



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:29 PM UTC

PDB ID : 4ECK / pdb\_00004eck  
Title : Crystal Structure of the Toxoplasma gondii TS-DHFR  
Authors : Sharma, H.; Anderson, K.S.  
Deposited on : 2012-03-26  
Resolution : 3.52 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

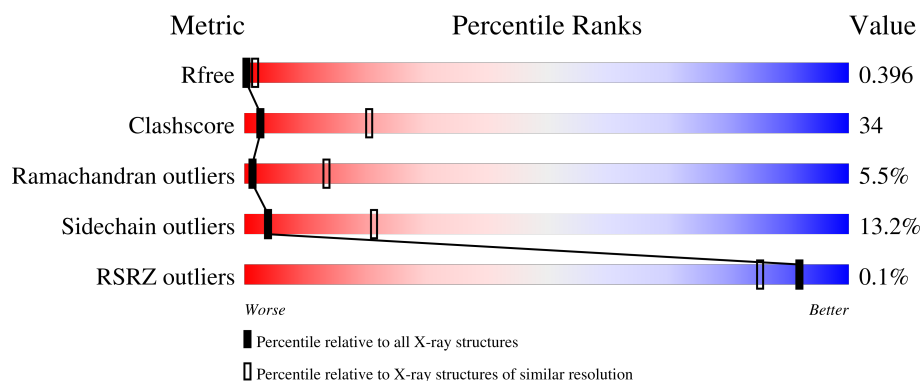
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.52 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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

Mol	Chain	Length	Quality of chain
1	A	610	
1	B	610	

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
2	UMP	A	701	-	-	X	-
2	UMP	B	701	-	-	X	-
3	CB3	A	702	-	-	X	-
3	CB3	B	702	-	-	X	-
4	FOL	A	703	-	-	X	-
4	FOL	B	703	-	-	X	-

## 2 Entry composition [i](#)

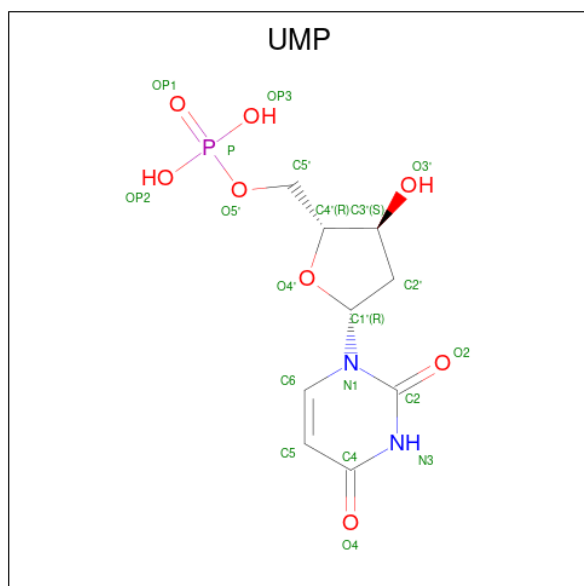
There are 5 unique types of molecules in this entry. The entry contains 8248 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional dihydrofolate reductase-thymidylate synthase.

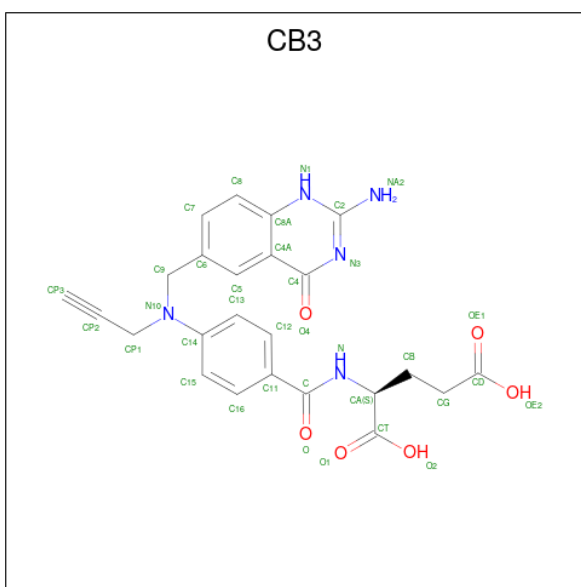
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3989	2550	697	717	25			
1	B	498	Total	C	N	O	S	0	0	0
			3989	2550	697	717	25			

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: C<sub>9</sub>H<sub>13</sub>N<sub>2</sub>O<sub>8</sub>P).



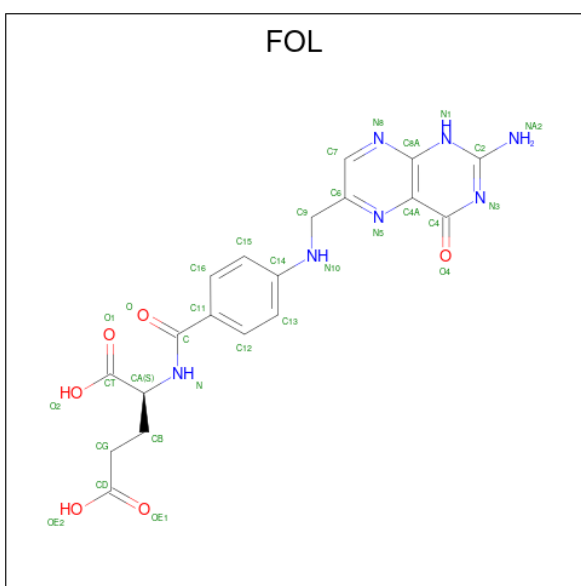
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (CCD ID: CB3) (formula: C<sub>24</sub>H<sub>23</sub>N<sub>5</sub>O<sub>6</sub>).



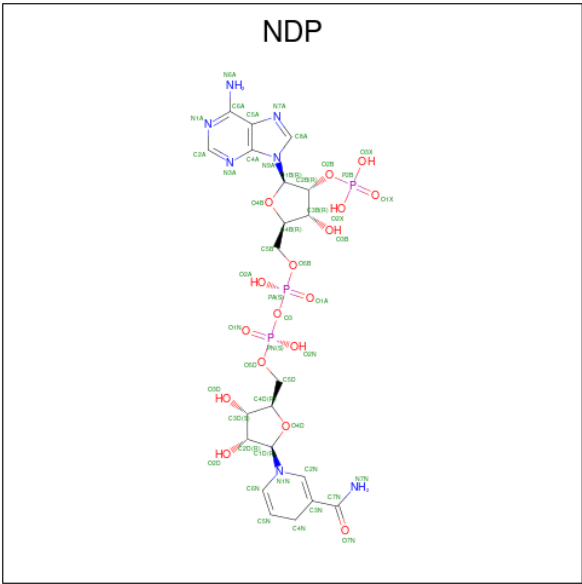
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is FOLIC ACID (CCD ID: FOL) (formula:  $C_{19}H_{19}N_7O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	19	7	6		
4	B	1	Total	C	N	O	0	0
			32	19	7	6		

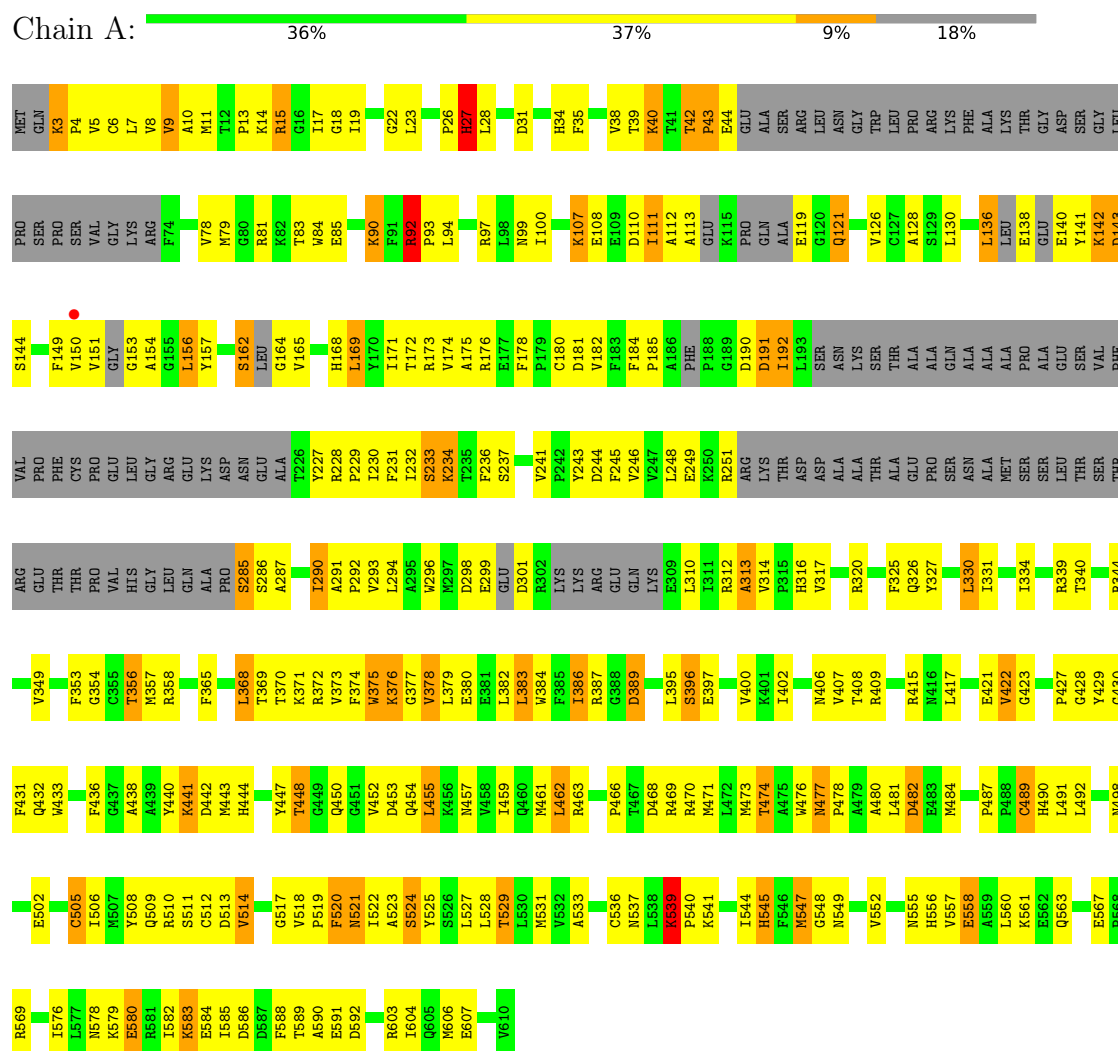
- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



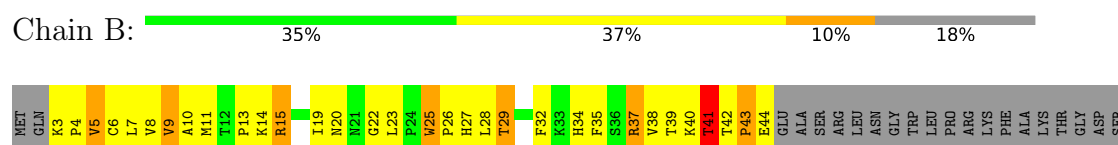
### 3 Residue-property plots

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: Bifunctional dihydrofolate reductase-thymidylate synthase



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P568	Q500	D424	I331	SER	GLN	L134	GLY
R569	C506	P427	I334	ASN	ALA	S135	LEU
P570	I506	W433	I335	ALA	ALA	L136	PRO
I573	M507	F436	R339	MET	PRO	LEU	SER
R578	Y508	Y440	R344	SER	ALA	E138	SER
K579	Q509	Y447	T345	LEU	GLU	GLU	VAL
E580	R510	K441	I350	THR	SER	E140	GLY
R581	S511	D442	F353	THR	VAL	Y141	LYS
I582	C512	M443	G354	ARG	PHE	K142	ARG
I585	D513	H444	C355	GLU	VAL	D143	F74
D586	V514	T445	T356	THR	PRO	S144	N75
D587	G515	D446	R357	THR	PHE	V145	A76
F588	L516	Y447	L361	THR	CYS	I148	V77
T589	G517	D453	P366	PRO	GLU	F149	V78
A590	G519	Q454	L367	VAL	LEU	M79	M79
E591	V518	L455	L368	HIS	GLY	V150	G80
D592	P519	K456	T369	GLY	ARG	V151	R81
I599	F520	M457	T370	LEU	GLY	GLY	K82
E591	M521	V458	K371	GLN	GLU	G153	
D592	M522	M461	R372	ALA	LYS	A154	
P599	A523	L462	F373	ASP	ASP	G155	M87
P600	S524	M465	F374	PRO	ASN	L156	P88
H601	Y525	M468	V378	S285	GLU	Y157	R89
G602	S526	R469	L379	S286	ALA	E158	K90
R603	L527	M470	E380	A287		S162	F91
I604	L528	M471	E299	I290	Y226	LEU	R92
Q605	M530	L472	E381	V293	Y227	GLU	P93
M606	C536	M473	L382	W296	R228	G164	L94
E607		T474	L383	M297	P229	V165	V95
Y610	K539	A475	L384	D298	I230	A166	D96
	P540	M476	F385	E299	F231	S167	R97
		M477	I386	GLU	I232	H168	L98
	F543	P478	N391	D301	S233	L169	N99
I544	H545	A479	A392	R302	K234	Y170	I100
H545	F546	A480	N393	LYS	F236	I171	V101
F546	M547	L481	H394	LYS	S237	T172	
M547	G548	M484	L395	LYS	V241	R173	K107
M549	T550	A485	S396	LYS	P242	V174	E108
H551	V552	L486	I402	LYS	Y243		E109
V552		P487	W403	LYS	D244		D110
H556		C488	K405	LYS	F245	D181	I111
		H489	R409	LYS	V246	F184	A112
A559	L491	L490	E421	LYS	V247	P185	A113
L560	L492	L491	G423	LYS	L248	A186	GLU
K561	C493	C494		LYS	E249	PHE	K115
F562	Q494	F495		LYS	K250	PRO	PRO
Q563	F495	Y496		LYS	R251	GLN	GLN
L564	F496	V497		LYS	ARG	ALA	ALA
R565	R566	N498		LYS	LYS	D190	E119
R566	E567	D499		LYS	THR	D191	G120
E567				LYS	THR	I192	Q121
				LYS	ASP	L193	Q122
				LYS	ASP	SER	R123
				LYS	ALA	ASN	
				LYS	ALA	LYS	C127
				LYS	THR	SER	A128
				LYS	ALA	THR	S129
				LYS	GLU	ALA	L130
				LYS	PRO	ALA	P131



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.94Å 143.01Å 59.84Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	46.18 – 3.52 46.18 – 3.52	Depositor EDS
% Data completeness (in resolution range)	95.9 (46.18-3.52) 95.9 (46.18-3.52)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.332 , 0.395 0.328 , 0.396	Depositor DCC
$R_{free}$ test set	982 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.5	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 150.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.387 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	8248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2797e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UMP, FOL, NDP, CB3

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.79	0/4078	1.03	11/5510 (0.2%)
1	B	0.80	0/4078	1.02	13/5510 (0.2%)
All	All	0.79	0/8156	1.03	24/11020 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	111	ILE	N-CA-C	-9.94	104.27	113.71
1	A	539	LYS	CA-C-N	8.88	130.28	119.98
1	A	539	LYS	C-N-CA	8.88	130.28	119.98
1	B	233	SER	N-CA-C	8.29	120.09	111.14
1	A	365	PHE	CA-C-N	7.01	128.60	119.84
1	A	365	PHE	C-N-CA	7.01	128.60	119.84
1	B	92	ARG	CA-C-N	-6.59	111.60	119.84
1	B	92	ARG	C-N-CA	-6.59	111.60	119.84
1	B	539	LYS	CA-C-N	6.20	126.14	119.76
1	B	539	LYS	C-N-CA	6.20	126.14	119.76
1	B	228	ARG	CA-C-N	5.91	127.23	119.84
1	B	228	ARG	C-N-CA	5.91	127.23	119.84
1	B	108	GLU	N-CA-C	5.79	118.55	108.76
1	A	233	SER	N-CA-C	5.79	120.40	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	477	ASN	CA-C-N	5.55	125.38	119.28
1	A	477	ASN	C-N-CA	5.55	125.38	119.28
1	B	287	ALA	N-CA-C	-5.47	99.15	110.80
1	A	505	CYS	N-CA-C	5.44	118.33	109.24
1	B	486	LEU	CA-C-N	5.42	125.96	120.38
1	B	486	LEU	C-N-CA	5.42	125.96	120.38
1	A	192	ILE	N-CA-C	-5.39	100.93	108.80
1	A	514	VAL	N-CA-C	5.21	115.99	110.72
1	B	505	CYS	N-CA-C	5.08	117.69	109.06
1	A	356	THR	N-CA-C	5.05	116.08	108.46

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	THR	Peptide
1	A	92	ARG	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	3989	0	3939	269	0
1	B	3989	0	3940	304	0
2	A	20	0	11	25	0
2	B	20	0	11	15	0
3	A	35	0	21	15	0
3	B	35	0	21	18	0
4	A	32	0	17	10	0
4	B	32	0	17	24	0
5	A	48	0	26	7	0
5	B	48	0	26	16	0
All	All	8248	0	8029	554	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 34.

All (554) 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:B:402:ILE:HG22	3:B:702:CB3:C16	1.09	1.56
1:B:402:ILE:CG2	3:B:702:CB3:C16	1.91	1.46
1:B:510:ARG:HH12	2:B:701:UMP:P	1.40	1.41
1:A:489:CYS:SG	2:A:701:UMP:C6	2.28	1.25
1:A:344:ARG:NH2	2:A:701:UMP:OP3	1.72	1.21
1:B:23:LEU:CD2	5:B:704:NDP:H2N	1.74	1.17
1:A:151:VAL:HG12	4:A:703:FOL:H7	1.22	1.16
1:B:402:ILE:CG2	3:B:702:CB3:C11	2.24	1.16
1:A:83:THR:OG1	5:A:704:NDP:O2A	1.66	1.12
1:B:510:ARG:NH1	2:B:701:UMP:OP2	1.82	1.11
1:B:156:LEU:HD12	5:B:704:NDP:N7A	1.65	1.10
1:B:35:PHE:CE2	4:B:703:FOL:H12	1.86	1.09
1:B:23:LEU:HD21	5:B:704:NDP:H2N	1.30	1.09
1:B:91:PHE:CD1	4:B:703:FOL:O	2.05	1.09
1:B:402:ILE:HG22	3:B:702:CB3:H16	1.31	1.09
1:B:402:ILE:CG2	3:B:702:CB3:C15	2.31	1.09
1:B:510:ARG:NH1	2:B:701:UMP:P	2.25	1.07
1:B:402:ILE:HG22	3:B:702:CB3:C11	1.82	1.07
1:A:344:ARG:HH21	2:A:701:UMP:P	1.81	1.04
1:B:402:ILE:HG22	3:B:702:CB3:C15	1.89	1.03
1:B:35:PHE:HE2	4:B:703:FOL:H12	1.27	0.99
1:A:433:TRP:HZ2	1:A:525:TYR:HH	1.04	0.98
1:A:94:LEU:HB2	1:A:99:ASN:HD21	1.22	0.98
1:A:521:ASN:ND2	3:A:702:CB3:CP3	2.27	0.98
1:A:151:VAL:CG1	4:A:703:FOL:H7	1.94	0.97
1:A:8:VAL:HG22	4:A:703:FOL:HN1	1.30	0.94
2:A:701:UMP:OP3	1:B:470:ARG:NH2	2.01	0.93
1:A:470:ARG:NH2	2:B:701:UMP:OP2	2.03	0.91
1:A:136:LEU:O	1:A:141:TYR:HB2	1.69	0.91
1:A:151:VAL:CG1	4:A:703:FOL:C7	2.48	0.91
1:B:81:ARG:NE	5:B:704:NDP:O1X	2.04	0.91
1:A:402:ILE:HB	3:A:702:CB3:C15	2.01	0.90
1:B:402:ILE:HG21	3:B:702:CB3:C11	2.02	0.89
1:B:89:ARG:HA	1:B:92:ARG:HG3	1.56	0.88
1:A:489:CYS:SG	2:A:701:UMP:C5	2.68	0.87
1:B:156:LEU:HD12	5:B:704:NDP:C8A	2.03	0.87
1:A:40:LYS:HG2	1:A:97:ARG:HD3	1.57	0.86
1:B:23:LEU:HD21	5:B:704:NDP:C2N	2.05	0.86
1:A:470:ARG:HH21	2:B:701:UMP:P	1.98	0.85
2:A:701:UMP:P	1:B:470:ARG:NH2	2.49	0.85
1:A:151:VAL:HG12	4:A:703:FOL:C7	2.03	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG23	1:A:171:ILE:HG12	1.60	0.83
1:A:344:ARG:NH2	2:A:701:UMP:P	2.47	0.83
1:B:427:PRO:HD2	1:B:484:MET:HG2	1.59	0.82
1:B:229:PRO:O	1:B:230:ILE:HB	1.78	0.82
1:B:244:ASP:HB2	1:B:570:PRO:HG3	1.62	0.81
1:A:344:ARG:NH2	2:A:701:UMP:C5'	2.44	0.81
1:B:87:MET:HE1	4:B:703:FOL:C11	2.11	0.81
1:B:344:ARG:HG3	1:B:345:THR:N	1.97	0.80
1:B:156:LEU:CD1	5:B:704:NDP:C8A	2.59	0.80
1:B:402:ILE:HB	3:B:702:CB3:C15	2.12	0.80
1:B:402:ILE:HG21	3:B:702:CB3:C12	2.11	0.80
1:B:76:ALA:HB3	1:B:148:ILE:HG22	1.64	0.80
1:B:138:GLU:HA	1:B:142:LYS:HB2	1.64	0.80
1:A:375:TRP:CH2	1:A:379:LEU:HD22	2.17	0.79
1:B:87:MET:CE	4:B:703:FOL:C16	2.60	0.79
1:B:87:MET:HE3	4:B:703:FOL:C15	2.13	0.79
1:A:344:ARG:HH22	2:A:701:UMP:H5''	1.46	0.78
1:B:8:VAL:HG12	4:B:703:FOL:HN1	1.45	0.78
1:A:233:SER:O	1:A:234:LYS:HB3	1.84	0.78
1:A:521:ASN:OD1	2:A:701:UMP:N3	2.16	0.77
1:A:22:GLY:O	5:A:704:NDP:O2D	2.02	0.77
1:B:87:MET:CE	4:B:703:FOL:C11	2.61	0.77
1:B:227:TYR:HB3	1:B:248:LEU:HB3	1.67	0.77
1:A:8:VAL:HG22	4:A:703:FOL:N1	2.00	0.76
1:B:489:CYS:SG	2:B:701:UMP:C6	2.79	0.76
1:A:489:CYS:SG	2:A:701:UMP:N1	2.58	0.76
1:B:510:ARG:NH2	2:B:701:UMP:OP1	2.20	0.74
1:B:402:ILE:CB	3:B:702:CB3:C15	2.65	0.74
1:B:560:LEU:O	1:B:561:LYS:HB3	1.87	0.74
1:A:580:GLU:H	1:A:580:GLU:CD	1.95	0.74
1:A:344:ARG:HH22	2:A:701:UMP:C5'	2.02	0.73
1:B:322:HIS:O	1:B:323:GLU:HB2	1.87	0.73
1:B:87:MET:HE1	4:B:703:FOL:C12	2.19	0.73
1:A:84:TRP:CH2	1:A:92:ARG:O	2.42	0.72
1:B:81:ARG:HE	5:B:704:NDP:P2B	2.11	0.72
2:A:701:UMP:P	1:B:470:ARG:HH22	2.12	0.72
1:B:510:ARG:NH1	2:B:701:UMP:OP1	2.19	0.72
1:B:140:GLU:O	1:B:141:TYR:HB2	1.89	0.71
1:B:8:VAL:HG12	4:B:703:FOL:N1	2.05	0.71
1:B:402:ILE:HG21	3:B:702:CB3:C16	2.09	0.70
1:B:94:LEU:HB2	1:B:99:ASN:HD21	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LEU:HD11	1:B:601:HIS:HA	1.72	0.70
1:A:533:ALA:HB1	1:A:540:PRO:HD3	1.74	0.69
1:B:233:SER:O	1:B:234:LYS:HB3	1.92	0.69
1:B:42:THR:O	1:B:43:PRO:C	2.35	0.69
1:A:469:ARG:HB2	1:B:510:ARG:NH2	2.07	0.69
1:A:436:PHE:CZ	1:A:477:ASN:HB2	2.28	0.69
1:B:9:VAL:CG2	1:B:171:ILE:HG12	2.22	0.68
1:B:9:VAL:HG23	1:B:171:ILE:HG12	1.76	0.68
1:A:344:ARG:CZ	2:A:701:UMP:OP3	2.41	0.68
1:B:507:MET:HB2	1:B:525:TYR:CD2	2.29	0.68
1:A:521:ASN:CG	3:A:702:CB3:CP3	2.67	0.68
1:B:91:PHE:CE1	4:B:703:FOL:O	2.47	0.68
1:A:151:VAL:HG13	4:A:703:FOL:C7	2.23	0.68
1:A:107:LYS:HD2	1:A:108:GLU:HG3	1.74	0.68
1:A:402:ILE:HG22	3:A:702:CB3:C16	2.23	0.68
1:B:381:GLU:OE1	1:B:520:PHE:HE1	1.77	0.68
1:A:173:ARG:HD3	1:A:244:ASP:OD1	1.95	0.67
1:B:10:ALA:O	1:B:25:TRP:HZ2	1.76	0.67
1:B:389:ASP:OD2	1:B:394:HIS:ND1	2.26	0.67
1:A:190:ASP:O	1:A:191:ASP:HB2	1.95	0.67
1:B:344:ARG:HG3	1:B:345:THR:H	1.58	0.67
1:A:296:TRP:CZ2	1:B:34:HIS:HB2	2.29	0.67
1:A:505:CYS:SG	1:A:506:ILE:N	2.68	0.67
1:B:94:LEU:HB2	1:B:99:ASN:ND2	2.10	0.67
1:A:589:THR:O	1:A:591:GLU:N	2.28	0.66
1:B:589:THR:O	1:B:591:GLU:N	2.28	0.66
1:A:107:LYS:HG2	1:A:126:VAL:HB	1.78	0.66
1:B:510:ARG:HG3	1:B:511:SER:N	2.10	0.66
1:A:22:GLY:C	5:A:704:NDP:HO2N	2.00	0.66
1:A:84:TRP:HH2	1:A:92:ARG:O	1.78	0.66
1:B:313:ALA:O	1:B:320:ARG:NH1	2.28	0.66
1:A:18:GLY:HA3	5:A:704:NDP:H1D	1.75	0.66
1:B:151:VAL:HB	4:B:703:FOL:H7	1.78	0.66
1:B:23:LEU:HD13	1:B:25:TRP:CZ3	2.30	0.66
1:A:287:ALA:O	1:A:290:ILE:HD13	1.94	0.66
1:A:427:PRO:HD2	1:A:484:MET:HG2	1.78	0.66
1:A:502:GLU:HB3	1:A:541:LYS:HB2	1.78	0.66
1:A:528:LEU:O	1:A:531:MET:HB2	1.94	0.66
1:A:138:GLU:HA	1:A:142:LYS:HG2	1.78	0.65
1:B:89:ARG:HA	1:B:92:ARG:CG	2.24	0.65
1:B:35:PHE:CE2	4:B:703:FOL:C12	2.74	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LEU:HD11	1:A:528:LEU:HD13	1.79	0.65
1:B:6:CYS:SG	1:B:168:HIS:HB2	2.36	0.65
1:B:402:ILE:HG21	3:B:702:CB3:C13	2.26	0.65
1:B:433:TRP:HZ2	1:B:525:TYR:HH	1.44	0.65
1:B:5:VAL:CG2	1:B:6:CYS:N	2.60	0.65
1:A:358:ARG:HB2	1:A:544:ILE:HG12	1.80	0.64
1:A:233:SER:OG	1:A:244:ASP:HB2	1.98	0.64
1:B:19:ILE:HG13	1:B:181:ASP:OD2	1.96	0.64
1:A:162:SER:O	1:A:164:GLY:N	2.30	0.64
1:A:181:ASP:OD1	1:A:182:VAL:HG23	1.98	0.64
1:B:166:ALA:O	1:B:167:SER:HB3	1.98	0.64
1:A:9:VAL:CG2	1:A:171:ILE:HG12	2.27	0.64
1:B:371:LYS:HG2	1:B:563:GLN:NE2	2.14	0.63
1:B:358:ARG:HB2	1:B:544:ILE:HG12	1.79	0.63
1:B:154:ALA:O	5:B:704:NDP:O1A	2.16	0.63
1:A:511:SER:OG	1:B:469:ARG:HD2	1.98	0.63
1:A:94:LEU:HB2	1:A:99:ASN:ND2	2.06	0.63
1:A:470:ARG:NH2	2:B:701:UMP:P	2.69	0.62
1:B:8:VAL:HG11	1:B:35:PHE:HD1	1.63	0.62
1:A:466:PRO:HA	1:A:471:MET:HE1	1.81	0.62
1:B:531:MET:HB3	1:B:588:PHE:CE2	2.34	0.62
1:B:167:SER:O	1:B:249:GLU:HA	1.99	0.62
1:A:508:TYR:HD2	1:B:508:TYR:HD2	1.48	0.62
1:A:368:LEU:HD22	1:A:368:LEU:H	1.64	0.61
1:A:438:ALA:HB1	1:A:450:GLN:HE21	1.64	0.61
1:A:455:LEU:HD22	1:A:473:MET:SD	2.40	0.61
1:A:489:CYS:HB3	1:A:509:GLN:HE21	1.65	0.61
1:A:291:ALA:HA	1:A:294:LEU:HD12	1.82	0.61
1:B:233:SER:O	1:B:234:LYS:CB	2.49	0.61
1:B:421:GLU:O	1:B:422:VAL:C	2.43	0.61
1:B:391:ASN:HB2	1:B:443:MET:HB2	1.82	0.61
1:B:5:VAL:HG23	1:B:6:CYS:H	1.65	0.61
1:A:13:PRO:HG3	1:A:175:ALA:HA	1.82	0.61
1:A:290:ILE:HG12	1:A:290:ILE:O	2.01	0.61
1:A:536:CYS:O	1:A:537:ASN:HB3	2.01	0.60
1:B:91:PHE:CE1	4:B:703:FOL:HA	2.36	0.60
1:A:228:ARG:HG3	1:A:251:ARG:HG3	1.83	0.60
1:B:14:LYS:O	1:B:15:ARG:HB2	2.01	0.60
1:B:368:LEU:H	1:B:368:LEU:HD22	1.65	0.60
1:B:402:ILE:HG21	3:B:702:CB3:C15	2.26	0.60
1:B:514:VAL:HB	1:B:552:VAL:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:GLU:CA	1:B:142:LYS:HB2	2.32	0.60
1:B:166:ALA:O	1:B:167:SER:CB	2.50	0.60
1:A:331:ILE:HD13	1:A:560:LEU:HD22	1.82	0.60
1:B:508:TYR:CD1	1:B:508:TYR:C	2.79	0.60
1:A:463:ARG:HH12	1:A:584:GLU:CD	2.09	0.60
1:A:34:HIS:HB2	1:B:296:TRP:CZ2	2.37	0.59
1:A:384:TRP:NE1	1:A:389:ASP:HB3	2.16	0.59
1:B:140:GLU:N	1:B:140:GLU:OE1	2.35	0.59
1:B:87:MET:HE3	4:B:703:FOL:C16	2.31	0.59
1:B:509:GLN:NE2	1:B:512:CYS:SG	2.75	0.59
1:A:431:PHE:CE2	1:A:440:TYR:HD2	2.19	0.59
1:B:154:ALA:HB3	5:B:704:NDP:O1N	2.03	0.59
1:B:39:THR:O	1:B:75:ASN:HB2	2.03	0.59
1:B:493:CYS:HB3	1:B:525:TYR:HE2	1.68	0.59
1:A:402:ILE:CG2	3:A:702:CB3:C16	2.81	0.58
1:B:560:LEU:O	1:B:561:LYS:CB	2.50	0.58
1:A:233:SER:O	1:A:234:LYS:CB	2.51	0.58
1:A:3:LYS:N	1:A:4:PRO:HD3	2.18	0.58
1:A:521:ASN:CG	3:A:702:CB3:HP3	2.28	0.58
1:A:287:ALA:O	1:A:290:ILE:CD1	2.52	0.57
1:A:525:TYR:O	1:A:529:THR:OG1	2.21	0.57
1:A:154:ALA:HB3	5:A:704:NDP:O1N	2.04	0.57
1:A:402:ILE:HG22	3:A:702:CB3:C11	2.34	0.57
1:B:87:MET:HE3	4:B:703:FOL:C14	2.33	0.57
1:B:531:MET:O	1:B:535:VAL:HG22	2.04	0.57
1:B:334:ILE:O	1:B:350:ILE:HG22	2.05	0.57
1:B:510:ARG:CZ	2:B:701:UMP:OP1	2.52	0.57
1:A:521:ASN:HD21	3:A:702:CB3:CP3	2.12	0.57
1:B:131:PRO:HA	1:B:134:LEU:HD12	1.86	0.57
1:A:17:ILE:HD11	1:A:154:ALA:HB2	1.86	0.57
1:A:517:GLY:O	1:A:520:PHE:HB3	2.04	0.57
1:A:330:LEU:O	1:A:334:ILE:HG13	2.04	0.57
1:B:344:ARG:HD3	2:B:701:UMP:OP3	2.05	0.57
1:B:433:TRP:HZ2	1:B:525:TYR:OH	1.87	0.57
1:B:10:ALA:O	1:B:25:TRP:CZ2	2.57	0.56
1:B:15:ARG:HD2	1:B:184:PHE:HB3	1.87	0.56
1:B:402:ILE:HG21	3:B:702:CB3:C14	2.35	0.56
1:A:241:VAL:HG12	1:A:243:TYR:HD2	1.69	0.56
1:B:15:ARG:HB3	1:B:184:PHE:HB3	1.87	0.56
1:B:81:ARG:CD	5:B:704:NDP:O1X	2.52	0.56
1:A:138:GLU:HA	1:A:142:LYS:CG	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:O	1:B:334:ILE:HD12	2.05	0.56
1:B:384:TRP:NE1	1:B:389:ASP:HB3	2.20	0.56
1:A:370:THR:HG23	1:A:563:GLN:NE2	2.20	0.56
1:A:556:HIS:CD2	1:A:606:MET:HB3	2.40	0.56
1:A:474:THR:HG21	1:B:476:TRP:O	2.06	0.56
1:B:136:LEU:O	1:B:141:TYR:HB2	2.06	0.56
1:B:322:HIS:O	1:B:323:GLU:CB	2.52	0.56
1:B:381:GLU:OE1	1:B:520:PHE:CE1	2.59	0.56
1:B:461:MET:SD	1:B:468:ASP:OD2	2.63	0.56
1:B:241:VAL:HG12	1:B:243:TYR:HD2	1.71	0.56
1:A:11:MET:SD	1:A:15:ARG:HG2	2.46	0.56
1:A:107:LYS:HD2	1:A:108:GLU:CD	2.30	0.55
1:A:90:LYS:NZ	1:A:90:LYS:H	2.04	0.55
1:A:407:VAL:O	1:A:422:VAL:HG13	2.06	0.55
1:B:491:LEU:HD21	1:B:510:ARG:HB3	1.87	0.55
1:A:356:THR:HA	1:A:545:HIS:O	2.07	0.55
1:A:370:THR:HG23	1:A:563:GLN:HE21	1.72	0.55
1:B:390:THR:HG21	1:B:440:TYR:CE2	2.42	0.55
1:B:505:CYS:SG	1:B:506:ILE:N	2.75	0.55
1:B:543:PHE:CD1	1:B:543:PHE:C	2.85	0.55
1:A:26:PRO:O	1:A:28:LEU:HD23	2.07	0.55
1:A:312:ARG:HG2	1:A:313:ALA:H	1.71	0.55
1:B:454:GLN:NE2	1:B:474:THR:O	2.37	0.55
1:A:229:PRO:HB2	1:A:317:VAL:HG22	1.89	0.55
1:A:34:HIS:HA	1:B:296:TRP:NE1	2.21	0.55
1:A:589:THR:C	1:A:591:GLU:H	2.14	0.55
1:A:35:PHE:CE2	4:A:703:FOL:H12	2.42	0.55
1:A:107:LYS:HD2	1:A:108:GLU:CG	2.36	0.55
1:B:390:THR:HG21	1:B:440:TYR:HE2	1.72	0.55
1:B:556:HIS:CD2	1:B:606:MET:HB3	2.42	0.55
1:A:111:ILE:O	1:A:112:ALA:HB3	2.08	0.54
1:B:458:VAL:HG11	1:B:495:PHE:CE2	2.43	0.54
1:B:455:LEU:HD21	1:B:585:ILE:HG21	1.88	0.54
1:B:508:TYR:C	1:B:508:TYR:HD1	2.16	0.54
1:B:531:MET:HB3	1:B:588:PHE:HE2	1.71	0.54
1:A:384:TRP:CE2	1:A:389:ASP:HB3	2.43	0.54
1:B:491:LEU:CD2	1:B:510:ARG:HB3	2.38	0.54
1:A:110:ASP:O	1:A:113:ALA:HB3	2.08	0.53
1:A:9:VAL:HG11	1:A:184:PHE:CE2	2.43	0.53
1:B:11:MET:SD	1:B:15:ARG:HA	2.49	0.53
1:B:119:GLU:HG3	1:B:121:GLN:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LYS:N	1:B:4:PRO:HD3	2.24	0.53
1:A:11:MET:O	1:A:174:VAL:HB	2.08	0.53
1:A:169:LEU:HD12	1:A:248:LEU:HD12	1.90	0.53
1:A:415:ARG:HH11	1:A:487:PRO:HD3	1.74	0.53
1:B:510:ARG:HG3	1:B:511:SER:H	1.72	0.53
1:A:138:GLU:HA	1:A:142:LYS:CB	2.39	0.53
1:B:156:LEU:HD12	5:B:704:NDP:C5A	2.36	0.53
1:A:521:ASN:OD1	2:A:701:UMP:C4	2.61	0.53
1:B:335:ILE:HA	1:B:350:ILE:HG21	1.91	0.53
1:A:374:PHE:O	1:A:378:VAL:CG1	2.57	0.52
1:A:461:MET:SD	1:A:468:ASP:OD2	2.66	0.52
1:A:514:VAL:HB	1:A:552:VAL:HG12	1.92	0.52
1:A:521:ASN:ND2	3:A:702:CB3:CP2	2.70	0.52
1:B:22:GLY:O	5:B:704:NDP:O2D	2.19	0.52
1:A:10:ALA:HA	1:A:172:THR:HB	1.91	0.52
1:B:507:MET:HB2	1:B:525:TYR:HD2	1.71	0.52
1:B:26:PRO:O	1:B:27:HIS:C	2.52	0.52
1:B:5:VAL:CG2	1:B:6:CYS:H	2.23	0.52
1:B:156:LEU:HD13	5:B:704:NDP:C8A	2.38	0.52
1:A:433:TRP:CD1	1:A:473:MET:HG2	2.45	0.51
1:B:497:VAL:HG12	1:B:498:ASN:O	2.10	0.51
1:B:569:ARG:HD2	1:B:599:VAL:O	2.09	0.51
1:B:165:VAL:O	1:B:166:ALA:HB2	2.10	0.51
1:A:421:GLU:O	1:A:422:VAL:C	2.52	0.51
1:A:521:ASN:HD21	3:A:702:CB3:CP2	2.23	0.51
1:B:525:TYR:O	1:B:529:THR:OG1	2.29	0.51
1:B:589:THR:C	1:B:591:GLU:H	2.18	0.51
1:A:227:TYR:HB3	1:A:248:LEU:HB3	1.92	0.51
1:B:8:VAL:HB	1:B:151:VAL:HG12	1.92	0.51
1:B:168:HIS:O	1:B:169:LEU:HD23	2.10	0.51
1:B:326:GLN:O	1:B:330:LEU:HB2	2.11	0.51
1:A:430:GLY:HA2	1:A:433:TRP:HB2	1.93	0.51
1:A:508:TYR:CD2	1:B:508:TYR:HD2	2.28	0.51
1:B:533:ALA:HB1	1:B:540:PRO:HD3	1.91	0.51
1:B:586:ASP:C	1:B:588:PHE:H	2.19	0.51
1:A:249:GLU:OE2	1:A:251:ARG:HD3	2.11	0.51
1:B:28:LEU:O	1:B:32:PHE:HD1	1.93	0.51
1:B:158:GLU:HB3	1:B:185:PRO:HG3	1.93	0.51
1:A:427:PRO:O	1:A:432:GLN:HG2	2.10	0.51
1:B:559:ALA:HB1	1:B:604:ILE:HG21	1.93	0.51
1:B:472:LEU:HG	1:B:494:GLN:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LYS:HG2	1:B:142:LYS:HZ1	1.75	0.50
1:B:402:ILE:CG2	3:B:702:CB3:C14	2.89	0.50
1:B:505:CYS:O	1:B:544:ILE:N	2.45	0.50
1:B:578:ASN:O	1:B:582:ILE:HD12	2.12	0.50
1:A:474:THR:HB	1:B:476:TRP:CD1	2.47	0.50
1:B:9:VAL:HG21	1:B:171:ILE:HG12	1.93	0.50
1:A:173:ARG:HD2	1:A:246:VAL:CG1	2.42	0.49
1:A:344:ARG:NH2	2:A:701:UMP:O5'	2.44	0.49
1:A:344:ARG:NH2	2:A:701:UMP:H5''	2.13	0.49
1:A:375:TRP:O	1:A:378:VAL:HG13	2.12	0.49
2:A:701:UMP:P	1:B:469:ARG:HH21	2.34	0.49
1:B:7:LEU:HD13	1:B:157:TYR:HD1	1.77	0.49
1:A:26:PRO:O	1:A:27:HIS:C	2.55	0.49
1:A:232:ILE:HD12	1:A:325:PHE:HZ	1.77	0.49
1:A:344:ARG:NE	2:A:701:UMP:OP3	2.45	0.49
1:A:580:GLU:O	1:A:583:LYS:NZ	2.44	0.49
1:B:35:PHE:HE2	4:B:703:FOL:HN	1.61	0.49
1:A:42:THR:C	1:A:43:PRO:O	2.56	0.49
1:A:402:ILE:CG2	3:A:702:CB3:C11	2.91	0.49
1:B:561:LYS:HA	1:B:564:LEU:HG	1.94	0.49
1:A:330:LEU:O	1:A:330:LEU:HD22	2.12	0.49
1:A:375:TRP:O	1:A:376:LYS:C	2.56	0.49
1:B:374:PHE:O	1:B:378:VAL:HG23	2.13	0.49
1:A:441:LYS:N	1:A:447:TYR:OH	2.46	0.49
1:A:90:LYS:H	1:A:90:LYS:HZ1	1.60	0.48
1:A:455:LEU:HD13	1:A:473:MET:SD	2.53	0.48
1:B:527:LEU:O	1:B:531:MET:HG3	2.12	0.48
1:A:604:ILE:HG22	1:A:606:MET:HG3	1.94	0.48
1:B:331:ILE:HD13	1:B:560:LEU:HD22	1.94	0.48
1:B:453:ASP:O	1:B:454:GLN:C	2.56	0.48
1:B:512:CYS:O	1:B:551:HIS:CE1	2.66	0.48
1:A:490:HIS:HD2	2:A:701:UMP:O4	1.96	0.48
1:B:409:ARG:HD2	1:B:422:VAL:HG22	1.95	0.48
1:B:531:MET:HE2	1:B:588:PHE:CD2	2.48	0.48
1:A:291:ALA:N	1:A:292:PRO:HD2	2.28	0.48
1:B:91:PHE:HE1	4:B:703:FOL:HA	1.78	0.48
1:A:313:ALA:HB3	1:A:320:ARG:HH22	1.78	0.48
1:A:474:THR:HB	1:B:476:TRP:HD1	1.77	0.48
1:A:517:GLY:O	1:A:521:ASN:N	2.44	0.48
1:B:34:HIS:O	1:B:38:VAL:HG23	2.13	0.48
1:A:229:PRO:HG2	1:A:316:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ARG:CB	1:B:15:ARG:HH21	2.25	0.48
1:B:514:VAL:HB	1:B:552:VAL:CG2	2.42	0.48
1:B:10:ALA:HA	1:B:172:THR:HB	1.96	0.48
1:B:10:ALA:HB2	4:B:703:FOL:C2	2.44	0.48
1:B:102:VAL:HA	1:B:127:CYS:HB3	1.94	0.48
1:A:480:ALA:O	1:A:482:ASP:N	2.47	0.48
1:B:40:LYS:O	1:B:41:THR:HG23	2.13	0.48
1:B:91:PHE:CD1	4:B:703:FOL:HA	2.49	0.48
1:B:361:LEU:HD23	1:B:366:PRO:HD3	1.95	0.48
1:A:31:ASP:OD2	4:A:703:FOL:N3	2.47	0.47
1:A:11:MET:SD	1:A:15:ARG:HA	2.54	0.47
1:A:312:ARG:HG2	1:A:313:ALA:N	2.29	0.47
2:A:701:UMP:OP3	1:B:469:ARG:NH2	2.33	0.47
1:B:7:LEU:HD13	1:B:157:TYR:CD1	2.50	0.47
1:B:13:PRO:HD3	1:B:174:VAL:O	2.15	0.47
1:B:75:ASN:HA	1:B:145:VAL:HG23	1.95	0.47
1:B:296:TRP:O	1:B:299:GLU:HB2	2.14	0.47
1:B:192:ILE:HD12	1:B:193:LEU:H	1.80	0.47
1:B:368:LEU:H	1:B:368:LEU:CD2	2.26	0.47
1:A:459:ILE:HG22	1:A:463:ARG:NE	2.29	0.47
1:A:523:ALA:O	1:A:524:SER:C	2.56	0.47
1:A:548:GLY:O	1:A:549:ASN:C	2.57	0.47
1:B:518:VAL:O	1:B:522:ILE:HG13	2.15	0.47
1:A:586:ASP:C	1:A:588:PHE:H	2.22	0.47
1:A:5:VAL:HG22	1:A:6:CYS:N	2.29	0.47
1:A:469:ARG:HB2	1:B:510:ARG:HH22	1.76	0.47
1:B:409:ARG:HH11	1:B:422:VAL:HG22	1.80	0.47
1:A:22:GLY:N	5:A:704:NDP:O3D	2.46	0.47
1:A:327:TYR:CZ	1:A:331:ILE:HD11	2.49	0.47
1:B:234:LYS:O	1:B:236:PHE:CE1	2.68	0.47
1:B:441:LYS:N	1:B:447:TYR:OH	2.47	0.47
1:A:407:VAL:HG21	1:A:423:GLY:HA2	1.96	0.47
1:A:107:LYS:HA	1:A:126:VAL:HG21	1.97	0.47
1:B:19:ILE:O	1:B:20:ASN:C	2.58	0.47
1:A:354:GLY:HA2	1:A:547:MET:O	2.15	0.46
1:B:3:LYS:HG2	1:B:142:LYS:NZ	2.30	0.46
1:A:231:PHE:HD2	1:B:290:ILE:HG23	1.81	0.46
1:A:326:GLN:OE1	1:A:357:MET:HB3	2.15	0.46
1:B:81:ARG:NH2	1:B:82:LYS:HD2	2.31	0.46
1:A:353:PHE:HB2	1:B:496:TYR:CE2	2.50	0.46
1:A:39:THR:HA	1:A:149:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:PRO:HG2	1:B:91:PHE:HB2	1.97	0.46
1:B:385:PHE:HB3	1:B:433:TRP:CZ3	2.50	0.46
1:A:237:SER:HA	1:A:241:VAL:O	2.14	0.46
1:B:87:MET:CE	4:B:703:FOL:C12	2.90	0.46
1:B:151:VAL:HB	4:B:703:FOL:C7	2.43	0.46
1:B:586:ASP:C	1:B:588:PHE:N	2.72	0.46
1:B:299:GLU:O	1:B:301:ASP:HA	2.15	0.46
1:B:370:THR:O	1:B:566:ARG:HD3	2.16	0.46
1:B:232:ILE:HD12	1:B:325:PHE:HZ	1.81	0.46
1:B:474:THR:HA	1:B:492:LEU:HG	1.98	0.46
1:A:14:LYS:O	1:A:15:ARG:HB2	2.15	0.46
1:A:142:LYS:O	1:A:143:ASP:CG	2.59	0.46
1:A:544:ILE:HG22	1:A:545:HIS:N	2.30	0.46
1:B:471:MET:HE3	1:B:495:PHE:O	2.16	0.46
1:B:489:CYS:SG	2:B:701:UMP:C5	3.08	0.46
1:A:299:GLU:O	1:A:301:ASP:HA	2.16	0.45
1:A:428:GLY:HA2	1:A:484:MET:SD	2.56	0.45
1:A:489:CYS:CB	2:A:701:UMP:C5	2.99	0.45
1:A:520:PHE:CD1	3:A:702:CB3:CP2	2.99	0.45
1:A:539:LYS:HD2	1:A:539:LYS:C	2.41	0.45
1:B:19:ILE:HB	1:B:180:CYS:HA	1.98	0.45
1:B:230:ILE:O	1:B:247:VAL:HB	2.16	0.45
1:B:356:THR:O	1:B:357:MET:HG2	2.16	0.45
1:A:19:ILE:HG13	1:A:181:ASP:OD2	2.16	0.45
1:A:436:PHE:HB3	1:A:452:VAL:HB	1.97	0.45
1:A:462:LEU:HG	1:A:471:MET:SD	2.56	0.45
1:A:294:LEU:O	1:A:298:ASP:HB2	2.15	0.45
1:A:407:VAL:HG11	1:A:423:GLY:O	2.17	0.45
1:B:81:ARG:HD3	5:B:704:NDP:O1X	2.16	0.45
1:B:356:THR:CG2	1:B:357:MET:N	2.80	0.45
1:B:380:GLU:HA	1:B:383:LEU:HD12	1.99	0.45
1:A:78:VAL:HG22	1:A:100:ILE:HB	1.99	0.45
1:A:520:PHE:CE1	3:A:702:CB3:HP12	2.51	0.45
1:B:188:PRO:O	1:B:190:ASP:N	2.50	0.45
1:A:442:ASP:C	1:A:444:HIS:H	2.25	0.45
1:A:453:ASP:O	1:A:454:GLN:C	2.58	0.45
1:A:344:ARG:HE	1:B:470:ARG:NH2	2.15	0.45
1:A:40:LYS:HG2	1:A:97:ARG:CD	2.38	0.45
1:A:153:GLY:O	1:A:157:TYR:N	2.47	0.45
1:A:293:VAL:HA	1:A:296:TRP:CD1	2.52	0.45
1:A:344:ARG:HE	1:B:470:ARG:HH22	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:THR:O	1:A:409:ARG:C	2.59	0.45
1:A:518:VAL:HB	1:A:519:PRO:HD3	1.99	0.45
1:B:403:TRP:C	1:B:405:LYS:H	2.24	0.45
1:B:461:MET:HG2	1:B:471:MET:HG2	1.99	0.45
1:B:516:LEU:HD13	1:B:606:MET:HB2	1.99	0.45
4:A:703:FOL:C7	5:A:704:NDP:H42N	2.47	0.45
1:A:513:ASP:HB2	2:A:701:UMP:H2''	1.99	0.45
1:B:39:THR:OG1	1:B:97:ARG:NH1	2.48	0.45
1:B:136:LEU:HD22	1:B:141:TYR:CD2	2.52	0.45
1:B:484:MET:HE1	1:B:488:PRO:HD3	1.98	0.45
1:A:454:GLN:NE2	1:A:474:THR:O	2.45	0.44
1:B:461:MET:O	1:B:465:ASN:N	2.50	0.44
1:A:518:VAL:O	1:A:522:ILE:HG13	2.16	0.44
1:B:356:THR:O	1:B:357:MET:CG	2.65	0.44
1:B:442:ASP:OD1	1:B:445:THR:N	2.48	0.44
1:A:3:LYS:N	1:A:4:PRO:CD	2.81	0.44
1:A:478:PRO:HD2	1:B:436:PHE:CE1	2.52	0.44
1:B:5:VAL:HG22	1:B:6:CYS:N	2.30	0.44
1:B:102:VAL:HG21	1:B:129:SER:HA	1.99	0.44
1:B:384:TRP:CD1	1:B:389:ASP:HB3	2.53	0.44
1:A:234:LYS:HD2	1:A:236:PHE:CE1	2.52	0.44
1:A:469:ARG:NH1	2:B:701:UMP:OP3	2.51	0.44
1:B:87:MET:HE2	4:B:703:FOL:C16	2.45	0.44
1:B:138:GLU:O	1:B:140:GLU:N	2.50	0.44
1:B:173:ARG:HD2	1:B:246:VAL:CG1	2.48	0.44
1:A:5:VAL:HG22	1:A:6:CYS:H	1.82	0.44
1:A:8:VAL:HG21	1:A:35:PHE:HD1	1.83	0.44
1:A:111:ILE:O	1:A:112:ALA:CB	2.66	0.44
1:A:558:GLU:O	1:A:561:LYS:HB2	2.18	0.44
1:B:313:ALA:O	1:B:314:VAL:C	2.61	0.44
1:A:168:HIS:HA	1:A:248:LEU:O	2.18	0.43
1:B:40:LYS:HB3	1:B:97:ARG:HG3	1.98	0.43
1:B:136:LEU:HD22	1:B:141:TYR:HD2	1.82	0.43
1:A:78:VAL:HG22	1:A:100:ILE:HD12	1.98	0.43
1:A:130:LEU:HD22	1:A:156:LEU:HD22	2.00	0.43
1:B:526:SER:O	1:B:530:LEU:HD13	2.19	0.43
1:A:168:HIS:NE2	1:A:249:GLU:HG3	2.33	0.43
1:A:296:TRP:HB2	1:B:37:ARG:CZ	2.48	0.43
1:A:586:ASP:C	1:A:588:PHE:N	2.74	0.43
1:B:344:ARG:HG3	1:B:345:THR:HG23	2.00	0.43
1:A:296:TRP:C	1:A:298:ASP:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LYS:HA	1:A:540:PRO:HD2	1.76	0.43
1:B:79:MET:HG2	1:B:101:VAL:HG22	2.00	0.43
1:B:78:VAL:HB	1:B:150:VAL:HG22	1.99	0.43
1:B:167:SER:HA	1:B:250:LYS:HB2	2.00	0.43
1:B:534:HIS:NE2	1:B:579:LYS:HB3	2.33	0.43
1:B:27:HIS:HE1	1:B:29:THR:HG23	1.83	0.43
1:A:141:TYR:O	1:A:144:SER:OG	2.27	0.43
1:A:373:VAL:HG12	1:A:374:PHE:N	2.33	0.43
1:B:5:VAL:N	1:B:166:ALA:O	2.43	0.43
1:B:91:PHE:CG	4:B:703:FOL:O	2.67	0.43
1:B:293:VAL:HG12	1:B:297:MET:SD	2.59	0.43
1:B:490:HIS:HD2	2:B:701:UMP:O4	2.02	0.43
1:A:375:TRP:O	1:A:377:GLY:N	2.52	0.42
1:A:233:SER:HB3	1:A:245:PHE:O	2.18	0.42
1:A:291:ALA:N	1:A:292:PRO:CD	2.83	0.42
1:B:462:LEU:CB	1:B:536:CYS:SG	3.07	0.42
1:A:79:MET:HE1	1:A:94:LEU:HD12	2.00	0.42
1:A:296:TRP:HB2	1:B:37:ARG:NH1	2.33	0.42
1:A:374:PHE:CE1	1:A:376:LYS:HB3	2.54	0.42
1:A:173:ARG:HD2	1:A:246:VAL:HG13	2.01	0.42
1:A:374:PHE:O	1:A:378:VAL:HG12	2.18	0.42
1:B:586:ASP:O	1:B:588:PHE:N	2.52	0.42
1:A:26:PRO:O	1:A:28:LEU:N	2.52	0.42
1:B:168:HIS:HA	1:B:248:LEU:O	2.19	0.42
1:B:461:MET:HE2	1:B:461:MET:HB2	1.93	0.42
1:A:154:ALA:HB3	1:A:182:VAL:HG13	2.02	0.42
1:A:589:THR:C	1:A:591:GLU:N	2.78	0.42
1:B:391:ASN:OD1	1:B:393:ASN:HB2	2.19	0.42
1:B:325:PHE:O	1:B:326:GLN:C	2.61	0.42
1:B:517:GLY:O	1:B:520:PHE:HB3	2.19	0.42
1:A:560:LEU:O	1:A:561:LYS:C	2.63	0.42
1:B:122:GLN:O	1:B:123:ARG:HB2	2.19	0.42
1:B:374:PHE:HD1	1:B:603:ARG:NH1	2.18	0.42
1:B:511:SER:OG	1:B:551:HIS:HE1	2.03	0.42
1:A:339:ARG:HH12	1:B:500:GLN:HG2	1.84	0.42
1:B:395:LEU:O	1:B:396:SER:C	2.63	0.42
1:B:442:ASP:OD2	1:B:444:HIS:HD2	2.02	0.42
1:A:314:VAL:H	1:A:320:ARG:NH2	2.17	0.42
1:A:578:ASN:O	1:A:582:ILE:HD12	2.20	0.42
1:B:23:LEU:HD22	5:B:704:NDP:H2N	1.85	0.42
1:B:102:VAL:CG2	1:B:129:SER:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ALA:C	1:B:156:LEU:H	2.28	0.42
1:A:81:ARG:HE	1:A:81:ARG:HB3	1.71	0.41
1:A:371:LYS:O	1:A:372:ARG:C	2.62	0.41
1:A:382:LEU:HD23	1:A:527:LEU:HG	2.02	0.41
1:A:490:HIS:CD2	2:A:701:UMP:O4	2.73	0.41
1:B:229:PRO:HB2	1:B:317:VAL:HG22	2.01	0.41
1:A:382:LEU:O	1:A:386:ILE:N	2.40	0.41
1:A:518:VAL:O	1:A:519:PRO:C	2.62	0.41
1:B:242:PRO:HB3	1:B:573:ILE:HG23	2.02	0.41
1:B:372:ARG:HD2	1:B:603:ARG:HG2	2.02	0.41
1:A:7:LEU:HG	1:A:150:VAL:HB	2.02	0.41
1:A:509:GLN:O	1:A:548:GLY:N	2.44	0.41
1:B:237:SER:HA	1:B:241:VAL:O	2.20	0.41
1:B:486:LEU:HA	1:B:487:PRO:HD3	1.90	0.41
1:A:508:TYR:CD1	1:A:508:TYR:C	2.99	0.41
1:B:78:VAL:HA	1:B:100:ILE:O	2.21	0.41
1:B:368:LEU:HD22	1:B:368:LEU:N	2.33	0.41
1:B:374:PHE:CE1	3:B:702:CB3:OE2	2.73	0.41
1:A:81:ARG:HD2	1:A:85:GLU:OE2	2.21	0.41
1:A:138:GLU:O	1:A:140:GLU:N	2.53	0.41
1:A:498:ASN:HB2	1:B:339:ARG:HG3	2.01	0.41
1:A:603:ARG:NH1	3:A:702:CB3:O2	2.53	0.41
1:B:378:VAL:HG11	1:B:523:ALA:HB3	2.01	0.41
1:B:382:LEU:O	1:B:386:ILE:N	2.48	0.41
1:B:433:TRP:CZ2	1:B:525:TYR:OH	2.63	0.41
1:A:138:GLU:HA	1:A:142:LYS:HB2	2.02	0.41
1:B:15:ARG:HB2	1:B:15:ARG:NH2	2.36	0.41
1:A:285:SER:OG	1:A:286:SER:N	2.53	0.41
1:A:369:THR:HG21	1:A:569:ARG:O	2.21	0.41
1:A:555:ASN:HD21	1:A:607:GLU:HB2	1.85	0.41
1:B:462:LEU:HB3	1:B:536:CYS:SG	2.60	0.41
1:B:481:LEU:H	1:B:481:LEU:HG	1.69	0.41
1:A:119:GLU:O	1:A:121:GLN:N	2.53	0.41
1:A:176:ARG:NH1	1:A:178:PHE:HE1	2.18	0.41
1:A:327:TYR:CE2	1:A:331:ILE:HD11	2.55	0.41
1:A:372:ARG:HB3	1:A:603:ARG:HG2	2.03	0.41
1:A:576:ILE:HB	1:A:579:LYS:HE2	2.02	0.41
1:B:3:LYS:N	1:B:4:PRO:CD	2.84	0.41
1:B:74:PHE:O	1:B:145:VAL:HA	2.21	0.41
1:B:478:PRO:C	1:B:480:ALA:H	2.29	0.41
1:B:520:PHE:CG	3:B:702:CB3:H13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLU:CD	1:A:580:GLU:N	2.68	0.40
3:A:702:CB3:C6	3:A:702:CB3:H15	2.51	0.40
1:B:173:ARG:NH1	1:B:570:PRO:HD3	2.37	0.40
1:A:19:ILE:HA	1:A:181:ASP:OD2	2.22	0.40
1:A:327:TYR:O	1:A:330:LEU:HB3	2.21	0.40
1:A:520:PHE:O	1:A:522:ILE:N	2.54	0.40
1:B:109:GLU:C	1:B:109:GLU:CD	2.90	0.40
1:B:521:ASN:HD22	1:B:521:ASN:HA	1.76	0.40
1:A:19:ILE:HB	1:A:180:CYS:HA	2.02	0.40
1:A:190:ASP:O	1:A:191:ASP:CB	2.67	0.40
1:A:293:VAL:HA	1:A:296:TRP:HD1	1.87	0.40
1:A:395:LEU:O	1:A:396:SER:C	2.64	0.40
1:A:469:ARG:HH11	2:B:701:UMP:P	2.44	0.40
1:A:489:CYS:HB2	2:A:701:UMP:C5	2.57	0.40
1:B:96:ASP:H	1:B:122:GLN:HE21	1.70	0.40
1:B:499:ASP:N	1:B:499:ASP:OD1	2.53	0.40
1:B:549:ASN:OD1	1:B:549:ASN:C	2.64	0.40
1:A:383:LEU:O	1:A:387:ARG:N	2.39	0.40
1:A:432:GLN:HE22	1:A:477:ASN:HD22	1.70	0.40
1:A:459:ILE:HG22	1:A:463:ARG:CZ	2.51	0.40
1:A:476:TRP:O	1:B:474:THR:HG21	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	474/610 (78%)	379 (80%)	68 (14%)	27 (6%)	1	13
1	B	474/610 (78%)	385 (81%)	64 (14%)	25 (5%)	1	14
All	All	948/1220 (78%)	764 (81%)	132 (14%)	52 (6%)	1	13

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PRO
1	A	92	ARG
1	A	128	ALA
1	A	165	VAL
1	A	313	ALA
1	A	376	LYS
1	A	481	LEU
1	A	524	SER
1	A	590	ALA
1	B	43	PRO
1	B	166	ALA
1	B	167	SER
1	B	189	GLY
1	B	229	PRO
1	B	234	LYS
1	B	422	VAL
1	B	590	ALA
1	A	27	HIS
1	A	93	PRO
1	A	191	ASP
1	A	422	VAL
1	A	429	TYR
1	A	443	MET
1	B	41	THR
1	B	141	TYR
1	B	144	SER
1	B	287	ALA
1	B	323	GLU
1	B	561	LYS
1	A	121	GLN
1	A	375	TRP
1	A	489	CYS
1	A	592	ASP
1	B	424	ASP
1	B	587	ASP
1	A	234	LYS
1	A	396	SER
1	A	520	PHE
1	A	521	ASN
1	B	15	ARG
1	B	123	ARG
1	B	230	ILE

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Mol	Chain	Res	Type
1	B	353	PHE
1	B	592	ASP
1	A	448	THR
1	B	231	PHE
1	B	314	VAL
1	B	605	GLN
1	A	15	ARG
1	A	185	PRO
1	B	489	CYS
1	A	557	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	433/525 (82%)	379 (88%)	54 (12%)	4	22
1	B	433/525 (82%)	373 (86%)	60 (14%)	3	20
All	All	866/1050 (82%)	752 (87%)	114 (13%)	4	21

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	9	VAL
1	A	23	LEU
1	A	27	HIS
1	A	38	VAL
1	A	40	LYS
1	A	44	GLU
1	A	90	LYS
1	A	107	LYS
1	A	111	ILE
1	A	136	LEU
1	A	142	LYS
1	A	143	ASP

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Mol	Chain	Res	Type
1	A	156	LEU
1	A	162	SER
1	A	169	LEU
1	A	192	ILE
1	A	230	ILE
1	A	285	SER
1	A	290	ILE
1	A	310	LEU
1	A	330	LEU
1	A	340	THR
1	A	349	VAL
1	A	368	LEU
1	A	378	VAL
1	A	380	GLU
1	A	383	LEU
1	A	386	ILE
1	A	389	ASP
1	A	397	GLU
1	A	400	VAL
1	A	406	ASN
1	A	417	LEU
1	A	441	LYS
1	A	448	THR
1	A	455	LEU
1	A	457	ASN
1	A	462	LEU
1	A	474	THR
1	A	482	ASP
1	A	491	LEU
1	A	492	LEU
1	A	510	ARG
1	A	512	CYS
1	A	529	THR
1	A	539	LYS
1	A	545	HIS
1	A	547	MET
1	A	558	GLU
1	A	567	GLU
1	A	580	GLU
1	A	583	LYS
1	A	585	ILE
1	B	5	VAL

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Mol	Chain	Res	Type
1	B	9	VAL
1	B	25	TRP
1	B	29	THR
1	B	37	ARG
1	B	41	THR
1	B	44	GLU
1	B	79	MET
1	B	82	LYS
1	B	89	ARG
1	B	98	LEU
1	B	102	VAL
1	B	107	LYS
1	B	108	GLU
1	B	110	ASP
1	B	111	ILE
1	B	156	LEU
1	B	162	SER
1	B	192	ILE
1	B	193	LEU
1	B	228	ARG
1	B	230	ILE
1	B	249	GLU
1	B	251	ARG
1	B	302	ARG
1	B	318	HIS
1	B	320	ARG
1	B	334	ILE
1	B	344	ARG
1	B	355	CYS
1	B	356	THR
1	B	368	LEU
1	B	371	LYS
1	B	386	ILE
1	B	395	LEU
1	B	402	ILE
1	B	404	ASP
1	B	409	ARG
1	B	422	VAL
1	B	456	LYS
1	B	470	ARG
1	B	474	THR
1	B	491	LEU

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Mol	Chain	Res	Type
1	B	492	LEU
1	B	526	SER
1	B	529	THR
1	B	535	VAL
1	B	539	LYS
1	B	543	PHE
1	B	545	HIS
1	B	547	MET
1	B	552	VAL
1	B	564	LEU
1	B	567	GLU
1	B	579	LYS
1	B	580	GLU
1	B	589	THR
1	B	599	VAL
1	B	603	ARG
1	B	607	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	99	ASN
1	A	239	ASN
1	A	393	ASN
1	A	406	ASN
1	A	432	GLN
1	A	435	HIS
1	A	450	GLN
1	A	465	ASN
1	A	490	HIS
1	B	21	ASN
1	B	99	ASN
1	B	460	GLN
1	B	490	HIS
1	B	509	GLN
1	B	537	ASN
1	B	578	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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$
2	UMP	B	701	-	21,21,21	1.32	4 (19%)	30,31,31	1.90	8 (26%)
4	FOL	A	703	-	34,34,34	1.06	2 (5%)	43,47,47	1.32	2 (4%)
2	UMP	A	701	-	21,21,21	1.26	4 (19%)	30,31,31	1.79	6 (20%)
4	FOL	B	703	-	34,34,34	1.13	3 (8%)	43,47,47	1.44	4 (9%)
3	CB3	A	702	-	37,37,37	1.41	3 (8%)	50,51,51	1.47	7 (14%)
5	NDP	B	704	-	51,52,52	1.82	8 (15%)	71,80,80	2.27	11 (15%)
5	NDP	A	704	-	51,52,52	1.82	8 (15%)	71,80,80	2.26	11 (15%)
3	CB3	B	702	-	37,37,37	1.40	3 (8%)	50,51,51	1.36	6 (12%)

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
2	UMP	B	701	-	-	5/10/22/22	0/2/2/2
4	FOL	A	703	-	-	6/22/22/22	0/3/3/3
2	UMP	A	701	-	-	5/10/22/22	0/2/2/2
4	FOL	B	703	-	-	5/22/22/22	0/3/3/3
3	CB3	A	702	-	-	10/27/28/28	0/3/3/3
5	NDP	B	704	-	-	3/34/77/77	0/5/5/5
5	NDP	A	704	-	-	3/34/77/77	0/5/5/5
3	CB3	B	702	-	-	9/27/28/28	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	NDP	C6A-N6A	5.45	1.48	1.34
5	A	704	NDP	C6A-N6A	5.25	1.47	1.34
5	A	704	NDP	C2N-C3N	4.93	1.48	1.35
3	A	702	CB3	C4A-C8A	4.91	1.48	1.41
5	B	704	NDP	C6N-C5N	4.90	1.48	1.33
3	B	702	CB3	C4A-C8A	4.89	1.48	1.41
5	B	704	NDP	C2N-C3N	4.88	1.48	1.35
5	A	704	NDP	C6N-C5N	4.82	1.47	1.33
5	B	704	NDP	C3B-C2B	-4.17	1.43	1.53
5	A	704	NDP	C3B-C2B	-4.02	1.44	1.53
5	A	704	NDP	C7N-N7N	3.76	1.44	1.33
5	B	704	NDP	C7N-N7N	3.61	1.43	1.33
3	B	702	CB3	C8A-N1	-3.39	1.34	1.39
3	A	702	CB3	C8A-N1	-3.36	1.34	1.39
5	A	704	NDP	C2D-C3D	-3.28	1.44	1.53
3	A	702	CB3	CP2-CP3	3.17	1.27	1.18
5	B	704	NDP	C2D-C3D	-3.17	1.44	1.53
5	B	704	NDP	C6N-N1N	2.99	1.44	1.37
5	A	704	NDP	C6N-N1N	2.88	1.44	1.37
3	B	702	CB3	CP2-CP3	2.87	1.26	1.18
4	B	703	FOL	C8A-N1	-2.79	1.34	1.38
2	B	701	UMP	C2-N1	2.70	1.42	1.38
2	A	701	UMP	C2-N1	2.60	1.42	1.38
4	A	703	FOL	C4A-C8A	2.57	1.49	1.42
2	B	701	UMP	C2-N3	-2.51	1.33	1.38
4	A	703	FOL	C8A-N1	-2.51	1.34	1.38
2	B	701	UMP	C4-N3	-2.47	1.34	1.38
2	A	701	UMP	C2-N3	-2.41	1.33	1.38
2	A	701	UMP	C4-N3	-2.36	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	704	NDP	C5A-N7A	-2.26	1.35	1.39
2	B	701	UMP	C5-C4	-2.17	1.39	1.43
4	B	703	FOL	C4A-C8A	2.13	1.48	1.42
4	B	703	FOL	C7-C6	2.13	1.43	1.39
5	B	704	NDP	C5A-N7A	-2.09	1.35	1.39
2	A	701	UMP	C5-C4	-2.08	1.39	1.43

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	704	NDP	C1D-N1N-C2N	10.23	137.99	121.14
5	B	704	NDP	C1D-N1N-C2N	9.73	137.16	121.14
5	A	704	NDP	C1D-N1N-C6N	-8.04	103.77	120.77
5	B	704	NDP	C1D-N1N-C6N	-7.40	105.12	120.77
5	B	704	NDP	O4D-C1D-N1N	6.45	120.39	108.08
5	A	704	NDP	O4D-C1D-N1N	6.10	119.71	108.08
3	A	702	CB3	CP2-CP1-N10	-5.80	108.10	113.45
5	B	704	NDP	C5A-C4A-N3A	-5.51	119.14	126.72
5	A	704	NDP	C5A-C4A-N3A	-5.36	119.34	126.72
4	B	703	FOL	N1-C8A-N8	5.32	124.33	116.38
3	B	702	CB3	CP2-CP1-N10	-5.17	108.68	113.45
4	A	703	FOL	N1-C8A-N8	4.99	123.83	116.38
5	A	704	NDP	N3A-C2A-N1A	-4.78	121.35	128.58
5	B	704	NDP	N3A-C2A-N1A	-4.61	121.60	128.58
2	B	701	UMP	C5-C4-N3	4.59	121.23	114.80
2	A	701	UMP	C5-C4-N3	4.40	120.97	114.80
2	B	701	UMP	C4-N3-C2	-4.32	121.24	126.61
2	A	701	UMP	C4-N3-C2	-4.20	121.40	126.61
2	B	701	UMP	O4-C4-C5	-3.65	118.86	125.16
2	A	701	UMP	O4-C4-C5	-3.63	118.89	125.16
5	B	704	NDP	N3A-C4A-N9A	3.60	133.30	127.17
5	A	704	NDP	N3A-C4A-N9A	3.42	132.99	127.17
5	B	704	NDP	C2A-N3A-C4A	3.42	120.18	111.83
5	A	704	NDP	C3N-C2N-N1N	-3.33	118.31	123.20
5	A	704	NDP	C2A-N3A-C4A	3.33	119.97	111.83
2	B	701	UMP	N3-C2-N1	3.15	118.99	114.89
5	B	704	NDP	C3N-C2N-N1N	-3.05	118.73	123.20
2	A	701	UMP	N3-C2-N1	3.01	118.81	114.89
5	B	704	NDP	N9A-C8A-N7A	-2.96	109.74	113.94
3	A	702	CB3	C11-C-N	2.93	122.47	117.04
5	B	704	NDP	C4A-C5A-N7A	-2.87	107.31	110.58
5	B	704	NDP	C5A-N7A-C8A	2.75	107.77	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	CB3	OE2-CD-CG	2.59	122.18	114.00
3	B	702	CB3	CP1-N10-C9	-2.57	114.60	117.19
3	B	702	CB3	CT-CA-N	2.50	116.37	110.57
3	A	702	CB3	CT-CA-N	2.50	116.37	110.57
4	A	703	FOL	O4-C4-N3	2.45	123.96	120.23
5	A	704	NDP	C4A-C5A-N7A	-2.44	107.80	110.58
3	A	702	CB3	O-C-C11	-2.41	116.13	120.90
2	B	701	UMP	O5'-C5'-C4'	2.39	117.12	108.99
4	B	703	FOL	CA-N-C	2.37	127.26	121.56
3	A	702	CB3	OE1-CD-CG	-2.36	115.59	123.09
5	A	704	NDP	N9A-C8A-N7A	-2.34	110.61	113.94
3	B	702	CB3	C11-C-N	2.33	121.36	117.04
2	B	701	UMP	O4'-C1'-N1	2.31	111.97	107.86
3	B	702	CB3	O2-CT-CA	2.27	121.19	113.51
2	A	701	UMP	O5'-C5'-C4'	2.27	116.72	108.99
5	A	704	NDP	C5A-N7A-C8A	2.23	106.95	103.45
3	A	702	CB3	O2-CT-CA	2.21	120.98	113.51
3	B	702	CB3	O-C-C11	-2.21	116.53	120.90
2	A	701	UMP	O4'-C4'-C5'	2.17	116.27	109.33
2	B	701	UMP	O4'-C4'-C5'	2.14	116.19	109.33
4	B	703	FOL	O4-C4-N3	2.08	123.39	120.23
4	B	703	FOL	O2-CT-CA	2.05	120.45	113.51
2	B	701	UMP	OP3-P-OP2	2.02	115.37	107.80

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	UMP	C5'-O5'-P-OP1
2	A	701	UMP	C5'-O5'-P-OP2
2	B	701	UMP	C5'-O5'-P-OP1
4	A	703	FOL	N-CA-CB-CG
4	B	703	FOL	N-CA-CB-CG
4	B	703	FOL	CT-CA-CB-CG
3	A	702	CB3	CT-CA-CB-CG
3	B	702	CB3	CT-CA-CB-CG
4	A	703	FOL	CT-CA-CB-CG
5	A	704	NDP	O4D-C4D-C5D-O5D
3	B	702	CB3	N-CA-CB-CG
3	A	702	CB3	N-CA-CT-O2
3	B	702	CB3	N-CA-CT-O1
3	B	702	CB3	N-CA-CT-O2

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Mol	Chain	Res	Type	Atoms
5	A	704	NDP	C3D-C4D-C5D-O5D
3	A	702	CB3	N-CA-CT-O1
2	B	701	UMP	C5'-O5'-P-OP2
2	B	701	UMP	C2'-C1'-N1-C2
3	B	702	CB3	CB-CA-N-C
3	A	702	CB3	N-CA-CB-CG
2	A	701	UMP	C2'-C1'-N1-C2
3	A	702	CB3	CB-CA-CT-O2
3	B	702	CB3	CB-CA-CT-O1
3	B	702	CB3	CB-CA-CT-O2
4	B	703	FOL	CA-CB-CG-CD
3	A	702	CB3	CB-CA-N-C
5	B	704	NDP	O4D-C4D-C5D-O5D
5	B	704	NDP	C3D-C4D-C5D-O5D
3	A	702	CB3	CB-CA-CT-O1
4	A	703	FOL	CA-CB-CG-CD
5	B	704	NDP	O4D-C1D-N1N-C2N
5	A	704	NDP	O4D-C1D-N1N-C2N
4	A	703	FOL	OE2-CD-CG-CB
3	A	702	CB3	OE1-CD-CG-CB
4	B	703	FOL	OE1-CD-CG-CB
4	B	703	FOL	OE2-CD-CG-CB
2	B	701	UMP	C2'-C1'-N1-C6
3	A	702	CB3	OE2-CD-CG-CB
3	B	702	CB3	OE2-CD-CG-CB
4	A	703	FOL	OE1-CD-CG-CB
3	B	702	CB3	OE1-CD-CG-CB
2	A	701	UMP	C5'-O5'-P-OP3
2	B	701	UMP	C5'-O5'-P-OP3
3	A	702	CB3	CA-CB-CG-CD
2	A	701	UMP	C2'-C1'-N1-C6
4	A	703	FOL	N-CA-CT-O1

There are no ring outliers.

8 monomers are involved in 129 short contacts:

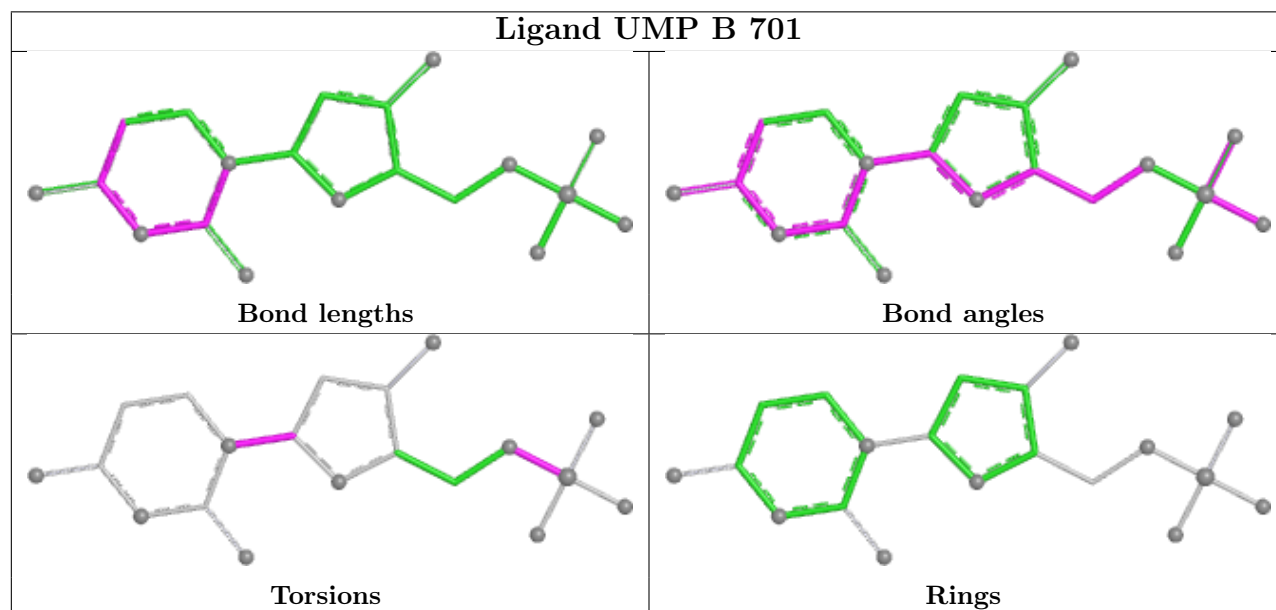
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	UMP	15	0
4	A	703	FOL	10	0
2	A	701	UMP	25	0
4	B	703	FOL	24	0
3	A	702	CB3	15	0

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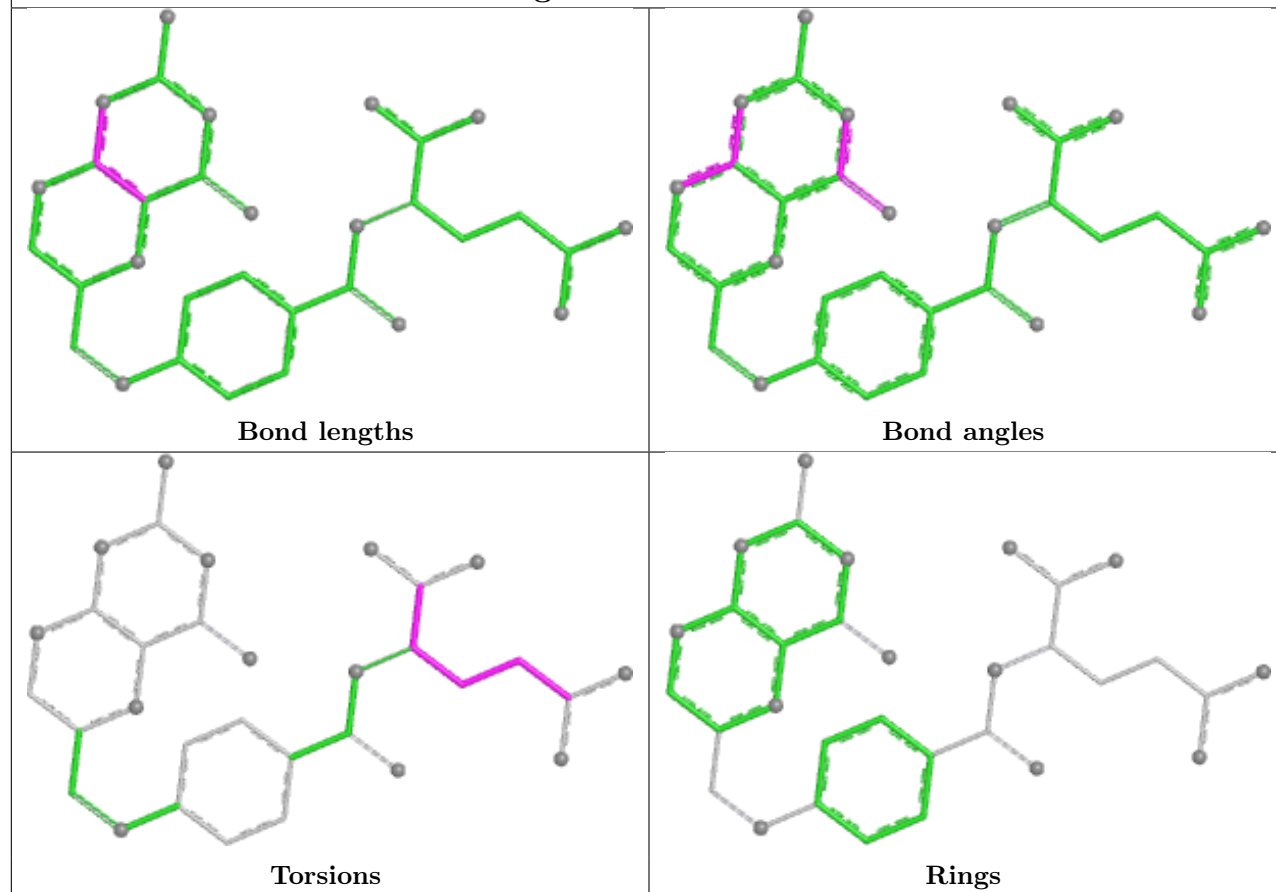
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	704	NDP	16	0
5	A	704	NDP	7	0
3	B	702	CB3	18	0

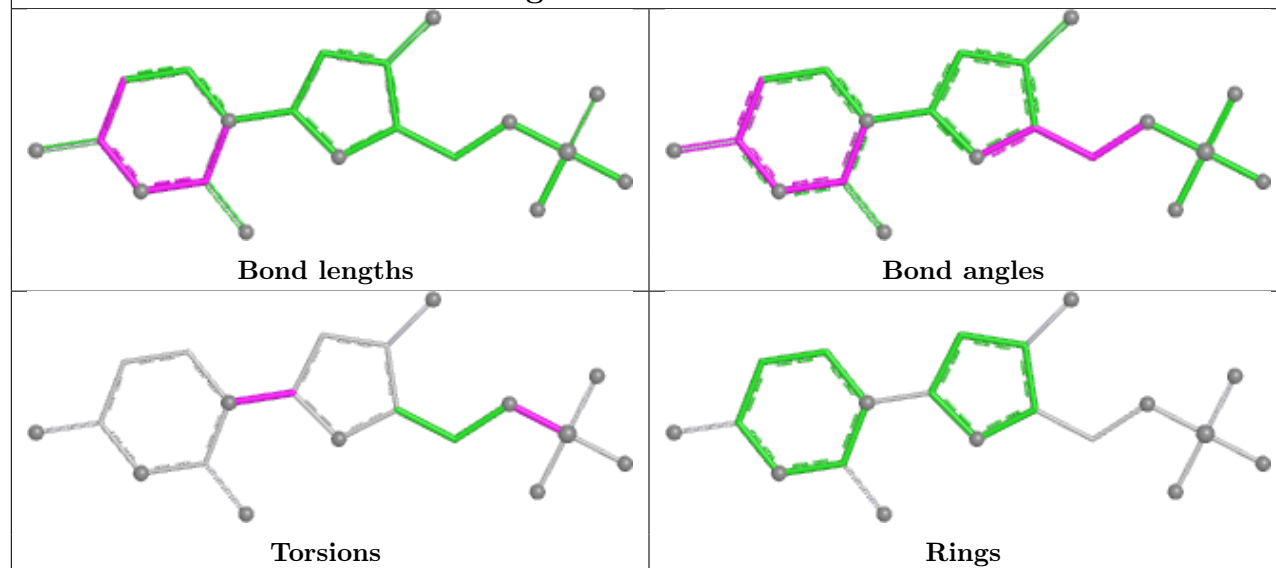
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



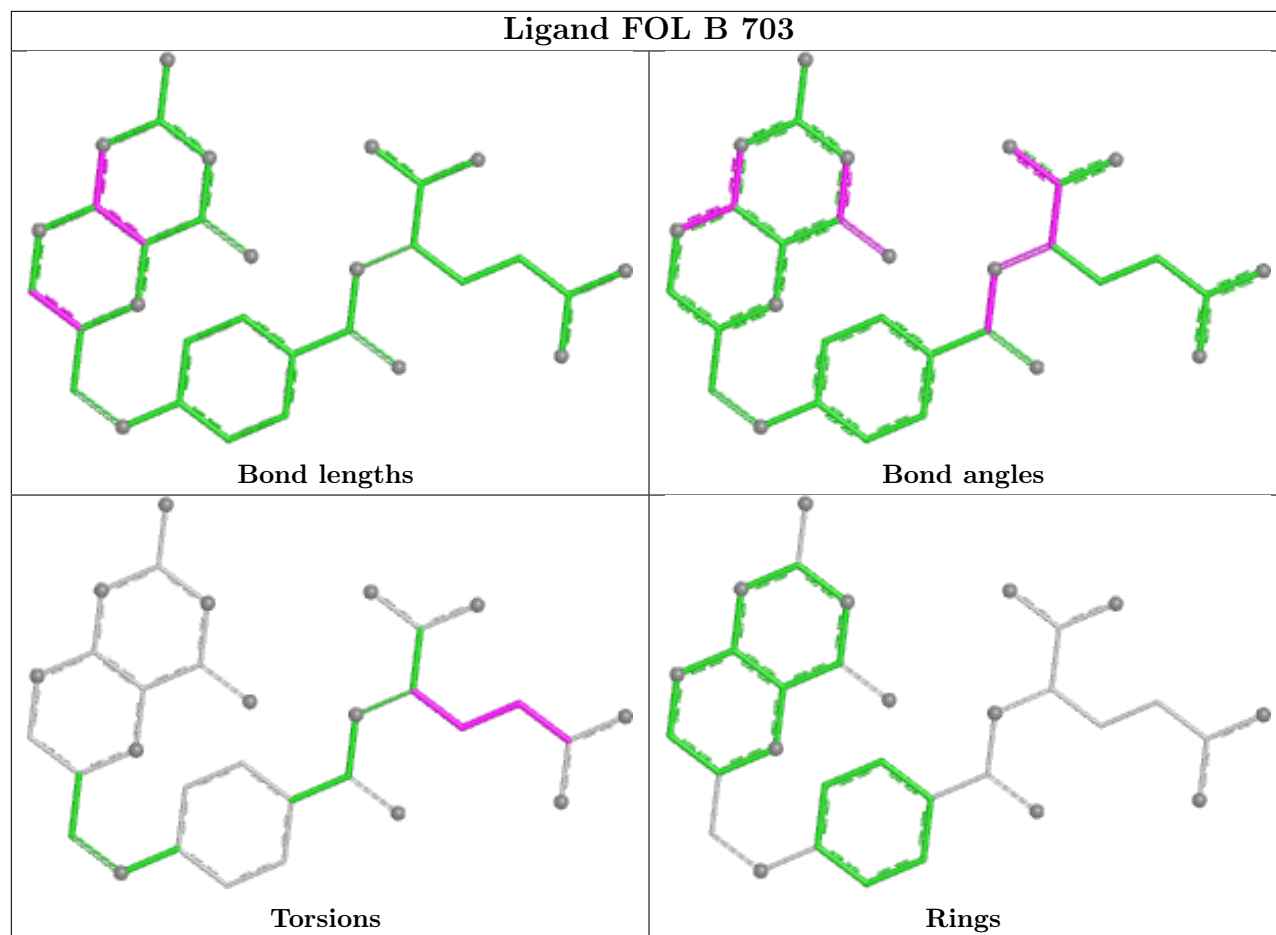
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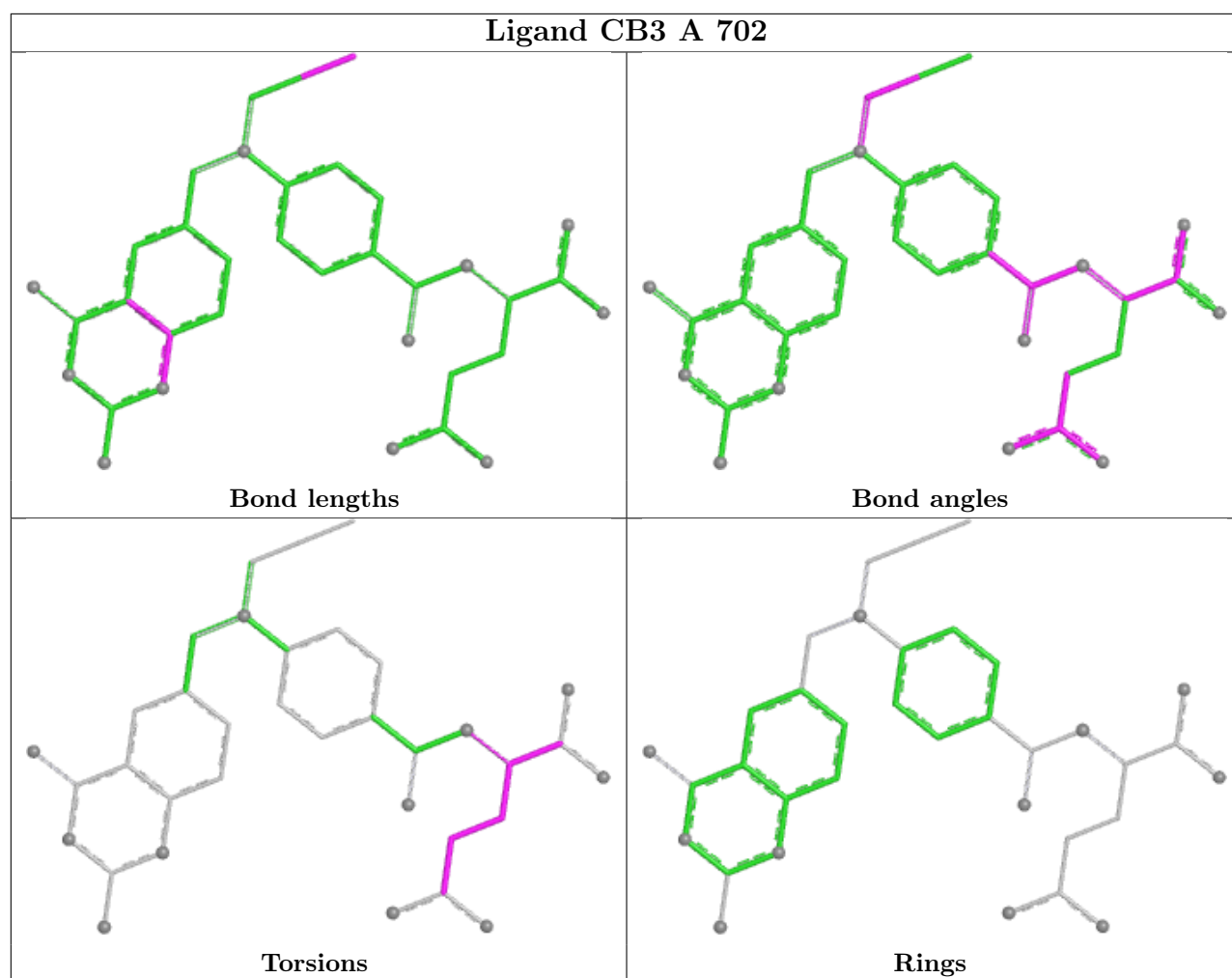


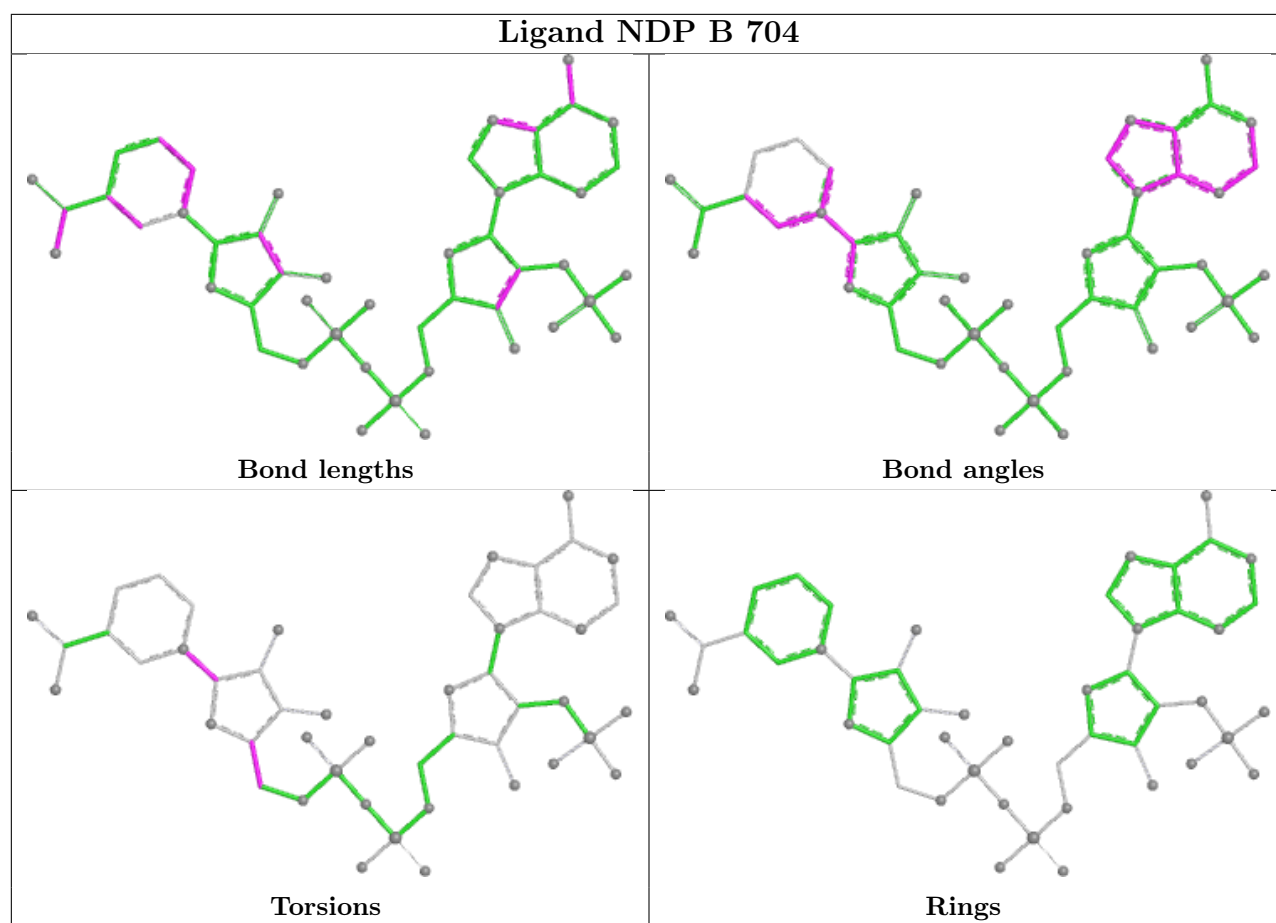
## Ligand UMP A 701



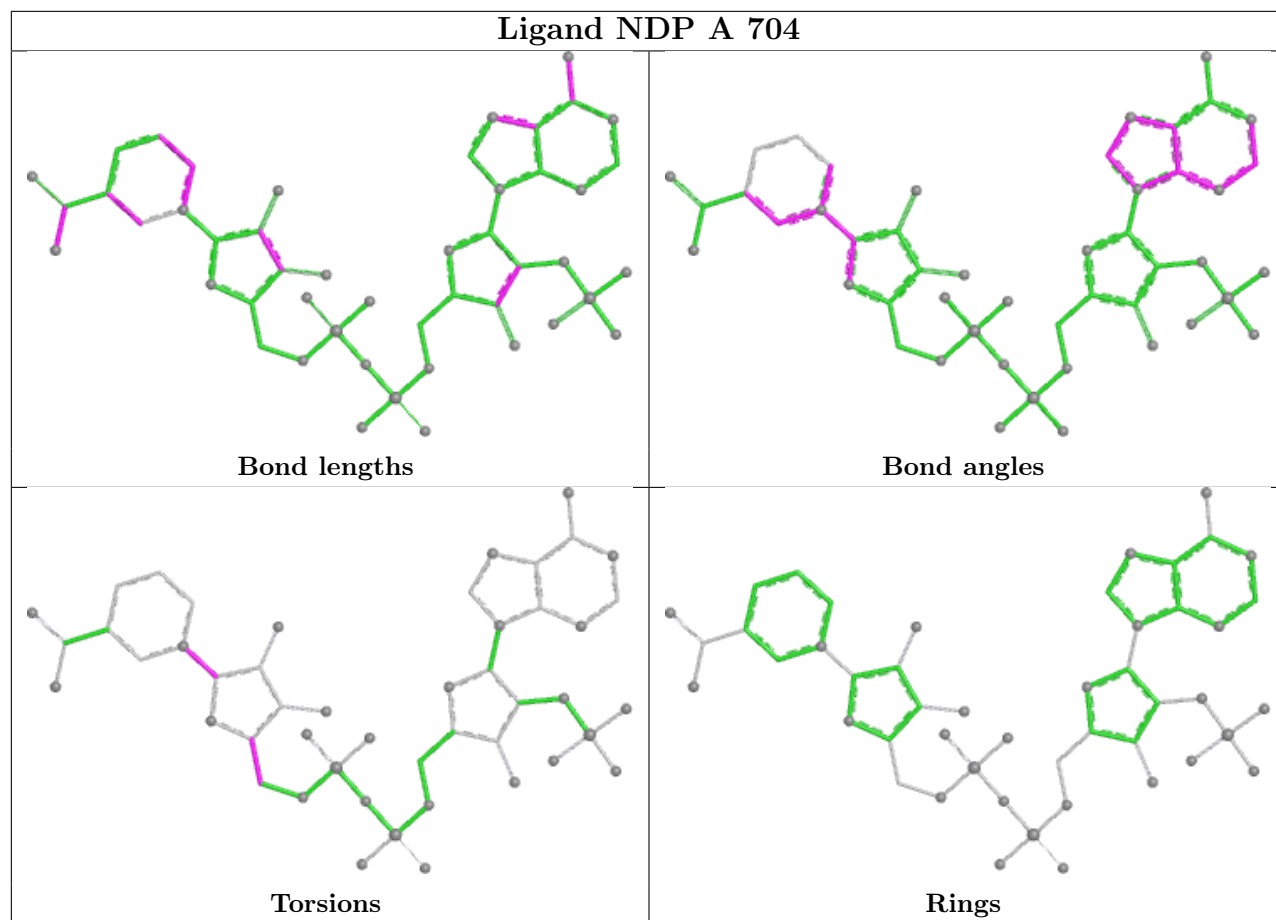
## Ligand FOL B 703

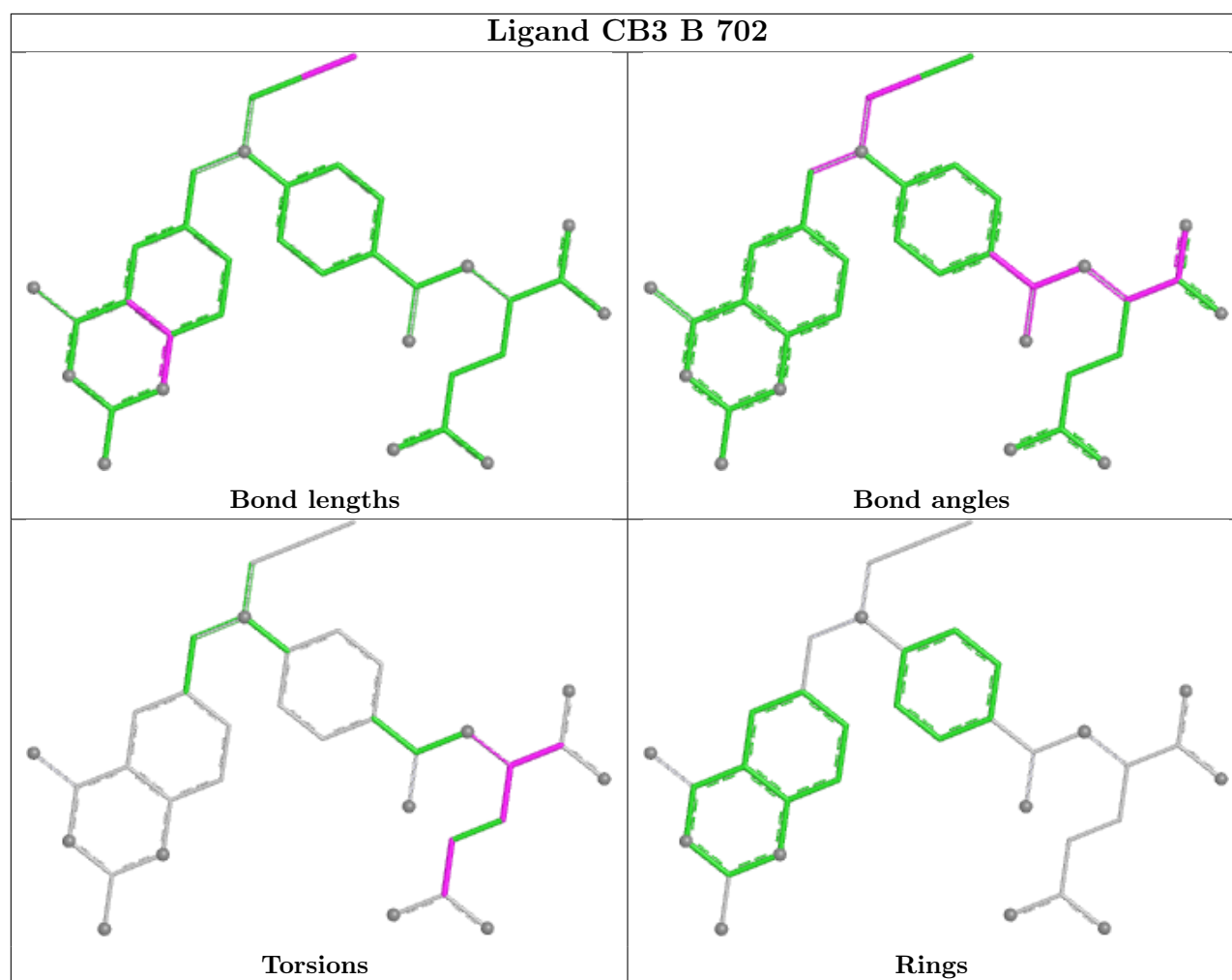












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	498/610 (81%)	-0.99	1 (0%) 91 81	16, 57, 83, 115	2 (0%)
1	B	498/610 (81%)	-1.01	0 100 100	26, 57, 79, 103	2 (0%)
All	All	996/1220 (81%)	-1.00	1 (0%) 92 85	16, 57, 81, 115	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	VAL	2.3

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CB3	A	702	35/35	0.98	0.07	80,90,105,105	0
3	CB3	B	702	35/35	0.98	0.08	72,92,110,116	0
2	UMP	A	701	20/20	0.99	0.06	71,78,95,97	0
2	UMP	B	701	20/20	0.99	0.05	68,79,103,105	0

*Continued on next page...*

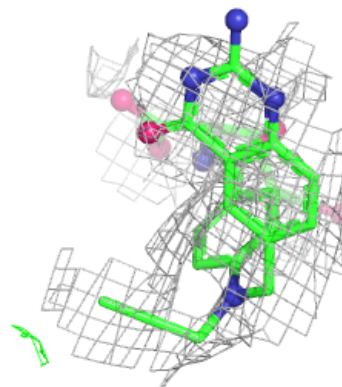
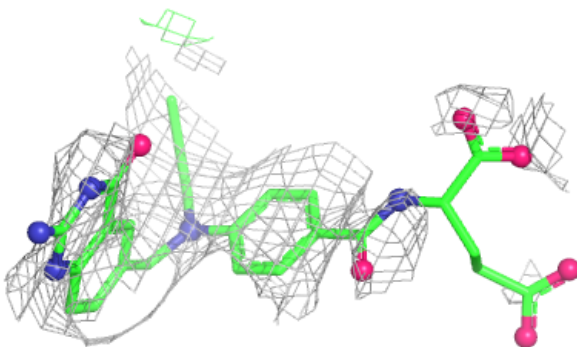
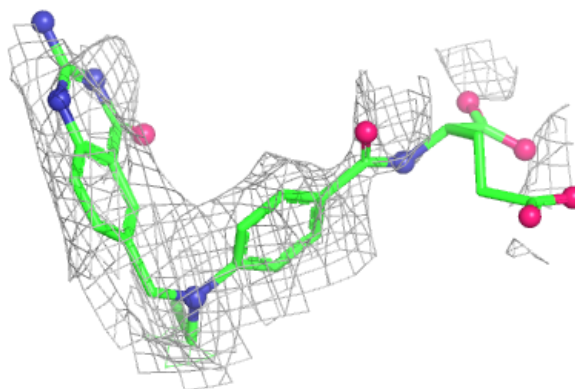
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FOL	A	703	32/32	0.99	0.05	72,86,94,98	0
4	FOL	B	703	32/32	0.99	0.05	72,82,105,110	0
5	NDP	A	704	48/48	0.99	0.06	75,83,100,104	0
5	NDP	B	704	48/48	0.99	0.06	75,84,99,102	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.

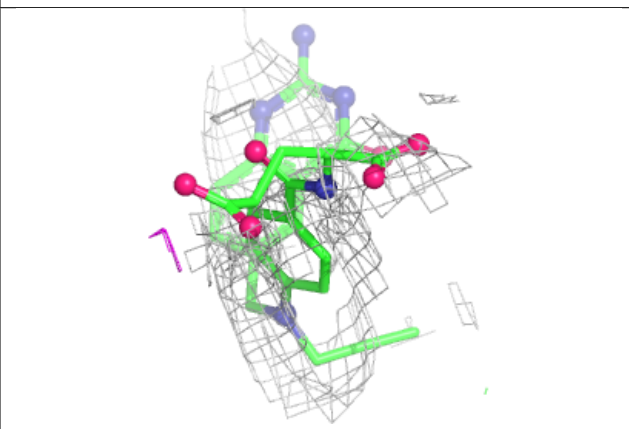
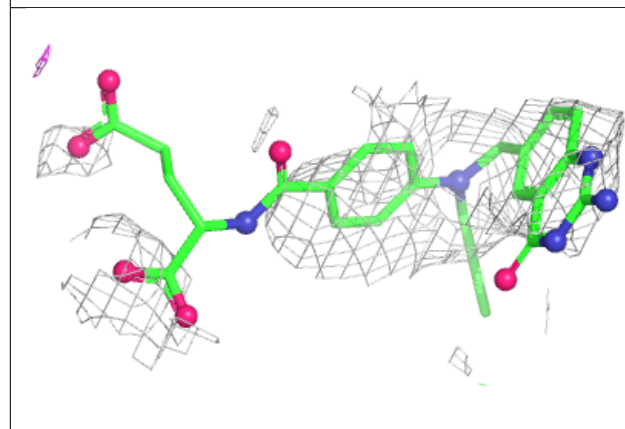
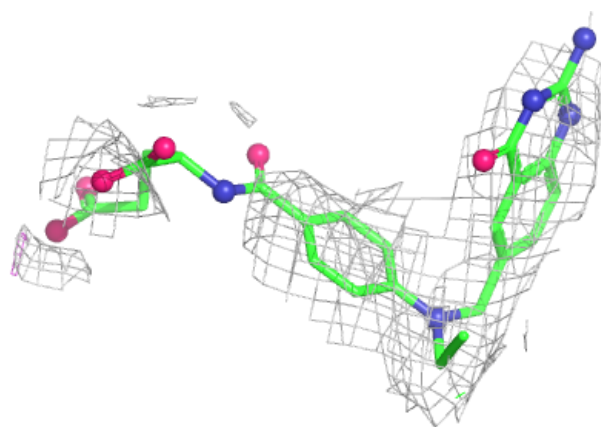
**Electron density around CB3 A 702:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

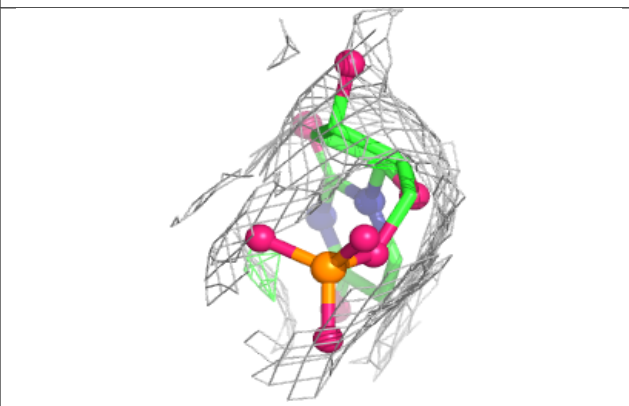
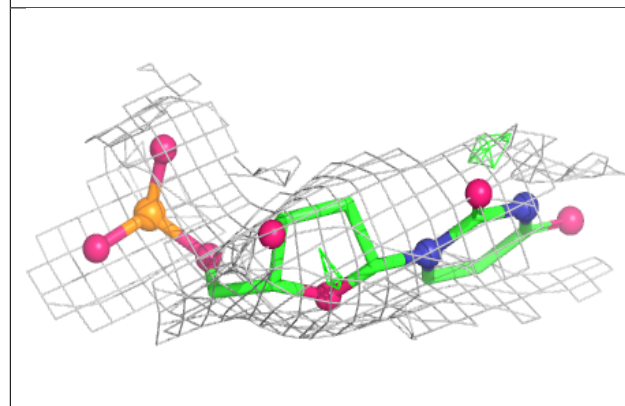
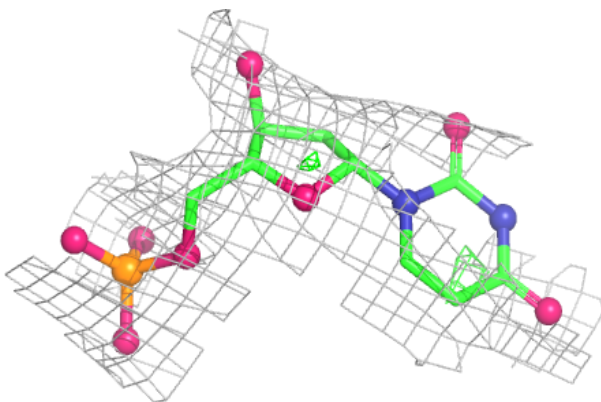


**Electron density around CB3 B 702:**

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

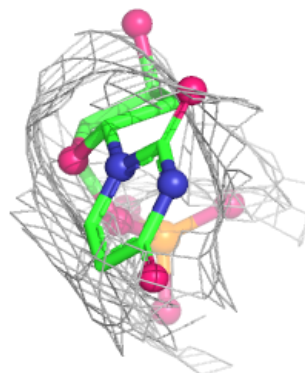
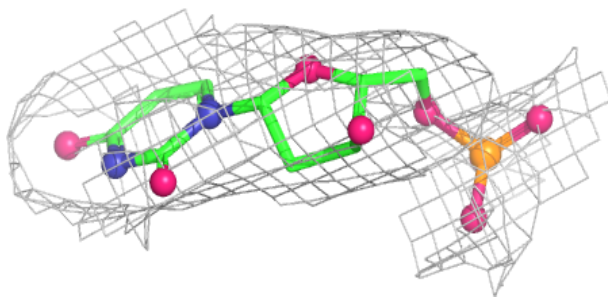
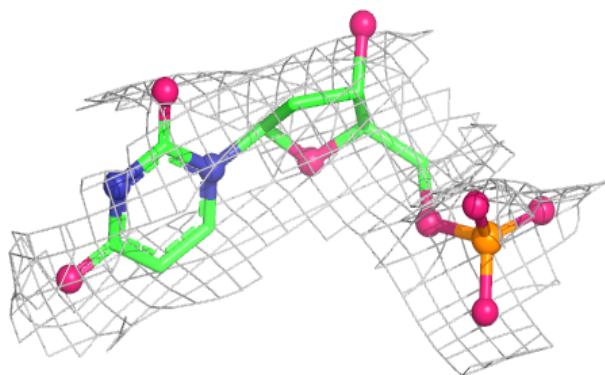
**Electron density around UMP A 701:**

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



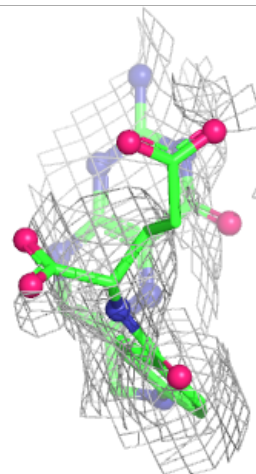
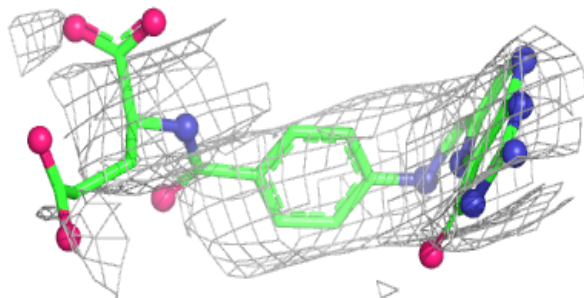
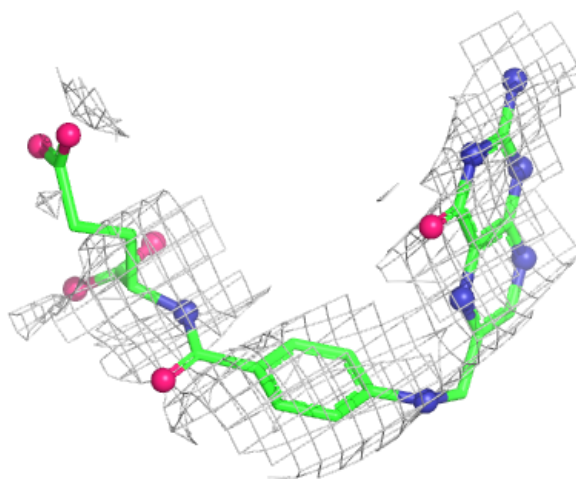
**Electron density around UMP B 701:**

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



**Electron density around FOL A 703:**

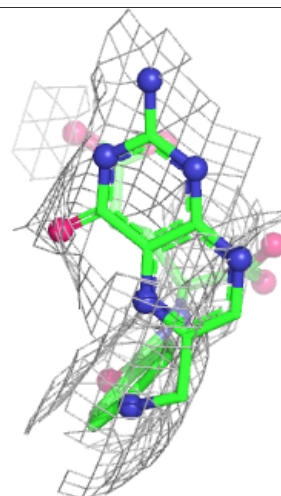
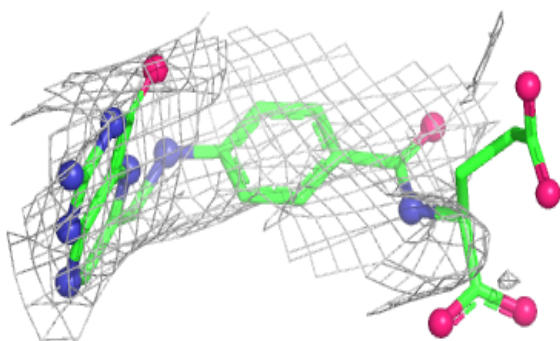
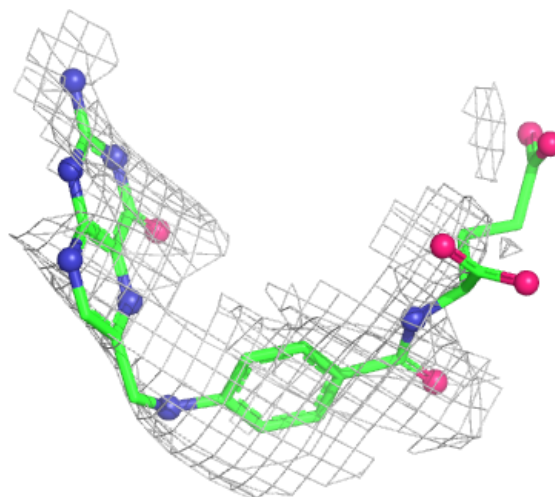
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around FOL B 703:**

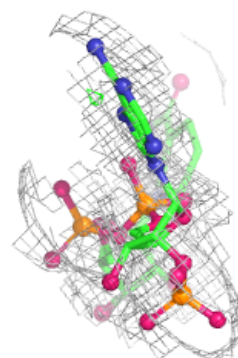
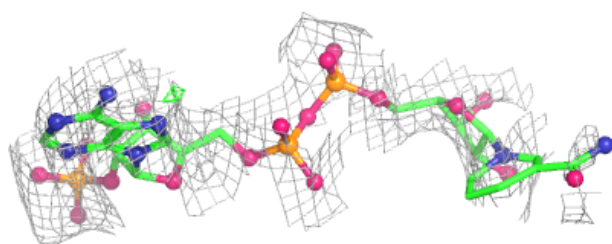
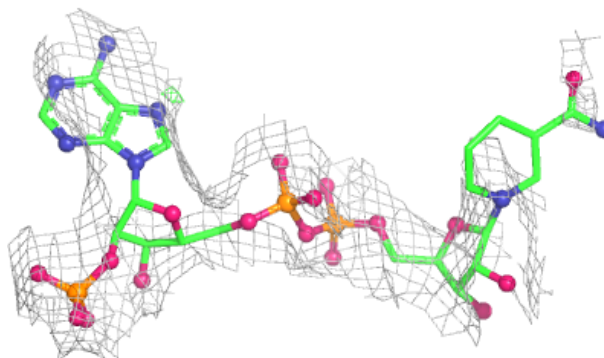
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



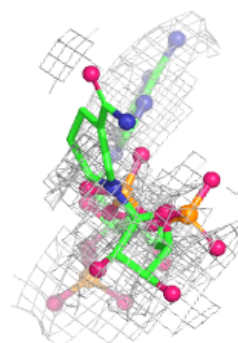
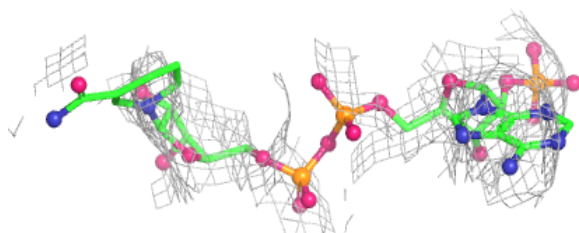
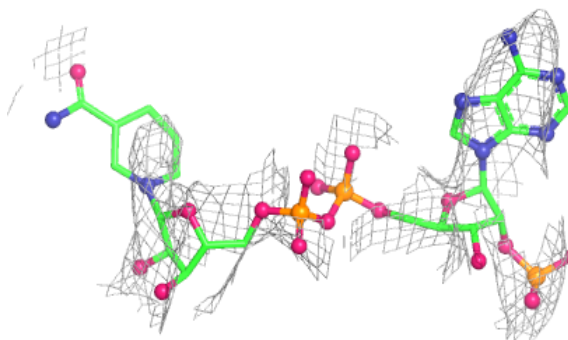


**Electron density around NDP A 704:**

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

**Electron density around NDP B 704:**

$2mF_o-DF_c$  (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.