



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 07:44 AM EDT

PDB ID : 3HKD / pdb_00003hkd
Title : Tubulin-TN16 : RB3 stathmin-like domain complex
Authors : Dorleans, A.; Gigant, B.; Ravelli, R.B.G.; Mailliet, P.; Mikol, V.; Knossow, M.
Deposited on : 2009-05-23
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

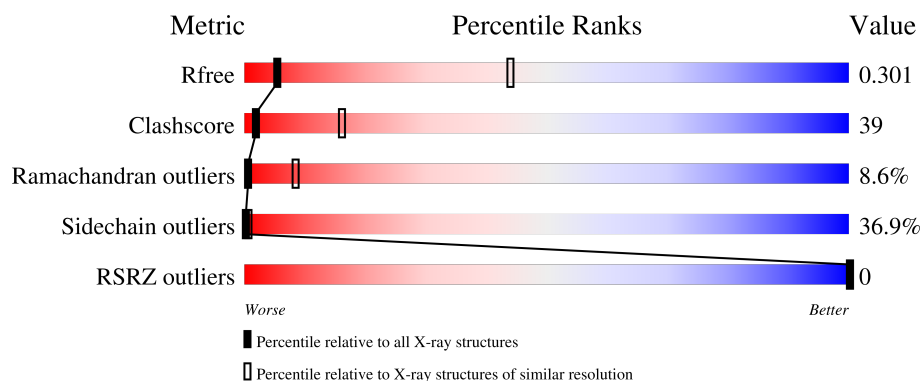
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
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
6	GDP	B	600	-	-	X	-
6	GDP	D	600	-	-	X	-
7	N16	D	700	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14223 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	420	Total	C	N	O	S	0	0	0
			3251	2046	547	633	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 (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

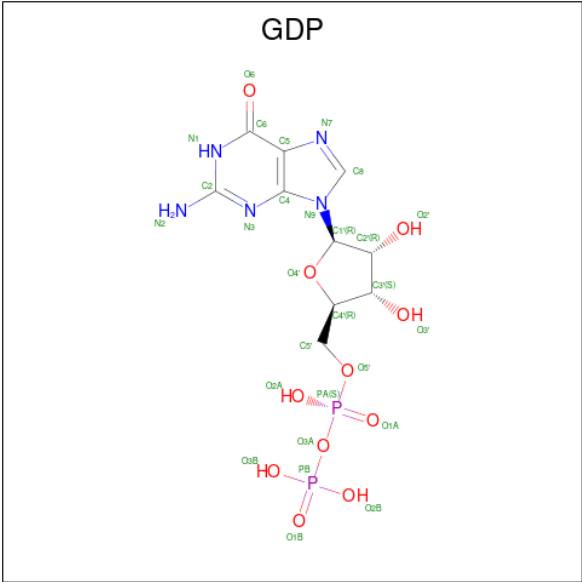


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

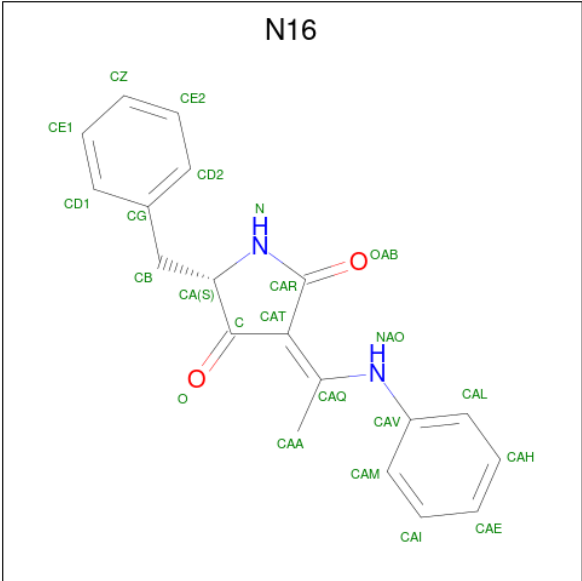
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 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 (3Z,5S)-5-benzyl-3-[1-(phenylamino)ethylidene]pyrrolidine-2,4-dione (CCD ID: N16) (formula: C₁₉H₁₈N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			23	19	2	2		

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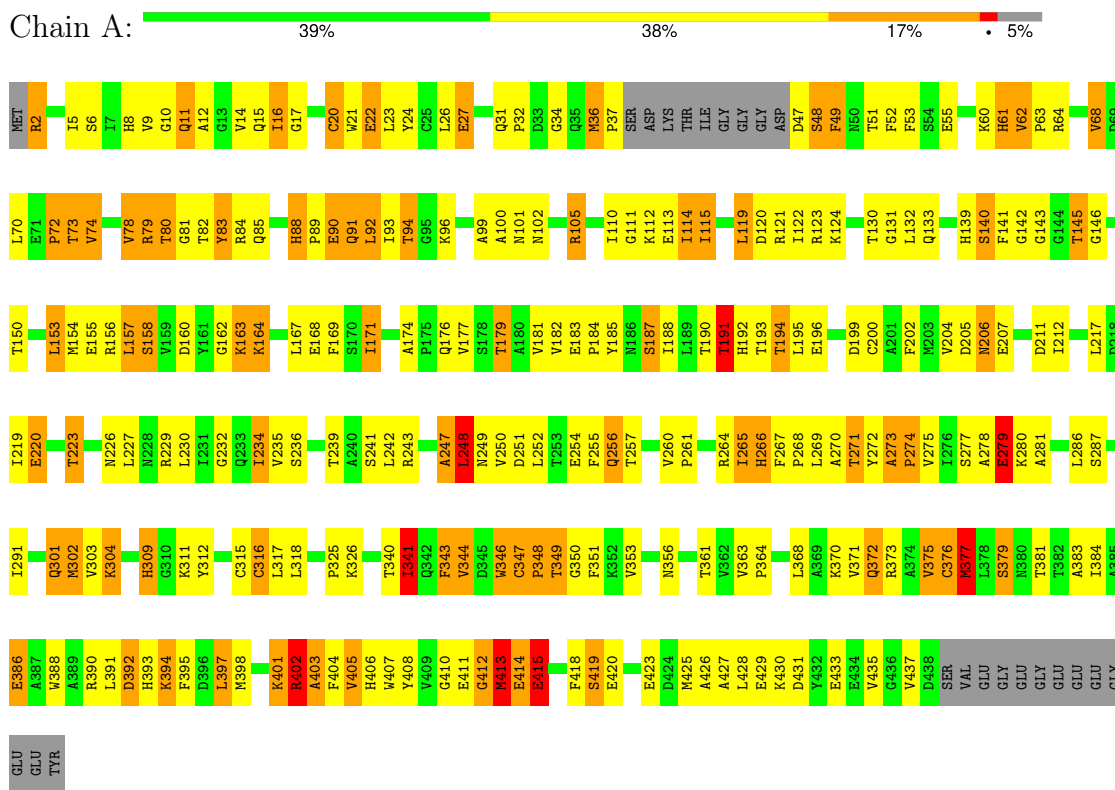
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			23	19	2	2		

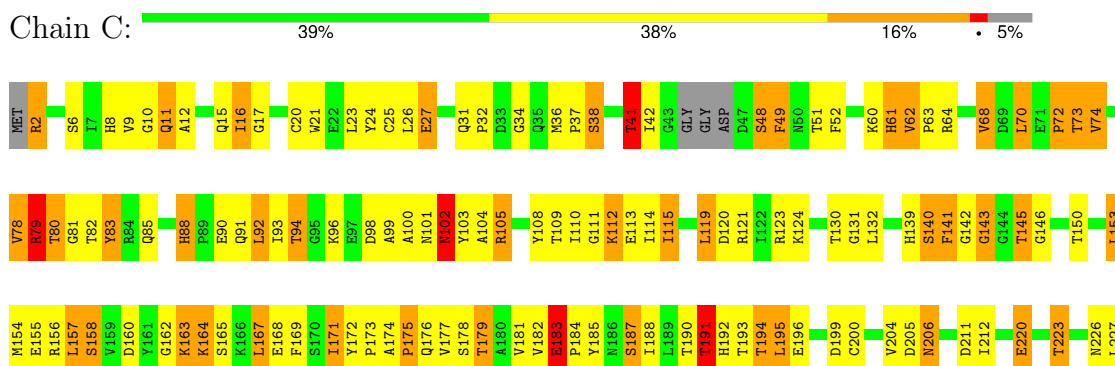
3 Residue-property plots

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

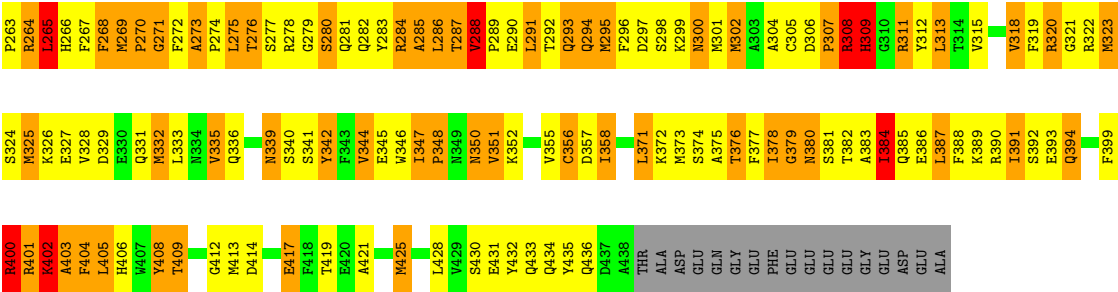
• Molecule 1: Tubulin alpha chain



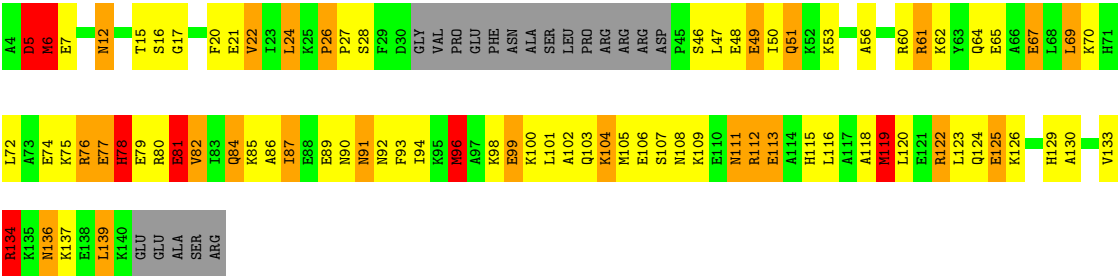
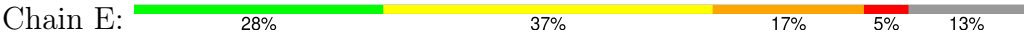
• Molecule 1: Tubulin alpha chain







● Molecule 3: Stathmin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	328.53Å 328.53Å 54.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.70 20.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-3.70) 97.8 (20.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.209 , 0.264 0.267 , 0.301	Depositor DCC
R_{free} test set	1852 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	152.5	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.127 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14223	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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: MG, N16, GDP, GTP

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	0.88	5/3377 (0.1%)	1.18	7/4593 (0.2%)
1	C	0.79	2/3360 (0.1%)	1.16	8/4572 (0.2%)
2	B	0.91	2/3323 (0.1%)	1.19	19/4512 (0.4%)
2	D	1.20	16/3370 (0.5%)	1.30	24/4574 (0.5%)
3	E	1.05	3/928 (0.3%)	1.30	10/1243 (0.8%)
All	All	0.96	28/14358 (0.2%)	1.22	68/19494 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	3
2	B	0	3
2	D	0	4
3	E	0	1
All	All	0	13

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	96	MET	SD-CE	10.20	2.05	1.79
2	D	379	GLY	C-O	9.73	1.37	1.23
3	E	119	MET	SD-CE	8.97	2.02	1.79
2	D	269	MET	C-O	7.70	1.34	1.24
3	E	105	MET	SD-CE	7.08	1.97	1.79
1	A	36	MET	SD-CE	6.80	1.96	1.79
2	D	302	MET	SD-CE	6.57	1.96	1.79
2	D	318	VAL	CA-CB	6.28	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	THR	CA-CB	6.19	1.60	1.52
1	A	302	MET	SD-CE	6.14	1.94	1.79
2	B	325	MET	SD-CE	5.97	1.94	1.79
2	D	305	CYS	C-O	5.70	1.31	1.24
2	D	177	VAL	CA-C	5.67	1.59	1.52
1	C	349	THR	CA-CB	5.62	1.59	1.53
2	D	308	ARG	NE-CZ	5.50	1.39	1.33
1	A	62	VAL	CA-CB	5.47	1.61	1.54
2	D	384	ILE	CA-CB	5.47	1.61	1.54
2	D	259	MET	SD-CE	5.46	1.93	1.79
2	D	288	VAL	CA-CB	5.45	1.61	1.54
2	B	216	THR	CA-CB	5.42	1.61	1.53
2	D	48	ARG	NE-CZ	5.42	1.39	1.33
2	D	300	ASN	C-O	5.39	1.30	1.24
2	D	235	MET	SD-CE	5.35	1.93	1.79
1	A	114	ILE	CA-CB	5.29	1.61	1.54
1	C	302	MET	SD-CE	5.20	1.92	1.79
2	D	269	MET	CG-SD	5.09	1.93	1.80
2	D	271	GLY	C-O	5.04	1.29	1.24
2	D	379	GLY	CA-C	5.04	1.58	1.51

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	51	GLN	N-CA-C	-9.46	102.83	114.75
2	D	91	ASN	N-CA-C	-7.35	102.58	113.61
3	E	104	LYS	N-CA-C	-7.28	104.20	113.23
2	B	431	GLU	N-CA-C	-7.26	104.41	113.55
3	E	96	MET	N-CA-C	-7.25	104.30	113.43
1	C	42	ILE	N-CA-C	-7.19	99.75	108.53
1	C	102	ASN	N-CA-C	7.16	120.15	108.26
1	C	41	THR	N-CA-C	7.08	121.23	108.48
2	D	144	GLY	N-CA-C	7.00	120.96	112.49
3	E	6	MET	N-CA-C	6.96	122.56	114.62
1	A	376	CYS	N-CA-C	6.80	124.64	114.09
2	D	244	PHE	N-CA-C	6.62	124.45	109.81
2	D	243	ARG	N-CA-C	6.62	121.00	112.26
3	E	56	ALA	N-CA-C	-6.44	105.55	113.41
1	A	24	TYR	N-CA-C	-6.42	104.20	111.07
2	D	250	ALA	N-CA-C	6.37	120.45	111.92
2	B	4	ILE	N-CA-C	6.35	117.26	108.12
2	D	260	VAL	N-CA-C	6.26	117.60	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	244	PHE	N-CA-C	6.22	123.55	109.81
2	D	346	TRP	CA-C-N	-6.17	116.60	123.02
2	D	346	TRP	C-N-CA	-6.17	116.60	123.02
2	B	254	LYS	N-CA-C	-6.09	103.59	111.02
2	D	99	ALA	N-CA-C	-6.04	105.00	112.72
3	E	100	LYS	N-CA-C	-6.00	105.68	112.87
2	D	379	GLY	N-CA-C	5.96	127.30	113.18
2	B	328	VAL	N-CA-C	5.94	116.41	110.23
2	B	144	GLY	N-CA-C	5.89	119.62	112.49
2	B	427	ASP	N-CA-C	-5.83	103.72	111.24
1	C	24	TYR	N-CA-C	-5.83	104.83	111.07
1	C	352	LYS	N-CA-C	-5.78	101.85	110.23
2	D	431	GLU	N-CA-C	-5.78	106.27	113.55
2	B	275	LEU	N-CA-C	5.77	118.88	109.06
2	B	228	ASN	N-CA-C	-5.72	105.12	111.36
2	D	130	ASP	N-CA-C	5.72	118.46	111.82
1	C	62	VAL	N-CA-C	5.70	115.23	108.96
2	D	318	VAL	CB-CA-C	5.65	118.58	110.33
2	D	62	VAL	N-CA-C	5.59	120.96	108.88
2	D	414	ASP	N-CA-C	5.59	118.73	109.46
2	B	91	ASN	N-CA-C	-5.58	105.23	113.61
2	D	185	TYR	N-CA-C	-5.57	105.11	111.07
3	E	78	HIS	N-CA-C	-5.57	106.16	113.12
2	B	414	ASP	N-CA-C	5.56	118.30	109.24
2	D	272	PHE	N-CA-C	5.56	118.14	109.52
2	B	288	VAL	N-CA-CB	5.47	118.87	111.21
3	E	17	GLY	N-CA-C	5.43	117.92	110.69
2	B	62	VAL	N-CA-C	5.42	120.58	108.88
1	A	5	ILE	N-CA-C	5.41	116.10	108.36
2	D	163	ASP	N-CA-C	5.39	122.29	110.80
1	A	20	CYS	CB-CA-C	5.32	117.96	109.02
2	D	4	ILE	N-CA-C	5.32	115.78	108.12
1	A	122	ILE	N-CA-C	-5.30	105.68	110.82
1	C	250	VAL	N-CA-C	5.28	120.33	109.34
3	E	26	PRO	N-CA-C	5.26	117.12	110.70
2	B	260	VAL	N-CA-C	5.25	116.01	107.71
1	A	346	TRP	N-CA-C	5.24	120.46	112.54
2	D	197	ASN	N-CA-C	5.24	120.54	114.04
1	A	413	MET	N-CA-C	5.23	117.57	110.35
2	D	169	PHE	N-CA-C	-5.21	100.24	108.73
2	B	338	LYS	N-CA-C	-5.21	106.19	112.54
2	D	254	LYS	N-CA-C	-5.18	102.87	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	376	CYS	N-CA-C	5.18	122.51	114.64
2	B	44	LEU	N-CA-C	5.14	118.65	112.38
3	E	134	ARG	N-CA-C	-5.14	107.08	113.55
2	D	160	GLU	N-CA-C	-5.08	105.45	111.69
2	D	165	ILE	N-CA-C	5.06	116.56	108.87
2	B	163	ASP	N-CA-C	5.03	121.52	110.80
2	B	272	PHE	N-CA-C	5.02	117.04	109.41
2	B	243	ARG	N-CA-C	5.01	118.87	112.26

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLY	Peptide
1	A	266	HIS	Peptide
2	B	162	PRO	Peptide
2	B	248	LEU	Peptide
2	B	249	ASN	Peptide
1	C	143	GLY	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 [i](#)

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	186	0
1	C	3286	0	3133	203	0
2	B	3251	0	3074	293	0
2	D	3297	0	3116	388	0
3	E	920	0	816	64	0
4	A	32	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	10	0
6	D	28	0	12	19	0
7	B	23	0	18	8	0
7	D	23	0	18	16	0
All	All	14223	0	13385	1078	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 39.

All (1078) 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)
3:E:119:MET:SD	3:E:119:MET:CE	2.02	1.47
3:E:96:MET:CE	3:E:96:MET:SD	2.05	1.44
2:D:140:SER:CB	6:D:600:GDP:H5'	1.59	1.31
2:D:387:LEU:O	2:D:390:ARG:HG2	1.31	1.26
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.16	1.14
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.22	1.13
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.27	1.12
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.80	1.11
2:B:142:GLY:O	6:B:600:GDP:H5'	1.52	1.10
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.22	1.09
2:D:223:THR:HB	2:D:225:GLY:H	1.16	1.08
2:B:308:ARG:HG3	2:B:308:ARG:HH11	1.16	1.07
2:D:140:SER:HB2	6:D:600:GDP:H5'	1.15	1.07
2:B:387:LEU:O	2:B:390:ARG:HG2	1.53	1.07
1:C:105:ARG:NH2	2:D:253:ARG:HH21	1.53	1.06
2:D:270:PRO:HD2	2:D:302:MET:HB2	1.33	1.05
2:D:135:PHE:HB2	2:D:166:MET:CE	1.87	1.05
2:D:319:PHE:HB2	2:D:355:VAL:HG12	1.39	1.04
2:B:223:THR:HB	2:B:225:GLY:H	1.16	1.04
2:D:171:VAL:HG12	2:D:206:ASN:HD21	1.23	1.04
2:D:133:GLN:HE21	2:D:252:LEU:HD22	1.21	1.03
2:B:401:ARG:NH2	1:C:434:GLU:O	1.90	1.03
3:E:118:ALA:O	3:E:122:ARG:NH1	1.91	1.02
1:A:105:ARG:HH22	2:B:253:ARG:HH21	1.02	1.01
2:D:171:VAL:HG12	2:D:206:ASN:ND2	1.74	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:PHE:HB2	2:B:355:VAL:HG12	1.44	1.00
2:B:135:PHE:HB2	2:B:166:MET:CE	1.91	0.99
2:D:287:THR:HG23	2:D:290:GLU:HB2	1.41	0.99
2:B:133:GLN:HE21	2:B:252:LEU:HD22	1.26	0.99
2:D:231:VAL:HG12	2:D:235:MET:HE2	1.46	0.98
2:D:171:VAL:CG1	2:D:206:ASN:HD21	1.75	0.97
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.44	0.97
1:C:206:ASN:HD21	4:C:600:GTP:N2	1.63	0.97
2:D:287:THR:CG2	2:D:290:GLU:HB2	1.94	0.97
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.95	0.95
2:D:262:PHE:HB2	2:D:265:LEU:HD11	1.48	0.95
1:C:404:PHE:HE1	2:D:347:ILE:HG21	1.28	0.94
1:A:273:ALA:CB	1:A:274:PRO:HD3	1.96	0.94
2:B:287:THR:HG23	2:B:290:GLU:HB2	1.49	0.94
2:D:242:LEU:HD11	7:D:700:N16:HD1	1.49	0.94
1:C:206:ASN:HD21	4:C:600:GTP:HN22	0.94	0.94
2:D:135:PHE:HB2	2:D:166:MET:HE1	1.50	0.93
2:B:5:VAL:HG22	2:B:135:PHE:HD2	1.32	0.93
2:B:262:PHE:HB2	2:B:265:LEU:HD11	1.50	0.93
2:D:200:GLU:HB3	2:D:268:PHE:CE1	2.03	0.93
2:B:273:ALA:HB3	2:B:274:PRO:CD	1.98	0.93
1:A:404:PHE:HE1	2:B:347:ILE:HG21	1.34	0.93
2:D:308:ARG:HG3	2:D:308:ARG:HH11	1.32	0.92
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.51	0.92
1:A:70:LEU:HD12	1:A:145:THR:HB	1.52	0.92
2:D:229:HIS:CE1	2:D:277:SER:HB3	2.05	0.91
2:D:223:THR:CB	2:D:225:GLY:H	1.84	0.91
1:C:315:CYS:SG	1:C:377:MET:HE2	2.10	0.91
2:D:255:LEU:HG	7:D:700:N16:HAAA	1.51	0.90
2:D:391:ILE:HG13	2:D:392:SER:N	1.84	0.90
2:D:296:PHE:HE1	2:D:332:MET:HE1	1.35	0.90
2:B:403:ALA:O	2:B:405:LEU:N	2.04	0.90
2:B:171:VAL:HG12	2:B:206:ASN:ND2	1.87	0.90
1:C:105:ARG:HH22	2:D:253:ARG:HH21	0.89	0.89
2:B:287:THR:CG2	2:B:290:GLU:HB2	2.02	0.89
1:C:273:ALA:CB	1:C:274:PRO:HD3	2.03	0.89
1:C:105:ARG:HH22	2:D:253:ARG:NH2	1.70	0.88
2:D:248:LEU:HD11	7:D:700:N16:CAH	2.03	0.88
2:D:223:THR:HB	2:D:225:GLY:N	1.88	0.88
2:D:350:ASN:HD22	2:D:350:ASN:H	1.17	0.88
2:B:270:PRO:HD2	2:B:302:MET:HB2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:VAL:HG22	1:A:302:MET:HE1	1.56	0.86
2:B:220:THR:O	2:B:222:PRO:HD3	1.76	0.86
2:B:242:LEU:HD21	7:B:700:N16:HD1	1.56	0.86
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.57	0.86
1:C:70:LEU:HD12	1:C:145:THR:HB	1.58	0.86
2:B:135:PHE:HB2	2:B:166:MET:HE1	1.57	0.85
2:D:5:VAL:HG22	2:D:135:PHE:HD2	1.42	0.85
2:D:16:ILE:HG23	2:D:235:MET:HE1	1.55	0.85
1:A:278:ALA:O	1:A:279:GLU:HB3	1.77	0.85
2:D:162:PRO:HD2	2:D:163:ASP:HB2	1.57	0.84
2:B:273:ALA:CB	2:B:274:PRO:CD	2.55	0.84
1:C:206:ASN:ND2	4:C:600:GTP:HN22	1.75	0.84
2:D:200:GLU:HB3	2:D:268:PHE:HE1	1.43	0.84
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.60	0.84
2:D:391:ILE:HG13	2:D:392:SER:H	1.39	0.83
2:D:99:ALA:HB1	2:D:145:THR:CG2	2.07	0.83
1:A:105:ARG:HH22	2:B:253:ARG:NH2	1.76	0.83
1:C:315:CYS:SG	1:C:377:MET:CE	2.66	0.83
2:D:140:SER:CB	6:D:600:GDP:C5'	2.52	0.83
1:A:79:ARG:NH2	1:A:94:THR:HG21	1.94	0.83
2:D:296:PHE:HE1	2:D:332:MET:CE	1.91	0.83
2:B:223:THR:HB	2:B:225:GLY:N	1.94	0.83
2:D:292:THR:HA	2:D:295:MET:CE	2.09	0.82
2:D:220:THR:O	2:D:222:PRO:HD3	1.79	0.82
2:B:145:THR:HG23	6:B:600:GDP:O3B	1.79	0.82
2:D:224:TYR:O	2:D:228:ASN:ND2	2.12	0.82
2:B:99:ALA:HB1	2:B:145:THR:HG22	1.61	0.81
2:D:123:ARG:O	2:D:127:GLU:HB2	1.80	0.81
2:B:200:GLU:HB3	2:B:268:PHE:CE1	2.15	0.81
2:B:16:ILE:HG23	2:B:235:MET:HE1	1.60	0.81
2:B:171:VAL:CG1	2:B:206:ASN:HD21	1.94	0.80
1:A:206:ASN:HD21	4:A:600:GTP:HN22	1.26	0.80
2:B:99:ALA:HB1	2:B:145:THR:CG2	2.12	0.80
1:C:79:ARG:NH2	1:C:94:THR:HG21	1.96	0.80
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.63	0.80
2:D:250:ALA:HA	2:D:255:LEU:HD13	1.64	0.80
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.63	0.80
2:D:191:VAL:HG11	2:D:425:MET:HE3	1.63	0.80
2:B:391:ILE:HG13	2:B:392:SER:N	1.95	0.79
2:D:403:ALA:O	2:D:405:LEU:N	2.14	0.79
2:D:151:THR:HB	2:D:193:GLN:HG2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:74:GLU:C	3:E:76:ARG:H	1.90	0.79
2:B:123:ARG:O	2:B:127:GLU:HB2	1.83	0.79
2:B:296:PHE:HE1	2:B:332:MET:HE1	1.48	0.78
1:C:41:THR:HG21	1:C:61:HIS:HE1	1.48	0.78
2:D:298:SER:C	2:D:300:ASN:H	1.90	0.78
1:C:343:PHE:CD1	1:C:349:THR:HG22	2.18	0.78
2:B:171:VAL:HG12	2:B:206:ASN:HD21	1.47	0.78
1:C:167:LEU:HD13	1:C:252:LEU:HD11	1.65	0.78
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.08	0.78
2:D:309:HIS:H	2:D:309:HIS:CD2	2.00	0.78
3:E:60:ARG:HH11	3:E:60:ARG:HB2	1.49	0.77
2:B:292:THR:HA	2:B:295:MET:HE3	1.67	0.77
2:D:312:TYR:HD2	2:D:315:VAL:CG2	1.97	0.77
2:B:276:THR:HG23	2:B:277:SER:N	1.99	0.77
2:D:261:PRO:HG3	2:D:313:LEU:HD12	1.64	0.77
2:D:296:PHE:CE1	2:D:332:MET:HE1	2.19	0.77
2:B:403:ALA:C	2:B:405:LEU:H	1.91	0.77
2:B:312:TYR:HE2	2:B:377:PHE:HZ	1.31	0.77
1:C:204:VAL:HG22	1:C:302:MET:HE1	1.66	0.77
2:D:195:VAL:HG21	2:D:428:LEU:HD22	1.65	0.77
2:D:265:LEU:CB	2:D:432:TYR:CE2	2.69	0.76
1:A:315:CYS:SG	1:A:377:MET:HE2	2.25	0.76
1:C:404:PHE:CE1	2:D:347:ILE:HG21	2.17	0.76
1:A:273:ALA:HB3	1:A:274:PRO:CD	2.10	0.76
1:A:145:THR:HG23	4:A:600:GTP:O2B	1.85	0.76
2:B:308:ARG:HG3	2:B:308:ARG:NH1	1.95	0.76
2:D:255:LEU:HG	7:D:700:N16:CAA	2.15	0.76
1:C:153:LEU:HD13	1:C:157:LEU:HD11	1.68	0.75
2:D:248:LEU:HD11	7:D:700:N16:CAL	2.15	0.75
2:D:159:GLU:HB2	3:E:123:LEU:HD13	1.67	0.75
1:C:167:LEU:HD13	1:C:252:LEU:CD1	2.16	0.75
1:C:406:HIS:CG	2:D:263:PRO:HG3	2.21	0.75
2:D:133:GLN:NE2	2:D:252:LEU:HD22	2.01	0.75
2:D:270:PRO:CD	2:D:302:MET:HB2	2.13	0.75
2:B:276:THR:HG23	2:B:277:SER:H	1.49	0.75
1:C:265:ILE:H	1:C:265:ILE:HD12	1.52	0.75
2:D:179:ASP:OD1	2:D:179:ASP:N	2.19	0.75
2:D:298:SER:O	2:D:300:ASN:N	2.18	0.75
2:D:345:GLU:N	2:D:345:GLU:OE1	2.19	0.75
2:D:292:THR:HA	2:D:295:MET:HE3	1.69	0.75
2:D:383:ALA:O	2:D:386:GLU:HB2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:312:TYR:CD2	2:D:315:VAL:CG2	2.70	0.74
2:D:250:ALA:HA	2:D:255:LEU:CD1	2.17	0.74
2:D:298:SER:HA	2:D:301:MET:HG2	1.67	0.74
1:A:153:LEU:HD13	1:A:157:LEU:HD11	1.69	0.74
1:A:401:LYS:C	1:A:403:ALA:H	1.94	0.74
1:C:101:ASN:HD22	2:D:254:LYS:HG2	1.53	0.74
1:A:265:ILE:HD12	1:A:265:ILE:H	1.51	0.74
1:C:256:GLN:C	1:C:258:ASN:H	1.96	0.74
2:B:292:THR:HA	2:B:295:MET:CE	2.18	0.74
1:C:273:ALA:HB3	1:C:375:VAL:H	1.52	0.73
3:E:22:VAL:HG13	3:E:22:VAL:O	1.86	0.73
1:C:256:GLN:C	1:C:258:ASN:N	2.44	0.73
3:E:72:LEU:C	3:E:74:GLU:H	1.96	0.73
2:D:312:TYR:CD2	2:D:315:VAL:HG21	2.23	0.73
2:B:151:THR:HB	2:B:193:GLN:HG2	1.71	0.72
1:C:183:GLU:HB3	1:C:184:PRO:CD	2.18	0.72
2:D:387:LEU:O	2:D:390:ARG:CG	2.24	0.72
1:A:343:PHE:CD1	1:A:349:THR:HG22	2.23	0.72
2:D:51:VAL:HG13	2:D:52:TYR:CD1	2.24	0.72
2:B:147:SER:O	2:B:151:THR:OG1	2.05	0.72
2:B:309:HIS:CD2	2:B:309:HIS:H	2.05	0.72
2:D:140:SER:HB3	6:D:600:GDP:H5'	1.67	0.72
2:D:265:LEU:HB3	2:D:432:TYR:CE2	2.25	0.72
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.25	0.72
2:B:231:VAL:HG12	2:B:235:MET:HE2	1.69	0.72
2:D:99:ALA:HB1	2:D:145:THR:HG22	1.71	0.71
2:B:224:TYR:O	2:B:228:ASN:ND2	2.20	0.71
1:A:181:VAL:H	2:B:258:ASN:ND2	1.87	0.71
2:D:276:THR:HG21	2:D:280:SER:CB	2.21	0.71
2:B:298:SER:C	2:B:300:ASN:H	1.99	0.71
2:D:51:VAL:O	2:D:64:ARG:NH2	2.24	0.71
1:A:101:ASN:HD22	2:B:254:LYS:HG2	1.55	0.71
2:B:223:THR:CB	2:B:225:GLY:H	1.99	0.71
2:D:12:CYS:SG	6:D:600:GDP:C4	2.84	0.71
2:D:36:TYR:OH	2:D:40:SER:O	2.07	0.71
3:E:60:ARG:HB2	3:E:60:ARG:NH1	2.05	0.70
2:D:295:MET:HG3	2:D:377:PHE:HB2	1.72	0.70
1:A:412:GLY:O	3:E:60:ARG:NH1	2.24	0.70
2:B:274:PRO:C	2:B:275:LEU:HG	2.16	0.70
1:C:260:VAL:HG23	1:C:260:VAL:O	1.92	0.70
2:D:265:LEU:HB2	2:D:432:TYR:CE2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:312:TYR:HE2	2:D:377:PHE:CZ	2.09	0.70
2:B:155:SER:CB	3:E:76:ARG:HH22	2.05	0.70
2:D:5:VAL:HG13	2:D:132:LEU:CD1	2.21	0.70
1:A:105:ARG:NH2	2:B:253:ARG:HH21	1.84	0.70
2:D:208:ALA:O	2:D:211:ASP:N	2.23	0.70
2:D:89:PRO:O	2:D:92:PHE:HD1	1.74	0.70
2:D:273:ALA:HB2	2:D:375:ALA:H	1.57	0.70
2:D:306:ASP:C	2:D:308:ARG:H	1.99	0.70
1:A:270:ALA:O	1:A:302:MET:HB2	1.92	0.70
2:D:295:MET:O	2:D:295:MET:HG2	1.92	0.69
2:D:312:TYR:HE2	2:D:377:PHE:HZ	1.41	0.69
2:B:200:GLU:HB3	2:B:268:PHE:HE1	1.55	0.69
2:D:51:VAL:CG1	2:D:52:TYR:HD1	2.06	0.69
2:B:296:PHE:HE1	2:B:332:MET:CE	2.06	0.69
2:D:285:ALA:O	2:D:287:THR:HG22	1.93	0.69
1:A:99:ALA:CB	1:A:145:THR:HG22	2.22	0.68
1:C:273:ALA:CB	1:C:375:VAL:H	2.06	0.68
2:D:202:TYR:OH	7:D:700:N16:HA	1.93	0.68
2:D:273:ALA:CB	2:D:375:ALA:H	2.05	0.68
1:A:273:ALA:HB3	1:A:375:VAL:H	1.59	0.68
1:A:273:ALA:CB	1:A:274:PRO:CD	2.70	0.68
1:C:8:HIS:CD2	1:C:17:GLY:HA3	2.28	0.68
3:E:120:LEU:O	3:E:123:LEU:HB2	1.94	0.68
2:D:135:PHE:HZ	2:D:161:TYR:CD1	2.11	0.68
1:C:401:LYS:C	1:C:403:ALA:H	2.00	0.68
1:C:85:GLN:HA	1:C:85:GLN:HE21	1.59	0.68
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.15	0.68
2:D:325:MET:HE3	2:D:326:LYS:N	2.09	0.68
2:B:151:THR:HG21	2:B:190:SER:HB3	1.75	0.68
1:C:99:ALA:HB2	1:C:145:THR:HG22	1.75	0.68
2:B:54:ASN:HB2	2:B:64:ARG:HD3	1.76	0.67
2:D:135:PHE:CZ	2:D:161:TYR:CD1	2.82	0.67
2:D:384:ILE:HG22	2:D:432:TYR:CE1	2.30	0.67
2:B:401:ARG:O	1:C:262:TYR:OH	2.12	0.67
3:E:84:GLN:C	3:E:86:ALA:H	2.02	0.67
1:A:85:GLN:HE21	1:A:85:GLN:HA	1.59	0.67
1:C:190:THR:HG23	1:C:191:THR:H	1.60	0.67
2:D:234:THR:HG21	2:D:302:MET:HG3	1.75	0.67
1:A:411:GLU:O	3:E:61:ARG:NH1	2.26	0.67
2:B:179:ASP:N	2:B:179:ASP:OD1	2.28	0.67
2:B:135:PHE:HZ	2:B:161:TYR:CD1	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:ALA:HA	2:B:255:LEU:HD13	1.78	0.66
2:D:140:SER:HB2	6:D:600:GDP:C5'	2.09	0.66
1:A:70:LEU:CD1	1:A:145:THR:HB	2.24	0.66
2:D:224:TYR:CE2	6:D:600:GDP:C4	2.84	0.66
3:E:74:GLU:C	3:E:76:ARG:N	2.54	0.66
2:D:224:TYR:OH	6:D:600:GDP:H2'	1.94	0.65
2:D:350:ASN:HD22	2:D:350:ASN:N	1.89	0.65
2:B:89:PRO:O	2:B:92:PHE:HD1	1.78	0.65
2:B:133:GLN:HE21	2:B:252:LEU:CD2	2.07	0.65
2:B:312:TYR:HE2	2:B:377:PHE:CZ	2.12	0.65
2:D:162:PRO:CD	2:D:163:ASP:HB2	2.24	0.65
2:D:252:LEU:HD13	7:D:700:N16:CD1	2.26	0.65
1:A:404:PHE:CE1	2:B:347:ILE:HG21	2.24	0.65
2:B:2:ARG:N	2:B:133:GLN:OE1	2.29	0.65
2:D:171:VAL:CG1	2:D:206:ASN:ND2	2.47	0.65
2:D:412:GLY:O	3:E:133:VAL:HB	1.96	0.65
2:B:224:TYR:CE2	6:B:600:GDP:C4	2.84	0.65
2:D:325:MET:HE3	2:D:326:LYS:H	1.61	0.65
2:D:229:HIS:ND1	2:D:277:SER:HB3	2.12	0.65
1:A:404:PHE:HE1	2:B:347:ILE:CG2	2.10	0.65
2:B:51:VAL:HG13	2:B:52:TYR:CD1	2.32	0.65
2:B:192:HIS:O	2:B:195:VAL:HG12	1.97	0.65
2:D:384:ILE:CG2	2:D:432:TYR:CE1	2.80	0.65
2:B:273:ALA:HB1	2:B:274:PRO:HD3	1.78	0.64
3:E:123:LEU:C	3:E:125:GLU:H	2.05	0.64
1:C:181:VAL:H	2:D:258:ASN:ND2	1.94	0.64
1:C:187:SER:O	1:C:191:THR:HB	1.98	0.64
3:E:78:HIS:C	3:E:78:HIS:CD2	2.74	0.64
1:A:133:GLN:NE2	1:A:252:LEU:HG	2.13	0.64
2:D:255:LEU:HG	7:D:700:N16:CAQ	2.28	0.64
1:A:79:ARG:NH2	1:A:94:THR:CG2	2.60	0.64
2:D:154:ILE:HA	2:D:157:ILE:HB	1.80	0.64
1:A:406:HIS:CG	2:B:263:PRO:HG3	2.33	0.63
2:D:403:ALA:C	2:D:405:LEU:H	2.05	0.63
2:B:296:PHE:CE1	2:B:332:MET:HE1	2.31	0.63
2:D:55:GLU:HB3	2:D:61:TYR:HD2	1.61	0.63
2:D:147:SER:O	2:D:151:THR:OG1	2.09	0.63
1:C:270:ALA:O	1:C:302:MET:HB2	1.99	0.63
1:C:404:PHE:HE1	2:D:347:ILE:CG2	2.08	0.63
2:D:266:HIS:H	2:D:267:PHE:HD1	1.45	0.63
2:D:273:ALA:CB	2:D:274:PRO:CD	2.74	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:67:GLU:C	3:E:69:LEU:H	2.07	0.63
1:A:34:GLY:O	1:A:61:HIS:HB2	1.98	0.63
2:B:135:PHE:CZ	2:B:161:TYR:CD1	2.87	0.63
1:A:88:HIS:HB2	1:A:91:GLN:NE2	2.14	0.63
2:B:298:SER:HA	2:B:301:MET:HG2	1.78	0.63
1:C:108:TYR:HB3	3:E:108:ASN:OD1	1.99	0.63
1:C:143:GLY:HA3	4:C:600:GTP:H5'	1.80	0.63
2:B:345:GLU:N	2:B:345:GLU:OE1	2.32	0.63
2:B:412:GLY:HA3	3:E:86:ALA:HB2	1.80	0.63
2:D:245:PRO:HG2	2:D:246:GLY:H	1.64	0.63
2:D:252:LEU:HD13	7:D:700:N16:HD1	1.79	0.63
2:D:336:GLN:O	2:D:340:SER:HA	1.98	0.62
3:E:118:ALA:O	3:E:122:ARG:CZ	2.47	0.62
2:D:114:LEU:O	2:D:116:ASP:N	2.31	0.62
2:D:54:ASN:HB2	2:D:64:ARG:HD3	1.81	0.62
3:E:81:GLU:O	3:E:82:VAL:C	2.42	0.62
1:C:88:HIS:HB2	1:C:91:GLN:NE2	2.13	0.62
2:D:251:ASP:HB2	2:D:254:LYS:HB2	1.81	0.62
1:A:167:LEU:HD13	1:A:252:LEU:HD13	1.81	0.62
2:D:51:VAL:HG13	2:D:52:TYR:HD1	1.63	0.62
2:D:306:ASP:O	2:D:308:ARG:N	2.33	0.62
3:E:48:GLU:O	3:E:50:ILE:N	2.32	0.62
1:A:273:ALA:CB	1:A:375:VAL:H	2.13	0.62
1:C:256:GLN:O	1:C:259:LEU:N	2.32	0.62
3:E:99:GLU:C	3:E:101:LEU:H	2.06	0.62
1:C:79:ARG:NH2	1:C:94:THR:CG2	2.63	0.61
1:A:266:HIS:O	1:A:268:PRO:HD3	1.99	0.61
1:A:398:MET:HE2	2:B:348:PRO:CD	2.30	0.61
1:C:111:GLY:O	1:C:113:GLU:N	2.33	0.61
1:C:266:HIS:O	1:C:268:PRO:HD3	1.99	0.61
1:A:260:VAL:O	1:A:260:VAL:HG23	1.99	0.61
2:D:381:SER:O	2:D:384:ILE:HB	2.00	0.61
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.24	0.61
2:B:245:PRO:HB2	2:B:247:GLN:HG3	1.82	0.61
2:B:306:ASP:C	2:B:308:ARG:H	2.08	0.61
1:A:271:THR:HG23	1:A:301:GLN:HA	1.83	0.61
2:B:159:GLU:HB2	3:E:72:LEU:HD23	1.83	0.61
2:B:191:VAL:HG11	2:B:425:MET:HE3	1.82	0.61
2:B:251:ASP:HB2	2:B:254:LYS:HB2	1.83	0.61
2:B:308:ARG:HH11	2:B:308:ARG:CG	2.05	0.61
2:D:2:ARG:NH1	2:D:133:GLN:HB2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LEU:HD12	1:A:286:LEU:H	1.64	0.61
2:B:155:SER:HB3	3:E:76:ARG:HH22	1.65	0.61
1:C:315:CYS:SG	1:C:377:MET:HE1	2.39	0.61
1:A:133:GLN:HE21	1:A:252:LEU:HG	1.66	0.60
1:A:249:ASN:HD22	1:A:254:GLU:HG2	1.66	0.60
2:B:131:CYS:O	2:B:131:CYS:SG	2.58	0.60
2:B:265:LEU:CB	2:B:432:TYR:CE2	2.84	0.60
1:A:256:GLN:HG3	1:A:260:VAL:CG2	2.31	0.60
2:B:114:LEU:HB3	2:B:149:MET:HE1	1.83	0.60
2:D:101:ASN:HD22	2:D:143:GLY:HA2	1.65	0.60
2:D:242:LEU:HD11	7:D:700:N16:CD1	2.29	0.60
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.65	0.60
2:D:118:VAL:O	2:D:122:VAL:HG13	2.01	0.60
1:A:105:ARG:HD3	1:A:411:GLU:OE1	2.01	0.60
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.35	0.60
1:A:291:ILE:HD12	1:A:375:VAL:CG2	2.32	0.60
1:A:344:VAL:HG13	1:A:346:TRP:H	1.67	0.60
2:B:55:GLU:HB3	2:B:61:TYR:HD2	1.66	0.60
2:D:262:PHE:CE1	2:D:435:TYR:CZ	2.90	0.60
1:A:275:VAL:O	1:A:275:VAL:HG23	2.02	0.60
2:B:172:MET:HE1	2:B:203:SER:HA	1.84	0.60
2:B:114:LEU:O	2:B:116:ASP:N	2.35	0.59
2:B:245:PRO:HG3	2:B:247:GLN:HE21	1.67	0.59
1:C:343:PHE:HD1	1:C:349:THR:HG22	1.67	0.59
7:B:700:N16:HAA	7:B:700:N16:CAL	2.31	0.59
1:C:101:ASN:ND2	2:D:254:LYS:HG2	2.16	0.59
2:D:70:LEU:HD11	2:D:149:MET:HG3	1.84	0.59
2:D:210:TYR:CE2	2:D:222:PRO:HG2	2.37	0.59
1:C:165:SER:OG	1:C:252:LEU:HD12	2.02	0.59
2:D:10:GLY:O	2:D:14:ASN:N	2.31	0.59
2:B:195:VAL:HG21	2:B:428:LEU:HD22	1.83	0.59
2:D:307:PRO:HB2	2:D:312:TYR:OH	2.03	0.59
3:E:78:HIS:O	3:E:81:GLU:HB2	2.03	0.59
3:E:99:GLU:C	3:E:101:LEU:N	2.54	0.59
1:C:229:ARG:HG2	1:C:229:ARG:HH11	1.66	0.59
1:C:34:GLY:O	1:C:61:HIS:HB2	2.03	0.59
2:D:4:ILE:HD11	2:D:136:GLN:HG2	1.85	0.59
2:D:276:THR:HG21	2:D:280:SER:HB3	1.84	0.59
2:D:358:ILE:HG23	2:D:358:ILE:O	2.01	0.59
2:D:42:LEU:O	2:D:44:LEU:N	2.36	0.59
2:B:306:ASP:O	2:B:308:ARG:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.18	0.58
2:D:262:PHE:CD1	2:D:435:TYR:CE1	2.91	0.58
2:D:309:HIS:CD2	2:D:309:HIS:N	2.70	0.58
2:D:265:LEU:HB2	2:D:432:TYR:OH	2.03	0.58
3:E:84:GLN:C	3:E:86:ALA:N	2.60	0.58
2:D:52:TYR:OH	2:D:239:THR:HG22	2.03	0.58
2:D:391:ILE:HA	2:D:394:GLN:NE2	2.18	0.58
2:B:192:HIS:HD2	2:B:421:ALA:HA	1.68	0.58
1:C:72:PRO:O	1:C:74:VAL:N	2.36	0.58
1:C:177:VAL:HG13	1:C:177:VAL:O	2.03	0.58
2:D:192:HIS:CD2	2:D:421:ALA:CB	2.87	0.58
2:D:226:ASP:OD1	2:D:226:ASP:N	2.37	0.58
2:D:332:MET:O	2:D:335:VAL:HG23	2.02	0.58
2:D:205:ASP:OD1	2:D:207:GLU:HB3	2.02	0.58
2:D:313:LEU:HD13	2:D:347:ILE:HD11	1.86	0.58
1:C:102:ASN:C	1:C:102:ASN:ND2	2.62	0.58
1:C:190:THR:HG23	1:C:191:THR:N	2.18	0.58
1:C:344:VAL:HG13	1:C:346:TRP:H	1.69	0.58
2:D:192:HIS:HD2	2:D:421:ALA:CB	2.16	0.58
2:D:200:GLU:OE2	2:D:268:PHE:HE1	1.87	0.58
2:D:292:THR:HA	2:D:295:MET:HE1	1.85	0.58
2:D:295:MET:CG	2:D:377:PHE:HB2	2.34	0.58
2:D:298:SER:C	2:D:300:ASN:N	2.57	0.58
2:D:269:MET:HE1	2:D:307:PRO:HG3	1.85	0.58
3:E:130:ALA:O	3:E:134:ARG:HD3	2.03	0.58
2:B:171:VAL:CG1	2:B:206:ASN:ND2	2.58	0.57
1:C:99:ALA:CB	1:C:145:THR:HG22	2.33	0.57
2:B:350:ASN:H	2:B:350:ASN:HD22	1.52	0.57
2:D:245:PRO:HB2	2:D:247:GLN:HG3	1.86	0.57
2:D:270:PRO:HD2	2:D:302:MET:CB	2.21	0.57
2:B:384:ILE:HG22	2:B:432:TYR:CE1	2.39	0.57
1:C:271:THR:HG23	1:C:301:GLN:HA	1.87	0.57
2:D:2:ARG:HH12	2:D:133:GLN:HA	1.67	0.57
2:D:142:GLY:O	6:D:600:GDP:H5''	2.04	0.57
2:D:350:ASN:H	2:D:350:ASN:ND2	1.96	0.57
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.40	0.57
2:D:261:PRO:HG3	2:D:313:LEU:CD1	2.32	0.57
2:D:265:LEU:HB2	2:D:432:TYR:HE2	1.70	0.57
2:B:42:LEU:O	2:B:44:LEU:N	2.38	0.57
2:D:55:GLU:HB3	2:D:61:TYR:CD2	2.38	0.57
3:E:101:LEU:O	3:E:103:GLN:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:CZ	2:B:133:GLN:HB2	2.35	0.57
2:B:158:ARG:O	2:B:159:GLU:HB3	2.04	0.57
2:D:351:VAL:HG22	2:D:351:VAL:O	2.05	0.57
2:B:2:ARG:NH1	2:B:133:GLN:HB2	2.20	0.57
2:B:76:ASP:O	2:B:80:SER:HB2	2.05	0.56
2:B:210:TYR:CE2	2:B:222:PRO:HG2	2.39	0.56
1:A:88:HIS:O	1:A:90:GLU:N	2.38	0.56
2:B:239:THR:O	2:B:240:THR:C	2.48	0.56
2:B:245:PRO:HG2	2:B:246:GLY:H	1.70	0.56
2:B:265:LEU:HB2	2:B:432:TYR:CE2	2.40	0.56
1:C:100:ALA:O	1:C:102:ASN:N	2.38	0.56
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.86	0.56
1:A:397:LEU:HG	2:B:346:TRP:HA	1.87	0.56
2:B:5:VAL:HG13	2:B:132:LEU:CD1	2.35	0.56
2:B:21:TRP:CH2	2:B:63:PRO:HB3	2.41	0.56
2:B:265:LEU:HB3	2:B:432:TYR:CE2	2.40	0.56
1:C:20:CYS:HB3	1:C:232:GLY:HA2	1.87	0.56
1:C:188:ILE:HG23	1:C:425:MET:HG3	1.86	0.56
2:D:21:TRP:O	2:D:25:SER:HB2	2.05	0.56
2:D:284:ARG:HD3	2:D:372:LYS:HD2	1.85	0.56
2:D:320:ARG:HA	2:D:356:CYS:O	2.05	0.56
2:B:70:LEU:C	2:B:95:GLY:HA3	2.31	0.56
2:B:205:ASP:OD2	2:B:387:LEU:HD12	2.05	0.56
2:D:224:TYR:CE2	6:D:600:GDP:C5	2.92	0.56
1:C:105:ARG:CZ	2:D:253:ARG:HH21	2.16	0.56
2:D:229:HIS:CE1	2:D:277:SER:CB	2.84	0.56
2:D:236:SER:O	2:D:240:THR:HG23	2.05	0.56
1:A:52:PHE:O	1:A:64:ARG:HB2	2.05	0.56
2:B:135:PHE:HB2	2:B:166:MET:HE2	1.82	0.56
2:B:295:MET:CG	2:B:377:PHE:HB2	2.32	0.56
2:B:325:MET:HE3	2:B:326:LYS:H	1.70	0.56
2:B:325:MET:HE3	2:B:326:LYS:N	2.20	0.56
2:D:192:HIS:HD2	2:D:421:ALA:HA	1.71	0.56
2:D:296:PHE:CE1	2:D:332:MET:CE	2.82	0.56
2:B:101:ASN:HD22	2:B:143:GLY:HA2	1.70	0.56
2:B:102:ASN:OD1	2:B:102:ASN:C	2.48	0.56
2:B:208:ALA:O	2:B:211:ASP:N	2.38	0.56
1:A:22:GLU:HB2	1:A:83:TYR:HE1	1.71	0.56
1:C:68:VAL:HG12	1:C:93:ILE:HB	1.88	0.56
1:A:183:GLU:HB3	1:A:184:PRO:CD	2.33	0.55
2:D:308:ARG:HG3	2:D:308:ARG:NH1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:TRP:O	2:B:25:SER:HB2	2.06	0.55
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.70	0.55
2:D:2:ARG:CZ	2:D:133:GLN:HB2	2.35	0.55
2:D:253:ARG:O	2:D:254:LYS:C	2.49	0.55
1:A:388:TRP:CE3	1:A:388:TRP:HA	2.41	0.55
3:E:77:GLU:HG2	3:E:80:ARG:HB2	1.87	0.55
2:B:115:VAL:HG12	2:B:116:ASP:N	2.21	0.55
2:B:118:VAL:O	2:B:122:VAL:HG13	2.06	0.55
2:B:51:VAL:CG1	2:B:52:TYR:HD1	2.18	0.55
2:B:276:THR:CG2	2:B:277:SER:N	2.68	0.55
2:D:164:ARG:HE	2:D:164:ARG:HA	1.71	0.55
3:E:120:LEU:HA	3:E:123:LEU:HD12	1.88	0.55
2:B:55:GLU:HB3	2:B:61:TYR:CD2	2.42	0.55
2:B:110:GLU:O	2:B:113:GLU:HB3	2.07	0.55
2:B:261:PRO:HG3	2:B:313:LEU:HD12	1.87	0.55
2:B:10:GLY:O	2:B:14:ASN:N	2.37	0.55
2:D:266:HIS:N	2:D:267:PHE:HD1	2.05	0.55
2:D:406:HIS:HA	2:D:409:THR:HB	1.88	0.55
2:D:2:ARG:N	2:D:133:GLN:OE1	2.40	0.55
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.41	0.55
1:A:312:TYR:HE2	1:A:379:SER:HB3	1.72	0.55
1:C:190:THR:CG2	1:C:191:THR:H	2.20	0.55
2:D:137:LEU:HD21	2:D:139:HIS:CE1	2.41	0.55
2:D:165:ILE:CG2	2:D:253:ARG:HH11	2.20	0.55
1:A:72:PRO:O	1:A:74:VAL:N	2.39	0.54
1:C:78:VAL:C	1:C:80:THR:H	2.15	0.54
1:C:286:LEU:H	1:C:286:LEU:HD12	1.72	0.54
1:C:427:ALA:O	1:C:430:LYS:HB3	2.08	0.54
2:B:51:VAL:HG13	2:B:52:TYR:HD1	1.72	0.54
2:B:309:HIS:CD2	2:B:309:HIS:N	2.75	0.54
1:C:70:LEU:CD1	1:C:145:THR:HB	2.35	0.54
1:A:154:MET:O	1:A:158:SER:HB2	2.07	0.54
2:B:292:THR:C	2:B:294:GLN:H	2.14	0.54
2:B:391:ILE:HG13	2:B:392:SER:H	1.71	0.54
2:B:234:THR:HG21	2:B:302:MET:HG3	1.89	0.54
2:D:48:ARG:NH1	2:D:242:LEU:O	2.40	0.54
3:E:6:MET:HE3	3:E:24:LEU:HD21	1.89	0.54
1:A:101:ASN:ND2	2:B:254:LYS:HG2	2.23	0.54
2:B:273:ALA:CB	2:B:375:ALA:H	2.21	0.54
2:B:312:TYR:CD2	2:B:315:VAL:HG21	2.43	0.54
1:C:401:LYS:C	1:C:403:ALA:N	2.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:387:LEU:C	2:D:390:ARG:HG2	2.26	0.54
2:B:383:ALA:O	2:B:386:GLU:HB2	2.08	0.54
1:C:80:THR:HG22	1:C:81:GLY:N	2.23	0.54
2:D:4:ILE:HG23	2:D:51:VAL:HG22	1.89	0.54
2:D:255:LEU:CG	7:D:700:N16:HAAA	2.31	0.54
2:B:64:ARG:HG3	2:B:125:GLU:OE1	2.08	0.54
2:B:270:PRO:CD	2:B:302:MET:HB2	2.35	0.54
2:B:319:PHE:CB	2:B:355:VAL:HG12	2.29	0.54
2:D:384:ILE:CG2	2:D:432:TYR:HE1	2.21	0.54
1:A:8:HIS:CD2	1:A:17:GLY:CA	2.90	0.54
2:D:192:HIS:CD2	2:D:421:ALA:HB2	2.43	0.53
2:B:12:CYS:SG	6:B:600:GDP:C4	3.01	0.53
1:A:79:ARG:HH21	1:A:94:THR:HG21	1.73	0.53
1:A:187:SER:O	1:A:191:THR:HB	2.06	0.53
2:B:312:TYR:CD2	2:B:315:VAL:CG2	2.91	0.53
1:A:315:CYS:SG	1:A:377:MET:CE	2.95	0.53
2:D:245:PRO:CG	2:D:246:GLY:H	2.21	0.53
2:D:242:LEU:CD1	7:D:700:N16:HD1	2.33	0.53
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.91	0.53
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.15	0.53
2:B:155:SER:HB2	3:E:76:ARG:HH22	1.74	0.53
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.42	0.53
2:D:158:ARG:O	2:D:160:GLU:N	2.32	0.53
1:A:317:LEU:HD23	1:A:377:MET:HE3	1.91	0.53
1:A:351:PHE:HB2	3:E:22:VAL:HG12	1.91	0.53
1:C:291:ILE:HD12	1:C:375:VAL:CG2	2.38	0.53
2:D:158:ARG:HA	2:D:161:TYR:O	2.07	0.52
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.91	0.52
2:D:171:VAL:HG11	2:D:206:ASN:HD21	1.66	0.52
3:E:118:ALA:O	3:E:122:ARG:NH2	2.43	0.52
1:A:85:GLN:HA	1:A:85:GLN:NE2	2.22	0.52
1:A:133:GLN:CD	1:A:252:LEU:H	2.18	0.52
2:B:133:GLN:NE2	2:B:252:LEU:HB2	2.24	0.52
2:B:408:TYR:O	2:B:409:THR:C	2.52	0.52
1:A:88:HIS:O	1:A:89:PRO:C	2.51	0.52
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.90	0.52
2:D:11:GLN:HB3	6:D:600:GDP:O1A	2.09	0.52
2:D:12:CYS:SG	6:D:600:GDP:N3	2.83	0.52
2:D:265:LEU:CB	2:D:432:TYR:CZ	2.92	0.52
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.75	0.52
2:B:70:LEU:HD11	2:B:149:MET:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:LEU:O	1:C:392:ASP:C	2.52	0.52
2:D:151:THR:HG21	2:D:190:SER:HB3	1.92	0.52
2:D:226:ASP:O	2:D:227:LEU:HB2	2.10	0.52
1:C:383:ALA:O	1:C:386:GLU:HB2	2.10	0.52
2:B:400:ARG:C	2:B:402:LYS:H	2.18	0.52
3:E:74:GLU:O	3:E:76:ARG:N	2.43	0.52
3:E:133:VAL:HA	3:E:136:ASN:HB3	1.92	0.52
2:B:70:LEU:HA	2:B:95:GLY:HA3	1.92	0.52
2:B:177:VAL:HG12	2:B:177:VAL:O	2.10	0.52
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.45	0.52
2:B:2:ARG:HD2	2:B:131:CYS:SG	2.50	0.51
2:B:406:HIS:HA	2:B:409:THR:HB	1.91	0.51
1:C:102:ASN:HD22	1:C:103:TYR:N	2.08	0.51
2:D:209:LEU:HD21	2:D:231:VAL:HG22	1.92	0.51
1:A:190:THR:HG23	1:A:191:THR:N	2.25	0.51
2:D:224:TYR:CD2	6:D:600:GDP:C5	2.98	0.51
2:B:295:MET:O	2:B:295:MET:HG2	2.11	0.51
2:D:153:LEU:O	2:D:157:ILE:N	2.43	0.51
2:B:298:SER:C	2:B:300:ASN:N	2.68	0.51
1:C:154:MET:O	1:C:158:SER:HB2	2.10	0.51
1:C:376:CYS:O	1:C:376:CYS:SG	2.69	0.51
1:C:387:ALA:HB2	1:C:390:ARG:HH12	1.75	0.51
2:D:21:TRP:CH2	2:D:63:PRO:HB3	2.46	0.51
2:D:150:GLY:HA2	2:D:153:LEU:HB2	1.91	0.51
2:D:383:ALA:O	2:D:386:GLU:CB	2.57	0.51
2:B:224:TYR:CD2	6:B:600:GDP:C6	2.98	0.51
2:B:248:LEU:O	2:B:249:ASN:HB3	2.09	0.51
1:C:163:LYS:O	1:C:164:LYS:C	2.53	0.51
2:D:2:ARG:HD2	2:D:131:CYS:SG	2.51	0.51
2:D:145:THR:O	2:D:149:MET:HB2	2.10	0.51
3:E:72:LEU:C	3:E:74:GLU:N	2.64	0.51
2:B:245:PRO:CG	2:B:247:GLN:HE21	2.24	0.51
2:D:284:ARG:HB2	2:D:372:LYS:HE3	1.91	0.51
2:D:402:LYS:HB3	2:D:405:LEU:HD22	1.92	0.51
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.46	0.51
2:D:237:GLY:CA	2:D:376:THR:HG21	2.41	0.51
2:D:283:TYR:C	2:D:285:ALA:H	2.19	0.51
2:B:145:THR:O	2:B:149:MET:HB2	2.11	0.51
2:B:171:VAL:HG11	2:B:206:ASN:HD21	1.73	0.51
2:B:237:GLY:CA	2:B:376:THR:HG21	2.41	0.51
2:B:403:ALA:C	2:B:405:LEU:N	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:391:ILE:CG1	2:D:392:SER:N	2.68	0.51
1:A:88:HIS:O	1:A:91:GLN:N	2.40	0.51
1:C:48:SER:O	1:C:243:ARG:O	2.29	0.51
2:D:133:GLN:HE21	2:D:252:LEU:CD2	2.08	0.51
2:D:182:VAL:HG23	2:D:186:ASN:ND2	2.26	0.51
2:D:114:LEU:HD12	2:D:117:SER:HB2	1.92	0.51
2:B:138:THR:O	2:B:139:HIS:HB3	2.11	0.50
2:D:141:LEU:HA	2:D:147:SER:HB3	1.92	0.50
2:D:287:THR:OG1	2:D:289:PRO:HD2	2.11	0.50
1:A:47:ASP:O	1:A:48:SER:HB2	2.12	0.50
2:B:7:ILE:O	2:B:137:LEU:HA	2.10	0.50
2:D:265:LEU:CB	2:D:432:TYR:OH	2.59	0.50
1:A:163:LYS:O	1:A:164:LYS:C	2.54	0.50
1:A:179:THR:O	2:B:352:LYS:HG3	2.11	0.50
2:D:164:ARG:HE	2:D:164:ARG:CA	2.21	0.50
2:D:264:ARG:O	2:D:265:LEU:C	2.55	0.50
2:D:312:TYR:CE2	2:D:377:PHE:HZ	2.24	0.50
3:E:78:HIS:HA	3:E:81:GLU:OE2	2.10	0.50
2:B:224:TYR:CE2	6:B:600:GDP:C5	2.99	0.50
1:C:431:ASP:O	1:C:435:VAL:HG23	2.12	0.50
1:A:111:GLY:O	1:A:113:GLU:N	2.44	0.50
1:C:109:THR:HG21	3:E:112:ARG:NH2	2.27	0.50
2:D:52:TYR:OH	2:D:136:GLN:NE2	2.45	0.50
2:D:108:TYR:HE1	2:D:413:MET:HE3	1.77	0.50
2:D:191:VAL:HG11	2:D:425:MET:CE	2.39	0.50
1:A:190:THR:HG23	1:A:191:THR:H	1.75	0.50
1:C:191:THR:HG23	1:C:425:MET:CE	2.41	0.50
2:B:350:ASN:HD22	2:B:350:ASN:N	2.09	0.50
2:B:114:LEU:HB3	2:B:149:MET:CE	2.41	0.50
2:B:200:GLU:OE2	2:B:268:PHE:HE1	1.94	0.50
2:B:255:LEU:HD23	7:B:700:N16:HB	1.94	0.50
1:C:12:ALA:HB3	1:C:140:SER:OG	2.12	0.50
1:C:190:THR:O	1:C:192:HIS:N	2.45	0.50
1:A:181:VAL:N	2:B:258:ASN:ND2	2.59	0.50
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.94	0.50
2:D:202:TYR:CD1	2:D:202:TYR:N	2.79	0.50
1:A:398:MET:HE2	2:B:348:PRO:HD2	1.93	0.49
2:B:51:VAL:O	2:B:64:ARG:NH2	2.44	0.49
2:B:287:THR:HG21	2:B:290:GLU:HB2	1.92	0.49
2:D:70:LEU:HD11	2:D:149:MET:HE3	1.94	0.49
3:E:123:LEU:C	3:E:125:GLU:N	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:TYR:O	1:C:104:ALA:C	2.54	0.49
3:E:22:VAL:O	3:E:22:VAL:CG1	2.55	0.49
1:A:312:TYR:CE2	1:A:379:SER:HB3	2.47	0.49
1:A:401:LYS:C	1:A:403:ALA:N	2.61	0.49
1:C:49:PHE:C	1:C:49:PHE:CD2	2.90	0.49
2:D:319:PHE:CB	2:D:355:VAL:HG12	2.27	0.49
2:D:225:GLY:O	2:D:228:ASN:N	2.46	0.49
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.48	0.49
1:C:90:GLU:O	1:C:121:ARG:CD	2.60	0.49
2:D:158:ARG:C	2:D:160:GLU:H	2.19	0.49
1:A:247:ALA:O	1:A:248:LEU:HB3	2.12	0.49
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.93	0.49
2:D:276:THR:HG21	2:D:280:SER:HB2	1.94	0.49
2:D:385:GLN:HG2	2:D:389:LYS:HD2	1.95	0.49
1:A:177:VAL:O	1:A:177:VAL:HG13	2.13	0.49
1:A:309:HIS:ND1	1:A:309:HIS:C	2.71	0.49
1:A:376:CYS:O	1:A:376:CYS:SG	2.70	0.49
2:B:118:VAL:O	2:B:119:LEU:C	2.54	0.49
2:D:205:ASP:OD2	2:D:387:LEU:HD12	2.12	0.49
3:E:49:GLU:O	3:E:49:GLU:HG3	2.11	0.49
1:A:317:LEU:CD2	1:A:377:MET:HE3	2.43	0.49
2:B:88:ARG:HB3	2:B:91:ASN:OD1	2.13	0.49
2:B:149:MET:O	2:B:152:LEU:HB3	2.13	0.49
2:B:261:PRO:HG2	2:B:262:PHE:H	1.78	0.49
1:C:253:THR:O	1:C:256:GLN:N	2.40	0.49
2:D:275:LEU:O	2:D:276:THR:HB	2.11	0.49
2:D:413:MET:HE2	2:D:417:GLU:OE2	2.13	0.49
1:A:55:GLU:HG2	1:A:61:HIS:CE1	2.48	0.49
1:A:68:VAL:HG12	1:A:93:ILE:HB	1.94	0.49
1:A:420:GLU:HA	1:A:423:GLU:HG3	1.95	0.49
2:B:164:ARG:NH2	2:B:253:ARG:HH22	2.11	0.49
2:B:261:PRO:HG3	2:B:313:LEU:CD1	2.43	0.49
1:A:383:ALA:O	1:A:386:GLU:HB2	2.12	0.48
2:B:255:LEU:HG	7:B:700:N16:CAQ	2.43	0.48
2:D:88:ARG:HB3	2:D:91:ASN:OD1	2.13	0.48
2:D:287:THR:HG21	2:D:290:GLU:HB2	1.88	0.48
1:C:115:ILE:O	1:C:119:LEU:HB2	2.13	0.48
1:C:139:HIS:HD2	1:C:146:GLY:O	1.95	0.48
1:C:167:LEU:HD13	1:C:252:LEU:HD13	1.96	0.48
1:C:408:TYR:C	1:C:410:GLY:N	2.69	0.48
1:A:202:PHE:CE2	1:A:268:PRO:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:399:PHE:O	2:B:400:ARG:O	2.30	0.48
1:C:167:LEU:CD1	1:C:252:LEU:HD13	2.44	0.48
1:C:184:PRO:O	1:C:185:TYR:C	2.57	0.48
2:D:195:VAL:CG2	2:D:428:LEU:HD22	2.41	0.48
2:D:267:PHE:CD2	2:D:388:PHE:HZ	2.31	0.48
1:A:312:TYR:HE2	1:A:379:SER:CB	2.27	0.48
2:B:251:ASP:HB3	2:B:254:LYS:H	1.78	0.48
1:C:183:GLU:O	1:C:184:PRO:C	2.54	0.48
1:A:343:PHE:HD1	1:A:349:THR:HG22	1.76	0.48
1:C:8:HIS:CD2	1:C:17:GLY:CA	2.96	0.48
2:D:276:THR:CG2	2:D:277:SER:N	2.77	0.48
2:D:292:THR:C	2:D:294:GLN:H	2.21	0.48
1:A:6:SER:HB3	1:A:8:HIS:HE1	1.79	0.48
1:A:278:ALA:HA	1:A:281:ALA:HB2	1.95	0.48
2:B:217:LEU:HB3	2:B:219:LEU:HG	1.95	0.48
2:B:224:TYR:CD2	6:B:600:GDP:C5	3.02	0.48
1:C:260:VAL:O	1:C:260:VAL:CG2	2.61	0.48
2:D:15:GLN:HG3	2:D:15:GLN:O	2.13	0.48
2:D:307:PRO:HB2	2:D:312:TYR:CZ	2.49	0.48
1:A:49:PHE:C	1:A:49:PHE:CD2	2.92	0.48
1:C:395:PHE:C	1:C:395:PHE:CD2	2.91	0.48
2:D:239:THR:O	2:D:240:THR:C	2.56	0.48
2:D:265:LEU:HB2	2:D:432:TYR:CZ	2.49	0.48
2:D:403:ALA:C	2:D:405:LEU:N	2.67	0.48
2:B:102:ASN:OD1	2:B:102:ASN:O	2.31	0.48
2:B:164:ARG:HE	2:B:164:ARG:HA	1.79	0.48
2:B:202:TYR:OH	7:B:700:N16:HA	2.14	0.48
1:C:49:PHE:C	1:C:49:PHE:HD2	2.22	0.48
1:C:181:VAL:N	2:D:258:ASN:ND2	2.62	0.48
1:A:53:PHE:CD1	1:A:53:PHE:N	2.81	0.48
1:A:182:VAL:HG22	1:A:182:VAL:O	2.14	0.48
1:A:425:MET:O	1:A:426:ALA:C	2.56	0.48
2:B:141:LEU:HA	2:B:147:SER:HB3	1.94	0.48
1:C:402:ARG:O	1:C:403:ALA:C	2.56	0.48
2:D:251:ASP:HB2	2:D:254:LYS:HD3	1.96	0.48
1:A:190:THR:O	1:A:192:HIS:N	2.47	0.47
2:B:273:ALA:HB2	2:B:375:ALA:H	1.79	0.47
2:B:306:ASP:C	2:B:308:ARG:N	2.72	0.47
2:D:205:ASP:OD1	2:D:207:GLU:CB	2.62	0.47
1:A:391:LEU:O	1:A:392:ASP:C	2.57	0.47
2:B:298:SER:O	2:B:300:ASN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:CYS:O	1:C:377:MET:HA	2.14	0.47
2:D:200:GLU:OE2	2:D:268:PHE:CE1	2.66	0.47
2:D:298:SER:CB	2:D:307:PRO:HD2	2.43	0.47
3:E:90:ASN:O	3:E:93:PHE:HB3	2.14	0.47
2:B:202:TYR:N	2:B:202:TYR:CD1	2.82	0.47
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.96	0.47
1:C:105:ARG:NH2	2:D:253:ARG:NH2	2.39	0.47
2:D:291:LEU:HD11	2:D:374:SER:HA	1.95	0.47
1:A:408:TYR:C	1:A:410:GLY:N	2.69	0.47
2:B:114:LEU:HD12	2:B:117:SER:HB2	1.95	0.47
2:B:357:ASP:OD2	2:B:357:ASP:N	2.46	0.47
1:C:428:LEU:C	1:C:430:LYS:N	2.70	0.47
2:D:177:VAL:HG12	2:D:177:VAL:O	2.14	0.47
1:C:102:ASN:C	1:C:102:ASN:HD22	2.23	0.47
1:C:223:THR:O	1:C:227:LEU:HD13	2.15	0.47
2:D:27:GLU:OE2	2:D:243:ARG:NH2	2.38	0.47
2:D:262:PHE:CE1	2:D:435:TYR:CE1	3.03	0.47
1:A:6:SER:HB3	1:A:8:HIS:CE1	2.50	0.47
1:A:431:ASP:O	1:A:435:VAL:HG23	2.14	0.47
2:B:62:VAL:HA	2:B:63:PRO:HD2	1.83	0.47
1:C:187:SER:HB2	1:C:391:LEU:HD21	1.97	0.47
1:C:275:VAL:O	1:C:275:VAL:HG23	2.13	0.47
1:C:341:ILE:HD13	1:C:341:ILE:H	1.79	0.47
2:D:192:HIS:HD2	2:D:421:ALA:CA	2.28	0.47
1:A:256:GLN:HG3	1:A:260:VAL:HG22	1.96	0.47
2:B:7:ILE:HG22	2:B:137:LEU:HD13	1.96	0.47
2:D:200:GLU:HA	2:D:266:HIS:HB2	1.96	0.47
2:D:207:GLU:O	2:D:211:ASP:HB2	2.15	0.47
2:D:260:VAL:HG11	2:D:266:HIS:HB3	1.95	0.47
2:B:153:LEU:O	2:B:157:ILE:N	2.43	0.47
2:D:202:TYR:H	2:D:202:TYR:HD1	1.63	0.47
2:D:273:ALA:HB2	2:D:375:ALA:N	2.28	0.47
2:D:400:ARG:C	2:D:402:LYS:H	2.22	0.47
1:A:402:ARG:O	1:A:403:ALA:C	2.58	0.46
1:C:372:GLN:HB2	1:C:373:ARG:HE	1.80	0.46
1:C:391:LEU:O	1:C:393:HIS:N	2.49	0.46
2:D:158:ARG:O	2:D:159:GLU:HB3	2.15	0.46
2:D:336:GLN:O	2:D:340:SER:CA	2.63	0.46
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.49	0.46
1:A:316:CYS:O	1:A:377:MET:HA	2.14	0.46
2:B:154:ILE:HA	2:B:157:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:PRO:HD2	2:B:163:ASP:HB2	1.97	0.46
2:B:321:GLY:O	2:B:323:MET:N	2.48	0.46
2:B:407:TRP:CE2	1:C:257:THR:HA	2.51	0.46
2:D:202:TYR:HE2	2:D:378:ILE:HG12	1.80	0.46
2:B:312:TYR:CE2	2:B:377:PHE:CZ	3.00	0.46
1:C:6:SER:HB3	1:C:8:HIS:CE1	2.50	0.46
1:C:111:GLY:O	1:C:112:LYS:C	2.57	0.46
2:D:408:TYR:O	2:D:409:THR:C	2.58	0.46
1:A:223:THR:O	1:A:227:LEU:HD13	2.16	0.46
2:D:115:VAL:HG12	2:D:116:ASP:N	2.29	0.46
2:D:226:ASP:O	2:D:227:LEU:CB	2.63	0.46
2:D:406:HIS:CD2	2:D:406:HIS:C	2.92	0.46
3:E:119:MET:HA	3:E:122:ARG:NH2	2.31	0.46
2:B:236:SER:O	2:B:240:THR:HG23	2.16	0.46
2:B:239:THR:HG22	7:B:700:N16:HE1	1.96	0.46
1:C:405:VAL:CG1	1:C:406:HIS:N	2.78	0.46
2:D:255:LEU:HA	7:D:700:N16:HAAA	1.98	0.46
2:D:286:LEU:H	2:D:286:LEU:HG	1.38	0.46
1:A:190:THR:O	1:A:194:THR:HB	2.15	0.46
2:D:4:ILE:CD1	2:D:136:GLN:HG2	2.46	0.46
2:D:251:ASP:HB3	2:D:254:LYS:H	1.79	0.46
2:D:321:GLY:O	2:D:323:MET:N	2.49	0.46
1:A:20:CYS:HB3	1:A:232:GLY:HA2	1.96	0.46
2:B:312:TYR:HD2	2:B:315:VAL:CG2	2.29	0.46
2:D:76:ASP:O	2:D:80:SER:HB2	2.15	0.46
1:A:249:ASN:H	1:A:254:GLU:CD	2.24	0.46
1:A:347:CYS:O	1:A:348:PRO:C	2.59	0.46
2:B:122:VAL:CG2	2:B:123:ARG:N	2.79	0.46
2:B:142:GLY:O	6:B:600:GDP:C5'	2.43	0.46
2:D:223:THR:HB	2:D:225:GLY:CA	2.44	0.46
1:A:10:GLY:O	1:A:11:GLN:C	2.59	0.46
1:A:12:ALA:HB3	1:A:140:SER:OG	2.16	0.46
1:A:115:ILE:O	1:A:119:LEU:HB2	2.15	0.46
2:B:36:TYR:OH	2:B:40:SER:O	2.27	0.46
2:B:172:MET:CE	2:B:203:SER:HB3	2.46	0.46
2:B:205:ASP:HB2	2:B:304:ALA:H	1.80	0.46
1:C:100:ALA:O	1:C:101:ASN:C	2.58	0.46
1:C:142:GLY:HA3	1:C:183:GLU:HG3	1.98	0.46
1:A:341:ILE:HD13	1:A:341:ILE:H	1.81	0.46
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.72	0.46
2:B:52:TYR:OH	2:B:136:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:MET:O	2:D:152:LEU:HB3	2.16	0.46
2:D:413:MET:CE	2:D:417:GLU:OE2	2.64	0.46
1:A:260:VAL:O	1:A:260:VAL:CG2	2.64	0.45
2:B:4:ILE:HG23	2:B:51:VAL:HG22	1.97	0.45
1:C:27:GLU:OE2	1:C:243:ARG:NH2	2.48	0.45
1:C:169:PHE:CE2	1:C:235:VAL:HG22	2.51	0.45
1:C:251:ASP:OD1	1:C:252:LEU:N	2.50	0.45
3:E:76:ARG:C	3:E:78:HIS:H	2.24	0.45
3:E:77:GLU:HG2	3:E:80:ARG:CB	2.46	0.45
2:B:191:VAL:HG11	2:B:425:MET:CE	2.44	0.45
2:B:253:ARG:O	2:B:254:LYS:C	2.58	0.45
2:B:265:LEU:HB2	2:B:432:TYR:HE2	1.80	0.45
1:C:102:ASN:HD21	1:C:104:ALA:HB3	1.81	0.45
1:C:248:LEU:HD22	1:C:249:ASN:H	1.81	0.45
2:D:140:SER:OG	6:D:600:GDP:H5'	2.12	0.45
2:D:351:VAL:O	2:D:351:VAL:CG2	2.64	0.45
1:A:88:HIS:C	1:A:90:GLU:N	2.71	0.45
1:A:185:TYR:CD1	1:A:418:PHE:HE2	2.34	0.45
2:B:12:CYS:SG	6:B:600:GDP:N3	2.89	0.45
2:B:198:THR:OG1	2:B:266:HIS:CE1	2.69	0.45
1:C:256:GLN:O	1:C:258:ASN:N	2.49	0.45
2:D:51:VAL:CG1	2:D:52:TYR:CD1	2.89	0.45
2:B:260:VAL:HG11	2:B:266:HIS:HB3	1.98	0.45
1:A:8:HIS:HD2	1:A:17:GLY:HA3	1.80	0.45
2:B:16:ILE:HG22	2:B:17:GLY:N	2.32	0.45
2:B:308:ARG:HA	2:B:308:ARG:HD2	1.76	0.45
1:C:190:THR:O	1:C:194:THR:HB	2.16	0.45
1:C:229:ARG:HD3	1:C:363:VAL:HG21	1.99	0.45
2:D:99:ALA:CB	2:D:145:THR:CG2	2.89	0.45
2:B:172:MET:HG2	2:B:387:LEU:HD21	1.97	0.45
7:B:700:N16:CAL	7:B:700:N16:CAA	2.94	0.45
1:C:2:ARG:HB2	1:C:131:GLY:O	2.16	0.45
1:C:41:THR:CG2	1:C:61:HIS:HE1	2.24	0.45
1:C:79:ARG:HD3	1:C:92:LEU:HD13	1.99	0.45
1:C:139:HIS:CG	1:C:150:THR:HG21	2.51	0.45
2:D:114:LEU:HD23	2:D:149:MET:HE1	1.97	0.45
3:E:67:GLU:C	3:E:69:LEU:N	2.74	0.45
2:B:20:PHE:HD2	2:B:235:MET:HB3	1.80	0.45
2:B:20:PHE:O	2:B:24:ILE:HG23	2.16	0.45
2:B:381:SER:O	2:B:384:ILE:HB	2.16	0.45
1:C:85:GLN:HA	1:C:85:GLN:NE2	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:TYR:CD1	1:C:418:PHE:HE2	2.35	0.45
1:C:273:ALA:CB	1:C:274:PRO:CD	2.76	0.45
1:C:309:HIS:ND1	1:C:310:GLY:N	2.64	0.45
2:D:192:HIS:O	2:D:195:VAL:HG12	2.16	0.45
3:E:101:LEU:O	3:E:104:LYS:N	2.47	0.45
1:A:78:VAL:C	1:A:80:THR:H	2.24	0.45
2:D:295:MET:HE2	2:D:295:MET:HB3	1.65	0.45
2:D:308:ARG:HH21	2:D:339:ASN:HD21	1.64	0.45
2:B:248:LEU:HD23	2:B:248:LEU:HA	1.46	0.45
2:D:5:VAL:HG22	2:D:135:PHE:CD2	2.34	0.45
2:D:42:LEU:O	2:D:43:GLN:C	2.59	0.45
2:D:223:THR:CG2	2:D:225:GLY:H	2.29	0.45
3:E:76:ARG:O	3:E:79:GLU:HB2	2.17	0.45
2:B:4:ILE:HD11	2:B:136:GLN:HG2	1.99	0.45
2:B:407:TRP:NE1	1:C:257:THR:HA	2.32	0.45
2:D:250:ALA:HA	2:D:255:LEU:HD11	1.95	0.45
2:B:192:HIS:CD2	2:B:421:ALA:CB	3.00	0.44
1:C:153:LEU:HD13	1:C:157:LEU:CD1	2.44	0.44
1:C:153:LEU:HD23	1:C:153:LEU:HA	1.84	0.44
3:E:137:LYS:C	3:E:139:LEU:H	2.25	0.44
1:C:82:THR:O	1:C:83:TYR:CG	2.69	0.44
2:D:245:PRO:CG	2:D:246:GLY:N	2.81	0.44
2:D:325:MET:HA	2:D:328:VAL:HG23	1.99	0.44
2:B:239:THR:O	2:B:241:CYS:N	2.50	0.44
1:C:167:LEU:CD1	1:C:252:LEU:CD1	2.91	0.44
2:D:282:GLN:HG3	2:D:286:LEU:HD21	1.98	0.44
2:D:289:PRO:HA	2:D:331:GLN:NE2	2.31	0.44
2:D:313:LEU:HD23	2:D:382:THR:CG2	2.47	0.44
2:D:404:PHE:HD1	2:D:404:PHE:H	1.66	0.44
1:A:49:PHE:C	1:A:49:PHE:HD2	2.25	0.44
2:D:145:THR:HG23	6:D:600:GDP:O3B	2.17	0.44
2:D:165:ILE:HD11	2:D:167:ASN:ND2	2.33	0.44
2:D:174:SER:HB2	2:D:390:ARG:NH2	2.32	0.44
1:A:169:PHE:CE2	1:A:235:VAL:HG22	2.51	0.44
1:A:174:ALA:HB1	1:A:207:GLU:HB2	1.99	0.44
1:A:428:LEU:C	1:A:430:LYS:N	2.73	0.44
2:D:229:HIS:HE1	2:D:277:SER:HB3	1.72	0.44
2:D:306:ASP:C	2:D:308:ARG:N	2.68	0.44
3:E:91:ASN:C	3:E:93:PHE:H	2.25	0.44
1:A:2:ARG:HB2	1:A:131:GLY:O	2.17	0.44
1:A:394:LYS:HG2	2:B:348:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLN:OE1	2:B:67:LEU:HD23	2.17	0.44
2:B:150:GLY:HA2	2:B:153:LEU:HB2	1.98	0.44
2:B:174:SER:HB2	2:B:390:ARG:NH2	2.32	0.44
1:C:68:VAL:CG1	1:C:93:ILE:HB	2.48	0.44
2:D:224:TYR:CD2	6:D:600:GDP:C6	3.06	0.44
1:A:372:GLN:H	1:A:372:GLN:HG2	1.42	0.44
2:B:332:MET:O	2:B:335:VAL:HG23	2.18	0.44
2:D:104:ALA:O	2:D:105:LYS:C	2.61	0.44
2:D:114:LEU:HB3	2:D:149:MET:HE1	1.98	0.44
2:D:237:GLY:HA2	2:D:376:THR:HG21	2.00	0.44
2:D:245:PRO:CB	2:D:247:GLN:HG3	2.47	0.44
2:D:384:ILE:HG22	2:D:432:TYR:CD1	2.52	0.44
2:D:252:LEU:CD1	7:D:700:N16:CD1	2.95	0.44
2:D:311:ARG:HG2	2:D:342:TYR:HD2	1.82	0.44
2:D:358:ILE:O	2:D:358:ILE:CG2	2.66	0.44
1:A:205:ASP:CB	1:A:303:VAL:HA	2.48	0.44
1:A:277:SER:O	1:A:280:LYS:HB2	2.18	0.44
2:B:42:LEU:O	2:B:43:GLN:C	2.61	0.44
1:C:16:ILE:HD13	1:C:171:ILE:HD11	2.00	0.44
1:C:260:VAL:HA	1:C:261:PRO:HD3	1.84	0.44
2:D:28:HIS:HA	2:D:43:GLN:HB3	2.00	0.44
2:D:31:ASP:C	2:D:33:THR:N	2.76	0.44
1:A:205:ASP:HB3	1:A:303:VAL:HA	2.00	0.43
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.50	0.43
2:B:224:TYR:OH	6:B:600:GDP:H2'	2.18	0.43
1:C:52:PHE:O	1:C:64:ARG:HB2	2.19	0.43
2:D:379:GLY:O	2:D:381:SER:N	2.51	0.43
1:C:420:GLU:HA	1:C:423:GLU:HG3	1.99	0.43
2:B:158:ARG:C	2:B:160:GLU:H	2.26	0.43
1:C:10:GLY:O	1:C:11:GLN:C	2.61	0.43
1:A:80:THR:HG22	1:A:81:GLY:N	2.34	0.43
1:A:304:LYS:O	1:A:390:ARG:NH1	2.51	0.43
2:B:320:ARG:HA	2:B:356:CYS:O	2.18	0.43
1:C:100:ALA:O	1:C:102:ASN:HB3	2.18	0.43
2:D:70:LEU:C	2:D:95:GLY:HA3	2.43	0.43
2:D:174:SER:OG	2:D:176:LYS:N	2.51	0.43
1:C:105:ARG:HH12	2:D:253:ARG:NH2	2.16	0.43
1:C:234:ILE:HG12	1:C:272:TYR:HB2	2.00	0.43
2:D:107:HIS:O	2:D:152:LEU:HD22	2.19	0.43
1:A:68:VAL:CG1	1:A:93:ILE:HB	2.48	0.43
2:B:177:VAL:O	2:B:177:VAL:CG1	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:PHE:CE1	2:B:435:TYR:CZ	3.06	0.43
2:D:55:GLU:H	2:D:55:GLU:HG3	1.57	0.43
1:A:82:THR:O	1:A:83:TYR:CG	2.72	0.43
1:A:188:ILE:HG23	1:A:425:MET:HG3	2.00	0.43
1:A:81:GLY:O	1:A:82:THR:C	2.61	0.43
1:A:217:LEU:HB3	1:A:219:ILE:HG12	2.00	0.43
1:C:81:GLY:O	1:C:82:THR:C	2.62	0.43
1:C:172:TYR:HA	1:C:173:PRO:HD3	1.78	0.43
1:C:317:LEU:HD23	1:C:377:MET:HE3	2.00	0.43
1:C:407:TRP:CD2	2:D:257:VAL:HG22	2.53	0.43
1:A:419:SER:O	1:A:423:GLU:HG2	2.19	0.43
1:C:90:GLU:O	1:C:121:ARG:HD3	2.19	0.43
1:C:100:ALA:CB	2:D:253:ARG:HG2	2.49	0.43
1:C:190:THR:CG2	1:C:191:THR:N	2.81	0.43
2:D:102:ASN:OD1	2:D:102:ASN:C	2.60	0.43
1:A:391:LEU:HB3	1:A:392:ASP:H	1.70	0.43
1:C:70:LEU:HD12	1:C:145:THR:CB	2.41	0.43
1:A:36:MET:HA	1:A:37:PRO:HD3	1.89	0.42
1:A:267:PHE:CD1	1:A:267:PHE:N	2.87	0.42
1:A:407:TRP:CD2	2:B:257:VAL:HG22	2.54	0.42
2:B:55:GLU:H	2:B:55:GLU:HG3	1.56	0.42
2:B:211:ASP:O	2:B:215:ARG:HG2	2.19	0.42
2:B:316:ALA:HB1	7:B:700:N16:CAM	2.49	0.42
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.01	0.42
1:C:376:CYS:O	1:C:377:MET:C	2.62	0.42
1:C:407:TRP:CG	2:D:257:VAL:HG22	2.54	0.42
2:D:164:ARG:CA	2:D:164:ARG:NE	2.82	0.42
2:D:192:HIS:ND1	2:D:192:HIS:C	2.77	0.42
2:D:248:LEU:HD23	2:D:248:LEU:HA	1.53	0.42
2:D:311:ARG:HH21	2:D:344:VAL:CG2	2.32	0.42
1:A:185:TYR:OH	1:A:403:ALA:HB3	2.19	0.42
1:A:247:ALA:HB1	3:E:12:ASN:HB3	2.01	0.42
2:B:336:GLN:O	2:B:340:SER:HA	2.19	0.42
2:B:398:MET:HE3	1:C:348:PRO:HD2	1.99	0.42
1:C:6:SER:HB3	1:C:8:HIS:HE1	1.83	0.42
1:C:250:VAL:HG22	1:C:250:VAL:O	2.19	0.42
1:C:389:ALA:HA	1:C:392:ASP:HB2	2.01	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.18	0.42
2:D:265:LEU:HB3	2:D:432:TYR:CZ	2.52	0.42
1:A:79:ARG:HD3	1:A:92:LEU:HD13	2.02	0.42
1:A:90:GLU:O	1:A:121:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLN:HB2	1:A:373:ARG:HE	1.84	0.42
2:B:401:ARG:HH11	2:B:401:ARG:CG	2.32	0.42
1:C:174:ALA:O	1:C:175:PRO:C	2.61	0.42
2:D:288:VAL:HB	2:D:289:PRO:HD3	2.01	0.42
2:D:297:ASP:OD1	2:D:298:SER:N	2.52	0.42
2:B:15:GLN:HG3	2:B:15:GLN:O	2.18	0.42
2:B:295:MET:HE2	2:B:295:MET:HB3	1.85	0.42
1:C:179:THR:O	2:D:352:LYS:HG3	2.19	0.42
1:C:191:THR:O	1:C:195:LEU:HB3	2.20	0.42
2:D:5:VAL:HG23	2:D:6:HIS:N	2.34	0.42
2:D:177:VAL:O	2:D:177:VAL:CG1	2.67	0.42
2:D:308:ARG:HD2	2:D:308:ARG:HA	1.78	0.42
1:A:70:LEU:HD12	1:A:145:THR:CB	2.34	0.42
1:A:376:CYS:O	1:A:377:MET:C	2.63	0.42
2:B:406:HIS:CD2	2:B:406:HIS:C	2.95	0.42
1:C:119:LEU:HD22	1:C:156:ARG:NH2	2.35	0.42
1:C:183:GLU:CB	1:C:184:PRO:CD	2.91	0.42
2:D:70:LEU:HA	2:D:95:GLY:HA3	2.00	0.42
2:D:102:ASN:OD1	2:D:102:ASN:O	2.37	0.42
2:D:165:ILE:CG2	2:D:253:ARG:NH1	2.82	0.42
3:E:116:LEU:O	3:E:119:MET:HB3	2.19	0.42
1:A:348:PRO:HA	3:E:27:PRO:HD3	2.01	0.42
2:B:2:ARG:CB	2:B:131:CYS:SG	3.07	0.42
2:B:245:PRO:CG	2:B:246:GLY:H	2.25	0.42
2:B:347:ILE:HA	2:B:348:PRO:HD3	1.81	0.42
1:C:239:THR:OG1	1:C:243:ARG:NH1	2.53	0.42
1:C:402:ARG:HD3	1:C:402:ARG:HA	1.89	0.42
1:C:406:HIS:CD2	2:D:263:PRO:HG3	2.53	0.42
2:D:51:VAL:CG1	2:D:52:TYR:N	2.83	0.42
2:B:5:VAL:HG13	2:B:132:LEU:HD11	2.01	0.42
2:B:31:ASP:C	2:B:33:THR:N	2.76	0.42
2:B:118:VAL:C	2:B:120:ASP:N	2.75	0.42
2:B:384:ILE:CG2	2:B:432:TYR:CE1	3.02	0.42
1:C:178:SER:HB3	2:D:352:LYS:NZ	2.35	0.42
1:C:372:GLN:H	1:C:372:GLN:HG2	1.47	0.42
2:D:151:THR:HA	2:D:154:ILE:HG12	2.02	0.42
1:A:325:PRO:HB3	3:E:20:PHE:CE2	2.54	0.42
1:C:79:ARG:H	1:C:79:ARG:HG2	1.40	0.42
1:C:100:ALA:C	1:C:102:ASN:N	2.76	0.42
1:C:291:ILE:HD12	1:C:375:VAL:HG23	2.00	0.42
1:C:416:GLY:O	1:C:419:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:SER:C	2:D:204:ILE:HG13	2.44	0.42
2:D:245:PRO:HG2	2:D:246:GLY:N	2.32	0.42
1:A:402:ARG:HD2	1:A:415:GLU:OE2	2.20	0.42
2:B:44:LEU:HA	2:B:49:ILE:HB	2.02	0.42
2:B:118:VAL:O	2:B:120:ASP:N	2.53	0.42
2:D:385:GLN:HE21	2:D:389:LYS:CD	2.32	0.42
1:A:119:LEU:HD22	1:A:156:ARG:HH21	1.85	0.42
1:A:174:ALA:CB	1:A:207:GLU:HB2	2.50	0.42
2:B:172:MET:HE3	2:B:203:SER:HB3	2.02	0.42
1:C:317:LEU:CD2	1:C:377:MET:HE3	2.50	0.42
2:D:210:TYR:CD1	2:D:210:TYR:C	2.98	0.42
1:A:100:ALA:O	1:A:101:ASN:C	2.63	0.41
1:A:153:LEU:HD13	1:A:157:LEU:CD1	2.46	0.41
1:A:184:PRO:O	1:A:185:TYR:C	2.63	0.41
1:A:402:ARG:HD3	1:A:402:ARG:HA	1.80	0.41
2:D:110:GLU:O	2:D:113:GLU:HB3	2.20	0.41
2:D:133:GLN:HG3	2:D:252:LEU:HD23	2.00	0.41
2:D:269:MET:HA	2:D:270:PRO:HD3	1.93	0.41
2:D:401:ARG:CG	2:D:401:ARG:HH11	2.33	0.41
3:E:84:GLN:O	3:E:86:ALA:N	2.53	0.41
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.92	0.41
2:D:5:VAL:CG2	2:D:135:PHE:HD2	2.23	0.41
2:D:255:LEU:HD23	7:D:700:N16:HB	2.01	0.41
2:D:384:ILE:HD13	2:D:384:ILE:HA	1.89	0.41
3:E:101:LEU:C	3:E:103:GLN:H	2.28	0.41
1:C:36:MET:HA	1:C:37:PRO:HD3	1.90	0.41
1:C:251:ASP:O	1:C:255:PHE:CB	2.68	0.41
2:D:48:ARG:HB2	2:D:243:ARG:C	2.44	0.41
2:D:158:ARG:C	2:D:160:GLU:N	2.77	0.41
2:D:176:LYS:HD2	2:D:207:GLU:OE2	2.20	0.41
2:D:433:GLN:HA	2:D:433:GLN:OE1	2.20	0.41
1:A:234:ILE:HG12	1:A:272:TYR:HB2	2.02	0.41
1:A:398:MET:HG3	2:B:348:PRO:HD3	2.02	0.41
2:B:116:ASP:O	2:B:120:ASP:OD1	2.38	0.41
1:C:398:MET:HE2	2:D:348:PRO:CD	2.50	0.41
2:D:263:PRO:C	2:D:264:ARG:O	2.62	0.41
1:A:139:HIS:CG	1:A:150:THR:HG21	2.55	0.41
2:B:2:ARG:HB3	2:B:131:CYS:SG	2.60	0.41
2:B:31:ASP:O	2:B:33:THR:N	2.54	0.41
2:B:151:THR:CG2	2:B:190:SER:HB3	2.47	0.41
1:C:98:ASP:OD1	1:C:99:ALA:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:SER:O	1:C:291:ILE:HG12	2.20	0.41
2:D:204:ILE:HG22	2:D:209:LEU:HD22	2.01	0.41
6:D:600:GDP:C3'	6:D:600:GDP:C8	3.03	0.41
1:A:16:ILE:HD13	1:A:171:ILE:HD11	2.02	0.41
2:B:164:ARG:HE	2:B:164:ARG:CA	2.32	0.41
2:B:351:VAL:HG22	2:B:351:VAL:O	2.20	0.41
1:C:174:ALA:HA	1:C:175:PRO:HD2	1.63	0.41
2:D:8:GLN:OE1	2:D:14:ASN:ND2	2.54	0.41
2:D:34:GLY:HA2	2:D:60:LYS:HE2	2.03	0.41
1:C:297:GLU:HA	1:C:298:PRO:HD2	1.79	0.41
2:D:224:TYR:HE2	6:D:600:GDP:C4	2.34	0.41
1:A:395:PHE:CD2	1:A:395:PHE:C	2.99	0.41
2:B:245:PRO:CB	2:B:247:GLN:HG3	2.50	0.41
2:D:5:VAL:HG13	2:D:132:LEU:HD11	2.01	0.41
2:D:48:ARG:HH12	2:D:242:LEU:C	2.28	0.41
2:D:245:PRO:HG3	2:D:247:GLN:HE21	1.85	0.41
6:D:600:GDP:H8	6:D:600:GDP:H3'	1.86	0.41
1:A:49:PHE:C	1:A:51:THR:H	2.28	0.41
1:A:405:VAL:CG1	1:A:406:HIS:N	2.84	0.41
1:A:413:MET:HG2	1:A:414:GLU:H	1.84	0.41
2:B:70:LEU:HD12	2:B:145:THR:HB	2.03	0.41
2:B:163:ASP:HB3	2:B:164:ARG:HG2	2.02	0.41
2:B:217:LEU:HD11	2:B:276:THR:HB	2.02	0.41
2:B:325:MET:HA	2:B:328:VAL:HG23	2.03	0.41
2:B:401:ARG:NH1	2:B:401:ARG:HG3	2.36	0.41
1:C:178:SER:HB3	2:D:352:LYS:HZ3	1.85	0.41
2:D:67:LEU:O	2:D:93:VAL:HG23	2.20	0.41
2:D:209:LEU:HD12	2:D:209:LEU:HA	1.87	0.41
2:D:240:THR:O	2:D:243:ARG:N	2.53	0.41
2:D:253:ARG:O	2:D:256:ALA:N	2.54	0.41
2:D:262:PHE:O	2:D:264:ARG:O	2.38	0.41
2:D:399:PHE:O	2:D:400:ARG:O	2.39	0.41
3:E:48:GLU:C	3:E:50:ILE:H	2.28	0.41
3:E:107:SER:O	3:E:111:ASN:HB2	2.21	0.41
2:B:99:ALA:CB	2:B:145:THR:CG2	2.93	0.41
2:B:242:LEU:N	2:B:242:LEU:HD23	2.36	0.41
1:C:119:LEU:HD22	1:C:156:ARG:HH21	1.86	0.41
1:C:182:VAL:O	1:C:182:VAL:HG22	2.21	0.41
2:D:138:THR:O	2:D:139:HIS:HB3	2.21	0.41
2:D:205:ASP:HB2	2:D:304:ALA:H	1.86	0.41
1:A:84:ARG:HE	1:A:84:ARG:HB3	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ALA:O	1:A:430:LYS:HB3	2.21	0.40
2:B:70:LEU:CA	2:B:95:GLY:HA3	2.51	0.40
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.82	0.40
2:B:152:LEU:O	2:B:153:LEU:C	2.64	0.40
2:B:385:GLN:HG2	2:B:389:LYS:HD2	2.02	0.40
1:C:36:MET:SD	1:C:38:SER:HB2	2.61	0.40
1:C:83:TYR:C	1:C:85:GLN:N	2.77	0.40
2:D:271:GLY:HA2	2:D:302:MET:HG2	2.02	0.40
1:A:139:HIS:HD2	1:A:146:GLY:O	2.04	0.40
1:A:391:LEU:O	1:A:393:HIS:N	2.54	0.40
2:B:8:GLN:OE1	2:B:14:ASN:ND2	2.54	0.40
1:C:345:ASP:OD2	1:C:438:ASP:HB2	2.21	0.40
1:C:428:LEU:C	1:C:430:LYS:H	2.30	0.40
2:D:2:ARG:NH2	2:D:251:ASP:O	2.54	0.40
2:D:255:LEU:HD11	7:D:700:N16:HAL	2.03	0.40
3:E:84:GLN:HA	3:E:87:ILE:HG22	2.02	0.40
1:A:260:VAL:HA	1:A:261:PRO:HD3	1.90	0.40
1:A:264:ARG:O	1:A:266:HIS:N	2.55	0.40
2:D:347:ILE:HA	2:D:348:PRO:HD3	1.72	0.40
1:A:22:GLU:HB2	1:A:83:TYR:CE1	2.55	0.40
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.21	0.40
2:B:2:ARG:HH12	2:B:133:GLN:HA	1.86	0.40
2:B:292:THR:C	2:B:294:GLN:N	2.79	0.40
1:C:36:MET:HE1	1:C:38:SER:O	2.22	0.40
1:C:204:VAL:HG22	1:C:302:MET:CE	2.43	0.40
1:C:265:ILE:O	1:C:265:ILE:HG22	2.21	0.40
2:D:114:LEU:HB3	2:D:149:MET:CE	2.52	0.40
2:D:265:LEU:CB	2:D:432:TYR:HE2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/451 (94%)	324 (76%)	72 (17%)	28 (7%)	1	13
1	C	423/451 (94%)	337 (80%)	54 (13%)	32 (8%)	1	10
2	B	416/445 (94%)	302 (73%)	80 (19%)	34 (8%)	0	9
2	D	425/445 (96%)	291 (68%)	88 (21%)	46 (11%)	0	5
3	E	119/142 (84%)	73 (61%)	30 (25%)	16 (13%)	0	3
All	All	1807/1934 (93%)	1327 (73%)	324 (18%)	156 (9%)	0	8

All (156) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	PRO
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	392	ASP
1	A	403	ALA
1	A	437	VAL
2	B	42	LEU
2	B	43	GLN
2	B	62	VAL
2	B	73	GLY
2	B	82	PRO
2	B	163	ASP
2	B	227	LEU
2	B	245	PRO
2	B	273	ALA
2	B	288	VAL
2	B	299	LYS
2	B	371	LEU
2	B	400	ARG
2	B	404	PHE
1	C	72	PRO
1	C	73	THR
1	C	112	LYS
1	C	191	THR
1	C	257	THR
1	C	265	ILE
1	C	341	ILE

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Mol	Chain	Res	Type
1	C	348	PRO
1	C	377	MET
1	C	392	ASP
1	C	403	ALA
1	C	437	VAL
2	D	43	GLN
2	D	62	VAL
2	D	73	GLY
2	D	82	PRO
2	D	162	PRO
2	D	163	ASP
2	D	245	PRO
2	D	251	ASP
2	D	288	VAL
2	D	299	LYS
2	D	380	ASN
2	D	400	ARG
3	E	49	GLU
3	E	81	GLU
3	E	82	VAL
3	E	102	ALA
3	E	139	LEU
1	A	48	SER
1	A	83	TYR
1	A	162	GLY
1	A	164	LYS
1	A	191	THR
1	A	273	ALA
1	A	279	GLU
2	B	3	GLU
2	B	34	GLY
2	B	60	LYS
2	B	162	PRO
2	B	226	ASP
2	B	264	ARG
2	B	276	THR
2	B	309	HIS
2	B	348	PRO
1	C	83	TYR
1	C	162	GLY
1	C	164	LYS
1	C	253	THR

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Mol	Chain	Res	Type
1	C	273	ALA
1	C	350	GLY
1	C	429	GLU
2	D	3	GLU
2	D	34	GLY
2	D	115	VAL
2	D	227	LEU
2	D	244	PHE
2	D	264	ARG
2	D	265	LEU
2	D	278	ARG
2	D	285	ALA
2	D	309	HIS
2	D	322	ARG
2	D	348	PRO
2	D	371	LEU
2	D	403	ALA
2	D	404	PHE
3	E	12	ASN
3	E	26	PRO
3	E	28	SER
3	E	46	SER
3	E	75	LYS
3	E	124	GLN
1	A	32	PRO
1	A	247	ALA
1	A	350	GLY
1	A	415	GLU
1	A	429	GLU
2	B	115	VAL
2	B	240	THR
2	B	244	PHE
2	B	249	ASN
2	B	403	ALA
1	C	32	PRO
1	C	245	ASP
2	D	42	LEU
2	D	60	LYS
2	D	195	VAL
2	D	279	GLY
3	E	85	LYS
3	E	113	GLU

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Mol	Chain	Res	Type
1	A	402	ARG
1	C	183	GLU
1	C	220	GLU
2	D	167	ASN
2	D	220	THR
2	D	226	ASP
2	D	240	THR
2	D	293	GLN
3	E	7	GLU
3	E	47	LEU
1	A	220	GLU
2	B	119	LEU
2	B	307	PRO
2	B	322	ARG
1	C	48	SER
1	C	79	ARG
1	C	141	PHE
1	C	351	PHE
2	D	249	ASN
2	D	268	PHE
2	D	273	ALA
2	D	402	LYS
1	A	248	LEU
2	B	293	GLN
1	C	254	GLU
1	C	402	ARG
2	D	270	PRO
2	D	342	TYR
3	E	5	ASP
2	D	261	PRO
1	A	364	PRO
1	C	364	PRO
1	C	412	GLY
1	A	412	GLY
2	B	32	PRO
1	C	175	PRO
2	D	84	GLY
2	D	177	VAL
2	D	307	PRO
1	A	274	PRO
2	B	177	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/378 (92%)	231 (67%)	115 (33%)	0	1
1	C	344/378 (91%)	225 (65%)	119 (35%)	0	1
2	B	350/383 (91%)	220 (63%)	130 (37%)	0	0
2	D	353/383 (92%)	215 (61%)	138 (39%)	0	0
3	E	82/126 (65%)	40 (49%)	42 (51%)	0	0
All	All	1475/1648 (90%)	931 (63%)	544 (37%)	0	1

All (544) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	9	VAL
1	A	11	GLN
1	A	14	VAL
1	A	15	GLN
1	A	16	ILE
1	A	22	GLU
1	A	23	LEU
1	A	26	LEU
1	A	27	GLU
1	A	31	GLN
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	78	VAL
1	A	79	ARG
1	A	80	THR
1	A	88	HIS
1	A	90	GLU

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Mol	Chain	Res	Type
1	A	91	GLN
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	114	ILE
1	A	115	ILE
1	A	119	LEU
1	A	120	ASP
1	A	123	ARG
1	A	124	LYS
1	A	130	THR
1	A	132	LEU
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	168	GLU
1	A	171	ILE
1	A	176	GLN
1	A	179	THR
1	A	187	SER
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	212	ILE
1	A	220	GLU
1	A	223	THR
1	A	226	ASN

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Mol	Chain	Res	Type
1	A	230	LEU
1	A	234	ILE
1	A	236	SER
1	A	241	SER
1	A	242	LEU
1	A	248	LEU
1	A	250	VAL
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	287	SER
1	A	301	GLN
1	A	304	LYS
1	A	309	HIS
1	A	311	LYS
1	A	316	CYS
1	A	318	LEU
1	A	326	LYS
1	A	341	ILE
1	A	343	PHE
1	A	344	VAL
1	A	347	CYS
1	A	349	THR
1	A	353	VAL
1	A	356	ASN
1	A	361	THR
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	381	THR
1	A	384	ILE
1	A	386	GLU
1	A	394	LYS
1	A	397	LEU

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Mol	Chain	Res	Type
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	60	LYS
2	B	61	TYR
2	B	62	VAL
2	B	68	VAL
2	B	70	LEU
2	B	71	GLU
2	B	78	VAL
2	B	80	SER
2	B	85	GLN
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	110	GLU
2	B	113	GLU
2	B	118	VAL
2	B	119	LEU
2	B	120	ASP
2	B	122	VAL

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Mol	Chain	Res	Type
2	B	129	CYS
2	B	130	ASP
2	B	131	CYS
2	B	132	LEU
2	B	133	GLN
2	B	137	LEU
2	B	141	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	163	ASP
2	B	164	ARG
2	B	165	ILE
2	B	166	MET
2	B	170	SER
2	B	171	VAL
2	B	174	SER
2	B	177	VAL
2	B	179	ASP
2	B	181	VAL
2	B	188	THR
2	B	190	SER
2	B	196	GLU
2	B	200	GLU
2	B	209	LEU
2	B	212	ILE
2	B	216	THR
2	B	217	LEU
2	B	219	LEU
2	B	223	THR
2	B	227	LEU
2	B	230	LEU
2	B	231	VAL
2	B	239	THR
2	B	242	LEU
2	B	248	LEU
2	B	251	ASP
2	B	254	LYS
2	B	255	LEU

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Mol	Chain	Res	Type
2	B	257	VAL
2	B	260	VAL
2	B	265	LEU
2	B	275	LEU
2	B	276	THR
2	B	277	SER
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	308	ARG
2	B	309	HIS
2	B	311	ARG
2	B	313	LEU
2	B	315	VAL
2	B	318	VAL
2	B	320	ARG
2	B	323	MET
2	B	324	SER
2	B	325	MET
2	B	329	ASP
2	B	332	MET
2	B	333	LEU
2	B	335	VAL
2	B	339	ASN
2	B	341	SER
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	371	LEU
2	B	373	MET
2	B	376	THR
2	B	384	ILE
2	B	387	LEU
2	B	391	ILE
2	B	393	GLU

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Mol	Chain	Res	Type
2	B	394	GLN
2	B	400	ARG
2	B	401	ARG
2	B	405	LEU
2	B	408	TYR
2	B	409	THR
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	9	VAL
1	C	11	GLN
1	C	15	GLN
1	C	16	ILE
1	C	23	LEU
1	C	25	CYS
1	C	26	LEU
1	C	27	GLU
1	C	31	GLN
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	70	LEU
1	C	73	THR
1	C	74	VAL
1	C	78	VAL
1	C	79	ARG
1	C	80	THR
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	114	ILE
1	C	115	ILE
1	C	119	LEU
1	C	120	ASP
1	C	123	ARG
1	C	124	LYS
1	C	130	THR
1	C	132	LEU
1	C	140	SER
1	C	141	PHE
1	C	145	THR
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	167	LEU
1	C	168	GLU
1	C	171	ILE
1	C	176	GLN
1	C	179	THR
1	C	183	GLU
1	C	187	SER
1	C	191	THR
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	212	ILE
1	C	220	GLU
1	C	223	THR
1	C	226	ASN
1	C	230	LEU
1	C	234	ILE
1	C	236	SER
1	C	241	SER

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Mol	Chain	Res	Type
1	C	242	LEU
1	C	245	ASP
1	C	248	LEU
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	311	LYS
1	C	316	CYS
1	C	318	LEU
1	C	334	THR
1	C	341	ILE
1	C	344	VAL
1	C	347	CYS
1	C	349	THR
1	C	353	VAL
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	381	THR
1	C	384	ILE
1	C	386	GLU
1	C	394	LYS
1	C	397	LEU
1	C	401	LYS
1	C	402	ARG
1	C	405	VAL
1	C	413	MET

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Mol	Chain	Res	Type
1	C	414	GLU
1	C	415	GLU
1	C	419	SER
1	C	420	GLU
1	C	433	GLU
2	D	4	ILE
2	D	5	VAL
2	D	7	ILE
2	D	14	ASN
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	61	TYR
2	D	62	VAL
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	86	ILE
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	113	GLU
2	D	115	VAL
2	D	118	VAL
2	D	119	LEU
2	D	120	ASP

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Mol	Chain	Res	Type
2	D	122	VAL
2	D	124	LYS
2	D	129	CYS
2	D	130	ASP
2	D	132	LEU
2	D	133	GLN
2	D	137	LEU
2	D	141	LEU
2	D	145	THR
2	D	149	MET
2	D	151	THR
2	D	156	LYS
2	D	157	ILE
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	177	VAL
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	212	ILE
2	D	216	THR
2	D	227	LEU
2	D	230	LEU
2	D	231	VAL
2	D	239	THR
2	D	241	CYS
2	D	242	LEU
2	D	248	LEU
2	D	251	ASP
2	D	253	ARG
2	D	254	LYS

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Mol	Chain	Res	Type
2	D	257	VAL
2	D	260	VAL
2	D	265	LEU
2	D	275	LEU
2	D	276	THR
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
2	D	295	MET
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	327	GLU
2	D	329	ASP
2	D	332	MET
2	D	333	LEU
2	D	335	VAL
2	D	339	ASN
2	D	341	SER
2	D	344	VAL
2	D	347	ILE
2	D	350	ASN
2	D	351	VAL
2	D	356	CYS
2	D	357	ASP
2	D	358	ILE
2	D	371	LEU
2	D	373	MET
2	D	376	THR
2	D	378	ILE
2	D	380	ASN

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Mol	Chain	Res	Type
2	D	384	ILE
2	D	387	LEU
2	D	391	ILE
2	D	393	GLU
2	D	394	GLN
2	D	400	ARG
2	D	401	ARG
2	D	402	LYS
2	D	405	LEU
2	D	408	TYR
2	D	409	THR
2	D	417	GLU
2	D	419	THR
2	D	425	MET
2	D	430	SER
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	61	ARG
3	E	62	LYS
3	E	64	GLN
3	E	65	GLU
3	E	67	GLU
3	E	69	LEU
3	E	70	LYS
3	E	76	ARG
3	E	77	GLU
3	E	78	HIS
3	E	81	GLU
3	E	84	GLN
3	E	87	ILE
3	E	89	GLU
3	E	91	ASN
3	E	92	ASN

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Mol	Chain	Res	Type
3	E	94	ILE
3	E	96	MET
3	E	98	LYS
3	E	99	GLU
3	E	106	GLU
3	E	109	LYS
3	E	111	ASN
3	E	112	ARG
3	E	113	GLU
3	E	115	HIS
3	E	119	MET
3	E	122	ARG
3	E	125	GLU
3	E	126	LYS
3	E	129	HIS
3	E	134	ARG
3	E	136	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	50	ASN
1	A	85	GLN
1	A	91	GLN
1	A	101	ASN
1	A	102	ASN
1	A	139	HIS
1	A	176	GLN
1	A	206	ASN
1	A	249	ASN
1	A	258	ASN
1	A	329	ASN
1	A	356	ASN
2	B	8	GLN
2	B	14	ASN
2	B	54	ASN
2	B	85	GLN
2	B	101	ASN
2	B	133	GLN
2	B	136	GLN
2	B	192	HIS

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Mol	Chain	Res	Type
2	B	197	ASN
2	B	206	ASN
2	B	247	GLN
2	B	258	ASN
2	B	266	HIS
2	B	294	GLN
2	B	309	HIS
2	B	331	GLN
2	B	339	ASN
2	B	349	ASN
2	B	350	ASN
2	B	380	ASN
2	B	385	GLN
2	B	406	HIS
2	B	424	ASN
2	B	436	GLN
1	C	8	HIS
1	C	50	ASN
1	C	85	GLN
1	C	91	GLN
1	C	101	ASN
1	C	102	ASN
1	C	139	HIS
1	C	206	ASN
1	C	258	ASN
1	C	329	ASN
2	D	8	GLN
2	D	14	ASN
2	D	85	GLN
2	D	101	ASN
2	D	133	GLN
2	D	136	GLN
2	D	192	HIS
2	D	193	GLN
2	D	206	ASN
2	D	258	ASN
2	D	266	HIS
2	D	294	GLN
2	D	309	HIS
2	D	331	GLN
2	D	339	ASN
2	D	349	ASN

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Mol	Chain	Res	Type
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
2	D	394	GLN
2	D	406	HIS
2	D	424	ASN
2	D	434	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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GTP	A	600	-	33,34,34	1.31	6 (18%)	50,54,54	1.78	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GTP	C	600	-	33,34,34	1.04	3 (9%)	50,54,54	1.81	13 (26%)
7	N16	B	700	-	24,25,25	1.39	3 (12%)	28,34,34	1.52	5 (17%)
6	GDP	D	600	-	29,30,30	0.87	1 (3%)	45,47,47	1.99	9 (20%)
6	GDP	B	600	-	29,30,30	0.97	2 (6%)	45,47,47	1.85	11 (24%)
7	N16	D	700	-	24,25,25	2.02	6 (25%)	28,34,34	2.05	9 (32%)

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	A	600	-	-	6/22/38/38	0/3/3/3
4	GTP	C	600	-	-	8/22/38/38	0/3/3/3
7	N16	B	700	-	-	1/12/28/28	0/3/3/3
6	GDP	D	600	-	-	2/16/32/32	0/3/3/3
6	GDP	B	600	-	-	2/16/32/32	0/3/3/3
7	N16	D	700	-	-	3/12/28/28	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	N16	CAV-NAO	-4.75	1.32	1.41
7	D	700	N16	CAV-NAO	-4.10	1.33	1.41
7	D	700	N16	CB-CG	3.84	1.60	1.51
4	A	600	GTP	PB-O3A	3.56	1.63	1.59
7	D	700	N16	CAA-CAQ	3.48	1.55	1.49
4	A	600	GTP	PA-O3A	3.17	1.62	1.59
4	A	600	GTP	PB-O3B	3.00	1.62	1.59
7	B	700	N16	CAA-CAQ	2.85	1.54	1.49
4	C	600	GTP	PA-O3A	2.81	1.62	1.59
7	D	700	N16	CD2-CG	2.67	1.44	1.38
6	D	600	GDP	C2-N3	2.63	1.39	1.33
4	C	600	GTP	C2-N3	2.46	1.39	1.33
4	A	600	GTP	C5-N7	-2.43	1.34	1.39
7	D	700	N16	CAI-CAE	2.29	1.43	1.38
6	B	600	GDP	PA-O3A	2.28	1.62	1.59
6	B	600	GDP	C2-N3	2.22	1.38	1.33
7	B	700	N16	CAT-CAR	-2.19	1.40	1.47
4	A	600	GTP	C2-N3	2.13	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	600	GTP	PB-O3A	2.12	1.61	1.59
7	D	700	N16	CAL-CAV	2.06	1.42	1.39
4	A	600	GTP	O4'-C4'	-2.04	1.40	1.45

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	GTP	C5-C4-N3	-5.89	119.02	128.39
7	D	700	N16	CB-CA-N	-5.79	107.59	113.84
6	D	600	GDP	C5-C4-N3	-5.64	119.41	128.39
6	D	600	GDP	C2-N3-C4	5.51	121.79	112.30
4	C	600	GTP	C2-N3-C4	5.35	121.51	112.30
6	B	600	GDP	C5-C4-N3	-5.29	119.97	128.39
4	C	600	GTP	C5-C4-N3	-5.28	119.98	128.39
4	A	600	GTP	C2-N3-C4	5.02	120.95	112.30
6	B	600	GDP	C2-N3-C4	4.75	120.49	112.30
6	D	600	GDP	O6-C6-C5	-4.58	114.43	126.53
4	A	600	GTP	N9-C4-N3	4.19	134.33	125.95
6	D	600	GDP	N9-C4-N3	3.99	133.93	125.95
6	B	600	GDP	O6-C6-C5	-3.89	116.26	126.53
7	B	700	N16	CB-CA-N	-3.87	109.66	113.84
4	A	600	GTP	C2-N1-C6	-3.55	118.68	125.11
4	C	600	GTP	N9-C4-N3	3.49	132.93	125.95
6	B	600	GDP	N9-C4-N3	3.44	132.83	125.95
7	D	700	N16	CAT-CAQ-NAO	-3.44	113.55	119.15
7	B	700	N16	CA-N-CAR	-3.37	108.24	113.42
6	D	600	GDP	N9-C8-N7	-3.36	107.17	113.40
6	D	600	GDP	C8-N7-C5	3.35	110.22	104.26
4	C	600	GTP	N9-C8-N7	-3.28	107.33	113.40
7	B	700	N16	CAT-CAR-N	3.26	113.60	107.35
4	A	600	GTP	O6-C6-C5	-3.22	118.02	126.53
7	D	700	N16	OAB-CAR-N	-3.20	121.62	126.02
4	C	600	GTP	C8-N7-C5	3.04	109.67	104.26
7	D	700	N16	CAI-CAM-CAV	-3.00	116.27	119.73
4	C	600	GTP	C5-C6-N1	2.97	120.82	113.25
6	D	600	GDP	N1-C2-N3	-2.88	118.06	123.32
4	C	600	GTP	C2-N1-C6	-2.83	119.98	125.11
4	A	600	GTP	N9-C8-N7	-2.76	108.28	113.40
4	A	600	GTP	C5-C6-N1	2.73	120.20	113.25
4	A	600	GTP	C8-N7-C5	2.63	108.95	104.26
7	D	700	N16	CA-N-CAR	-2.59	109.44	113.42
7	D	700	N16	CAM-CAV-CAL	2.58	122.47	119.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	GDP	O2B-PB-O3A	2.53	113.14	104.64
7	D	700	N16	CAT-CAR-N	2.46	112.06	107.35
6	B	600	GDP	N2-C2-N3	-2.44	114.90	119.67
6	B	600	GDP	C8-N7-C5	2.38	108.50	104.26
7	B	700	N16	OAB-CAR-N	-2.35	122.79	126.02
4	C	600	GTP	N1-C2-N3	-2.34	119.03	123.32
6	B	600	GDP	O3A-PA-O1A	-2.33	103.69	110.70
6	B	600	GDP	C2-N1-C6	-2.30	120.94	125.11
7	D	700	N16	CAE-CAH-CAL	-2.28	117.43	120.24
6	B	600	GDP	N9-C8-N7	-2.24	109.24	113.40
4	C	600	GTP	O2G-PG-O3B	2.22	112.08	104.64
4	C	600	GTP	O6-C6-C5	-2.22	120.68	126.53
6	D	600	GDP	O2B-PB-O3A	2.21	112.03	104.64
4	C	600	GTP	C4-C5-N7	-2.18	107.22	110.67
7	D	700	N16	CAA-CAQ-NAO	2.16	122.06	118.52
4	C	600	GTP	C2'-C1'-N9	2.14	119.21	113.25
7	B	700	N16	CAV-NAO-CAQ	-2.13	124.39	128.35
6	B	600	GDP	C5-C6-N1	2.13	118.67	113.25
6	D	600	GDP	C4-C5-N7	-2.11	107.33	110.67
4	C	600	GTP	C6-C5-N7	2.10	134.12	130.29

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	GTP	PB-O3B-PG-O3G
4	C	600	GTP	PB-O3B-PG-O3G
6	B	600	GDP	O4'-C4'-C5'-O5'
6	B	600	GDP	C3'-C4'-C5'-O5'
6	D	600	GDP	PA-O3A-PB-O2B
4	A	600	GTP	PB-O3B-PG-O1G
4	A	600	GTP	C3'-C4'-C5'-O5'
7	D	700	N16	CA-CB-CG-CD1
7	D	700	N16	CA-CB-CG-CD2
4	C	600	GTP	C3'-C4'-C5'-O5'
4	C	600	GTP	C5'-O5'-PA-O2A
4	C	600	GTP	C4'-C5'-O5'-PA
4	A	600	GTP	PG-O3B-PB-O1B
4	C	600	GTP	PB-O3A-PA-O1A
6	D	600	GDP	PA-O3A-PB-O1B
4	C	600	GTP	PB-O3B-PG-O2G
4	C	600	GTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	A	600	GTP	PG-O3B-PB-O2B
4	C	600	GTP	PB-O3A-PA-O2A
7	B	700	N16	N-CA-CB-CG
7	D	700	N16	N-CA-CB-CG
4	A	600	GTP	O4'-C4'-C5'-O5'

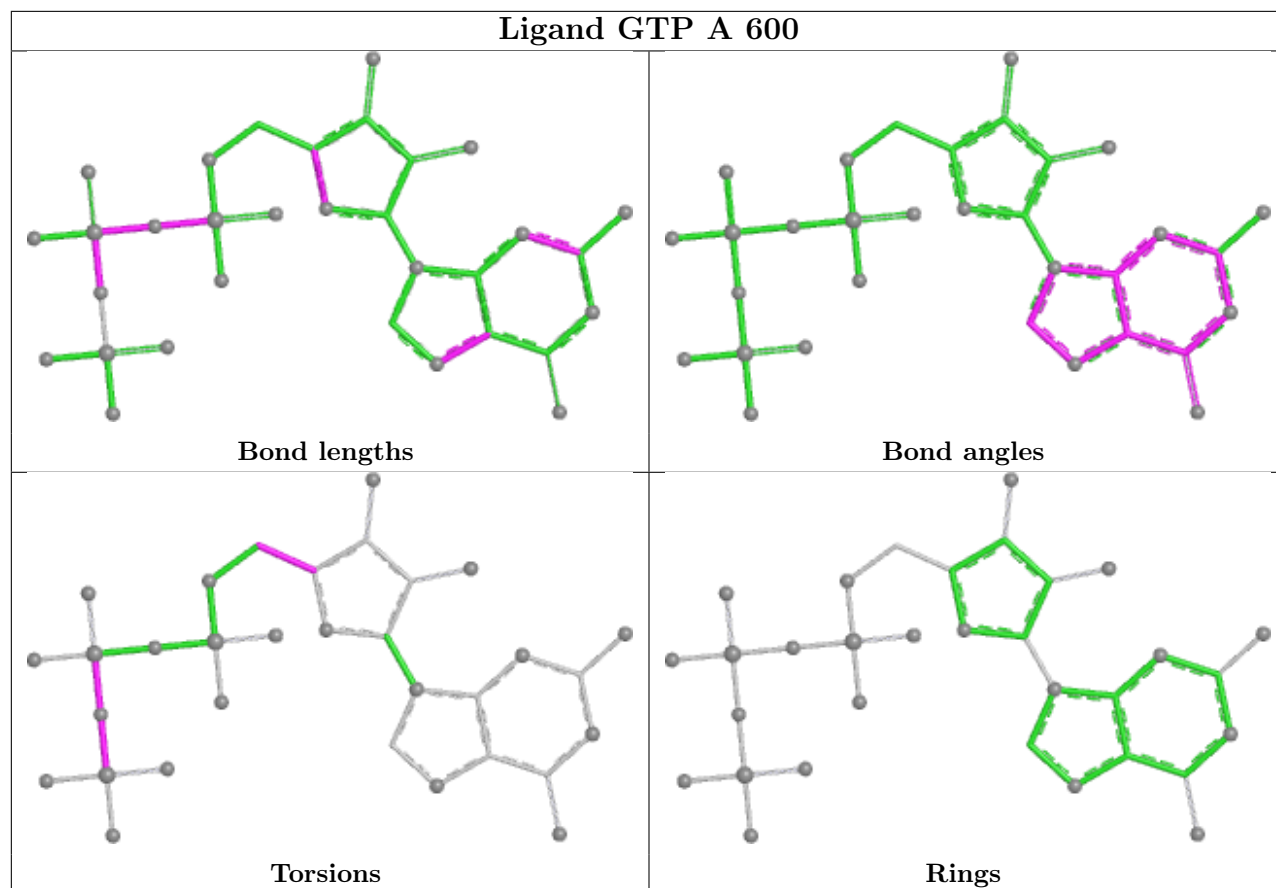
There are no ring outliers.

6 monomers are involved in 59 short contacts:

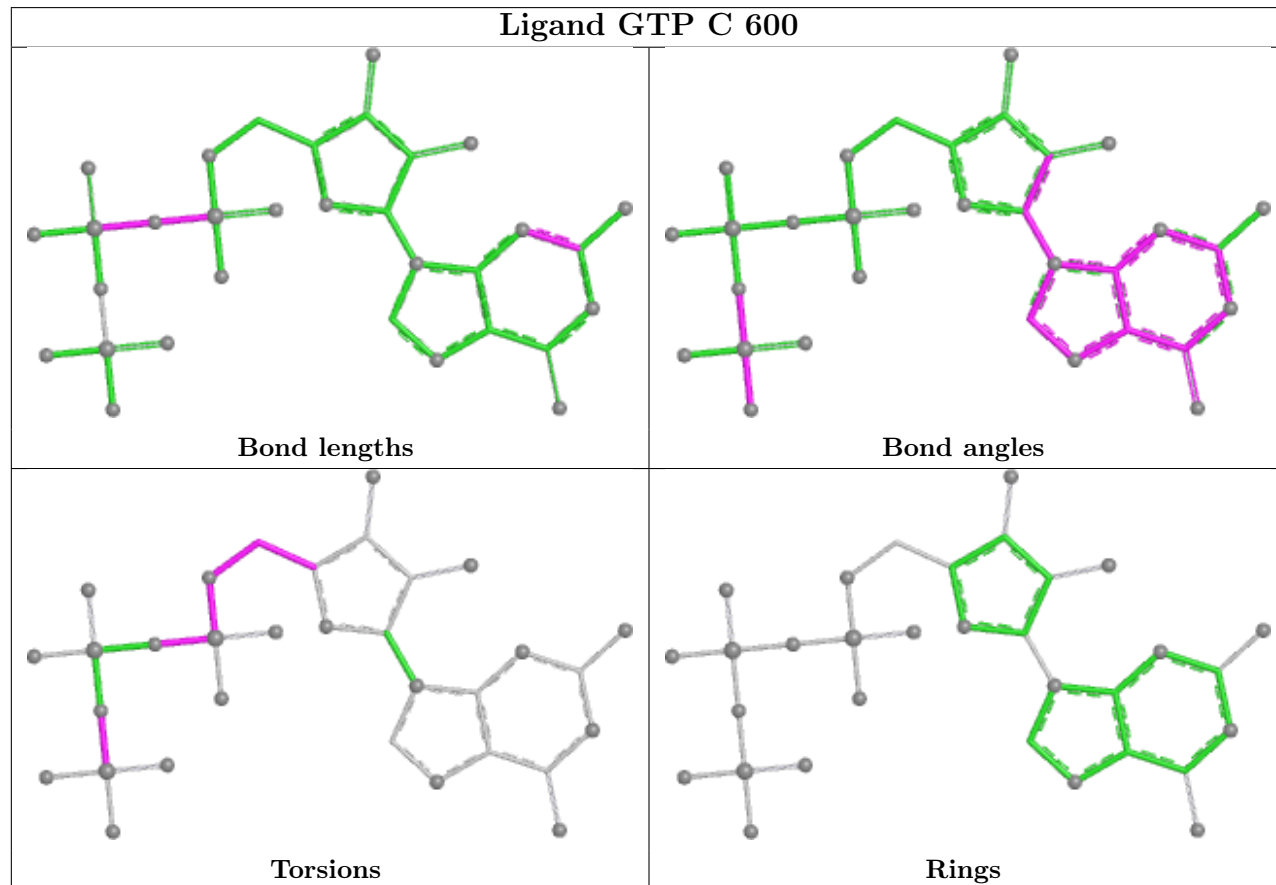
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GTP	2	0
4	C	600	GTP	4	0
7	B	700	N16	8	0
6	D	600	GDP	19	0
6	B	600	GDP	10	0
7	D	700	N16	16	0

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.

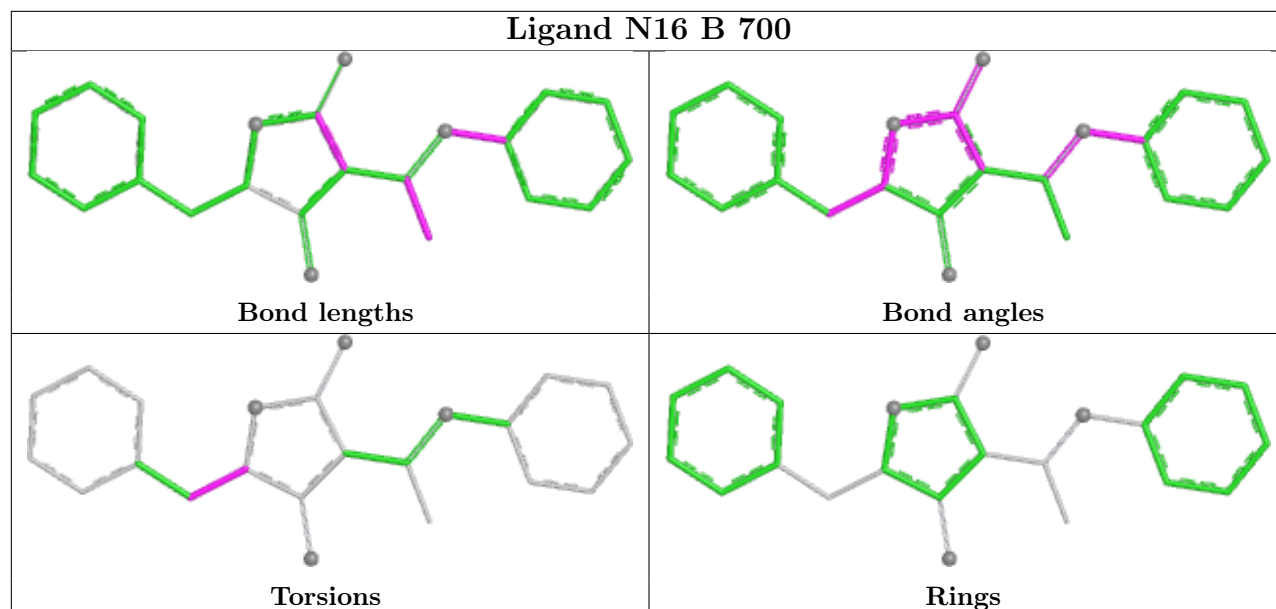
Ligand GTP A 600



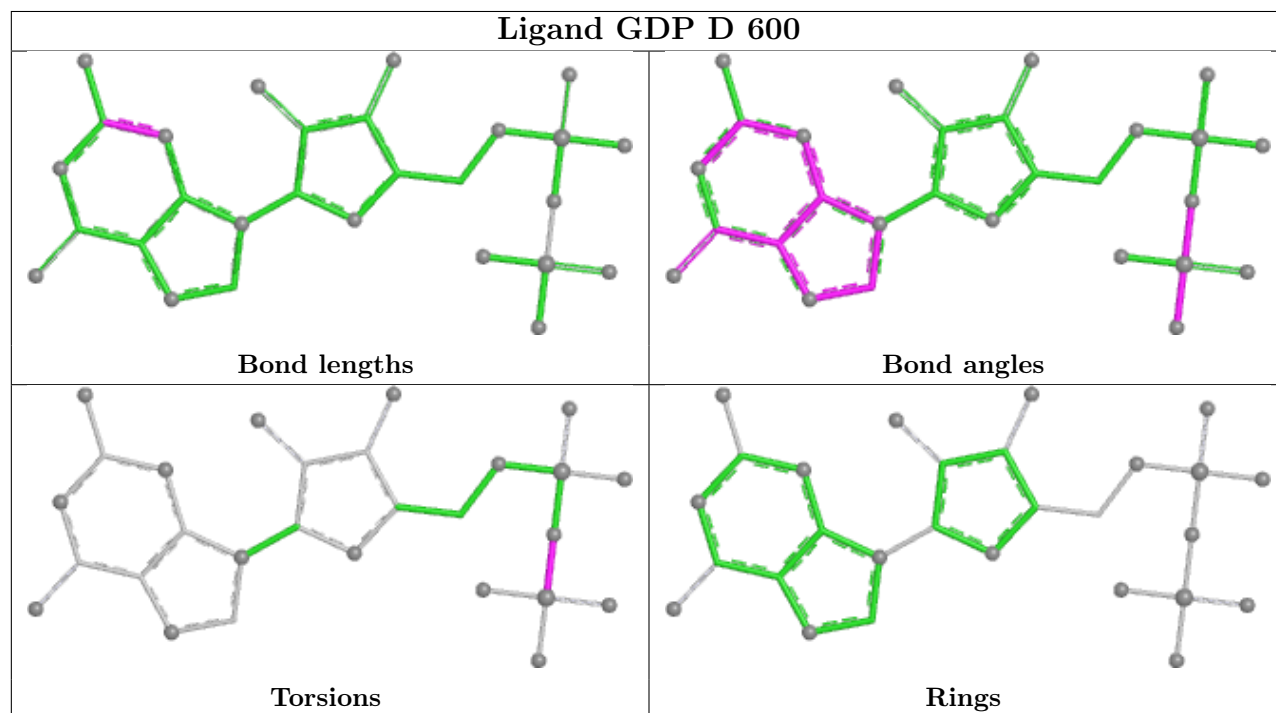
Ligand GTP C 600

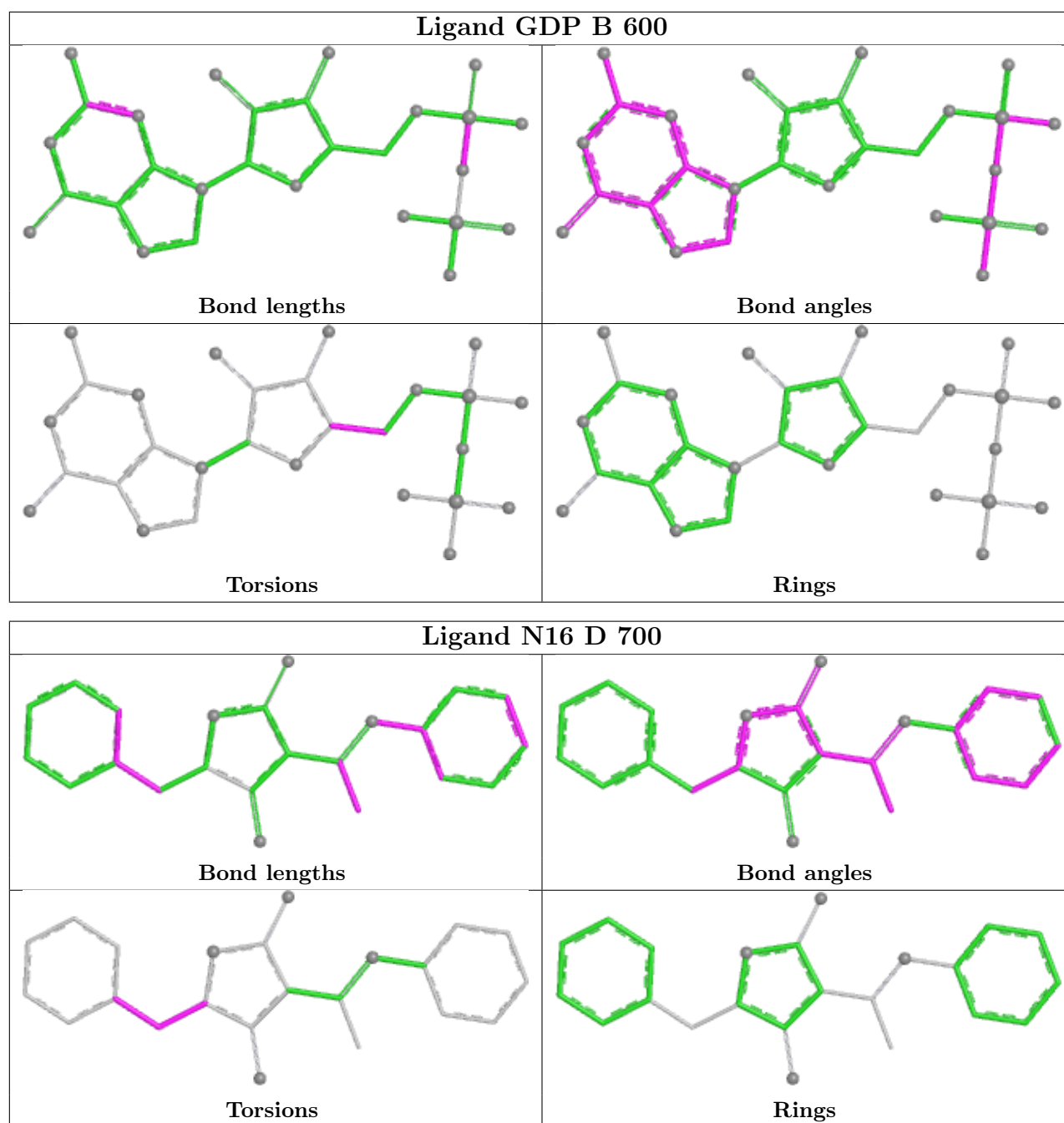


Ligand N16 B 700



Ligand GDP D 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%)	-0.58	0 100 100	39, 43, 44, 47	0
1	C	429/451 (95%)	-0.62	0 100 100	40, 43, 44, 52	0
2	B	420/445 (94%)	-0.62	0 100 100	41, 43, 45, 50	0
2	D	427/445 (95%)	-0.46	0 100 100	41, 43, 45, 48	0
3	E	123/142 (86%)	-0.72	0 100 100	34, 43, 49, 53	0
All	All	1827/1934 (94%)	-0.58	0 100 100	34, 43, 45, 53	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	N16	D	700	23/23	0.85	0.15	79,83,85,85	0
6	GDP	D	600	28/28	0.89	0.09	40,49,56,57	0
5	MG	B	601	1/1	0.93	0.32	15,15,15,15	0

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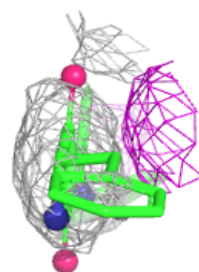
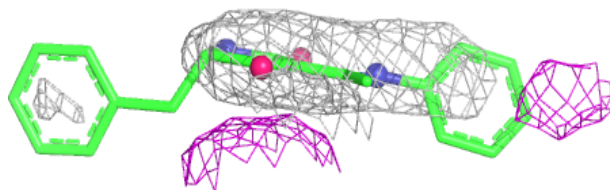
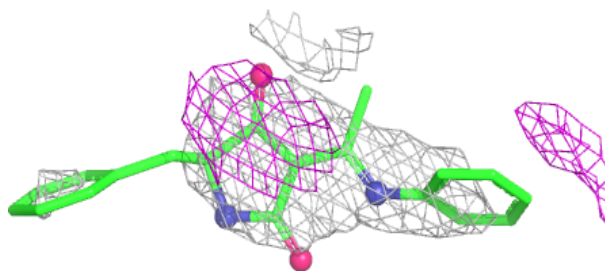
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GDP	B	600	28/28	0.94	0.07	34,42,49,50	0
4	GTP	A	600	32/32	0.96	0.07	33,35,38,40	0
7	N16	B	700	23/23	0.96	0.08	48,49,50,51	0
5	MG	A	601	1/1	0.96	0.15	5,5,5,5	0
4	GTP	C	600	32/32	0.97	0.06	24,32,36,37	0
5	MG	C	601	1/1	0.98	0.07	5,5,5,5	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.

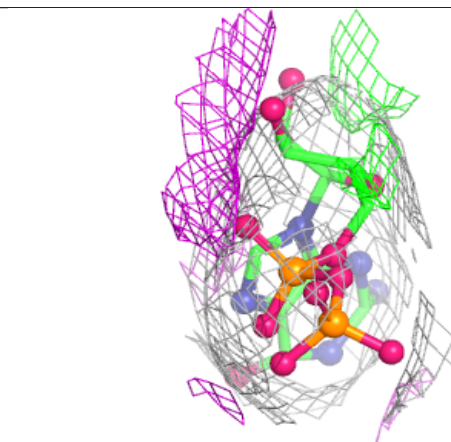
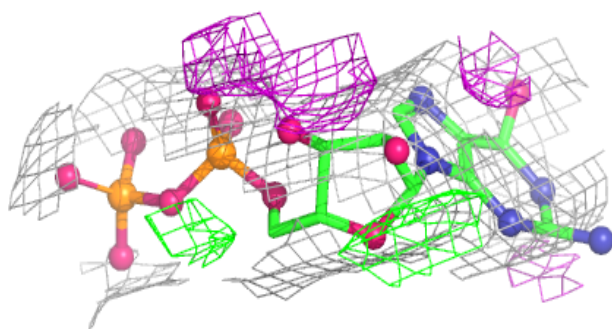
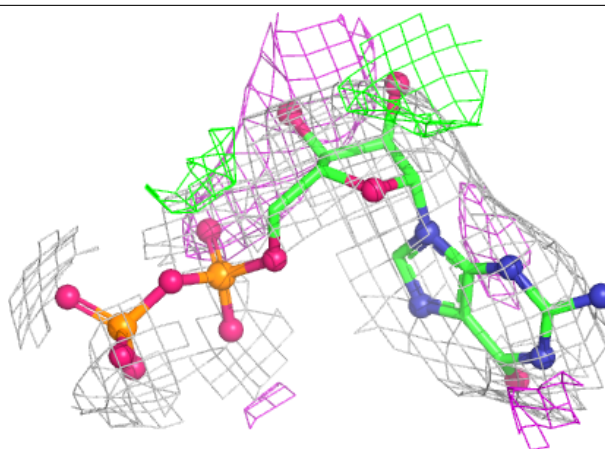
Electron density around N16 D 700:

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

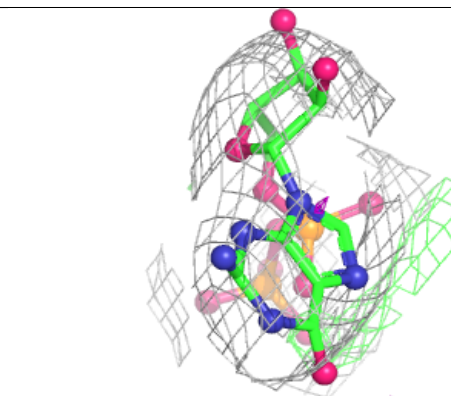
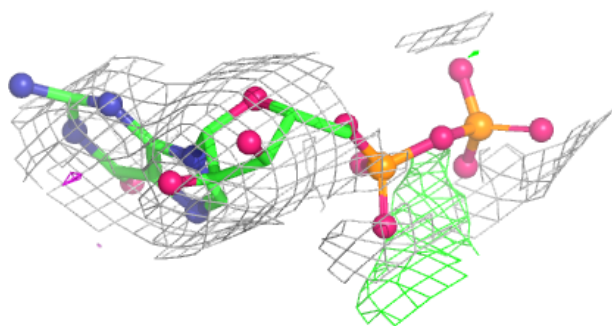
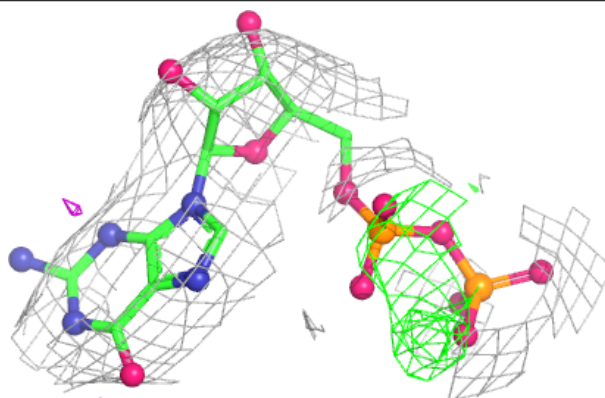


Electron density around GDP D 600:

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

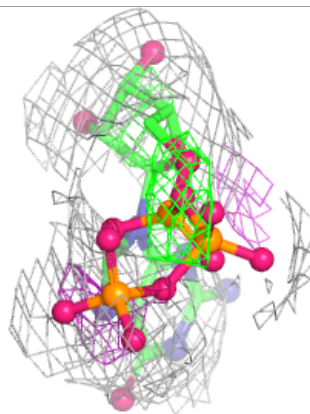
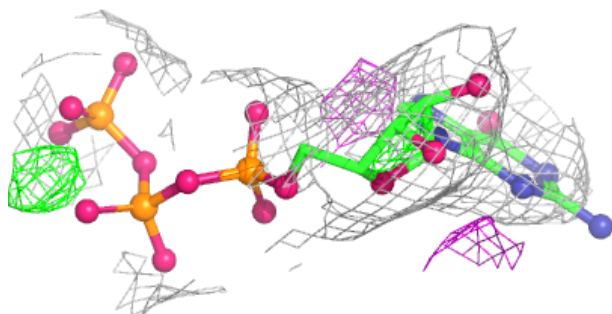
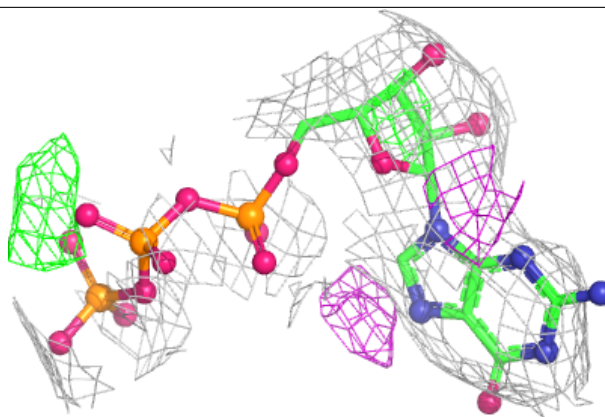
**Electron density around GDP B 600:**

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

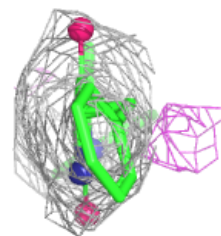
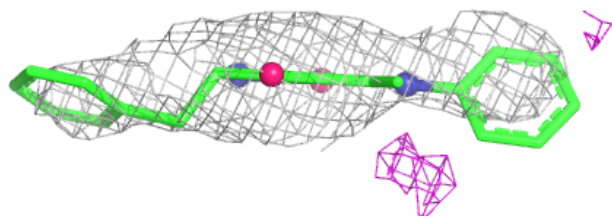
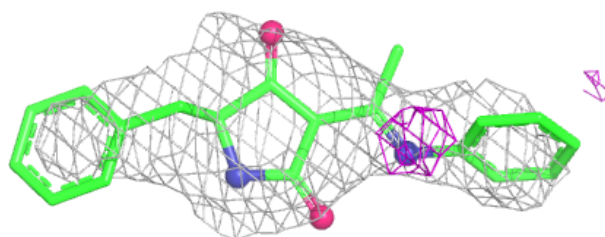


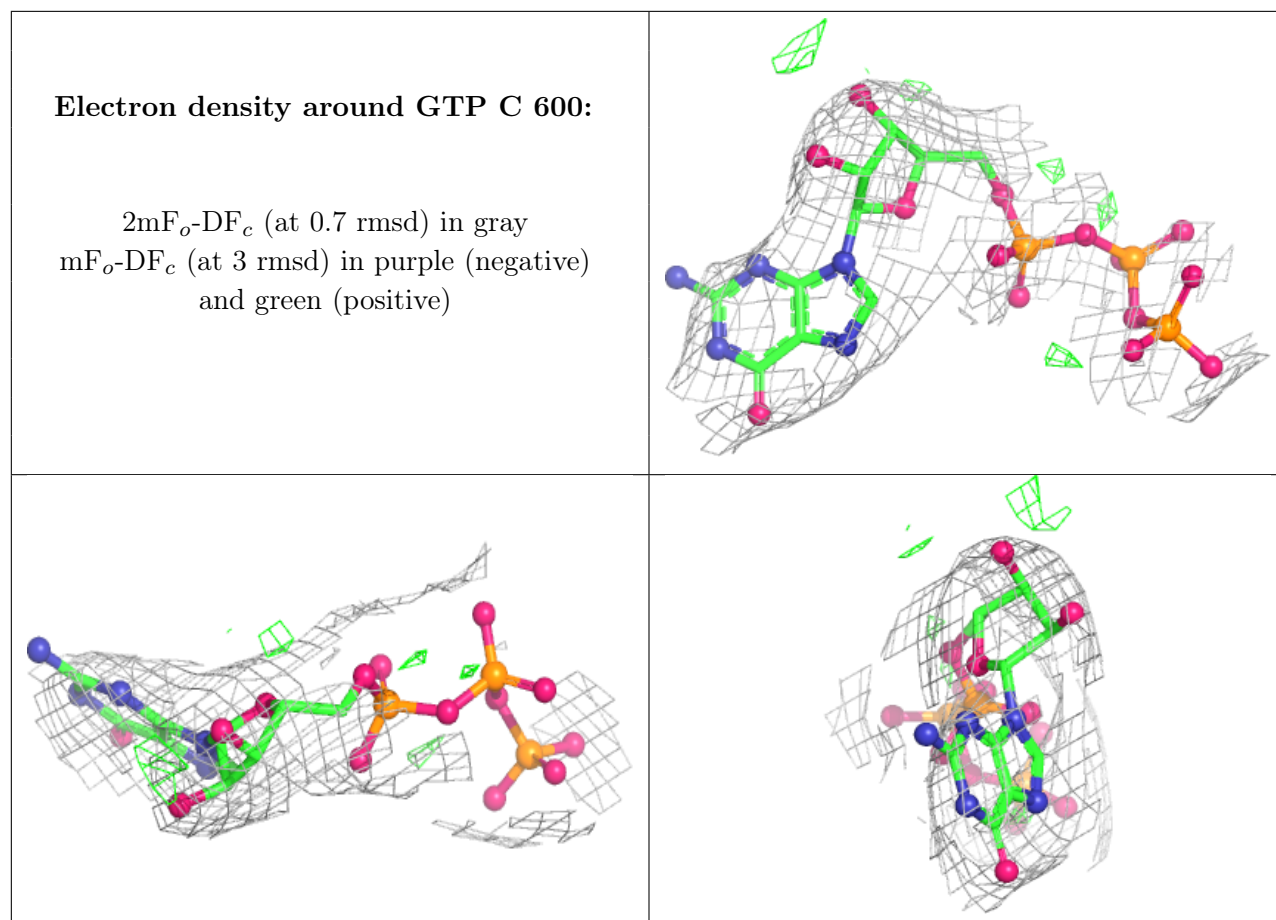
Electron density around GTP A 600:

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

**Electron density around N16 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.