



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:23 AM UTC

PDB ID : 1Z2B / pdb_00001z2b
Title : Tubulin-colchicine-vinblastine: stathmin-like domain complex
Authors : Gigant, B.; Wang, C.; Ravelli, R.B.G.; Roussi, F.; Steinmetz, M.O.; Curmi, P.A.; Sobel, A.; Knossow, M.
Deposited on : 2005-03-08
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

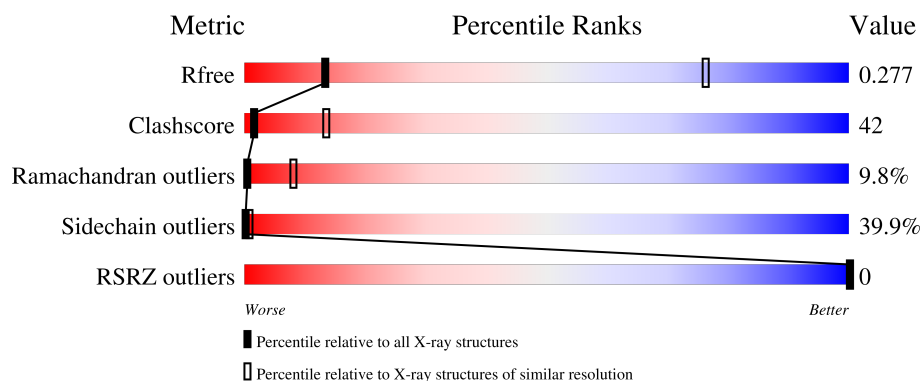
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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	448	
1	C	448	
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
8	VLB	C	800	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14173 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tubulin alpha chain.

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

There are 22 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Tubulin beta chain.

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

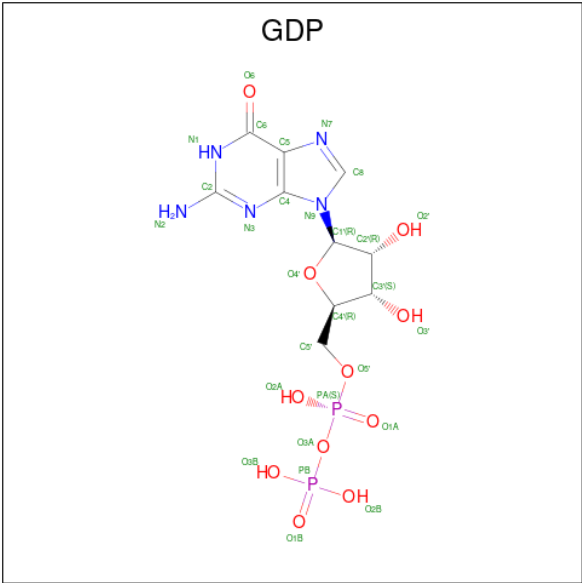
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



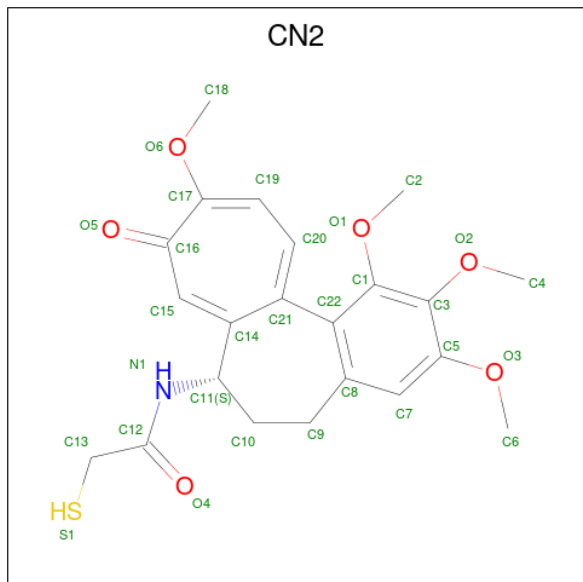
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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



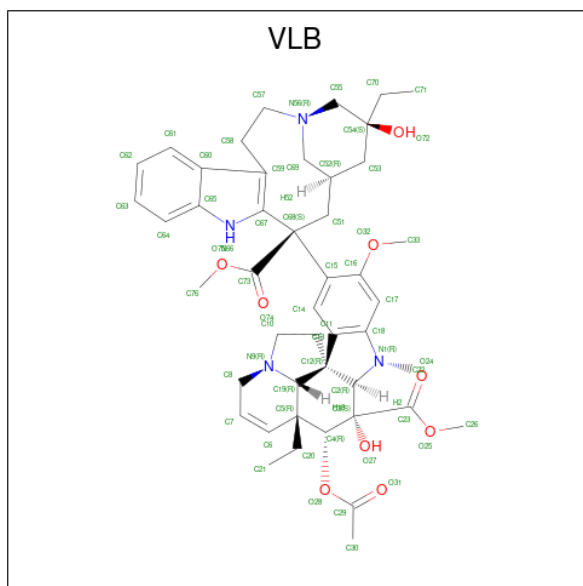
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



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

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

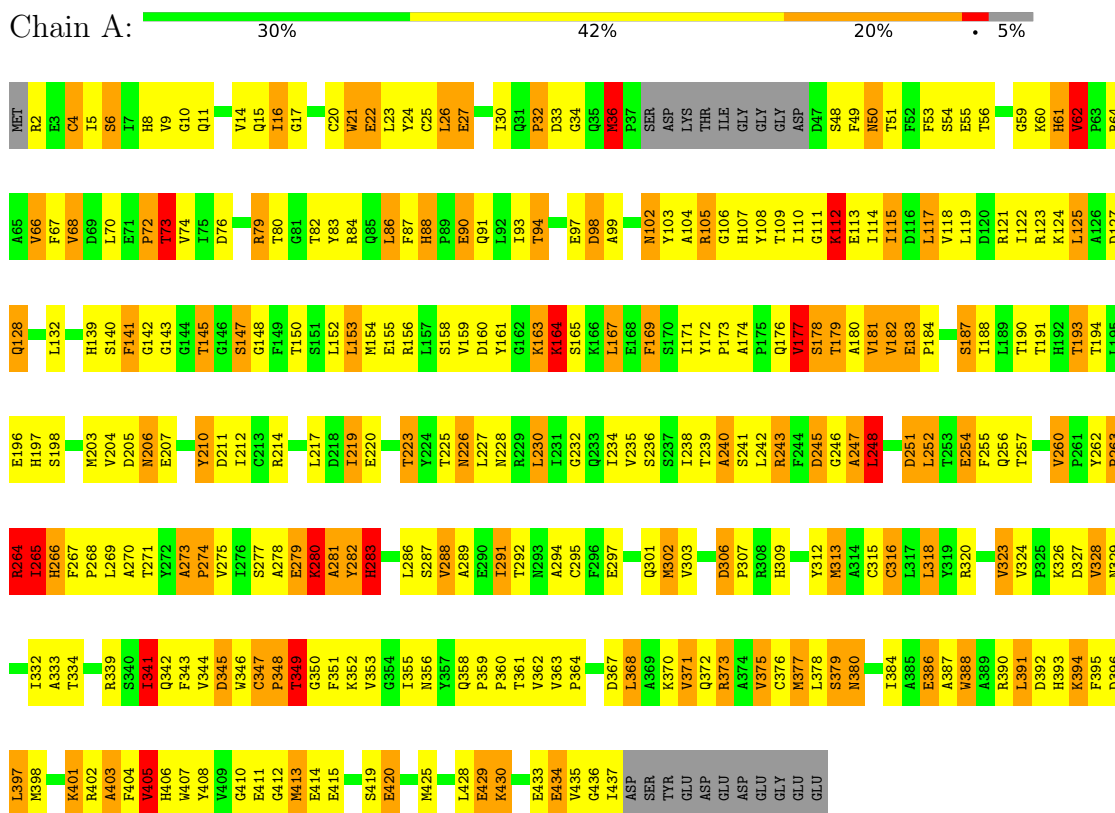


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			59	46	4	9		

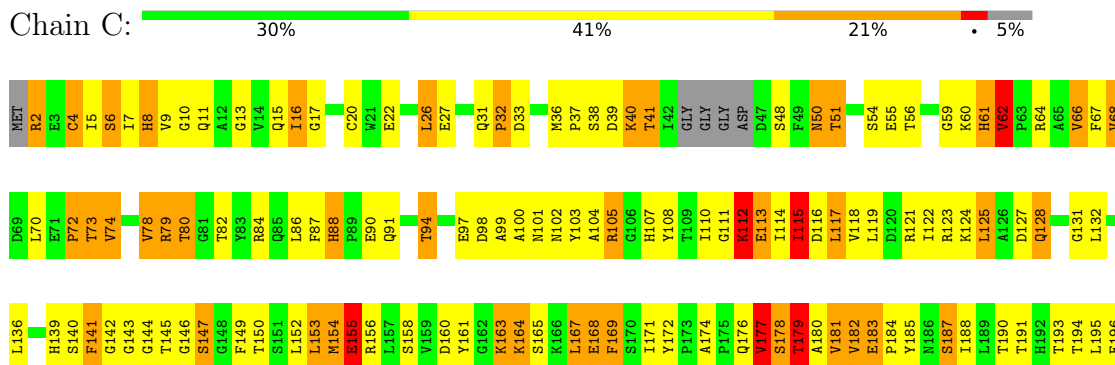
3 Residue-property plots

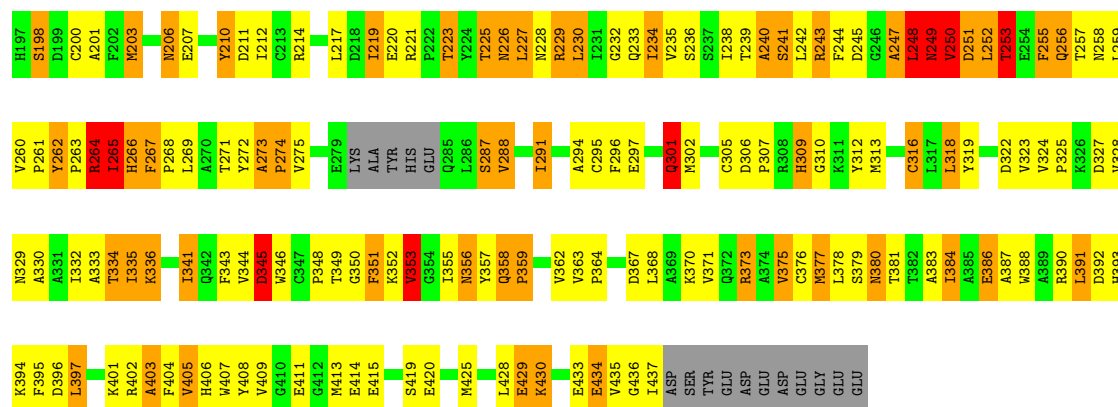
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



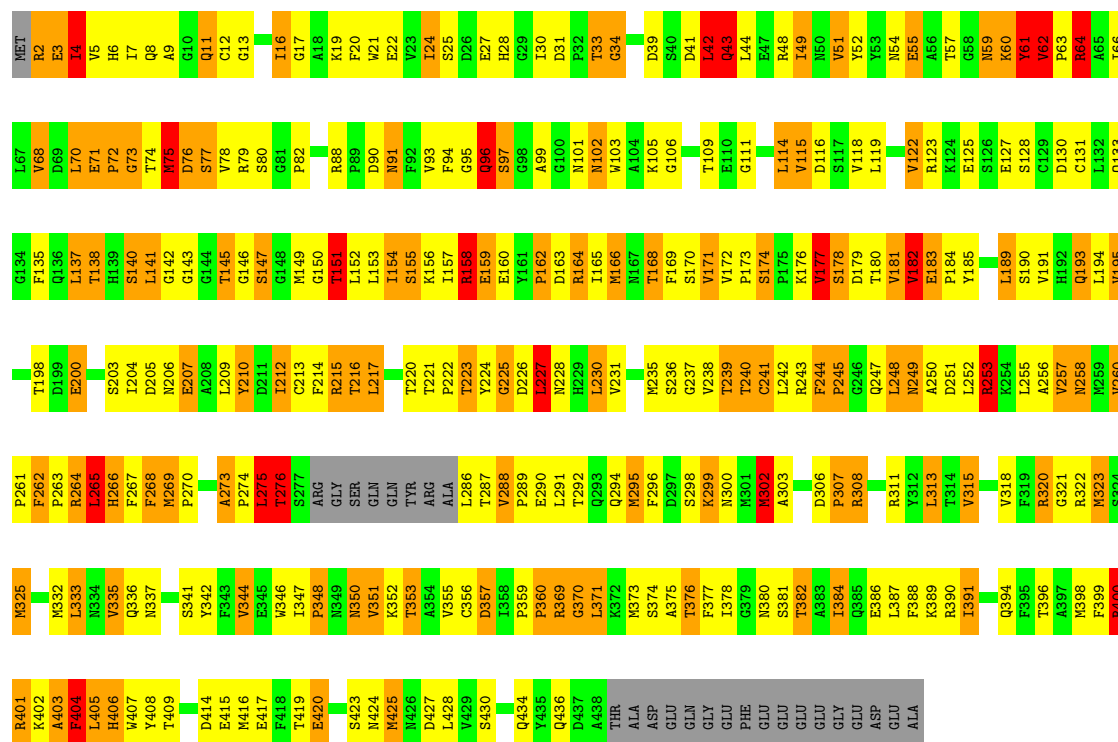
• Molecule 1: Tubulin alpha chain





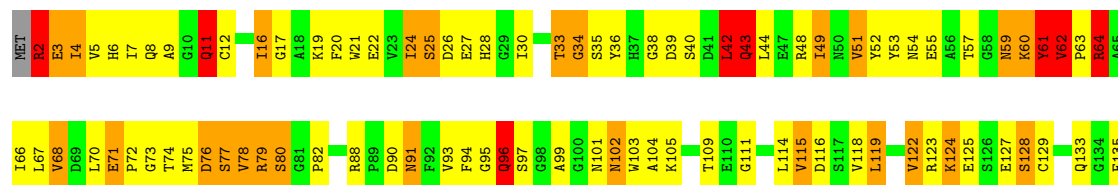
• Molecule 2: Tubulin beta chain

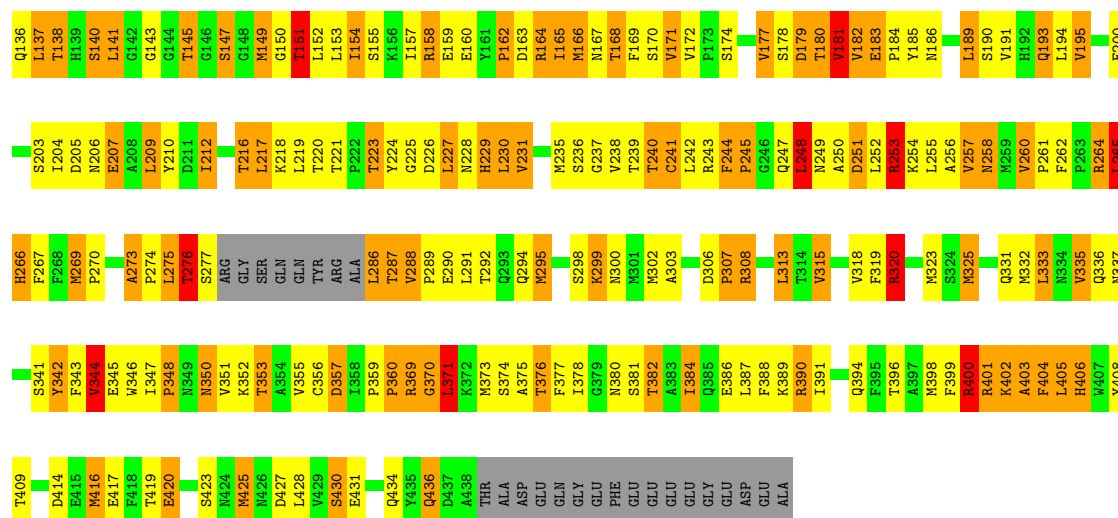
Chain B: 28% 38% 23% 6%



• Molecule 2: Tubulin beta chain

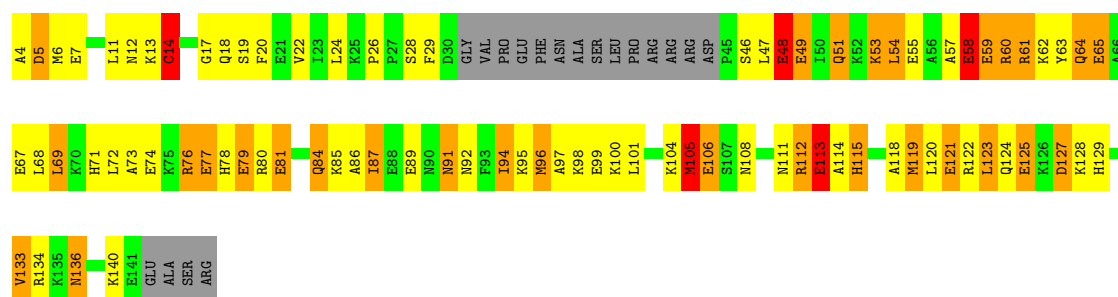
Chain D: 29% 38% 24% 6%





• Molecule 3: RB3 STATHMIN-LIKE DOMAIN 4

Chain E: 27% 36% 21% • 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	324.85Å 324.85Å 54.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.10 20.00 – 4.10	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-4.10) 94.4 (20.00-4.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 4.13Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.209 , 0.269 0.212 , 0.277	Depositor DCC
R_{free} test set	1283 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	197.5	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 189.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14173	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CN2, VLB, 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	1.00	4/3367 (0.1%)	1.21	11/4579 (0.2%)
1	C	1.00	5/3320 (0.2%)	1.29	23/4520 (0.5%)
2	B	0.99	8/3312 (0.2%)	1.23	16/4498 (0.4%)
2	D	0.95	3/3309 (0.1%)	1.27	22/4494 (0.5%)
3	E	1.02	3/925 (0.3%)	1.39	9/1241 (0.7%)
All	All	0.99	23/14233 (0.2%)	1.26	81/19332 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	4
2	B	0	1
2	D	0	1
3	E	0	1
All	All	0	8

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	105	MET	SD-CE	11.52	2.08	1.79
1	A	36	MET	SD-CE	11.45	2.08	1.79
1	C	203	MET	SD-CE	11.29	2.07	1.79
2	B	325	MET	SD-CE	8.58	2.00	1.79
3	E	119	MET	SD-CE	7.35	1.98	1.79
1	A	62	VAL	CA-CB	7.31	1.63	1.54
2	B	391	ILE	CA-CB	7.09	1.64	1.54
1	A	193	THR	CA-CB	6.30	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	MET	SD-CE	6.27	1.95	1.79
1	C	309	HIS	CA-C	6.23	1.58	1.52
1	C	253	THR	CA-CB	6.07	1.63	1.53
3	E	96	MET	SD-CE	5.77	1.94	1.79
2	D	359	PRO	CA-C	5.74	1.57	1.52
2	B	182	VAL	CA-CB	5.63	1.61	1.54
2	B	75	MET	SD-CE	5.51	1.93	1.79
2	D	2	ARG	NE-CZ	5.50	1.39	1.33
1	A	14	VAL	CA-CB	-5.43	1.48	1.54
2	B	62	VAL	CA-CB	5.29	1.60	1.54
2	B	114	LEU	CA-C	-5.25	1.49	1.52
2	D	276	THR	CA-CB	5.22	1.62	1.53
1	C	353	VAL	CA-CB	-5.10	1.47	1.54
1	C	62	VAL	CA-CB	5.05	1.60	1.54
2	B	276	THR	CA-CB	5.02	1.61	1.53

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	301	GLN	O-C-N	-16.80	99.77	121.78
3	E	106	GLU	N-CA-C	-14.74	95.84	114.56
3	E	78	HIS	N-CA-C	-10.23	100.42	113.72
1	A	339	ARG	N-CA-C	9.74	120.75	108.19
1	C	250	VAL	N-CA-C	9.51	129.12	109.34
3	E	6	MET	N-CA-C	9.09	122.97	111.24
2	D	180	THR	N-CA-C	8.56	121.90	109.14
2	D	253	ARG	N-CA-C	-7.98	101.36	112.45
3	E	48	GLU	N-CA-C	7.83	119.45	111.07
3	E	134	ARG	N-CA-C	-7.76	104.71	114.56
1	C	359	PRO	O-C-N	7.39	124.71	121.31
1	C	249	ASN	N-CA-C	7.34	126.44	110.80
2	B	253	ARG	N-CA-C	-7.30	102.71	111.69
3	E	118	ALA	N-CA-C	-7.29	104.42	113.38
1	A	349	THR	N-CA-C	-7.18	95.50	110.80
1	C	155	GLU	N-CA-C	-7.17	103.39	111.07
2	B	158	ARG	N-CA-C	-7.17	101.03	110.43
2	D	181	VAL	CB-CA-C	-6.97	102.91	112.04
2	D	62	VAL	N-CA-C	6.94	123.86	108.88
3	E	54	LEU	N-CA-C	-6.89	106.07	114.75
1	C	301	GLN	CA-C-N	6.81	132.41	121.98
1	C	301	GLN	C-N-CA	6.81	132.41	121.98
2	D	275	LEU	N-CA-C	6.76	118.07	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	62	VAL	N-CA-C	6.74	123.44	108.88
2	D	248	LEU	O-C-N	6.69	126.73	120.71
1	A	280	LYS	N-CA-C	-6.65	104.31	112.88
3	E	17	GLY	N-CA-C	6.61	120.49	110.18
2	D	359	PRO	N-CA-C	6.46	118.58	110.70
2	D	260	VAL	N-CA-C	6.20	114.28	108.15
1	C	4	CYS	N-CA-C	6.10	117.38	107.32
2	D	431	GLU	N-CA-C	-6.08	105.52	113.12
2	B	168	THR	N-CA-C	6.00	118.53	109.23
2	D	436	GLN	N-CA-C	-6.00	100.08	108.54
1	C	39	ASP	N-CA-C	6.00	123.57	110.80
1	C	264	ARG	CA-C-N	5.90	132.59	121.97
1	C	264	ARG	C-N-CA	5.90	132.59	121.97
1	A	98	ASP	N-CA-C	5.84	117.59	110.41
1	A	169	PHE	CB-CA-C	-5.83	102.91	111.77
1	C	267	PHE	CB-CA-C	5.76	116.20	110.33
2	B	275	LEU	N-CA-C	5.73	116.65	108.74
2	B	61	TYR	N-CA-C	5.73	122.69	114.39
1	C	345	ASP	N-CA-C	5.68	122.91	110.80
1	A	4	CYS	N-CA-C	5.58	116.53	107.32
2	D	179	ASP	N-CA-C	-5.57	105.99	112.89
1	C	255	PHE	N-CA-C	-5.56	105.30	111.36
2	D	168	THR	N-CA-C	5.55	117.83	109.23
2	D	35	SER	CA-C-O	5.54	121.15	117.94
2	D	53	TYR	N-CA-C	5.53	119.22	107.67
2	B	265	LEU	N-CA-C	5.52	122.56	110.80
2	B	260	VAL	N-CA-C	5.51	113.60	108.15
1	C	169	PHE	CB-CA-C	-5.50	102.39	111.51
1	C	74	VAL	CB-CA-C	-5.46	104.76	111.92
1	C	168	GLU	CB-CA-C	5.42	118.78	109.51
2	D	264	ARG	CA-C-N	5.39	131.83	121.54
2	D	264	ARG	C-N-CA	5.39	131.83	121.54
1	C	250	VAL	CB-CA-C	-5.33	102.55	111.29
1	A	62	VAL	N-CA-C	5.32	120.37	108.88
1	C	249	ASN	CA-C-N	5.32	131.54	121.97
1	C	249	ASN	C-N-CA	5.32	131.54	121.97
2	D	265	LEU	N-CA-C	5.32	122.12	110.80
2	B	359	PRO	N-CA-C	5.28	117.14	110.70
2	D	244	PHE	N-CA-C	5.24	121.38	109.81
1	C	62	VAL	N-CA-C	5.21	120.14	108.88
2	B	268	PHE	CA-C-N	-5.21	114.37	121.61
2	B	268	PHE	C-N-CA	-5.21	114.37	121.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	353	VAL	CB-CA-C	-5.21	102.75	111.29
3	E	51	GLN	N-CA-C	-5.21	107.60	114.31
2	D	287	THR	N-CA-C	5.18	119.87	113.50
2	B	264	ARG	CA-C-N	5.16	131.39	121.54
2	B	264	ARG	C-N-CA	5.16	131.39	121.54
1	A	21	TRP	N-CA-C	-5.15	105.36	111.69
2	D	371	LEU	N-CA-C	5.13	121.72	110.80
1	A	264	ARG	CA-C-N	5.12	131.19	121.97
1	A	264	ARG	C-N-CA	5.12	131.19	121.97
2	B	244	PHE	N-CA-C	5.12	121.12	109.81
1	C	262	TYR	N-CA-C	5.10	117.44	108.82
2	D	61	TYR	N-CA-C	5.10	121.78	114.39
2	B	262	PHE	N-CA-C	5.10	118.36	107.91
1	A	102	ASN	N-CA-C	5.09	117.64	108.48
2	D	320	ARG	N-CA-C	5.03	116.61	108.26
2	B	4	ILE	N-CA-C	5.00	115.91	108.46

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	VAL	Peptide
2	B	162	PRO	Peptide
1	C	177	VAL	Peptide
1	C	248	LEU	Peptide
1	C	249	ASN	Peptide
1	C	301	GLN	Mainchain
2	D	162	PRO	Peptide
3	E	5	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3290	0	3154	250	0
1	C	3248	0	3087	273	0
2	B	3240	0	3056	320	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3237	0	3054	284	0
3	E	917	0	803	73	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	12	4	0
5	C	32	0	12	5	0
6	B	28	0	12	5	0
6	D	28	0	12	7	0
7	B	30	0	23	7	0
7	D	30	0	23	8	0
8	C	59	0	58	22	0
All	All	14173	0	13306	1157	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 42.

All (1157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.37	1.04
1:C:8:HIS:CD2	1:C:17:GLY:HA3	1.93	1.04
1:C:8:HIS:HD2	1:C:17:GLY:HA3	1.21	1.03
2:D:133:GLN:HE21	2:D:252:LEU:HB3	1.22	1.02
1:C:79:ARG:HH22	1:C:94:THR:CG2	1.72	1.01
1:A:346:TRP:O	1:A:346:TRP:CE3	2.14	1.00
2:D:241:CYS:HB3	2:D:247:GLN:HE21	1.18	1.00
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.90	0.99
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.44	0.98
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.94	0.97
1:C:206:ASN:HD21	5:C:601:GTP:N2	1.62	0.97
2:B:135:PHE:HB2	2:B:166:MET:HE1	1.46	0.97
1:C:79:ARG:NH2	1:C:94:THR:HG21	1.80	0.96
2:B:156:LYS:HG2	3:E:76:ARG:NH2	1.80	0.96
1:A:8:HIS:HD2	1:A:17:GLY:HA3	1.19	0.95
1:C:273:ALA:CB	1:C:274:PRO:HD3	1.94	0.95
1:A:273:ALA:HB3	1:A:274:PRO:CD	1.96	0.95
1:A:79:ARG:HH22	1:A:94:THR:CG2	1.78	0.95
1:C:206:ASN:HD21	5:C:601:GTP:HN22	0.97	0.95
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.28	0.95
2:B:241:CYS:CB	2:B:247:GLN:HE21	1.80	0.94
1:C:264:ARG:O	1:C:266:HIS:CD2	2.21	0.94
2:B:241:CYS:HB3	2:B:247:GLN:HE21	1.17	0.94
1:A:79:ARG:NH2	1:A:94:THR:HG21	1.83	0.93
2:B:352:LYS:HG3	7:B:700:CN2:O5	1.69	0.93
2:D:231:VAL:HG12	2:D:235:MET:HE2	1.49	0.93
2:D:165:ILE:HD11	2:D:252:LEU:HG	1.52	0.91
2:B:247:GLN:HG3	2:B:248:LEU:HG	1.50	0.91
1:A:206:ASN:HD21	5:A:600:GTP:HN22	0.96	0.91
2:B:287:THR:HG22	2:B:290:GLU:HB2	1.53	0.91
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.52	0.91
2:D:247:GLN:HG3	2:D:248:LEU:HG	1.53	0.90
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.34	0.90
2:D:172:VAL:HG11	2:D:387:LEU:HD21	1.51	0.90
2:D:401:ARG:HG3	2:D:401:ARG:NH1	1.72	0.90
1:A:273:ALA:CB	1:A:375:VAL:H	1.84	0.90
8:C:800:VLB:O72	8:C:800:VLB:H572	1.70	0.90
2:B:401:ARG:HG3	2:B:401:ARG:NH1	1.75	0.89
1:C:99:ALA:HB2	1:C:145:THR:HG22	1.55	0.89
1:A:115:ILE:HG13	1:A:152:LEU:HD23	1.54	0.89
2:B:54:ASN:HB2	2:B:64:ARG:HD3	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ILE:HG23	1:C:267:PHE:CZ	2.08	0.89
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.55	0.88
2:B:133:GLN:NE2	2:B:252:LEU:HB3	1.88	0.88
2:B:177:VAL:HA	8:C:800:VLB:H532	1.56	0.87
1:C:98:ASP:OD1	1:C:99:ALA:N	2.06	0.87
1:A:270:ALA:HB3	1:A:302:MET:CE	2.05	0.86
2:D:291:LEU:HD21	2:D:375:ALA:CB	2.03	0.86
1:A:99:ALA:HB2	1:A:145:THR:CG2	2.05	0.86
1:A:206:ASN:HD21	5:A:600:GTP:N2	1.73	0.86
1:C:178:SER:HB3	7:D:701:CN2:S1	2.16	0.86
2:D:287:THR:HG22	2:D:290:GLU:HB2	1.57	0.86
1:C:206:ASN:ND2	5:C:601:GTP:HN22	1.74	0.86
1:C:234:ILE:HD11	1:C:272:TYR:HB2	1.57	0.86
1:A:98:ASP:OD1	1:A:99:ALA:N	2.09	0.85
1:C:329:ASN:HA	8:C:800:VLB:C21	2.03	0.85
2:D:401:ARG:HH11	2:D:401:ARG:CG	1.85	0.85
1:A:270:ALA:O	1:A:302:MET:HB2	1.75	0.85
2:B:140:SER:HA	2:B:171:VAL:HG23	1.59	0.85
1:A:238:ILE:HG12	1:A:378:LEU:HD11	1.59	0.84
1:C:273:ALA:CB	1:C:375:VAL:H	1.91	0.84
2:D:350:ASN:HD22	2:D:350:ASN:H	1.22	0.84
2:D:241:CYS:CB	2:D:247:GLN:HE21	1.91	0.84
2:B:216:THR:CG2	2:B:299:LYS:HD3	2.09	0.83
2:D:164:ARG:HE	2:D:164:ARG:HA	1.42	0.83
1:C:115:ILE:HG13	1:C:152:LEU:HD23	1.58	0.83
2:B:180:THR:HB	2:B:183:GLU:OE2	1.76	0.83
8:C:800:VLB:H572	8:C:800:VLB:H511	1.60	0.83
3:E:4:ALA:HB3	3:E:24:LEU:HD11	1.60	0.82
2:B:241:CYS:CB	2:B:247:GLN:NE2	2.40	0.82
2:D:223:THR:HB	2:D:225:GLY:N	1.94	0.82
2:B:336:GLN:OE1	2:B:351:VAL:HG11	1.78	0.82
2:B:265:LEU:HD12	2:B:265:LEU:O	1.80	0.82
1:A:36:MET:HG2	1:A:61:HIS:NE2	1.94	0.82
1:C:41:THR:HG21	1:C:61:HIS:HE1	1.45	0.82
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.60	0.81
2:B:165:ILE:HD11	2:B:252:LEU:HG	1.61	0.81
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.05	0.81
2:B:401:ARG:HH11	2:B:401:ARG:CG	1.88	0.81
2:D:224:TYR:O	2:D:228:ASN:ND2	2.13	0.81
2:D:205:ASP:OD1	2:D:207:GLU:HB3	1.81	0.80
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:VAL:HG22	8:C:800:VLB:H532	1.64	0.80
1:C:97:GLU:HG2	1:C:110:ILE:HD11	1.64	0.80
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.12	0.79
2:B:88:ARG:O	2:B:91:ASN:HB2	1.82	0.79
2:B:216:THR:HG23	2:B:299:LYS:HD3	1.63	0.79
1:C:99:ALA:HB2	1:C:145:THR:CG2	2.13	0.79
1:C:238:ILE:HG12	1:C:378:LEU:HD11	1.64	0.79
2:B:231:VAL:HG12	2:B:235:MET:HE2	1.63	0.79
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.64	0.78
2:D:336:GLN:OE1	2:D:351:VAL:HG11	1.83	0.78
2:B:350:ASN:H	2:B:350:ASN:HD22	1.32	0.78
1:A:128:GLN:O	1:A:128:GLN:HG2	1.80	0.78
1:C:241:SER:HB2	1:C:250:VAL:O	1.83	0.78
2:D:135:PHE:HB2	2:D:166:MET:HE1	1.66	0.78
2:D:250:ALA:CB	7:D:701:CN2:H7	2.14	0.78
2:D:70:LEU:HA	2:D:95:GLY:HA3	1.64	0.77
2:D:70:LEU:HD12	2:D:145:THR:HB	1.66	0.77
2:D:332:MET:HG3	2:D:353:THR:HG21	1.66	0.77
2:D:265:LEU:HD12	2:D:265:LEU:O	1.84	0.77
1:A:294:ALA:O	1:A:297:GLU:HB3	1.84	0.77
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.49	0.77
2:D:333:LEU:O	2:D:337:ASN:ND2	2.18	0.77
1:A:265:ILE:HG23	1:A:267:PHE:CZ	2.20	0.77
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.66	0.77
2:D:2:ARG:NH1	2:D:133:GLN:HA	2.01	0.76
2:D:133:GLN:NE2	2:D:252:LEU:HB3	2.01	0.76
1:A:388:TRP:CE3	1:A:388:TRP:HA	2.21	0.76
2:B:332:MET:HG3	2:B:353:THR:HG21	1.66	0.76
1:C:329:ASN:CA	8:C:800:VLB:H211	2.09	0.76
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.67	0.76
1:A:178:SER:HB3	7:B:700:CN2:S1	2.25	0.76
2:B:2:ARG:NH1	2:B:133:GLN:HA	2.01	0.76
2:B:264:ARG:O	2:B:266:HIS:CD2	2.40	0.75
2:D:245:PRO:HG2	2:D:247:GLN:HG2	1.68	0.75
2:D:264:ARG:O	2:D:266:HIS:CD2	2.40	0.75
1:A:260:VAL:HB	1:A:266:HIS:HB2	1.68	0.75
3:E:123:LEU:C	3:E:125:GLU:H	1.95	0.75
1:C:252:LEU:O	1:C:253:THR:HB	1.86	0.74
1:A:318:LEU:HB2	1:A:376:CYS:HB3	1.68	0.74
3:E:55:GLU:HA	3:E:58:GLU:HB2	1.69	0.74
2:B:291:LEU:HD21	2:B:375:ALA:CB	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:TRP:CD2	2:D:257:VAL:HG23	2.22	0.74
1:A:292:THR:O	1:A:295:CYS:HB2	1.88	0.74
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.70	0.74
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.23	0.73
2:D:180:THR:HG22	2:D:182:VAL:H	1.52	0.73
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.28	0.73
2:B:70:LEU:HA	2:B:95:GLY:HA3	1.70	0.73
2:B:205:ASP:OD1	2:B:207:GLU:HB3	1.89	0.73
2:D:48:ARG:NH1	2:D:245:PRO:HD2	2.03	0.73
1:A:206:ASN:ND2	5:A:600:GTP:HN22	1.80	0.73
2:D:88:ARG:O	2:D:91:ASN:HB2	1.89	0.73
1:C:330:ALA:O	1:C:334:THR:OG1	2.07	0.72
2:D:414:ASP:HB3	2:D:416:MET:HE2	1.71	0.72
3:E:127:ASP:C	3:E:129:HIS:H	1.95	0.72
2:B:123:ARG:O	2:B:127:GLU:HB2	1.88	0.72
2:D:48:ARG:HH12	2:D:245:PRO:HD2	1.55	0.72
2:D:99:ALA:HB1	2:D:145:THR:HG21	1.70	0.72
2:D:140:SER:HA	2:D:171:VAL:HG23	1.70	0.72
2:B:99:ALA:HB1	2:B:145:THR:HG21	1.70	0.72
2:B:151:THR:HB	2:B:193:GLN:HG2	1.71	0.72
1:C:288:VAL:HG11	1:C:327:ASP:HB3	1.69	0.72
1:C:288:VAL:HG21	1:C:327:ASP:OD2	1.90	0.72
1:C:328:VAL:HG12	1:C:332:ILE:HD12	1.72	0.72
1:C:191:THR:HG23	1:C:425:MET:HE3	1.71	0.71
2:B:414:ASP:HB3	2:B:416:MET:HE2	1.72	0.71
2:D:257:VAL:HG13	2:D:257:VAL:O	1.87	0.71
2:B:176:LYS:HB3	8:C:800:VLB:H222	1.72	0.71
2:D:16:ILE:HG23	2:D:235:MET:HE1	1.70	0.71
2:B:273:ALA:CB	2:B:274:PRO:CD	2.66	0.71
1:C:90:GLU:HB3	1:C:121:ARG:HD3	1.73	0.71
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.19	0.71
2:B:156:LYS:HG2	3:E:76:ARG:HH21	1.56	0.71
1:A:273:ALA:HB2	1:A:375:VAL:H	1.53	0.71
2:D:315:VAL:HG12	2:D:351:VAL:HG23	1.71	0.71
1:C:6:SER:HB3	1:C:8:HIS:HE1	1.55	0.71
2:B:403:ALA:C	2:B:405:LEU:H	1.97	0.70
2:B:336:GLN:OE1	2:B:351:VAL:CG1	2.39	0.70
1:C:40:LYS:O	1:C:41:THR:HB	1.89	0.70
1:C:66:VAL:HG11	1:C:122:ILE:HG22	1.72	0.70
2:B:33:THR:O	2:B:34:GLY:O	2.09	0.70
2:D:2:ARG:O	2:D:3:GLU:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:VAL:HG22	2:D:135:PHE:CD2	2.27	0.70
1:C:128:GLN:O	1:C:128:GLN:HG2	1.92	0.70
2:B:181:VAL:O	2:B:398:MET:HE1	1.91	0.70
1:A:99:ALA:CB	1:A:145:THR:HG22	2.16	0.69
2:B:403:ALA:O	2:B:405:LEU:N	2.25	0.69
1:C:288:VAL:HG13	1:C:323:VAL:HG13	1.73	0.69
2:B:221:THR:HA	8:C:800:VLB:H761	1.74	0.69
1:C:68:VAL:HG11	1:C:118:VAL:CG2	2.22	0.69
1:C:115:ILE:HG13	1:C:152:LEU:CD2	2.23	0.69
1:C:265:ILE:HG12	1:C:265:ILE:O	1.92	0.69
2:D:5:VAL:HG12	2:D:64:ARG:HG2	1.74	0.69
2:B:220:THR:O	2:B:222:PRO:HD3	1.93	0.69
1:A:8:HIS:CD2	1:A:17:GLY:CA	2.74	0.69
1:C:328:VAL:HG12	1:C:332:ILE:CD1	2.22	0.69
1:A:191:THR:HG23	1:A:425:MET:HE3	1.74	0.69
1:A:273:ALA:CB	1:A:274:PRO:CD	2.56	0.69
2:B:269:MET:HG2	2:B:384:ILE:HG12	1.75	0.69
1:A:291:ILE:HB	1:A:375:VAL:HG23	1.75	0.68
1:A:323:VAL:HG12	1:A:355:ILE:HD13	1.75	0.68
1:A:388:TRP:HA	1:A:388:TRP:HE3	1.58	0.68
1:C:68:VAL:HG11	1:C:118:VAL:HG22	1.76	0.68
2:B:212:ILE:HG22	2:B:230:LEU:HD21	1.75	0.68
2:D:111:GLY:HA2	2:D:149:MET:CE	2.23	0.68
2:D:237:GLY:CA	2:D:376:THR:HG21	2.24	0.68
1:C:88:HIS:HB2	1:C:91:GLN:NE2	2.04	0.68
1:A:68:VAL:HG11	1:A:118:VAL:HG22	1.75	0.68
1:A:341:ILE:HG12	1:A:342:GLN:H	1.59	0.68
2:B:133:GLN:HE21	2:B:252:LEU:CB	1.98	0.68
2:D:159:GLU:HB2	3:E:123:LEU:HD23	1.76	0.68
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.29	0.68
2:D:273:ALA:CB	2:D:274:PRO:CD	2.70	0.68
1:A:68:VAL:HG11	1:A:118:VAL:CG2	2.24	0.68
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.76	0.68
2:B:250:ALA:CB	7:B:700:CN2:H7	2.24	0.67
1:C:265:ILE:CG2	1:C:267:PHE:CZ	2.77	0.67
2:D:33:THR:O	2:D:34:GLY:O	2.12	0.67
1:A:6:SER:HB3	1:A:8:HIS:HE1	1.59	0.67
1:A:115:ILE:HG13	1:A:152:LEU:CD2	2.23	0.67
2:D:251:ASP:C	2:D:253:ARG:H	2.01	0.67
2:D:266:HIS:HB3	2:D:380:ASN:HD21	1.58	0.67
1:C:210:TYR:CE1	1:C:214:ARG:HD2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:ILE:HG22	2:D:133:GLN:HB3	1.77	0.67
2:B:251:ASP:C	2:B:253:ARG:H	2.01	0.67
3:E:112:ARG:O	3:E:115:HIS:N	2.21	0.67
2:D:145:THR:HG23	6:D:603:GDP:O3B	1.95	0.67
1:A:407:TRP:CD2	2:B:257:VAL:HG23	2.30	0.67
2:B:114:LEU:O	2:B:116:ASP:N	2.28	0.67
1:C:350:GLY:O	1:C:351:PHE:HB2	1.93	0.67
1:C:316:CYS:O	1:C:377:MET:HA	1.95	0.66
1:C:41:THR:HG21	1:C:61:HIS:CE1	2.30	0.66
2:D:195:VAL:HA	2:D:265:LEU:HD23	1.76	0.66
2:B:154:ILE:HG12	2:B:155:SER:N	2.08	0.66
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.77	0.66
1:C:234:ILE:CD1	1:C:272:TYR:HB2	2.26	0.66
1:A:98:ASP:HB3	2:B:251:ASP:OD2	1.96	0.66
2:D:250:ALA:HB1	7:D:701:CN2:H7	1.77	0.66
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.78	0.66
2:B:12:CYS:SG	2:B:171:VAL:HG21	2.35	0.65
1:C:294:ALA:O	1:C:297:GLU:HB3	1.96	0.65
2:B:176:LYS:O	2:B:177:VAL:HB	1.96	0.65
2:B:111:GLY:HA2	2:B:149:MET:CE	2.25	0.65
2:D:164:ARG:HE	2:D:164:ARG:CA	2.03	0.65
2:B:177:VAL:HG22	8:C:800:VLB:C53	2.25	0.65
2:B:308:ARG:HH11	2:B:308:ARG:CG	2.08	0.65
1:C:181:VAL:HG23	2:D:258:ASN:HD22	1.62	0.65
2:D:191:VAL:HG11	2:D:425:MET:HE3	1.78	0.65
2:B:210:TYR:HD1	2:B:210:TYR:C	2.04	0.65
2:B:224:TYR:OH	6:B:602:GDP:H2'	1.96	0.65
1:C:240:ALA:O	1:C:243:ARG:N	2.30	0.65
2:D:315:VAL:CG1	2:D:351:VAL:HG23	2.27	0.65
3:E:115:HIS:C	3:E:115:HIS:HD1	2.04	0.65
1:C:407:TRP:CG	2:D:257:VAL:HG23	2.32	0.65
2:B:250:ALA:HB1	7:B:700:CN2:H7	1.78	0.65
1:C:48:SER:C	1:C:50:ASN:H	2.02	0.64
1:C:334:THR:C	1:C:336:LYS:H	2.04	0.64
1:C:20:CYS:HB3	1:C:232:GLY:HA2	1.79	0.64
2:D:158:ARG:O	2:D:159:GLU:CB	2.46	0.64
2:D:5:VAL:CG2	2:D:135:PHE:HD2	2.10	0.64
1:A:8:HIS:HD2	1:A:17:GLY:CA	2.04	0.64
2:B:48:ARG:HH12	2:B:245:PRO:HD2	1.63	0.64
1:C:36:MET:C	1:C:38:SER:H	2.05	0.64
2:D:141:LEU:HD23	2:D:172:VAL:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:ALA:HB1	2:B:145:THR:CG2	2.29	0.63
2:D:42:LEU:O	2:D:44:LEU:N	2.31	0.63
1:A:407:TRP:HZ2	2:B:260:VAL:HG23	1.62	0.63
1:C:8:HIS:CD2	1:C:17:GLY:CA	2.77	0.63
2:B:333:LEU:O	2:B:337:ASN:ND2	2.31	0.63
2:D:114:LEU:O	2:D:116:ASP:N	2.31	0.63
1:A:273:ALA:HB2	1:A:375:VAL:N	2.14	0.63
1:C:253:THR:H	1:C:256:GLN:HB2	1.62	0.63
2:D:9:ALA:HA	2:D:68:VAL:O	1.99	0.63
2:D:95:GLY:O	2:D:96:GLN:HB2	1.97	0.63
2:D:336:GLN:OE1	2:D:351:VAL:CG1	2.46	0.63
1:C:262:TYR:O	1:C:263:PRO:C	2.42	0.63
1:A:190:THR:CG2	1:A:191:THR:N	2.62	0.63
2:B:147:SER:O	2:B:151:THR:OG1	2.15	0.63
2:B:414:ASP:HB3	2:B:416:MET:CE	2.28	0.63
1:C:221:ARG:CB	2:D:325:MET:HE2	2.29	0.63
2:D:347:ILE:O	2:D:348:PRO:O	2.17	0.63
2:B:95:GLY:O	2:B:96:GLN:HB2	1.98	0.62
2:B:210:TYR:C	2:B:210:TYR:CD1	2.77	0.62
2:D:54:ASN:HB2	2:D:64:ARG:HD3	1.80	0.62
2:B:159:GLU:HB2	3:E:72:LEU:HD23	1.81	0.62
2:B:195:VAL:HA	2:B:265:LEU:HD23	1.82	0.62
2:B:212:ILE:CG2	2:B:230:LEU:HD21	2.29	0.62
1:C:288:VAL:CG1	1:C:327:ASP:HB3	2.30	0.62
2:D:185:TYR:HE2	2:D:398:MET:HB3	1.65	0.62
1:A:262:TYR:O	1:A:266:HIS:HD2	1.82	0.62
1:A:265:ILE:HG12	1:A:265:ILE:O	1.99	0.62
1:A:266:HIS:O	1:A:268:PRO:HD3	1.99	0.62
2:B:4:ILE:HG22	2:B:133:GLN:HB3	1.81	0.62
2:B:135:PHE:HB2	2:B:166:MET:CE	2.25	0.62
1:C:181:VAL:CG2	2:D:258:ASN:HD22	2.11	0.62
1:A:66:VAL:HG11	1:A:122:ILE:HG22	1.82	0.62
2:B:156:LYS:HA	3:E:76:ARG:HH21	1.62	0.62
2:B:226:ASP:O	2:B:227:LEU:CB	2.47	0.62
1:C:8:HIS:HD2	1:C:17:GLY:CA	2.06	0.62
2:B:141:LEU:HD23	2:B:172:VAL:HG22	1.82	0.62
3:E:84:GLN:HA	3:E:87:ILE:HG22	1.82	0.61
1:A:88:HIS:HB2	1:A:91:GLN:NE2	2.11	0.61
2:B:42:LEU:O	2:B:44:LEU:N	2.33	0.61
1:C:388:TRP:HA	1:C:388:TRP:HE3	1.64	0.61
2:B:320:ARG:HA	2:B:356:CYS:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLU:OE1	1:A:197:HIS:CE1	2.54	0.61
2:B:265:LEU:O	2:B:266:HIS:O	2.19	0.61
1:C:244:PHE:CZ	1:C:358:GLN:HG2	2.35	0.61
1:C:407:TRP:CG	2:D:257:VAL:CG2	2.83	0.61
1:A:177:VAL:HG22	1:A:210:TYR:CD2	2.35	0.61
1:C:260:VAL:HG12	1:C:266:HIS:HB2	1.82	0.61
2:B:236:SER:O	2:B:240:THR:HG23	2.01	0.61
2:B:315:VAL:HG12	2:B:351:VAL:HG23	1.82	0.61
2:B:20:PHE:O	2:B:24:ILE:HG23	2.01	0.61
2:B:70:LEU:HD12	2:B:145:THR:HB	1.82	0.61
2:B:177:VAL:HG22	8:C:800:VLB:H712	1.81	0.61
1:C:312:TYR:HB3	1:C:343:PHE:CE2	2.36	0.61
8:C:800:VLB:H511	8:C:800:VLB:C57	2.31	0.61
2:D:70:LEU:CD1	2:D:145:THR:HB	2.30	0.61
2:D:404:PHE:HD1	2:D:404:PHE:N	1.99	0.60
1:C:6:SER:HB3	1:C:8:HIS:CE1	2.36	0.60
3:E:51:GLN:C	3:E:53:LYS:H	2.09	0.60
3:E:67:GLU:C	3:E:69:LEU:H	2.07	0.60
2:D:287:THR:HG22	2:D:290:GLU:H	1.66	0.60
3:E:94:ILE:CG2	3:E:95:LYS:N	2.63	0.60
2:B:48:ARG:NH1	2:B:245:PRO:HD2	2.16	0.60
2:D:298:SER:C	2:D:300:ASN:H	2.10	0.60
1:A:273:ALA:CB	1:A:375:VAL:N	2.62	0.60
1:A:179:THR:O	7:B:700:CN2:H132	2.00	0.60
7:B:700:CN2:C12	7:B:700:CN2:H15	2.31	0.60
1:C:230:LEU:HD12	1:C:230:LEU:O	2.02	0.60
1:C:273:ALA:CB	1:C:375:VAL:N	2.63	0.60
2:D:99:ALA:HB1	2:D:145:THR:CG2	2.32	0.60
6:D:603:GDP:O2B	6:D:603:GDP:O1A	2.20	0.60
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.82	0.60
2:B:151:THR:HG22	2:B:193:GLN:HB3	1.83	0.60
2:B:216:THR:HG21	2:B:299:LYS:HD3	1.84	0.60
2:B:266:HIS:HB3	2:B:380:ASN:HD21	1.65	0.59
1:C:142:GLY:HA3	1:C:183:GLU:HG3	1.84	0.59
1:A:246:GLY:O	1:A:247:ALA:O	2.20	0.59
2:B:59:ASN:O	2:B:60:LYS:O	2.20	0.59
2:B:185:TYR:HE2	2:B:398:MET:HB3	1.67	0.59
1:C:183:GLU:HB3	1:C:184:PRO:CD	2.32	0.59
2:B:306:ASP:O	2:B:308:ARG:N	2.35	0.59
1:C:111:GLY:O	1:C:113:GLU:N	2.35	0.59
2:D:123:ARG:O	2:D:127:GLU:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:352:LYS:HG3	7:D:701:CN2:O5	2.00	0.59
1:A:27:GLU:HG3	1:A:361:THR:OG1	2.02	0.59
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.37	0.59
2:B:237:GLY:CA	2:B:376:THR:HG21	2.32	0.59
2:B:4:ILE:HD11	2:B:52:TYR:CE2	2.38	0.59
2:B:287:THR:HG22	2:B:290:GLU:CB	2.31	0.59
1:C:125:LEU:HD23	1:C:128:GLN:HE22	1.67	0.59
1:A:163:LYS:H	1:A:163:LYS:HE3	1.67	0.59
2:B:158:ARG:O	2:B:159:GLU:CB	2.49	0.59
1:C:324:VAL:HG13	1:C:325:PRO:HD2	1.85	0.59
1:C:387:ALA:HA	1:C:390:ARG:NH1	2.18	0.59
2:D:154:ILE:HG12	2:D:155:SER:N	2.15	0.59
2:D:308:ARG:HH11	2:D:308:ARG:CG	2.16	0.59
2:B:262:PHE:O	2:B:266:HIS:CD2	2.56	0.59
2:D:151:THR:HA	2:D:154:ILE:HD13	1.85	0.59
1:C:143:GLY:O	1:C:147:SER:OG	2.20	0.59
1:C:177:VAL:HG22	1:C:210:TYR:CD2	2.37	0.59
1:C:346:TRP:HZ2	1:C:435:VAL:CG1	2.15	0.59
2:D:183:GLU:O	2:D:184:PRO:C	2.44	0.59
2:D:291:LEU:HD21	2:D:375:ALA:HB3	1.83	0.59
1:A:176:GLN:HG2	1:A:177:VAL:H	1.68	0.58
1:A:411:GLU:O	3:E:61:ARG:HD3	2.03	0.58
2:D:190:SER:O	2:D:193:GLN:N	2.36	0.58
2:D:306:ASP:O	2:D:308:ARG:N	2.36	0.58
2:B:407:TRP:CD1	1:C:257:THR:HG23	2.37	0.58
2:B:287:THR:HG22	2:B:290:GLU:H	1.68	0.58
2:B:347:ILE:CG2	2:B:350:ASN:HB3	2.26	0.58
1:C:51:THR:HG21	1:C:242:LEU:HD13	1.85	0.58
1:A:371:VAL:HG12	1:A:372:GLN:H	1.68	0.58
2:B:70:LEU:C	2:B:95:GLY:HA3	2.29	0.58
2:B:287:THR:O	2:B:288:VAL:HB	2.04	0.58
1:C:41:THR:O	1:C:41:THR:HG23	2.03	0.58
1:A:198:SER:O	1:A:265:ILE:HG13	2.03	0.58
2:D:404:PHE:N	2:D:404:PHE:CD1	2.70	0.58
2:B:156:LYS:HG2	3:E:76:ARG:CZ	2.32	0.58
1:C:223:THR:N	1:C:226:ASN:HB2	2.18	0.58
2:D:209:LEU:HD21	2:D:231:VAL:HG22	1.84	0.58
2:D:226:ASP:O	2:D:227:LEU:CB	2.51	0.58
1:A:167:LEU:HD13	1:A:252:LEU:HD13	1.85	0.58
3:E:125:GLU:C	3:E:127:ASP:H	2.12	0.58
1:A:315:CYS:HB3	1:A:351:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:87:ILE:O	3:E:91:ASN:ND2	2.37	0.58
1:A:271:THR:O	1:A:376:CYS:O	2.22	0.58
1:C:125:LEU:HD23	1:C:128:GLN:NE2	2.19	0.58
2:B:264:ARG:O	2:B:266:HIS:N	2.34	0.58
1:C:356:ASN:O	1:C:358:GLN:N	2.36	0.58
2:B:183:GLU:N	2:B:184:PRO:HD2	2.19	0.57
1:C:181:VAL:HG23	2:D:258:ASN:ND2	2.19	0.57
2:D:151:THR:HG22	2:D:193:GLN:HB3	1.86	0.57
1:C:182:VAL:CG2	1:C:408:TYR:OH	2.53	0.57
1:A:204:VAL:HG22	1:A:302:MET:HE1	1.86	0.57
2:B:298:SER:C	2:B:300:ASN:H	2.13	0.57
1:C:291:ILE:HB	1:C:375:VAL:HG23	1.84	0.57
3:E:115:HIS:O	3:E:115:HIS:ND1	2.33	0.57
1:A:341:ILE:HD13	1:A:341:ILE:H	1.69	0.57
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.40	0.57
1:C:325:PRO:HB2	8:C:800:VLB:H763	1.86	0.57
1:A:190:THR:HG23	1:A:191:THR:N	2.18	0.57
2:B:262:PHE:O	2:B:266:HIS:HD2	1.87	0.57
1:C:288:VAL:HG11	1:C:327:ASP:CB	2.33	0.57
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.85	0.57
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.85	0.57
1:C:54:SER:HB3	1:C:64:ARG:HE	1.70	0.57
2:D:136:GLN:HA	2:D:167:ASN:O	2.05	0.57
1:A:180:ALA:O	1:A:181:VAL:C	2.48	0.57
2:B:190:SER:O	2:B:191:VAL:C	2.48	0.57
1:C:48:SER:C	1:C:50:ASN:N	2.63	0.57
1:C:266:HIS:O	1:C:268:PRO:HD3	2.03	0.57
2:B:6:HIS:CE1	2:B:8:GLN:HB2	2.40	0.57
2:B:183:GLU:O	2:B:184:PRO:C	2.47	0.57
8:C:800:VLB:O72	8:C:800:VLB:C57	2.50	0.57
2:D:133:GLN:HE21	2:D:252:LEU:CB	2.08	0.57
1:C:182:VAL:HG23	1:C:408:TYR:OH	2.05	0.56
1:C:176:GLN:HG2	1:C:177:VAL:H	1.69	0.56
1:A:6:SER:HB3	1:A:8:HIS:CE1	2.41	0.56
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.39	0.56
2:D:265:LEU:O	2:D:266:HIS:O	2.23	0.56
2:B:2:ARG:O	2:B:3:GLU:HB2	2.04	0.56
2:B:145:THR:HG23	6:B:602:GDP:O3B	2.06	0.56
1:C:102:ASN:OD1	1:C:105:ARG:HB2	2.05	0.56
1:C:248:LEU:O	1:C:249:ASN:HB2	2.05	0.56
2:D:159:GLU:HB2	3:E:123:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:ASP:OD1	1:C:429:GLU:OE1	2.24	0.56
2:D:180:THR:HG22	2:D:181:VAL:N	2.20	0.56
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.87	0.56
3:E:94:ILE:HG22	3:E:95:LYS:H	1.69	0.56
1:C:264:ARG:C	1:C:266:HIS:CD2	2.84	0.56
2:B:4:ILE:HD11	2:B:52:TYR:CZ	2.40	0.56
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.87	0.56
2:B:262:PHE:O	2:B:264:ARG:N	2.38	0.56
3:E:76:ARG:O	3:E:79:GLU:HB2	2.05	0.56
1:A:265:ILE:CG2	1:A:267:PHE:CZ	2.89	0.56
2:B:191:VAL:HG11	2:B:425:MET:HE3	1.88	0.56
1:C:111:GLY:O	1:C:112:LYS:C	2.49	0.56
2:D:224:TYR:CE2	6:D:603:GDP:C5	2.94	0.56
3:E:123:LEU:C	3:E:125:GLU:N	2.64	0.55
1:A:72:PRO:O	1:A:74:VAL:N	2.38	0.55
1:A:102:ASN:ND2	1:A:104:ALA:HB3	2.21	0.55
2:B:64:ARG:HG3	2:B:125:GLU:OE1	2.05	0.55
2:B:177:VAL:CG2	8:C:800:VLB:H532	2.33	0.55
3:E:67:GLU:O	3:E:71:HIS:HB2	2.05	0.55
1:C:111:GLY:C	1:C:113:GLU:N	2.62	0.55
3:E:127:ASP:C	3:E:129:HIS:N	2.64	0.55
2:B:164:ARG:HE	2:B:164:ARG:HA	1.71	0.55
2:B:223:THR:HB	2:B:225:GLY:N	2.21	0.55
2:B:71:GLU:O	2:B:71:GLU:HG2	2.07	0.55
1:A:265:ILE:O	1:A:266:HIS:O	2.25	0.55
2:B:414:ASP:CB	2:B:416:MET:HE2	2.36	0.55
1:C:70:LEU:CD2	1:C:110:ILE:HG23	2.37	0.55
1:C:265:ILE:HG23	1:C:267:PHE:CE1	2.42	0.55
2:D:226:ASP:O	2:D:227:LEU:HB2	2.07	0.55
2:D:264:ARG:O	2:D:266:HIS:N	2.32	0.55
1:A:412:GLY:O	3:E:60:ARG:NH1	2.40	0.55
2:B:158:ARG:HH11	2:B:158:ARG:CG	2.20	0.55
2:B:396:THR:O	2:B:400:ARG:HB2	2.07	0.55
2:D:147:SER:O	2:D:151:THR:OG1	2.15	0.55
2:B:213:CYS:HA	2:B:217:LEU:HD12	1.89	0.55
1:C:98:ASP:HB3	2:D:251:ASP:OD2	2.07	0.55
1:C:191:THR:HG23	1:C:425:MET:CE	2.35	0.55
1:C:54:SER:O	1:C:56:THR:N	2.40	0.55
2:D:152:LEU:O	2:D:153:LEU:C	2.50	0.55
1:C:288:VAL:CG1	1:C:323:VAL:HG13	2.37	0.55
2:D:141:LEU:CD2	2:D:172:VAL:HG22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:PRO:HG2	2:B:247:GLN:HG2	1.89	0.54
1:C:273:ALA:CB	1:C:274:PRO:CD	2.68	0.54
1:C:273:ALA:HB2	1:C:375:VAL:N	2.21	0.54
2:B:70:LEU:CA	2:B:95:GLY:HA3	2.38	0.54
2:B:416:MET:O	2:B:420:GLU:HB2	2.07	0.54
1:C:177:VAL:CG2	1:C:210:TYR:CD2	2.90	0.54
2:B:133:GLN:NE2	2:B:252:LEU:CB	2.65	0.54
1:C:318:LEU:HB2	1:C:376:CYS:HB3	1.89	0.54
1:A:313:MET:HG3	1:A:380:ASN:O	2.07	0.54
2:B:347:ILE:O	2:B:348:PRO:O	2.25	0.54
2:D:5:VAL:CG2	2:D:135:PHE:CD2	2.87	0.54
2:D:180:THR:HG21	2:D:182:VAL:HG22	1.89	0.54
2:D:369:ARG:O	2:D:370:GLY:C	2.51	0.54
2:B:228:ASN:HD21	6:B:602:GDP:HN1	1.55	0.54
2:D:124:LYS:O	2:D:128:SER:HB2	2.08	0.54
1:C:198:SER:O	1:C:265:ILE:HG13	2.08	0.54
2:D:241:CYS:CB	2:D:247:GLN:NE2	2.52	0.54
2:D:347:ILE:HG22	2:D:347:ILE:O	2.07	0.54
2:B:216:THR:O	2:B:217:LEU:HG	2.08	0.54
2:D:210:TYR:CD1	2:D:210:TYR:C	2.86	0.54
1:A:262:TYR:O	1:A:266:HIS:CD2	2.61	0.54
2:D:180:THR:HB	2:D:183:GLU:OE2	2.07	0.54
3:E:19:SER:O	3:E:20:PHE:HB3	2.07	0.54
1:A:205:ASP:CB	1:A:303:VAL:HA	2.38	0.54
1:A:230:LEU:HD12	1:A:230:LEU:O	2.07	0.54
1:C:344:VAL:O	1:C:346:TRP:N	2.35	0.54
2:D:59:ASN:O	2:D:60:LYS:O	2.25	0.54
1:A:387:ALA:HA	1:A:390:ARG:NH1	2.23	0.54
2:B:369:ARG:O	2:B:370:GLY:O	2.26	0.53
1:A:404:PHE:O	1:A:405:VAL:C	2.50	0.53
2:B:269:MET:HB3	2:B:303:ALA:HB3	1.89	0.53
2:D:7:ILE:HD13	2:D:153:LEU:HD13	1.90	0.53
1:A:182:VAL:HG23	1:A:408:TYR:OH	2.08	0.53
1:A:407:TRP:HZ2	2:B:260:VAL:CG2	2.20	0.53
2:B:152:LEU:O	2:B:153:LEU:C	2.47	0.53
1:C:404:PHE:O	1:C:405:VAL:C	2.51	0.53
2:D:51:VAL:HG12	2:D:52:TYR:CD1	2.43	0.53
2:D:114:LEU:O	2:D:115:VAL:C	2.51	0.53
1:A:239:THR:O	1:A:240:ALA:C	2.51	0.53
1:C:287:SER:O	1:C:291:ILE:HG12	2.08	0.53
2:D:6:HIS:HD2	2:D:136:GLN:HG3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:GLY:O	2:B:96:GLN:CB	2.57	0.53
2:B:102:ASN:OD1	2:B:105:LYS:HB2	2.08	0.53
2:B:205:ASP:OD1	2:B:207:GLU:N	2.42	0.53
1:C:79:ARG:NH2	1:C:94:THR:CG2	2.57	0.53
1:C:108:TYR:O	1:C:112:LYS:HB2	2.08	0.53
1:C:187:SER:O	1:C:191:THR:HG22	2.09	0.53
1:C:239:THR:O	1:C:240:ALA:C	2.52	0.53
2:B:70:LEU:HD11	2:B:149:MET:HE3	1.90	0.53
2:B:257:VAL:HG13	2:B:257:VAL:O	2.07	0.53
1:C:190:THR:CG2	1:C:191:THR:N	2.71	0.53
2:D:414:ASP:CB	2:D:416:MET:HE2	2.38	0.53
2:B:16:ILE:HG23	2:B:235:MET:HE1	1.90	0.53
1:C:332:ILE:O	1:C:335:ILE:N	2.42	0.53
2:D:236:SER:O	2:D:240:THR:HG23	2.09	0.53
2:D:382:THR:HB	2:D:436:GLN:HE21	1.74	0.53
2:B:296:PHE:CE2	2:B:377:PHE:CE1	2.97	0.53
1:C:70:LEU:HD22	1:C:110:ILE:HG23	1.90	0.53
1:C:180:ALA:O	1:C:181:VAL:C	2.50	0.53
2:D:70:LEU:CA	2:D:95:GLY:HA3	2.37	0.53
2:D:224:TYR:CD2	6:D:603:GDP:C6	2.97	0.53
7:D:701:CN2:H62	7:D:701:CN2:H43	1.91	0.53
1:A:177:VAL:CG2	1:A:210:TYR:CD2	2.93	0.52
2:D:11:GLN:CG	2:D:74:THR:HG21	2.34	0.52
2:D:250:ALA:C	2:D:252:LEU:H	2.17	0.52
2:B:295:MET:SD	2:B:377:PHE:HB2	2.49	0.52
1:C:88:HIS:H	1:C:91:GLN:NE2	2.07	0.52
1:C:190:THR:HG23	1:C:191:THR:N	2.23	0.52
2:D:153:LEU:O	2:D:157:ILE:HG12	2.09	0.52
2:D:183:GLU:O	2:D:186:ASN:N	2.42	0.52
2:D:185:TYR:CE2	2:D:398:MET:HB3	2.43	0.52
1:A:66:VAL:C	1:A:67:PHE:HD1	2.18	0.52
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.44	0.52
2:B:118:VAL:HG11	2:B:153:LEU:HD11	1.91	0.52
2:B:185:TYR:CE2	2:B:398:MET:HB3	2.45	0.52
2:B:251:ASP:C	2:B:253:ARG:N	2.67	0.52
1:A:402:ARG:O	1:A:403:ALA:C	2.51	0.52
2:B:404:PHE:N	2:B:404:PHE:CD1	2.75	0.52
1:C:177:VAL:HG22	1:C:210:TYR:HD2	1.73	0.52
1:C:264:ARG:O	1:C:266:HIS:N	2.42	0.52
2:D:194:LEU:O	2:D:265:LEU:CD2	2.57	0.52
2:D:273:ALA:CB	2:D:375:ALA:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:57:ALA:O	3:E:59:GLU:N	2.42	0.52
1:C:402:ARG:O	1:C:403:ALA:C	2.51	0.52
1:A:32:PRO:O	1:A:33:ASP:C	2.52	0.52
2:B:7:ILE:O	2:B:137:LEU:HA	2.10	0.52
1:C:68:VAL:CG1	1:C:118:VAL:HG22	2.39	0.52
1:C:310:GLY:HA3	1:C:383:ALA:HB2	1.92	0.52
2:D:408:TYR:O	2:D:409:THR:C	2.53	0.52
3:E:51:GLN:O	3:E:54:LEU:HB3	2.09	0.52
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.92	0.52
2:B:404:PHE:N	2:B:404:PHE:HD1	2.08	0.52
1:C:247:ALA:C	1:C:249:ASN:H	2.17	0.52
2:D:151:THR:HB	2:D:193:GLN:HG2	1.90	0.52
2:D:287:THR:HG22	2:D:290:GLU:CB	2.35	0.52
2:D:287:THR:O	2:D:288:VAL:HB	2.10	0.52
2:D:360:PRO:C	2:D:369:ARG:O	2.53	0.52
1:A:277:SER:O	1:A:280:LYS:HB2	2.10	0.52
2:B:238:VAL:HG13	2:B:378:ILE:HD11	1.91	0.52
1:A:49:PHE:HA	1:A:243:ARG:O	2.10	0.52
1:A:393:HIS:O	1:A:394:LYS:C	2.51	0.52
2:B:237:GLY:O	2:B:240:THR:OG1	2.27	0.52
1:C:152:LEU:O	1:C:153:LEU:C	2.50	0.52
2:D:205:ASP:OD2	2:D:390:ARG:NH1	2.42	0.52
3:E:115:HIS:C	3:E:115:HIS:ND1	2.67	0.52
1:A:87:PHE:N	1:A:87:PHE:CD2	2.78	0.51
1:A:251:ASP:C	1:A:251:ASP:OD1	2.53	0.51
2:B:251:ASP:O	2:B:252:LEU:HB3	2.10	0.51
1:C:7:ILE:HD13	1:C:153:LEU:HD11	1.92	0.51
1:C:36:MET:O	1:C:38:SER:N	2.43	0.51
2:D:416:MET:O	2:D:420:GLU:HB2	2.10	0.51
3:E:69:LEU:C	3:E:71:HIS:H	2.17	0.51
1:C:161:TYR:HB3	1:C:164:LYS:HG3	1.92	0.51
1:C:425:MET:O	1:C:429:GLU:HB2	2.09	0.51
3:E:63:TYR:O	3:E:64:GLN:C	2.53	0.51
1:A:281:ALA:O	1:A:283:HIS:N	2.42	0.51
1:A:347:CYS:O	1:A:348:PRO:C	2.54	0.51
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.25	0.51
2:B:347:ILE:HG22	2:B:347:ILE:O	2.10	0.51
1:C:435:VAL:HG12	1:C:435:VAL:O	2.10	0.51
2:D:182:VAL:O	2:D:185:TYR:HB2	2.11	0.51
1:A:90:GLU:O	1:A:121:ARG:CD	2.59	0.51
2:B:369:ARG:O	2:B:370:GLY:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:256:ALA:O	2:D:260:VAL:HG22	2.10	0.51
2:D:266:HIS:CD2	2:D:266:HIS:H	2.29	0.51
2:D:267:PHE:CD1	2:D:267:PHE:N	2.78	0.51
2:B:142:GLY:HA3	2:B:173:PRO:HG3	1.91	0.51
1:C:155:GLU:O	1:C:158:SER:HB2	2.11	0.51
1:C:313:MET:HG3	1:C:380:ASN:O	2.10	0.51
2:D:223:THR:CB	2:D:225:GLY:H	2.05	0.51
1:C:68:VAL:HG11	1:C:118:VAL:HG21	1.93	0.51
1:C:251:ASP:C	1:C:252:LEU:O	2.51	0.51
1:C:273:ALA:HB2	1:C:375:VAL:H	1.70	0.51
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.92	0.51
2:B:31:ASP:HB2	2:B:34:GLY:CA	2.40	0.51
2:B:265:LEU:O	2:B:266:HIS:C	2.53	0.51
7:B:700:CN2:H43	7:B:700:CN2:H62	1.92	0.51
2:B:158:ARG:HG3	2:B:158:ARG:NH1	2.26	0.51
1:C:100:ALA:HB1	2:D:253:ARG:HG2	1.93	0.51
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.41	0.51
2:D:76:ASP:OD1	2:D:76:ASP:N	2.44	0.51
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.46	0.50
1:A:177:VAL:HG22	1:A:210:TYR:HD2	1.76	0.50
1:A:210:TYR:CD1	1:A:210:TYR:C	2.89	0.50
1:A:392:ASP:OD1	1:A:429:GLU:OE1	2.29	0.50
2:B:176:LYS:HB3	8:C:800:VLB:C22	2.40	0.50
1:A:407:TRP:CZ2	2:B:260:VAL:HG23	2.45	0.50
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.24	0.50
1:C:201:ALA:O	1:C:268:PRO:HD2	2.11	0.50
1:C:405:VAL:CG1	1:C:406:HIS:N	2.73	0.50
7:D:701:CN2:C12	7:D:701:CN2:H15	2.39	0.50
1:A:262:TYR:O	1:A:264:ARG:N	2.45	0.50
2:D:165:ILE:HG23	2:D:253:ARG:NH1	2.26	0.50
3:E:13:LYS:HG3	3:E:18:GLN:HG3	1.92	0.50
2:B:7:ILE:HG22	2:B:137:LEU:CD1	2.42	0.50
2:B:11:GLN:CG	2:B:74:THR:HG21	2.36	0.50
2:B:342:TYR:N	2:B:342:TYR:CD2	2.80	0.50
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.47	0.50
2:D:115:VAL:HG21	2:D:152:LEU:CD2	2.41	0.50
2:D:270:PRO:HA	2:D:377:PHE:O	2.12	0.50
1:A:117:LEU:HD11	1:A:121:ARG:NH2	2.27	0.50
1:A:183:GLU:HB3	1:A:184:PRO:CD	2.42	0.50
1:A:247:ALA:O	1:A:248:LEU:O	2.29	0.50
1:A:327:ASP:O	1:A:328:VAL:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:VAL:HG11	2:B:387:LEU:HD21	1.92	0.50
1:C:325:PRO:HB3	8:C:800:VLB:C65	2.40	0.50
1:C:136:LEU:HD23	1:C:167:LEU:HB3	1.94	0.50
2:D:295:MET:SD	2:D:377:PHE:HB2	2.51	0.50
3:E:51:GLN:C	3:E:53:LYS:N	2.68	0.50
1:A:174:ALA:CB	1:A:207:GLU:HB2	2.41	0.50
1:A:288:VAL:HG13	1:A:323:VAL:HG22	1.92	0.50
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.60	0.50
1:C:87:PHE:N	1:C:87:PHE:CD2	2.78	0.50
1:C:328:VAL:O	1:C:332:ILE:HD12	2.11	0.50
2:D:360:PRO:O	2:D:369:ARG:O	2.30	0.50
1:A:54:SER:O	1:A:56:THR:N	2.45	0.49
1:A:223:THR:N	1:A:226:ASN:HB2	2.27	0.49
1:A:291:ILE:HB	1:A:375:VAL:CG2	2.41	0.49
1:A:316:CYS:O	1:A:377:MET:HA	2.12	0.49
1:A:332:ILE:O	1:A:333:ALA:C	2.54	0.49
1:A:344:VAL:O	1:A:346:TRP:N	2.45	0.49
1:C:11:GLN:HB3	5:C:601:GTP:O2A	2.12	0.49
2:D:4:ILE:HD11	2:D:52:TYR:CE2	2.47	0.49
2:D:7:ILE:O	2:D:137:LEU:HA	2.13	0.49
1:A:155:GLU:OE1	1:A:197:HIS:HE1	1.95	0.49
1:A:176:GLN:HG2	1:A:177:VAL:N	2.27	0.49
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.92	0.49
1:A:398:MET:HE2	2:B:348:PRO:HD2	1.93	0.49
1:A:111:GLY:O	1:A:112:LYS:C	2.55	0.49
2:B:146:GLY:N	6:B:602:GDP:O1B	2.41	0.49
2:B:401:ARG:O	1:C:262:TYR:OH	2.29	0.49
1:C:72:PRO:O	1:C:74:VAL:N	2.44	0.49
2:D:396:THR:O	2:D:400:ARG:HB2	2.12	0.49
1:A:184:PRO:O	1:A:188:ILE:HG12	2.12	0.49
2:B:408:TYR:O	2:B:409:THR:C	2.55	0.49
2:D:224:TYR:CD2	6:D:603:GDP:C5	3.00	0.49
2:D:250:ALA:O	2:D:252:LEU:N	2.44	0.49
2:D:414:ASP:HB3	2:D:416:MET:CE	2.41	0.49
1:A:405:VAL:CG1	1:A:406:HIS:N	2.75	0.49
1:C:149:PHE:O	1:C:150:THR:C	2.55	0.49
1:C:191:THR:O	1:C:195:LEU:HB2	2.12	0.49
2:B:291:LEU:HD21	2:B:375:ALA:HB3	1.94	0.49
2:B:357:ASP:OD2	2:B:357:ASP:N	2.46	0.49
3:E:105:MET:CE	3:E:105:MET:HB3	2.43	0.49
1:A:16:ILE:HG22	1:A:17:GLY:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ALA:C	1:A:283:HIS:H	2.20	0.49
2:D:224:TYR:HD2	6:D:603:GDP:C6	2.30	0.49
2:D:250:ALA:CB	7:D:701:CN2:C7	2.88	0.49
2:D:320:ARG:HA	2:D:356:CYS:O	2.12	0.49
1:A:68:VAL:CG1	1:A:118:VAL:HG22	2.41	0.49
2:B:177:VAL:O	2:B:177:VAL:CG1	2.61	0.49
2:B:194:LEU:O	2:B:265:LEU:CD2	2.61	0.49
2:B:266:HIS:CD2	2:B:266:HIS:H	2.29	0.49
1:A:264:ARG:HB2	1:A:266:HIS:NE2	2.28	0.49
2:B:270:PRO:HA	2:B:377:PHE:O	2.12	0.49
1:C:329:ASN:HD21	8:C:800:VLB:H66	1.60	0.49
2:D:8:GLN:OE1	2:D:67:LEU:CD2	2.61	0.49
2:D:210:TYR:C	2:D:210:TYR:HD1	2.21	0.49
1:A:90:GLU:O	1:A:121:ARG:HD3	2.12	0.48
1:C:36:MET:C	1:C:38:SER:N	2.71	0.48
1:C:261:PRO:HB2	1:C:262:TYR:CD1	2.48	0.48
1:C:395:PHE:C	1:C:395:PHE:CD2	2.91	0.48
3:E:79:GLU:C	3:E:81:GLU:H	2.21	0.48
1:A:401:LYS:C	1:A:403:ALA:H	2.21	0.48
2:B:335:VAL:C	2:B:337:ASN:H	2.21	0.48
1:A:105:ARG:HH22	2:B:253:ARG:HH21	1.61	0.48
1:A:106:GLY:O	1:A:111:GLY:HA3	2.14	0.48
2:B:44:LEU:HA	2:B:49:ILE:HB	1.95	0.48
2:B:150:GLY:O	2:B:152:LEU:N	2.45	0.48
3:E:4:ALA:HB3	3:E:24:LEU:CD1	2.37	0.48
2:B:150:GLY:C	2:B:152:LEU:N	2.69	0.48
2:B:226:ASP:O	2:B:227:LEU:HB2	2.12	0.48
2:B:267:PHE:N	2:B:267:PHE:CD1	2.81	0.48
1:C:108:TYR:HB3	3:E:108:ASN:OD1	2.13	0.48
1:C:309:HIS:ND1	1:C:386:GLU:OE1	2.47	0.48
2:D:2:ARG:HH12	2:D:133:GLN:HA	1.76	0.48
1:A:22:GLU:HB2	1:A:83:TYR:CE1	2.49	0.48
1:A:159:VAL:HG11	3:E:48:GLU:HB2	1.94	0.48
2:B:62:VAL:HA	2:B:63:PRO:HD2	1.72	0.48
2:B:114:LEU:O	2:B:115:VAL:C	2.55	0.48
3:E:73:ALA:HA	3:E:76:ARG:HB2	1.94	0.48
1:A:145:THR:N	5:A:600:GTP:O2B	2.45	0.48
1:A:254:GLU:HA	1:A:257:THR:HB	1.95	0.48
2:B:360:PRO:C	2:B:369:ARG:O	2.56	0.48
2:D:164:ARG:NH2	2:D:253:ARG:HH22	2.11	0.48
1:C:247:ALA:C	1:C:249:ASN:N	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ILE:O	1:C:266:HIS:O	2.31	0.48
1:C:266:HIS:HB3	1:C:380:ASN:OD1	2.13	0.48
1:A:182:VAL:CG2	1:A:408:TYR:OH	2.62	0.48
1:A:198:SER:HB3	1:A:265:ILE:CD1	2.43	0.48
2:B:3:GLU:OE2	2:B:130:ASP:HB3	2.14	0.48
1:C:178:SER:OG	2:D:352:LYS:HD2	2.14	0.48
2:D:36:TYR:OH	2:D:40:SER:O	2.32	0.48
2:D:42:LEU:O	2:D:43:GLN:C	2.56	0.48
2:D:250:ALA:C	2:D:252:LEU:N	2.72	0.48
2:B:155:SER:C	3:E:76:ARG:HH22	2.21	0.48
2:B:308:ARG:NH1	2:B:308:ARG:HG3	2.29	0.48
1:C:146:GLY:N	5:C:601:GTP:O1B	2.42	0.48
1:C:273:ALA:HB2	1:C:375:VAL:CA	2.43	0.48
2:D:138:THR:HG22	2:D:169:PHE:HB2	1.95	0.48
2:D:269:MET:HE1	2:D:307:PRO:HG3	1.96	0.48
1:C:296:PHE:HZ	1:C:351:PHE:HE2	1.62	0.48
1:A:105:ARG:NH2	2:B:253:ARG:HH21	2.11	0.47
2:B:16:ILE:HG22	2:B:17:GLY:N	2.29	0.47
1:A:139:HIS:CG	1:A:150:THR:HG21	2.49	0.47
2:B:5:VAL:CG2	2:B:135:PHE:CD2	2.97	0.47
2:B:7:ILE:HG22	2:B:137:LEU:HD12	1.96	0.47
2:B:51:VAL:HG12	2:B:52:TYR:CD1	2.49	0.47
2:B:155:SER:O	3:E:76:ARG:NH2	2.47	0.47
2:B:399:PHE:O	2:B:400:ARG:O	2.33	0.47
1:C:309:HIS:CE1	1:C:386:GLU:OE1	2.67	0.47
1:A:111:GLY:O	1:A:113:GLU:N	2.48	0.47
1:A:309:HIS:CE1	1:A:386:GLU:OE1	2.67	0.47
1:C:179:THR:HB	1:C:180:ALA:H	1.57	0.47
2:D:238:VAL:HG13	2:D:378:ILE:HD11	1.96	0.47
1:A:435:VAL:HG12	1:A:435:VAL:O	2.12	0.47
2:B:70:LEU:CD1	2:B:145:THR:HB	2.43	0.47
1:C:54:SER:HB3	1:C:64:ARG:NE	2.28	0.47
2:D:251:ASP:O	2:D:252:LEU:HB3	2.13	0.47
1:A:54:SER:HB3	1:A:64:ARG:HE	1.80	0.47
1:A:97:GLU:HG2	1:A:110:ILE:CD1	2.45	0.47
2:B:12:CYS:O	2:B:13:GLY:C	2.57	0.47
1:C:26:LEU:HD21	1:C:364:PRO:HD3	1.95	0.47
2:D:103:TRP:CZ3	2:D:189:LEU:HD22	2.50	0.47
1:A:152:LEU:O	1:A:153:LEU:C	2.58	0.47
2:B:41:ASP:O	2:B:42:LEU:C	2.56	0.47
2:B:106:GLY:O	2:B:111:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:THR:O	2:B:182:VAL:N	2.47	0.47
2:B:181:VAL:O	2:B:398:MET:CE	2.61	0.47
2:B:256:ALA:O	2:B:260:VAL:HG22	2.15	0.47
2:B:381:SER:O	2:B:384:ILE:HB	2.14	0.47
2:B:407:TRP:NE1	1:C:257:THR:HG23	2.30	0.47
1:C:78:VAL:C	1:C:80:THR:H	2.23	0.47
1:C:111:GLY:C	1:C:113:GLU:H	2.22	0.47
1:C:267:PHE:N	1:C:267:PHE:CD1	2.82	0.47
1:C:319:TYR:CZ	1:C:328:VAL:HG13	2.50	0.47
1:C:407:TRP:HZ2	2:D:260:VAL:HG23	1.78	0.47
2:D:273:ALA:HB3	2:D:375:ALA:H	1.79	0.47
1:A:88:HIS:H	1:A:91:GLN:NE2	2.13	0.47
2:B:190:SER:O	2:B:193:GLN:N	2.48	0.47
1:C:66:VAL:HG12	1:C:125:LEU:HD12	1.97	0.47
2:B:308:ARG:HH11	2:B:308:ARG:HG2	1.77	0.47
2:B:388:PHE:HD2	2:B:425:MET:CE	2.28	0.47
1:C:40:LYS:O	1:C:41:THR:CB	2.60	0.47
1:C:97:GLU:HG2	1:C:110:ILE:CD1	2.40	0.47
1:C:163:LYS:O	1:C:164:LYS:C	2.58	0.47
1:C:407:TRP:HZ2	2:D:260:VAL:CG2	2.28	0.47
2:D:335:VAL:C	2:D:337:ASN:H	2.23	0.47
3:E:112:ARG:HG2	3:E:113:GLU:N	2.28	0.47
2:B:360:PRO:O	2:B:369:ARG:O	2.32	0.47
3:E:85:LYS:O	3:E:89:GLU:HB2	2.15	0.47
2:B:102:ASN:OD1	2:B:105:LYS:N	2.36	0.46
2:B:263:PRO:O	2:B:265:LEU:N	2.48	0.46
2:B:416:MET:HE3	2:B:417:GLU:N	2.30	0.46
2:D:70:LEU:C	2:D:95:GLY:HA3	2.40	0.46
2:D:308:ARG:HH11	2:D:308:ARG:HG2	1.80	0.46
1:A:51:THR:CB	1:A:243:ARG:HA	2.45	0.46
1:A:97:GLU:HG2	1:A:110:ILE:HD11	1.96	0.46
2:B:102:ASN:OD1	2:B:102:ASN:O	2.32	0.46
2:B:118:VAL:O	2:B:122:VAL:HG13	2.15	0.46
2:B:158:ARG:HH11	2:B:158:ARG:HG3	1.79	0.46
2:D:95:GLY:O	2:D:96:GLN:CB	2.63	0.46
2:D:150:GLY:C	2:D:152:LEU:N	2.72	0.46
2:D:261:PRO:HG3	2:D:313:LEU:HG	1.97	0.46
2:D:381:SER:O	2:D:384:ILE:HB	2.15	0.46
2:D:403:ALA:C	2:D:405:LEU:H	2.23	0.46
2:D:239:THR:O	2:D:240:THR:C	2.58	0.46
2:D:399:PHE:O	2:D:400:ARG:O	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:VAL:CG1	2:B:351:VAL:HG23	2.44	0.46
2:B:333:LEU:HA	2:B:336:GLN:HE21	1.81	0.46
1:C:249:ASN:HB3	1:C:250:VAL:HG22	1.96	0.46
1:C:407:TRP:CD1	2:D:257:VAL:HG22	2.49	0.46
2:D:209:LEU:HD12	2:D:209:LEU:HA	1.71	0.46
1:A:105:ARG:HH22	2:B:253:ARG:NH2	2.14	0.46
1:C:411:GLU:OE2	1:C:411:GLU:HA	2.15	0.46
2:D:212:ILE:HG22	2:D:230:LEU:HD21	1.97	0.46
1:A:102:ASN:OD1	1:A:105:ARG:HB2	2.15	0.46
1:A:368:LEU:H	1:A:368:LEU:HG	1.29	0.46
1:A:395:PHE:C	1:A:395:PHE:CD2	2.93	0.46
2:B:9:ALA:HA	2:B:68:VAL:O	2.16	0.46
2:B:342:TYR:N	2:B:342:TYR:HD2	2.14	0.46
2:D:6:HIS:CE1	2:D:8:GLN:HB2	2.51	0.46
1:A:99:ALA:CB	1:A:145:THR:CG2	2.87	0.46
1:A:181:VAL:O	1:A:398:MET:HE1	2.15	0.46
1:A:203:MET:HE2	1:A:303:VAL:HG21	1.97	0.46
1:A:393:HIS:CE1	1:A:397:LEU:HD13	2.51	0.46
2:D:177:VAL:HG12	2:D:177:VAL:O	2.16	0.46
3:E:13:LYS:O	3:E:14:CYS:O	2.33	0.46
3:E:67:GLU:O	3:E:69:LEU:N	2.49	0.46
1:A:36:MET:HG2	1:A:61:HIS:CD2	2.51	0.46
1:A:251:ASP:OD1	1:A:252:LEU:N	2.48	0.46
2:B:177:VAL:O	2:B:178:SER:HB3	2.16	0.46
2:B:403:ALA:C	2:B:405:LEU:N	2.61	0.46
2:D:190:SER:O	2:D:191:VAL:C	2.59	0.46
1:A:20:CYS:HB3	1:A:232:GLY:HA2	1.98	0.46
1:A:315:CYS:HB3	1:A:351:PHE:HE2	1.81	0.46
2:B:209:LEU:HD21	2:B:231:VAL:HG22	1.97	0.46
2:B:308:ARG:CG	2:B:308:ARG:NH1	2.70	0.46
1:C:172:TYR:HE2	1:C:391:LEU:HD22	1.81	0.46
1:A:143:GLY:O	1:A:147:SER:OG	2.34	0.46
1:A:312:TYR:O	1:A:344:VAL:HG12	2.16	0.46
2:B:313:LEU:HD11	2:B:346:TRP:CH2	2.51	0.46
1:C:100:ALA:HB3	1:C:105:ARG:HE	1.81	0.46
2:D:262:PHE:O	2:D:266:HIS:CD2	2.69	0.46
2:D:342:TYR:CD2	2:D:342:TYR:N	2.84	0.46
1:A:181:VAL:HG23	2:B:258:ASN:HD22	1.81	0.45
1:A:395:PHE:O	1:A:396:ASP:C	2.59	0.45
1:C:316:CYS:O	1:C:377:MET:HE3	2.16	0.45
2:D:195:VAL:HG21	2:D:428:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLY:O	1:A:11:GLN:C	2.59	0.45
1:A:30:ILE:HG23	1:A:34:GLY:O	2.16	0.45
2:B:5:VAL:HG12	2:B:64:ARG:HG2	1.98	0.45
2:B:228:ASN:ND2	6:B:602:GDP:HN1	2.14	0.45
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.98	0.45
1:C:184:PRO:O	1:C:188:ILE:HG12	2.15	0.45
2:D:343:PHE:O	2:D:344:VAL:C	2.59	0.45
1:A:82:THR:O	1:A:83:TYR:HB2	2.17	0.45
1:A:190:THR:CG2	1:A:191:THR:H	2.30	0.45
2:B:74:THR:HA	2:B:77:SER:HB2	1.99	0.45
1:A:82:THR:O	1:A:83:TYR:CB	2.65	0.45
2:D:115:VAL:HG12	2:D:116:ASP:N	2.30	0.45
2:D:245:PRO:HG3	2:D:247:GLN:CD	2.41	0.45
2:D:269:MET:HG2	2:D:384:ILE:HG12	1.98	0.45
2:D:401:ARG:O	2:D:402:LYS:C	2.59	0.45
2:B:171:VAL:HA	2:B:204:ILE:O	2.16	0.45
1:C:334:THR:C	1:C:336:LYS:N	2.74	0.45
2:D:416:MET:HE3	2:D:417:GLU:N	2.32	0.45
2:D:427:ASP:O	2:D:430:SER:N	2.50	0.45
1:A:312:TYR:HE2	1:A:379:SER:HB2	1.82	0.45
2:B:135:PHE:CD1	2:B:135:PHE:N	2.83	0.45
2:B:382:THR:HB	2:B:436:GLN:HE21	1.81	0.45
1:C:102:ASN:O	1:C:103:TYR:C	2.59	0.45
1:C:141:PHE:HD1	1:C:172:TYR:HA	1.81	0.45
1:C:346:TRP:O	1:C:348:PRO:HD3	2.17	0.45
2:D:289:PRO:HA	2:D:331:GLN:NE2	2.32	0.45
1:C:183:GLU:CB	1:C:184:PRO:CD	2.94	0.45
2:D:8:GLN:NE2	2:D:17:GLY:HA3	2.32	0.45
2:D:118:VAL:O	2:D:122:VAL:HG13	2.16	0.45
2:D:260:VAL:HA	2:D:261:PRO:HD2	1.82	0.45
1:A:289:ALA:O	1:A:292:THR:HB	2.17	0.45
1:A:320:ARG:O	1:A:373:ARG:HA	2.17	0.45
1:A:348:PRO:HB2	1:A:349:THR:H	1.50	0.45
2:B:140:SER:HA	2:B:171:VAL:CG2	2.37	0.45
2:B:248:LEU:HB2	2:B:249:ASN:H	1.50	0.45
1:C:100:ALA:CB	2:D:253:ARG:HG2	2.47	0.45
1:C:107:HIS:HD2	1:C:108:TYR:CE2	2.35	0.45
1:C:115:ILE:HD12	1:C:156:ARG:HD3	1.99	0.45
2:D:20:PHE:O	2:D:24:ILE:HG23	2.17	0.45
1:A:68:VAL:HG11	1:A:118:VAL:HG21	1.98	0.45
2:B:212:ILE:HD12	2:B:215:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:PHE:CD2	2:B:425:MET:CE	2.99	0.45
1:C:358:GLN:HA	1:C:359:PRO:HD3	1.89	0.45
2:D:223:THR:C	2:D:225:GLY:H	2.24	0.45
2:D:308:ARG:CG	2:D:308:ARG:NH1	2.76	0.45
2:B:141:LEU:CD2	2:B:172:VAL:HG22	2.46	0.45
2:D:62:VAL:O	2:D:62:VAL:CG2	2.63	0.45
2:D:135:PHE:HB2	2:D:166:MET:CE	2.40	0.45
1:C:154:MET:HB3	1:C:154:MET:HE3	1.55	0.44
1:C:181:VAL:HG11	1:C:404:PHE:CZ	2.51	0.44
3:E:67:GLU:C	3:E:69:LEU:N	2.75	0.44
1:C:244:PHE:CE2	1:C:358:GLN:HG2	2.51	0.44
2:D:102:ASN:OD1	2:D:105:LYS:HB2	2.16	0.44
3:E:76:ARG:HD3	3:E:76:ARG:HA	1.43	0.44
1:A:125:LEU:HD23	1:A:128:GLN:NE2	2.32	0.44
1:C:31:GLN:O	1:C:32:PRO:C	2.59	0.44
1:C:393:HIS:CE1	1:C:397:LEU:HD13	2.52	0.44
2:D:143:GLY:O	2:D:147:SER:HB3	2.17	0.44
1:A:26:LEU:HD21	1:A:364:PRO:HD3	1.99	0.44
1:A:108:TYR:CE1	1:A:413:MET:HG3	2.52	0.44
1:A:112:LYS:HG3	3:E:54:LEU:HD11	1.99	0.44
2:B:262:PHE:O	2:B:263:PRO:C	2.61	0.44
2:B:287:THR:O	2:B:288:VAL:CB	2.66	0.44
2:D:36:TYR:CZ	2:D:38:GLY:O	2.71	0.44
2:D:150:GLY:O	2:D:152:LEU:N	2.51	0.44
2:B:143:GLY:O	2:B:147:SER:HB3	2.16	0.44
2:D:406:HIS:ND1	2:D:406:HIS:C	2.75	0.44
1:A:410:GLY:HA2	3:E:64:GLN:NE2	2.32	0.44
1:C:180:ALA:O	1:C:183:GLU:HB2	2.18	0.44
1:C:223:THR:CG2	1:C:225:THR:HG23	2.48	0.44
2:B:274:PRO:C	2:B:275:LEU:HG	2.42	0.44
2:B:332:MET:HG3	2:B:353:THR:CG2	2.43	0.44
1:C:223:THR:HB	1:C:226:ASN:H	1.83	0.44
1:C:381:THR:HG23	1:C:384:ILE:H	1.83	0.44
3:E:77:GLU:HG2	3:E:80:ARG:HB2	1.98	0.44
1:A:265:ILE:O	1:A:266:HIS:C	2.61	0.44
2:B:403:ALA:HB1	2:B:404:PHE:HD1	1.82	0.44
2:D:269:MET:HA	2:D:270:PRO:HD3	1.83	0.44
2:D:404:PHE:HD1	2:D:404:PHE:H	1.64	0.44
3:E:57:ALA:O	3:E:60:ARG:N	2.50	0.44
3:E:129:HIS:O	3:E:133:VAL:HG23	2.18	0.44
2:B:75:MET:HE2	2:B:94:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:CG	2:B:158:ARG:NH1	2.81	0.44
1:C:70:LEU:HB2	1:C:145:THR:HG21	1.99	0.44
2:D:135:PHE:CD1	2:D:135:PHE:N	2.85	0.44
3:E:92:ASN:O	3:E:96:MET:HB2	2.18	0.44
1:A:407:TRP:CG	2:B:257:VAL:CG2	3.02	0.43
2:B:164:ARG:HE	2:B:164:ARG:CA	2.31	0.43
2:B:182:VAL:O	2:B:185:TYR:HB2	2.17	0.43
1:C:176:GLN:HG2	1:C:177:VAL:N	2.31	0.43
1:C:383:ALA:O	1:C:386:GLU:HB2	2.18	0.43
2:D:9:ALA:CB	2:D:68:VAL:HB	2.48	0.43
2:D:319:PHE:CD1	2:D:319:PHE:N	2.86	0.43
1:A:21:TRP:HZ3	1:A:53:PHE:CZ	2.36	0.43
1:A:205:ASP:HB3	1:A:303:VAL:HA	2.01	0.43
1:A:359:PRO:HA	1:A:360:PRO:HD3	1.91	0.43
2:B:195:VAL:HG21	2:B:428:LEU:HD13	2.00	0.43
1:C:8:HIS:ND1	1:C:8:HIS:N	2.66	0.43
1:C:346:TRP:CZ2	1:C:435:VAL:HG13	2.40	0.43
2:D:191:VAL:HG11	2:D:425:MET:CE	2.47	0.43
2:D:269:MET:HB3	2:D:303:ALA:HB3	2.00	0.43
1:A:24:TYR:CE2	1:A:243:ARG:NH1	2.86	0.43
1:A:158:SER:HB3	3:E:46:SER:CB	2.48	0.43
1:A:180:ALA:HB1	2:B:258:ASN:HD21	1.84	0.43
1:A:420:GLU:O	1:A:420:GLU:HG2	2.18	0.43
1:C:322:ASP:O	1:C:373:ARG:HD3	2.18	0.43
2:D:61:TYR:HD2	2:D:61:TYR:HA	1.72	0.43
1:A:169:PHE:CE2	1:A:235:VAL:HG22	2.53	0.43
2:B:61:TYR:HD2	2:B:61:TYR:HA	1.69	0.43
1:C:405:VAL:HG13	1:C:406:HIS:N	2.33	0.43
1:C:430:LYS:O	1:C:434:GLU:HB2	2.18	0.43
1:A:306:ASP:HA	1:A:307:PRO:HD3	1.83	0.43
2:B:321:GLY:O	2:B:323:MET:N	2.51	0.43
2:D:224:TYR:HE2	6:D:603:GDP:C4	2.36	0.43
2:D:307:PRO:O	2:D:308:ARG:HD2	2.18	0.43
2:D:357:ASP:OD2	2:D:357:ASP:N	2.50	0.43
3:E:79:GLU:C	3:E:81:GLU:N	2.76	0.43
3:E:84:GLN:C	3:E:86:ALA:H	2.25	0.43
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.54	0.43
2:B:270:PRO:HG2	2:B:302:MET:CB	2.49	0.43
1:C:229:ARG:HG2	1:C:229:ARG:HH11	1.83	0.43
1:C:324:VAL:O	1:C:327:ASP:HB2	2.18	0.43
1:A:108:TYR:HE1	1:A:413:MET:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:ALA:CB	2:B:375:ALA:H	2.32	0.43
1:C:169:PHE:CE2	1:C:235:VAL:HG22	2.54	0.43
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.01	0.43
2:B:158:ARG:O	2:B:159:GLU:HB3	2.19	0.43
2:B:216:THR:HG21	2:B:299:LYS:CD	2.49	0.43
2:B:222:PRO:O	8:C:800:VLB:H713	2.19	0.43
2:B:399:PHE:O	2:B:400:ARG:C	2.61	0.43
8:C:800:VLB:N9	8:C:800:VLB:O27	2.52	0.43
3:E:97:ALA:HA	3:E:100:LYS:CB	2.49	0.43
1:A:270:ALA:CB	1:A:302:MET:CE	2.88	0.43
2:D:332:MET:HG3	2:D:353:THR:CG2	2.45	0.43
1:A:273:ALA:HB2	1:A:375:VAL:CA	2.49	0.43
1:A:425:MET:O	1:A:429:GLU:HB2	2.19	0.43
2:B:166:MET:HB3	2:B:198:THR:HA	2.01	0.43
1:C:352:LYS:C	1:C:353:VAL:HG22	2.44	0.43
2:D:78:VAL:O	2:D:79:ARG:C	2.62	0.43
3:E:123:LEU:O	3:E:125:GLU:N	2.52	0.43
1:A:118:VAL:O	1:A:121:ARG:N	2.51	0.42
1:A:262:TYR:O	1:A:263:PRO:C	2.62	0.42
1:A:280:LYS:HG2	1:A:283:HIS:CE1	2.54	0.42
1:A:320:ARG:HH21	1:A:358:GLN:HG3	1.84	0.42
2:B:55:GLU:H	2:B:55:GLU:HG3	1.71	0.42
1:A:141:PHE:HD2	1:A:141:PHE:HA	1.74	0.42
2:B:115:VAL:HG12	2:B:116:ASP:N	2.32	0.42
1:C:249:ASN:HB2	1:C:355:ILE:H	1.83	0.42
1:C:436:GLY:O	1:C:437:ILE:C	2.61	0.42
2:D:251:ASP:HB2	2:D:254:LYS:H	1.85	0.42
3:E:112:ARG:C	3:E:114:ALA:N	2.77	0.42
3:E:77:GLU:OE2	3:E:80:ARG:HG3	2.19	0.42
1:A:107:HIS:HD2	1:A:108:TYR:CE2	2.37	0.42
1:A:436:GLY:O	1:A:437:ILE:C	2.62	0.42
2:B:241:CYS:SG	2:B:247:GLN:NE2	2.93	0.42
1:C:16:ILE:HG22	1:C:17:GLY:N	2.33	0.42
1:C:70:LEU:HD13	1:C:145:THR:HB	2.00	0.42
1:C:101:ASN:ND2	2:D:254:LYS:HE3	2.34	0.42
1:C:198:SER:HB3	1:C:265:ILE:CD1	2.50	0.42
1:C:395:PHE:O	1:C:396:ASP:C	2.62	0.42
1:A:181:VAL:HG11	1:A:404:PHE:CZ	2.55	0.42
1:A:265:ILE:HG23	1:A:267:PHE:CE1	2.54	0.42
2:B:33:THR:O	2:B:34:GLY:C	2.63	0.42
2:B:102:ASN:OD1	2:B:105:LYS:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:ARG:C	2:B:266:HIS:H	2.26	0.42
2:D:74:THR:HA	2:D:77:SER:HB2	2.00	0.42
2:D:216:THR:O	2:D:217:LEU:CB	2.68	0.42
7:D:701:CN2:C12	7:D:701:CN2:C15	2.97	0.42
1:A:398:MET:HG3	2:B:348:PRO:CD	2.50	0.42
2:B:151:THR:CG2	2:B:193:GLN:HB3	2.48	0.42
2:B:416:MET:H	2:B:416:MET:HG3	1.68	0.42
2:D:64:ARG:HG3	2:D:125:GLU:OE1	2.19	0.42
2:D:264:ARG:C	2:D:266:HIS:H	2.23	0.42
2:D:295:MET:HB3	2:D:295:MET:HE3	1.81	0.42
1:C:255:PHE:O	1:C:259:LEU:HG	2.20	0.42
1:A:271:THR:HB	1:A:377:MET:HB3	2.00	0.42
1:A:309:HIS:ND1	1:A:386:GLU:OE1	2.53	0.42
2:B:2:ARG:HH12	2:B:133:GLN:HA	1.79	0.42
1:C:183:GLU:O	1:C:184:PRO:C	2.61	0.42
1:C:227:LEU:O	1:C:228:ASN:C	2.63	0.42
2:D:164:ARG:HH21	2:D:253:ARG:HH22	1.67	0.42
2:D:399:PHE:O	2:D:400:ARG:C	2.63	0.42
1:A:54:SER:HB3	1:A:64:ARG:NE	2.34	0.42
1:A:109:THR:OG1	1:A:411:GLU:HB3	2.19	0.42
1:A:294:ALA:O	1:A:297:GLU:CB	2.63	0.42
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.79	0.42
1:A:398:MET:HG3	2:B:348:PRO:HD3	2.00	0.42
1:C:2:ARG:HB2	1:C:131:GLY:O	2.20	0.42
1:C:177:VAL:CG2	1:C:210:TYR:HD2	2.31	0.42
1:C:223:THR:H	1:C:226:ASN:HB2	1.83	0.42
2:D:21:TRP:O	2:D:25:SER:HB2	2.19	0.42
2:D:298:SER:C	2:D:300:ASN:N	2.78	0.42
1:A:187:SER:O	1:A:191:THR:HG22	2.20	0.42
2:B:239:THR:O	2:B:240:THR:C	2.63	0.42
2:B:424:ASN:O	2:B:427:ASP:HB2	2.19	0.42
1:C:248:LEU:O	1:C:249:ASN:CB	2.67	0.42
1:C:350:GLY:O	1:C:351:PHE:CB	2.63	0.42
2:D:119:LEU:HD23	2:D:123:ARG:HH21	1.85	0.42
3:E:19:SER:O	3:E:20:PHE:CB	2.67	0.42
1:A:111:GLY:C	1:A:113:GLU:N	2.78	0.41
1:A:405:VAL:HG13	1:A:406:HIS:N	2.34	0.41
2:B:111:GLY:HA2	2:B:149:MET:HE3	2.00	0.41
2:B:122:VAL:CG2	2:B:123:ARG:N	2.82	0.41
1:C:219:ILE:HD12	1:C:226:ASN:HD21	1.85	0.41
1:C:229:ARG:HH11	1:C:229:ARG:CG	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:THR:HG21	2:D:299:LYS:HD3	2.01	0.41
2:D:274:PRO:HG3	2:D:286:LEU:HD22	2.00	0.41
3:E:63:TYR:O	3:E:65:GLU:N	2.53	0.41
3:E:84:GLN:C	3:E:86:ALA:N	2.77	0.41
1:C:163:LYS:HE3	1:C:163:LYS:H	1.85	0.41
1:C:174:ALA:HB1	1:C:176:GLN:NE2	2.35	0.41
1:A:102:ASN:O	1:A:103:TYR:C	2.63	0.41
1:A:181:VAL:CG2	2:B:258:ASN:HD22	2.33	0.41
1:A:430:LYS:O	1:A:434:GLU:HB2	2.20	0.41
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.38	0.41
2:B:141:LEU:HA	2:B:147:SER:HB2	2.02	0.41
2:B:273:ALA:HB1	2:B:274:PRO:HD3	1.94	0.41
1:C:10:GLY:O	1:C:11:GLN:C	2.63	0.41
2:D:28:HIS:CG	2:D:49:ILE:HD12	2.54	0.41
2:D:229:HIS:NE2	2:D:277:SER:HB3	2.35	0.41
3:E:129:HIS:O	3:E:133:VAL:CG2	2.68	0.41
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.35	0.41
2:B:42:LEU:O	2:B:43:GLN:C	2.63	0.41
2:B:177:VAL:O	2:B:177:VAL:HG13	2.20	0.41
1:C:185:TYR:OH	1:C:403:ALA:HB3	2.21	0.41
1:C:260:VAL:HA	1:C:261:PRO:HD3	1.73	0.41
1:C:271:THR:HG21	1:C:295:CYS:O	2.21	0.41
2:D:261:PRO:HB2	2:D:262:PHE:CD1	2.56	0.41
1:A:16:ILE:CG2	1:A:17:GLY:N	2.82	0.41
1:A:323:VAL:HG12	1:A:355:ILE:CD1	2.47	0.41
1:C:182:VAL:CG2	1:C:182:VAL:O	2.68	0.41
2:D:111:GLY:HA2	2:D:149:MET:HE3	2.00	0.41
2:D:287:THR:CG2	2:D:290:GLU:H	2.32	0.41
3:E:121:GLU:O	3:E:121:GLU:HG3	2.21	0.41
2:B:2:ARG:HH11	2:B:133:GLN:HA	1.80	0.41
1:C:291:ILE:O	1:C:294:ALA:HB3	2.21	0.41
2:D:71:GLU:O	2:D:71:GLU:HG2	2.19	0.41
2:D:141:LEU:HD12	2:D:141:LEU:HA	1.67	0.41
2:D:251:ASP:C	2:D:253:ARG:N	2.68	0.41
1:A:50:ASN:O	1:A:51:THR:C	2.62	0.41
1:A:73:THR:O	1:A:76:ASP:HB2	2.21	0.41
1:A:125:LEU:HD23	1:A:128:GLN:HE22	1.85	0.41
1:A:155:GLU:O	1:A:158:SER:HB2	2.21	0.41
1:A:171:ILE:HD12	1:A:171:ILE:N	2.36	0.41
1:A:219:ILE:HD12	1:A:226:ASN:HD21	1.86	0.41
2:B:200:GLU:HB3	2:B:268:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:TRP:CD1	1:C:257:THR:CG2	3.03	0.41
1:C:210:TYR:CD1	1:C:210:TYR:C	2.98	0.41
1:C:273:ALA:HB2	1:C:375:VAL:C	2.46	0.41
2:D:75:MET:HE2	2:D:94:PHE:CD2	2.55	0.41
2:D:104:ALA:O	2:D:105:LYS:C	2.63	0.41
2:D:333:LEU:HA	2:D:336:GLN:HE21	1.85	0.41
2:B:19:LYS:O	2:B:20:PHE:C	2.61	0.41
1:C:272:TYR:CE2	1:C:274:PRO:HD2	2.56	0.41
2:D:76:ASP:O	2:D:80:SER:HB2	2.21	0.41
1:A:98:ASP:CB	2:B:251:ASP:OD2	2.65	0.41
1:A:282:TYR:N	1:A:282:TYR:CD1	2.89	0.41
1:A:286:LEU:HD12	1:A:286:LEU:H	1.86	0.41
2:B:76:ASP:OD1	2:B:76:ASP:N	2.52	0.41
2:B:150:GLY:C	2:B:152:LEU:H	2.28	0.41
2:B:262:PHE:C	2:B:264:ARG:N	2.79	0.41
2:B:348:PRO:O	2:B:350:ASN:N	2.54	0.41
2:B:388:PHE:CD2	2:B:425:MET:HE2	2.55	0.41
1:C:265:ILE:HD13	1:C:267:PHE:CE2	2.56	0.41
1:C:332:ILE:O	1:C:333:ALA:C	2.63	0.41
1:C:403:ALA:O	2:D:261:PRO:O	2.39	0.41
1:C:420:GLU:HG2	1:C:420:GLU:O	2.19	0.41
2:D:158:ARG:O	2:D:159:GLU:HB2	2.19	0.41
2:D:205:ASP:OD1	2:D:207:GLU:N	2.54	0.41
2:D:217:LEU:C	2:D:219:LEU:H	2.28	0.41
2:D:262:PHE:O	2:D:264:ARG:N	2.54	0.41
2:D:387:LEU:O	2:D:390:ARG:HG3	2.21	0.41
3:E:94:ILE:CG2	3:E:95:LYS:H	2.28	0.41
2:B:28:HIS:CG	2:B:49:ILE:HD12	2.56	0.41
2:B:287:THR:CG2	2:B:290:GLU:H	2.32	0.41
1:C:66:VAL:C	1:C:67:PHE:HD1	2.29	0.41
1:C:103:TYR:O	1:C:104:ALA:C	2.63	0.41
1:C:168:GLU:HG2	1:C:201:ALA:HB2	2.03	0.41
1:C:171:ILE:O	1:C:171:ILE:HG22	2.21	0.41
2:D:171:VAL:HA	2:D:204:ILE:O	2.20	0.41
2:D:178:SER:HB2	2:D:183:GLU:OE2	2.21	0.41
2:D:237:GLY:HA2	2:D:376:THR:HG21	2.00	0.41
2:D:262:PHE:O	2:D:266:HIS:HD2	2.03	0.41
2:D:388:PHE:CD2	2:D:425:MET:HE2	2.56	0.41
1:A:115:ILE:HD12	1:A:156:ARG:HD3	2.02	0.40
1:A:141:PHE:CD1	1:A:172:TYR:HB2	2.55	0.40
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:TRP:HZ3	1:A:347:CYS:HG	1.64	0.40
1:A:408:TYR:C	1:A:410:GLY:N	2.76	0.40
2:B:72:PRO:O	2:B:73:GLY:C	2.63	0.40
2:B:103:TRP:CZ3	2:B:189:LEU:HD22	2.56	0.40
2:B:177:VAL:HA	8:C:800:VLB:C53	2.38	0.40
2:B:406:HIS:ND1	2:B:406:HIS:C	2.78	0.40
1:C:31:GLN:H	1:C:31:GLN:HG3	1.76	0.40
1:A:404:PHE:O	1:A:406:HIS:N	2.54	0.40
2:B:155:SER:C	3:E:76:ARG:NH2	2.79	0.40
2:B:269:MET:HG2	2:B:384:ILE:CG1	2.48	0.40
1:A:70:LEU:HB2	1:A:145:THR:HG21	2.02	0.40
1:A:228:ASN:O	1:A:232:GLY:N	2.45	0.40
1:A:318:LEU:CB	1:A:376:CYS:HB3	2.45	0.40
2:B:103:TRP:HD1	2:B:147:SER:OG	2.05	0.40
1:C:328:VAL:HG12	1:C:332:ILE:HD11	2.00	0.40
2:D:164:ARG:CA	2:D:164:ARG:NE	2.77	0.40
2:D:342:TYR:N	2:D:342:TYR:HD2	2.19	0.40
2:D:344:VAL:HG13	2:D:346:TRP:H	1.86	0.40
3:E:112:ARG:HA	3:E:115:HIS:HB3	2.02	0.40
2:B:62:VAL:O	2:B:62:VAL:CG2	2.69	0.40
1:C:10:GLY:O	1:C:13:GLY:N	2.55	0.40
2:D:150:GLY:O	2:D:153:LEU:N	2.55	0.40
3:E:48:GLU:O	3:E:49:GLU:C	2.64	0.40
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.62	0.40
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.56	0.40
1:C:329:ASN:CG	8:C:800:VLB:H211	2.46	0.40
2:D:388:PHE:CE1	2:D:428:LEU:HD21	2.56	0.40
3:E:84:GLN:HE21	3:E:84:GLN:HB2	1.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	423/448 (94%)	317 (75%)	75 (18%)	31 (7%)	1	13
1	C	421/448 (94%)	315 (75%)	68 (16%)	38 (9%)	0	10
2	B	415/445 (93%)	298 (72%)	71 (17%)	46 (11%)	0	6
2	D	415/445 (93%)	297 (72%)	73 (18%)	45 (11%)	0	6
3	E	120/142 (84%)	68 (57%)	36 (30%)	16 (13%)	0	3
All	All	1794/1928 (93%)	1295 (72%)	323 (18%)	176 (10%)	0	8

All (176) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	62	VAL
1	A	72	PRO
1	A	112	LYS
1	A	240	ALA
1	A	247	ALA
1	A	248	LEU
1	A	345	ASP
1	A	348	PRO
1	A	403	ALA
2	B	3	GLU
2	B	34	GLY
2	B	43	GLN
2	B	60	LYS
2	B	62	VAL
2	B	72	PRO
2	B	82	PRO
2	B	115	VAL
2	B	163	ASP
2	B	177	VAL
2	B	245	PRO
2	B	249	ASN
2	B	265	LEU
2	B	266	HIS
2	B	273	ALA
2	B	288	VAL
2	B	348	PRO
2	B	369	ARG
2	B	370	GLY
2	B	371	LEU
2	B	400	ARG

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Mol	Chain	Res	Type
2	B	403	ALA
1	C	41	THR
1	C	62	VAL
1	C	72	PRO
1	C	73	THR
1	C	112	LYS
1	C	240	ALA
1	C	249	ASN
1	C	250	VAL
1	C	266	HIS
1	C	341	ILE
1	C	345	ASP
1	C	357	TYR
1	C	403	ALA
2	D	3	GLU
2	D	34	GLY
2	D	43	GLN
2	D	60	LYS
2	D	62	VAL
2	D	64	ARG
2	D	72	PRO
2	D	82	PRO
2	D	96	GLN
2	D	115	VAL
2	D	163	ASP
2	D	217	LEU
2	D	227	LEU
2	D	245	PRO
2	D	249	ASN
2	D	265	LEU
2	D	266	HIS
2	D	273	ALA
2	D	288	VAL
2	D	348	PRO
2	D	369	ARG
2	D	370	GLY
2	D	400	ARG
2	D	403	ALA
3	E	14	CYS
3	E	28	SER
3	E	29	PHE
3	E	47	LEU

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Mol	Chain	Res	Type
3	E	58	GLU
3	E	124	GLN
3	E	128	LYS
1	A	73	THR
1	A	164	LYS
1	A	241	SER
1	A	264	ARG
1	A	273	ALA
1	A	282	TYR
1	A	341	ILE
1	A	350	GLY
2	B	42	LEU
2	B	64	ARG
2	B	73	GLY
2	B	96	GLN
2	B	151	THR
2	B	178	SER
2	B	181	VAL
2	B	217	LEU
2	B	225	GLY
2	B	227	LEU
2	B	244	PHE
2	B	276	THR
2	B	299	LYS
2	B	404	PHE
1	C	33	ASP
1	C	55	GLU
1	C	164	LYS
1	C	241	SER
1	C	252	LEU
1	C	265	ILE
1	C	335	ILE
1	C	351	PHE
1	C	377	MET
2	D	42	LEU
2	D	57	THR
2	D	73	GLY
2	D	151	THR
2	D	229	HIS
2	D	244	PHE
2	D	251	ASP
2	D	276	THR

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Mol	Chain	Res	Type
2	D	299	LYS
2	D	371	LEU
3	E	7	GLU
3	E	12	ASN
3	E	64	GLN
3	E	68	LEU
3	E	113	GLU
3	E	140	LYS
1	A	59	GLY
1	A	181	VAL
1	A	263	PRO
1	A	266	HIS
1	A	274	PRO
1	A	281	ALA
1	A	283	HIS
2	B	57	THR
2	B	360	PRO
1	C	59	GLY
1	C	181	VAL
1	C	247	ALA
1	C	248	LEU
1	C	273	ALA
1	C	274	PRO
1	C	305	CYS
2	D	344	VAL
2	D	360	PRO
3	E	136	ASN
1	A	245	ASP
1	A	349	THR
2	B	97	SER
2	B	159	GLU
2	B	322	ARG
1	C	179	THR
1	C	349	THR
2	D	59	ASN
2	D	129	CYS
2	D	218	LYS
2	D	402	LYS
1	A	32	PRO
2	B	59	ASN
2	B	307	PRO
2	B	402	LYS

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Mol	Chain	Res	Type
1	C	37	PRO
1	C	40	LYS
1	C	307	PRO
2	D	11	GLN
2	D	220	THR
3	E	26	PRO
3	E	49	GLU
1	A	377	MET
1	C	32	PRO
2	D	307	PRO
1	A	405	VAL
1	C	115	ILE
2	D	177	VAL
2	B	162	PRO
1	C	405	VAL
1	A	265	ILE
2	B	344	VAL
1	C	144	GLY
2	D	162	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/377 (92%)	205 (59%)	140 (41%)	0	1
1	C	336/377 (89%)	207 (62%)	129 (38%)	0	1
2	B	348/383 (91%)	211 (61%)	137 (39%)	0	1
2	D	348/383 (91%)	213 (61%)	135 (39%)	0	1
3	E	80/126 (64%)	39 (49%)	41 (51%)	0	0
All	All	1457/1646 (88%)	875 (60%)	582 (40%)	0	1

All (582) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	4	CYS
1	A	5	ILE
1	A	6	SER
1	A	9	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	36	MET
1	A	48	SER
1	A	50	ASN
1	A	60	LYS
1	A	61	HIS
1	A	62	VAL
1	A	66	VAL
1	A	68	VAL
1	A	73	THR
1	A	79	ARG
1	A	80	THR
1	A	84	ARG
1	A	86	LEU
1	A	88	HIS
1	A	90	GLU
1	A	93	ILE
1	A	94	THR
1	A	105	ARG
1	A	112	LYS
1	A	114	ILE
1	A	115	ILE
1	A	117	LEU
1	A	119	LEU
1	A	123	ARG
1	A	124	LYS
1	A	125	LEU
1	A	127	ASP
1	A	128	GLN
1	A	132	LEU
1	A	140	SER
1	A	141	PHE
1	A	145	THR

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Mol	Chain	Res	Type
1	A	147	SER
1	A	153	LEU
1	A	154	MET
1	A	160	ASP
1	A	163	LYS
1	A	164	LYS
1	A	165	SER
1	A	167	LEU
1	A	177	VAL
1	A	178	SER
1	A	179	THR
1	A	182	VAL
1	A	183	GLU
1	A	187	SER
1	A	193	THR
1	A	194	THR
1	A	196	GLU
1	A	206	ASN
1	A	210	TYR
1	A	211	ASP
1	A	212	ILE
1	A	217	LEU
1	A	219	ILE
1	A	220	GLU
1	A	223	THR
1	A	225	THR
1	A	226	ASN
1	A	227	LEU
1	A	230	LEU
1	A	234	ILE
1	A	236	SER
1	A	242	LEU
1	A	243	ARG
1	A	245	ASP
1	A	248	LEU
1	A	251	ASP
1	A	252	LEU
1	A	254	GLU
1	A	255	PHE
1	A	256	GLN
1	A	260	VAL
1	A	265	ILE

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Mol	Chain	Res	Type
1	A	269	LEU
1	A	275	VAL
1	A	279	GLU
1	A	280	LYS
1	A	283	HIS
1	A	287	SER
1	A	288	VAL
1	A	291	ILE
1	A	301	GLN
1	A	302	MET
1	A	306	ASP
1	A	313	MET
1	A	316	CYS
1	A	318	LEU
1	A	323	VAL
1	A	324	VAL
1	A	326	LYS
1	A	328	VAL
1	A	329	ASN
1	A	334	THR
1	A	341	ILE
1	A	343	PHE
1	A	345	ASP
1	A	347	CYS
1	A	349	THR
1	A	352	LYS
1	A	356	ASN
1	A	362	VAL
1	A	363	VAL
1	A	367	ASP
1	A	368	LEU
1	A	370	LYS
1	A	371	VAL
1	A	373	ARG
1	A	375	VAL
1	A	379	SER
1	A	380	ASN
1	A	384	ILE
1	A	386	GLU
1	A	388	TRP
1	A	391	LEU
1	A	394	LYS

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Mol	Chain	Res	Type
1	A	397	LEU
1	A	401	LYS
1	A	405	VAL
1	A	413	MET
1	A	414	GLU
1	A	415	GLU
1	A	419	SER
1	A	420	GLU
1	A	428	LEU
1	A	429	GLU
1	A	430	LYS
1	A	433	GLU
1	A	434	GLU
2	B	2	ARG
2	B	4	ILE
2	B	11	GLN
2	B	16	ILE
2	B	22	GLU
2	B	24	ILE
2	B	25	SER
2	B	27	GLU
2	B	30	ILE
2	B	33	THR
2	B	39	ASP
2	B	42	LEU
2	B	43	GLN
2	B	49	ILE
2	B	51	VAL
2	B	55	GLU
2	B	61	TYR
2	B	62	VAL
2	B	64	ARG
2	B	66	ILE
2	B	68	VAL
2	B	70	LEU
2	B	71	GLU
2	B	75	MET
2	B	76	ASP
2	B	77	SER
2	B	78	VAL
2	B	79	ARG
2	B	80	SER

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Mol	Chain	Res	Type
2	B	90	ASP
2	B	91	ASN
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	119	LEU
2	B	122	VAL
2	B	128	SER
2	B	131	CYS
2	B	137	LEU
2	B	138	THR
2	B	140	SER
2	B	141	LEU
2	B	145	THR
2	B	147	SER
2	B	151	THR
2	B	154	ILE
2	B	155	SER
2	B	157	ILE
2	B	158	ARG
2	B	160	GLU
2	B	164	ARG
2	B	166	MET
2	B	168	THR
2	B	170	SER
2	B	171	VAL
2	B	174	SER
2	B	177	VAL
2	B	179	ASP
2	B	182	VAL
2	B	183	GLU
2	B	189	LEU
2	B	193	GLN
2	B	195	VAL
2	B	200	GLU
2	B	203	SER
2	B	206	ASN
2	B	207	GLU
2	B	210	TYR

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Mol	Chain	Res	Type
2	B	212	ILE
2	B	214	PHE
2	B	215	ARG
2	B	216	THR
2	B	223	THR
2	B	227	LEU
2	B	230	LEU
2	B	239	THR
2	B	240	THR
2	B	241	CYS
2	B	242	LEU
2	B	243	ARG
2	B	248	LEU
2	B	253	ARG
2	B	255	LEU
2	B	257	VAL
2	B	258	ASN
2	B	265	LEU
2	B	269	MET
2	B	275	LEU
2	B	276	THR
2	B	286	LEU
2	B	292	THR
2	B	294	GLN
2	B	295	MET
2	B	302	MET
2	B	308	ARG
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	325	MET
2	B	333	LEU
2	B	335	VAL
2	B	341	SER
2	B	344	VAL
2	B	350	ASN
2	B	351	VAL
2	B	353	THR
2	B	355	VAL

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Mol	Chain	Res	Type
2	B	357	ASP
2	B	371	LEU
2	B	373	MET
2	B	374	SER
2	B	376	THR
2	B	382	THR
2	B	384	ILE
2	B	386	GLU
2	B	389	LYS
2	B	390	ARG
2	B	391	ILE
2	B	394	GLN
2	B	400	ARG
2	B	401	ARG
2	B	404	PHE
2	B	405	LEU
2	B	406	HIS
2	B	415	GLU
2	B	419	THR
2	B	420	GLU
2	B	423	SER
2	B	425	MET
2	B	430	SER
2	B	434	GLN
1	C	2	ARG
1	C	4	CYS
1	C	5	ILE
1	C	6	SER
1	C	8	HIS
1	C	9	VAL
1	C	15	GLN
1	C	16	ILE
1	C	22	GLU
1	C	26	LEU
1	C	27	GLU
1	C	50	ASN
1	C	51	THR
1	C	60	LYS
1	C	61	HIS
1	C	62	VAL
1	C	66	VAL
1	C	68	VAL

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Mol	Chain	Res	Type
1	C	73	THR
1	C	78	VAL
1	C	79	ARG
1	C	80	THR
1	C	82	THR
1	C	84	ARG
1	C	86	LEU
1	C	88	HIS
1	C	94	THR
1	C	105	ARG
1	C	112	LYS
1	C	113	GLU
1	C	114	ILE
1	C	115	ILE
1	C	116	ASP
1	C	117	LEU
1	C	119	LEU
1	C	123	ARG
1	C	124	LYS
1	C	125	LEU
1	C	127	ASP
1	C	128	GLN
1	C	132	LEU
1	C	140	SER
1	C	141	PHE
1	C	147	SER
1	C	153	LEU
1	C	154	MET
1	C	155	GLU
1	C	160	ASP
1	C	163	LYS
1	C	165	SER
1	C	167	LEU
1	C	177	VAL
1	C	178	SER
1	C	179	THR
1	C	182	VAL
1	C	183	GLU
1	C	187	SER
1	C	193	THR
1	C	194	THR
1	C	196	GLU

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Mol	Chain	Res	Type
1	C	198	SER
1	C	200	CYS
1	C	206	ASN
1	C	210	TYR
1	C	211	ASP
1	C	212	ILE
1	C	217	LEU
1	C	219	ILE
1	C	220	GLU
1	C	223	THR
1	C	225	THR
1	C	226	ASN
1	C	227	LEU
1	C	229	ARG
1	C	230	LEU
1	C	233	GLN
1	C	234	ILE
1	C	236	SER
1	C	243	ARG
1	C	245	ASP
1	C	251	ASP
1	C	253	THR
1	C	256	GLN
1	C	258	ASN
1	C	264	ARG
1	C	265	ILE
1	C	269	LEU
1	C	275	VAL
1	C	287	SER
1	C	288	VAL
1	C	291	ILE
1	C	301	GLN
1	C	302	MET
1	C	306	ASP
1	C	316	CYS
1	C	318	LEU
1	C	334	THR
1	C	336	LYS
1	C	341	ILE
1	C	345	ASP
1	C	353	VAL
1	C	356	ASN

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Mol	Chain	Res	Type
1	C	358	GLN
1	C	362	VAL
1	C	363	VAL
1	C	367	ASP
1	C	368	LEU
1	C	370	LYS
1	C	371	VAL
1	C	373	ARG
1	C	375	VAL
1	C	379	SER
1	C	380	ASN
1	C	384	ILE
1	C	386	GLU
1	C	391	LEU
1	C	394	LYS
1	C	397	LEU
1	C	401	LYS
1	C	409	VAL
1	C	413	MET
1	C	414	GLU
1	C	415	GLU
1	C	419	SER
1	C	428	LEU
1	C	429	GLU
1	C	430	LYS
1	C	433	GLU
1	C	434	GLU
2	D	2	ARG
2	D	4	ILE
2	D	11	GLN
2	D	16	ILE
2	D	19	LYS
2	D	22	GLU
2	D	24	ILE
2	D	25	SER
2	D	26	ASP
2	D	27	GLU
2	D	30	ILE
2	D	33	THR
2	D	39	ASP
2	D	42	LEU
2	D	43	GLN

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Mol	Chain	Res	Type
2	D	49	ILE
2	D	51	VAL
2	D	55	GLU
2	D	61	TYR
2	D	62	VAL
2	D	64	ARG
2	D	66	ILE
2	D	68	VAL
2	D	71	GLU
2	D	76	ASP
2	D	77	SER
2	D	78	VAL
2	D	79	ARG
2	D	80	SER
2	D	90	ASP
2	D	91	ASN
2	D	93	VAL
2	D	96	GLN
2	D	97	SER
2	D	101	ASN
2	D	102	ASN
2	D	109	THR
2	D	119	LEU
2	D	122	VAL
2	D	124	LYS
2	D	128	SER
2	D	137	LEU
2	D	138	THR
2	D	140	SER
2	D	141	LEU
2	D	145	THR
2	D	147	SER
2	D	149	MET
2	D	151	THR
2	D	154	ILE
2	D	158	ARG
2	D	160	GLU
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	171	VAL
2	D	174	SER
2	D	179	ASP
2	D	181	VAL
2	D	182	VAL
2	D	183	GLU
2	D	189	LEU
2	D	193	GLN
2	D	195	VAL
2	D	200	GLU
2	D	203	SER
2	D	206	ASN
2	D	207	GLU
2	D	209	LEU
2	D	212	ILE
2	D	216	THR
2	D	221	THR
2	D	223	THR
2	D	230	LEU
2	D	231	VAL
2	D	240	THR
2	D	241	CYS
2	D	242	LEU
2	D	243	ARG
2	D	248	LEU
2	D	253	ARG
2	D	255	LEU
2	D	257	VAL
2	D	258	ASN
2	D	265	LEU
2	D	269	MET
2	D	275	LEU
2	D	276	THR
2	D	286	LEU
2	D	292	THR
2	D	294	GLN
2	D	295	MET
2	D	302	MET
2	D	308	ARG
2	D	313	LEU
2	D	315	VAL
2	D	318	VAL

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Mol	Chain	Res	Type
2	D	320	ARG
2	D	323	MET
2	D	325	MET
2	D	333	LEU
2	D	335	VAL
2	D	341	SER
2	D	342	TYR
2	D	344	VAL
2	D	345	GLU
2	D	350	ASN
2	D	353	THR
2	D	355	VAL
2	D	357	ASP
2	D	371	LEU
2	D	373	MET
2	D	374	SER
2	D	376	THR
2	D	382	THR
2	D	384	ILE
2	D	386	GLU
2	D	389	LYS
2	D	390	ARG
2	D	391	ILE
2	D	394	GLN
2	D	400	ARG
2	D	401	ARG
2	D	404	PHE
2	D	405	LEU
2	D	406	HIS
2	D	416	MET
2	D	419	THR
2	D	420	GLU
2	D	423	SER
2	D	425	MET
2	D	430	SER
2	D	434	GLN
3	E	5	ASP
3	E	11	LEU
3	E	14	CYS
3	E	22	VAL
3	E	48	GLU
3	E	53	LYS

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Mol	Chain	Res	Type
3	E	58	GLU
3	E	59	GLU
3	E	60	ARG
3	E	61	ARG
3	E	62	LYS
3	E	65	GLU
3	E	69	LEU
3	E	74	GLU
3	E	76	ARG
3	E	77	GLU
3	E	79	GLU
3	E	81	GLU
3	E	84	GLN
3	E	87	ILE
3	E	91	ASN
3	E	94	ILE
3	E	98	LYS
3	E	99	GLU
3	E	101	LEU
3	E	104	LYS
3	E	105	MET
3	E	106	GLU
3	E	111	ASN
3	E	112	ARG
3	E	113	GLU
3	E	115	HIS
3	E	119	MET
3	E	120	LEU
3	E	121	GLU
3	E	122	ARG
3	E	123	LEU
3	E	125	GLU
3	E	127	ASP
3	E	133	VAL
3	E	136	ASN

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

Mol	Chain	Res	Type
1	A	8	HIS
1	A	88	HIS
1	A	91	GLN

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Mol	Chain	Res	Type
1	A	107	HIS
1	A	133	GLN
1	A	197	HIS
1	A	206	ASN
1	A	216	ASN
1	A	226	ASN
1	A	249	ASN
1	A	329	ASN
1	A	393	HIS
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	133	GLN
2	B	136	GLN
2	B	139	HIS
2	B	228	ASN
2	B	247	GLN
2	B	258	ASN
2	B	266	HIS
2	B	294	GLN
2	B	300	ASN
2	B	331	GLN
2	B	334	ASN
2	B	337	ASN
2	B	339	ASN
2	B	350	ASN
2	B	380	ASN
2	B	424	ASN
2	B	436	GLN
1	C	8	HIS
1	C	61	HIS
1	C	91	GLN
1	C	101	ASN
1	C	107	HIS
1	C	176	GLN
1	C	197	HIS
1	C	206	ASN
1	C	226	ASN
1	C	256	GLN
1	C	266	HIS
1	C	329	ASN
1	C	393	HIS

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Mol	Chain	Res	Type
2	D	6	HIS
2	D	133	GLN
2	D	136	GLN
2	D	139	HIS
2	D	193	GLN
2	D	249	ASN
2	D	258	ASN
2	D	266	HIS
2	D	294	GLN
2	D	300	ASN
2	D	309	HIS
2	D	334	ASN
2	D	337	ASN
2	D	339	ASN
2	D	350	ASN
2	D	380	ASN
2	D	424	ASN
2	D	436	GLN
3	E	12	ASN
3	E	64	GLN
3	E	71	HIS
3	E	84	GLN
3	E	91	ASN
3	E	124	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CN2	D	701	-	32,32,32	2.73	10 (31%)	44,45,45	4.72	20 (45%)
5	GTP	A	600	4	33,34,34	1.26	6 (18%)	50,54,54	1.68	11 (22%)
8	VLB	C	800	-	66,67,67	1.70	13 (19%)	82,108,108	2.57	27 (32%)
6	GDP	D	603	-	29,30,30	0.81	0	45,47,47	1.90	12 (26%)
5	GTP	C	601	4	33,34,34	1.10	3 (9%)	50,54,54	1.68	13 (26%)
6	GDP	B	602	-	29,30,30	0.84	0	45,47,47	1.93	12 (26%)
7	CN2	B	700	-	32,32,32	2.93	11 (34%)	44,45,45	4.43	23 (52%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CN2	D	701	-	-	5/12/27/27	0/3/3/3
5	GTP	A	600	4	-	5/22/38/38	0/3/3/3
8	VLB	C	800	-	-	18/40/131/131	0/7/9/9
6	GDP	D	603	-	-	3/16/32/32	0/3/3/3
5	GTP	C	601	4	-	6/22/38/38	0/3/3/3
6	GDP	B	602	-	-	4/16/32/32	0/3/3/3
7	CN2	B	700	-	-	4/12/27/27	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	CN2	C20-C21	-8.36	1.23	1.37
7	B	700	CN2	C19-C20	-7.66	1.19	1.41
7	D	701	CN2	C20-C21	-7.61	1.24	1.37
7	D	701	CN2	C19-C20	-7.11	1.21	1.41
7	B	700	CN2	C21-C14	-6.32	1.34	1.43
8	C	800	VLB	C5-C6	-6.32	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	701	CN2	C21-C14	-5.81	1.35	1.43
7	B	700	CN2	C19-C17	-5.66	1.24	1.39
7	D	701	CN2	C19-C17	-5.64	1.24	1.39
7	B	700	CN2	O6-C17	4.71	1.45	1.36
7	D	701	CN2	O6-C17	4.37	1.44	1.36
8	C	800	VLB	C6-C7	4.29	1.40	1.32
8	C	800	VLB	C8-C7	-4.28	1.38	1.49
8	C	800	VLB	C65-N66	-3.94	1.31	1.38
8	C	800	VLB	C18-N1	-3.57	1.33	1.39
5	A	600	GTP	PA-O3A	3.44	1.63	1.59
8	C	800	VLB	C60-C59	-3.42	1.37	1.44
7	D	701	CN2	C22-C8	3.38	1.47	1.41
5	A	600	GTP	PB-O3A	3.26	1.63	1.59
7	B	700	CN2	C15-C16	3.25	1.54	1.44
5	C	601	GTP	PA-O3A	3.11	1.62	1.59
7	D	701	CN2	C15-C16	3.08	1.53	1.44
8	C	800	VLB	C30-C29	-2.94	1.39	1.49
8	C	800	VLB	C3-C23	2.87	1.59	1.52
8	C	800	VLB	O25-C23	2.77	1.38	1.33
7	B	700	CN2	C15-C14	2.62	1.41	1.36
5	A	600	GTP	C5-N7	-2.57	1.33	1.39
7	D	701	CN2	C15-C14	2.55	1.41	1.36
8	C	800	VLB	C60-C65	-2.53	1.38	1.41
7	B	700	CN2	C22-C21	-2.51	1.47	1.50
8	C	800	VLB	C67-C59	2.47	1.40	1.37
8	C	800	VLB	O28-C4	-2.45	1.39	1.44
8	C	800	VLB	C67-N66	-2.29	1.34	1.38
5	A	600	GTP	PB-O3B	2.29	1.62	1.59
5	C	601	GTP	O4'-C4'	-2.26	1.40	1.45
5	A	600	GTP	O4'-C4'	-2.20	1.40	1.45
5	A	600	GTP	C5-C6	-2.15	1.36	1.44
7	B	700	CN2	O3-C5	2.14	1.40	1.37
7	D	701	CN2	C11-C14	-2.14	1.50	1.53
7	B	700	CN2	C22-C1	-2.13	1.36	1.40
5	C	601	GTP	PB-O3A	2.13	1.61	1.59
7	D	701	CN2	O2-C3	2.04	1.42	1.38
7	B	700	CN2	C13-C12	-2.04	1.48	1.51

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	701	CN2	O6-C17-C16	18.15	126.28	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	CN2	O6-C17-C16	14.28	122.72	109.60
7	D	701	CN2	C20-C21-C14	-12.36	112.13	124.67
7	B	700	CN2	C19-C17-C16	-11.81	109.53	128.57
7	D	701	CN2	C19-C17-C16	-11.01	110.84	128.57
7	B	700	CN2	C20-C21-C14	-10.90	113.61	124.67
8	C	800	VLB	C4-O28-C29	-9.74	102.87	117.65
7	D	701	CN2	C19-C20-C21	8.48	147.72	131.06
7	B	700	CN2	C19-C20-C21	8.45	147.65	131.06
8	C	800	VLB	C57-C58-C59	8.43	127.27	113.65
7	D	701	CN2	C20-C19-C17	7.52	145.96	130.27
7	B	700	CN2	C20-C19-C17	7.42	145.74	130.27
7	B	700	CN2	C22-C21-C14	7.15	124.48	118.62
7	D	701	CN2	C22-C21-C14	6.48	123.93	118.62
8	C	800	VLB	O25-C23-C3	6.20	122.41	112.21
7	B	700	CN2	C15-C14-C21	-5.76	122.65	127.56
6	B	602	GDP	C5-C4-N3	-5.65	119.39	128.39
8	C	800	VLB	C22-N1-C18	-5.42	104.13	120.94
7	D	701	CN2	O3-C5-C7	-5.40	114.77	124.08
6	B	602	GDP	C2-N3-C4	5.33	121.48	112.30
6	D	603	GDP	C5-C4-N3	-5.15	120.19	128.39
8	C	800	VLB	C22-N1-C2	-5.14	106.69	119.14
6	D	603	GDP	C2-N3-C4	5.13	121.14	112.30
8	C	800	VLB	O75-C73-C68	5.10	119.45	111.21
5	A	600	GTP	C5-C4-N3	-5.03	120.38	128.39
8	C	800	VLB	O28-C29-C30	4.78	119.61	111.09
7	B	700	CN2	C9-C10-C11	4.73	117.86	112.13
8	C	800	VLB	O32-C16-C15	4.63	121.18	116.59
5	C	601	GTP	C2-N3-C4	4.59	120.20	112.30
5	A	600	GTP	C2-N3-C4	4.51	120.08	112.30
7	D	701	CN2	C4-O2-C3	4.48	126.90	114.74
7	D	701	CN2	O3-C5-C3	4.35	122.59	115.14
7	B	700	CN2	C11-C14-C15	4.34	120.89	117.06
8	C	800	VLB	O25-C23-O24	-4.27	116.60	123.95
7	D	701	CN2	C22-C21-C20	4.18	123.75	116.95
7	B	700	CN2	O3-C5-C3	4.05	122.08	115.14
7	D	701	CN2	C11-C14-C15	4.03	120.61	117.06
7	D	701	CN2	C14-C11-N1	-3.99	111.16	114.31
7	D	701	CN2	C10-C11-N1	-3.96	102.50	109.76
7	B	700	CN2	C6-O3-C5	3.81	123.10	117.51
7	B	700	CN2	O6-C17-C19	3.75	127.73	122.29
5	C	601	GTP	N9-C8-N7	-3.70	106.54	113.40
8	C	800	VLB	C76-O75-C73	-3.64	109.94	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	701	CN2	C13-C12-N1	-3.55	110.95	115.33
5	C	601	GTP	C5-C4-N3	-3.44	122.92	128.39
6	D	603	GDP	N9-C4-N3	3.40	132.76	125.95
8	C	800	VLB	C4-C3-C2	-3.36	102.31	109.23
7	B	700	CN2	C10-C9-C8	-3.32	106.25	113.48
7	D	701	CN2	O4-C12-N1	3.31	128.56	122.95
7	B	700	CN2	C10-C11-C14	3.26	114.82	110.71
8	C	800	VLB	O32-C16-C17	-3.24	118.49	124.08
6	B	602	GDP	N9-C4-N3	3.22	132.40	125.95
8	C	800	VLB	C69-N56-C55	-3.19	106.55	110.87
5	A	600	GTP	C2-N1-C6	-3.16	119.38	125.11
6	D	603	GDP	O6-C6-C5	-3.16	118.19	126.53
5	C	601	GTP	O6-C6-C5	-3.10	118.34	126.53
6	B	602	GDP	N2-C2-N3	-3.08	113.66	119.67
8	C	800	VLB	C12-C19-C5	-3.07	115.92	118.20
7	B	700	CN2	C22-C21-C20	3.05	121.90	116.95
6	B	602	GDP	O6-C6-C5	-3.04	118.51	126.53
5	A	600	GTP	O6-C6-C5	-3.02	118.57	126.53
7	B	700	CN2	C10-C11-N1	-3.01	104.24	109.76
8	C	800	VLB	C33-O32-C16	-2.99	113.13	117.51
7	B	700	CN2	O4-C12-N1	2.97	127.98	122.95
6	B	602	GDP	C8-N7-C5	2.93	109.48	104.26
7	B	700	CN2	O3-C5-C7	-2.91	119.06	124.08
5	C	601	GTP	C5-C6-N1	2.88	120.58	113.25
6	D	603	GDP	N9-C8-N7	-2.86	108.09	113.40
7	D	701	CN2	C6-O3-C5	2.84	121.67	117.51
7	B	700	CN2	O4-C12-C13	-2.83	116.66	121.44
6	D	603	GDP	C8-N7-C5	2.81	109.26	104.26
5	A	600	GTP	N9-C4-N3	2.68	131.31	125.95
8	C	800	VLB	C7-C8-N9	-2.67	104.54	110.94
6	D	603	GDP	O3A-PA-O1A	-2.61	102.84	110.70
8	C	800	VLB	C59-C67-N66	-2.61	107.18	109.95
8	C	800	VLB	C13-C12-C19	-2.60	106.62	115.26
5	C	601	GTP	N1-C2-N3	-2.59	118.58	123.32
5	A	600	GTP	N2-C2-N1	2.58	122.21	116.76
5	C	601	GTP	C2-N1-C6	-2.57	120.45	125.11
7	D	701	CN2	C9-C10-C11	2.56	115.23	112.13
8	C	800	VLB	C17-C18-C13	-2.54	119.08	121.99
8	C	800	VLB	C58-C59-C60	-2.52	117.09	123.91
6	D	603	GDP	C2'-C3'-C4'	2.49	107.43	102.61
6	D	603	GDP	N1-C2-N3	-2.48	118.78	123.32
6	B	602	GDP	N9-C8-N7	-2.48	108.81	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	GTP	C8-N7-C5	2.47	108.66	104.26
7	D	701	CN2	C11-C14-C21	-2.47	113.12	115.37
5	C	601	GTP	N9-C4-N3	2.45	130.86	125.95
6	B	602	GDP	O2B-PB-O3A	2.40	112.69	104.64
5	C	601	GTP	C1'-N9-C4	-2.40	119.40	126.49
5	C	601	GTP	N2-C2-N1	2.40	121.82	116.76
8	C	800	VLB	O28-C29-O31	-2.39	118.37	122.99
6	B	602	GDP	C4-C5-N7	-2.38	106.89	110.67
7	B	700	CN2	C9-C8-C7	2.36	124.47	119.35
6	D	603	GDP	C5-C6-N1	2.35	119.24	113.25
5	A	600	GTP	N9-C8-N7	-2.35	109.04	113.40
8	C	800	VLB	C21-C20-C5	-2.32	111.32	115.79
8	C	800	VLB	O74-C73-C68	-2.31	119.31	124.81
8	C	800	VLB	C64-C65-C60	-2.30	119.96	122.19
5	A	600	GTP	C5-C6-N1	2.29	119.09	113.25
5	A	600	GTP	O3G-PG-O3B	2.29	112.31	104.64
8	C	800	VLB	C8-N9-C19	-2.27	106.72	112.48
5	A	600	GTP	C8-N7-C5	2.19	108.15	104.26
8	C	800	VLB	C61-C60-C65	2.17	121.09	118.84
7	D	701	CN2	C7-C5-C3	2.16	122.63	120.22
6	B	602	GDP	N1-C2-N3	-2.15	119.38	123.32
7	D	701	CN2	O2-C3-C5	2.15	123.20	120.12
5	A	600	GTP	O2B-PB-O3A	2.14	113.05	107.27
6	D	603	GDP	C2-N1-C6	-2.13	121.26	125.11
6	D	603	GDP	O2B-PB-O3A	2.12	111.76	104.64
7	B	700	CN2	C8-C22-C21	-2.12	117.85	120.20
6	B	602	GDP	C2-N1-C6	-2.11	121.28	125.11
7	B	700	CN2	C4-O2-C3	2.11	120.48	114.74
7	B	700	CN2	C9-C8-C22	-2.10	116.43	119.88
6	B	602	GDP	C5-C6-N1	2.07	118.53	113.25
5	C	601	GTP	C8-N9-C4	2.07	109.90	106.03
5	C	601	GTP	C6-C5-N7	2.06	134.03	130.29
8	C	800	VLB	C4-C3-C23	2.04	116.05	110.85

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	600	GTP	C5'-O5'-PA-O3A
5	A	600	GTP	C5'-O5'-PA-O1A
5	C	601	GTP	C5'-O5'-PA-O3A
5	C	601	GTP	C5'-O5'-PA-O1A

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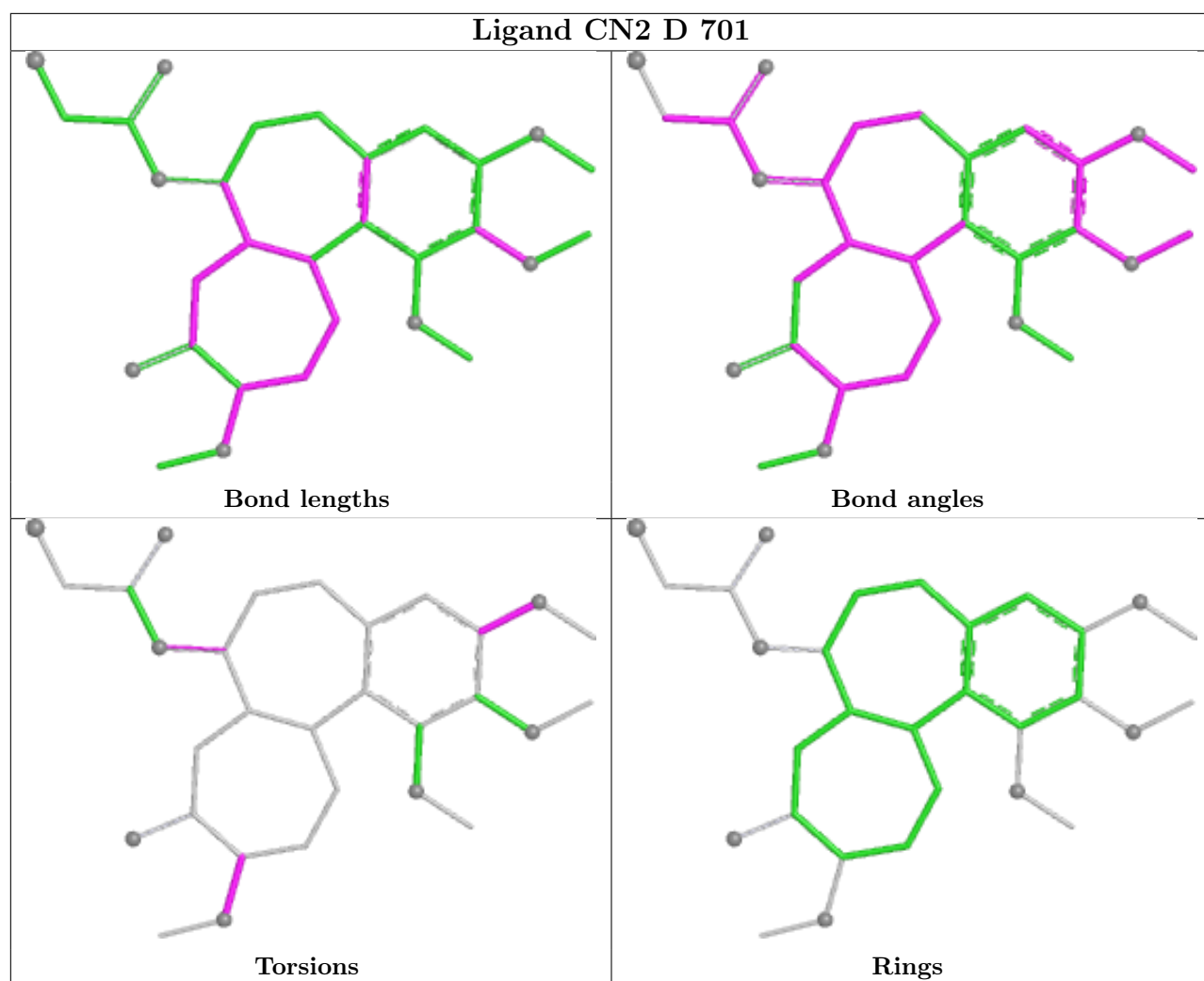
Mol	Chain	Res	Type	Atoms
6	B	602	GDP	PA-O3A-PB-O2B
6	B	602	GDP	O4'-C4'-C5'-O5'
6	D	603	GDP	O4'-C4'-C5'-O5'
6	D	603	GDP	C3'-C4'-C5'-O5'
7	B	700	CN2	C19-C17-O6-C18
7	B	700	CN2	C16-C17-O6-C18
7	D	701	CN2	C19-C17-O6-C18
7	D	701	CN2	C16-C17-O6-C18
8	C	800	VLB	C57-C58-C59-C60
8	C	800	VLB	C21-C20-C5-C19
8	C	800	VLB	C21-C20-C5-C6
8	C	800	VLB	C21-C20-C5-C4
8	C	800	VLB	O24-C23-C3-C4
8	C	800	VLB	O25-C23-C3-C4
8	C	800	VLB	O24-C23-C3-O27
8	C	800	VLB	O25-C23-C3-O27
8	C	800	VLB	O24-C23-C3-C2
8	C	800	VLB	O25-C23-C3-C2
8	C	800	VLB	C30-C29-O28-C4
6	B	602	GDP	C3'-C4'-C5'-O5'
7	B	700	CN2	C7-C5-O3-C6
7	D	701	CN2	C7-C5-O3-C6
7	B	700	CN2	C3-C5-O3-C6
8	C	800	VLB	O31-C29-O28-C4
7	D	701	CN2	C3-C5-O3-C6
5	C	601	GTP	PG-O3B-PB-O1B
7	D	701	CN2	C14-C11-N1-C12
5	A	600	GTP	C5'-O5'-PA-O2A
5	C	601	GTP	C5'-O5'-PA-O2A
6	D	603	GDP	PA-O3A-PB-O1B
8	C	800	VLB	C15-C68-C73-O75
8	C	800	VLB	C67-C68-C73-O75
5	A	600	GTP	PB-O3A-PA-O2A
8	C	800	VLB	C15-C68-C73-O74
6	B	602	GDP	PA-O3A-PB-O1B
8	C	800	VLB	C67-C68-C73-O74
5	A	600	GTP	PB-O3A-PA-O1A
5	C	601	GTP	PG-O3B-PB-O2B
5	C	601	GTP	PB-O3A-PA-O2A
8	C	800	VLB	C58-C57-N56-C55
8	C	800	VLB	C57-C58-C59-C67

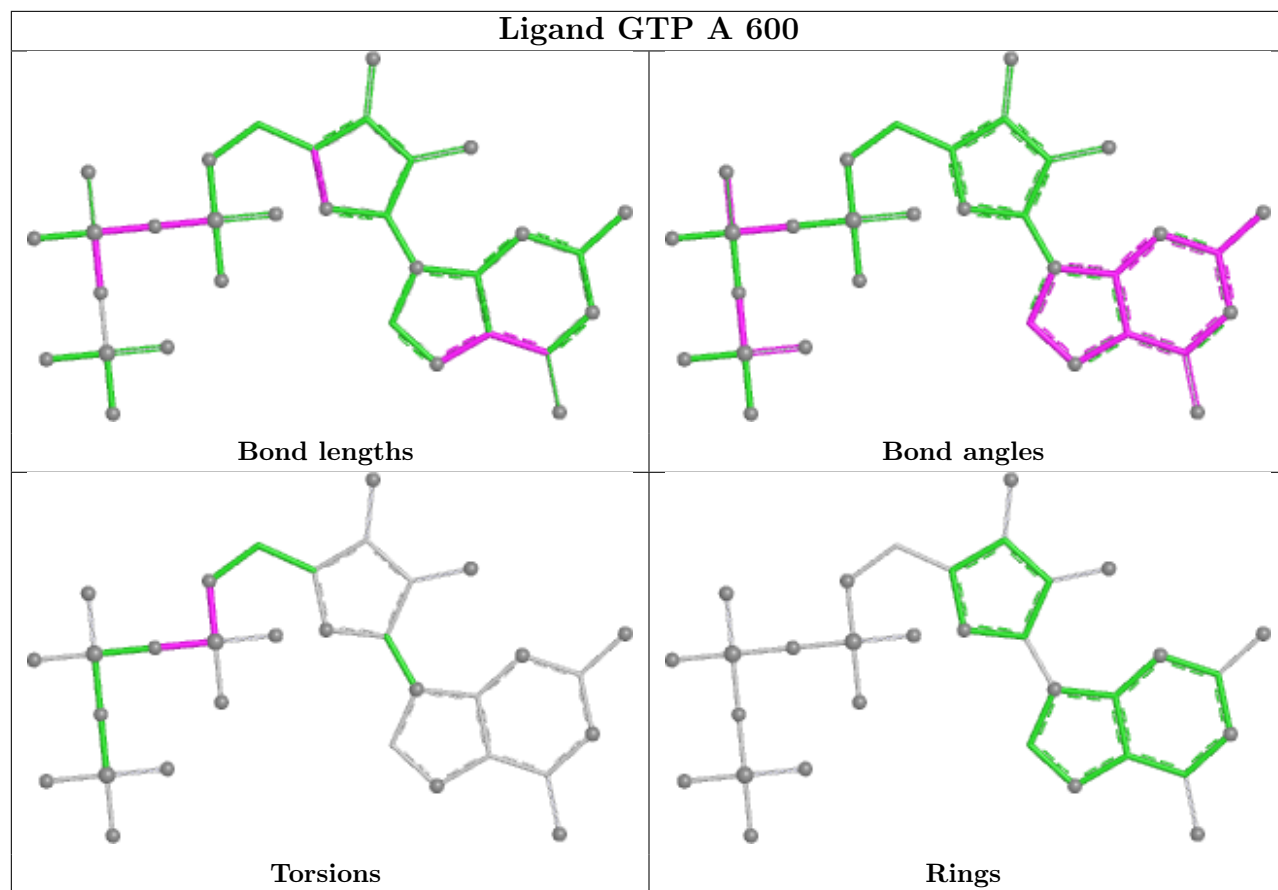
There are no ring outliers.

7 monomers are involved in 58 short contacts:

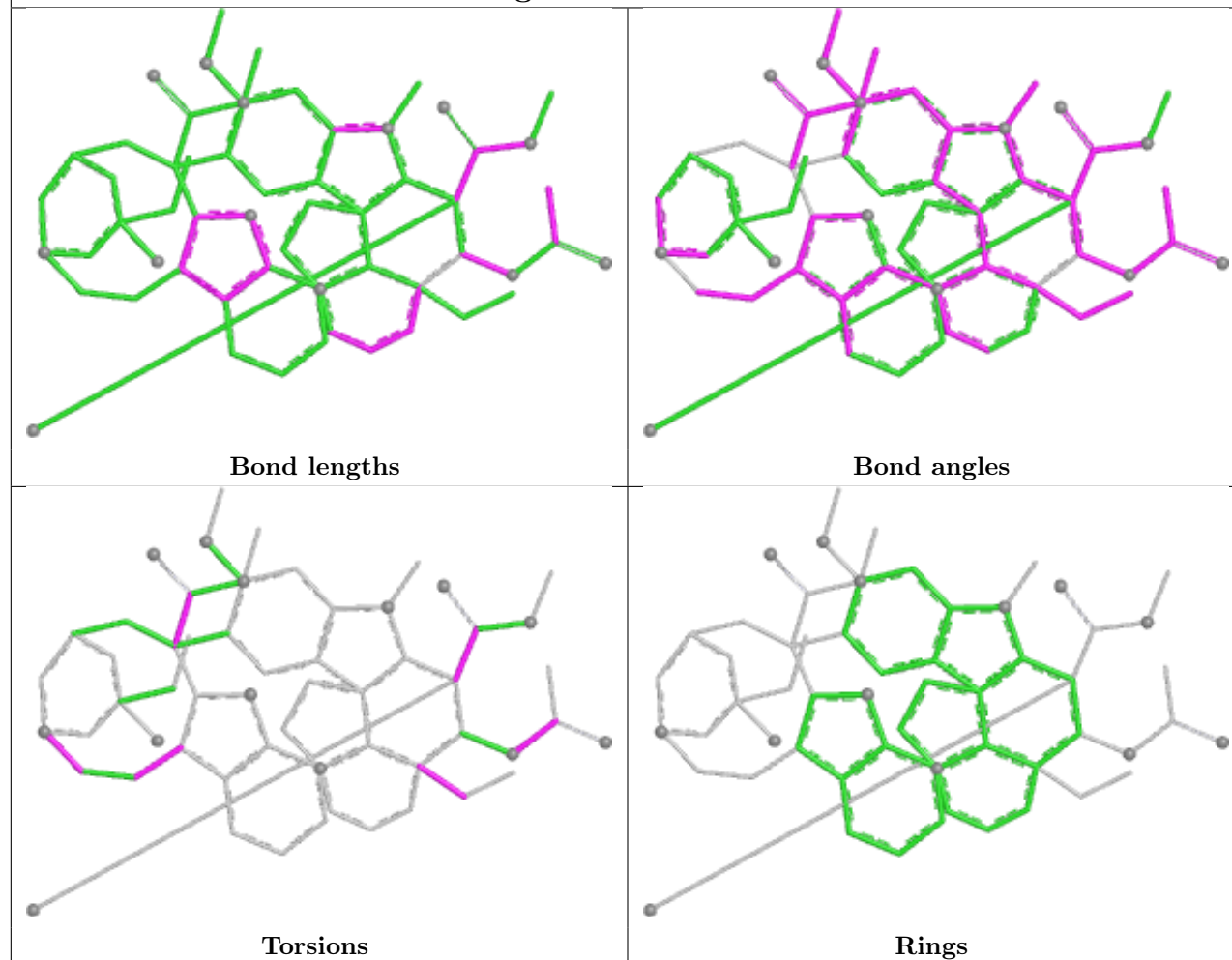
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	701	CN2	8	0
5	A	600	GTP	4	0
8	C	800	VLB	22	0
6	D	603	GDP	7	0
5	C	601	GTP	5	0
6	B	602	GDP	5	0
7	B	700	CN2	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

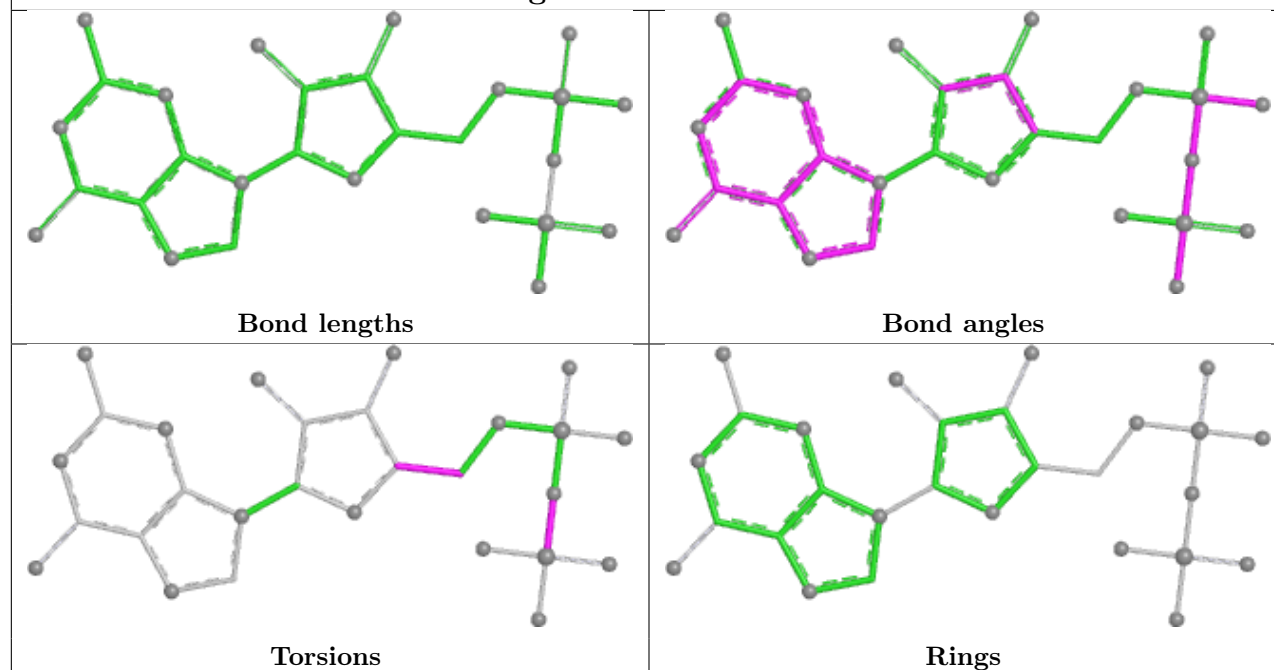




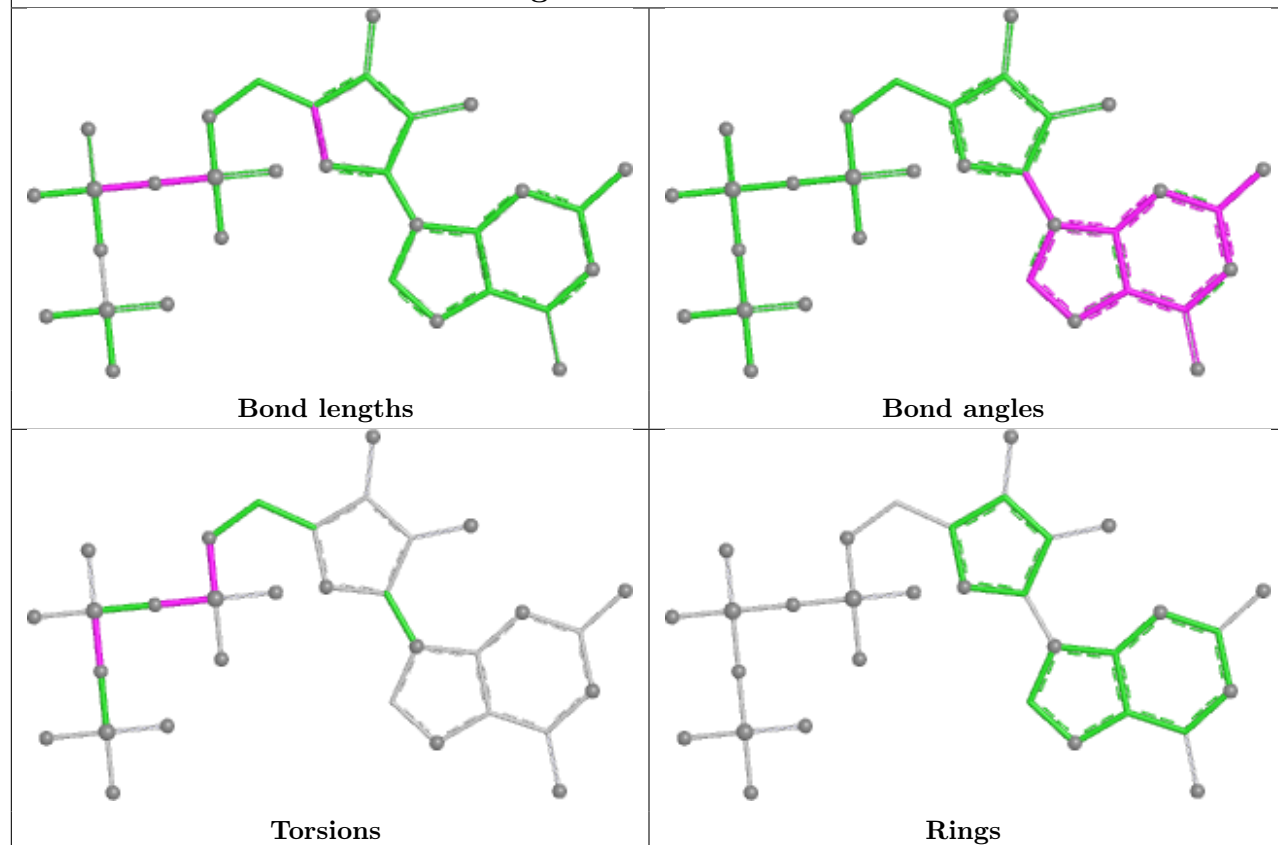
Ligand VLB C 800



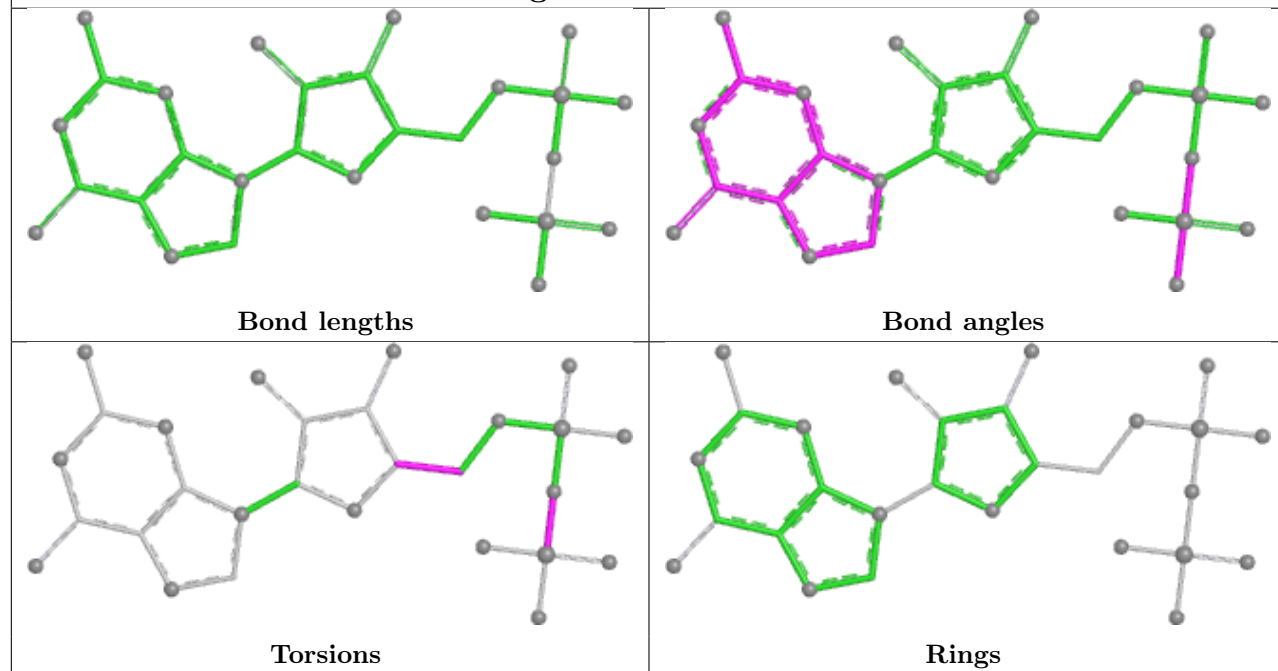
Ligand GDP D 603

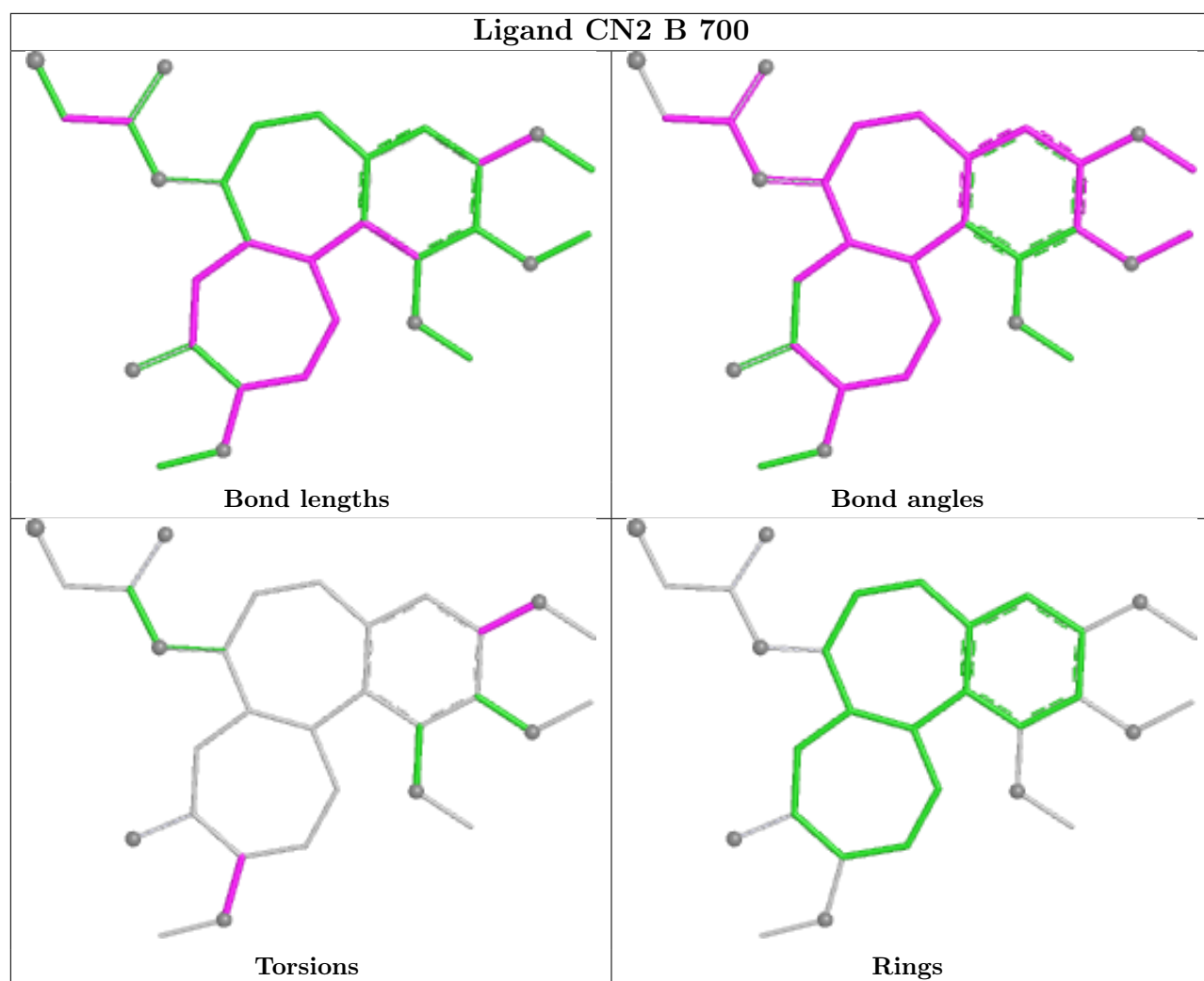


Ligand GTP C 601



Ligand GDP B 602





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	427/448 (95%)	-0.75	0 100 100	88, 118, 118, 118	1 (0%)
1	C	422/448 (94%)	-0.67	0 100 100	118, 118, 118, 118	0
2	B	419/445 (94%)	-0.88	0 100 100	118, 118, 118, 118	0
2	D	419/445 (94%)	-0.78	0 100 100	118, 118, 118, 118	0
3	E	124/142 (87%)	-0.79	0 100 100	118, 118, 118, 118	0
All	All	1811/1928 (93%)	-0.77	0 100 100	88, 118, 118, 118	1 (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.

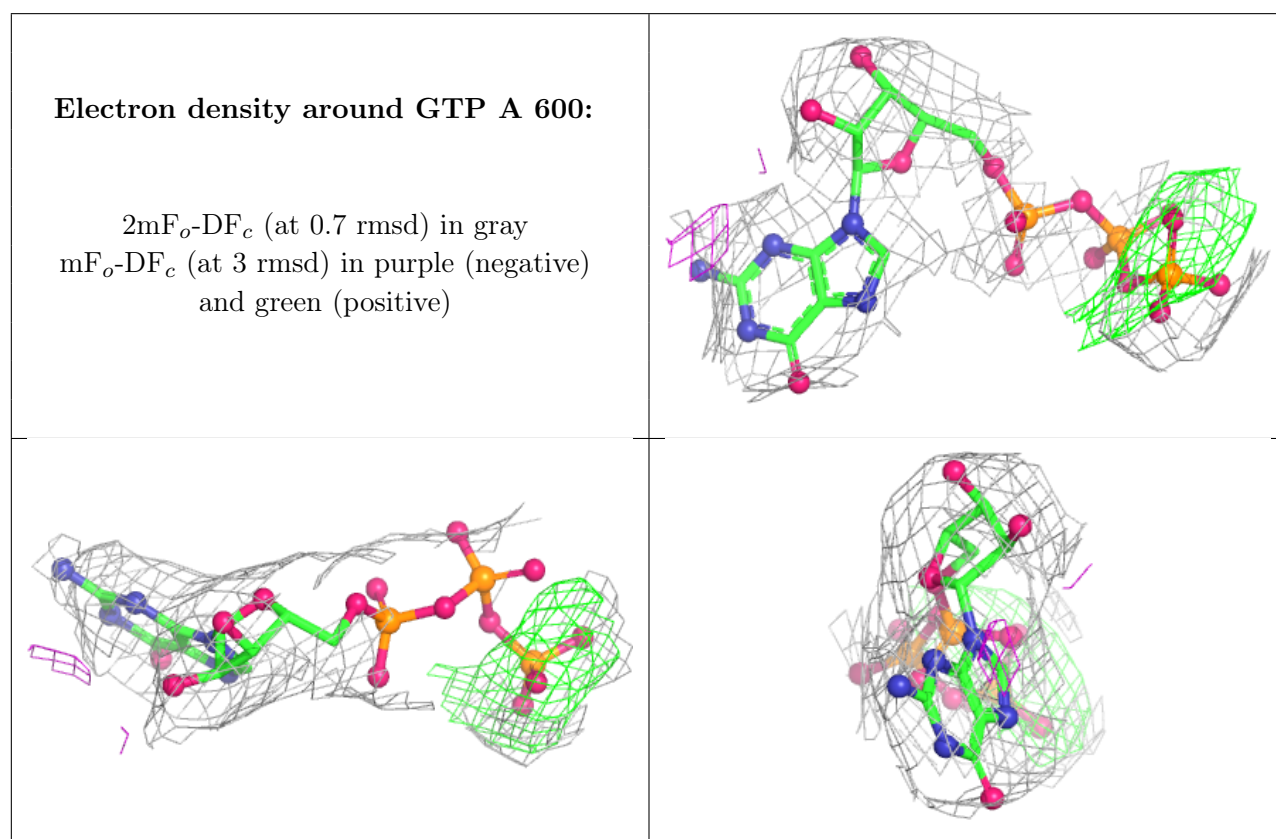
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	500	1/1	0.80	0.15	117,117,117,117	0
5	GTP	A	600	32/32	0.89	0.07	117,117,117,117	0
8	VLB	C	800	59/59	0.92	0.07	117,117,117,117	0

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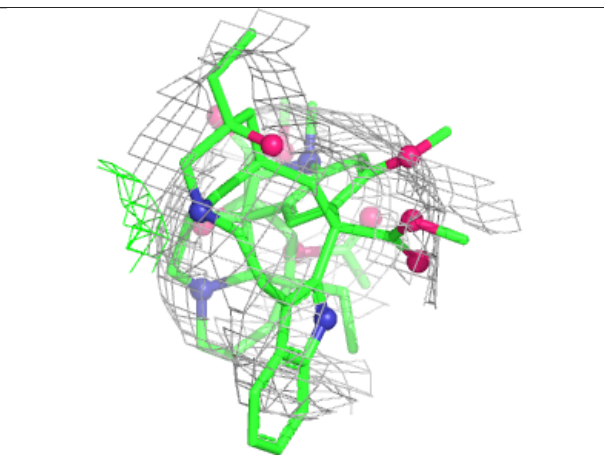
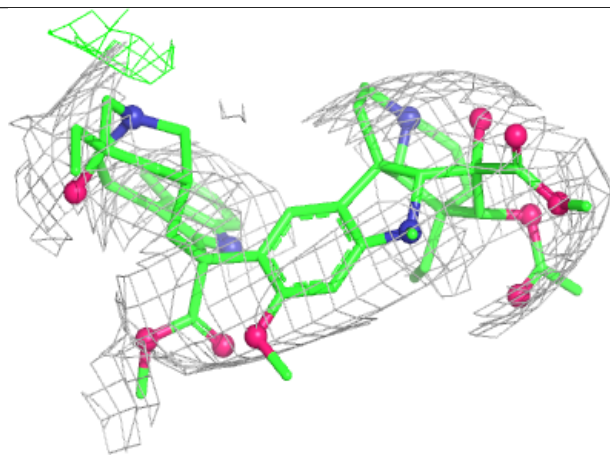
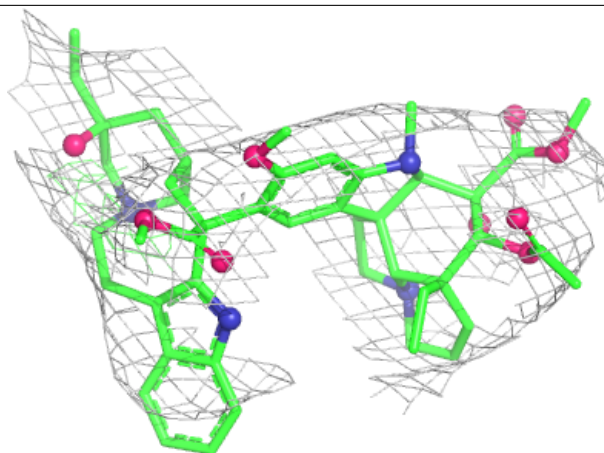
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GDP	B	602	28/28	0.93	0.06	117,117,117,117	0
4	MG	C	501	1/1	0.95	0.10	117,117,117,117	0
6	GDP	D	603	28/28	0.95	0.04	117,117,117,117	0
7	CN2	D	701	30/30	0.95	0.06	117,117,117,117	0
5	GTP	C	601	32/32	0.95	0.06	117,117,117,117	0
7	CN2	B	700	30/30	0.96	0.05	117,117,117,117	0

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

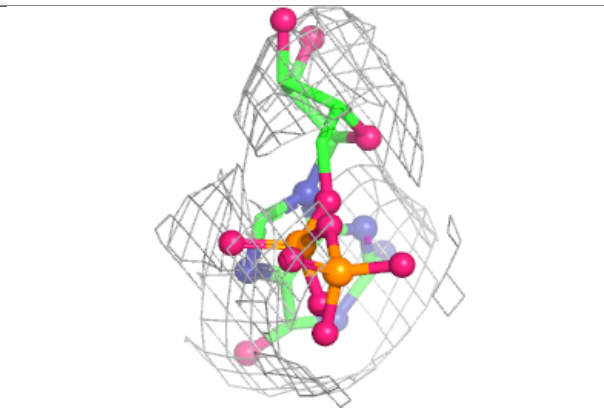
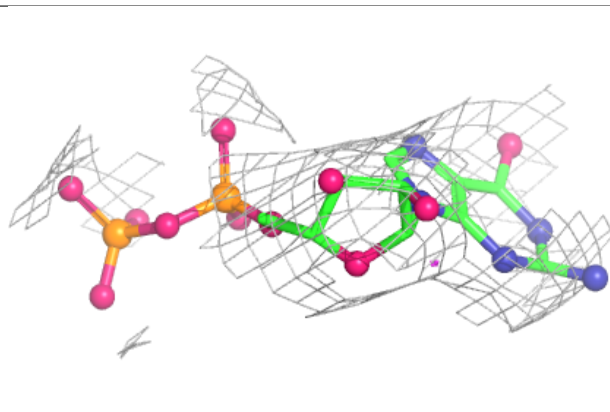
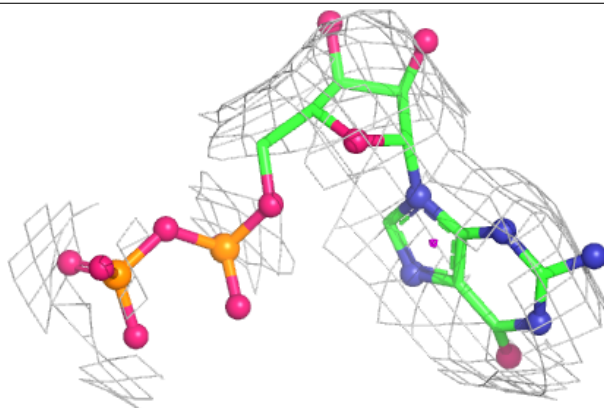


Electron density around VLB C 800:

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

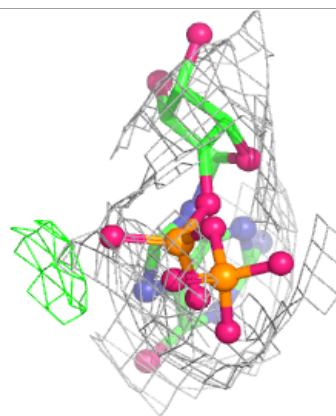
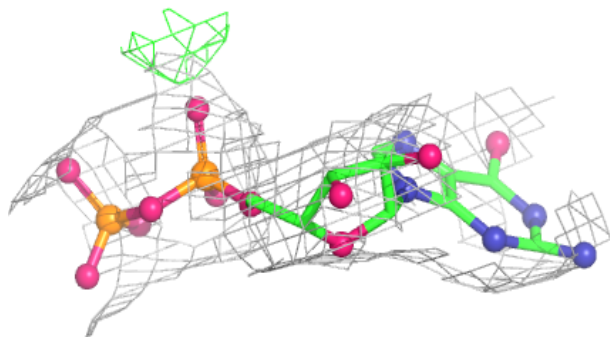
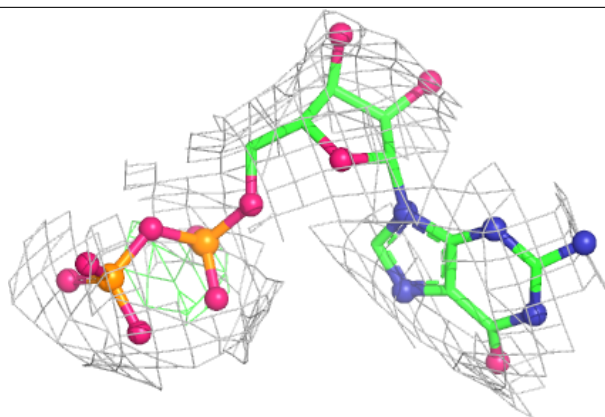
**Electron density around GDP B 602:**

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



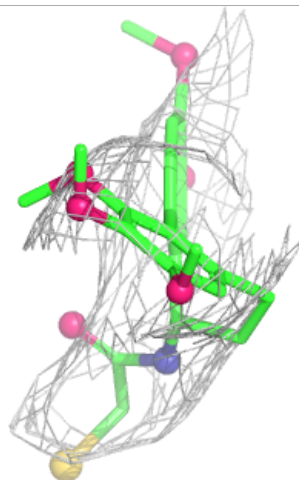
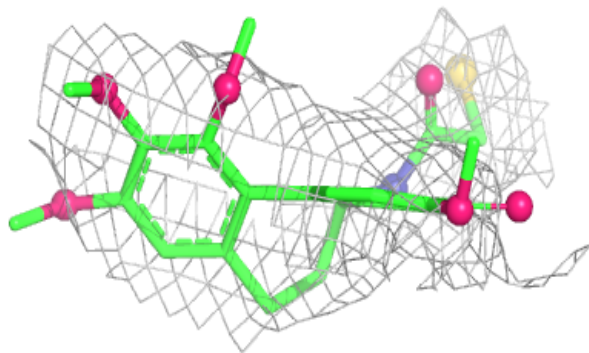
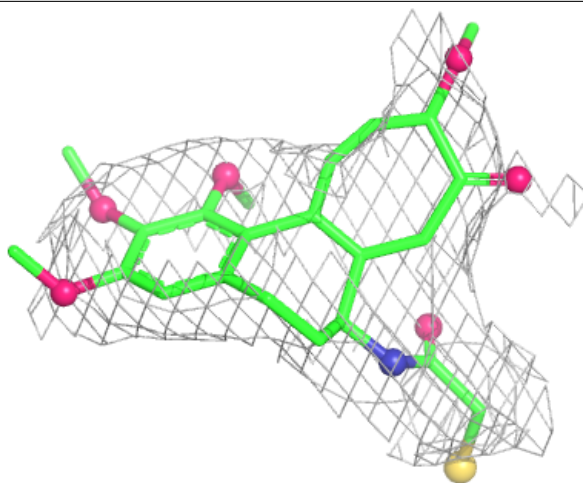
Electron density around GDP D 603:

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



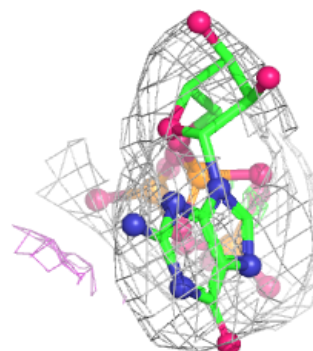
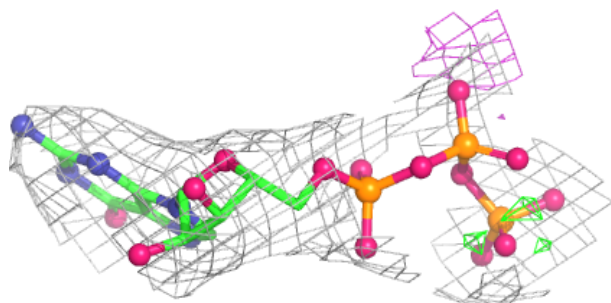
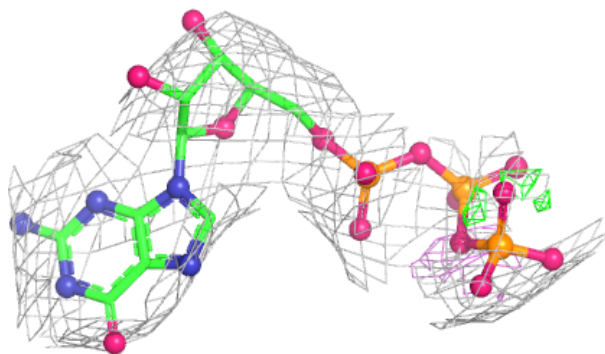
Electron density around CN2 D 701:

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



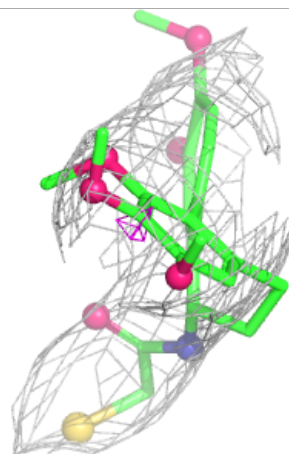
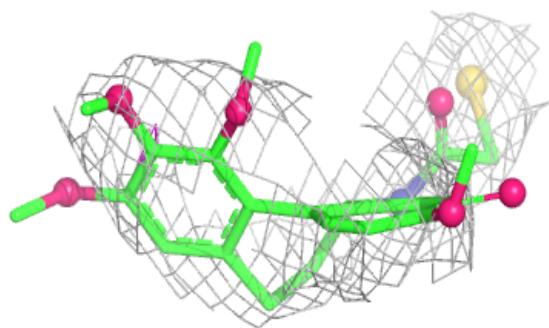
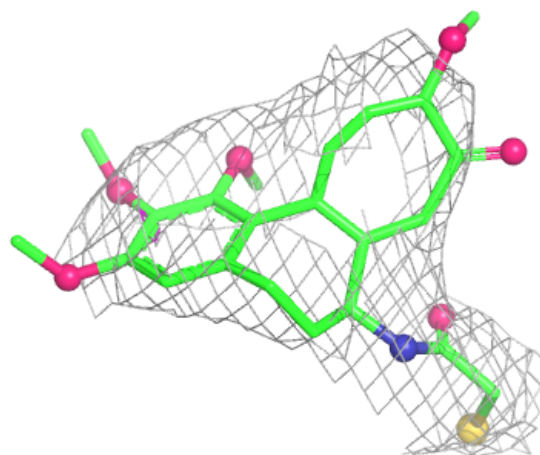
Electron density around GTP C 601:

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



Electron density around CN2 B 700:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.