Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 07:27 AM EDT

PDB ID	:	3N2K
Title	:	TUBULIN-NSC 613862: 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 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:

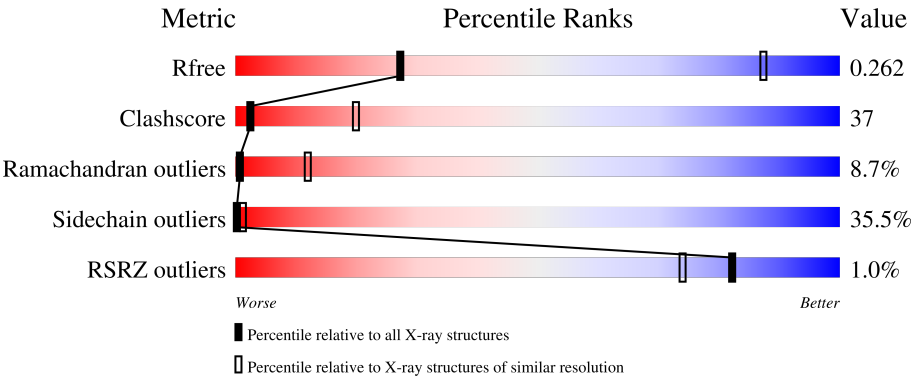
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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 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 <=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	41% 37% 15% • 5%
1	C	451	% 44% 33% 15% • 5%
2	B	445	% 27% 46% 19% • 6%
2	D	445	% 24% 45% 22% 5% •
3	E	142	% 32% 32% 19% • 13%

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	K2N	D	700	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14225 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			

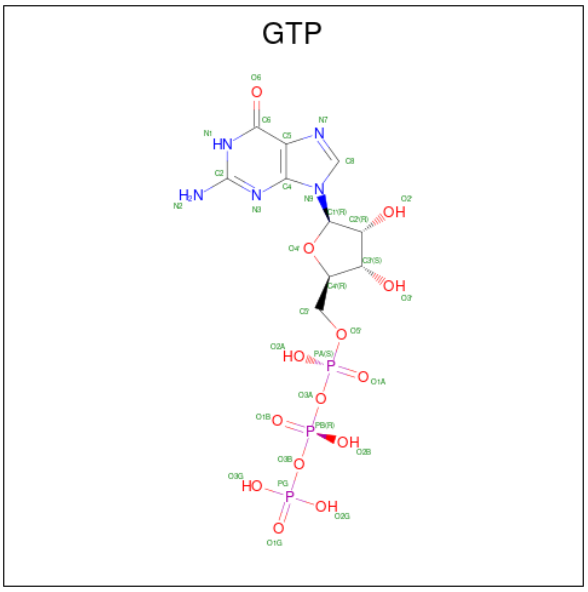
- Molecule 3 is a protein called Stathmin-4.

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 (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

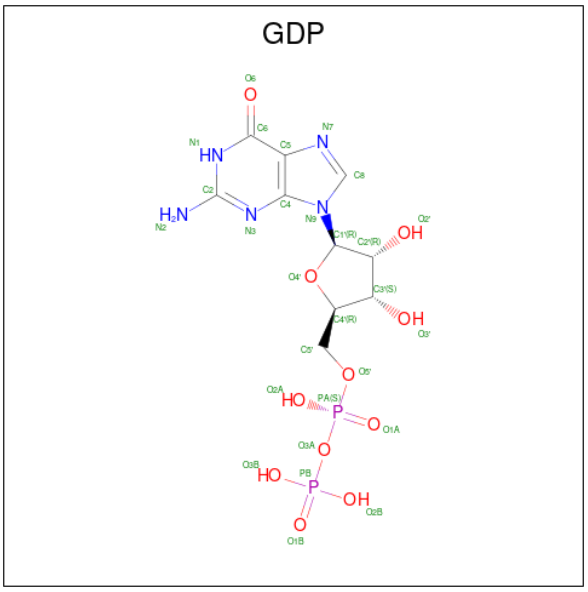


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 32 10 5 14 3	0	0
4	C	1	Total C N O P 32 10 5 14 3	0	0

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

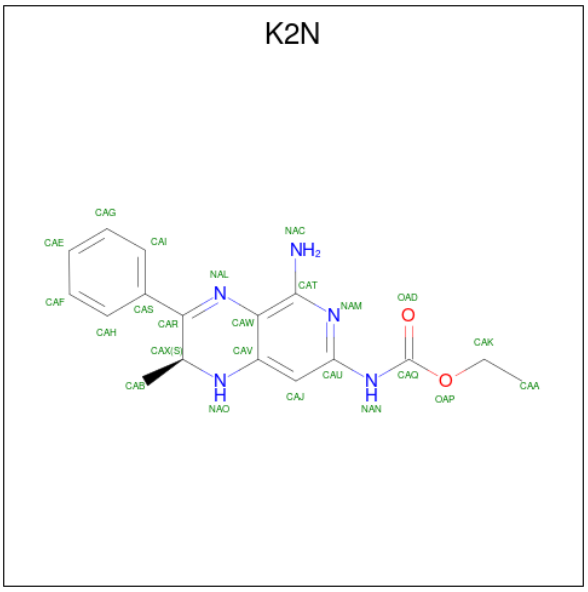
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

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



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

- Molecule 7 is ethyl [(2S)-5-amino-2-methyl-3-phenyl-1,2-dihydropyrido[3,4-b]pyrazin-7-yl]carbamate (three-letter code: K2N) (formula: $C_{17}H_{19}N_5O_2$).



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

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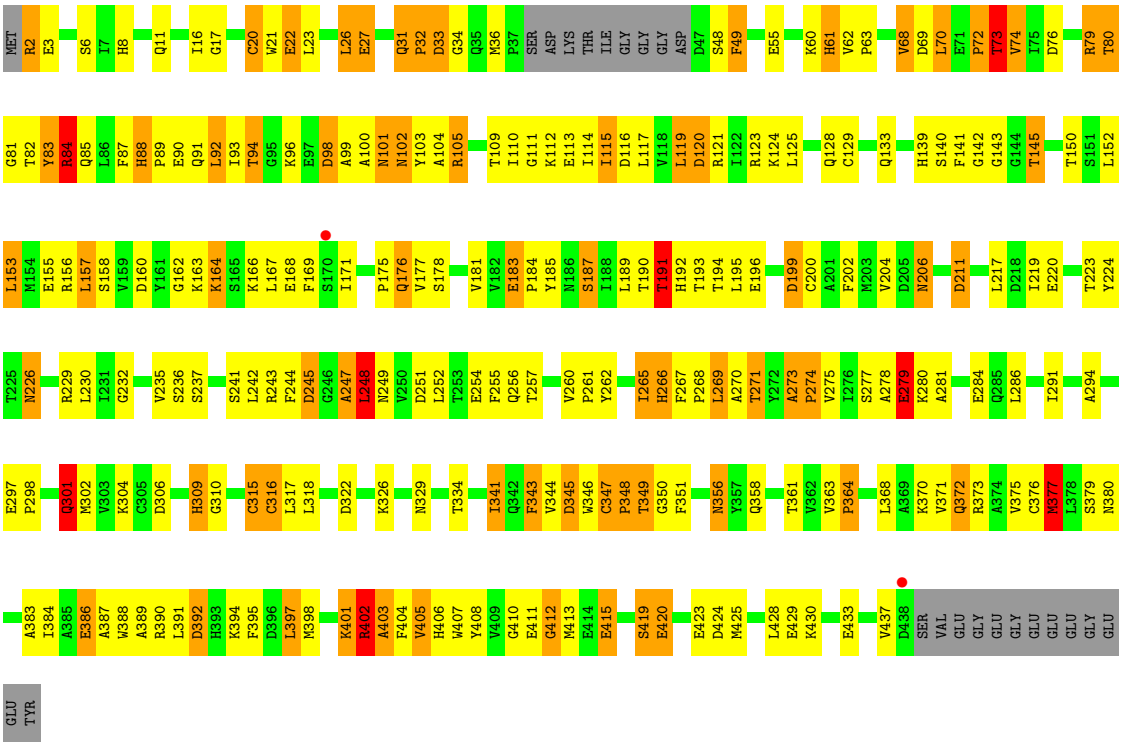
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			24	17	5	2		

3 Residue-property plots (i)

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.

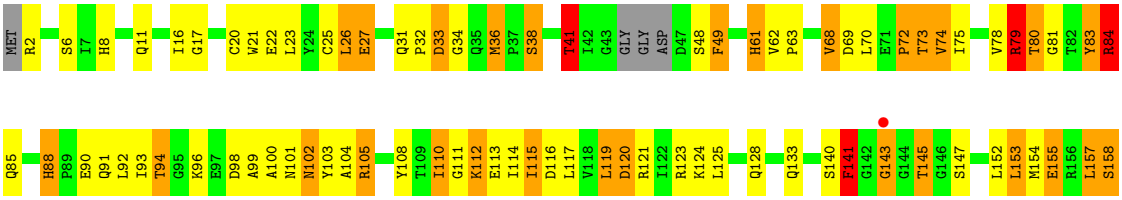
• Molecule 1: Tubulin alpha chain

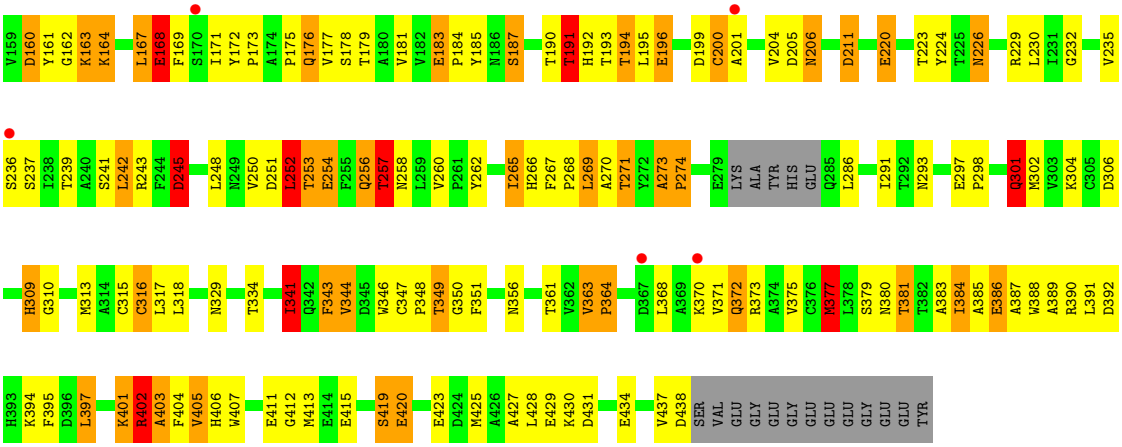
Chain A:



• Molecule 1: Tubulin alpha chain

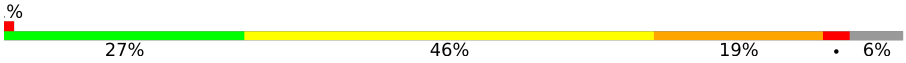
Chain C:

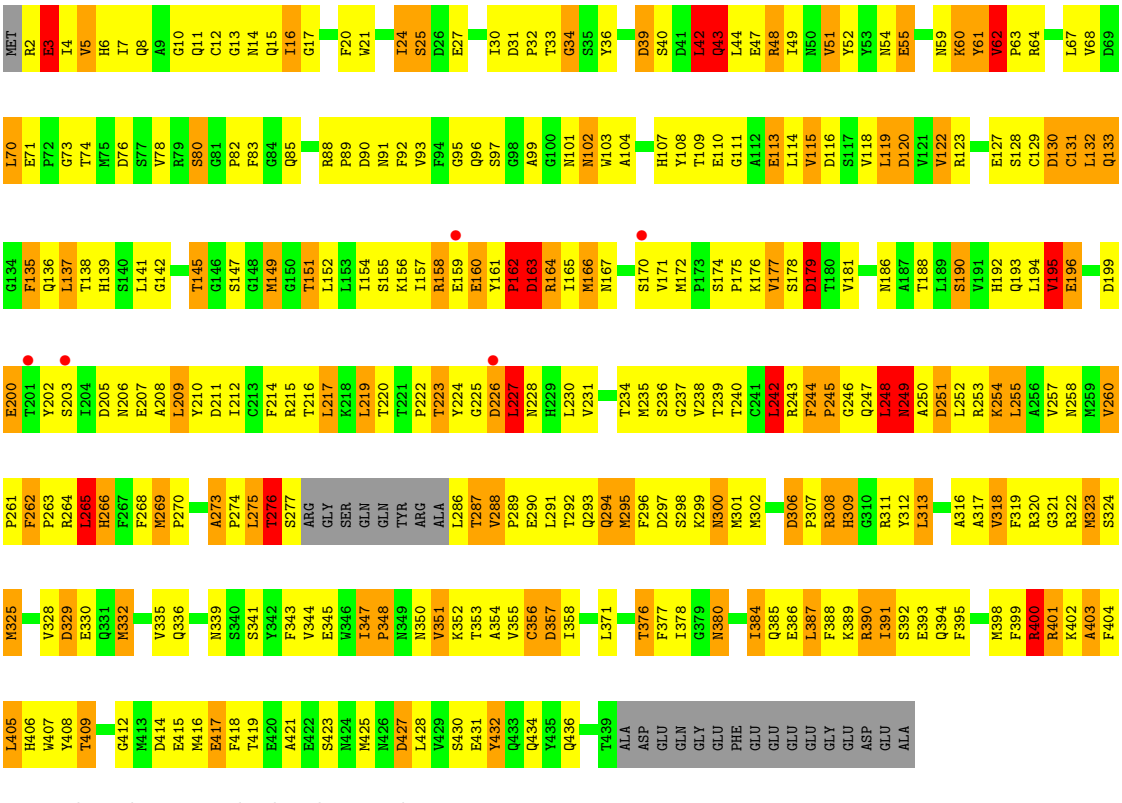




• Molecule 2: Tubulin beta chain

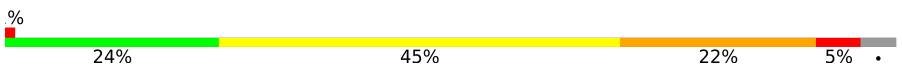
Chain B:

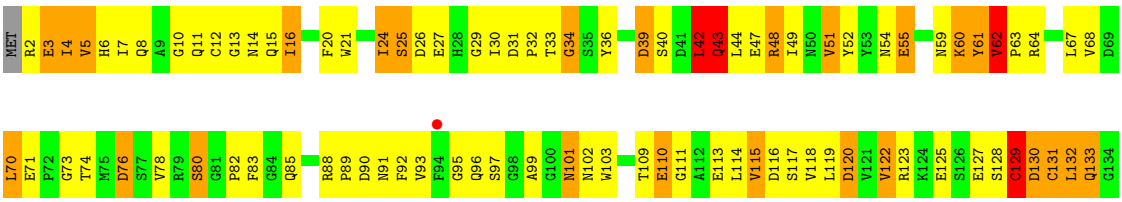


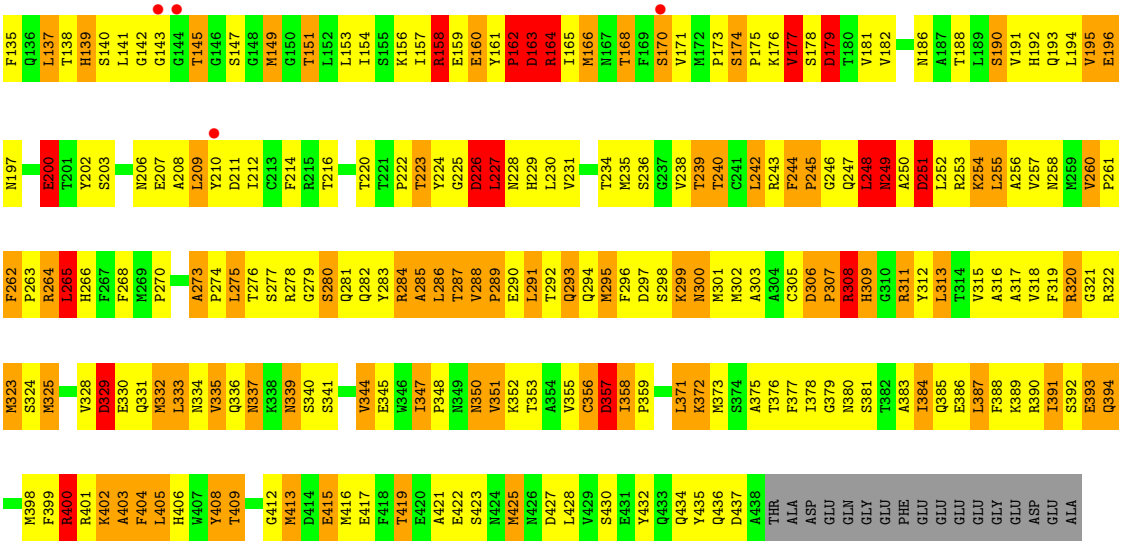


• Molecule 2: Tubulin beta chain

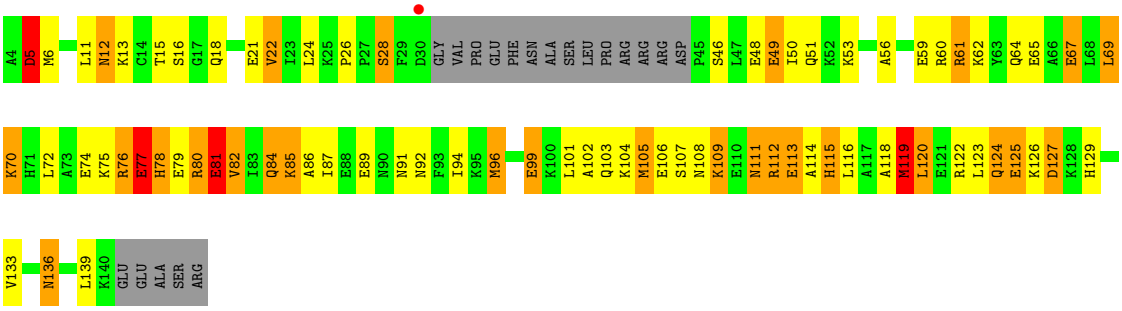
Chain D:







- Molecule 3: Stathmin-4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	326.32Å 326.32Å 54.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.00 29.73 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-4.00) 99.6 (29.73-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 3.98Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.223 , 0.250 0.250 , 0.262	Depositor DCC
R_{free} test set	1435 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	162.7	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 190.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14225	wwPDB-VP
Average B, all atoms (Å^2)	232.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: K2N, MG, GTP, GDP

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	0.96	17/4593 (0.4%)
1	C	0.71	1/3360 (0.0%)	0.95	12/4572 (0.3%)
2	B	0.78	0/3323	0.97	11/4512 (0.2%)
2	D	0.85	2/3370 (0.1%)	1.01	14/4574 (0.3%)
3	E	0.82	2/928 (0.2%)	0.94	1/1243 (0.1%)
All	All	0.79	5/14358 (0.0%)	0.97	55/19494 (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	1
1	C	0	2
2	B	0	4
2	D	0	4
3	E	0	1
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	200	GLU	CD-OE1	7.30	1.33	1.25
1	C	168	GLU	CD-OE1	5.61	1.31	1.25
3	E	119	MET	SD-CE	5.50	2.08	1.77
3	E	105	MET	SD-CE	5.48	2.08	1.77
2	D	177	VAL	CB-CG2	5.39	1.64	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	160	ASP	CB-CG-OD2	7.46	125.01	118.30
1	C	120	ASP	CB-CG-OD2	7.32	124.88	118.30
1	A	248	LEU	CA-CB-CG	7.22	131.91	115.30
1	C	397	LEU	CA-CB-CG	7.10	131.63	115.30
2	D	297	ASP	CB-CG-OD2	7.06	124.65	118.30
1	A	397	LEU	CA-CB-CG	6.97	131.32	115.30
1	A	160	ASP	CB-CG-OD2	6.96	124.57	118.30
1	C	269	LEU	CA-CB-CG	6.94	131.26	115.30
2	D	179	ASP	CB-CG-OD2	6.88	124.50	118.30
1	C	211	ASP	CB-CG-OD2	6.68	124.31	118.30
2	B	130	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	269	LEU	CA-CB-CG	6.55	130.37	115.30
2	B	306	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	322	ASP	CB-CG-OD2	6.49	124.14	118.30
1	C	245	ASP	CB-CG-OD2	6.47	124.12	118.30
2	B	39	ASP	CB-CG-OD2	6.41	124.06	118.30
2	B	120	ASP	CB-CG-OD2	6.38	124.04	118.30
2	B	199	ASP	CB-CG-OD1	6.35	124.02	118.30
1	C	33	ASP	CB-CG-OD2	6.32	123.98	118.30
1	A	211	ASP	CB-CG-OD2	6.26	123.94	118.30
1	C	69	ASP	CB-CG-OD2	6.26	123.93	118.30
2	D	308	ARG	NE-CZ-NH1	6.25	123.43	120.30
2	D	226	ASP	CB-CG-OD2	6.20	123.88	118.30
2	D	357	ASP	CB-CG-OD2	6.19	123.87	118.30
2	B	242	LEU	CA-CB-CG	6.19	129.53	115.30
2	D	242	LEU	CA-CB-CG	6.12	129.37	115.30
1	A	69	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	120	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	266	HIS	CB-CA-C	-6.03	98.34	110.40
1	A	116	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	33	ASP	CB-CG-OD2	6.00	123.70	118.30
2	B	179	ASP	CB-CG-OD2	5.93	123.64	118.30
2	D	164	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	20	CYS	CA-CB-SG	5.82	124.47	114.00
2	D	130	ASP	CB-CG-OD2	5.78	123.50	118.30
3	E	127	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	306	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	424	ASP	CB-CG-OD2	5.69	123.42	118.30
1	C	306	ASP	CB-CG-OD2	5.62	123.36	118.30
2	B	205	ASP	CB-CG-OD2	5.61	123.35	118.30
2	B	427	ASP	CB-CG-OD2	5.54	123.28	118.30
2	B	297	ASP	CB-CG-OD2	5.49	123.24	118.30
2	D	39	ASP	CB-CG-OD2	5.48	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	252	LEU	CA-CB-CG	5.43	127.78	115.30
2	D	427	ASP	CB-CG-OD2	5.42	123.18	118.30
2	D	306	ASP	CB-CG-OD2	5.38	123.15	118.30
2	D	120	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	205	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	98	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	431	ASP	CB-CG-OD2	5.25	123.03	118.30
2	D	329	ASP	CB-CG-OD2	5.18	122.96	118.30
2	D	379	GLY	N-CA-C	5.10	125.86	113.10
2	B	329	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	251	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	345	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLY	Peptide
2	B	162	PRO	Peptide
2	B	248	LEU	Peptide
2	B	249	ASN	Peptide
2	B	262	PHE	Peptide
1	C	143	GLY	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	186	0
2	B	3251	0	3074	276	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3297	0	3116	358	0
3	E	920	0	816	61	0
4	A	32	0	12	5	0
4	C	32	0	12	7	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	7	0
6	D	28	0	12	12	0
7	B	24	0	19	8	0
7	D	24	0	19	23	0
All	All	14225	0	13387	1032	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 37.

All (1032) 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:96:MET:CE	3:E:96:MET:SD	2.01	1.47
3:E:105:MET:SD	3:E:105:MET:CE	2.08	1.42
3:E:119:MET:SD	3:E:119:MET:CE	2.08	1.41
2:D:387:LEU:O	2:D:390:ARG:HG2	1.41	1.18
2:D:287:THR:HG23	2:D:290:GLU:HB2	1.20	1.17
2:D:319:PHE:HB2	2:D:355:VAL:HG12	1.24	1.15
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.28	1.11
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.19	1.10
2:D:252:LEU:HD13	7:D:700:K2N:HAK	1.12	1.09
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.82	1.09
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.32	1.08
2:D:223:THR:HB	2:D:225:GLY:H	1.11	1.06
2:D:135:PHE:HB2	2:D:166:MET:CE	1.85	1.05
2:D:308:ARG:HG3	2:D:308:ARG:HH11	1.14	1.05
1:A:278:ALA:O	1:A:279:GLU:HB3	1.53	1.05
2:B:135:PHE:HB2	2:B:166:MET:CE	1.86	1.05
2:D:252:LEU:HD13	7:D:700:K2N:CAK	1.88	1.03
2:D:252:LEU:CD1	7:D:700:K2N:HAK	1.88	1.03
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.06	1.03
2:B:223:THR:HB	2:B:225:GLY:H	1.19	1.02
2:B:308:ARG:HG3	2:B:308:ARG:HH11	1.23	1.01
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.88	1.00
2:D:140:SER:HB2	6:D:600:GDP:H5'	1.41	1.00
2:D:252:LEU:CD1	7:D:700:K2N:CAK	2.40	0.99
1:C:105:ARG:NH2	2:D:253:ARG:HH21	1.60	0.99
2:D:295:MET:HG3	2:D:377:PHE:HB2	1.46	0.97
2:D:229:HIS:CE1	2:D:277:SER:HB3	2.00	0.96
1:C:70:LEU:HD12	1:C:145:THR:HB	1.47	0.96
2:D:273:ALA:HB3	2:D:274:PRO:CD	1.95	0.96
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.46	0.95
1:A:206:ASN:HD21	4:A:600:GTP:HN22	1.14	0.95
2:D:261:PRO:HG3	2:D:313:LEU:HD12	1.48	0.95
2:D:378:ILE:HD12	7:D:700:K2N:HABA	1.47	0.94
1:C:206:ASN:HD21	4:C:600:GTP:N2	1.66	0.94
1:C:41:THR:HG21	1:C:61:HIS:HE1	1.32	0.93
2:D:287:THR:CG2	2:D:290:GLU:HB2	1.97	0.93
1:C:105:ARG:HH22	2:D:253:ARG:HH21	0.94	0.93
2:B:403:ALA:O	2:B:405:LEU:N	2.03	0.92
1:C:206:ASN:HD21	4:C:600:GTP:HN22	0.96	0.92
2:D:99:ALA:HB1	2:D:145:THR:CG2	2.01	0.91
2:D:5:VAL:HG22	2:D:135:PHE:HD2	1.36	0.91
2:D:311:ARG:HH21	2:D:344:VAL:HG22	1.37	0.90
1:A:249:ASN:HD22	1:A:254:GLU:HG2	1.38	0.89
2:B:133:GLN:HE21	2:B:252:LEU:HD22	1.35	0.89
2:B:99:ALA:HB1	2:B:145:THR:HG22	1.51	0.89
1:A:70:LEU:HD12	1:A:145:THR:HB	1.55	0.89
2:B:123:ARG:O	2:B:127:GLU:HB2	1.74	0.89
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.03	0.88
2:B:151:THR:HB	2:B:193:GLN:HG2	1.56	0.88
2:B:135:PHE:HB2	2:B:166:MET:HE2	1.54	0.88
1:C:79:ARG:NH2	1:C:94:THR:HG21	1.89	0.88
1:A:273:ALA:CB	1:A:274:PRO:HD3	2.03	0.88
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.56	0.87
2:B:403:ALA:C	2:B:405:LEU:H	1.76	0.87
2:D:316:ALA:HB1	7:D:700:K2N:CAI	2.05	0.87
2:B:270:PRO:HD2	2:B:302:MET:HB2	1.57	0.87
2:D:223:THR:HB	2:D:225:GLY:N	1.90	0.86
1:A:105:ARG:HH22	2:B:253:ARG:HH21	1.16	0.86
2:D:319:PHE:CB	2:D:355:VAL:HG12	2.05	0.86
1:C:153:LEU:HD13	1:C:157:LEU:HD11	1.58	0.85
2:B:155:SER:HB3	3:E:76:ARG:HH22	1.40	0.85
2:B:5:VAL:HG22	2:B:135:PHE:HD2	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:ALA:HB1	2:D:145:THR:HG22	1.57	0.85
2:D:252:LEU:HD11	7:D:700:K2N:H19	1.59	0.85
2:D:123:ARG:O	2:D:127:GLU:HB2	1.75	0.85
2:D:265:LEU:HB2	2:D:432:TYR:CE2	2.12	0.84
2:D:133:GLN:HE21	2:D:252:LEU:HD22	1.40	0.84
1:C:105:ARG:HH22	2:D:253:ARG:NH2	1.75	0.84
2:B:248:LEU:O	2:B:249:ASN:HB3	1.78	0.83
2:D:135:PHE:HB2	2:D:166:MET:HE1	1.59	0.83
1:A:79:ARG:NH2	1:A:94:THR:HG21	1.93	0.83
1:C:404:PHE:HE1	2:D:347:ILE:HG21	1.44	0.83
7:B:700:K2N:OAD	7:B:700:K2N:H3	1.79	0.82
1:C:273:ALA:CB	1:C:274:PRO:HD3	2.10	0.82
2:D:308:ARG:HG3	2:D:308:ARG:NH1	1.92	0.82
2:D:262:PHE:HB2	2:D:265:LEU:HD11	1.61	0.82
2:D:151:THR:HB	2:D:193:GLN:HG2	1.61	0.82
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.61	0.82
1:C:183:GLU:HB3	1:C:184:PRO:CD	2.09	0.82
2:B:223:THR:HB	2:B:225:GLY:N	1.96	0.81
3:E:116:LEU:O	3:E:119:MET:HB3	1.79	0.81
2:D:308:ARG:HH21	2:D:339:ASN:HD21	1.29	0.81
1:C:265:ILE:H	1:C:265:ILE:HD12	1.44	0.80
1:C:206:ASN:ND2	4:C:600:GTP:HN22	1.79	0.80
2:D:171:VAL:HG12	2:D:206:ASN:ND2	1.96	0.80
2:D:200:GLU:HB3	2:D:268:PHE:CE1	2.17	0.80
3:E:118:ALA:O	3:E:122:ARG:NH1	2.16	0.79
2:D:252:LEU:CD1	7:D:700:K2N:H19	2.11	0.79
2:B:99:ALA:HB1	2:B:145:THR:CG2	2.13	0.79
2:B:320:ARG:HA	2:B:356:CYS:O	1.82	0.79
2:D:270:PRO:HD2	2:D:302:MET:HB2	1.64	0.78
2:B:401:ARG:HG3	2:B:401:ARG:HH11	1.48	0.78
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.18	0.78
2:D:273:ALA:HB2	2:D:375:ALA:H	1.47	0.78
2:B:133:GLN:HE21	2:B:252:LEU:CD2	1.97	0.78
2:D:312:TYR:CD2	2:D:315:VAL:CG2	2.67	0.78
2:D:391:ILE:HG13	2:D:392:SER:H	1.47	0.78
1:C:8:HIS:CD2	1:C:17:GLY:HA3	2.18	0.78
2:D:309:HIS:H	2:D:309:HIS:CD2	2.01	0.78
2:D:391:ILE:HG13	2:D:392:SER:N	1.99	0.78
2:B:2:ARG:N	2:B:133:GLN:OE1	2.17	0.78
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.65	0.78
2:D:378:ILE:CD1	7:D:700:K2N:HABA	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:316:ALA:HB1	7:D:700:K2N:HAI	1.65	0.77
1:A:105:ARG:HH22	2:B:253:ARG:NH2	1.83	0.77
2:B:220:THR:O	2:B:222:PRO:HD3	1.83	0.77
2:B:311:ARG:HH21	2:B:344:VAL:HG22	1.48	0.77
2:D:140:SER:CB	6:D:600:GDP:H5'	2.13	0.77
2:D:223:THR:CB	2:D:225:GLY:H	1.94	0.77
2:B:200:GLU:HB3	2:B:268:PHE:CE1	2.20	0.77
2:B:224:TYR:O	2:B:228:ASN:ND2	2.18	0.77
2:B:319:PHE:HB2	2:B:355:VAL:HG12	1.67	0.76
2:D:200:GLU:OE2	2:D:268:PHE:HE1	1.68	0.76
2:D:224:TYR:O	2:D:228:ASN:ND2	2.19	0.76
2:D:319:PHE:HB2	2:D:355:VAL:CG1	2.12	0.76
2:D:162:PRO:HD2	2:D:163:ASP:HB2	1.66	0.76
2:B:42:LEU:O	2:B:44:LEU:N	2.19	0.76
2:D:383:ALA:O	2:D:386:GLU:HB2	1.86	0.76
1:C:343:PHE:CD1	1:C:349:THR:HG22	2.21	0.75
2:B:171:VAL:HG12	2:B:206:ASN:ND2	2.00	0.75
2:D:403:ALA:O	2:D:405:LEU:N	2.20	0.75
2:B:142:GLY:O	6:B:600:GDP:H5'	1.86	0.75
2:B:298:SER:C	2:B:300:ASN:H	1.90	0.75
2:B:298:SER:HA	2:B:301:MET:HG2	1.67	0.75
2:B:145:THR:HG23	6:B:600:GDP:O3B	1.87	0.75
1:C:101:ASN:HD22	2:D:254:LYS:HG2	1.52	0.74
1:A:265:ILE:HD12	1:A:265:ILE:H	1.50	0.74
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.35	0.74
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.69	0.74
1:A:401:LYS:C	1:A:403:ALA:H	1.90	0.74
2:D:224:TYR:OH	6:D:600:GDP:H2'	1.87	0.74
1:A:270:ALA:O	1:A:302:MET:HB2	1.87	0.74
2:D:42:LEU:O	2:D:44:LEU:N	2.20	0.74
2:D:306:ASP:O	2:D:308:ARG:N	2.19	0.73
1:A:266:HIS:O	1:A:268:PRO:HD3	1.87	0.73
2:B:387:LEU:HA	2:B:390:ARG:HG2	1.70	0.73
2:D:2:ARG:N	2:D:133:GLN:OE1	2.21	0.73
1:A:273:ALA:HB3	1:A:375:VAL:H	1.53	0.73
1:A:343:PHE:CD1	1:A:349:THR:HG22	2.23	0.73
2:D:133:GLN:HE21	2:D:252:LEU:CD2	2.02	0.73
1:C:273:ALA:HB3	1:C:375:VAL:H	1.52	0.72
2:B:76:ASP:O	2:B:80:SER:HB2	1.87	0.72
1:C:270:ALA:O	1:C:302:MET:HB2	1.90	0.72
2:D:345:GLU:N	2:D:345:GLU:OE1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:SER:O	1:C:191:THR:HB	1.90	0.72
2:B:287:THR:HG23	2:B:290:GLU:HB2	1.72	0.72
2:D:273:ALA:CB	2:D:375:ALA:H	2.02	0.72
1:C:79:ARG:NH2	1:C:94:THR:CG2	2.52	0.72
2:D:114:LEU:O	2:D:116:ASP:N	2.22	0.72
2:D:220:THR:O	2:D:222:PRO:HD3	1.90	0.72
7:B:700:K2N:OAD	7:B:700:K2N:CAA	2.36	0.71
1:C:404:PHE:CE1	2:D:347:ILE:HG21	2.24	0.71
2:D:192:HIS:CD2	2:D:421:ALA:CB	2.73	0.71
1:A:273:ALA:HB3	1:A:274:PRO:CD	2.16	0.71
2:D:321:GLY:O	2:D:323:MET:N	2.24	0.71
2:D:171:VAL:HG12	2:D:206:ASN:HD21	1.54	0.71
2:B:295:MET:CG	2:B:377:PHE:HB2	2.18	0.71
2:D:312:TYR:HD2	2:D:315:VAL:CG2	2.04	0.71
2:B:135:PHE:HB2	2:B:166:MET:HE1	1.70	0.70
1:C:41:THR:HG21	1:C:61:HIS:CE1	2.22	0.70
1:C:70:LEU:CD1	1:C:145:THR:HB	2.21	0.70
2:D:311:ARG:HH21	2:D:344:VAL:CG2	2.05	0.70
2:D:350:ASN:HD22	2:D:350:ASN:H	1.37	0.70
2:B:273:ALA:CB	2:B:274:PRO:CD	2.64	0.70
3:E:72:LEU:C	3:E:74:GLU:H	1.95	0.70
2:B:345:GLU:N	2:B:345:GLU:OE1	2.25	0.69
2:B:378:ILE:HD12	7:B:700:K2N:HABA	1.74	0.69
2:D:265:LEU:CB	2:D:432:TYR:CE2	2.74	0.69
3:E:77:GLU:HG2	3:E:80:ARG:HB2	1.74	0.69
2:B:21:TRP:O	2:B:25:SER:HB2	1.93	0.69
1:C:344:VAL:HG13	1:C:346:TRP:H	1.58	0.69
2:D:276:THR:HG21	2:D:280:SER:CB	2.22	0.69
3:E:123:LEU:C	3:E:125:GLU:H	1.95	0.69
1:C:271:THR:HG23	1:C:301:GLN:HA	1.75	0.69
1:C:315:CYS:SG	1:C:377:MET:HE2	2.32	0.69
2:D:135:PHE:HB2	2:D:166:MET:HE2	1.74	0.69
1:A:273:ALA:CB	1:A:375:VAL:H	2.06	0.69
2:D:171:VAL:CG1	2:D:206:ASN:HD21	2.06	0.69
2:D:179:ASP:OD1	2:D:179:ASP:N	2.25	0.69
2:D:192:HIS:HD2	2:D:421:ALA:CB	2.06	0.69
7:D:700:K2N:H3	7:D:700:K2N:OAD	1.92	0.69
2:D:311:ARG:NH2	2:D:344:VAL:HG22	2.07	0.69
3:E:107:SER:O	3:E:111:ASN:HB2	1.93	0.69
2:D:385:GLN:HG2	2:D:389:LYS:HD2	1.75	0.69
2:B:7:ILE:HG22	2:B:137:LEU:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:CD1	1:A:145:THR:HB	2.24	0.68
1:C:99:ALA:HB2	1:C:145:THR:HG22	1.74	0.68
2:D:402:LYS:HD2	2:D:415:GLU:OE1	1.92	0.68
1:A:79:ARG:NH2	1:A:94:THR:CG2	2.56	0.68
1:A:271:THR:HG23	1:A:301:GLN:HA	1.75	0.68
1:A:99:ALA:CB	1:A:145:THR:HG22	2.24	0.68
2:B:51:VAL:HG13	2:B:52:TYR:CD1	2.28	0.68
2:D:238:VAL:HG12	7:D:700:K2N:HAJ	1.76	0.68
2:B:262:PHE:HB2	2:B:265:LEU:HD11	1.76	0.68
3:E:101:LEU:O	3:E:103:GLN:N	2.26	0.68
2:B:151:THR:HG21	2:B:190:SER:HB3	1.76	0.68
2:D:135:PHE:HZ	2:D:161:TYR:CD1	2.11	0.68
2:D:252:LEU:HD11	7:D:700:K2N:CAK	2.14	0.68
2:D:141:LEU:HA	2:D:147:SER:HB3	1.75	0.68
2:D:164:ARG:HE	2:D:164:ARG:HA	1.57	0.68
1:C:273:ALA:CB	1:C:375:VAL:H	2.06	0.67
2:D:295:MET:O	2:D:295:MET:HG2	1.94	0.67
2:B:12:CYS:SG	6:B:600:GDP:C4	2.87	0.67
1:A:412:GLY:O	3:E:60:ARG:NH1	2.27	0.67
2:D:333:LEU:CD2	2:D:337:ASN:HD21	2.06	0.67
2:B:308:ARG:HG3	2:B:308:ARG:NH1	2.00	0.67
2:D:51:VAL:HG13	2:D:52:TYR:CD1	2.29	0.67
2:B:401:ARG:HG3	2:B:401:ARG:NH1	2.08	0.67
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.59	0.67
2:D:312:TYR:HE2	2:D:377:PHE:HZ	1.43	0.67
2:D:273:ALA:CB	2:D:274:PRO:CD	2.61	0.67
1:C:102:ASN:HD21	1:C:104:ALA:HB3	1.60	0.66
3:E:48:GLU:O	3:E:50:ILE:N	2.28	0.66
1:A:153:LEU:HD13	1:A:157:LEU:HD11	1.77	0.66
2:B:54:ASN:HB2	2:B:64:ARG:HD3	1.76	0.66
2:B:306:ASP:O	2:B:308:ARG:N	2.26	0.66
2:D:357:ASP:OD2	2:D:357:ASP:N	2.29	0.66
1:C:88:HIS:HB2	1:C:91:GLN:NE2	2.11	0.66
1:A:85:GLN:HE21	1:A:85:GLN:HA	1.61	0.66
2:D:162:PRO:CD	2:D:163:ASP:HB2	2.26	0.66
2:D:306:ASP:C	2:D:308:ARG:H	1.98	0.66
2:D:21:TRP:O	2:D:25:SER:HB2	1.95	0.66
1:A:178:SER:HB3	2:B:352:LYS:NZ	2.11	0.66
2:B:155:SER:CB	3:E:76:ARG:HH22	2.07	0.66
1:C:315:CYS:SG	1:C:377:MET:CE	2.84	0.66
2:D:298:SER:O	2:D:300:ASN:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:NH2	2:B:253:ARG:HH21	1.93	0.65
2:D:76:ASP:O	2:D:80:SER:HB2	1.96	0.65
2:B:179:ASP:N	2:B:179:ASP:OD1	2.29	0.65
2:D:135:PHE:CZ	2:D:161:TYR:CD1	2.84	0.65
2:D:320:ARG:HA	2:D:356:CYS:O	1.96	0.65
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.19	0.65
2:D:12:CYS:SG	6:D:600:GDP:C4	2.90	0.65
2:B:114:LEU:O	2:B:116:ASP:N	2.30	0.65
1:C:105:ARG:NH2	2:D:253:ARG:NH2	2.41	0.65
2:D:114:LEU:HB3	2:D:149:MET:HE1	1.78	0.65
2:D:399:PHE:O	2:D:400:ARG:O	2.14	0.65
2:B:223:THR:CB	2:B:225:GLY:H	2.04	0.64
1:A:270:ALA:HB3	1:A:302:MET:HE2	1.79	0.64
2:D:151:THR:HG21	2:D:190:SER:HB3	1.80	0.64
2:D:312:TYR:CD2	2:D:315:VAL:HG21	2.32	0.64
1:A:101:ASN:HD22	2:B:254:LYS:HG2	1.62	0.64
1:C:229:ARG:HG2	1:C:229:ARG:HH11	1.62	0.64
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.78	0.64
2:B:141:LEU:HA	2:B:147:SER:HB3	1.78	0.64
2:B:387:LEU:O	2:B:390:ARG:HG2	1.97	0.64
1:C:102:ASN:C	1:C:102:ASN:ND2	2.51	0.64
1:A:388:TRP:CE3	1:A:388:TRP:HA	2.32	0.64
2:D:251:ASP:HB2	2:D:254:LYS:HB2	1.78	0.64
1:A:145:THR:HG23	4:A:600:GTP:O2B	1.98	0.64
1:A:344:VAL:HG13	1:A:346:TRP:H	1.62	0.64
2:B:399:PHE:O	2:B:400:ARG:O	2.15	0.64
2:B:238:VAL:HG13	2:B:378:ILE:HD11	1.79	0.64
2:B:242:LEU:HD11	7:B:700:K2N:HAK	1.79	0.64
2:B:325:MET:HA	2:B:328:VAL:HB	1.80	0.64
3:E:74:GLU:C	3:E:76:ARG:H	2.01	0.64
2:B:401:ARG:NH2	1:C:434:GLU:O	2.24	0.64
2:B:384:ILE:HG22	2:B:432:TYR:CE1	2.33	0.63
3:E:22:VAL:HG13	3:E:22:VAL:O	1.98	0.63
2:B:114:LEU:HB3	2:B:149:MET:HE1	1.79	0.63
1:C:34:GLY:O	1:C:61:HIS:HB2	1.98	0.63
2:D:51:VAL:O	2:D:64:ARG:NH2	2.31	0.63
2:D:192:HIS:CD2	2:D:421:ALA:HB2	2.32	0.63
2:B:164:ARG:HE	2:B:164:ARG:HA	1.62	0.63
2:D:333:LEU:HD23	2:D:337:ASN:HD21	1.61	0.63
3:E:133:VAL:HA	3:E:136:ASN:HB3	1.81	0.63
2:D:55:GLU:HB3	2:D:61:TYR:HD2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:THR:HA	2:D:295:MET:CE	2.28	0.63
2:B:131:CYS:O	2:B:131:CYS:SG	2.56	0.62
2:D:265:LEU:HB2	2:D:432:TYR:CZ	2.32	0.62
3:E:49:GLU:O	3:E:49:GLU:HG3	1.99	0.62
3:E:112:ARG:O	3:E:115:HIS:N	2.24	0.62
1:A:278:ALA:O	1:A:279:GLU:CB	2.36	0.62
2:B:217:LEU:HD22	2:B:219:LEU:HD21	1.81	0.62
2:D:5:VAL:HG22	2:D:135:PHE:CD2	2.27	0.62
2:B:171:VAL:CG1	2:B:206:ASN:HD21	2.12	0.62
2:D:118:VAL:O	2:D:122:VAL:HG13	1.99	0.62
2:B:295:MET:O	2:B:295:MET:HG2	1.99	0.62
1:C:266:HIS:O	1:C:268:PRO:HD3	2.00	0.62
1:C:85:GLN:HA	1:C:85:GLN:HE21	1.63	0.62
2:D:261:PRO:HG3	2:D:313:LEU:CD1	2.25	0.62
2:B:51:VAL:HG13	2:B:52:TYR:HD1	1.64	0.62
1:C:99:ALA:CB	1:C:145:THR:HG22	2.29	0.62
2:D:36:TYR:OH	2:D:40:SER:O	2.13	0.62
2:D:142:GLY:O	6:D:600:GDP:H5”	2.00	0.62
2:B:12:CYS:SG	6:B:600:GDP:N3	2.72	0.62
2:B:147:SER:O	2:B:151:THR:OG1	2.16	0.62
2:D:312:TYR:HD2	2:D:315:VAL:HG23	1.64	0.62
3:E:81:GLU:O	3:E:82:VAL:C	2.38	0.62
1:A:273:ALA:CB	1:A:274:PRO:CD	2.76	0.61
2:B:7:ILE:O	2:B:137:LEU:HA	2.00	0.61
2:B:8:GLN:OE1	2:B:67:LEU:HD23	2.00	0.61
2:D:34:GLY:HA2	2:D:60:LYS:HE2	1.82	0.61
2:D:255:LEU:HG	7:D:700:K2N:NAL	2.15	0.61
3:E:60:ARG:HH11	3:E:60:ARG:HB2	1.64	0.61
2:D:51:VAL:CG1	2:D:52:TYR:HD1	2.13	0.61
1:A:34:GLY:O	1:A:61:HIS:HB2	2.01	0.60
2:B:408:TYR:O	2:B:409:THR:C	2.38	0.60
2:D:229:HIS:HE1	2:D:277:SER:HB3	1.63	0.60
2:B:162:PRO:HD2	2:B:163:ASP:HB2	1.83	0.60
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.49	0.60
2:D:10:GLY:O	2:D:14:ASN:N	2.31	0.60
2:B:51:VAL:CG1	2:B:52:TYR:HD1	2.14	0.60
2:B:295:MET:HG3	2:B:377:PHE:CB	2.27	0.60
2:D:384:ILE:HG22	2:D:432:TYR:CE1	2.36	0.60
3:E:22:VAL:O	3:E:22:VAL:CG1	2.49	0.60
1:C:20:CYS:HB3	1:C:232:GLY:HA2	1.84	0.60
2:D:101:ASN:HD22	2:D:143:GLY:HA2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:384:ILE:CG2	2:D:432:TYR:CE1	2.84	0.60
2:B:20:PHE:O	2:B:24:ILE:HG23	2.02	0.60
2:D:312:TYR:HE2	2:D:377:PHE:CZ	2.20	0.60
1:A:406:HIS:CG	2:B:263:PRO:HG3	2.36	0.59
2:B:158:ARG:O	2:B:159:GLU:HB3	2.01	0.59
1:C:401:LYS:C	1:C:403:ALA:H	2.03	0.59
2:B:135:PHE:HZ	2:B:161:TYR:CD1	2.20	0.59
2:B:209:LEU:HD21	2:B:231:VAL:HG22	1.83	0.59
1:C:79:ARG:HH21	1:C:94:THR:HG21	1.67	0.59
1:A:90:GLU:HB2	1:A:121:ARG:HD3	1.84	0.59
2:D:54:ASN:HB2	2:D:64:ARG:HD3	1.84	0.59
2:B:7:ILE:HG22	2:B:137:LEU:CD1	2.32	0.59
2:B:55:GLU:HB3	2:B:61:TYR:HD2	1.66	0.59
2:B:325:MET:HG2	2:B:355:VAL:HG21	1.84	0.59
2:D:154:ILE:HA	2:D:157:ILE:HB	1.84	0.59
1:A:187:SER:O	1:A:191:THR:HB	2.02	0.59
1:A:315:CYS:SG	1:A:377:MET:HE1	2.43	0.59
2:B:276:THR:HG23	2:B:277:SER:N	2.17	0.59
2:B:401:ARG:HH11	2:B:401:ARG:CG	2.16	0.59
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.38	0.59
2:B:242:LEU:HD11	7:B:700:K2N:CAK	2.32	0.59
2:D:164:ARG:HE	2:D:164:ARG:CA	2.13	0.59
1:A:181:VAL:H	2:B:258:ASN:ND2	2.01	0.58
1:C:256:GLN:C	1:C:258:ASN:N	2.55	0.58
1:C:404:PHE:HE1	2:D:347:ILE:CG2	2.16	0.58
3:E:84:GLN:C	3:E:86:ALA:H	2.05	0.58
1:C:169:PHE:CE2	1:C:235:VAL:HG22	2.38	0.58
2:D:159:GLU:HB2	3:E:123:LEU:HD13	1.84	0.58
2:D:295:MET:CG	2:D:377:PHE:HB2	2.26	0.58
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.68	0.58
1:C:427:ALA:O	1:C:430:LYS:HB3	2.04	0.58
2:D:274:PRO:C	2:D:275:LEU:HG	2.23	0.58
2:B:200:GLU:OE2	2:B:268:PHE:HE1	1.87	0.58
1:C:389:ALA:HA	1:C:392:ASP:HB2	1.86	0.58
3:E:74:GLU:C	3:E:76:ARG:N	2.56	0.58
2:B:164:ARG:HE	2:B:164:ARG:CA	2.15	0.58
2:D:158:ARG:O	2:D:160:GLU:N	2.27	0.58
2:D:234:THR:HG21	2:D:302:MET:HG3	1.86	0.58
2:B:245:PRO:CG	2:B:247:GLN:HE21	2.16	0.58
2:B:251:ASP:HB3	2:B:254:LYS:H	1.69	0.58
1:C:256:GLN:C	1:C:258:ASN:H	2.06	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:VAL:HG23	1:C:260:VAL:O	2.04	0.57
1:A:286:LEU:HD12	1:A:286:LEU:H	1.69	0.57
2:D:270:PRO:CD	2:D:302:MET:HB2	2.33	0.57
2:B:427:ASP:O	2:B:431:GLU:HG3	2.05	0.57
1:C:183:GLU:CB	1:C:184:PRO:CD	2.82	0.57
2:D:250:ALA:HA	2:D:255:LEU:HD13	1.85	0.57
2:D:276:THR:HG21	2:D:280:SER:HB2	1.85	0.57
1:A:315:CYS:SG	1:A:377:MET:CE	2.93	0.57
2:B:403:ALA:C	2:B:405:LEU:N	2.43	0.57
1:C:123:ARG:HD2	1:C:161:TYR:OH	2.03	0.57
1:A:117:LEU:HD11	1:A:121:ARG:NH2	2.19	0.57
1:C:343:PHE:HD1	1:C:349:THR:HG22	1.69	0.57
2:D:229:HIS:ND1	2:D:277:SER:HB3	2.17	0.57
2:D:309:HIS:CD2	2:D:309:HIS:N	2.73	0.57
2:D:5:VAL:CG2	2:D:135:PHE:HD2	2.15	0.57
2:B:274:PRO:C	2:B:275:LEU:HG	2.25	0.57
1:C:341:ILE:HD13	1:C:341:ILE:H	1.70	0.57
1:A:72:PRO:O	1:A:74:VAL:N	2.38	0.56
1:C:8:HIS:CD2	1:C:17:GLY:CA	2.88	0.56
2:D:289:PRO:HA	2:D:331:GLN:NE2	2.20	0.56
1:C:8:HIS:HD2	1:C:17:GLY:HA3	1.70	0.56
1:C:111:GLY:O	1:C:113:GLU:N	2.38	0.56
2:D:251:ASP:HB3	2:D:254:LYS:H	1.70	0.56
1:A:85:GLN:HA	1:A:85:GLN:NE2	2.20	0.56
2:B:357:ASP:OD2	2:B:357:ASP:N	2.36	0.56
1:C:70:LEU:HD12	1:C:145:THR:CB	2.29	0.56
1:A:133:GLN:HE21	1:A:252:LEU:HG	1.71	0.56
2:B:135:PHE:CZ	2:B:161:TYR:CD1	2.93	0.56
2:B:245:PRO:HG3	2:B:247:GLN:HE21	1.70	0.56
1:C:83:TYR:C	1:C:85:GLN:N	2.56	0.56
2:B:5:VAL:HG13	2:B:132:LEU:CD1	2.35	0.56
2:B:292:THR:HA	2:B:295:MET:CE	2.35	0.56
2:B:414:ASP:HB3	2:B:417:GLU:HB2	1.87	0.56
2:D:208:ALA:O	2:D:211:ASP:N	2.37	0.56
1:A:68:VAL:HG12	1:A:93:ILE:HB	1.88	0.56
1:A:102:ASN:HD21	1:A:104:ALA:HB3	1.69	0.56
2:D:298:SER:C	2:D:300:ASN:H	2.09	0.56
2:B:245:PRO:HB2	2:B:247:GLN:HG3	1.87	0.56
2:D:55:GLU:HB3	2:D:61:TYR:CD2	2.39	0.56
2:B:118:VAL:O	2:B:122:VAL:HG13	2.06	0.56
2:B:336:GLN:HA	2:B:343:PHE:HE1	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:CYS:O	1:C:377:MET:HA	2.06	0.56
2:B:34:GLY:HA2	2:B:60:LYS:HE2	1.88	0.56
2:B:251:ASP:HB2	2:B:254:LYS:HB2	1.88	0.56
1:C:406:HIS:CG	2:D:263:PRO:HG3	2.40	0.56
2:D:296:PHE:HE1	2:D:332:MET:CE	2.19	0.56
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.22	0.55
1:A:79:ARG:HH21	1:A:94:THR:HG21	1.68	0.55
2:B:2:ARG:CZ	2:B:133:GLN:HB2	2.36	0.55
2:B:6:HIS:CE1	2:B:8:GLN:HB2	2.42	0.55
2:B:88:ARG:HB3	2:B:91:ASN:OD1	2.07	0.55
2:D:2:ARG:NH1	2:D:133:GLN:HB2	2.20	0.55
2:B:110:GLU:O	2:B:113:GLU:HB3	2.07	0.55
2:D:260:VAL:HG11	2:D:266:HIS:HB3	1.87	0.55
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.20	0.55
1:C:41:THR:CG2	1:C:61:HIS:HE1	2.10	0.55
2:B:378:ILE:CD1	7:B:700:K2N:HABA	2.36	0.55
2:D:51:VAL:HG13	2:D:52:TYR:HD1	1.69	0.55
2:D:209:LEU:HD21	2:D:231:VAL:HG22	1.88	0.55
2:D:403:ALA:C	2:D:405:LEU:H	2.10	0.55
2:B:250:ALA:HA	2:B:255:LEU:HD13	1.88	0.55
1:C:177:VAL:HG13	1:C:177:VAL:O	2.07	0.55
2:D:308:ARG:NH2	2:D:339:ASN:HD21	2.00	0.55
1:A:102:ASN:C	1:A:102:ASN:ND2	2.60	0.55
1:A:247:ALA:O	1:A:248:LEU:HB3	2.06	0.55
1:C:407:TRP:CD2	2:D:257:VAL:HG22	2.42	0.55
1:C:253:THR:O	1:C:256:GLN:N	2.39	0.55
2:B:115:VAL:HG12	2:B:116:ASP:N	2.22	0.55
2:B:265:LEU:HB2	2:B:432:TYR:CE2	2.42	0.55
1:C:33:ASP:HA	1:C:85:GLN:HB3	1.89	0.55
2:D:282:GLN:O	2:D:282:GLN:HG2	2.06	0.55
2:B:2:ARG:NH1	2:B:133:GLN:HB2	2.22	0.55
1:C:88:HIS:HB3	1:C:90:GLU:OE1	2.06	0.55
1:C:133:GLN:NE2	1:C:252:LEU:HG	2.22	0.55
1:C:273:ALA:CB	1:C:274:PRO:CD	2.81	0.55
1:A:8:HIS:HD2	1:A:17:GLY:HA3	1.70	0.54
1:A:183:GLU:HB3	1:A:184:PRO:CD	2.32	0.54
1:A:404:PHE:HE1	2:B:347:ILE:HG21	1.71	0.54
2:B:30:ILE:HD11	2:B:49:ILE:HD11	1.89	0.54
2:B:55:GLU:HB3	2:B:61:TYR:CD2	2.41	0.54
2:B:70:LEU:HA	2:B:95:GLY:HA3	1.89	0.54
1:C:153:LEU:HD13	1:C:157:LEU:CD1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:THR:C	2:D:294:GLN:H	2.10	0.54
1:C:102:ASN:HD22	1:C:103:TYR:N	2.05	0.54
2:D:381:SER:O	2:D:384:ILE:HB	2.07	0.54
3:E:99:GLU:C	3:E:101:LEU:N	2.60	0.54
1:A:419:SER:O	1:A:423:GLU:HG2	2.08	0.54
2:D:192:HIS:HD2	2:D:421:ALA:HA	1.73	0.54
1:A:8:HIS:CD2	1:A:17:GLY:CA	2.90	0.54
1:C:191:THR:HG23	1:C:425:MET:CE	2.38	0.54
2:D:15:GLN:HG3	2:D:15:GLN:O	2.08	0.54
1:A:206:ASN:HD21	4:A:600:GTP:N2	1.95	0.54
2:B:171:VAL:CG1	2:B:206:ASN:ND2	2.67	0.54
2:D:115:VAL:HG12	2:D:116:ASP:N	2.22	0.54
2:B:260:VAL:HG11	2:B:266:HIS:HB3	1.89	0.54
2:B:311:ARG:HH21	2:B:344:VAL:CG2	2.18	0.54
2:D:174:SER:HB2	2:D:390:ARG:NH2	2.22	0.54
2:B:287:THR:CG2	2:B:290:GLU:HB2	2.37	0.54
3:E:60:ARG:NH1	3:E:60:ARG:HB2	2.23	0.54
1:A:88:HIS:HB2	1:A:91:GLN:NE2	2.22	0.54
2:B:306:ASP:C	2:B:308:ARG:H	2.09	0.54
1:C:100:ALA:O	1:C:102:ASN:N	2.40	0.54
2:D:70:LEU:HD11	2:D:149:MET:HG3	1.90	0.54
2:B:70:LEU:C	2:B:95:GLY:HA3	2.28	0.53
2:D:47:GLU:HB2	2:D:48:ARG:HG2	1.91	0.53
2:D:200:GLU:HA	2:D:266:HIS:HB2	1.89	0.53
1:A:191:THR:HG23	1:A:425:MET:CE	2.38	0.53
2:B:192:HIS:O	2:B:195:VAL:HG12	2.08	0.53
2:D:226:ASP:O	2:D:227:LEU:HB2	2.08	0.53
1:A:70:LEU:HD12	1:A:145:THR:CB	2.34	0.53
1:A:387:ALA:HB2	1:A:390:ARG:HH12	1.74	0.53
2:D:224:TYR:CE2	6:D:600:GDP:C4	2.96	0.53
1:C:68:VAL:HG12	1:C:93:ILE:HB	1.91	0.53
1:A:190:THR:HG23	1:A:191:THR:N	2.24	0.53
2:B:321:GLY:O	2:B:323:MET:N	2.41	0.53
2:B:321:GLY:H	2:B:357:ASP:HA	1.73	0.53
2:D:350:ASN:H	2:D:350:ASN:ND2	2.06	0.53
1:C:6:SER:HB3	1:C:8:HIS:CE1	2.44	0.53
1:A:33:ASP:HA	1:A:85:GLN:HB3	1.91	0.53
1:C:85:GLN:HA	1:C:85:GLN:NE2	2.24	0.53
1:A:133:GLN:CD	1:A:252:LEU:H	2.12	0.53
2:B:15:GLN:HG3	2:B:15:GLN:O	2.09	0.53
1:C:102:ASN:C	1:C:102:ASN:HD22	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:GLN:NE2	2:B:252:LEU:HD22	2.16	0.53
2:B:248:LEU:O	2:B:249:ASN:CB	2.55	0.53
2:B:387:LEU:CA	2:B:390:ARG:HG2	2.37	0.53
1:C:190:THR:HG23	1:C:191:THR:N	2.23	0.53
3:E:99:GLU:C	3:E:101:LEU:H	2.11	0.53
1:A:167:LEU:HD13	1:A:252:LEU:HD13	1.91	0.53
1:A:343:PHE:HD1	1:A:349:THR:HG22	1.71	0.53
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.44	0.53
1:C:80:THR:HG22	1:C:81:GLY:N	2.24	0.53
1:C:181:VAL:H	2:D:258:ASN:ND2	2.07	0.53
2:D:2:ARG:CZ	2:D:133:GLN:HB2	2.39	0.53
2:D:388:PHE:CE1	2:D:428:LEU:HD21	2.44	0.53
2:B:89:PRO:O	2:B:92:PHE:HD1	1.92	0.52
2:D:3:GLU:HG2	2:D:64:ARG:NH2	2.24	0.52
2:B:175:PRO:HD2	2:B:390:ARG:NH2	2.24	0.52
2:B:192:HIS:HD2	2:B:421:ALA:HA	1.74	0.52
1:C:125:LEU:HD23	1:C:128:GLN:NE2	2.23	0.52
2:D:133:GLN:NE2	2:D:252:LEU:HB2	2.25	0.52
1:A:278:ALA:HA	1:A:281:ALA:HB2	1.90	0.52
2:D:99:ALA:CB	2:D:145:THR:HG22	2.36	0.52
2:B:202:TYR:CD1	2:B:202:TYR:N	2.75	0.52
2:B:298:SER:C	2:B:300:ASN:N	2.63	0.52
2:B:309:HIS:CD2	2:B:309:HIS:H	2.27	0.52
2:B:336:GLN:HA	2:B:343:PHE:CE1	2.45	0.52
1:A:83:TYR:C	1:A:85:GLN:N	2.61	0.52
1:C:265:ILE:H	1:C:265:ILE:CD1	2.17	0.52
1:C:291:ILE:HD12	1:C:375:VAL:CG2	2.38	0.52
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.28	0.52
3:E:78:HIS:C	3:E:78:HIS:CD2	2.82	0.52
2:B:3:GLU:HG2	2:B:64:ARG:NH2	2.23	0.52
2:B:318:VAL:HA	2:B:354:ALA:O	2.09	0.52
3:E:67:GLU:C	3:E:69:LEU:H	2.13	0.52
1:A:119:LEU:HD22	1:A:156:ARG:NH2	2.25	0.52
1:C:6:SER:HB3	1:C:8:HIS:HE1	1.73	0.52
1:C:36:MET:SD	1:C:38:SER:HB2	2.49	0.52
1:C:115:ILE:HD11	1:C:119:LEU:HD13	1.91	0.52
2:D:284:ARG:HH11	2:D:284:ARG:HB2	1.72	0.52
1:A:88:HIS:CD2	1:A:90:GLU:OE1	2.63	0.52
1:C:48:SER:O	1:C:243:ARG:O	2.28	0.52
2:B:133:GLN:NE2	2:B:252:LEU:HB2	2.25	0.51
2:D:264:ARG:O	2:D:265:LEU:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.45	0.51
2:B:237:GLY:CA	2:B:376:THR:HG21	2.40	0.51
2:D:8:GLN:OE1	2:D:67:LEU:HD23	2.11	0.51
2:D:12:CYS:SG	6:D:600:GDP:N3	2.83	0.51
2:D:200:GLU:OE2	2:D:268:PHE:CE1	2.58	0.51
2:D:383:ALA:O	2:D:386:GLU:CB	2.58	0.51
2:D:389:LYS:O	2:D:393:GLU:HB3	2.09	0.51
1:A:401:LYS:C	1:A:403:ALA:N	2.56	0.51
2:D:48:ARG:HB2	2:D:243:ARG:C	2.31	0.51
1:A:317:LEU:CD2	1:A:377:MET:HE3	2.40	0.51
2:B:103:TRP:HB2	2:B:186:ASN:OD1	2.11	0.51
2:B:138:THR:O	2:B:139:HIS:HB3	2.11	0.51
2:B:296:PHE:HE1	2:B:332:MET:CE	2.24	0.51
2:B:401:ARG:O	1:C:262:TYR:OH	2.26	0.51
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.31	0.51
2:B:31:ASP:O	2:B:33:THR:N	2.44	0.51
2:B:311:ARG:NH2	2:B:344:VAL:HG22	2.23	0.51
2:D:384:ILE:CG2	2:D:432:TYR:HE1	2.23	0.51
1:A:275:VAL:O	1:A:275:VAL:HG23	2.11	0.51
2:D:2:ARG:HH12	2:D:133:GLN:HA	1.75	0.51
2:D:265:LEU:CB	2:D:432:TYR:CZ	2.93	0.51
2:D:283:TYR:C	2:D:285:ALA:H	2.13	0.51
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.75	0.51
1:A:383:ALA:O	1:A:386:GLU:HB2	2.11	0.51
2:B:162:PRO:CD	2:B:163:ASP:HB2	2.40	0.51
1:C:315:CYS:SG	1:C:377:MET:HE1	2.51	0.51
2:D:313:LEU:HD13	2:D:347:ILE:HD11	1.93	0.51
3:E:123:LEU:C	3:E:125:GLU:N	2.62	0.51
2:B:208:ALA:O	2:B:211:ASP:N	2.43	0.50
2:D:140:SER:CB	6:D:600:GDP:C5'	2.88	0.50
3:E:109:LYS:O	3:E:113:GLU:HB2	2.10	0.50
2:B:325:MET:CA	2:B:328:VAL:HB	2.41	0.50
2:D:312:TYR:CD2	2:D:315:VAL:HG23	2.41	0.50
1:A:20:CYS:HB3	1:A:232:GLY:HA2	1.91	0.50
2:B:99:ALA:CB	2:B:145:THR:HG22	2.33	0.50
2:D:99:ALA:CB	2:D:145:THR:CG2	2.81	0.50
2:D:245:PRO:HB2	2:D:247:GLN:HG3	1.92	0.50
1:A:291:ILE:HD12	1:A:375:VAL:CG2	2.42	0.50
1:C:78:VAL:C	1:C:80:THR:H	2.14	0.50
2:D:153:LEU:O	2:D:157:ILE:N	2.42	0.50
2:D:103:TRP:HB2	2:D:186:ASN:OD1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:276:THR:CG2	2:D:277:SER:N	2.74	0.50
1:A:169:PHE:CE2	1:A:235:VAL:HG22	2.47	0.50
2:B:159:GLU:HB2	3:E:72:LEU:HD23	1.93	0.50
1:C:309:HIS:ND1	1:C:310:GLY:N	2.60	0.50
1:C:402:ARG:O	1:C:403:ALA:C	2.50	0.50
1:A:55:GLU:HG2	1:A:61:HIS:CE1	2.47	0.50
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.30	0.50
2:D:265:LEU:HB2	2:D:432:TYR:OH	2.12	0.50
2:D:262:PHE:CE1	2:D:435:TYR:CZ	3.00	0.50
1:A:102:ASN:HD22	1:A:103:TYR:N	2.10	0.49
1:A:389:ALA:HA	1:A:392:ASP:HB2	1.92	0.49
2:B:407:TRP:NE1	1:C:257:THR:HA	2.27	0.49
1:C:401:LYS:C	1:C:403:ALA:N	2.66	0.49
2:D:176:LYS:HD2	2:D:207:GLU:OE2	2.12	0.49
2:D:265:LEU:HB2	2:D:432:TYR:HE2	1.72	0.49
1:A:401:LYS:O	1:A:403:ALA:N	2.45	0.49
2:D:70:LEU:HA	2:D:95:GLY:HA3	1.93	0.49
2:D:284:ARG:HD3	2:D:372:LYS:NZ	2.27	0.49
2:D:384:ILE:HG21	2:D:432:TYR:HE1	1.77	0.49
3:E:81:GLU:O	3:E:84:GLN:N	2.45	0.49
2:B:51:VAL:O	2:B:64:ARG:NH2	2.44	0.49
1:C:90:GLU:HB3	1:C:121:ARG:HD3	1.94	0.49
1:A:125:LEU:HD23	1:A:128:GLN:NE2	2.27	0.49
1:A:395:PHE:C	1:A:395:PHE:CD2	2.86	0.49
2:B:226:ASP:O	2:B:227:LEU:HB2	2.12	0.49
2:D:5:VAL:HG13	2:D:132:LEU:CD1	2.43	0.49
3:E:56:ALA:HA	3:E:59:GLU:HB2	1.95	0.49
3:E:123:LEU:O	3:E:125:GLU:N	2.46	0.49
1:A:260:VAL:O	1:A:260:VAL:HG23	2.13	0.49
1:C:26:LEU:HD21	1:C:364:PRO:HD3	1.93	0.49
1:A:26:LEU:HD21	1:A:364:PRO:HD3	1.94	0.49
1:C:395:PHE:C	1:C:395:PHE:CD2	2.85	0.49
1:C:420:GLU:HA	1:C:423:GLU:HG3	1.93	0.49
2:D:158:ARG:C	2:D:160:GLU:H	2.13	0.49
3:E:81:GLU:O	3:E:85:LYS:N	2.40	0.49
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.45	0.49
1:C:200:CYS:HA	1:C:266:HIS:HB3	1.95	0.49
1:C:419:SER:O	1:C:423:GLU:HG2	2.12	0.49
2:B:2:ARG:HH12	2:B:133:GLN:HA	1.78	0.49
2:B:36:TYR:OH	2:B:40:SER:O	2.24	0.49
1:C:291:ILE:HD12	1:C:375:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:VAL:HG22	2:D:377:PHE:HE1	1.77	0.49
2:D:328:VAL:O	2:D:332:MET:HB2	2.12	0.49
2:D:384:ILE:HG21	2:D:432:TYR:CE1	2.48	0.49
1:C:123:ARG:NH1	1:C:161:TYR:HE2	2.11	0.49
2:D:30:ILE:HD11	2:D:49:ILE:HD11	1.95	0.49
1:C:154:MET:O	1:C:158:SER:HB2	2.13	0.49
2:D:226:ASP:O	2:D:227:LEU:CB	2.60	0.49
1:A:405:VAL:CG1	1:A:406:HIS:N	2.76	0.48
2:B:318:VAL:HG22	2:B:318:VAL:O	2.12	0.48
1:A:204:VAL:HG22	1:A:302:MET:HE3	1.94	0.48
1:C:372:GLN:HB2	1:C:373:ARG:HE	1.78	0.48
1:C:229:ARG:HD3	1:C:363:VAL:HG21	1.95	0.48
2:D:192:HIS:HD2	2:D:421:ALA:CA	2.26	0.48
2:B:51:VAL:CG1	2:B:52:TYR:N	2.75	0.48
2:D:276:THR:HG21	2:D:280:SER:HB3	1.95	0.48
2:D:6:HIS:CE1	2:D:8:GLN:HB2	2.49	0.48
2:D:276:THR:HG22	2:D:277:SER:N	2.28	0.48
2:D:200:GLU:HB3	2:D:268:PHE:HE1	1.73	0.48
2:D:255:LEU:HD11	7:D:700:K2N:HAH	1.95	0.48
1:A:244:PHE:CZ	1:A:358:GLN:HG2	2.49	0.48
2:B:316:ALA:HB1	7:B:700:K2N:CAI	2.43	0.48
2:B:391:ILE:HG13	2:B:392:SER:N	2.29	0.48
2:D:20:PHE:O	2:D:24:ILE:HG23	2.14	0.48
2:D:51:VAL:CG1	2:D:52:TYR:N	2.77	0.48
2:D:250:ALA:O	2:D:252:LEU:N	2.46	0.48
2:B:200:GLU:HA	2:B:266:HIS:HB2	1.94	0.48
2:B:224:TYR:OH	6:B:600:GDP:H2'	2.14	0.48
2:B:355:VAL:HG23	2:B:355:VAL:O	2.14	0.48
2:B:70:LEU:HD11	2:B:149:MET:HG3	1.95	0.48
2:B:171:VAL:HG11	2:B:206:ASN:HD21	1.78	0.48
2:D:210:TYR:CE2	2:D:222:PRO:HG2	2.49	0.48
1:A:100:ALA:O	1:A:102:ASN:N	2.46	0.48
2:D:52:TYR:OH	2:D:239:THR:CG2	2.62	0.48
1:A:105:ARG:HD3	1:A:411:GLU:OE1	2.13	0.47
2:B:210:TYR:CE2	2:B:222:PRO:HG2	2.49	0.47
1:C:101:ASN:ND2	2:D:254:LYS:HG2	2.26	0.47
3:E:76:ARG:O	3:E:79:GLU:N	2.47	0.47
1:A:372:GLN:HB2	1:A:373:ARG:HE	1.79	0.47
2:B:47:GLU:HB2	2:B:48:ARG:HG2	1.96	0.47
1:C:105:ARG:HD3	1:C:411:GLU:OE1	2.14	0.47
1:C:183:GLU:CB	1:C:184:PRO:HD3	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:MET:O	2:D:329:ASP:OD2	2.32	0.47
1:A:133:GLN:NE2	1:A:252:LEU:HG	2.29	0.47
2:D:202:TYR:HE2	2:D:378:ILE:HG12	1.79	0.47
1:A:98:ASP:OD1	1:A:99:ALA:N	2.47	0.47
1:C:383:ALA:O	1:C:386:GLU:HB2	2.15	0.47
3:E:72:LEU:C	3:E:74:GLU:N	2.66	0.47
3:E:101:LEU:C	3:E:103:GLN:H	2.17	0.47
1:A:115:ILE:HG13	1:A:152:LEU:HD23	1.96	0.47
1:C:204:VAL:HG22	1:C:302:MET:HE3	1.96	0.47
2:D:307:PRO:HB2	2:D:312:TYR:CZ	2.50	0.47
1:A:183:GLU:CB	1:A:184:PRO:HD3	2.38	0.47
1:A:420:GLU:HA	1:A:423:GLU:HG3	1.97	0.47
2:B:154:ILE:HA	2:B:157:ILE:HB	1.97	0.47
2:B:298:SER:O	2:B:300:ASN:N	2.45	0.47
1:C:204:VAL:HG22	1:C:302:MET:CE	2.44	0.47
4:C:600:GTP:O3G	2:D:254:LYS:NZ	2.48	0.47
2:D:2:ARG:HD2	2:D:131:CYS:SG	2.54	0.47
2:D:21:TRP:CH2	2:D:63:PRO:HB3	2.50	0.47
2:D:163:ASP:HB3	2:D:164:ARG:HG2	1.96	0.47
2:D:236:SER:O	2:D:240:THR:HG23	2.15	0.47
3:E:76:ARG:O	3:E:79:GLU:CB	2.63	0.47
3:E:112:ARG:HG2	3:E:113:GLU:N	2.21	0.47
1:A:22:GLU:HB2	1:A:83:TYR:HE1	1.80	0.47
1:A:80:THR:HG22	1:A:81:GLY:N	2.28	0.47
2:B:20:PHE:HD2	2:B:235:MET:HB3	1.78	0.47
2:B:296:PHE:HE1	2:B:332:MET:HE3	1.80	0.47
2:B:399:PHE:O	2:B:400:ARG:C	2.52	0.47
2:D:14:ASN:HD21	2:D:67:LEU:HB3	1.80	0.47
1:A:72:PRO:HB2	1:A:76:ASP:OD2	2.14	0.47
2:D:389:LYS:O	2:D:393:GLU:CB	2.63	0.47
3:E:11:LEU:O	3:E:12:ASN:CB	2.62	0.47
2:B:154:ILE:HG13	2:B:155:SER:N	2.30	0.47
1:C:178:SER:OG	1:C:183:GLU:OE2	2.30	0.47
2:D:202:TYR:OH	7:D:700:K2N:CAU	2.63	0.47
2:D:282:GLN:HE21	2:D:286:LEU:HD11	1.80	0.47
1:A:111:GLY:O	1:A:113:GLU:N	2.48	0.46
1:A:294:ALA:O	1:A:297:GLU:HB3	2.15	0.46
1:A:309:HIS:ND1	1:A:310:GLY:N	2.63	0.46
2:B:62:VAL:HG22	2:B:62:VAL:O	2.15	0.46
2:B:253:ARG:O	2:B:254:LYS:C	2.52	0.46
2:D:151:THR:HA	2:D:154:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:408:TYR:N	2:D:408:TYR:CD1	2.82	0.46
1:A:79:ARG:HD3	1:A:92:LEU:HD13	1.96	0.46
1:A:119:LEU:HD22	1:A:156:ARG:HH21	1.78	0.46
1:A:171:ILE:O	1:A:171:ILE:HG22	2.15	0.46
2:B:224:TYR:CE2	6:B:600:GDP:C4	3.03	0.46
2:B:292:THR:HA	2:B:295:MET:HE3	1.97	0.46
2:B:407:TRP:CE2	1:C:257:THR:HA	2.51	0.46
1:C:405:VAL:CG1	1:C:406:HIS:N	2.77	0.46
2:D:125:GLU:O	2:D:129:CYS:HB2	2.15	0.46
2:D:238:VAL:HG12	7:D:700:K2N:CAJ	2.44	0.46
3:E:76:ARG:O	3:E:79:GLU:HB2	2.15	0.46
1:A:277:SER:O	1:A:280:LYS:HB2	2.15	0.46
1:A:317:LEU:HD21	1:A:377:MET:HE3	1.97	0.46
1:C:111:GLY:O	1:C:112:LYS:C	2.52	0.46
2:B:48:ARG:HB2	2:B:243:ARG:C	2.35	0.46
1:A:408:TYR:C	1:A:410:GLY:N	2.67	0.46
2:D:238:VAL:CG1	7:D:700:K2N:CAJ	2.93	0.46
2:B:313:LEU:HB2	2:B:380:ASN:O	2.16	0.46
2:B:385:GLN:HB2	2:B:432:TYR:HB3	1.96	0.46
2:D:52:TYR:OH	2:D:239:THR:HG22	2.15	0.46
1:A:316:CYS:O	1:A:377:MET:HA	2.16	0.46
1:C:72:PRO:O	1:C:74:VAL:N	2.48	0.46
1:C:115:ILE:CD1	1:C:119:LEU:HD13	2.45	0.46
2:D:177:VAL:HG12	2:D:177:VAL:O	2.15	0.46
2:D:298:SER:HA	2:D:301:MET:HG2	1.96	0.46
1:C:27:GLU:OE2	1:C:243:ARG:NH2	2.48	0.46
1:C:372:GLN:H	1:C:372:GLN:HG2	1.45	0.46
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.50	0.46
2:D:202:TYR:CD1	2:D:202:TYR:N	2.84	0.46
2:D:402:LYS:HB3	2:D:405:LEU:HD22	1.98	0.46
1:A:204:VAL:HG22	1:A:302:MET:CE	2.46	0.46
2:B:209:LEU:HD12	2:B:209:LEU:HA	1.86	0.46
2:B:395:PHE:C	2:B:395:PHE:CD2	2.89	0.46
1:C:167:LEU:HD13	1:C:252:LEU:HD13	1.97	0.46
2:D:16:ILE:HG23	2:D:235:MET:CE	2.45	0.46
2:D:298:SER:C	2:D:300:ASN:N	2.68	0.46
2:B:236:SER:O	2:B:240:THR:HG23	2.16	0.46
2:D:122:VAL:CG2	2:D:123:ARG:N	2.79	0.46
2:D:287:THR:OG1	2:D:289:PRO:HD2	2.16	0.46
2:D:292:THR:HA	2:D:295:MET:HE1	1.98	0.46
1:A:73:THR:O	1:A:76:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:O	1:A:199:ASP:HB2	2.16	0.45
2:B:412:GLY:HA3	3:E:86:ALA:HB2	1.98	0.45
1:C:266:HIS:O	1:C:268:PRO:CD	2.64	0.45
2:D:412:GLY:O	3:E:133:VAL:HB	2.15	0.45
1:A:402:ARG:HD3	1:A:402:ARG:HA	1.73	0.45
2:B:31:ASP:C	2:B:33:THR:N	2.68	0.45
1:C:224:TYR:CD2	4:C:600:GTP:C6	3.04	0.45
2:D:419:THR:HA	2:D:422:GLU:HB3	1.98	0.45
1:A:88:HIS:HB3	1:A:90:GLU:OE1	2.17	0.45
1:C:185:TYR:OH	1:C:403:ALA:HB3	2.16	0.45
1:C:315:CYS:HG	1:C:351:PHE:HE2	1.65	0.45
2:D:89:PRO:O	2:D:92:PHE:HD1	2.00	0.45
2:D:336:GLN:O	2:D:340:SER:HA	2.16	0.45
2:B:149:MET:O	2:B:152:LEU:HB3	2.16	0.45
2:D:7:ILE:O	2:D:137:LEU:HA	2.17	0.45
2:D:26:ASP:O	2:D:29:GLY:N	2.50	0.45
2:D:248:LEU:HD23	2:D:248:LEU:HA	1.56	0.45
2:D:256:ALA:O	2:D:257:VAL:C	2.55	0.45
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.75	0.45
1:A:372:GLN:H	1:A:372:GLN:HG2	1.38	0.45
2:B:265:LEU:CB	2:B:432:TYR:CE2	2.99	0.45
2:B:399:PHE:HE1	2:B:418:PHE:HB2	1.81	0.45
1:C:187:SER:HB2	1:C:391:LEU:HD21	1.98	0.45
1:C:196:GLU:H	1:C:196:GLU:HG3	1.64	0.45
2:D:296:PHE:HE1	2:D:332:MET:HE1	1.80	0.45
2:B:292:THR:C	2:B:294:GLN:H	2.19	0.45
2:D:4:ILE:HG23	2:D:51:VAL:HG22	1.99	0.45
3:E:84:GLN:C	3:E:86:ALA:N	2.70	0.45
1:A:82:THR:O	1:A:83:TYR:CG	2.70	0.45
1:A:351:PHE:HB2	3:E:22:VAL:HG12	1.98	0.45
2:B:317:ALA:HB3	2:B:353:THR:HG22	1.99	0.45
2:B:336:GLN:NE2	2:B:351:VAL:HG13	2.31	0.45
1:C:190:THR:HG23	1:C:191:THR:H	1.82	0.45
1:C:190:THR:O	1:C:194:THR:HB	2.16	0.45
2:D:195:VAL:HG21	2:D:428:LEU:HD22	1.99	0.45
1:A:79:ARG:H	1:A:79:ARG:HG2	1.59	0.45
1:A:102:ASN:ND2	1:A:104:ALA:N	2.65	0.45
1:A:266:HIS:O	1:A:268:PRO:CD	2.63	0.45
2:B:145:THR:O	2:B:149:MET:HB2	2.17	0.45
2:D:55:GLU:H	2:D:55:GLU:HG3	1.52	0.45
2:D:231:VAL:O	2:D:235:MET:HE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:402:LYS:HB2	2:D:402:LYS:HE2	1.66	0.45
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.98	0.45
1:A:344:VAL:HG22	1:A:345:ASP:H	1.82	0.45
1:C:90:GLU:O	1:C:121:ARG:HD2	2.16	0.45
1:C:108:TYR:HB3	3:E:108:ASN:OD1	2.16	0.45
2:D:177:VAL:O	2:D:177:VAL:CG1	2.64	0.45
2:B:118:VAL:O	2:B:119:LEU:C	2.55	0.44
2:B:176:LYS:HD2	2:B:207:GLU:OE2	2.17	0.44
2:B:432:TYR:HD2	2:B:432:TYR:HA	1.65	0.44
2:D:42:LEU:O	2:D:43:GLN:C	2.55	0.44
2:D:385:GLN:HE21	2:D:389:LYS:HD2	1.82	0.44
2:B:172:MET:HG2	2:B:387:LEU:HD21	1.99	0.44
2:B:194:LEU:O	2:B:196:GLU:N	2.51	0.44
2:B:203:SER:O	2:B:270:PRO:HD3	2.17	0.44
2:B:261:PRO:HG3	2:B:313:LEU:HD12	1.98	0.44
1:C:298:PRO:O	1:C:301:GLN:HB2	2.17	0.44
2:D:145:THR:O	2:D:149:MET:HB2	2.16	0.44
1:A:404:PHE:HE1	2:B:347:ILE:CG2	2.31	0.44
2:B:252:LEU:HD13	7:B:700:K2N:H19	1.99	0.44
1:C:98:ASP:OD1	1:C:99:ALA:N	2.49	0.44
2:D:110:GLU:O	2:D:113:GLU:HB3	2.17	0.44
2:D:226:ASP:OD1	2:D:226:ASP:N	2.51	0.44
2:D:384:ILE:HG22	2:D:432:TYR:CD1	2.51	0.44
2:D:391:ILE:CG1	2:D:392:SER:N	2.76	0.44
1:A:177:VAL:O	1:A:177:VAL:HG13	2.16	0.44
1:C:22:GLU:HB2	1:C:83:TYR:HE1	1.82	0.44
1:C:223:THR:N	1:C:226:ASN:HB2	2.32	0.44
2:B:7:ILE:CG2	2:B:137:LEU:HD13	2.47	0.44
2:B:102:ASN:O	2:B:102:ASN:OD1	2.36	0.44
2:B:309:HIS:CD2	2:B:386:GLU:OE2	2.71	0.44
1:C:428:LEU:C	1:C:430:LYS:N	2.71	0.44
2:D:111:GLY:HA2	2:D:149:MET:HE2	2.00	0.44
2:D:164:ARG:CA	2:D:164:ARG:NE	2.80	0.44
2:D:248:LEU:HD11	7:D:700:K2N:CAF	2.47	0.44
2:D:296:PHE:HE1	2:D:332:MET:HE3	1.82	0.44
1:A:175:PRO:HG2	1:A:176:GLN:NE2	2.32	0.44
1:A:190:THR:HG23	1:A:191:THR:H	1.82	0.44
1:A:224:TYR:CE2	4:A:600:GTP:C4	3.05	0.44
1:C:163:LYS:O	1:C:164:LYS:C	2.56	0.44
2:D:406:HIS:HA	2:D:409:THR:HB	1.97	0.44
3:E:111:ASN:HD22	3:E:111:ASN:HA	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:O	1:A:104:ALA:C	2.56	0.44
2:B:42:LEU:O	2:B:43:GLN:C	2.55	0.44
2:B:163:ASP:HB3	2:B:164:ARG:HG2	1.98	0.44
2:B:200:GLU:HB3	2:B:268:PHE:HE1	1.77	0.44
2:D:203:SER:O	2:D:270:PRO:HD3	2.18	0.44
3:E:74:GLU:O	3:E:76:ARG:N	2.50	0.44
1:A:100:ALA:O	1:A:101:ASN:C	2.56	0.44
1:C:83:TYR:C	1:C:85:GLN:H	2.21	0.44
1:C:317:LEU:CD2	1:C:377:MET:HE3	2.48	0.44
1:A:407:TRP:CD2	2:B:257:VAL:HG22	2.52	0.44
2:B:158:ARG:O	2:B:160:GLU:N	2.47	0.44
1:A:315:CYS:SG	1:A:377:MET:HE2	2.58	0.43
1:A:356:ASN:HD22	1:A:358:GLN:H	1.65	0.43
2:B:103:TRP:N	2:B:186:ASN:OD1	2.51	0.43
1:C:297:GLU:HA	1:C:298:PRO:HD2	1.76	0.43
2:D:273:ALA:HB2	2:D:375:ALA:N	2.24	0.43
2:D:308:ARG:HA	2:D:308:ARG:HD2	1.64	0.43
2:D:311:ARG:NH2	2:D:344:VAL:CG2	2.75	0.43
3:E:76:ARG:HA	3:E:76:ARG:HD3	1.46	0.43
1:A:265:ILE:HD12	1:A:265:ILE:N	2.26	0.43
2:B:217:LEU:HD13	2:B:219:LEU:HD11	2.00	0.43
2:B:270:PRO:CD	2:B:302:MET:HB2	2.37	0.43
1:C:143:GLY:HA3	4:C:600:GTP:H5'	1.98	0.43
1:C:168:GLU:HG2	1:C:201:ALA:HB1	1.99	0.43
2:D:13:GLY:CA	2:D:139:HIS:HA	2.48	0.43
2:D:62:VAL:HA	2:D:63:PRO:HD2	1.74	0.43
2:D:192:HIS:O	2:D:195:VAL:HG12	2.19	0.43
2:B:292:THR:HG23	2:B:295:MET:HE1	2.00	0.43
1:C:190:THR:CG2	1:C:191:THR:N	2.82	0.43
2:D:255:LEU:HG	7:D:700:K2N:CAW	2.48	0.43
2:D:307:PRO:HB2	2:D:312:TYR:CE1	2.52	0.43
2:D:358:ILE:HG23	2:D:358:ILE:O	2.19	0.43
2:D:387:LEU:O	2:D:390:ARG:CG	2.35	0.43
7:D:700:K2N:OAD	7:D:700:K2N:CAA	2.62	0.43
1:A:185:TYR:OH	1:A:403:ALA:HB3	2.18	0.43
2:B:70:LEU:CA	2:B:95:GLY:HA3	2.48	0.43
2:B:151:THR:CG2	2:B:190:SER:HB3	2.45	0.43
1:C:103:TYR:O	1:C:104:ALA:C	2.54	0.43
1:C:175:PRO:HG2	1:C:176:GLN:NE2	2.33	0.43
1:C:267:PHE:CD1	1:C:267:PHE:N	2.86	0.43
2:D:158:ARG:O	2:D:159:GLU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:HE	1:A:84:ARG:HB3	1.74	0.43
1:A:317:LEU:HA	1:A:317:LEU:HD23	1.87	0.43
2:B:102:ASN:OD1	2:B:102:ASN:C	2.56	0.43
2:B:136:GLN:HA	2:B:167:ASN:O	2.19	0.43
1:C:141:PHE:O	1:C:147:SER:HB3	2.17	0.43
1:C:191:THR:HG23	1:C:425:MET:HE1	2.00	0.43
2:D:202:TYR:OH	7:D:700:K2N:NAM	2.52	0.43
2:D:295:MET:HG3	2:D:377:PHE:CB	2.33	0.43
1:A:83:TYR:C	1:A:85:GLN:H	2.21	0.43
1:C:223:THR:HG22	1:C:224:TYR:H	1.84	0.43
2:D:110:GLU:H	2:D:110:GLU:HG2	1.66	0.43
2:D:231:VAL:HG12	2:D:235:MET:CE	2.49	0.43
2:D:384:ILE:HD13	2:D:384:ILE:HA	1.85	0.43
1:A:31:GLN:O	1:A:32:PRO:C	2.56	0.43
1:A:217:LEU:HB3	1:A:219:ILE:HG12	2.01	0.43
2:B:387:LEU:O	2:B:390:ARG:CG	2.66	0.43
1:C:125:LEU:CD2	1:C:128:GLN:NE2	2.81	0.43
2:D:192:HIS:CD2	2:D:421:ALA:HB1	2.52	0.43
1:A:31:GLN:HA	1:A:32:PRO:HD2	1.82	0.43
1:A:83:TYR:O	1:A:85:GLN:N	2.51	0.43
1:A:428:LEU:C	1:A:430:LYS:N	2.72	0.43
2:B:234:THR:HG21	2:B:302:MET:HG3	1.99	0.43
2:B:248:LEU:HA	2:B:248:LEU:HD23	1.39	0.43
1:C:83:TYR:O	1:C:84:ARG:C	2.57	0.43
2:D:268:PHE:CD2	2:D:268:PHE:N	2.83	0.43
2:D:385:GLN:HE21	2:D:389:LYS:CD	2.31	0.43
2:B:10:GLY:O	2:B:14:ASN:N	2.37	0.43
1:C:8:HIS:HD2	1:C:17:GLY:CA	2.30	0.43
1:C:190:THR:CG2	1:C:191:THR:H	2.31	0.43
1:C:317:LEU:HD23	1:C:377:MET:HE3	2.00	0.43
2:D:62:VAL:O	2:D:62:VAL:HG22	2.17	0.43
2:D:88:ARG:HB3	2:D:91:ASN:OD1	2.19	0.43
2:D:154:ILE:HD12	2:D:197:ASN:HB2	2.01	0.43
2:D:175:PRO:HD2	2:D:390:ARG:NH2	2.33	0.43
2:D:251:ASP:HB2	2:D:254:LYS:HD3	2.01	0.43
1:A:49:PHE:C	1:A:49:PHE:CD2	2.93	0.43
1:A:88:HIS:O	1:A:89:PRO:C	2.56	0.43
1:A:388:TRP:O	1:A:392:ASP:CG	2.57	0.43
2:D:8:GLN:OE1	2:D:14:ASN:ND2	2.52	0.43
2:D:12:CYS:HB3	2:D:140:SER:HB3	2.01	0.43
1:A:3:GLU:HG2	1:A:129:CYS:SG	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:H	1:A:265:ILE:CD1	2.24	0.42
2:D:158:ARG:C	2:D:160:GLU:N	2.71	0.42
2:D:224:TYR:CD2	6:D:600:GDP:C5	3.06	0.42
1:A:405:VAL:HG13	1:A:406:HIS:N	2.34	0.42
2:B:55:GLU:H	2:B:55:GLU:HG3	1.53	0.42
2:D:305:CYS:HB3	2:D:383:ALA:O	2.19	0.42
3:E:112:ARG:O	3:E:114:ALA:N	2.51	0.42
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.88	0.42
2:D:31:ASP:C	2:D:33:THR:N	2.72	0.42
2:B:13:GLY:CA	2:B:139:HIS:HA	2.49	0.42
1:C:242:LEU:H	1:C:242:LEU:HG	1.67	0.42
1:C:286:LEU:H	1:C:286:LEU:HD12	1.84	0.42
2:D:138:THR:O	2:D:139:HIS:HB3	2.20	0.42
2:D:296:PHE:CE1	2:D:332:MET:CE	3.01	0.42
2:D:303:ALA:HB1	2:D:387:LEU:HD13	2.01	0.42
6:D:600:GDP:O2B	6:D:600:GDP:O1A	2.37	0.42
1:A:79:ARG:HH22	1:A:94:THR:CG2	2.30	0.42
1:A:223:THR:N	1:A:226:ASN:HB2	2.34	0.42
1:A:298:PRO:O	1:A:301:GLN:HB2	2.18	0.42
2:B:61:TYR:HD2	2:B:61:TYR:HA	1.75	0.42
2:D:70:LEU:C	2:D:95:GLY:HA3	2.40	0.42
2:B:14:ASN:HD21	2:B:67:LEU:HB3	1.85	0.42
2:B:388:PHE:CE1	2:B:428:LEU:HD21	2.55	0.42
1:C:102:ASN:HD21	1:C:104:ALA:CB	2.32	0.42
2:D:253:ARG:O	2:D:254:LYS:C	2.58	0.42
2:D:306:ASP:C	2:D:308:ARG:N	2.69	0.42
3:E:124:GLN:HA	3:E:127:ASP:HB2	2.02	0.42
1:A:2:ARG:HA	1:A:2:ARG:NH1	2.34	0.42
1:A:88:HIS:O	1:A:91:GLN:N	2.48	0.42
2:B:288:VAL:HB	2:B:289:PRO:HD3	2.01	0.42
1:C:190:THR:O	1:C:192:HIS:N	2.53	0.42
1:C:239:THR:OG1	1:C:243:ARG:NH1	2.53	0.42
2:D:137:LEU:HD21	2:D:139:HIS:CE1	2.55	0.42
2:D:224:TYR:CE2	6:D:600:GDP:C5	3.07	0.42
2:D:51:VAL:CG1	2:D:52:TYR:CD1	2.94	0.42
2:D:209:LEU:HD12	2:D:209:LEU:HA	1.70	0.42
1:A:101:ASN:ND2	2:B:254:LYS:HG2	2.30	0.42
1:A:190:THR:O	1:A:192:HIS:N	2.53	0.42
2:B:16:ILE:HG22	2:B:17:GLY:N	2.35	0.42
2:B:387:LEU:HD23	2:B:388:PHE:CD2	2.55	0.42
1:C:123:ARG:HH11	1:C:161:TYR:HE2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:SER:HB3	1:A:8:HIS:HE1	1.85	0.42
2:B:308:ARG:NH1	2:B:308:ARG:CG	2.76	0.42
2:D:47:GLU:OE2	2:D:47:GLU:HA	2.20	0.42
2:D:288:VAL:HB	2:D:289:PRO:HD3	2.02	0.42
2:D:317:ALA:HB3	2:D:353:THR:HG22	2.02	0.42
2:D:408:TYR:O	2:D:413:MET:HB2	2.20	0.42
1:A:142:GLY:HA3	1:A:183:GLU:HG3	2.01	0.41
1:A:189:LEU:HA	1:A:189:LEU:HD23	1.88	0.41
1:A:375:VAL:HG12	1:A:376:CYS:H	1.85	0.41
2:D:31:ASP:O	2:D:33:THR:N	2.53	0.41
2:D:168:THR:OG1	2:D:170:SER:OG	2.31	0.41
2:D:255:LEU:CD1	7:D:700:K2N:HAH	2.50	0.41
1:A:87:PHE:N	1:A:87:PHE:CD2	2.88	0.41
1:A:249:ASN:ND2	1:A:254:GLU:HG2	2.19	0.41
2:B:387:LEU:C	2:B:390:ARG:HG2	2.40	0.41
2:D:291:LEU:HD21	2:D:375:ALA:HB2	2.02	0.41
1:A:102:ASN:HD21	1:A:104:ALA:CB	2.34	0.41
1:A:109:THR:HG23	3:E:61:ARG:NH1	2.34	0.41
1:A:262:TYR:HB2	1:A:265:ILE:HD13	2.02	0.41
2:D:114:LEU:HD12	2:D:117:SER:HB2	2.01	0.41
1:A:202:PHE:CE2	1:A:268:PRO:HG2	2.56	0.41
2:B:62:VAL:HA	2:B:63:PRO:HD2	1.80	0.41
2:D:292:THR:O	2:D:294:GLN:N	2.49	0.41
2:B:295:MET:HE2	2:B:295:MET:HB3	1.90	0.41
3:E:48:GLU:C	3:E:50:ILE:H	2.22	0.41
2:B:224:TYR:CD2	6:B:600:GDP:C5	3.09	0.41
2:B:287:THR:O	2:B:288:VAL:HG23	2.20	0.41
2:B:296:PHE:CE1	2:B:332:MET:CE	3.03	0.41
2:B:384:ILE:HG22	2:B:432:TYR:HE1	1.83	0.41
2:B:402:LYS:HE3	2:B:415:GLU:OE2	2.20	0.41
1:C:49:PHE:C	1:C:49:PHE:CD2	2.94	0.41
1:C:79:ARG:HH22	1:C:94:THR:CG2	2.27	0.41
1:C:179:THR:CA	2:D:352:LYS:HZ2	2.33	0.41
1:C:224:TYR:CE2	4:C:600:GTP:C5	3.08	0.41
2:D:16:ILE:HG23	2:D:235:MET:HE1	2.02	0.41
2:D:295:MET:HE2	2:D:295:MET:HB3	1.89	0.41
2:D:298:SER:O	2:D:301:MET:N	2.53	0.41
2:D:332:MET:O	2:D:335:VAL:HG23	2.20	0.41
1:A:309:HIS:ND1	1:A:309:HIS:C	2.73	0.41
1:C:172:TYR:HA	1:C:173:PRO:HD3	1.82	0.41
2:D:265:LEU:HB3	2:D:432:TYR:CE2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:120:LEU:O	3:E:123:LEU:HB2	2.21	0.41
1:A:224:TYR:CE2	4:A:600:GTP:C5	3.08	0.41
1:A:402:ARG:HD2	1:A:415:GLU:OE2	2.20	0.41
2:D:103:TRP:N	2:D:186:ASN:OD1	2.54	0.41
2:D:192:HIS:ND1	2:D:192:HIS:C	2.74	0.41
2:D:333:LEU:O	2:D:334:ASN:C	2.59	0.41
2:D:339:ASN:HD22	2:D:339:ASN:HA	1.77	0.41
3:E:13:LYS:HG2	3:E:18:GLN:HG3	2.03	0.41
2:B:31:ASP:HB2	2:B:34:GLY:N	2.36	0.41
2:B:141:LEU:HD22	2:B:172:MET:SD	2.61	0.41
2:B:276:THR:HG23	2:B:277:SER:H	1.85	0.41
2:B:287:THR:OG1	2:B:289:PRO:HD2	2.21	0.41
2:B:351:VAL:O	2:B:351:VAL:HG22	2.20	0.41
2:B:380:ASN:C	2:B:380:ASN:HD22	2.23	0.41
2:B:399:PHE:CE1	2:B:418:PHE:CB	3.03	0.41
1:C:102:ASN:ND2	1:C:104:ALA:N	2.69	0.41
1:C:115:ILE:HG23	1:C:116:ASP:N	2.34	0.41
1:C:387:ALA:HB2	1:C:390:ARG:HH12	1.86	0.41
2:D:194:LEU:O	2:D:196:GLU:N	2.54	0.41
2:D:255:LEU:HD12	2:D:255:LEU:HA	1.74	0.41
2:D:333:LEU:HD21	2:D:337:ASN:HD21	1.84	0.41
2:D:358:ILE:HA	2:D:359:PRO:HD3	1.75	0.41
2:D:391:ILE:HA	2:D:394:GLN:NE2	2.36	0.41
3:E:101:LEU:O	3:E:104:LYS:N	2.42	0.41
1:A:267:PHE:CD1	1:A:267:PHE:N	2.89	0.41
1:A:347:CYS:O	1:A:348:PRO:C	2.59	0.41
2:B:177:VAL:O	2:B:177:VAL:HG12	2.21	0.41
1:C:171:ILE:O	1:C:171:ILE:HG22	2.19	0.41
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.56	0.41
2:D:351:VAL:O	2:D:351:VAL:HG22	2.21	0.41
1:A:99:ALA:HB3	1:A:145:THR:HG22	2.03	0.40
1:A:187:SER:HB2	1:A:391:LEU:HD21	2.03	0.40
2:B:54:ASN:HD22	2:B:64:ARG:HD2	1.86	0.40
2:D:142:GLY:HA3	2:D:173:PRO:HG3	2.03	0.40
2:D:174:SER:HA	2:D:390:ARG:HH21	1.86	0.40
3:E:123:LEU:O	3:E:127:ASP:N	2.54	0.40
1:A:139:HIS:CG	1:A:150:THR:HG21	2.56	0.40
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.36	0.40
2:B:111:GLY:HA2	2:B:149:MET:HE2	2.03	0.40
1:C:75:ILE:HG21	1:C:94:THR:HG22	2.02	0.40
1:C:88:HIS:H	1:C:91:GLN:NE2	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ARG:O	1:C:110:ILE:HG22	2.21	0.40
1:C:381:THR:O	1:C:384:ILE:HG22	2.21	0.40
2:D:229:HIS:CE1	2:D:277:SER:CB	2.88	0.40
2:D:385:GLN:HE21	2:D:389:LYS:HE3	1.87	0.40
2:D:404:PHE:HD1	2:D:404:PHE:H	1.68	0.40
1:A:191:THR:HG23	1:A:425:MET:HE3	2.02	0.40
1:A:260:VAL:HA	1:A:261:PRO:HD3	1.93	0.40
2:B:21:TRP:CH2	2:B:63:PRO:HB3	2.57	0.40
2:B:276:THR:CG2	2:B:277:SER:N	2.84	0.40
1:C:229:ARG:HH11	1:C:229:ARG:CG	2.33	0.40
2:D:145:THR:HG23	6:D:600:GDP:O3B	2.20	0.40
2:D:182:VAL:HG12	2:D:404:PHE:CD2	2.57	0.40
2:D:191:VAL:HG11	2:D:425:MET:CG	2.51	0.40
1:A:394:LYS:HG2	2:B:348:PRO:HB3	2.02	0.40
2:B:107:HIS:O	2:B:152:LEU:HD22	2.21	0.40
1:C:152:LEU:HA	1:C:155:GLU:HG3	2.04	0.40
1:C:254:GLU:O	1:C:254:GLU:HG2	2.19	0.40
1:C:402:ARG:HD3	1:C:402:ARG:HA	1.88	0.40
2:D:122:VAL:HG22	2:D:123:ARG:N	2.36	0.40
1:A:88:HIS:O	1:A:90:GLU:N	2.54	0.40
1:A:398:MET:CG	2:B:348:PRO:HD3	2.52	0.40
2:B:104:ALA:O	2:B:108:TYR:N	2.40	0.40
2:B:226:ASP:N	2:B:226:ASP:OD1	2.54	0.40
2:B:269:MET:HG2	2:B:384:ILE:HG12	2.03	0.40
1:C:267:PHE:HA	1:C:268:PRO:HD3	1.93	0.40
3:E:70:LYS:HE2	3:E:70:LYS:HB3	2.00	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%)	327 (77%)	65 (15%)	32 (8%)	1 15
1	C	423/451 (94%)	331 (78%)	62 (15%)	30 (7%)	1 16
2	B	416/445 (94%)	306 (74%)	74 (18%)	36 (9%)	1 12
2	D	425/445 (96%)	295 (69%)	84 (20%)	46 (11%)	0 7
3	E	119/142 (84%)	80 (67%)	25 (21%)	14 (12%)	0 6
All	All	1807/1934 (93%)	1339 (74%)	310 (17%)	158 (9%)	1 12

All (158) 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	403	ALA
2	B	43	GLN
2	B	62	VAL
2	B	73	GLY
2	B	82	PRO
2	B	162	PRO
2	B	163	ASP
2	B	245	PRO
2	B	249	ASN
2	B	288	VAL
2	B	299	LYS
2	B	348	PRO
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	257	THR
1	C	265	ILE
1	C	341	ILE
1	C	348	PRO
1	C	377	MET
1	C	403	ALA

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Mol	Chain	Res	Type
1	C	437	VAL
2	D	43	GLN
2	D	62	VAL
2	D	73	GLY
2	D	82	PRO
2	D	163	ASP
2	D	249	ASN
2	D	251	ASP
2	D	285	ALA
2	D	288	VAL
2	D	299	LYS
2	D	322	ARG
2	D	371	LEU
2	D	400	ARG
3	E	26	PRO
3	E	28	SER
3	E	49	GLU
3	E	82	VAL
3	E	102	ALA
1	A	83	TYR
1	A	84	ARG
1	A	162	GLY
1	A	164	LYS
1	A	247	ALA
1	A	284	GLU
1	A	350	GLY
1	A	392	ASP
1	A	402	ARG
1	A	429	GLU
1	A	437	VAL
2	B	3	GLU
2	B	34	GLY
2	B	42	LEU
2	B	60	LYS
2	B	115	VAL
2	B	226	ASP
2	B	227	LEU
2	B	264	ARG
2	B	273	ALA
2	B	276	THR
1	C	83	TYR
1	C	162	GLY

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Mol	Chain	Res	Type
1	C	164	LYS
1	C	183	GLU
1	C	191	THR
1	C	253	THR
1	C	429	GLU
2	D	3	GLU
2	D	34	GLY
2	D	42	LEU
2	D	115	VAL
2	D	162	PRO
2	D	227	LEU
2	D	244	PHE
2	D	245	PRO
2	D	264	ARG
2	D	402	LYS
2	D	404	PHE
3	E	12	ASN
3	E	75	LYS
3	E	81	GLU
3	E	124	GLN
1	A	32	PRO
1	A	48	SER
1	A	191	THR
1	A	273	ALA
1	A	279	GLU
2	B	244	PHE
2	B	307	PRO
2	B	322	ARG
2	B	403	ALA
1	C	32	PRO
1	C	245	ASP
1	C	273	ALA
1	C	301	GLN
2	D	158	ARG
2	D	195	VAL
2	D	265	LEU
2	D	278	ARG
2	D	293	GLN
2	D	348	PRO
2	D	403	ALA
2	D	437	ASP
3	E	5	ASP

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Mol	Chain	Res	Type
3	E	46	SER
1	A	245	ASP
1	A	301	GLN
1	A	364	PRO
1	C	84	ARG
1	C	141	PHE
1	C	220	GLU
2	D	59	ASN
2	D	60	LYS
2	D	129	CYS
2	D	226	ASP
2	D	273	ALA
2	D	409	THR
3	E	85	LYS
1	A	101	ASN
1	A	183	GLU
1	A	248	LEU
2	B	59	ASN
2	B	217	LEU
2	B	265	LEU
2	B	409	THR
1	C	402	ARG
2	D	240	THR
2	D	246	GLY
2	D	279	GLY
2	D	307	PRO
3	E	139	LEU
2	B	246	GLY
1	C	79	ARG
1	C	274	PRO
1	C	364	PRO
1	C	412	GLY
2	D	139	HIS
3	E	77	GLU
1	A	274	PRO
2	B	32	PRO
2	B	195	VAL
2	D	289	PRO
1	A	412	GLY
1	C	350	GLY
2	D	32	PRO
2	B	177	VAL

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Mol	Chain	Res	Type
2	D	177	VAL

5.3.2 Protein sidechains (i)

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%)	243 (70%)	103 (30%)	0 2
1	C	344/378 (91%)	236 (69%)	108 (31%)	0 2
2	B	350/383 (91%)	217 (62%)	133 (38%)	0 0
2	D	353/383 (92%)	216 (61%)	137 (39%)	0 0
3	E	82/126 (65%)	40 (49%)	42 (51%)	0 0
All	All	1475/1648 (90%)	952 (64%)	523 (36%)	0 1

All (523) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	11	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	36	MET
1	A	49	PHE
1	A	60	LYS
1	A	61	HIS
1	A	62	VAL
1	A	68	VAL
1	A	70	LEU
1	A	73	THR
1	A	74	VAL
1	A	79	ARG

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Mol	Chain	Res	Type
1	A	80	THR
1	A	84	ARG
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	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	163	LYS
1	A	164	LYS
1	A	168	GLU
1	A	176	GLN
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	220	GLU
1	A	226	ASN
1	A	230	LEU
1	A	236	SER
1	A	237	SER
1	A	241	SER

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Mol	Chain	Res	Type
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	301	GLN
1	A	304	LYS
1	A	309	HIS
1	A	315	CYS
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
1	A	363	VAL
1	A	368	LEU
1	A	370	LYS
1	A	371	VAL
1	A	372	GLN
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	415	GLU
1	A	419	SER
1	A	420	GLU

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Mol	Chain	Res	Type
1	A	433	GLU
2	B	3	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	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
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	113	GLU
2	B	119	LEU
2	B	120	ASP
2	B	122	VAL
2	B	128	SER
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

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Mol	Chain	Res	Type
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	174	SER
2	B	178	SER
2	B	179	ASP
2	B	181	VAL
2	B	188	THR
2	B	190	SER
2	B	195	VAL
2	B	196	GLU
2	B	200	GLU
2	B	209	LEU
2	B	212	ILE
2	B	214	PHE
2	B	215	ARG
2	B	216	THR
2	B	219	LEU
2	B	223	THR
2	B	227	LEU
2	B	230	LEU
2	B	239	THR
2	B	242	LEU
2	B	244	PHE
2	B	248	LEU
2	B	249	ASN
2	B	251	ASP
2	B	254	LYS
2	B	255	LEU
2	B	260	VAL
2	B	265	LEU
2	B	266	HIS
2	B	269	MET
2	B	275	LEU

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Mol	Chain	Res	Type
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	324	SER
2	B	325	MET
2	B	329	ASP
2	B	330	GLU
2	B	332	MET
2	B	335	VAL
2	B	339	ASN
2	B	341	SER
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	376	THR
2	B	380	ASN
2	B	384	ILE
2	B	387	LEU
2	B	389	LYS
2	B	390	ARG
2	B	391	ILE
2	B	393	GLU
2	B	394	GLN
2	B	398	MET
2	B	400	ARG
2	B	401	ARG
2	B	405	LEU
2	B	406	HIS
2	B	416	MET

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Mol	Chain	Res	Type
2	B	417	GLU
2	B	419	THR
2	B	423	SER
2	B	425	MET
2	B	430	SER
2	B	432	TYR
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	25	CYS
1	C	26	LEU
1	C	27	GLU
1	C	31	GLN
1	C	36	MET
1	C	38	SER
1	C	41	THR
1	C	49	PHE
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	84	ARG
1	C	88	HIS
1	C	92	LEU
1	C	94	THR
1	C	96	LYS
1	C	102	ASN
1	C	105	ARG
1	C	110	ILE
1	C	114	ILE
1	C	115	ILE
1	C	119	LEU
1	C	120	ASP
1	C	124	LYS
1	C	140	SER
1	C	141	PHE

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Mol	Chain	Res	Type
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	176	GLN
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	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
1	C	250	VAL
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	293	ASN
1	C	301	GLN
1	C	304	LYS
1	C	309	HIS
1	C	313	MET

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Mol	Chain	Res	Type
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	344	VAL
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	377	MET
1	C	379	SER
1	C	380	ASN
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
1	C	415	GLU
1	C	419	SER
1	C	420	GLU
1	C	438	ASP
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

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Mol	Chain	Res	Type
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	76	ASP
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	122	VAL
2	D	128	SER
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
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	168	THR
2	D	170	SER

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Mol	Chain	Res	Type
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	212	ILE
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	255	LEU
2	D	260	VAL
2	D	265	LEU
2	D	275	LEU
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	295	MET
2	D	299	LYS
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

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Mol	Chain	Res	Type
2	D	323	MET
2	D	324	SER
2	D	325	MET
2	D	329	ASP
2	D	330	GLU
2	D	332	MET
2	D	333	LEU
2	D	335	VAL
2	D	337	ASN
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	372	LYS
2	D	373	MET
2	D	376	THR
2	D	380	ASN
2	D	384	ILE
2	D	387	LEU
2	D	391	ILE
2	D	393	GLU
2	D	394	GLN
2	D	398	MET
2	D	400	ARG
2	D	401	ARG
2	D	405	LEU
2	D	408	TYR
2	D	413	MET
2	D	415	GLU
2	D	416	MET
2	D	417	GLU
2	D	419	THR
2	D	423	SER
2	D	425	MET
2	D	430	SER
2	D	434	GLN

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Mol	Chain	Res	Type
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	28	SER
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	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	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	120	LEU
3	E	125	GLU
3	E	126	LYS
3	E	129	HIS

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Mol	Chain	Res	Type
3	E	136	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) 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	91	GLN
1	A	101	ASN
1	A	102	ASN
1	A	128	GLN
1	A	139	HIS
1	A	176	GLN
1	A	206	ASN
1	A	216	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
2	B	193	GLN
2	B	206	ASN
2	B	229	HIS
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	350	ASN
2	B	380	ASN
2	B	385	GLN

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Mol	Chain	Res	Type
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	128	GLN
1	C	139	HIS
1	C	176	GLN
1	C	197	HIS
1	C	206	ASN
1	C	216	ASN
1	C	258	ASN
1	C	329	ASN
1	C	356	ASN
2	D	8	GLN
2	D	14	ASN
2	D	43	GLN
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	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	337	ASN
2	D	339	ASN
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
2	D	434	GLN
3	E	78	HIS
3	E	90	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 monosaccharides 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	$\#\|Z\| > 2$
6	GDP	D	600	-	24,30,30	1.21	2 (8%)	30,47,47	1.61	6 (20%)
4	GTP	A	600	5	26,34,34	1.30	3 (11%)	32,54,54	1.63	7 (21%)
7	K2N	D	700	-	24,26,26	1.83	6 (25%)	27,36,36	2.84	12 (44%)
6	GDP	B	600	-	24,30,30	1.10	1 (4%)	30,47,47	1.72	7 (23%)
7	K2N	B	700	-	24,26,26	1.66	3 (12%)	27,36,36	3.22	13 (48%)
4	GTP	C	600	5	26,34,34	1.18	2 (7%)	32,54,54	1.73	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GDP	D	600	-	-	2/12/32/32	0/3/3/3
4	GTP	A	600	5	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	K2N	D	700	-	-	10/11/23/23	0/3/3/3
6	GDP	B	600	-	-	2/12/32/32	0/3/3/3
7	K2N	B	700	-	-	9/11/23/23	0/3/3/3
4	GTP	C	600	5	-	8/18/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	700	K2N	CAS-CAR	-6.69	1.38	1.48
7	B	700	K2N	CAS-CAR	-6.30	1.38	1.48
4	A	600	GTP	C5-C6	-4.40	1.38	1.47
4	C	600	GTP	C5-C6	-3.94	1.39	1.47
6	D	600	GDP	C5-C6	-3.89	1.39	1.47
6	B	600	GDP	C5-C6	-3.60	1.40	1.47
7	D	700	K2N	CAT-NAM	2.53	1.38	1.35
7	B	700	K2N	CAU-NAN	-2.36	1.35	1.40
6	D	600	GDP	C2-N3	2.33	1.38	1.33
4	C	600	GTP	C2-N3	2.32	1.38	1.33
4	A	600	GTP	O4'-C4'	-2.30	1.39	1.45
7	B	700	K2N	CAW-NAL	-2.26	1.34	1.38
7	D	700	K2N	CAW-NAL	-2.19	1.34	1.38
4	A	600	GTP	C5-C4	-2.15	1.37	1.43
7	D	700	K2N	CAU-NAM	2.13	1.38	1.34
7	D	700	K2N	OAD-CAQ	2.08	1.25	1.21
7	D	700	K2N	OAP-CAK	-2.03	1.40	1.46

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	700	K2N	OAP-CAQ-NAN	8.05	122.47	109.32
7	B	700	K2N	CAK-OAP-CAQ	-8.02	100.84	116.04
7	D	700	K2N	CAK-OAP-CAQ	-7.55	101.74	116.04
4	C	600	GTP	PB-O3B-PG	-5.80	112.93	132.83
7	D	700	K2N	NAN-CAU-NAM	5.48	126.27	113.24
7	B	700	K2N	OAP-CAQ-OAD	-5.23	114.21	124.25
7	B	700	K2N	CAB-CAX-NAO	-5.05	104.47	110.34
7	D	700	K2N	NAC-CAT-NAM	5.01	124.11	117.03
4	A	600	GTP	PB-O3B-PG	-4.46	117.51	132.83
6	D	600	GDP	PA-O3A-PB	-4.13	118.64	132.83
7	D	700	K2N	CAH-CAS-CAR	-4.08	115.92	120.75
7	B	700	K2N	NAC-CAT-NAM	4.04	122.74	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	700	K2N	CAJ-CAU-NAM	-3.74	115.49	123.41
6	D	600	GDP	C8-N7-C5	3.73	110.09	102.99
7	D	700	K2N	OAP-CAQ-NAN	3.67	115.32	109.32
7	B	700	K2N	CAI-CAS-CAR	3.45	124.84	120.75
6	B	600	GDP	C8-N7-C5	3.40	109.47	102.99
7	B	700	K2N	CAW-CAT-NAC	-3.37	116.11	123.43
4	A	600	GTP	C2-N1-C6	-3.36	118.91	125.10
7	B	700	K2N	CAH-CAS-CAR	-3.31	116.83	120.75
4	C	600	GTP	C8-N7-C5	3.31	109.29	102.99
4	A	600	GTP	C8-N7-C5	3.21	109.11	102.99
7	B	700	K2N	CAJ-CAU-NAM	-3.18	116.68	123.41
4	C	600	GTP	C5-C6-N1	3.10	119.43	113.95
4	A	600	GTP	C5-C6-N1	3.02	119.28	113.95
6	D	600	GDP	O6-C6-C5	-3.01	118.50	124.37
6	B	600	GDP	PA-O3A-PB	-3.01	122.51	132.83
7	D	700	K2N	CAW-CAT-NAC	-2.94	117.02	123.43
6	B	600	GDP	C5-C6-N1	2.88	119.04	113.95
6	B	600	GDP	N2-C2-N3	-2.84	114.21	119.74
4	A	600	GTP	PA-O3A-PB	-2.74	123.42	132.83
6	B	600	GDP	O6-C6-C5	-2.72	119.06	124.37
7	D	700	K2N	CAU-NAM-CAT	2.65	124.95	118.11
6	B	600	GDP	C3'-C2'-C1'	2.58	104.86	100.98
7	D	700	K2N	CAU-NAN-CAQ	2.58	133.60	127.36
4	A	600	GTP	N2-C2-N1	2.57	122.19	116.71
4	C	600	GTP	N1-C2-N3	-2.54	118.58	123.32
6	D	600	GDP	N1-C2-N3	-2.50	118.64	123.32
7	B	700	K2N	CAS-CAR-NAL	2.50	121.29	118.13
6	B	600	GDP	C2-N1-C6	-2.49	120.51	125.10
7	D	700	K2N	CAB-CAX-NAO	-2.40	107.56	110.34
4	C	600	GTP	C3'-C2'-C1'	-2.36	97.43	100.98
7	B	700	K2N	CAU-NAN-CAQ	2.31	132.95	127.36
7	B	700	K2N	CAU-NAM-CAT	2.30	124.02	118.11
4	C	600	GTP	C2-N1-C6	-2.18	121.09	125.10
6	D	600	GDP	C5-C6-N1	2.17	117.79	113.95
4	C	600	GTP	PA-O3A-PB	-2.12	125.56	132.83
7	B	700	K2N	OAP-CAK-CAA	2.10	116.15	108.42
7	D	700	K2N	CAG-CAI-CAS	-2.09	117.87	120.34
4	A	600	GTP	O6-C6-C5	-2.04	120.38	124.37
7	D	700	K2N	OAP-CAQ-OAD	-2.04	120.34	124.25
4	C	600	GTP	O6-C6-C5	-2.02	120.42	124.37
6	D	600	GDP	O2B-PB-O3A	2.01	111.37	104.64

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	GTP	PB-O3B-PG-O3G
4	A	600	GTP	C5'-O5'-PA-O1A
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
7	B	700	K2N	CAA-CAK-OAP-CAQ
7	B	700	K2N	OAD-CAQ-OAP-CAK
7	B	700	K2N	NAN-CAQ-OAP-CAK
7	D	700	K2N	CAJ-CAU-NAN-CAQ
7	D	700	K2N	NAM-CAU-NAN-CAQ
7	D	700	K2N	OAD-CAQ-OAP-CAK
7	D	700	K2N	NAN-CAQ-OAP-CAK
7	B	700	K2N	OAD-CAQ-NAN-CAU
7	B	700	K2N	OAP-CAQ-NAN-CAU
7	D	700	K2N	OAD-CAQ-NAN-CAU
7	D	700	K2N	OAP-CAQ-NAN-CAU
7	B	700	K2N	NAL-CAR-CAS-CAH
7	D	700	K2N	NAL-CAR-CAS-CAH
7	B	700	K2N	CAX-CAR-CAS-CAH
7	D	700	K2N	CAX-CAR-CAS-CAH
7	D	700	K2N	CAX-CAR-CAS-CAI
4	C	600	GTP	PB-O3A-PA-O1A
7	D	700	K2N	NAL-CAR-CAS-CAI
4	A	600	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O3A
7	B	700	K2N	NAL-CAR-CAS-CAI
4	A	600	GTP	C5'-O5'-PA-O2A
4	C	600	GTP	C3'-C4'-C5'-O5'
7	B	700	K2N	CAX-CAR-CAS-CAI
4	C	600	GTP	C4'-C5'-O5'-PA
6	D	600	GDP	PA-O3A-PB-O1B
4	C	600	GTP	PB-O3B-PG-O2G
4	A	600	GTP	PB-O3A-PA-O2A
4	C	600	GTP	PB-O3A-PA-O2A
4	C	600	GTP	C5'-O5'-PA-O2A
4	A	600	GTP	PB-O3B-PG-O1G

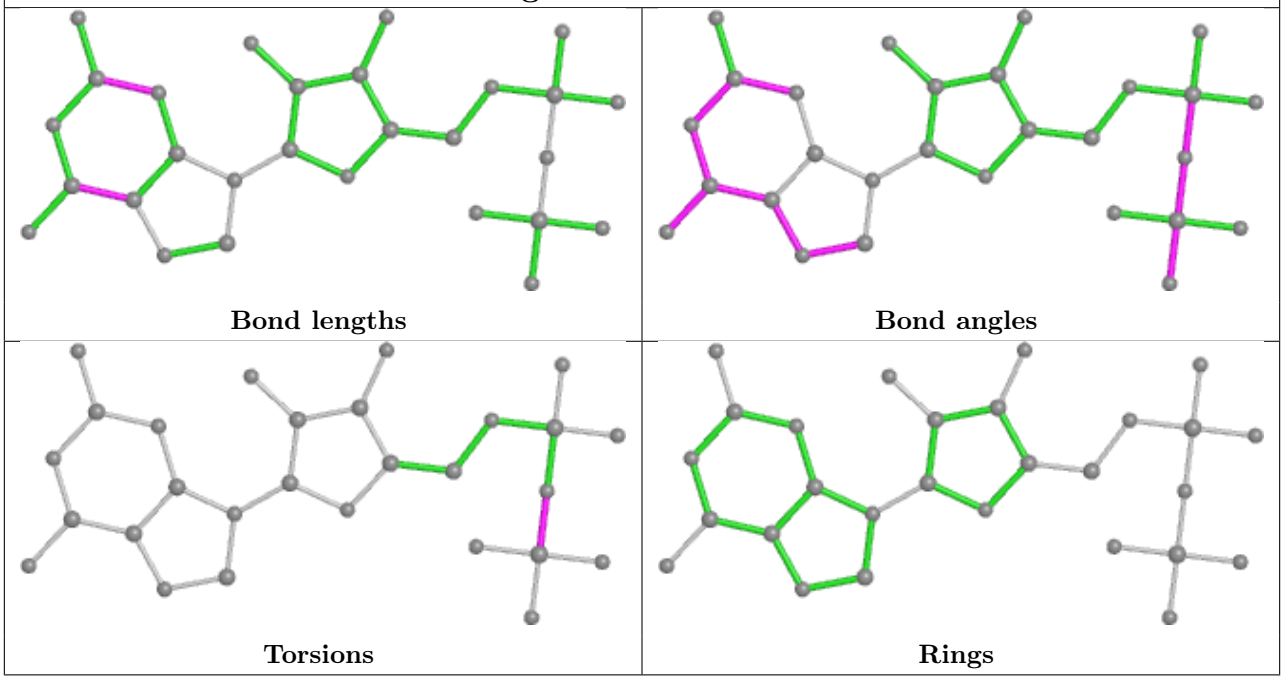
There are no ring outliers.

6 monomers are involved in 62 short contacts:

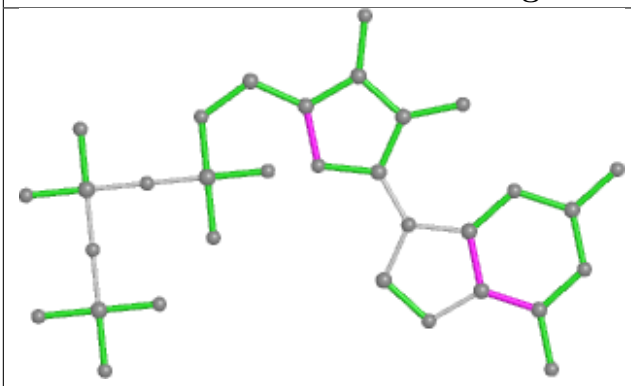
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	600	GDP	12	0
4	A	600	GTP	5	0
7	D	700	K2N	23	0
6	B	600	GDP	7	0
7	B	700	K2N	8	0
4	C	600	GTP	7	0

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

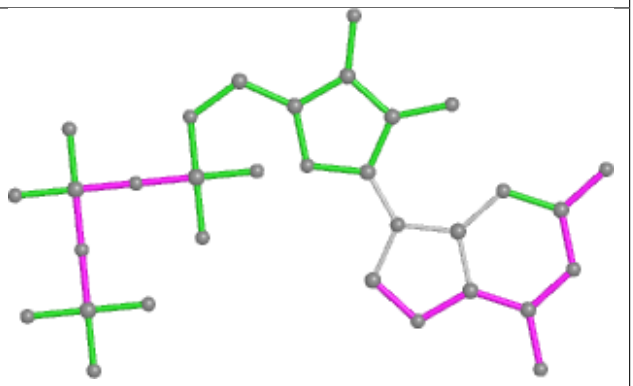
Ligand GDP D 600



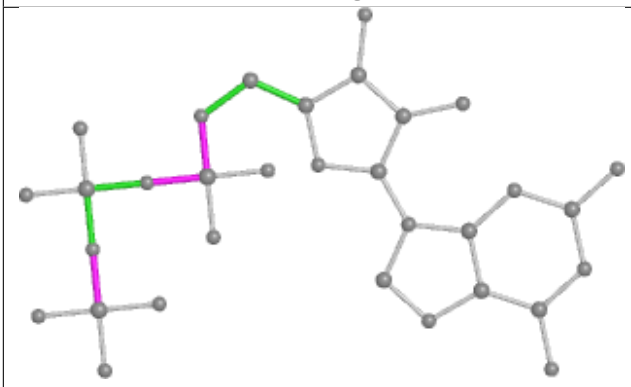
Ligand GTP A 600



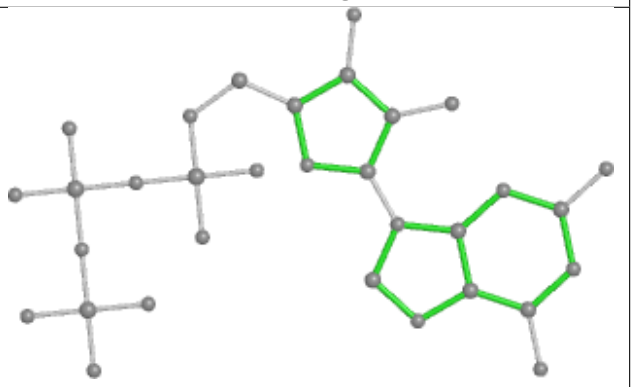
Bond lengths



Bond angles

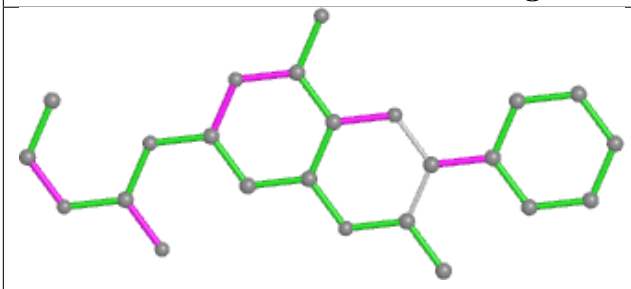


Torsions

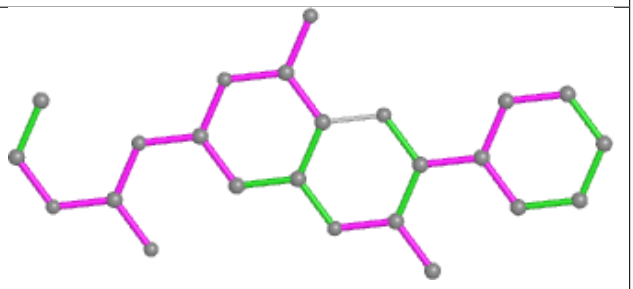


Rings

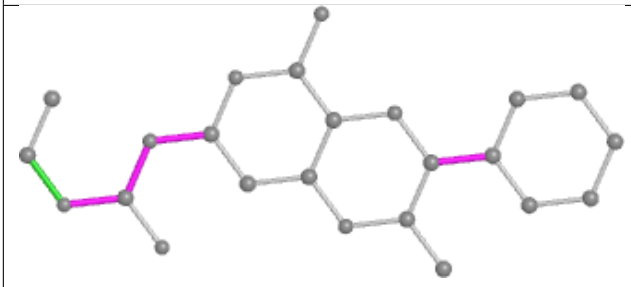
Ligand K2N D 700



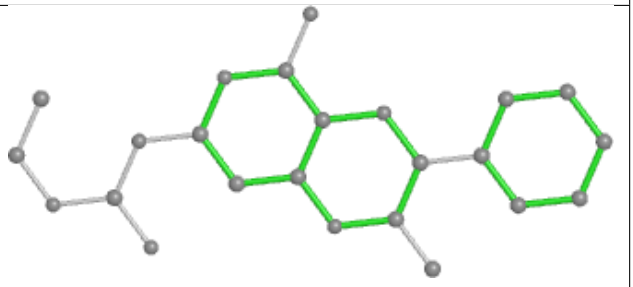
Bond lengths



Bond angles

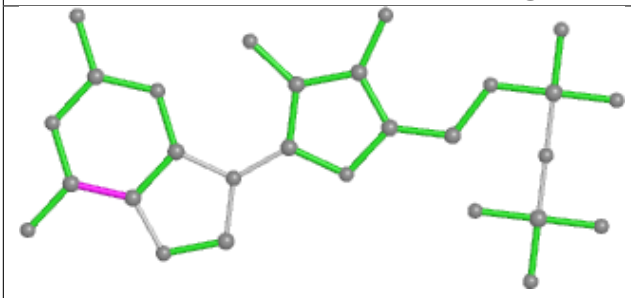


Torsions

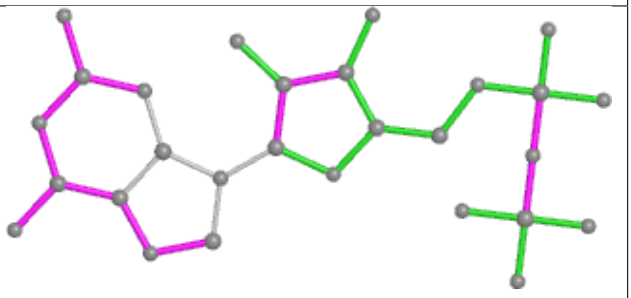


Rings

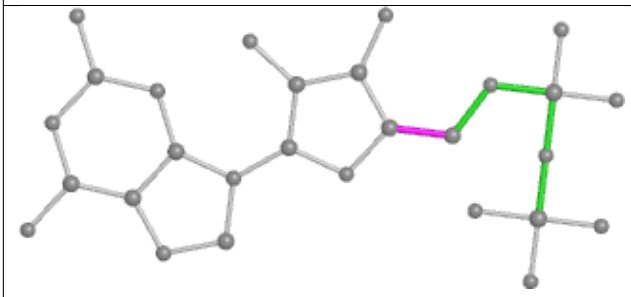
Ligand GDP B 600



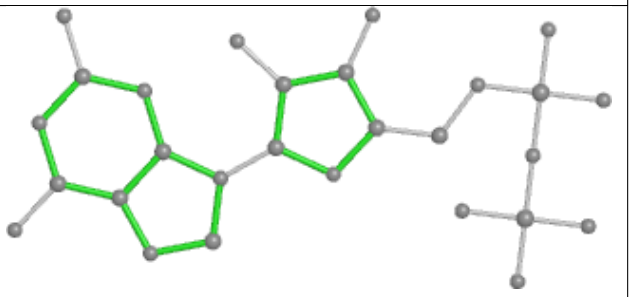
Bond lengths



Bond angles

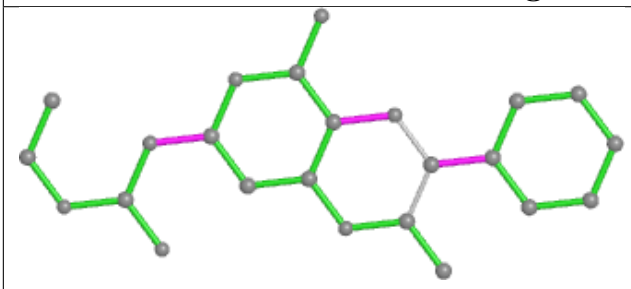


Torsions

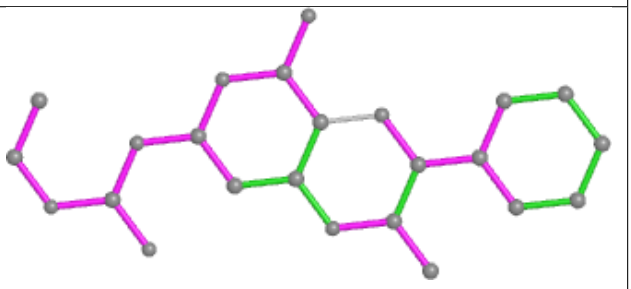


Rings

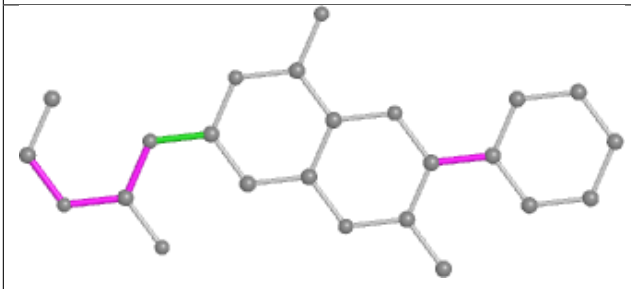
Ligand K2N B 700



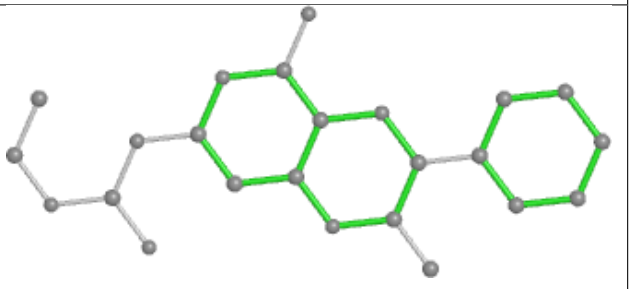
Bond lengths



Bond angles

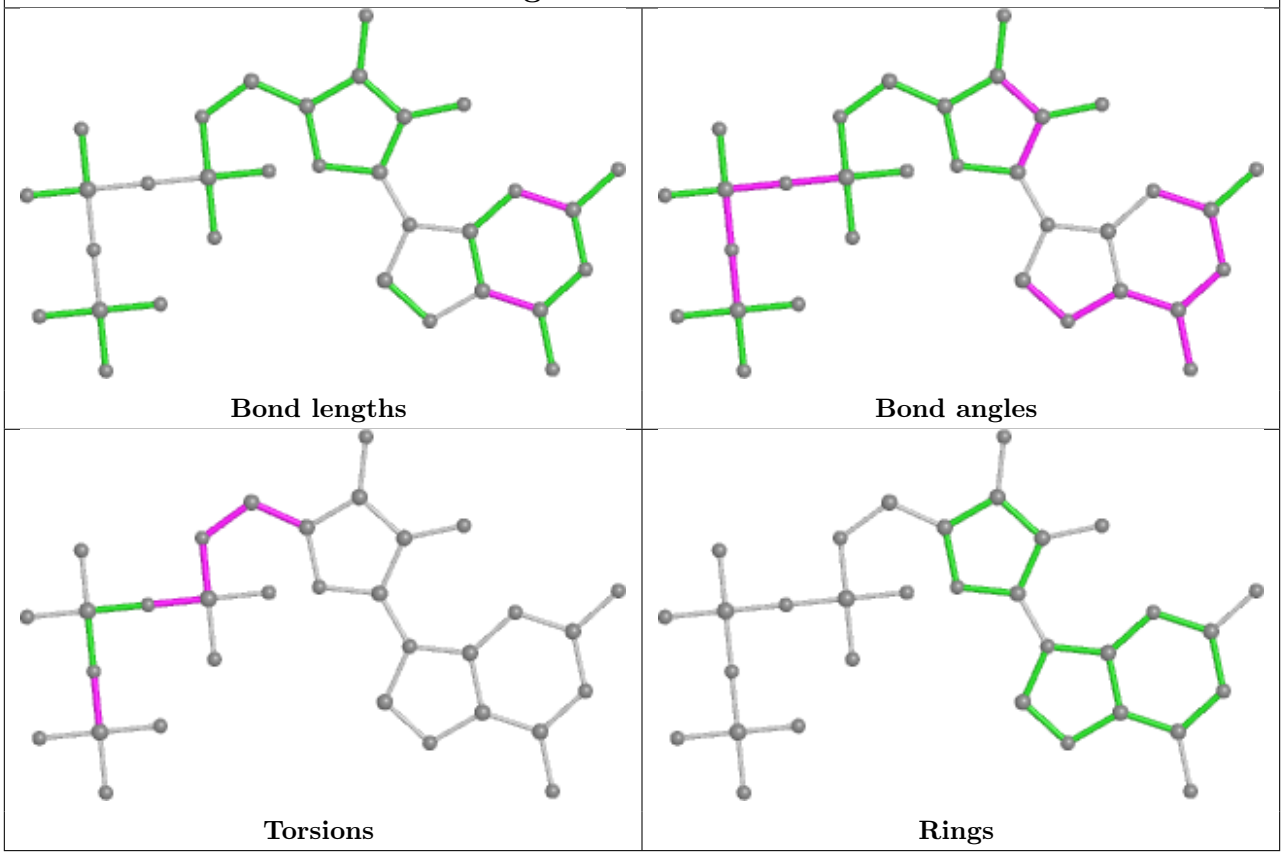


Torsions



Rings

Ligand GTP C 600



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.21	2 (0%)	91	85	173, 213, 260, 322	0
1	C	429/451 (95%)	-0.16	6 (1%)	75	65	190, 236, 318, 350	0
2	B	420/445 (94%)	-0.21	5 (1%)	79	70	176, 220, 277, 315	0
2	D	427/445 (95%)	-0.16	5 (1%)	79	70	189, 246, 315, 389	0
3	E	123/142 (86%)	0.06	1 (0%)	86	79	216, 250, 323, 363	0
All	All	1827/1934 (94%)	-0.17	19 (1%)	82	74	173, 229, 306, 389	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	30	ASP	5.1
1	C	367	ASP	3.3
1	C	170	SER	3.1
1	C	143	GLY	2.9
1	A	438	ASP	2.9
2	B	170	SER	2.8
1	A	170	SER	2.7
2	D	143	GLY	2.7
2	B	226	ASP	2.7
2	B	159	GLU	2.7
2	D	210	TYR	2.6
2	D	170	SER	2.3
2	D	144	GLY	2.3
1	C	370	LYS	2.2
2	D	94	PHE	2.1
2	B	203	SER	2.1
2	B	201	THR	2.1
1	C	236	SER	2.1
1	C	201	ALA	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

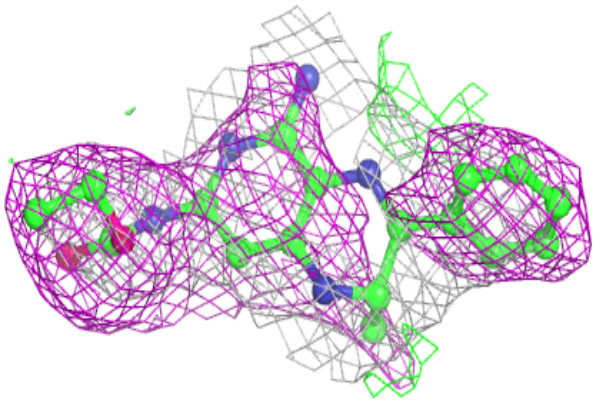
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

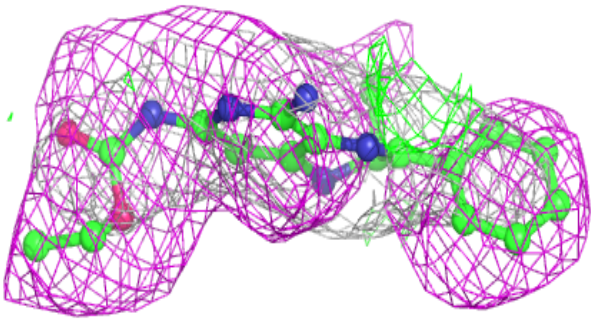
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	B	601	1/1	0.76	0.31	59,59,59,59	0
7	K2N	D	700	24/24	0.86	0.32	71,74,80,81	0
6	GDP	D	600	28/28	0.91	0.30	64,67,68,69	0
6	GDP	B	600	28/28	0.91	0.25	64,67,68,68	0
7	K2N	B	700	24/24	0.92	0.33	61,64,68,71	0
4	GTP	C	600	32/32	0.93	0.20	55,64,66,66	0
4	GTP	A	600	32/32	0.94	0.17	61,65,66,66	0
5	MG	C	601	1/1	0.97	0.10	43,43,43,43	0
5	MG	A	601	1/1	0.99	0.06	40,40,40,40	0

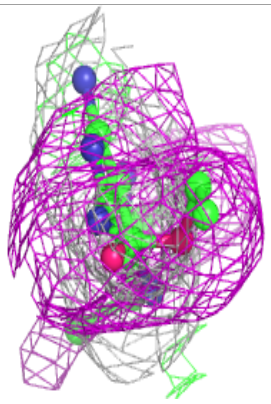
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around K2N 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)

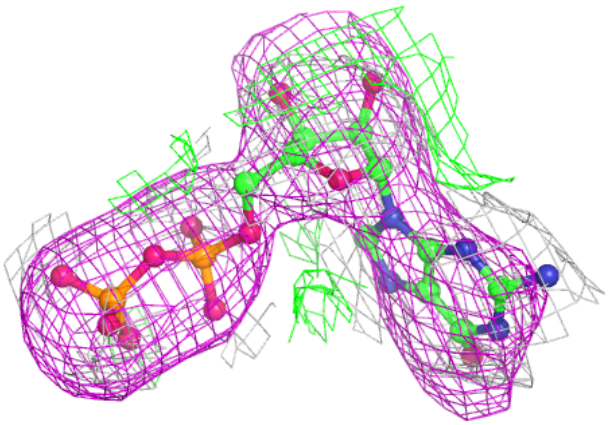


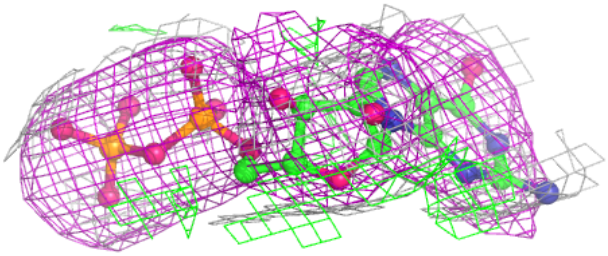


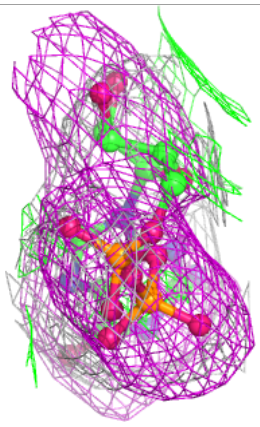


Electron density around GDP D 600:

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

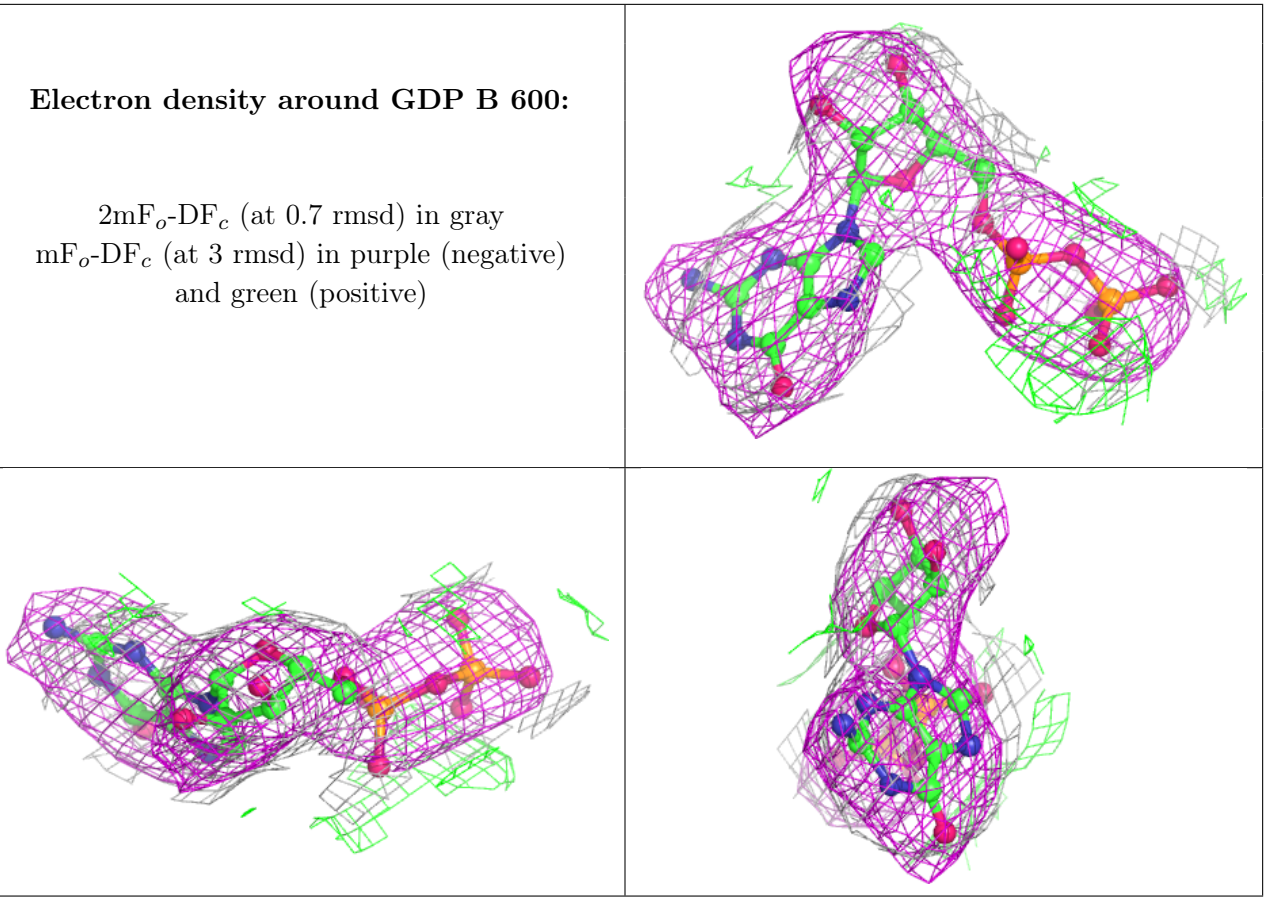






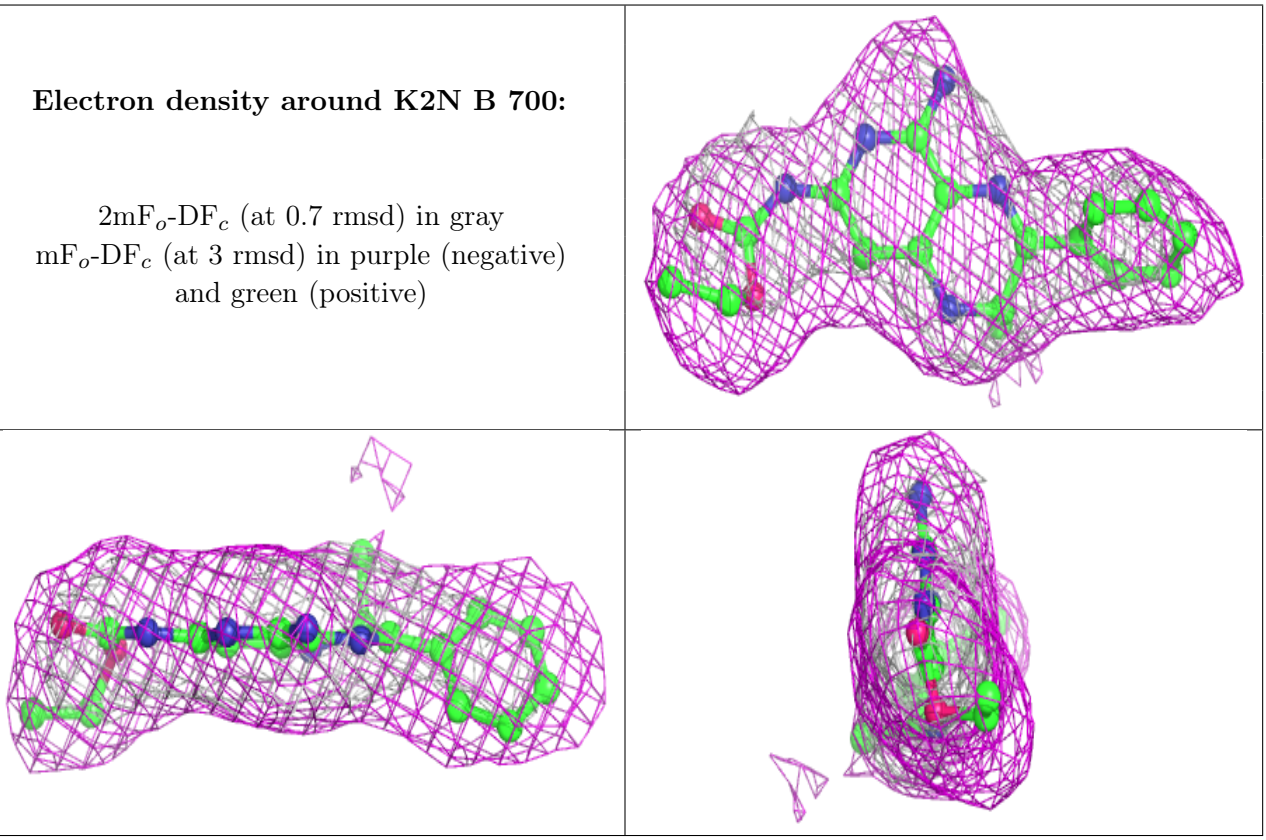
Electron density around GDP B 600:

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



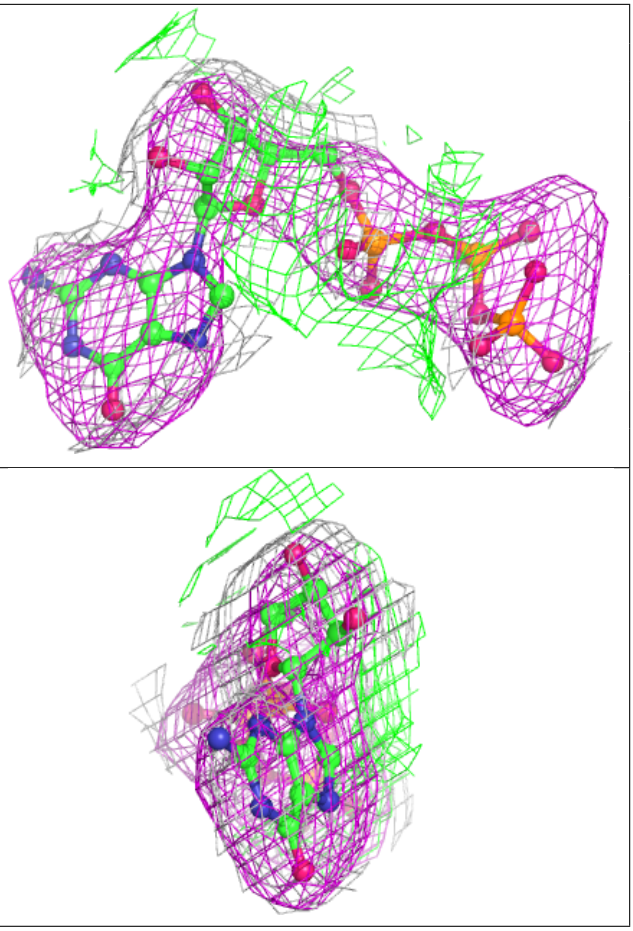
Electron density around K2N B 700:

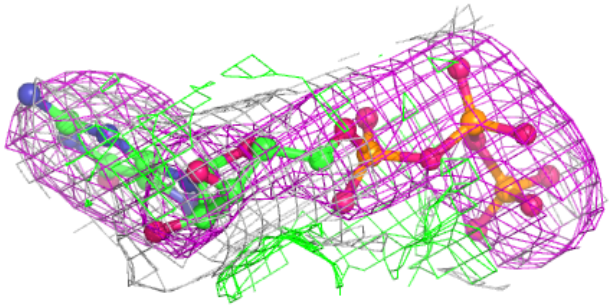
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GTP C 600:

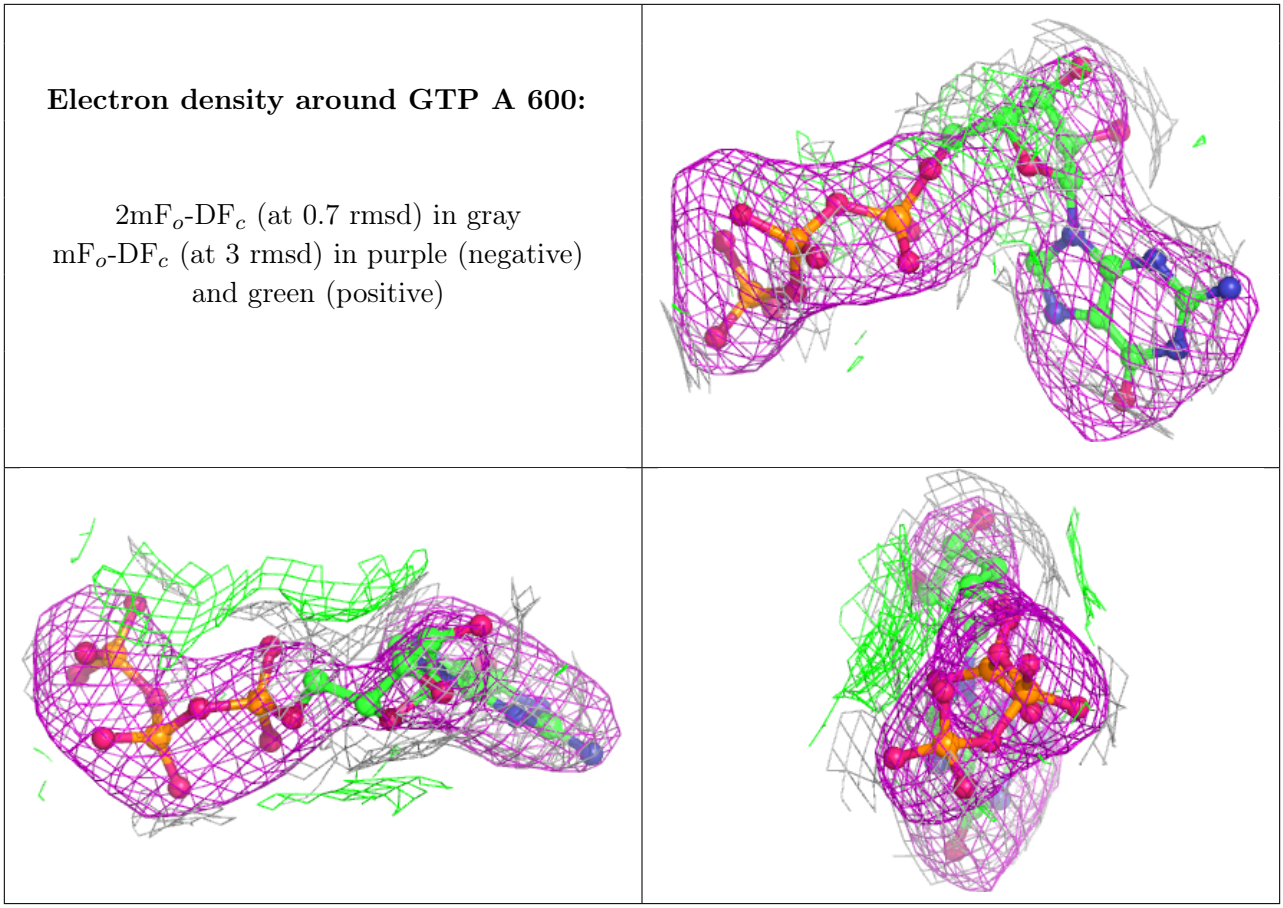
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around 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.