
1:A:312:TYR:HE2	1:A:379:SER:HB3	1.81	0.46
2:D:203:SER:C	2:D:204:ILE:HG13	2.36	0.46
2:D:350:ASN:HD22	2:D:350:ASN:N	2.02	0.46
1:A:88:HIS:CD2	1:A:90:GLU:OE1	2.69	0.46
2:B:135:PHE:CZ	2:B:161:TYR:CD1	3.04	0.46
2:B:401:ARG:NH2	1:C:434:GLU:O	2.38	0.46
2:D:131:CYS:O	2:D:131:CYS:SG	2.73	0.46
2:D:192:HIS:O	2:D:195:VAL:HG12	2.16	0.46
1:A:217:LEU:HB3	1:A:219:ILE:HG12	1.96	0.45
2:B:245:PRO:HG2	2:B:246:GLY:H	1.81	0.45
1:C:248:LEU:HD22	1:C:249:ASN:H	1.81	0.45
1:C:254:GLU:O	1:C:254:GLU:HG2	2.16	0.45
2:D:28:HIS:HA	2:D:43:GLN:HB3	1.98	0.45
2:D:30:ILE:HG22	2:D:31:ASP:O	2.17	0.45
2:D:312:TYR:CE2	2:D:377:PHE:CZ	2.95	0.45
3:E:49:GLU:HG3	3:E:49:GLU:O	2.16	0.45
1:A:187:SER:O	1:A:191:THR:HB	2.15	0.45
1:A:47:ASP:O	1:A:48:SER:HB2	2.15	0.45
1:C:97:GLU:OE1	2:D:164:ARG:NH2	2.43	0.45
2:D:122:VAL:CG2	2:D:123:ARG:N	2.79	0.45
2:D:274:PRO:C	2:D:275:LEU:HG	2.35	0.45
2:D:142:GLY:O	6:D:600:GDP:H5"	2.17	0.45
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.97	0.45
2:B:154:ILE:HG13	2:B:155:SER:N	2.31	0.45
2:D:344:VAL:HG22	2:D:346:TRP:NE1	2.31	0.45
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.73	0.45
2:B:342:TYR:HA	2:B:342:TYR:HD2	1.62	0.45
2:D:311:ARG:HH21	2:D:344:VAL:HG22	1.81	0.45
2:D:388:PHE:CD2	2:D:425:MET:CE	3.00	0.45
1:A:31:GLN:HA	1:A:32:PRO:HD2	1.83	0.45
1:A:6:SER:HB3	1:A:8:HIS:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLN:NE2	2:B:85:GLN:H	2.14	0.45
1:A:79:ARG:HD3	1:A:92:LEU:HD13	1.98	0.45
1:C:51:THR:HB	1:C:52:PHE:HD1	1.82	0.45
2:D:344:VAL:HG22	2:D:346:TRP:HE1	1.81	0.45
1:A:152:LEU:HA	1:A:155:GLU:HG3	1.99	0.45
1:A:343:PHE:HD1	1:A:349:THR:HG22	1.81	0.45
2:B:177:VAL:HG12	2:B:177:VAL:O	2.15	0.45
2:B:294:GLN:HE21	2:B:294:GLN:HB2	1.62	0.45
2:D:11:GLN:HB3	6:D:600:GDP:O1A	2.17	0.45
2:D:135:PHE:HB2	2:D:166:MET:HE2	1.90	0.45
2:D:253:ARG:O	2:D:254:LYS:C	2.55	0.45
2:B:16:ILE:HG22	2:B:17:GLY:N	2.32	0.45
1:C:102:ASN:C	1:C:102:ASN:HD22	2.20	0.45
1:C:251:ASP:O	1:C:255:PHE:HB2	2.16	0.45
2:D:385:GLN:HG2	2:D:389:LYS:HD2	1.97	0.45
1:A:229:ARG:NH1	1:A:229:ARG:CG	2.76	0.45
2:B:270:PRO:CD	2:B:302:MET:HB2	2.37	0.45
2:B:224:TYR:CD2	6:B:600:GDP:C6	3.05	0.45
1:C:123:ARG:HD2	1:C:161:TYR:OH	2.16	0.45
2:B:164:ARG:CA	2:B:164:ARG:HE	2.29	0.45
2:B:248:LEU:HD23	2:B:248:LEU:HA	1.54	0.45
2:B:165:ILE:HD11	2:B:252:LEU:HG	1.98	0.45
1:C:190:THR:CG2	1:C:191:THR:N	2.80	0.45
2:D:70:LEU:HD12	2:D:145:THR:HB	1.99	0.45
2:D:403:ALA:C	2:D:405:LEU:H	2.20	0.45
2:D:195:VAL:HG21	2:D:428:LEU:HD22	1.97	0.45
1:A:206:ASN:HD21	4:A:600:GTP:N2	2.06	0.44
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.81	0.44
2:B:209:LEU:HA	2:B:209:LEU:HD12	1.70	0.44
2:B:51:VAL:CG1	2:B:52:TYR:N	2.80	0.44
2:B:85:GLN:HE21	2:B:85:GLN:N	2.15	0.44
1:C:68:VAL:CG1	1:C:93:ILE:HB	2.47	0.44
2:D:153:LEU:O	2:D:157:ILE:N	2.46	0.44
2:D:388:PHE:CE1	2:D:428:LEU:HD21	2.53	0.44
2:D:55:GLU:HG3	2:D:55:GLU:H	1.50	0.44
2:D:70:LEU:C	2:D:95:GLY:HA3	2.37	0.44
2:B:30:ILE:HG22	2:B:31:ASP:O	2.17	0.44
2:D:261:PRO:HG2	2:D:262:PHE:H	1.82	0.44
3:E:99:GLU:C	3:E:101:LEU:N	2.70	0.44
2:B:102:ASN:OD1	2:B:102:ASN:O	2.35	0.44
2:B:298:SER:O	2:B:300:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:GLY:O	1:C:112:LYS:C	2.55	0.44
1:C:36:MET:HA	1:C:37:PRO:HD3	1.86	0.44
2:D:167:ASN:OD1	2:D:200:GLU:HG3	2.18	0.44
1:A:247:ALA:HB1	3:E:12:ASN:HB3	1.99	0.44
1:A:252:LEU:O	1:A:253:THR:C	2.55	0.44
1:A:260:VAL:HA	1:A:261:PRO:HD3	1.80	0.44
2:B:208:ALA:O	2:B:209:LEU:C	2.56	0.44
2:B:270:PRO:HA	2:B:377:PHE:O	2.18	0.44
1:C:153:LEU:HD13	1:C:157:LEU:CD1	2.43	0.44
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.99	0.44
2:B:408:TYR:O	2:B:409:THR:C	2.55	0.44
1:C:82:THR:O	1:C:83:TYR:CG	2.71	0.44
2:D:205:ASP:OD1	2:D:207:GLU:HB3	2.17	0.44
2:D:298:SER:C	2:D:300:ASN:N	2.71	0.44
2:D:62:VAL:HA	2:D:63:PRO:HD2	1.75	0.44
1:A:20:CYS:HB3	1:A:232:GLY:HA2	1.99	0.44
2:B:292:THR:C	2:B:294:GLN:H	2.21	0.44
1:C:133:GLN:NE2	1:C:252:LEU:HG	2.32	0.44
1:C:391:LEU:O	1:C:392:ASP:C	2.54	0.44
2:D:180:THR:HG22	2:D:182:VAL:H	1.82	0.44
2:D:251:ASP:CB	2:D:254:LYS:HB2	2.48	0.44
1:A:178:SER:OG	1:A:179:THR:N	2.51	0.44
2:D:151:THR:HA	2:D:154:ILE:HG12	1.98	0.44
2:D:51:VAL:O	2:D:64:ARG:NH2	2.51	0.44
2:B:118:VAL:O	2:B:122:VAL:HG13	2.18	0.44
1:C:163:LYS:O	1:C:164:LYS:C	2.56	0.44
3:E:76:ARG:O	3:E:79:GLU:N	2.51	0.44
2:D:239:THR:O	2:D:240:THR:C	2.56	0.43
2:D:248:LEU:HD23	2:D:248:LEU:HA	1.76	0.43
2:D:273:ALA:HB3	2:D:375:ALA:H	1.80	0.43
1:A:102:ASN:HD21	1:A:104:ALA:HB3	1.82	0.43
1:A:141:PHE:O	1:A:147:SER:HB3	2.18	0.43
1:A:183:GLU:CB	1:A:184:PRO:CD	2.88	0.43
1:A:79:ARG:HH22	1:A:94:THR:CG2	2.28	0.43
2:B:183:GLU:N	2:B:184:PRO:HD2	2.33	0.43
1:C:115:ILE:HG23	1:C:116:ASP:N	2.34	0.43
1:C:262:TYR:HB2	1:C:265:ILE:HD13	2.00	0.43
2:D:260:VAL:HA	2:D:261:PRO:HD2	1.78	0.43
2:D:325:MET:HA	2:D:328:VAL:HG23	2.01	0.43
1:C:102:ASN:HD22	1:C:103:TYR:N	2.17	0.43
2:D:308:ARG:NH1	2:D:308:ARG:HG3	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:84:GLN:HA	3:E:87:ILE:HG22	2.00	0.43
1:A:329:ASN:HD22	1:A:329:ASN:N	2.17	0.43
1:A:341:ILE:H	1:A:341:ILE:HD13	1.83	0.43
2:B:245:PRO:CG	2:B:246:GLY:H	2.31	0.43
1:C:178:SER:OG	1:C:179:THR:N	2.52	0.43
1:A:178:SER:HB3	2:B:352:LYS:NZ	2.34	0.43
1:A:190:THR:O	1:A:192:HIS:N	2.52	0.43
2:B:28:HIS:HA	2:B:43:GLN:HB3	1.99	0.43
1:C:115:ILE:CD1	1:C:156:ARG:HG3	2.48	0.43
1:C:294:ALA:O	1:C:297:GLU:HB3	2.18	0.43
2:B:224:TYR:CD2	6:B:600:GDP:C5	3.07	0.43
1:A:411:GLU:O	3:E:61:ARG:NH1	2.52	0.43
1:A:317:LEU:HD23	1:A:377:MET:HE3	1.99	0.42
1:A:8:HIS:CE1	1:A:67:PHE:HE1	2.37	0.42
2:B:251:ASP:CB	2:B:254:LYS:HB2	2.49	0.42
1:C:2:ARG:HB2	1:C:131:GLY:O	2.19	0.42
2:D:317:ALA:HB3	2:D:353:THR:HG22	2.00	0.42
1:C:185:TYR:CD1	1:C:418:PHE:HE2	2.37	0.42
2:D:383:ALA:O	2:D:386:GLU:CB	2.65	0.42
2:B:387:LEU:O	2:B:390:ARG:CG	2.60	0.42
1:C:141:PHE:O	1:C:147:SER:HB3	2.19	0.42
1:C:267:PHE:HA	1:C:268:PRO:HD3	1.85	0.42
1:C:391:LEU:HA	1:C:391:LEU:HD12	1.87	0.42
2:D:288:VAL:HG11	2:D:327:GLU:HG2	2.01	0.42
2:D:107:HIS:O	2:D:152:LEU:HD22	2.20	0.42
2:D:226:ASP:O	2:D:227:LEU:CB	2.67	0.42
1:A:163:LYS:O	1:A:164:LYS:C	2.58	0.42
1:A:344:VAL:HG13	1:A:346:TRP:H	1.85	0.42
2:B:138:THR:O	2:B:139:HIS:HB3	2.19	0.42
2:B:387:LEU:HA	2:B:390:ARG:HG2	2.01	0.42
1:C:168:GLU:HG2	1:C:201:ALA:CB	2.49	0.42
1:C:168:GLU:HG2	1:C:201:ALA:HB1	2.02	0.42
1:C:291:ILE:HB	1:C:375:VAL:HG23	2.00	0.42
2:D:122:VAL:HG22	2:D:123:ARG:N	2.34	0.42
2:D:7:ILE:HG21	2:D:153:LEU:HD13	2.02	0.42
1:A:8:HIS:HD2	1:A:17:GLY:CA	2.30	0.42
2:B:409:THR:HG22	2:B:410:GLY:N	2.34	0.42
1:C:171:ILE:HG22	1:C:171:ILE:O	2.18	0.42
1:C:172:TYR:HA	1:C:173:PRO:HD3	1.74	0.42
2:B:238:VAL:HG13	2:B:378:ILE:HD11	2.02	0.42
2:B:384:ILE:CG2	2:B:432:TYR:CE1	3.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ILE:HD11	1:C:119:LEU:HD13	2.02	0.42
1:C:3:GLU:HB2	1:C:132:LEU:HA	2.02	0.42
2:D:391:ILE:HA	2:D:394:GLN:NE2	2.35	0.42
1:A:312:TYR:HE2	1:A:379:SER:CB	2.33	0.42
2:B:205:ASP:HB3	2:B:208:ALA:H	1.84	0.42
1:A:174:ALA:HA	1:A:175:PRO:HD2	1.65	0.42
2:B:273:ALA:CB	2:B:375:ALA:H	2.33	0.42
2:B:400:ARG:C	2:B:402:LYS:N	2.72	0.42
2:B:5:VAL:HG23	2:B:6:HIS:N	2.33	0.42
2:D:308:ARG:NH2	2:D:339:ASN:HD21	2.18	0.42
1:A:247:ALA:CB	3:E:12:ASN:HB3	2.50	0.42
1:A:2:ARG:HB2	1:A:131:GLY:O	2.20	0.42
1:A:244:PHE:CZ	1:A:358:GLN:HG2	2.55	0.42
1:A:384:ILE:O	1:A:384:ILE:HG12	2.20	0.42
1:A:402:ARG:O	1:A:403:ALA:C	2.58	0.42
2:D:172:MET:HA	2:D:173:PRO:HD3	1.91	0.42
3:E:76:ARG:HA	3:E:76:ARG:HD3	1.61	0.42
1:A:291:ILE:HD12	1:A:375:VAL:CG2	2.50	0.41
1:A:88:HIS:O	1:A:89:PRO:C	2.57	0.41
2:B:55:GLU:H	2:B:55:GLU:HG3	1.50	0.41
2:D:384:ILE:HG22	2:D:432:TYR:CD1	2.54	0.41
1:A:387:ALA:HB2	1:A:390:ARG:NH1	2.32	0.41
2:B:325:MET:O	2:B:328:VAL:N	2.53	0.41
1:A:191:THR:HG23	1:A:425:MET:CE	2.50	0.41
1:A:242:LEU:HD23	1:A:249:ASN:O	2.20	0.41
2:B:102:ASN:OD1	2:B:102:ASN:C	2.58	0.41
2:B:85:GLN:HE21	2:B:85:GLN:H	1.67	0.41
2:D:226:ASP:N	2:D:226:ASP:OD1	2.51	0.41
2:D:20:PHE:HD2	2:D:235:MET:HB3	1.86	0.41
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.38	0.41
2:B:122:VAL:CG2	2:B:123:ARG:N	2.82	0.41
1:C:191:THR:O	1:C:195:LEU:HB3	2.20	0.41
1:C:395:PHE:C	1:C:395:PHE:CD2	2.93	0.41
3:E:76:ARG:C	3:E:78:HIS:H	2.24	0.41
3:E:77:GLU:HG2	3:E:80:ARG:CB	2.50	0.41
2:B:209:LEU:HB3	2:B:227:LEU:HD11	2.02	0.41
2:D:347:ILE:HD13	2:D:347:ILE:HG21	1.89	0.41
1:A:115:ILE:O	1:A:119:LEU:HB2	2.21	0.41
1:A:3:GLU:HB2	1:A:132:LEU:HA	2.03	0.41
1:A:49:PHE:CD2	1:A:49:PHE:C	2.94	0.41
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:VAL:HA	1:C:261:PRO:HD3	1.82	0.41
2:D:416:MET:O	2:D:420:GLU:N	2.49	0.41
2:D:47:GLU:HB2	2:D:48:ARG:HG2	2.03	0.41
2:B:135:PHE:HB2	2:B:166:MET:HE2	1.97	0.41
2:B:111:GLY:HA2	2:B:149:MET:HE2	2.03	0.41
2:B:309:HIS:CD2	2:B:386:GLU:OE2	2.74	0.41
2:D:114:LEU:HB3	2:D:149:MET:CE	2.48	0.41
2:D:99:ALA:CB	2:D:145:THR:HG22	2.44	0.41
2:D:229:HIS:O	2:D:232:SER:OG	2.32	0.41
2:D:133:GLN:NE2	2:D:252:LEU:HD22	2.18	0.41
2:D:164:ARG:NH2	2:D:253:ARG:HH22	2.18	0.41
1:A:408:TYR:C	1:A:410:GLY:H	2.24	0.41
2:D:177:VAL:CG1	2:D:177:VAL:O	2.69	0.41
2:B:224:TYR:CE2	6:B:600:GDP:C5	3.08	0.41
2:D:276:THR:HG22	2:D:277:SER:N	2.36	0.41
2:D:307:PRO:HB2	2:D:312:TYR:CE1	2.56	0.41
2:D:319:PHE:HD2	2:D:323:MET:HE2	1.86	0.41
1:A:153:LEU:HA	1:A:153:LEU:HD23	1.83	0.41
2:B:245:PRO:HB2	2:B:247:GLN:HG3	2.03	0.41
2:B:395:PHE:CD2	2:B:395:PHE:C	2.94	0.41
2:D:164:ARG:HA	2:D:164:ARG:NE	2.36	0.41
1:A:98:ASP:OD1	1:A:99:ALA:N	2.53	0.41
2:B:51:VAL:O	2:B:64:ARG:NH2	2.53	0.41
1:C:153:LEU:HA	1:C:153:LEU:HD23	1.84	0.41
2:B:407:TRP:NE1	1:C:257:THR:HA	2.36	0.41
2:D:284:ARG:HD3	2:D:372:LYS:HZ2	1.86	0.41
2:D:288:VAL:HB	2:D:289:PRO:CD	2.49	0.41
3:E:120:LEU:O	3:E:123:LEU:HB2	2.21	0.41
3:E:88:GLU:HA	3:E:91:ASN:HD21	1.85	0.41
2:B:385:GLN:HE21	2:B:389:LYS:HD2	1.85	0.40
2:D:205:ASP:HB3	2:D:208:ALA:H	1.85	0.40
2:D:408:TYR:HD1	2:D:408:TYR:N	2.19	0.40
3:E:84:GLN:O	3:E:86:ALA:N	2.54	0.40
2:B:2:ARG:CZ	2:B:133:GLN:HB2	2.51	0.40
1:C:242:LEU:HG	1:C:242:LEU:H	1.70	0.40
1:C:287:SER:O	1:C:291:ILE:HG12	2.21	0.40
2:D:54:ASN:ND2	2:D:64:ARG:HD2	2.36	0.40
1:A:49:PHE:C	1:A:49:PHE:HD2	2.25	0.40
2:B:293:GLN:H	2:B:293:GLN:HG3	1.60	0.40
2:B:6:HIS:CE1	2:B:8:GLN:HB2	2.56	0.40
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:LEU:HB3	1:C:219:ILE:HG12	2.02	0.40
1:C:41:THR:HG21	1:C:61:HIS:HE1	1.87	0.40
2:B:114:LEU:CD1	2:B:117:SER:HB2	2.51	0.40
2:B:158:ARG:HA	2:B:161:TYR:O	2.22	0.40
2:D:194:LEU:O	2:D:196:GLU:N	2.54	0.40
2:D:76:ASP:O	2:D:80:SER:HB2	2.22	0.40
2:D:81:GLY:HA3	2:D:82:PRO:HD3	1.93	0.40
1:A:358:GLN:HA	1:A:359:PRO:HD3	1.92	0.40
1:A:50:ASN:HA	1:A:50:ASN:HD22	1.75	0.40
1:A:53:PHE:CD1	1:A:53:PHE:N	2.89	0.40
1:A:55:GLU:HG2	1:A:61:HIS:CE1	2.56	0.40
2:B:153:LEU:O	2:B:157:ILE:N	2.51	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	424/451 (94%)	330 (78%)	68 (16%)	26 (6%)	1	19
1	C	423/451 (94%)	337 (80%)	61 (14%)	25 (6%)	1	19
2	B	415/445 (93%)	301 (72%)	80 (19%)	34 (8%)	1	13
2	D	425/445 (96%)	298 (70%)	85 (20%)	42 (10%)	0	9
3	E	119/142 (84%)	81 (68%)	24 (20%)	14 (12%)	0	6
All	All	1806/1934 (93%)	1347 (75%)	318 (18%)	141 (8%)	1	14

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	72	PRO

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Mol	Chain	Res	Type
1	A	73	THR
1	A	112	LYS
1	A	265	ILE
1	A	341	ILE
1	A	348	PRO
1	A	377	MET
1	A	403	ALA
2	B	34	GLY
2	B	42	LEU
2	B	43	GLN
2	B	62	VAL
2	B	82	PRO
2	B	162	PRO
2	B	163	ASP
2	B	227	LEU
2	B	245	PRO
2	B	288	VAL
2	B	299	LYS
2	B	348	PRO
2	B	400	ARG
2	B	403	ALA
2	B	404	PHE
1	C	72	PRO
1	C	73	THR
1	C	112	LYS
1	C	191	THR
1	C	253	THR
1	C	257	THR
1	C	265	ILE
1	C	341	ILE
1	C	348	PRO
1	C	377	MET
1	C	403	ALA
1	C	437	VAL
2	D	42	LEU
2	D	43	GLN
2	D	62	VAL
2	D	73	GLY
2	D	82	PRO
2	D	163	ASP
2	D	245	PRO
2	D	288	VAL

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Mol	Chain	Res	Type
2	D	348	PRO
2	D	371	LEU
2	D	400	ARG
2	D	403	ALA
3	E	46	SER
3	E	49	GLU
3	E	81	GLU
3	E	82	VAL
1	A	32	PRO
1	A	83	TYR
1	A	162	GLY
1	A	164	LYS
1	A	191	THR
1	A	247	ALA
1	A	279	GLU
1	A	350	GLY
1	A	392	ASP
1	A	429	GLU
1	A	437	VAL
2	B	3	GLU
2	B	60	LYS
2	B	73	GLY
2	B	226	ASP
2	B	244	PHE
2	B	249	ASN
2	B	322	ARG
2	B	371	LEU
2	B	401	ARG
2	B	415	GLU
1	C	83	TYR
1	C	162	GLY
1	C	164	LYS
1	C	429	GLU
2	D	3	GLU
2	D	34	GLY
2	D	60	LYS
2	D	115	VAL
2	D	162	PRO
2	D	227	LEU
2	D	244	PHE
2	D	249	ASN
2	D	264	ARG

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Mol	Chain	Res	Type
2	D	278	ARG
2	D	299	LYS
2	D	322	ARG
2	D	402	LYS
2	D	404	PHE
3	E	12	ASN
3	E	139	LEU
1	A	33	ASP
1	A	248	LEU
1	A	273	ALA
2	B	119	LEU
2	B	240	THR
2	B	264	ARG
2	B	276	THR
1	C	32	PRO
1	C	48	SER
1	C	273	ALA
1	C	350	GLY
2	D	85	GLN
2	D	240	THR
2	D	279	GLY
2	D	405	LEU
2	D	415	GLU
3	E	75	LYS
3	E	85	LYS
1	A	245	ASP
1	A	329	ASN
2	B	115	VAL
2	B	273	ALA
2	B	307	PRO
2	B	409	THR
1	C	392	ASP
2	D	220	THR
2	D	273	ALA
2	D	293	GLN
3	E	26	PRO
3	E	28	SER
3	E	102	ALA
3	E	124	GLN
1	C	79	ARG
1	C	245	ASP
2	D	195	VAL

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Mol	Chain	Res	Type
2	D	283	TYR
2	D	285	ALA
3	E	7	GLU
3	E	77	GLU
1	A	391	LEU
2	D	307	PRO
2	D	437	ASP
2	D	306	ASP
2	B	177	VAL
2	D	84	GLY
2	D	177	VAL
1	C	183	GLU
1	C	274	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/378 (92%)	236 (68%)	110 (32%)	0	2
1	C	344/378 (91%)	234 (68%)	110 (32%)	0	2
2	B	350/383 (91%)	228 (65%)	122 (35%)	0	1
2	D	353/383 (92%)	218 (62%)	135 (38%)	0	0
3	E	82/126 (65%)	43 (52%)	39 (48%)	0	0
All	All	1475/1648 (90%)	959 (65%)	516 (35%)	0	1

All (516) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	8	HIS
1	A	11	GLN
1	A	16	ILE
1	A	22	GLU
1	A	23	LEU

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Mol	Chain	Res	Type
1	A	26	LEU
1	A	27	GLU
1	A	36	MET
1	A	48	SER
1	A	49	PHE
1	A	60	LYS
1	A	61	HIS
1	A	62	VAL
1	A	68	VAL
1	A	73	THR
1	A	74	VAL
1	A	79	ARG
1	A	80	THR
1	A	85	GLN
1	A	88	HIS
1	A	92	LEU
1	A	94	THR
1	A	96	LYS
1	A	102	ASN
1	A	105	ARG
1	A	110	ILE
1	A	112	LYS
1	A	114	ILE
1	A	115	ILE
1	A	119	LEU
1	A	120	ASP
1	A	123	ARG
1	A	124	LYS
1	A	140	SER
1	A	141	PHE
1	A	145	THR
1	A	153	LEU
1	A	155	GLU
1	A	157	LEU
1	A	158	SER
1	A	160	ASP
1	A	163	LYS
1	A	164	LYS
1	A	167	LEU
1	A	176	GLN
1	A	179	THR
1	A	187	SER

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Mol	Chain	Res	Type
1	A	191	THR
1	A	193	THR
1	A	194	THR
1	A	195	LEU
1	A	196	GLU
1	A	199	ASP
1	A	200	CYS
1	A	206	ASN
1	A	211	ASP
1	A	220	GLU
1	A	223	THR
1	A	226	ASN
1	A	230	LEU
1	A	236	SER
1	A	237	SER
1	A	241	SER
1	A	242	LEU
1	A	245	ASP
1	A	248	LEU
1	A	255	PHE
1	A	256	GLN
1	A	257	THR
1	A	269	LEU
1	A	271	THR
1	A	279	GLU
1	A	284	GLU
1	A	287	SER
1	A	298	PRO
1	A	301	GLN
1	A	304	LYS
1	A	309	HIS
1	A	316	CYS
1	A	318	LEU
1	A	326	LYS
1	A	329	ASN
1	A	334	THR
1	A	341	ILE
1	A	343	PHE
1	A	347	CYS
1	A	349	THR
1	A	356	ASN
1	A	361	THR

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Mol	Chain	Res	Type
1	A	363	VAL
1	A	368	LEU
1	A	370	LYS
1	A	371	VAL
1	A	372	GLN
1	A	375	VAL
1	A	377	MET
1	A	379	SER
1	A	380	ASN
1	A	384	ILE
1	A	386	GLU
1	A	397	LEU
1	A	401	LYS
1	A	402	ARG
1	A	405	VAL
1	A	413	MET
1	A	414	GLU
1	A	415	GLU
1	A	419	SER
1	A	433	GLU
2	B	4	ILE
2	B	5	VAL
2	B	16	ILE
2	B	24	ILE
2	B	25	SER
2	B	27	GLU
2	B	39	ASP
2	B	42	LEU
2	B	43	GLN
2	B	48	ARG
2	B	51	VAL
2	B	55	GLU
2	B	61	TYR
2	B	62	VAL
2	B	67	LEU
2	B	68	VAL
2	B	70	LEU
2	B	71	GLU
2	B	78	VAL
2	B	80	SER
2	B	83	PHE
2	B	85	GLN

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Mol	Chain	Res	Type
2	B	88	ARG
2	B	90	ASP
2	B	93	VAL
2	B	96	GLN
2	B	97	SER
2	B	101	ASN
2	B	102	ASN
2	B	109	THR
2	B	116	ASP
2	B	119	LEU
2	B	120	ASP
2	B	129	CYS
2	B	130	ASP
2	B	131	CYS
2	B	132	LEU
2	B	133	GLN
2	B	135	PHE
2	B	137	LEU
2	B	145	THR
2	B	149	MET
2	B	151	THR
2	B	156	LYS
2	B	158	ARG
2	B	160	GLU
2	B	164	ARG
2	B	165	ILE
2	B	166	MET
2	B	170	SER
2	B	174	SER
2	B	178	SER
2	B	179	ASP
2	B	181	VAL
2	B	190	SER
2	B	196	GLU
2	B	200	GLU
2	B	205	ASP
2	B	209	LEU
2	B	214	PHE
2	B	216	THR
2	B	223	THR
2	B	227	LEU
2	B	230	LEU

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Mol	Chain	Res	Type
2	B	239	THR
2	B	242	LEU
2	B	244	PHE
2	B	248	LEU
2	B	251	ASP
2	B	254	LYS
2	B	260	VAL
2	B	265	LEU
2	B	275	LEU
2	B	276	THR
2	B	286	LEU
2	B	287	THR
2	B	291	LEU
2	B	293	GLN
2	B	294	GLN
2	B	295	MET
2	B	300	ASN
2	B	308	ARG
2	B	309	HIS
2	B	313	LEU
2	B	318	VAL
2	B	323	MET
2	B	325	MET
2	B	329	ASP
2	B	330	GLU
2	B	332	MET
2	B	333	LEU
2	B	335	VAL
2	B	339	ASN
2	B	344	VAL
2	B	347	ILE
2	B	350	ASN
2	B	351	VAL
2	B	356	CYS
2	B	357	ASP
2	B	358	ILE
2	B	374	SER
2	B	376	THR
2	B	380	ASN
2	B	384	ILE
2	B	387	LEU
2	B	389	LYS

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Mol	Chain	Res	Type
2	B	390	ARG
2	B	391	ILE
2	B	393	GLU
2	B	394	GLN
2	B	401	ARG
2	B	405	LEU
2	B	406	HIS
2	B	408	TYR
2	B	409	THR
2	B	416	MET
2	B	417	GLU
2	B	419	THR
2	B	425	MET
2	B	430	SER
2	B	434	GLN
2	B	436	GLN
1	C	2	ARG
1	C	11	GLN
1	C	16	ILE
1	C	23	LEU
1	C	26	LEU
1	C	27	GLU
1	C	36	MET
1	C	38	SER
1	C	41	THR
1	C	49	PHE
1	C	51	THR
1	C	60	LYS
1	C	61	HIS
1	C	62	VAL
1	C	68	VAL
1	C	73	THR
1	C	74	VAL
1	C	79	ARG
1	C	80	THR
1	C	85	GLN
1	C	88	HIS
1	C	92	LEU
1	C	94	THR
1	C	96	LYS
1	C	102	ASN
1	C	105	ARG

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Mol	Chain	Res	Type
1	C	110	ILE
1	C	112	LYS
1	C	114	ILE
1	C	115	ILE
1	C	116	ASP
1	C	119	LEU
1	C	120	ASP
1	C	123	ARG
1	C	124	LYS
1	C	132	LEU
1	C	140	SER
1	C	141	PHE
1	C	151	SER
1	C	153	LEU
1	C	155	GLU
1	C	157	LEU
1	C	158	SER
1	C	160	ASP
1	C	163	LYS
1	C	164	LYS
1	C	167	LEU
1	C	176	GLN
1	C	187	SER
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	199	ASP
1	C	200	CYS
1	C	206	ASN
1	C	211	ASP
1	C	220	GLU
1	C	226	ASN
1	C	230	LEU
1	C	236	SER
1	C	237	SER
1	C	241	SER
1	C	242	LEU
1	C	245	ASP
1	C	248	LEU

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Mol	Chain	Res	Type
1	C	251	ASP
1	C	252	LEU
1	C	254	GLU
1	C	256	GLN
1	C	257	THR
1	C	269	LEU
1	C	271	THR
1	C	287	SER
1	C	301	GLN
1	C	304	LYS
1	C	309	HIS
1	C	316	CYS
1	C	318	LEU
1	C	329	ASN
1	C	334	THR
1	C	341	ILE
1	C	343	PHE
1	C	347	CYS
1	C	349	THR
1	C	356	ASN
1	C	361	THR
1	C	363	VAL
1	C	368	LEU
1	C	370	LYS
1	C	371	VAL
1	C	372	GLN
1	C	375	VAL
1	C	377	MET
1	C	379	SER
1	C	380	ASN
1	C	384	ILE
1	C	386	GLU
1	C	397	LEU
1	C	401	LYS
1	C	402	ARG
1	C	405	VAL
1	C	413	MET
1	C	414	GLU
1	C	415	GLU
1	C	419	SER
1	C	433	GLU
1	C	438	ASP

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Mol	Chain	Res	Type
2	D	4	ILE
2	D	5	VAL
2	D	16	ILE
2	D	24	ILE
2	D	25	SER
2	D	27	GLU
2	D	39	ASP
2	D	42	LEU
2	D	43	GLN
2	D	48	ARG
2	D	51	VAL
2	D	55	GLU
2	D	60	LYS
2	D	61	TYR
2	D	62	VAL
2	D	67	LEU
2	D	68	VAL
2	D	70	LEU
2	D	71	GLU
2	D	78	VAL
2	D	80	SER
2	D	83	PHE
2	D	85	GLN
2	D	90	ASP
2	D	93	VAL
2	D	96	GLN
2	D	97	SER
2	D	101	ASN
2	D	102	ASN
2	D	109	THR
2	D	110	GLU
2	D	119	LEU
2	D	120	ASP
2	D	129	CYS
2	D	130	ASP
2	D	131	CYS
2	D	132	LEU
2	D	133	GLN
2	D	137	LEU
2	D	145	THR
2	D	149	MET
2	D	151	THR

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Mol	Chain	Res	Type
2	D	156	LYS
2	D	158	ARG
2	D	160	GLU
2	D	163	ASP
2	D	164	ARG
2	D	165	ILE
2	D	166	MET
2	D	170	SER
2	D	171	VAL
2	D	174	SER
2	D	178	SER
2	D	179	ASP
2	D	181	VAL
2	D	188	THR
2	D	190	SER
2	D	196	GLU
2	D	200	GLU
2	D	209	LEU
2	D	214	PHE
2	D	216	THR
2	D	223	THR
2	D	227	LEU
2	D	230	LEU
2	D	239	THR
2	D	242	LEU
2	D	244	PHE
2	D	248	LEU
2	D	249	ASN
2	D	251	ASP
2	D	254	LYS
2	D	260	VAL
2	D	265	LEU
2	D	275	LEU
2	D	277	SER
2	D	280	SER
2	D	281	GLN
2	D	284	ARG
2	D	286	LEU
2	D	287	THR
2	D	291	LEU
2	D	293	GLN
2	D	294	GLN

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Mol	Chain	Res	Type
2	D	295	MET
2	D	296	PHE
2	D	300	ASN
2	D	308	ARG
2	D	309	HIS
2	D	311	ARG
2	D	313	LEU
2	D	318	VAL
2	D	320	ARG
2	D	323	MET
2	D	324	SER
2	D	325	MET
2	D	329	ASP
2	D	332	MET
2	D	333	LEU
2	D	335	VAL
2	D	339	ASN
2	D	347	ILE
2	D	350	ASN
2	D	351	VAL
2	D	356	CYS
2	D	358	ILE
2	D	371	LEU
2	D	372	LYS
2	D	373	MET
2	D	376	THR
2	D	380	ASN
2	D	384	ILE
2	D	389	LYS
2	D	390	ARG
2	D	391	ILE
2	D	392	SER
2	D	393	GLU
2	D	394	GLN
2	D	396	THR
2	D	398	MET
2	D	400	ARG
2	D	401	ARG
2	D	402	LYS
2	D	405	LEU
2	D	408	TYR
2	D	409	THR

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Mol	Chain	Res	Type
2	D	411	GLU
2	D	413	MET
2	D	416	MET
2	D	417	GLU
2	D	419	THR
2	D	423	SER
2	D	425	MET
2	D	434	GLN
2	D	436	GLN
3	E	5	ASP
3	E	6	MET
3	E	15	THR
3	E	16	SER
3	E	21	GLU
3	E	22	VAL
3	E	24	LEU
3	E	51	GLN
3	E	53	LYS
3	E	62	LYS
3	E	65	GLU
3	E	67	GLU
3	E	76	ARG
3	E	77	GLU
3	E	78	HIS
3	E	80	ARG
3	E	81	GLU
3	E	84	GLN
3	E	87	ILE
3	E	89	GLU
3	E	91	ASN
3	E	92	ASN
3	E	94	ILE
3	E	96	MET
3	E	99	GLU
3	E	105	MET
3	E	106	GLU
3	E	109	LYS
3	E	111	ASN
3	E	112	ARG
3	E	115	HIS
3	E	119	MET
3	E	122	ARG

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Mol	Chain	Res	Type
3	E	124	GLN
3	E	125	GLU
3	E	126	LYS
3	E	129	HIS
3	E	134	ARG
3	E	136	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	50	ASN
1	A	85	GLN
1	A	88	HIS
1	A	101	ASN
1	A	102	ASN
1	A	139	HIS
1	A	176	GLN
1	A	206	ASN
1	A	249	ASN
1	A	258	ASN
1	A	283	HIS
1	A	329	ASN
1	A	356	ASN
1	A	380	ASN
1	A	393	HIS
2	B	8	GLN
2	B	14	ASN
2	B	43	GLN
2	B	54	ASN
2	B	85	GLN
2	B	101	ASN
2	B	133	GLN
2	B	136	GLN
2	B	192	HIS
2	B	206	ASN
2	B	229	HIS
2	B	258	ASN
2	B	266	HIS
2	B	294	GLN
2	B	309	HIS
2	B	350	ASN

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Mol	Chain	Res	Type
2	B	380	ASN
2	B	385	GLN
1	C	8	HIS
1	C	50	ASN
1	C	85	GLN
1	C	101	ASN
1	C	102	ASN
1	C	139	HIS
1	C	176	GLN
1	C	206	ASN
1	C	329	ASN
1	C	356	ASN
2	D	8	GLN
2	D	14	ASN
2	D	54	ASN
2	D	85	GLN
2	D	101	ASN
2	D	133	GLN
2	D	136	GLN
2	D	192	HIS
2	D	206	ASN
2	D	229	HIS
2	D	258	ASN
2	D	266	HIS
2	D	282	GLN
2	D	294	GLN
2	D	309	HIS
2	D	331	GLN
2	D	339	ASN
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
2	D	436	GLN
3	E	78	HIS
3	E	90	ASN
3	E	91	ASN
3	E	111	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GTP	C	600	5	26,34,34	1.12	3 (11%)	33,54,54	2.30	10 (30%)
4	GTP	A	600	5	26,34,34	0.97	2 (7%)	33,54,54	1.83	8 (24%)
7	G2N	B	700	-	24,26,26	1.99	3 (12%)	27,36,36	3.52	12 (44%)
7	G2N	D	700	-	24,26,26	1.57	2 (8%)	27,36,36	2.96	11 (40%)
6	GDP	B	600	-	24,30,30	1.06	1 (4%)	31,47,47	1.87	8 (25%)
6	GDP	D	600	-	24,30,30	1.19	3 (12%)	31,47,47	2.23	7 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	C	600	5	-	8/18/38/38	0/3/3/3
4	GTP	A	600	5	-	7/18/38/38	0/3/3/3
7	G2N	B	700	-	-	7/11/23/23	0/3/3/3
7	G2N	D	700	-	-	10/11/23/23	0/3/3/3
6	GDP	B	600	-	-	5/12/32/32	0/3/3/3
6	GDP	D	600	-	-	2/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	G2N	CAT-CAR	-7.03	1.37	1.48
7	D	700	G2N	CAT-CAR	-5.33	1.40	1.48
7	B	700	G2N	CAU-NAN	-4.09	1.31	1.40
7	B	700	G2N	CAW-NAL	-3.91	1.30	1.38
6	D	600	GDP	C6-N1	3.64	1.39	1.33
6	B	600	GDP	C6-N1	3.16	1.38	1.33
4	C	600	GTP	C6-N1	2.87	1.38	1.33
4	C	600	GTP	O4'-C4'	-2.43	1.39	1.45
4	A	600	GTP	O4'-C4'	-2.32	1.39	1.45
6	D	600	GDP	C2-N1	2.30	1.39	1.35
4	A	600	GTP	C6-N1	2.30	1.37	1.33
4	C	600	GTP	C6-C5	-2.19	1.37	1.41
6	D	600	GDP	C2'-C1'	-2.18	1.50	1.53
7	D	700	G2N	CAS-NAM	2.08	1.38	1.35

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	G2N	CAT-CAR-NAL	-9.90	105.60	118.13
7	D	700	G2N	OAP-CAQ-NAN	8.94	123.93	109.32
7	B	700	G2N	OAP-CAQ-NAN	8.16	122.65	109.32
4	C	600	GTP	N3-C2-N1	-7.21	117.61	127.22
6	D	600	GDP	N3-C2-N1	-6.88	118.05	127.22
7	B	700	G2N	CAH-CAT-CAR	-6.08	113.55	120.75
6	D	600	GDP	C2-N3-C4	5.51	121.66	115.36
4	C	600	GTP	C2-N3-C4	5.49	121.63	115.36
4	C	600	GTP	PB-O3B-PG	-5.38	114.36	132.83
7	D	700	G2N	NAN-CAU-NAM	5.27	125.77	113.24
6	B	600	GDP	N3-C2-N1	-5.26	120.21	127.22
7	B	700	G2N	OAP-CAK-CAA	4.80	126.06	108.42
7	B	700	G2N	NAC-CAS-NAM	4.69	123.67	117.03
7	D	700	G2N	CAK-OAP-CAQ	-4.66	107.21	116.04
7	B	700	G2N	CAB-CAX-NAO	-4.65	104.93	110.34
7	D	700	G2N	CAU-NAN-CAQ	4.62	138.53	127.36
4	A	600	GTP	C2-N3-C4	4.61	120.62	115.36
7	D	700	G2N	OAP-CAQ-OAD	-4.41	115.79	124.25
6	B	600	GDP	C2-N3-C4	4.23	120.19	115.36
4	A	600	GTP	PB-O3B-PG	-4.15	118.59	132.83
7	B	700	G2N	OAP-CAQ-OAD	-4.01	116.56	124.25
6	D	600	GDP	C5-C6-N1	-3.92	118.07	123.43
4	A	600	GTP	N3-C2-N1	-3.91	122.01	127.22
6	D	600	GDP	C6-N1-C2	3.90	122.13	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	600	GDP	PA-O3A-PB	-3.87	119.56	132.83
4	A	600	GTP	PA-O3A-PB	-3.69	120.17	132.83
7	D	700	G2N	CAJ-CAU-NAM	-3.32	116.39	123.41
7	B	700	G2N	CAI-CAT-CAR	3.15	124.48	120.75
4	C	600	GTP	C6-N1-C2	3.10	120.86	115.93
7	D	700	G2N	OAD-CAQ-NAN	-2.68	120.28	126.11
6	B	600	GDP	C6-N1-C2	2.66	120.15	115.93
6	D	600	GDP	O3B-PB-O3A	2.62	113.41	104.64
4	C	600	GTP	C3'-C2'-C1'	-2.60	97.07	100.98
6	B	600	GDP	C5-C6-N1	-2.59	119.89	123.43
4	A	600	GTP	C5-C6-N1	-2.56	119.92	123.43
7	D	700	G2N	NAC-CAS-NAM	2.52	120.59	117.03
7	D	700	G2N	CAH-CAT-CAR	-2.49	117.80	120.75
6	B	600	GDP	O2B-PB-O3A	2.46	112.89	104.64
7	B	700	G2N	OAD-CAQ-NAN	-2.45	120.78	126.11
4	A	600	GTP	C4-C5-N7	-2.44	106.86	109.40
6	D	600	GDP	C4-C5-N7	-2.36	106.94	109.40
4	C	600	GTP	N2-C2-N3	2.34	121.60	117.79
4	A	600	GTP	O3G-PG-O2G	2.31	116.48	107.64
7	B	700	G2N	CAI-CAT-CAH	2.28	121.83	118.59
4	C	600	GTP	N2-C2-N1	2.28	120.80	117.25
7	D	700	G2N	CAB-CAX-NAO	-2.28	107.70	110.34
4	C	600	GTP	C6-C5-C4	-2.26	118.64	120.80
6	B	600	GDP	PA-O3A-PB	-2.22	125.22	132.83
4	A	600	GTP	O4'-C4'-C5'	-2.21	102.11	109.37
4	C	600	GTP	C2'-C3'-C4'	2.19	106.89	102.64
7	B	700	G2N	CAG-CAI-CAT	-2.12	117.84	120.34
6	B	600	GDP	O4'-C4'-C3'	2.08	109.23	105.11
7	D	700	G2N	CAG-CAI-CAT	-2.07	117.90	120.34
4	C	600	GTP	C5-C6-N1	-2.02	120.67	123.43
6	B	600	GDP	C3'-C2'-C1'	2.02	104.02	100.98
7	B	700	G2N	CAW-CAS-NAC	-2.02	119.04	123.43

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	600	GTP	PB-O3B-PG-O3G
4	A	600	GTP	PB-O3B-PG-O3G
7	B	700	G2N	CAA-CAK-OAP-CAQ
7	B	700	G2N	CAX-CAR-CAT-CAH
7	B	700	G2N	CAX-CAR-CAT-CAI

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Mol	Chain	Res	Type	Atoms
6	D	600	GDP	PA-O3A-PB-O2B
6	B	600	GDP	O4'-C4'-C5'-O5'
6	B	600	GDP	C3'-C4'-C5'-O5'
7	D	700	G2N	CAJ-CAU-NAN-CAQ
7	D	700	G2N	NAM-CAU-NAN-CAQ
7	D	700	G2N	NAL-CAR-CAT-CAH
7	D	700	G2N	NAL-CAR-CAT-CAI
7	D	700	G2N	CAX-CAR-CAT-CAH
7	D	700	G2N	CAX-CAR-CAT-CAI
7	D	700	G2N	NAN-CAQ-OAP-CAK
7	D	700	G2N	OAD-CAQ-OAP-CAK
7	B	700	G2N	NAL-CAR-CAT-CAH
7	B	700	G2N	NAL-CAR-CAT-CAI
7	B	700	G2N	OAD-CAQ-NAN-CAU
7	B	700	G2N	OAP-CAQ-NAN-CAU
7	D	700	G2N	OAD-CAQ-NAN-CAU
7	D	700	G2N	OAP-CAQ-NAN-CAU
4	A	600	GTP	PB-O3B-PG-O1G
4	A	600	GTP	PG-O3B-PB-O1B
4	C	600	GTP	C4'-C5'-O5'-PA
4	A	600	GTP	C5'-O5'-PA-O3A
6	B	600	GDP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O2A
4	A	600	GTP	C5'-O5'-PA-O2A
4	C	600	GTP	PB-O3A-PA-O1A
4	C	600	GTP	PB-O3A-PA-O2A
4	A	600	GTP	C3'-C4'-C5'-O5'
4	C	600	GTP	PB-O3B-PG-O1G
4	C	600	GTP	PB-O3B-PG-O2G
6	D	600	GDP	PA-O3A-PB-O3B
4	C	600	GTP	C5'-O5'-PA-O3A
4	A	600	GTP	PG-O3B-PB-O2B
6	B	600	GDP	C5'-O5'-PA-O1A
6	B	600	GDP	C5'-O5'-PA-O2A

There are no ring outliers.

6 monomers are involved in 48 short contacts:

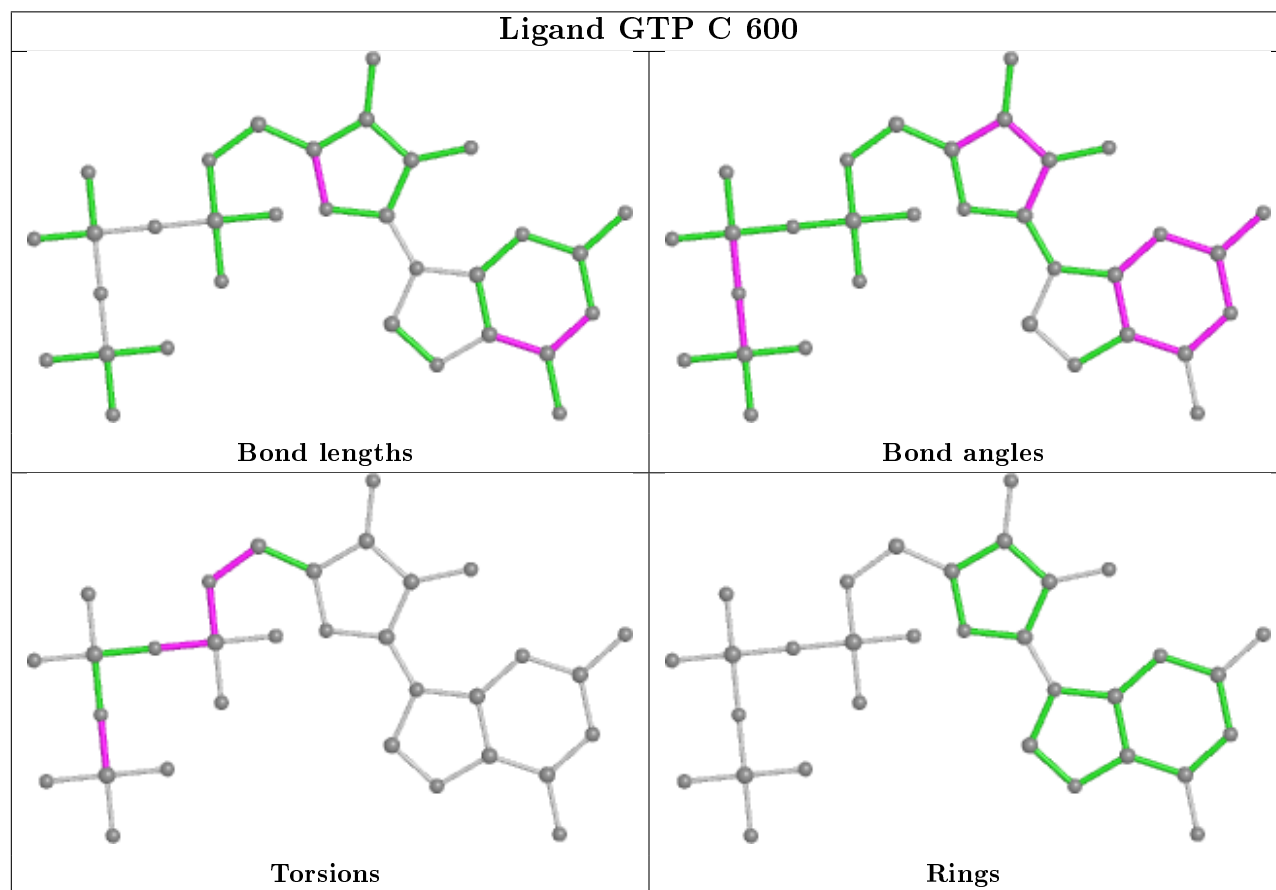
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	600	GTP	4	0
4	A	600	GTP	3	0
7	B	700	G2N	7	0

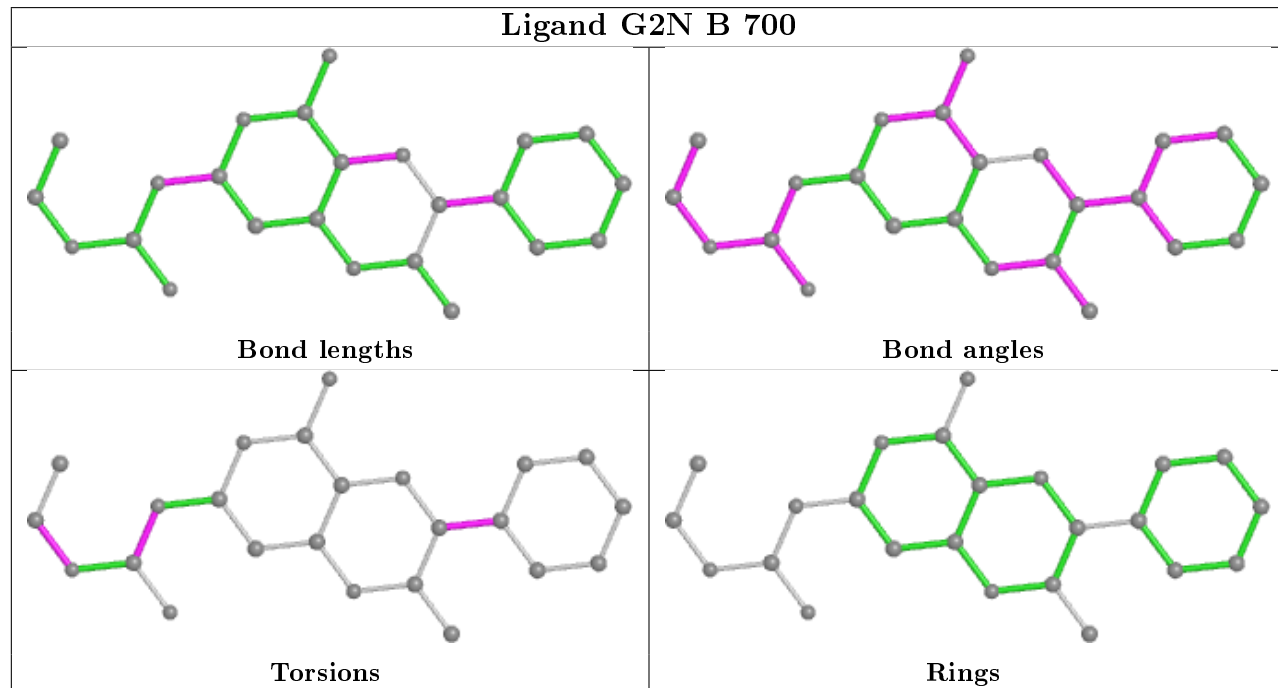
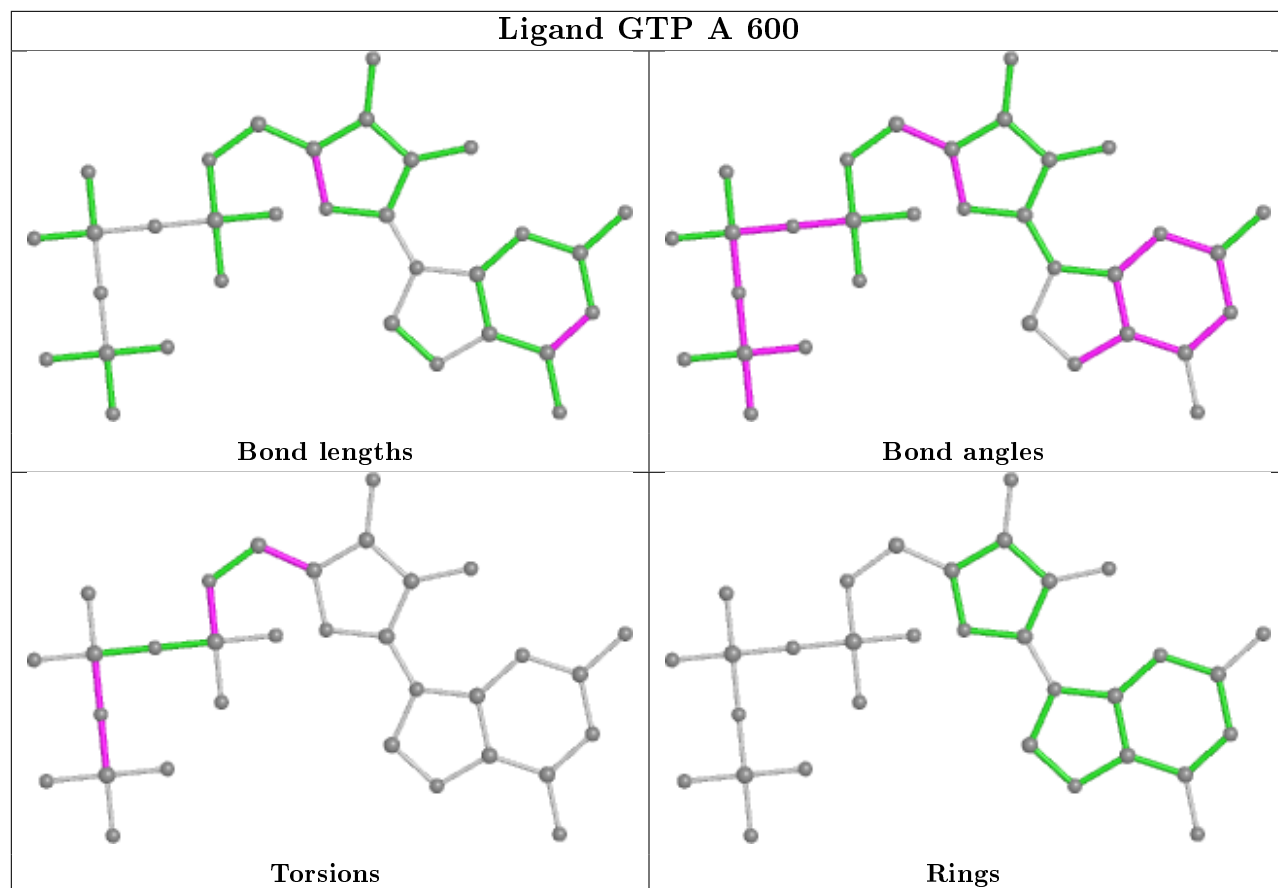
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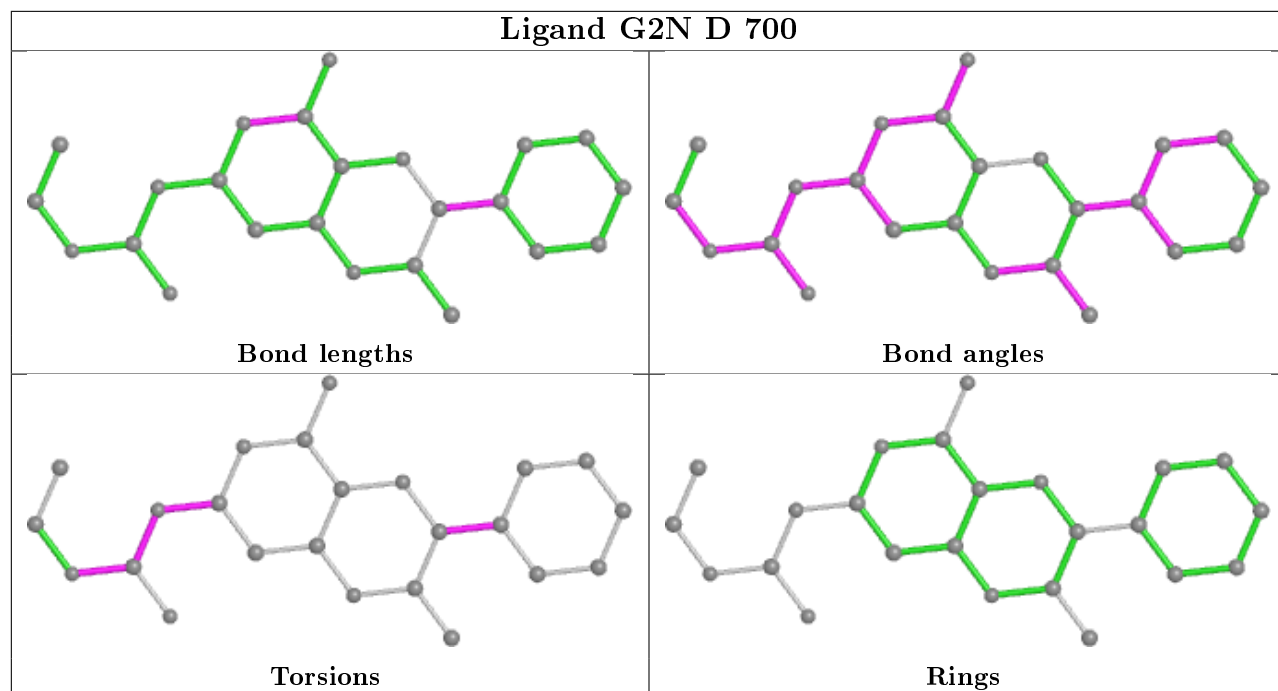
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	700	G2N	11	0
6	B	600	GDP	8	0
6	D	600	GDP	15	0

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.

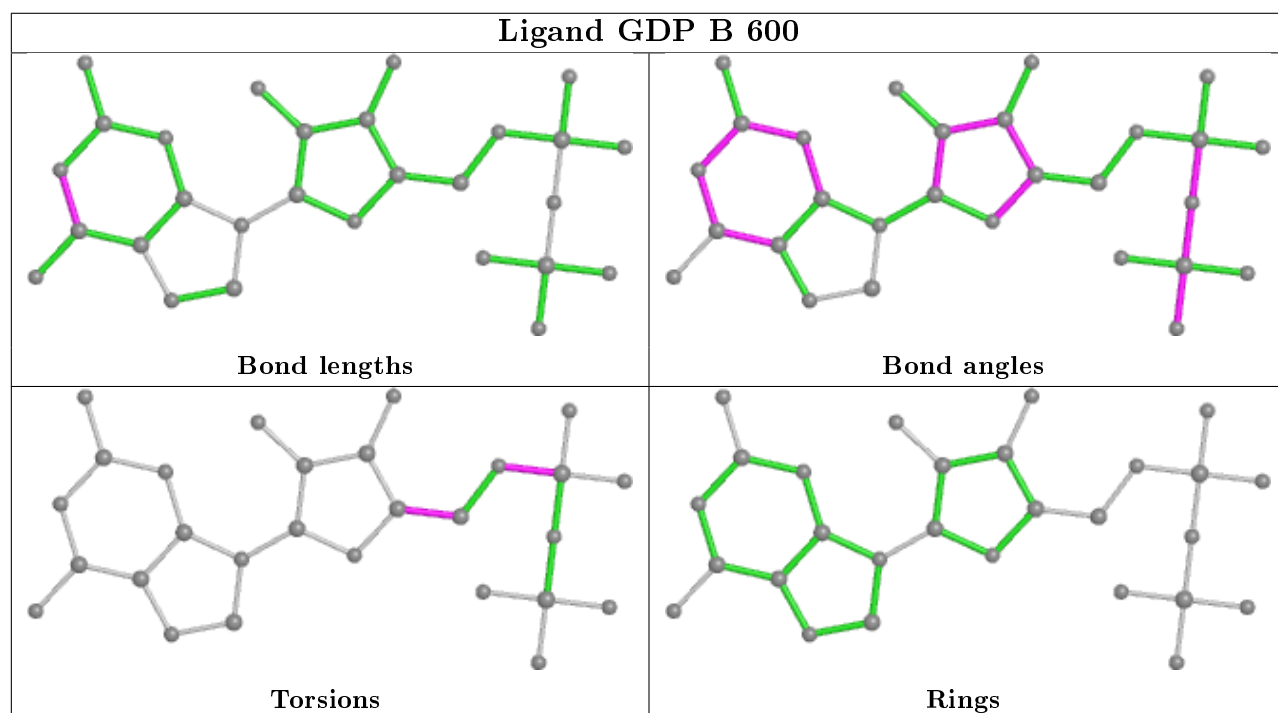


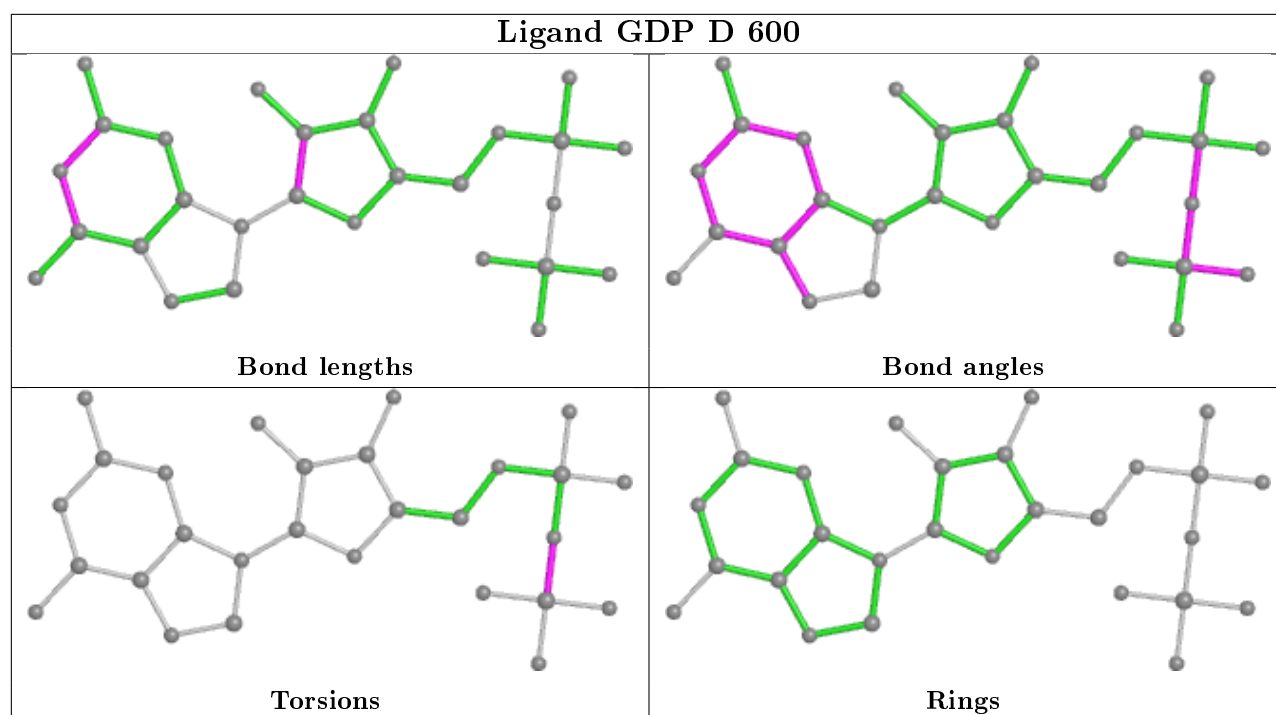


Ligand G2N D 700



Ligand GDP B 600





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	428/451 (94%)	-0.42	1 (0%) 95 93	78, 79, 80, 82	0
1	C	429/451 (95%)	-0.28	2 (0%) 91 85	79, 80, 80, 85	0
2	B	419/445 (94%)	-0.36	0 100 100	74, 79, 81, 86	0
2	D	427/445 (95%)	-0.27	3 (0%) 87 82	78, 80, 81, 83	0
3	E	123/142 (86%)	-0.29	1 (0%) 86 79	75, 80, 82, 84	0
All	All	1826/1934 (94%)	-0.33	7 (0%) 92 87	74, 80, 81, 86	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	143	GLY	3.3
2	D	201	THR	2.7
1	C	143	GLY	2.3
2	D	144	GLY	2.2
3	E	30	ASP	2.2
1	A	140	SER	2.1
1	C	170	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](#)

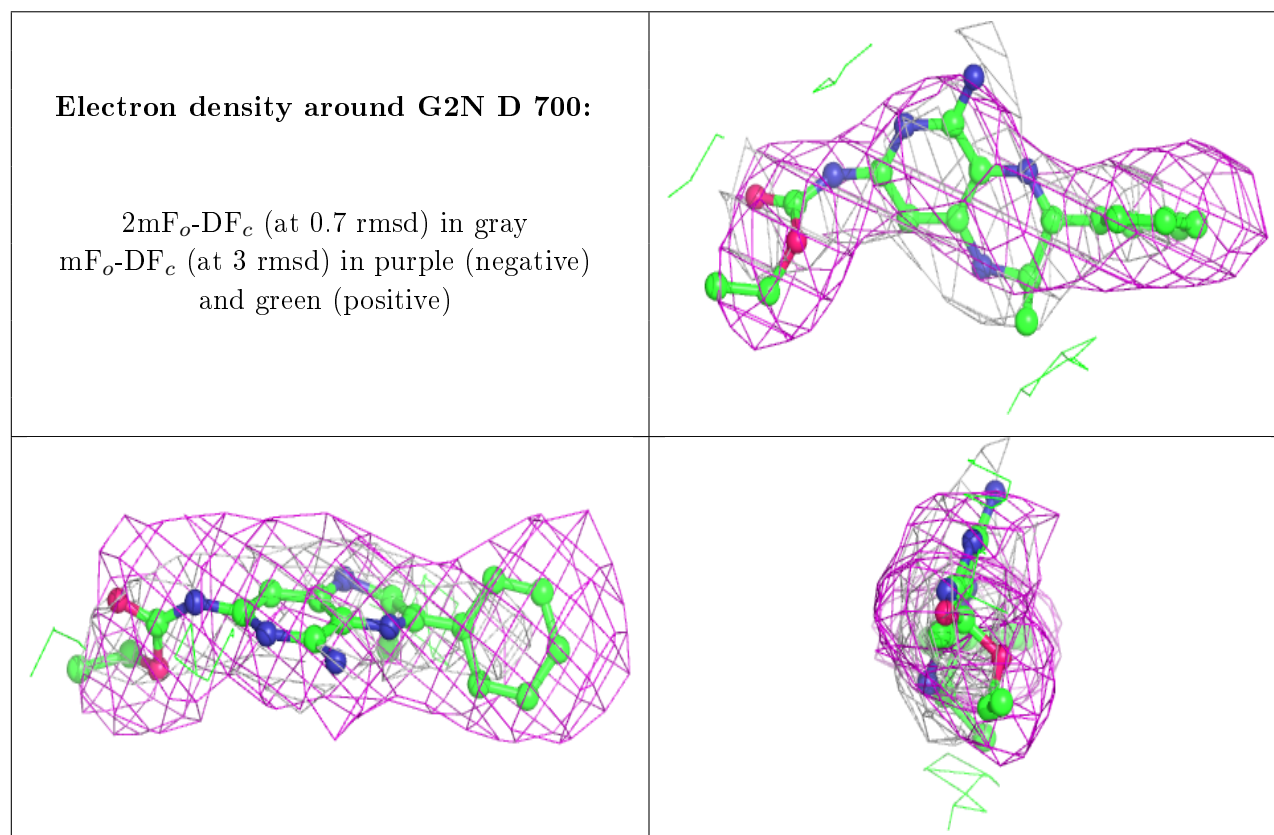
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

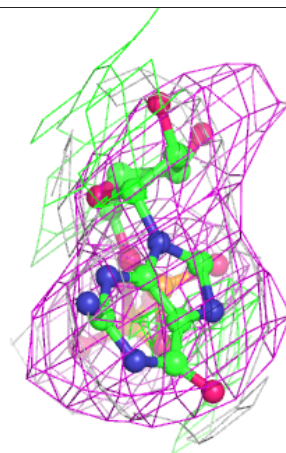
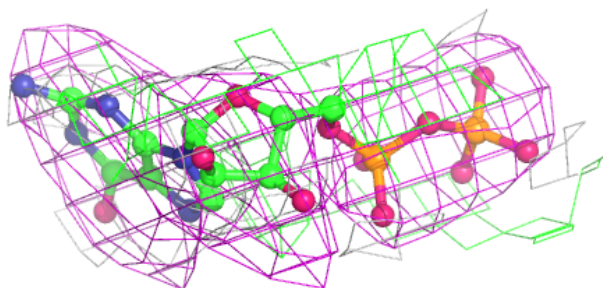
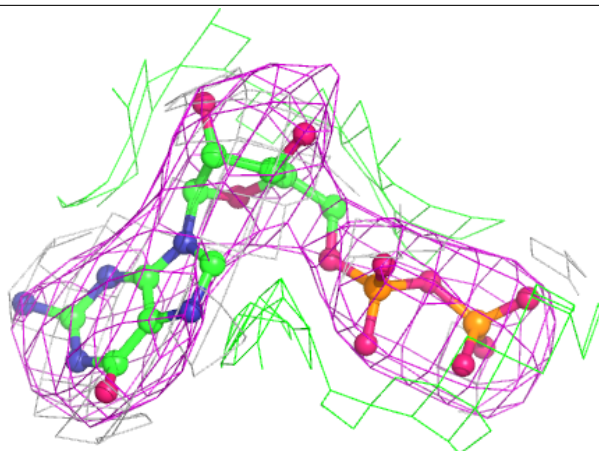
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	G2N	D	700	24/24	0.83	0.38	85,88,91,91	0
5	MG	B	601	1/1	0.86	0.66	81,81,81,81	0
6	GDP	D	600	28/28	0.88	0.25	77,78,80,80	0
4	GTP	C	600	32/32	0.91	0.20	72,75,76,77	0
6	GDP	B	600	28/28	0.92	0.19	76,80,81,81	0
7	G2N	B	700	24/24	0.92	0.27	75,78,79,82	0
4	GTP	A	600	32/32	0.94	0.15	71,75,76,76	0
5	MG	C	601	1/1	0.97	0.09	67,67,67,67	0
5	MG	A	601	1/1	0.98	0.12	46,46,46,46	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.



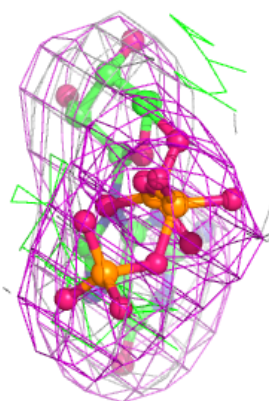
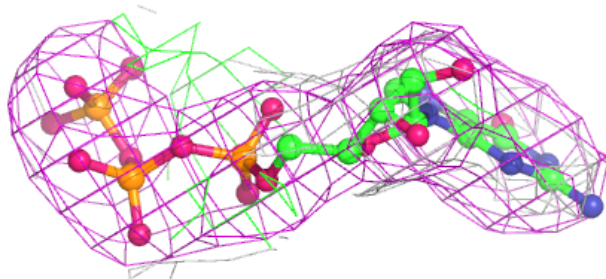
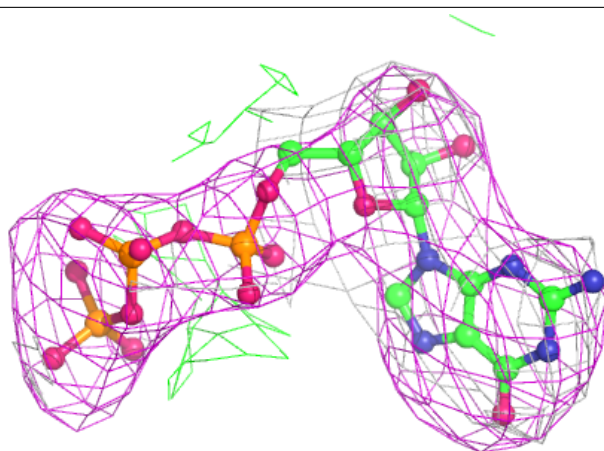
Electron density around GDP D 600:

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



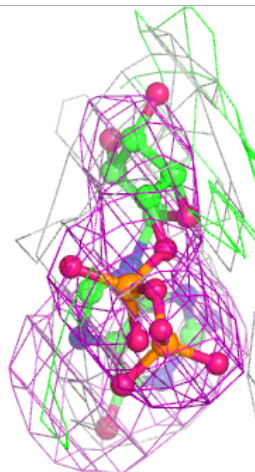
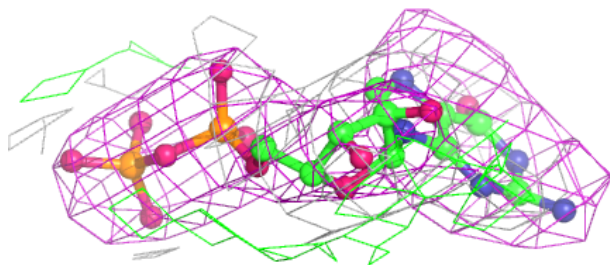
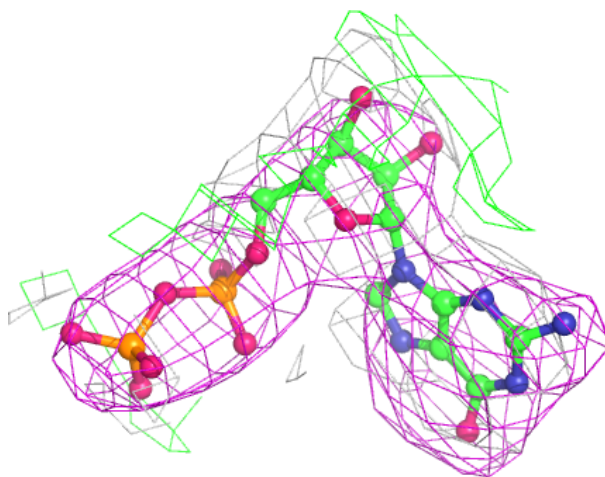
Electron density around GTP C 600:

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



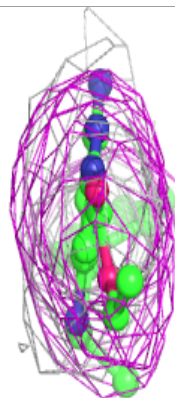
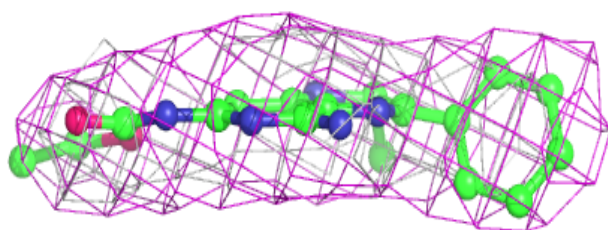
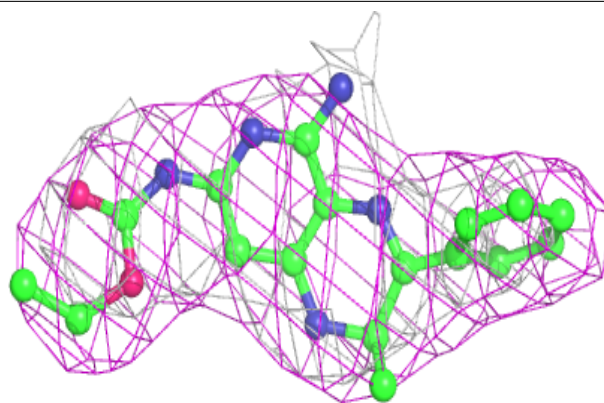
Electron density around GDP B 600:

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

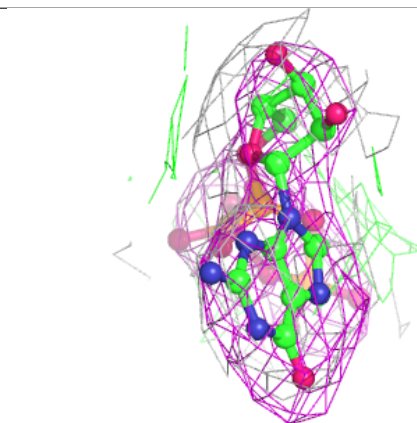
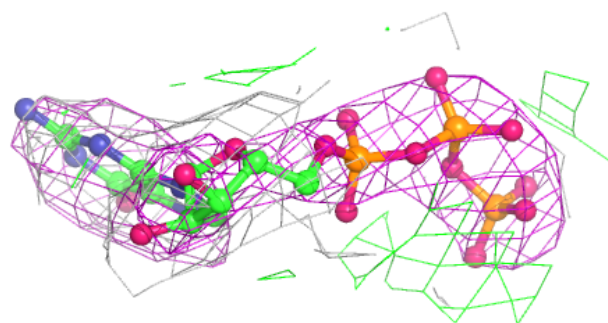
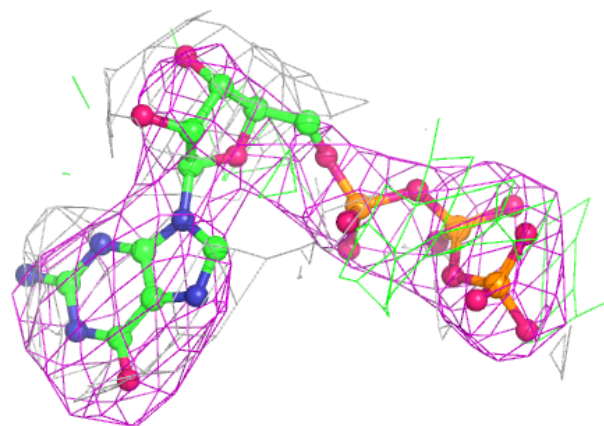


Electron density around G2N B 700:

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

**Electron density around GTP A 600:**

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



6.5 Other polymers

There are no such residues in this entry.